LARGE ATOMS AND QUANTUM DOTS

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Abstract

A functional integration approach – whose main ingredient is the Hubbard-Stratonovich transformation – for the quantum nonrelativistic many-fermion problem is investigated.

With this method, the ground state energy correponds to a systematic expansion in powers of a small parameter related to the number of fermions. It is a functional of a potential determined by a self-consistent equation. The semiclassical Hartree energy is obtained at lowest order of the expansion, the exchange energy at first order, and the correlation energy at second order.

This approach is applied to large neutral atoms, for which the correlation energy is computed.

This approach is also applied to many-electron quantum dots with harmonic confinement. The self-consistent equation is solved as a function of a small parameter depending on the confinement strength. The Hartree and exchange energies are computed in powers of this parameter, and the correlation energy is computed at lowest order. The energy oscillations, arising from the Hartree energy, are also evaluated; they are related to the periodic orbits of the classical dynamics of the self-consistent potential.

Keywords: Semiclassical quantum physics, quantum dots, large atoms, correlation energy.

Version abrégée

Une approche par l'intégrale fonctionnelle – dont le principal ingrédient est la transformation de Hubbard-Stratonovich – est investiguée pour le problème quantique non relativiste d'un système avec grand nombre de fermions.

Par cette méthode, l'énergie de l'état fondamental correspond à un développement en puissance d'un petit paramètre relié au nombre de fermions. C'est une fonctionnelle d'un potentiel déterminé par une équation autoconsistante. L'énergie de Hartree semiclassique est obtenue à l'ordre le plus bas du développement, l'énergie d'échange au premier ordre, et l'énergie de corrélation au deuxième ordre.

Cette approche est appliquée aux atomes neutre avec grand nombre d'électrons, pour lesquels l'énergie de corrélation est calculée.

Cette approche est aussi appliquée aux boîtes quantiques avec grand nombre d'électrons, avec confinement harmonique. L'équation autoconsistante est résolue comme fonction d'un petit paramètre relié à l'intensité du confinement. Les énergies de Hartree et d'échange sont calculées en puissance de ce paramètre, et l'énergie de corrélation est évaluée à l'ordre le plus bas. Les termes oscillants de l'énergie, provenant de l'énergie de Hartree, sont également évalués; ils sont reliés aux orbites périodiques de la dynamique classique du potentiel autoconsistant.

Mots-clés: Physique quantique semiclassique, boîtes quantiques, atomes lourds, énergie de corrélation.

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Introduction

The study of the atom is intimately related to the study of matter, which has been fascinating people for many centuries. The question of its existence goes back – in western culture – to the ancient Greeks, for whom it was a philosophical question. The presocratic philosophers, in the V$^{\text{th}}$ century BC (mainly Leucippus, Democritus, and later Epicurus), created atomism: all physical objects are constituted of atoms and void. Both are never created and never ending. Void creates space, in which atoms evolve. The packings and scatterings of these atoms are responsible for the sensations we feel. The atoms correspond to the smallest possible division of matter, the word describing it being $\alpha\tau o\mu o\zeta$ (atomos) in ancient Greek, and this word gave the name to the current atom.

At the time it was impossible to verify experimentally the discreteness of matter, and this theory was rejected by Aristotle (in the IV$^{\text{th}}$ century BC), who thought that matter was continuous. His ideas dominated through the middle ages in Europe.

In the XVI$^{\text{th}}$ and XVII$^{\text{th}}$ centuries, atomists (among them Galileo Galilei) met some success, and atomism really came back in the XVII$^{\text{th}}$ century with Descartes and Gassendi in France, and Boyle in England.

In the XVIII$^{\text{th}}$ century, experiments in chemistry led Lavoisier to postulate that nothing is created, nothing is lost, all is transformed. They model substance as constituted of elements, and the organization of these elements is modified during a chemical reaction to provide other substances.

During the same period, and following Descartes, Bernouilli (and also Hermann and Euler), suppose that gas is made of particles. They develop a kinetic theory of gases, which leads to results (for pressure and temperature) in agreement with experiment.

Another field of study, at this time, is crystallography: natural crystals present particular geometries, and to explain it, Haüy claims that these geometries are the consequence of an elementary piece (which is however not, at this time, related to atoms).

In the XIX$^{\text{th}}$ century, more experiments and postulates allow these three domains to have a common explanation: the existence of atoms and molecules. John Dalton, first, assumes that substance is made of spherical objects, the atoms, which are different for different elements. In parallel to this work, Gay-Lussac observes that during a chemical reaction, the ratios between the volumes in play are small integers. He too deduces that substance is made of discrete objects. A few years later, Avogadro is the first to make a clear distinction between atoms and molecules. Herapath develops a kinetic theory of gases to explain phase transitions. The kinetic theory of gases is improved mainly by Clausius, Maxwell, and Boltzmann, who provide the basis of statistical mechanics. During this century, crystallography also makes progress, and is related to the atomic point of view through the work of Delafosse, Pasteur, and Bravais. The elementary pieces consist of a lattice on which there are molecules.

Though there were strong arguments for the existence of atoms, the atomic point of view was still a subject of controversy. One of Einstein's papers of his miraculous year 1905 is considered the paper ending this controversy. He explains the brownian motion (observed by Brown in the XIX$^{\text{th}}$ century): pollen grains suspended in water have constant, apparently random, motion, and Einstein explained this motion by collisions with molecules of water, themselves moving because of thermal agitation.

A systematic classification of atoms, with increasing masses, is done by Mendeleïev, who identifies periodicities in properties of atoms. It leads to the periodic table of the elements, from which Mendeleïev predicts the existence of new atoms, which will be verified later. The periodicities of these properties could only be understood with quantum mechanics, as will be explained later in this chapter.

The atomistic point of view was then generally accepted. But the structure of the atom was not clearly understood. Electrodynamics was already known, and Thomson's experiments (at the end of the XIX$^{\text{th}}$ century) decompose the atom, leading to the discovery of the electron. A few years later, Rutherford projects alpha particles (which are positively charged) on gold foils, and observes that while the majority crosses, some are deviated and even come back. His conclusion is that matter is mainly empty, and that there are very concentrated clusters of positive charges. He derives a model for the atom, which consists of a positive nucleus with electrons orbiting around, like planets around the sun. This model is however in contradiction with one consequence of electrodynamics, the *Bremsstrahlung*: any accelerated charge loses energy by radiation. The electrons of a classical atom, having a centripetal acceleration due to the nucleus, should lose energy and crash very quickly on the nucleus. Classical physics can therefore not explain the stability of atoms. Moreover, the experiments show that the energy levels of atoms are quantized. This problem was solved with Bohr's model, which is the same kind of system, with certain orbits allowed only. He did not give an explanation to this quantization.

The problem of the stability of atoms could only be solved with the discovery of quantum mechanics, whose history is closely related to the history of atoms. The electron is described by a wave function, whose square corresponds to a probability of presence of the electron. The theoretical problem, describing the hydrogen atom, was solved analytically in quantum theory, and led to results in very good agreement with experimental data. For the treatment of other atoms, with more than one electron, the statistical properties (the wave function is antisymmetric under the exchange of particles, leading to Fermi-Dirac statistics) of electrons have to be taken into account. The computation of various properties of the atoms can be done analytically both for the hydrogen atom, and for atoms with a number of electrons tending to infinity. In between, approximation methods were developed to compute them, the main method being Hartree-Fock (described in chapter 1). But these numerical resolutions imply simplifications, and effects like correlation energy (which will be discussed below) are left out. The stability of atoms (and matter) was proven by Lieb in the 1970's, in the framework of quantum mechanics.

The quest for a deep understanding of matter led physicists to the current model, the standard model, a quantum field theory which describes the nucleus as constituted of protons and neutrons, which are constituted of quarks. We will not develop this theory in this introduction.

Since the eighties, technical developments in semiconductor physics allowed the creation of quantum dots, also called artificial atoms. A quantum dot consists of a set of electrons evolving in a bi-dimensional plane (a quantum well), and confined to a small region by an external potential, in the same way electrons of an atom are confined by the potential created by the nucleus. Quantum dots are of great importance both for scientific research and industrial applications.

In the case of an atom, the parameters like electron mass, confinement strength, electronic interaction strength, are fixed. In the case of quantum dots, these parameters are controllable through the choice of the semiconductor material – which allows a modification of the (effective) mass and the (effective) electronic interaction – and the strength and shape of the confinement. This allows a more systematic study. Moreover, the typical length, energy, and magnetic field in quantum dots are such that we can explore domains which are impossible to reach with atoms in a laboratory setting. For example, there are new effects found for atoms submitted to a huge magnetic field (of the order of 10^5 Tesla), which are impossible to produce in laboratory setting. But such strong magnetic fields exist in neutron stars, and this is why astrophysicists are interested in the properties of atoms in these regimes. This regime is attained for quantum dots in magnetic fields of the order of 1 Tesla, which are easily produced. The study of quantum dots can therefore lead to a better understanding of the behaviour of atoms in neutron stars.

Quantum dots have also important – existing and potential – technological applications, mainly due to their interesting transport and optical properties. There are potential applications in diode lasers, amplifiers, and biological sensors. Quantum dots are already used as blue lasers for DVD players.

Other very promising applications are in solar cells, where quantum dots based cells seem to have better efficiency than the current cells.

The quantum properties of quantum dots make them a hopeful candidate for q-bits in quantum computing. One possibility consists of having several dots, with one electron per dot. If they are close enough, their spins become automatically entangled, and they play the role of the q-bits.

The many-body problem is not limited to the study of atoms and artificial atoms. It appears in numerous situations, among them nuclear physics, where the particles studied are nucleons (protons and neutrons), chemistry, where the particles studied may be molecules, as well as biology, where the particles studied are large molecules.

Some effects in many-body systems are of great importance, although they are very weak. Among them, the correlation energy and the energy oscillations, which are discussed below.

Correlation energy

The correlation energy, which is defined as the energy beyond the Hartree-Fock approximations, is weak, but has deep physical consequences in some systems. The correlation energy explains, for example, the stability of certain systems, and, more exotically, the color of certain metals. This energy is negative, the Hartree-Fock energy being an upper limit to the true ground state energy.

For large atoms, it was proven by Teller's theorem (Teller, 1962) that the Thomas-Fermi energy (which is the asymptotic energy for atoms and molecules) is unstable under the decomposition of a big molecule into any smaller ones: it is the no-binding theorem. It is therefore necessary to go beyond the Thomas-Fermi model, and pay particular attention to the correlation energy.

The correlation energy of the neutral atom has been obtained experimentally for up to 18 electrons, as shown in Figure 1 (data is from Clementi (1963a,b); Chakravorty et al. (1993)). This data corresponds to the difference between experimental and numerical Hartree-Fock data, where some effects (like relativistic effects) are dropped – further details are given in chapter 3.

With so little data, it seems difficult to state that the correlation energy is a linear function of N, as resulting from our computations. If it were linear, a linear interpolation of this data provides, in Hartree,

$$-E_{corr} \simeq 0.043N. \tag{1}$$

Energy oscillations

A basic model of atoms consists of a system of independent particles evolving in the potential created by the nucleus at the origin. The Fermi-Dirac statistics is

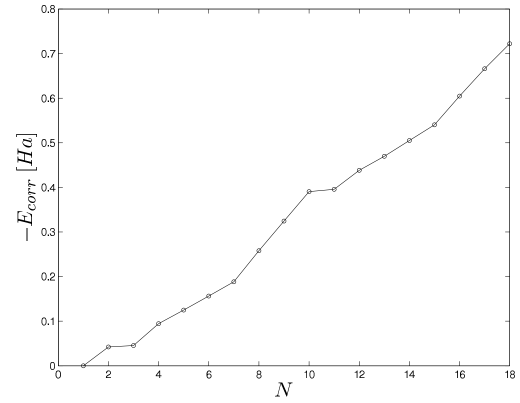


Figure 1: *Experimental correlation energy as a function of N for the neutral atom.*

therefore such that the electrons fill the first energy levels of the spectrum of the hydrogen atom.

The radial symmetry of this system (combined with an accidental degeneracy and the spin degeneracy) implies degeneracies, that is the electrons fill shells. The energy of a shell is $E_n = -\frac{1}{n^2}$ in Rydberg, and its degeneracy is $2n^2$. The two first shells (which contain 2 and 8 atoms respectively) are explained by the mentioned model. It is however too simple to explain the next shells, as can be seen in the periodic table of the elements.

The physical and chemical consequences of this shell structure are huge: it explains why the noble gases, their shells being completely filled, almost never interact; it explains the tendency of atoms to bind together (in order to "fill" their shells) to form molecules, which explains the existence of many molecules and chemical reactions.

This shell structure is observable in the ionization energy of neutral atoms: the atoms with filled shells are more stable, their ionization energy is therefore bigger than for other atoms. This can be characterized mathematically (as was done by Englert and Schwinger (1985a)). As shown in Figure 2 (experimental data from NIST – National Institute of Standards and Technology), the ionization energy shows variations. The same function, multiplied by $N^{\frac{1}{3}}$, as shown in Figure 2 as a function of $N^{\frac{1}{3}}$, shows a very interesting property: a periodicity, which led Englert and Schwinger (1985a) to compute the ground state energy of neutral atoms, and to identify these periodicities in the parameter $N^{\frac{1}{3}}$.

Quantum dots (seen as artificial atoms) have the same properties: by considering a system of independent particles evolving in an external potential as a basic model, the energy levels correspond to those of a two-dimensional harmonic oscillator. These energies are $E_{n_\rho,m} = 2n_\rho + |m| + 1 \doteq n + 1$ in appropriate units, and the degeneracy is $2n$. In this case, a quantum dot can be treated in the same way as an atom, as it was done by Kouwenhoven et al. (2001), from which Figure

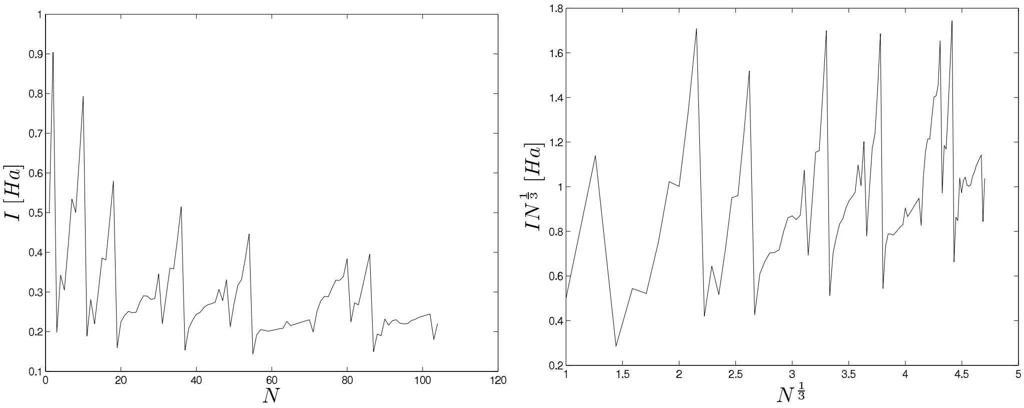


Figure 2: *Ionization energy of neutral atoms as a function of N, and ionization energy multiplied by $N^{\frac{1}{3}}$ as a function of $N^{\frac{1}{3}}$.*

3 is taken.

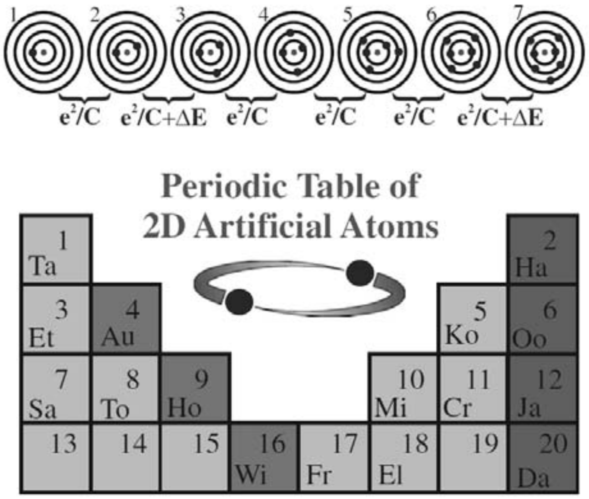


Figure 3: *Periodic table of quantum dots constructed by analogy with the periodic table of atoms, with typical electronic configurations shown above.*

This model is discussed in more detail in chapter 4. The values for which the shells are filled show a periodicity as a function of $\sqrt{N}$, as predicted by our computations done with a refined model.

Structure of the thesis

Some preliminary knowledge is required to understand this thesis: the reader should be familiar with quantum mechanics. A good book on this topic is "Quantum mechanics" by Schwinger (2001). The reader should also know functional integration over real and Grassmann variables. A nice book on functional integration is "Path integrals in quantum mechanics, statistics, polymer physics, and financial markets" by Kleinert (2004). For the Grassmann variables we recommend "Quantum many-particle systems" by Negele and Orland (1988), where the formalism we need is developed, and from which our notations are taken.

The thesis is divided in two parts: in part I, we develop the general method for the computation of the ground state energy of many-fermion systems, and compute the correlation energy for both atoms and quantum dots with the mentioned method. In part II, we proceed to the computation of the ground state energy of quantum dots (with radial symmetry), as an application of the method developed in part I.

Part I is organized as follows: we start with an introduction (chapter 1), where we define and discuss the model of the atom, and discuss the existing results on the subject. In chapter 2 we develop the new method, and obtain, for the ground state energy, the Hartree energy at lowest order, the exchange energy at first order, and the correlation energy at second order. These energies are expressed as functionals of a potential, which satisfies a self-consistent equation. The correlation energy is computed in chapter 3 for both atoms and quantum dots.

Part II is organized as follows: we start with an introduction (chapter 4), where we define and discuss the model of the quantum dot, and discuss the existing results (both theoretical and experimental) on the subject. In chapter 5 we proceed to a semiclassical Hartree-Fock development, with a specific discussion for its application to quantum dots. We derive the equation for the self-consistent potential, and obtain the Hartree and exchange energies as functionals of this potential. As this approach does not contain energy oscillations, those are obtained with the development of another approach, done in chapter 6, where the energy oscillations are related to the periodic orbits of the classical dynamics in the self-consistent potential. In chapter 7 we solve the self-consistent equation to find the density, which does not depend on N – after a scaling – but depends on a (small) parameter p related to the strength of the confining potential. The limit $p \to 0$ has an analytical solution, and the numerical solution is obtained in the small p regime, as a function of this parameter. In chapter 8, this solution is introduced in the Hartree, exchange, and correlation energies to obtain the smooth part of the energy of quantum dots. This smooth energy is a polynomial of N and p. We also compute the energy oscillations at lowest order, using the self-consistent potential at lowest order (for which we have an analytical solution). The smooth and oscillating energies are compared to experimental results.

The thesis ends with the conclusion and perspectives.

Part I

Many-fermion systems and semiclassical atoms

Chapter 1

Introduction

Contents

The objective of this chapter is to describe atoms, to describe and discuss its modeling, and to present existing approximations for the treatment of N-fermion systems, and theoretical results on the computation of the ground state energy of atoms.

We qualitatively describe an atom, before discussing its modeling. We discuss the existing results for the asymptotic smooth energy, as well as the theoretical treatment of the energy oscillations.

1.1 Atom description

As explained in the general introduction, it took a long time until the current understanding of the atom was reached. This model consists of a nucleus, constituted of A neutrons (no charge) and Z protons (positive charge), and a cloud of N electrons. For a neutral atom, as we will consider, $N = Z$.

The typical size of the nucleus is $10^{-15}m \doteq 1\ fermi$, and the typical size of the atom is $10^{-10}m \doteq 1$ *Angström*, which makes a ratio of 10^5 between the sizes of the nucleus and the atom.

The masses of a neutron and a proton are very similar $(1.67 \cdot 10^{-27}kg)$ while the mass of an electron is much smaller $(9.11 \cdot 10^{-31}kg)$. The ratio is of the order of 10^3.

In the atomic nucleus, the forces in play are the so called weak and strong interactions, and the energy excitations are of the order of $1MeV$. The electrons are submitted to electrostatic interactions, and the energy excitations are of the order of $1Ry \sim 10eV$, which corresponds to a ratio of 10^5 between the excitation energies.

1.2 The model

Considering the typical size of an atom, we will work in the framework of quantum mechanics (further considerations will allow us to work in the semiclassical regime).

The ratio between the masses of protons and electrons is so high that we will consider the protons to have an infinite mass, their position therefore being fixed.

Moreover, the ratio between the size of the nucleus and the electron cloud is so high that we will consider the nucleus to be a point, located at the origin.

The ratio between the energy excitations of the nucleus and the electrons is so high that we will only take the excitations due to the electrons into account.

We will consider that the atom is in the vacuum. Moreover we will neglect the gravitational interaction, as well as relativistic effects (even though Figure 1.2(a) shows that, for N large, they are not negligible). We will consider the classical electromagnetic field.

Based on these concepts, the system consists of a set of N electrons with mutual electronic interaction, evolving in three dimensions, and subjected to a confining potential produced by electrostatic interactions with the N protons located at the origin. The hamiltonian of this system is

$$\tilde{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\tilde{\Delta}_i - \sum_{i=1}^{N}\frac{e^2 N}{|\tilde{\boldsymbol{x}}_i|} + \frac{1}{2}\sum_{i,j=1,i\neq j}^{N}\frac{e^2}{|\tilde{\boldsymbol{x}}_i - \tilde{\boldsymbol{x}}_j|}, \tag{1.1}$$

where m is the electron mass, $e \doteq \frac{q}{\sqrt{4\pi\epsilon_0}}$, while q is the charge of an electron and ϵ_0 the dielectric constant (in the vacuum).

This hamiltonian is written in the (arbitrary) MKSA units. It is however more comfortable to work in atomic units. The energy unit is the Hartree (which equals two times the Rydberg)

$$E_H = 2Ry = \frac{me^4}{\hbar^2} = 27.2eV, \tag{1.2}$$

and the length unit is the Bohr radius

$$a_0 = \frac{\hbar^2}{me^2} = 0.53\mathring{A}. \tag{1.3}$$

The energy unit can be expressed in terms of the length unit

$$E_H = \frac{e^2}{a_0}. \tag{1.4}$$

The new variables are, writing them with a hat,

$$\hat{H} = \frac{\tilde{H}}{E_H}, \quad \hat{\boldsymbol{x}} = \frac{\tilde{\boldsymbol{x}}}{a_0}, \quad \frac{\partial^k}{\partial \hat{x}^k} = a_0^k \frac{\partial^k}{\partial \tilde{x}^k}. \tag{1.5}$$

The hamiltonian now has the very simple form

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N} \hat{\Delta}_i - \sum_{i=1}^{N} \frac{N}{|\hat{\boldsymbol{x}}_i|} + \frac{1}{2} \sum_{i,j=1, i\neq j}^{N} \frac{1}{|\hat{\boldsymbol{x}}_i - \hat{\boldsymbol{x}}_j|}. \tag{1.6}$$

This hamiltonian will be the starting point of our developments. The confining potential will be generalized to an arbitrary one, and the ground state energy of such a system will be computed for a large number of electrons in chapter 2.

1.3 Theoretical approaches of the N-body problem

The N-body problem (we will always consider fermions) cannot be solved exactly, and different approximation methods were developed to study properties of N-body systems. We will describe some of them.

The Thomas-Fermi model is a mean-field theory: the N-body system is simplified to a one-body system: one particle feels the average interaction from the other particles. The density is then computed through a self-consistent equation. This approach is adapted for a system with a large number of particles (and becomes exact in the limit of an infinite number of particles). One advantage of this approach is that we only deal with the density (a function of d variables), and not with a wave function of an N particle system (a function of dN variables).

Another approach is the Hartree-Fock approximation: it consists of writing the wave function as a product of one-particle wave functions, and finding the wave function which minimizes the energy. The hamiltonian itself depends on the wave function and the solution has to be found iteratively, numerically. It is possible to consider a simple product of wave functions (Hartree approximation) or an antisymmetrized product of wave functions (Hartree-Fock). As it is numerically demanding, this approach is best suited for systems with a low number of particles.

The semiclassical Hartree-Fock approach (as developed in detail in chapter 5) consists of considering the wave function to be an antisymmetrized product of wave functions. These are one-particle wave functions, the N first eigenfunctions of a one-particle hamiltonian, whose potential is determined self-consistently. More precisely, it is determined by minimizing the energy of the system in the semiclassical framework. This framework allows the expression of the potential as a function of the density, which leads to a self-consistent equation for the density. The energy can then be expressed as a functional of the density. At lowest order, this approach yields the Thomas-Fermi model. The advantage is that through a perturbative expansion, it can be extended beyond Thomas-Fermi.

The last approach we describe is the density functional theory (DFT). It is based on the Hohenberg-Kohn theorem, which states that there is a one to one correspondence between the ground state wave function and the ground state density, and that this density minimizes the ground state energy. However, this theorem does not provide the energy as a functional of the density, and approximations have to be made.

1.4 Theoretical results – atoms

The different techniques for the treatment of the N-body problem were very often developed to solve the problem of the atom. This is what Thomas (1927) and Fermi (1927) did independently. They used a mean-field theory: the many-body problem is simplified in a way that it becomes a one-body problem, and the electron considered is submitted to a mean-field potential, consisting of the confining potential, plus the mean potential the electron cloud produces. It therefore provides a self-consistent equation for this potential. This mean-field approach is now known as the Thomas-Fermi model. It was done rigorously by Lieb (see, for example, (Lieb, 1976)), who proved that the ground state energy obtained with the Thomas-Fermi model is asymptotically equal to the quantum ground state energy in the limit of an infinite number of electrons Z. The energy is proportional to $Z^{\frac{7}{3}}$.

This model was improved and many physicists provided smooth corrections (that is corrections in inverse powers of $Z^{\frac{1}{3}}$): Scott (1952) was the first to propose a $Z^{\frac{6}{3}}$ correction due to the innermost core electrons (where the confining potential is huge). Earlier, Dirac (1930) added the contribution of the exchange energy (of the order of $Z^{\frac{5}{3}}$), and von Weiszäcker (1935) the gradient contribution to the kinetic energy. These corrections provide the asymptotic ground state energy. A modification was done by Englert and Schwinger (1985b), who did the most comprehensive work on the topic. They worked in what we call the semiclassical Hartree-Fock model (as will be developed in detail in chapter 5), which provides, at lowest order, the Thomas-Fermi model. It also provides smooth corrections, given by inverse powers of $Z^{\frac{1}{3}}$. The innermost core electrons were treated outside this model, because the confining potential is divergent at the origin. It provides a term of the order of $Z^{\frac{6}{3}}$, as obtained by Scott. They obtain the exchange energy, like Dirac, but also a new term arising from quantum corrections to the kinetic energy, which are of the order $Z^{\frac{5}{3}}$. They obtain results which are in very good agreement with the reference solution (which are Hartree-Fock simulations, as there are no experimental results for $Z > 28$, up to which Hartree-Fock and experimental results agree very well), as shown in Figure 1.1, taken from (Englert and Schwinger, 1984). The final result provides the smooth energy (expressed in atomic units):

$$\frac{-E_{smooth}}{\frac{1}{2}Z^2} = 1.537Z^{\frac{1}{3}} - 1 + 0.540Z^{-\frac{1}{3}}. \tag{1.7}$$

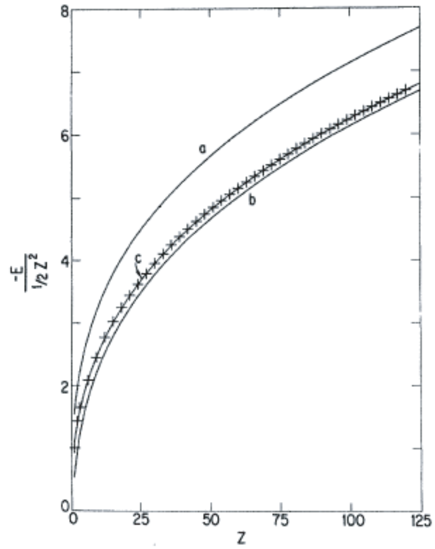
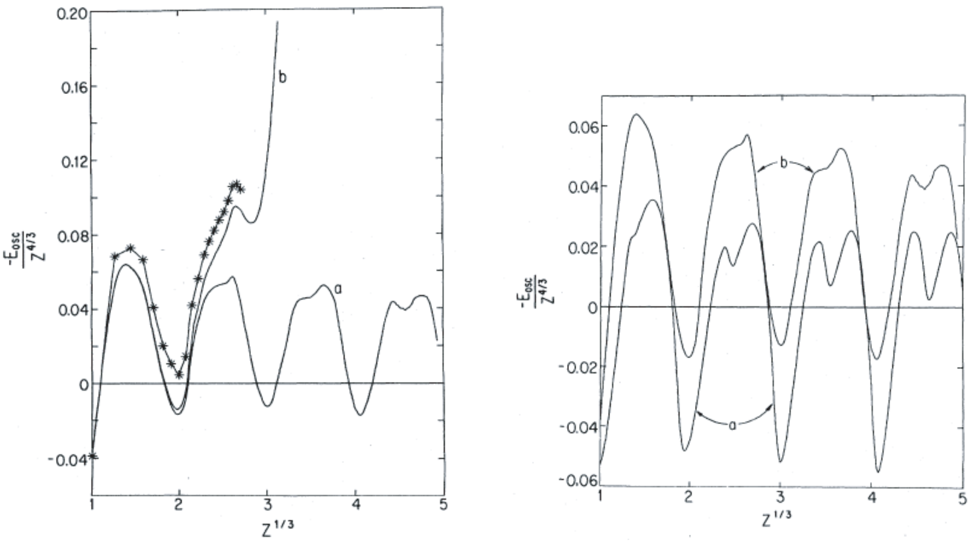


Figure 1.1: *Comparison of calculations of the total binding energy. Crosses are Hartree-Fock (HF) data; curve (a) is Thomas-Fermi (TF) energy; curve (b) is TF with corrections of relative order $Z^{-\frac{1}{3}}$; curve* c *is TF with corrections of relative order $Z^{-\frac{2}{3}}$.*

These smooth corrections were rigorously made by Feffermann and Seco, whose work is summarized in (Feffermann and Seco, 1997). They proved that Schwinger's correction is correct.

So far we have discussed the smooth contribution to the energy. But what about oscillatory terms? The energy oscillations were studied in detail by Englert and Schwinger (1985a) (computations are developed in more detail in (Englert, 1988)). The energy oscillations were computed analytically in the semiclassical Hartree-Fock approach and were compared to numerical Hartree-Fock results, considered as a reference solution. Comparison with experimental data is not easy: real atoms include relativistic effects. To verify the reference solution, Hartree-Fock simulations are compared to experimental results in Figure 1.2(a) for up to $Z = 20$. On this figure, relativistic numerical results are shown, and are in good agreement with experimental results (although not exact, numerical simulations being obtained by a simplification of the real problem). On the same figure, Hartree-Fock simulations (which are, of course, non relativistic) are shown. We observe that they are in very good agreement with relativistic results up to $Z^{\frac{1}{3}} = 2$. We also observe that the energy oscillations are a non relativistic effect. This is why Hartree-Fock results are a reference solution, and are used to validate semiclassical Hartree-Fock results. The comparison is shown in Figure 1.2(b), and we observe that the energy oscillations obtained this way are in good agreement with the reference solution. The oscillations are quasi-periodic functions of $Z^{\frac{1}{3}}$, and their magnitude is of the order of $Z^{\frac{4}{3}}$.



(a) Binding-energy oscillations. Stars are experimental values for $Z = 1, \ldots, 20$. Curve (a) shows non relativistic HF oscillations. Curve (b) shows relativistic simulations.

(b) Comparison of semiclassical predictions for the nonrelativistic binding-energy oscillations (curve (a)) with the HF prediction (curve (b)).

Figure 1.2: *Energy oscillations*

Feffermann and Seco (1997) tried to establish these oscillating terms rigorously but they could not prove it completely. They could prove that there are oscillating terms of the order of $Z^{\frac{4}{3}+\frac{1}{6}}$, and of a period of the order of $Z^{\frac{1}{3}}$, but they could not prove that the remaining terms (called the error terms) are of lower order in Z.

Chapter 2

Ground state energy of a many-fermion system

Contents

The objective of this chapter is to obtain a formula for the ground state energy of a system of many fermions, with a new approach using functional integration over Grassmann variables, up to a certain order in a small parameter (given by an inverse power of the number of electrons N). All developments are done in d dimensions.

This new formalism is developed in this chapter, and will be used in part II with an application to quantum dots.

We start this chapter by proceeding to a scaling of the energy and length, in order to see that we can work in the semiclassical regime. We proceed to the developments, whose main ingredient is the use of the Hubbard-Stratonovich transform. We then establish a formula for the grand-canonical partition function, from which we compute the pressure, as an expansion in an inverse power of N. We find that the lowest order term corresponds to the semiclassical Hartree pressure, while the first order provides the exchange term (their sum is therefore semiclassical Hartree-Fock). We then compute the second order corrections and find new terms. We take the limit of zero temperature to obtain the ground state pressure, from which we deduce, by a Legendre transformation, the energy of the ground state. The new corrections are universal, in the sense that they depend on the dimension of the system only, not on the specific properties of the problem.

The grand-canonical partition function is

$$Q(\beta, \mu) = \mathrm{Tr}_{\mathcal{F}} e^{-\beta(H-\mu N)}, \tag{2.1}$$

where $\mathrm{Tr}_{\mathcal{F}}$ is the trace over the Fock space of fermions, which will be explained later in this section. The pressure is

$$P_{GC}(\beta, \mu) = \frac{1}{\beta} \ln Q(\beta, \mu). \tag{2.2}$$

From this point we need some thermodynamics to obtain the energy of the system. The free energy is obtained from the pressure (which is the opposite of the grand potential) by a Legendre transformation with regards to μ:

$$F = E - TS = -P + \mu N. \tag{2.3}$$

In the zero temperature limit, the term with entropy S vanishes, and the energy is equal to the free energy.

The grand-canonical description corresponds to a system of particles in contact with a heat and particle reservoir. We however consider a physical system with a fixed number of particles N, in the ground state. In the grand-canonical ensemble the number of particles N is not fixed, there is a mean value $N_{GC}(\beta, \mu)$. In the zero temperature limit, we evaluate this mean value as a function of μ, leading to $N(\mu)$. We then impose this function to be an integer

$$N(\mu) = N. \tag{2.4}$$

This relation gives μ as a function of N.

A similar treatment could be done in the canonical ensemble, by writing the canonical partition function using

$$\delta_{N,M} = \int_{-\pi}^{\pi} \frac{\mathrm{d}\theta}{2\pi} e^{(i\theta+\beta\mu)(M-N)}. \tag{2.5}$$

The canonical partition function is then written as

$$Q_C = \sum_{M=1}^{\infty} \int_{-\pi}^{\pi} \frac{\mathrm{d}\theta}{2\pi} e^{(i\theta+\beta\mu)(M-N)} \mathrm{Tr} e^{-\beta H_M} = \int_{-\pi}^{\pi} \frac{\mathrm{d}\theta}{2\pi} e^{-(i\theta+\beta\mu)N} Q_{GC}(\beta, \mu + \frac{i\theta}{\beta}). \tag{2.6}$$

In the large N limit, the chemical potential is evaluated with a saddle point integration over θ, which leads to the same relation between N and μ, at lowest order, than what we find in the grand-canonical formalism. It remains to be verified if this relation is the same at higher orders.

Let's note that the usual Hartree Fock approach (used in Lieb (1976), for example) also makes use of the grand canonical ensemble: an energy functional is minimized, under the constraint $\int \mathrm{d}^d \boldsymbol{x} \rho(\boldsymbol{x}) = N$, making a chemical potential appear as a Lagrange multiplier.

2.1 Scaling

The general hamiltonian of a system of N interacting fermions is, in appropriate units,

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hat{\Delta}_i}{2} + \sum_{i=1}^{N} \hat{V}_{ext}(\hat{\boldsymbol{x}}_i) + \frac{1}{2} \sum_{i,j=1, i\neq j}^{N} \hat{V}(\hat{\boldsymbol{x}}_i, \hat{\boldsymbol{x}}_j), \tag{2.7}$$

where $\hat{V}_{ext}$ is the external confining potential, and $\hat{V}$ is the interacting potential, which will only depend on the interparticle distance:

$$\hat{V}(\hat{\boldsymbol{x}}_i, \hat{\boldsymbol{x}}_j) = \hat{V}(|\hat{\boldsymbol{x}}_i - \hat{\boldsymbol{x}}_j|), \tag{2.8}$$

and is therefore symmetric.

What does "appropriate units" mean? It means that we are working in a system of units in which all the fundamental constants of the system ($\hbar, m$, the confining potential constant, the interaction potential constant e) are set to 1, as it was done in equation (1.6) for the atoms. This can be performed for any system, and will be done in chapter 5 in the case of quantum dots.

To identify our framework we perform relevant scalings. Let's proceed to the scaling of the length unit

$$\hat{\boldsymbol{x}} \mapsto \boldsymbol{x} \doteq \frac{\hat{\boldsymbol{x}}}{N^{\lambda}} \quad \Rightarrow \quad \frac{\partial^k}{\partial \hat{x}_i^k} \mapsto \frac{\partial^k}{\partial x_i^k} = N^{k\lambda} \frac{\partial^k}{\partial \hat{x}_i^k}, \tag{2.9}$$

as well as the scaling of the energy

$$\hat{H} \mapsto H \doteq \frac{\hat{H}}{N^\gamma}. \tag{2.10}$$

We now want to find optimal values for λ and γ. The new hamiltonian H is

$$H = -\frac{1}{N^{(\gamma+2\lambda)}}\sum_{i=1}^{N}\frac{\Delta_i}{2} + \sum_{i=1}^{N}\frac{1}{N^\gamma}\hat{V}_{ext}(N^\lambda \boldsymbol{x}_i) + \frac{1}{2}\sum_{i,j=1, i\neq j}^{N}\frac{1}{N^\gamma}\hat{V}(N^\lambda \boldsymbol{x}_i, N^\lambda \boldsymbol{x}_j). \tag{2.11}$$

To proceed further we need some information on the confining and interacting potentials. We need to know how they scale. For simplification we will consider a special case: the three-dimensional electron-electron interaction:

$$V(\boldsymbol{x}_i, \boldsymbol{x}_j) = \frac{1}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}. \tag{2.12}$$

Let's note that this will be the interaction in the two cases we will study later (atom and quantum dot).

The energy (2.11) becomes

$$H = -\frac{1}{N^{(\gamma+2\lambda)}}\sum_{i=1}^{N}\frac{\Delta_i}{2} + \sum_{i=1}^{N}\frac{1}{N^\gamma}\hat{V}_{ext}(N^\lambda \boldsymbol{x}_i) + \frac{1}{2}\frac{1}{N^{\gamma+\lambda}}\sum_{i,j=1, i\neq j}^{N}\frac{1}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}. \tag{2.13}$$

The main idea of considering a large number of particles N is that one particle (the particle i) will feel the mean energy of all others, which will be

$$\frac{1}{N^{\gamma+\lambda}}\underbrace{\sum_{j=1, j\neq i}^{N}\frac{1}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}}_{\mathcal{O}(N)}. \tag{2.14}$$

This mean energy will be of the order of 1 if

$$\gamma + \lambda = 1. \tag{2.15}$$

This is the first condition on these parameters. The second one will be obtained by imposing the density to be normalized to N. We know from usual semiclassical results that the density is given by $\rho \sim \frac{1}{\hbar^d}$, where $\hbar^2$ is the prefactor of $\frac{\Delta}{2}$, which is $\hbar = \frac{1}{N^{\frac{\gamma}{2}+\lambda}}$ in our problem. Let's suppose that this value is small, which allows us to work in the semiclassical regime. This hypothesis will be verified *a posteriori.* Moreover we want the density to be of the order of N for an N-particle system. This leads to the second condition:

$$d\gamma + 2d\lambda = 2. \tag{2.16}$$

These two conditions lead to

$$\left\{ \begin{array}{lcl} \gamma & = & 2-\frac{2}{d}, \\ \lambda & = & \frac{2}{d}-1. \end{array} \right.$$

Returning to the hamiltonian (2.13) we find

$$H = -\frac{1}{N^{\frac{2}{d}}}\sum_{i=1}^{N}\frac{\Delta_i}{2} + \sum_{i=1}^{N}\frac{1}{N^{2-\frac{2}{d}}}\hat{V}_{ext}(N^{\frac{2}{d}-1}\boldsymbol{x}_i) + \frac{1}{2}\frac{1}{N}\sum_{i,j=1,i\neq j}^{N}\frac{1}{|\boldsymbol{x}_i-\boldsymbol{x}_j|}. \tag{2.17}$$

As supposed for the calculation, we are in the semiclassical regime: the prefactor of $\frac{\Delta}{2}$ is $\frac{1}{N^{\frac{2}{d}}} \ll 1$.

Let's have a look at the case of the neutral atom. In this case the dimension is $d = 3$, and the confining potential $\hat{V}_{ext}(\hat{\boldsymbol{x}}) = \frac{N}{|\hat{\boldsymbol{x}}|}$. Applying the scaling we find $V_{ext}(\boldsymbol{x}) = \frac{1}{N^{2-\frac{2}{d}}}\hat{V}_{ext}(N^{\frac{2}{d}-1}\boldsymbol{x}) = \frac{1}{|\boldsymbol{x}|}$. The scaling is perfect, in the sense that N has totally disappeared from the confining potential. For the atom we have $\hbar = N^{\frac{1}{3}}$, and the length scale is of the order of $N^{\frac{1}{3}}$. These are well-known results.

The case of quantum dots is treated in a similar way. It is a two-dimensional system (as will be explained later), the interacting potential is the same, and the confining potential is sometimes modeled as $\hat{V}(\hat{\boldsymbol{x}}) = \frac{1}{2}\kappa N\hat{\boldsymbol{x}}^2$. The factor N is "unnatural": the confining potential should not, *a priori*, depend on the number of electrons. We introduce it however, in order to have a system which scales as we want. We will justify this approach later (we can consider either (N, κ) or $(N, k = \kappa N)$, where k would be the real confining strength). We find $\hbar = N^{\frac{1}{2}}$, and the length scale is of the order of $N^0 = 1$. (We will see later that this length scale depends on κ, which, in the end, depends itself on N. We will find that the length scale is finally of the order of $N^{\frac{1}{2}}$.)

We want to determine the energy of the following hamiltonian (writing $\frac{1}{N^{2-\frac{2}{d}}}\hat{V}_{ext}(N^{\frac{2}{d}-1}\boldsymbol{x}) \doteq V_{ext}(\boldsymbol{x})$):

$$H = -\epsilon^2\sum_{i=1}^{N}\Delta_i + \sum_{i=1}^{N}V_{ext}(\boldsymbol{x}_i) + \frac{1}{2}\frac{1}{N}\sum_{i,j=1,i\neq j}^{N}\frac{1}{|\boldsymbol{x}_i-\boldsymbol{x}_j|}, \tag{2.18}$$

where $\epsilon^2 = \frac{1}{2N^{\frac{2}{d}}}$. We note $\hbar \doteq \epsilon$ to avoid a wrong physical interpretation.

2.2 Partition Function

As explained in the introduction, we first express the grand-canonical partition function. It consists of considering a system whose particle number is not fixed.

The second quantization is therefore best adapted, and the hamiltonian (2.18) becomes, in the $\{|\boldsymbol{x}\rangle\}$ representation, including the spin σ:

$$\begin{aligned}\hat{H} &= \sum_{\sigma=1}^{s} \int \mathrm{d}^d\boldsymbol{x} \hat{\psi}^\dagger(\boldsymbol{x},\sigma)[-\epsilon^2\Delta + V_{ext}(\boldsymbol{x})]\hat{\psi}(\boldsymbol{x},\sigma) \\ &+ \frac{1}{2}\frac{1}{N}\sum_{\sigma,\sigma'=1}^{s} \int \mathrm{d}^d\boldsymbol{x} \int \mathrm{d}^d\boldsymbol{y} \hat{\psi}^\dagger(\boldsymbol{x},\sigma)\hat{\psi}^\dagger(\boldsymbol{y},\sigma')V(\boldsymbol{x},\boldsymbol{y})\hat{\psi}(\boldsymbol{y},\sigma')\hat{\psi}(\boldsymbol{x},\sigma), \quad (2.19)\end{aligned}$$

where $\hat{\psi}^\dagger(\boldsymbol{x},\sigma)$, $\hat{\psi}(\boldsymbol{x},\sigma)$ are the creation and annihilation operators of the state $|\boldsymbol{x},\sigma\rangle$. The spin σ does not influence the energy; it only has an effect on the degeneracy of states. We consider a spin which can take an arbitrary number of values s. For the electrons we will take $s = 2$.

The grand-canonical partition function is given by the trace

$$Q(\beta,\mu) = \mathrm{Tr}_{\mathcal{F}} e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}, \quad (2.20)$$

where $\hat{N} = \sum_{\sigma=1}^{s} \int \mathrm{d}^d\boldsymbol{x}\hat{\psi}^\dagger(\boldsymbol{x},\sigma)\hat{\psi}(\boldsymbol{x},\sigma)$ is the operator which counts the number of particles. $\mathcal{F}$ is the Fock space (for fermions), which consists of all the possible antisymmetrized quantum states of N particles, N varying from 0 to ∞: $\mathcal{F} = \oplus_{N=0}^{\infty}\mathcal{F}_N$, where $\mathcal{F}_N$ is the space of states of an N-particle system. It is constructed from the one-particle Hilbert space $\mathcal{H}$ by antisymmetrizing its N-tensor product: $\mathcal{F}_N = \mathcal{A}\left(\mathcal{H}^{\otimes N}\right)$.

There are various techniques to evaluate this partition function. We will perform the Fock space integration by using functional integration over Grassmann variables, which are anticommuting variables. This approach consists of integrating over the set of all coherent states of the system, which forms a (overcomplete) basis. The coherent states have the strange property of not being states with a fixed number of particles (they are not eigenvectors of $\hat{N}$). Moreover, in the case of fermions, they do not even belong to the Fock space, which thus has to be extended. They also imply the necessity to introduce a new kind of object, the Grassmann variables. A good explanation is given in the book of Negele and Orland (1988), from which our notations are taken.

Using functional integration over Grassmann variables we find

$$Q(\beta,\mu) = \int \mathcal{D}\psi^\star\mathcal{D}\psi e^{-S[\psi^\star,\psi]}, \quad (2.21)$$

where the action is

$$\begin{aligned} S[\psi^\star,\psi] &= \sum_{\sigma=1}^{s}\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}t\psi^\star(\boldsymbol{x},\sigma,t)\left[\partial_t+(-\epsilon^2\Delta+V_{ext}(\boldsymbol{x}))-\mu\right]\psi(\boldsymbol{x},\sigma,t) \\ &\quad +\frac{1}{2}\frac{1}{N}\sum_{\sigma_1,\sigma_2=1}^{s}\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}t_1\mathrm{d}^d\boldsymbol{x}_2\mathrm{d}t_2\psi^\star(\boldsymbol{x}_1,\sigma_1,t_1)\psi^\star(\boldsymbol{x}_2,\sigma_2,t_2) \\ &\quad \times V(\boldsymbol{x}_1,\boldsymbol{x}_2)\delta(t_1-t_2)\psi(\boldsymbol{x}_2,\sigma_2,t_2)\psi(\boldsymbol{x}_1,\sigma_1,t_1). \end{aligned} \tag{2.22}$$

The integration over the positions $(\boldsymbol{x},\boldsymbol{x}_1,\boldsymbol{x}_2)$ runs over the entire space and the integration over the imaginary times (t,t_1,t_2) from 0 to β.

The boundary conditions are antiperiodic:

$$\psi(\boldsymbol{x},\sigma,0)=-\psi(\boldsymbol{x},\sigma,\beta) \tag{2.23}$$

in a continuous description of the problem.

Let's note that the integration is

$$\int\mathcal{D}\psi^\star\mathcal{D}\psi=\int\prod_{\sigma=1}^{s}\mathcal{D}\psi^\star(\cdot,\sigma,\cdot)\mathcal{D}\psi(\cdot,\sigma,\cdot). \tag{2.24}$$

We integrate over s fields, each corresponding to a given value of the spin.

If the action S were quadratic in $(\psi^\star,\psi)$, an exact solution could be found. Hence, using an integration equality for the second term, we will express this action as a quadratic form in those fields. This integration equality, known as the Hubbard-Stratonovich transform, is

$$e^{-\frac{1}{2}(\rho|\frac{V}{N}|\rho)}=\frac{\int\mathcal{D}\phi e^{-\frac{N}{2}(\phi|V^{-1}|\phi)+i(\rho|\,\phi)}}{\int\mathcal{D}\phi e^{-\frac{N}{2}(\phi|V^{-1}|\phi)}}, \tag{2.25}$$

where we used the notation

$$(f|\,A\,|g)\doteq\int\mathrm{d}^d\boldsymbol{x}_1\mathrm{d}t_1\mathrm{d}^d\boldsymbol{x}_2\mathrm{d}t_2 f(\boldsymbol{x}_1,t_1)A(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)g(\boldsymbol{x}_2,t_2) \tag{2.26}$$

and

$$(f|\,g)\doteq\int\mathrm{d}^d\boldsymbol{x}\mathrm{d}tf(\boldsymbol{x},t)g(\boldsymbol{x},t), \tag{2.27}$$

the real scalar product.

This equality is very well known in field theory and was already applied to systems of fermions by Blaizot and Orland (1981) and Rebei and Hitchon (2003), even to the specific problem of atoms by Dietz et al. (1982). In a non continuous formulation this equality states that the Fourier transform of a gaussian is a gaussian.

In this formula ϕ is a real variable, and ρ is chosen

$$\rho(\boldsymbol{x},t)=\sum_{\sigma=1}^{s}\psi^{\star}(\boldsymbol{x},\sigma,t)\psi(\boldsymbol{x},\sigma,t) \tag{2.28}$$

and has the physical interpretation of a density. The integral operator V is

$$V(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)=V(\boldsymbol{x}_1,\boldsymbol{x}_2)\delta(t_1-t_2), \tag{2.29}$$

its inverse being simply

$$V^{-1}(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)=V^{-1}(\boldsymbol{x}_1,\boldsymbol{x}_2)\delta(t_1-t_2). \tag{2.30}$$

Introducing equality (2.25) in equation (2.21) we find

$$Q=\frac{1}{\mathcal{N}}\int\mathcal{D}\phi\mathcal{D}\psi^{\star}\mathcal{D}\psi e^{-S[\phi,\psi^{\star},\psi]}, \tag{2.31}$$

where the action is

$$\begin{aligned} S[\phi,\psi^{\star},\psi] \;&=\; \frac{N}{2}\left(\phi\right|V^{-1}\left|\phi\right)+\sum_{\sigma=1}^{s}\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}t\psi^{\star}(\boldsymbol{x},\sigma,t)\big[\partial_t+ \\ &\qquad +(-\epsilon^2\Delta+V_{ext}(\boldsymbol{x}))-\mu-i\phi(\boldsymbol{x},t)\big]\psi(\boldsymbol{x},\sigma,t), \end{aligned} \tag{2.32}$$

and the normalization constant

$$\mathcal{N}=\int\mathcal{D}\phi e^{-\frac{N}{2}(\phi|V^{-1}|\phi)}. \tag{2.33}$$

The action is now a quadratic form in the Grassmann variables, its exact calculation could be performed. However, we would then have to evaluate a complicated expression of ϕ with a gaussian measure, which would be hard to treat. This is why we proceed, taking advantage of the large factor N of the gaussian measure, to the change of variables

$$\phi(\boldsymbol{x},t)\mapsto\theta(\boldsymbol{x},t),\quad \phi(\boldsymbol{x},t)\doteq\frac{\theta(\boldsymbol{x},t)}{\sqrt{N}}+iW(\boldsymbol{x}), \tag{2.34}$$

where the shift will be useful for canceling terms out, $W(\boldsymbol{x})$ being determined self-consistently later.

In these new variables, the partition function (2.31) becomes

$$Q=\frac{1}{\mathcal{N}}\int\mathcal{D}\theta\mathcal{D}\psi^{\star}\mathcal{D}\psi e^{-S[\theta,\psi^{\star},\psi]}, \tag{2.35}$$

where the action is

$$\begin{aligned} S[\theta,\psi^\star,\psi] &= \frac{1}{2}\left(\theta\right|V^{-1}\left|\theta\right) + i\sqrt{N}\left(\theta\right|V^{-1}\left|W\right) - \frac{N}{2}\left(W\right|V^{-1}\left|W\right) \\ &\quad + \sum_{\sigma=1}^{s}\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}t\psi^\star(\boldsymbol{x},\sigma,t)\Bigg[\partial_t + (-\epsilon^2\Delta + V_{ext}(\boldsymbol{x}) + W(\boldsymbol{x})) \\ &\qquad\qquad -\mu - i\frac{\theta(\boldsymbol{x},t)}{\sqrt{N}}\Bigg]\psi(\boldsymbol{x},\sigma,t), \end{aligned} \tag{2.36}$$

and the normalization constant is

$$\mathcal{N} = \int \mathcal{D}\theta e^{-\frac{1}{2}(\theta|V^{-1}|\theta)}. \tag{2.37}$$

The integration over the Grassmann variables can now be performed exactly. Writing

$$\frac{1}{\mathcal{N}}\int \mathcal{D}\theta e^{-\frac{1}{2}(\theta|V^{-1}|\theta)} f(\theta) \doteq \langle f(\theta)\rangle_{\theta,V^{-1}}, \tag{2.38}$$

we obtain

$$Q = e^{\frac{N}{2}(W|V^{-1}|W)}\left\langle e^{-i\sqrt{N}(\theta|V^{-1}|W)}\det{}^s\left(K - \frac{i\theta}{\sqrt{N}}\right)\right\rangle_{\theta,V^{-1}}, \tag{2.39}$$

where K is the integral operator with the kernel

$$K(\boldsymbol{x}_1,t_1\boldsymbol{x}_2,t_2) \doteq \delta(t_1-t_2)\delta(\boldsymbol{x}_1-\boldsymbol{x}_2)\Big(\partial_{t_1} + \underbrace{\left(-\epsilon^2\Delta_1 + V_{ext}(\boldsymbol{x}_1) + W(\boldsymbol{x}_1)\right)}_{\doteq h(\boldsymbol{x}_1)} - \mu\Big), \tag{2.40}$$

and θ is seen as a diagonal operator, whose kernel is

$$\theta(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2) = \delta(t_1-t_2)\delta(\boldsymbol{x}_1-\boldsymbol{x}_2)\theta(\boldsymbol{x}_1,t_1). \tag{2.41}$$

The expression (2.39) is a very good starting point for a perturbative expansion using the small parameter $\frac{1}{\sqrt{N}}$. We use

$$\begin{aligned} \det{}^s\left(K - i\frac{\theta}{\sqrt{N}}\right) &= \det{}^s K\det{}^s\left(\mathbb{1} - \frac{i}{\sqrt{N}}K^{-1}\theta\right) \\ &= \det{}^s K e^{s\mathrm{Tr}\ln\left(\mathbb{1} - \frac{i}{\sqrt{N}}K^{-1}\theta\right)} \\ &= \det{}^s K\exp\left(- \frac{is}{\sqrt{N}}\mathrm{Tr}\left(K^{-1}\theta\right) + \frac{s}{2N}\mathrm{Tr}\left(K^{-1}\theta\right)^2\right) \\ &\quad\times\exp\left(\frac{is}{3N^{\frac{3}{2}}}\mathrm{Tr}\left(K^{-1}\theta\right)^3 - \frac{s}{4N^2}\mathrm{Tr}\left(K^{-1}\theta\right)^4 + \mathcal{O}\left(N^{-\frac{5}{2}}\right)\right). \end{aligned} \tag{2.42}$$

The first term of the expansion will be used to compensate exactly the term linear in θ of the action of the partition function (2.39). This will lead to the self-consistent equation, which determines W.

The second term will be treated perturbatively, using the gaussian measure for the real variables θ. Its treatment is the one-loop expansion. The third term will not contribute: the measure is gaussian, hence at this order, an odd term in θ will be zero. The fourth term will also be treated perturbatively, using Wick's theorem. It corresponds to the two-loop expansion.

2.2.1 Propagator

Before proceeding to these developments, let's determine the inverse operator K^{-1}. It is a propagator, we note it G. More precisely it is the propagator of a one-body problem of fermions, with the hamiltonian (written in second quantization)

$$\hat{h} = \int \mathrm{d}^d\boldsymbol{x}\hat{\psi}^\dagger(\boldsymbol{x},\sigma)[-\epsilon^2\Delta + V_{ext}(\boldsymbol{x}) + W(\boldsymbol{x})]\hat{\psi}(\boldsymbol{x},\sigma). \tag{2.43}$$

Let's note that it is the hamiltonian of the system with fixed spin σ. In the following developments, the spin indices will be implicit.

We can already anticipate our results by giving a physical interpretation of W: it will correspond to the mean field potential.

h is a one-body hamiltonian, whose eigenvectors $\{\psi_\alpha\}_{\alpha\geq 1}$ clearly form a basis of the one-particle quantum states. A detailed study in the book of Negele and Orland (1988) leads to the result

$$\begin{aligned} G_{\alpha,\beta}(t_1,t_2) &= \langle\psi_\alpha|G(t_1,t_2)|\psi_\beta\rangle \\ &= e^{-(e_\alpha-\mu)(t_1-t_2)}\left[\theta(t_1-t_2-\epsilon) - \frac{1}{(e^{\beta(e_\alpha-\mu)}+1)}\right]\delta_{\alpha,\beta} \\ &= \langle\psi_\alpha|\sum_\gamma e^{-(e_\gamma-\mu)(t_1-t_2)}\left[\theta(t_1-t_2-\epsilon) - \frac{1}{(e^{\beta(e_\gamma-\mu)}+1)}\right]|\psi_\gamma\rangle\langle\psi_\gamma|\psi_\beta\rangle \\ &= \langle\psi_\alpha|e^{-(h-\mu)(t_1-t_2)}\left[\theta(t_1-t_2-\epsilon) - \frac{1}{(e^{\beta(h-\mu)}+1)}\right]|\psi_\beta\rangle \\ &= \langle\psi_\alpha|e^{-(h-\mu)(t_1-t_2)}\left[\theta(t_1-t_2-\epsilon) - f_\beta(h-\mu)\right]|\psi_\beta\rangle, \end{aligned} \tag{2.44}$$

where we introduced a small parameter $\epsilon \to 0$ to deal with the discontinuity problem at times $t_1 = t_2$. We introduced the Fermi-Dirac distribution

$$f_\beta(e-\mu) \doteq \frac{1}{e^{\beta(e-\mu)}+1}. \tag{2.45}$$

In an operator description, this result is

$$G(t_1,t_2) = e^{-(h-\mu)(t_1-t_2)}\left[\theta(t_1-t_2-\epsilon) - f_\beta(h-\mu)\right]. \tag{2.46}$$

It leads to

$$\begin{aligned}G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)&=\langle\boldsymbol{x}_1|G(t_1,t_2)|\boldsymbol{x}_2\rangle\\&=\langle\boldsymbol{x}_1|\sum_\alpha e^{-(e_\alpha-\mu)(t_1-t_2)}\left[\theta(t_1-t_2-\epsilon)-f_\beta(e_\alpha-\mu)\right]|\psi_\alpha\rangle\langle\psi_\alpha|\boldsymbol{x}_2\rangle\\&=\sum_\alpha e^{-(e_\alpha-\mu)(t_1-t_2)}\left[\theta(t_1-t_2-\epsilon)-f_\beta(e_\alpha-\mu)\right]\psi^\star_\alpha(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1).\end{aligned} \tag{2.47}$$

Hence, if $t_1 > t_2$ the propagator will be

$$G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)=\sum_\alpha e^{-(e_\alpha-\mu)(t_1-t_2)}\left[1-f_\beta(e_\alpha-\mu)\right]\psi^\star_\alpha(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1), \tag{2.48}$$

for $t_1 < t_2$

$$G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)=-\sum_\alpha e^{-(e_\alpha-\mu)(t_1-t_2)}f_\beta(e_\alpha-\mu)\psi^\star_\alpha(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1), \tag{2.49}$$

and for $t_1 = t_2 = t$

$$G(\boldsymbol{x}_1,t,\boldsymbol{x}_2,t)=-\sum_\alpha f_\beta(e_\alpha-\mu)\psi^\star_\alpha(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1)=-\rho^\sigma_{FD}(\boldsymbol{x}_2,\boldsymbol{x}_1), \tag{2.50}$$

where $\rho^\sigma_{FD}(\boldsymbol{x}_2,\boldsymbol{x}_1)$ is the two-body density matrix, with the Fermi-Dirac statistics, for particles with fixed spin σ. The total two-body density matrix is

$$\rho_{FD}(\boldsymbol{x}_2,\boldsymbol{x}_1)=\sum_{\sigma=1}^{s}\rho^\sigma_{FD}(\boldsymbol{x}_2,\boldsymbol{x}_1)=s\rho^\sigma_{FD}(\boldsymbol{x}_2,\boldsymbol{x}_1), \tag{2.51}$$

because $\rho^\sigma_{FD}(\boldsymbol{x}_2,\boldsymbol{x}_1)$ is independent of σ.

For times $t_1 = t_2 = t$ and positions $\boldsymbol{x}_1 = \boldsymbol{x}_2 = \boldsymbol{x}$ we find

$$G(\boldsymbol{x},t,\boldsymbol{x},t)=-\sum_\alpha f_\beta(e_\alpha-\mu)\psi^\star_\alpha(\boldsymbol{x})\psi_\alpha(\boldsymbol{x})=-\rho^\sigma_{FD}(\boldsymbol{x}), \tag{2.52}$$

where $\rho^\sigma_{FD}(\boldsymbol{x})$ is the fermion density with the Fermi-Dirac statistics, for particles with fixed spin σ. The total density is

$$\rho_{FD}(\boldsymbol{x})=\sum_{\sigma=1}^{s}\rho^\sigma_{FD}(\boldsymbol{x})=s\rho^\sigma_{FD}(\boldsymbol{x}). \tag{2.53}$$

In the zero temperature limit, using

$$f_\beta(e-\mu)\overset{\beta\to\infty}{\longrightarrow}\theta(\mu-e), \tag{2.54}$$

we obtain

$$G(\boldsymbol{x}_1,t,\boldsymbol{x}_2,t)\overset{\beta\to\infty}{\longrightarrow}-\rho^\sigma(\boldsymbol{x}_2,\boldsymbol{x}_1),\qquad G(\boldsymbol{x},t,\boldsymbol{x},t)\overset{\beta\to\infty}{\longrightarrow}-\rho^\sigma(\boldsymbol{x}),\tag{2.55}$$

which are the two-body density matrix and the density of a system of N particles in the ground state, for particles with fixed spin σ. The total density matrix is

$$\rho(\boldsymbol{x}_2,\boldsymbol{x}_1)=\sum_{\sigma=1}^{s}\rho^\sigma(\boldsymbol{x}_2,\boldsymbol{x}_1)=s\rho^\sigma(\boldsymbol{x}_2,\boldsymbol{x}_1).\tag{2.56}$$

The density $\rho^\sigma(\boldsymbol{x})$ is normalized to $\frac{N}{s}$, and the total density is given by

$$\rho(\boldsymbol{x})=\sum_{\sigma=1}^{s}\rho^\sigma(\boldsymbol{x})=s\rho^\sigma(\boldsymbol{x}).\tag{2.57}$$

We will also use the result

$$[1-f_\beta(e-\mu)]\overset{\beta\to\infty}{\longrightarrow}\theta(e-\mu).\tag{2.58}$$

Let's finally note that, when evaluated at equal times $t_1=t_2$, the propagator is time-independent.

2.2.2 Self-consistent equation

Introducing (2.42) in the partition function (2.39) we determine W such that the term linear in θ is eliminated.

To proceed we still need to have an explicit expression of the following objects (using (2.41) and (2.52)):

$$\begin{aligned}\mathrm{Tr}(G\theta)&=\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}t_1\mathrm{d}^d\boldsymbol{x}_2\mathrm{d}t_2G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)\theta(\boldsymbol{x}_2,t_2,\boldsymbol{x}_1,t_1)\\&=\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}tG(\boldsymbol{x},t,\boldsymbol{x},t)\theta(\boldsymbol{x},t)=-\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}t\rho^\sigma_{FD}(\boldsymbol{x})\theta(\boldsymbol{x},t),\end{aligned}\tag{2.59}$$

and

$$\begin{aligned}(\theta|\,V^{-1}\,|W)&=\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}t_1\mathrm{d}^d\boldsymbol{x}_2\mathrm{d}t_2\theta(\boldsymbol{x}_1,t_1)V^{-1}(\boldsymbol{x}_1,\boldsymbol{x}_2)\delta(t_1-t_2)W(\boldsymbol{x}_2)\\&=\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{x}_2\mathrm{d}t\theta(\boldsymbol{x}_1,t)V^{-1}(\boldsymbol{x}_1,\boldsymbol{x}_2)W(\boldsymbol{x}_2).\end{aligned}\tag{2.60}$$

It leads to the following self-consistent equation:

$$i\sqrt{N}\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}t\left\{-\int \mathrm{d}^d\boldsymbol{y}V^{-1}(\boldsymbol{x},\boldsymbol{y})W(\boldsymbol{y})+\frac{1}{N}\underbrace{s\rho^\sigma_{FD}(\boldsymbol{x})}_{=\rho_{FD}(\boldsymbol{x})}\right\}\theta(\boldsymbol{x},t)=0.\tag{2.61}$$

We impose this result to be verified for any function θ, hence the self-consistent equation is

$$\int \mathrm{d}^d\boldsymbol{y} V^{-1}(\boldsymbol{x},\boldsymbol{y})W(\boldsymbol{y}) = \frac{1}{N}\rho_{FD}(\boldsymbol{x}). \tag{2.62}$$

Applying V on the left we find

$$W(\boldsymbol{x}) = \frac{1}{N}\int \mathrm{d}^d\boldsymbol{y} V(\boldsymbol{x},\boldsymbol{y})\rho_{FD}(\boldsymbol{y}). \tag{2.63}$$

This is a self-consistent equation for W: the density ρ is the density of a one-body problem, with a one-body hamiltonian h depending itself on W (equation (2.43)). Let's replace W in this hamiltonian by its calculated value:

$$h = \int \mathrm{d}^d\boldsymbol{x}\hat{\psi}^\dagger(\boldsymbol{x})\left[-\epsilon^2\Delta + V_{ext}(\boldsymbol{x}) + \frac{1}{N}\int \mathrm{d}^d\boldsymbol{y} V(\boldsymbol{x},\boldsymbol{y})\rho_{FD}(\boldsymbol{y})\right]\hat{\psi}(\boldsymbol{x}). \tag{2.64}$$

The interpretation of this term is now completely clear: it consists of the mean potential produced by the other electrons, acting on an electron.

2.2.3 Final partition function

Let's replace W by its expression (2.63) in

$$\left(W\right| V^{-1} \left|W\right) = \frac{1}{N^2}\left(\rho_{FD}\right| V \left|\rho_{FD}\right) = \frac{\beta}{N^2}\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}^d\boldsymbol{y} V(\boldsymbol{x},\boldsymbol{y})\rho_{FD}(\boldsymbol{x})\rho_{FD}(\boldsymbol{y}), \tag{2.65}$$

where we performed explicitly the integration over the imaginary times (which provides a factor β).

We can now write the partition function (2.39), using (2.42) and (2.65). Moreover we do not write the term cubic in θ (which will not contribute at this order, as it is a gaussian process):

$$Q = \det{}^s K e^{\frac{\beta}{2N}\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}^d\boldsymbol{y} V(\boldsymbol{x},\boldsymbol{y})\rho_{FD}(\boldsymbol{x})\rho_{FD}(\boldsymbol{y})}\left\langle e^{\frac{s}{2N}\mathrm{Tr}(G\theta)^2 - \frac{s}{4N^2}\mathrm{Tr}(G\theta)^4 + \mathcal{O}(N^{-3})}\right\rangle_{\theta,V^{-1}}. \tag{2.66}$$

The remaining term is of the order of N^3, because the term of order $N^{\frac{5}{2}}$ is an odd power of θ (θ^5).

The term we have to evaluate with the gaussian measure contains a term which is an exponential of a quadratic form in θ. Let's write it explicitly:

$$\begin{aligned} s\mathrm{Tr}(G\theta)^2 &= s\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}t_1\mathrm{d}^d\boldsymbol{x}_2\mathrm{d}t_2 G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)G(\boldsymbol{x}_2,t_2,\boldsymbol{x}_1,t_1)\theta(\boldsymbol{x}_1,t_1)\theta(\boldsymbol{x}_2,t_2) \\ &\doteq \left(\theta\right|\Gamma\left|\theta\right), \end{aligned} \tag{2.67}$$

where we defined

$$\Gamma(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2) = sG(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)G(\boldsymbol{x}_2,t_2,\boldsymbol{x}_1,t_1). \tag{2.68}$$

The partition function can now be written as

$$\begin{aligned} Q \;=\; & \underbrace{\det{}^s K}_{\doteq Q_1}\, \underbrace{e^{\frac{\beta}{2N}\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}^d\boldsymbol{y} V(\boldsymbol{x},\boldsymbol{y})\rho_{FD}(\boldsymbol{x})\rho_{FD}(\boldsymbol{y})}}_{\doteq Q_2}\, \underbrace{\frac{\int \mathcal{D}\theta e^{-\frac{1}{2}(\theta|V^{-1}-\frac{\Gamma}{N}|\theta)}}{\int \mathcal{D}\theta e^{-\frac{1}{2}(\theta|V^{-1}|\theta)}}}_{\doteq Q_3} \\ & \times \underbrace{\left\langle e^{-\frac{s}{4N^2}\mathrm{Tr}(G\theta)^4+\mathcal{O}(N^{-3})} \right\rangle_{\theta,\left(V^{-1}-\frac{\Gamma}{N}\right)}}_{\doteq Q_4} . \end{aligned} \tag{2.69}$$

2.3 Ground state pressure

Introducing the partition function (2.69) in (2.2) we observe that the ground state pressure is a sum of four contributions:

$$P(N) = \lim_{\beta\to\infty} \frac{1}{\beta} \ln Q = \sum_{i=1}^{4} P_i = \sum_{i=1}^{4} \lim_{\beta\to\infty} \frac{1}{\beta} \ln Q_i. \tag{2.70}$$

Let's discuss and develop these four terms separately.

2.3.1 P_1

The first contribution to the pressure, P_1, is

$$P_1 = \lim_{\beta\to\infty} \frac{1}{\beta} \det{}^s K, \tag{2.71}$$

where K is the operator

$$K = \partial_t + h - \mu, \tag{2.72}$$

with h the one-body hamiltonian

$$h(\boldsymbol{x}) = -\epsilon^2\Delta + V(\boldsymbol{x}) + \frac{1}{N}\int \mathrm{d}^d\boldsymbol{y} V(\boldsymbol{x},\boldsymbol{y})\rho_{FD}(\boldsymbol{y}). \tag{2.73}$$

This pressure is simply the pressure of a system of free fermions, submitted to a mean-field potential. Due to the factor $\epsilon \ll 1$, the pressure can be treated in the semiclassical regime. This will be done in chapter 5 in the case of quantum dots. The limit of zero temperature implies $\rho_{FD} \to \rho$.

Let's note that the nature of the potential (in which only $\rho(\boldsymbol{x})$ is involved, not $\rho(\boldsymbol{x},\boldsymbol{y})$) is such that there is no exchange term. This exchange term will arise from the perturbative treatment[1].

---

[1] However, the exchange energy could arise from a one-body approach. A quite similar method including this exchange term was done by Dietz et al. (1982).

For $\beta \gg 1$, the determinant of K can be written as (Negele and Orland, 1988)

$$\det{}^s K = \prod_\alpha \left(1 + e^{-\beta(e_\alpha - \mu)}\right)^s \simeq \prod_{\{\alpha | e_\alpha < \mu\}} e^{-\beta s(e_\alpha - \mu)} \prod_{\{\beta | e_\beta > \mu\}} 1 = e^{-\beta \sum_{\{\alpha | e_\alpha < \mu\}} s(e_\alpha - \mu)}, \tag{2.74}$$

where e_α are the eigenvalues of the one-body operator h.

The pressure is therefore

$$P_1 = -s \left(\sum_{\alpha=1}^{N/s} e_\alpha \right) + \mu N. \tag{2.75}$$

A detailed treatment of this term, in the semiclassical limit, for a two-dimensional system, will be done in chapter 6 for the application to quantum dots.

2.3.2 P_2

The second contribution to the pressure, P_2, is

$$\begin{aligned} P_2 &= \lim_{\beta \to \infty} \frac{1}{\beta} \ln e^{\frac{\beta}{2N} \int \mathrm{d}^d\boldsymbol{x}\mathrm{d}^d\boldsymbol{y} V(\boldsymbol{x},\boldsymbol{y}) \rho_{FD}(\boldsymbol{x}) \rho_{FD}(\boldsymbol{y})} \\ &= \frac{1}{2N} \int \mathrm{d}^d\boldsymbol{x}\mathrm{d}^d\boldsymbol{y} V(\boldsymbol{x},\boldsymbol{y}) \rho(\boldsymbol{x}) \rho(\boldsymbol{y}). \end{aligned} \tag{2.76}$$

The interpretation of this term is simple: it corresponds to the opposite of the self-energy of the electrons. This self-energy is counted twice in P_1, it therefore has to be subtracted here.

The lowest order terms correspond to the Hartree approximation: it consists of the mean-field energy, without the exchange energy. Hence our approach (in which the expansion in inverse powers of N is controlled) shows that the dominant contribution is the semiclassical Hartree approximation. Let's note that it was proven by Lieb (1976) and Lieb et al. (1995) that the Hartree approximation is exact in the limit $N \to \infty$ for atoms as well as for dots.

These results ($P_1 + P_2$) can be obtained through another approach, as will be done later (see chapter 5), where we proceed to a semiclassical treatment of these terms.

2.3.3 P_3

The third contribution to the pressure, P_3, is obtained from Q_3, which we expand in powers of N^{-1} (by evaluating explicitly these gaussian integrals):

$$\begin{aligned}
Q_3 &= \frac{\int \mathcal{D}\theta e^{-\frac{1}{2}(\theta|V^{-1}-\frac{\Gamma}{N}|\theta)}}{\int \mathcal{D}\theta e^{-\frac{1}{2}(\theta|V^{-1}|\theta)}} \\
&= \left(\frac{\det(V^{-1})}{\det(V^{-1}-\frac{\Gamma}{N})}\right)^{\frac{1}{2}} \\
&= \frac{1}{\left(\det(\mathbb{1}-\frac{1}{N}V\Gamma)\right)^{\frac{1}{2}}} \\
&= \exp\left\{-\frac{1}{2}\mathrm{Tr}\ln\left(\mathbb{1}-\frac{1}{N}V\Gamma\right)\right\} \\
&= \exp\left\{\frac{1}{2N}\mathrm{Tr}(V\Gamma)+\frac{1}{4N^2}\mathrm{Tr}(V\Gamma)^2+\mathcal{O}(N^{-3})\right\}. \qquad (2.77)
\end{aligned}$$

The contribution to the pressure is therefore

$$P_3 = \lim_{\beta\to\infty}\frac{1}{\beta}\ln Q_3 = \lim_{\beta\to\infty}\frac{1}{\beta}\left(\frac{1}{2N}\mathrm{Tr}(V\Gamma)+\frac{1}{4N^2}\mathrm{Tr}(V\Gamma)^2+\mathcal{O}(N^{-3})\right). \qquad (2.78)$$

We have to calculate these terms explicitly. The first one is

$$\begin{aligned}
\mathrm{Tr}(V\Gamma) &= s\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}t_1\mathrm{d}^d\boldsymbol{x}_2\mathrm{d}t_2 V(\boldsymbol{x}_1,\boldsymbol{x}_2)\delta(t_1-t_2)G(\boldsymbol{x}_2,t_2,\boldsymbol{x}_1,t_1)G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2) \\
&= s\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{x}_2\mathrm{d}t V(\boldsymbol{x}_1,\boldsymbol{x}_2)\rho^\sigma_{FD}(\boldsymbol{x}_1,\boldsymbol{x}_2)\rho^\sigma_{FD}(\boldsymbol{x}_2,\boldsymbol{x}_1) \\
&= \beta s\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{x}_2 V(\boldsymbol{x}_1,\boldsymbol{x}_2)\rho^\sigma_{FD}(\boldsymbol{x}_1,\boldsymbol{x}_2)\rho^\sigma_{FD}(\boldsymbol{x}_2,\boldsymbol{x}_1), \qquad (2.79)
\end{aligned}$$

where we used the expression (2.50) for the propagator.

This term leads to the pressure

$$\begin{aligned}
P_3^1 &= \frac{s}{2N}\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}^d\boldsymbol{y}V(\boldsymbol{x},\boldsymbol{y})\rho^\sigma(\boldsymbol{x},\boldsymbol{y})\rho^\sigma(\boldsymbol{y},\boldsymbol{x}) \\
&= \frac{1}{2sN}\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}^d\boldsymbol{y}V(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{y},\boldsymbol{x}). \qquad (2.80)
\end{aligned}$$

The spin degeneracy was inserted in the density to obtain the total density. A factor $\frac{1}{s}$ appears.

The physical interpretation of this term is simple: it is the exchange energy of the system (with the right prefactor $\frac{1}{2s}$, as established in chapter 5 in the semiclassical Hartree-Fock developments). Hence, up to this order, the energy of the system is the Hartree-Fock energy. Our calculations therefore show that the semiclassical Hartree-Fock approach is exact up to a certain order in inverse powers of N.

Our approach shows that the Hartree-Fock approach is correct. But with this approach we can go beyond this, by calculating the next corrections. We will calculate corrections up to the order N^{-2}. The first one arises from Q_3. To calculate it we have to evaluate

$$\begin{aligned}\mathrm{Tr}(V\Gamma)^2 &= s^2\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\mathrm{d}t_i V(\boldsymbol{x}_1,\boldsymbol{x}_2)\delta(t_1-t_2)G(\boldsymbol{x}_2,t_2,\boldsymbol{x}_3,t_3)G(\boldsymbol{x}_3,t_3,\boldsymbol{x}_2,t_2)\\ &\qquad\times V(\boldsymbol{x}_3,\boldsymbol{x}_4)\delta(t_3-t_4)G(\boldsymbol{x}_4,t_4,\boldsymbol{x}_1,t_1)G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_4,t_4)\\ &= s^2\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\mathrm{d}t_1\mathrm{d}t_2 V(\boldsymbol{x}_1,\boldsymbol{x}_2)G(\boldsymbol{x}_2,t_1,\boldsymbol{x}_3,t_2)G(\boldsymbol{x}_3,t_2,\boldsymbol{x}_2,t_1)\\ &\qquad\times V(\boldsymbol{x}_3,\boldsymbol{x}_4)G(\boldsymbol{x}_4,t_2,\boldsymbol{x}_1,t_1)G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_4,t_2).\end{aligned}\tag{2.81}$$

We replace the propagator by its expression (2.47), and integrate over the imaginary times, separating the contributions for $t_1 > t_2$ and $t_2 < t_1$.

We have

$$\begin{aligned}I &= \int_0^\beta\mathrm{d}t_1\int_0^\beta\mathrm{d}t_2 G(\boldsymbol{x}_2,t_1,\boldsymbol{x}_3,t_2)G(\boldsymbol{x}_3,t_2,\boldsymbol{x}_2,t_1)G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_4,t_2)G(\boldsymbol{x}_4,t_2,\boldsymbol{x}_1,t_1)\\ &= \int_0^\beta\mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2 G(\boldsymbol{x}_2,t_1,\boldsymbol{x}_3,t_2)G(\boldsymbol{x}_3,t_2,\boldsymbol{x}_2,t_1)G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_4,t_2)G(\boldsymbol{x}_4,t_2,\boldsymbol{x}_1,t_1)\\ &\quad+\int_0^\beta\mathrm{d}t_1\int_{t_1}^\beta\mathrm{d}t_2 G(\boldsymbol{x}_2,t_1,\boldsymbol{x}_3,t_2)G(\boldsymbol{x}_3,t_2,\boldsymbol{x}_2,t_1)G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_4,t_2)G(\boldsymbol{x}_4,t_2,\boldsymbol{x}_1,t_1)\\ &\doteq I_1+I_2,\end{aligned}\tag{2.82}$$

with

$$\begin{aligned}I_1 = \sum_{\alpha,\beta,\gamma,\delta}\int_0^\beta\mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2 e^{-(e_\alpha+e_\gamma-e_\beta-e_\delta)(t_1-t_2)}\left[1-f_\beta(e_\alpha-\mu)\right]f_\beta(e_\beta-\mu)\\ \times\left[1-f_\beta(e_\gamma-\mu)\right]f_\beta(e_\delta-\mu)\psi_\alpha^\star(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\\ \times\psi_\beta^\star(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_3)\psi_\gamma^\star(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_1)\psi_\delta^\star(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4).\end{aligned}\tag{2.83}$$

We have to separate the terms $e_\alpha+e_\gamma\neq e_\beta+e_\delta$ and $e_\alpha+e_\gamma=e_\beta+e_\delta$.

Using the result

$$\int_0^\beta\mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2 e^{-\lambda(t_1-t_2)} = \frac{\beta}{\lambda}+\frac{e^{-\lambda\beta}-1}{\lambda^2},\tag{2.84}$$

we find

$$\begin{aligned} I_1 \;=\; & \sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{\beta}{(e_\alpha+e_\gamma-e_\beta-e_\delta)} \left[1-f_\beta(e_\alpha-\mu)\right] f_\beta(e_\beta-\mu) \\ & \times\left[1-f_\beta(e_\gamma-\mu)\right] f_\beta(e_\delta-\mu)\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2) \\ & \times\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_3)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_1)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4) \end{aligned} \tag{2.85}$$

$$\begin{aligned} + & \sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{e^{\beta(e_\beta+e_\delta-2\mu)}-e^{\beta(e_\alpha+e_\gamma-2\mu)}}{(e_\alpha+e_\gamma-e_\beta-e_\delta)^2} f_\beta(e_\alpha-\mu) \\ & \times f_\beta(e_\beta-\mu) f_\beta(e_\gamma-\mu) f_\beta(e_\delta-\mu)\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2) \\ & \times\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_3)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_1)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4) \end{aligned} \tag{2.86}$$

$$\begin{aligned} + & \frac{\beta^2}{2} \sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma=e_\beta+e_\delta\}} \left[1-f_\beta(e_\alpha-\mu)\right] f_\beta(e_\beta-\mu)\left[1-f_\beta(e_\gamma-\mu)\right] f_\beta(e_\delta-\mu) \\ & \times\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_3)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_1)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4), \end{aligned} \tag{2.87}$$

where we used the explicit expression of the Fermi-Dirac distribution (2.45).

We evaluate I_2 in the same way. Using the result

$$\int_0^\beta \mathrm{d}t_1 \int_{t_1}^\beta \mathrm{d}t_2 e^{-\lambda(t_1-t_2)} = -\frac{\beta}{\lambda}+\frac{e^{\lambda\beta}-1}{\lambda^2}, \tag{2.88}$$

we find

$$\begin{aligned} I_2 \;=\; & \sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{-\beta}{(e_\alpha+e_\gamma-e_\beta-e_\delta)} f_\beta(e_\alpha-\mu)\left[1-f_\beta(e_\beta-\mu)\right] \\ & \times f_\beta(e_\gamma-\mu)\left[1-f_\beta(e_\delta-\mu)\right]\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2) \\ & \times\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_3)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_1)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4) \end{aligned} \tag{2.89}$$

$$\begin{aligned} + & \sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{e^{\beta(e_\alpha+e_\gamma-2\mu)}-e^{\beta(e_\beta+e_\delta-2\mu)}}{(e_\alpha+e_\gamma-e_\beta-e_\delta)^2} f_\beta(e_\alpha-\mu) f_\beta(e_\beta-\mu) \\ & \times f_\beta(e_\gamma-\mu) f_\beta(e_\delta-\mu)\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2) \\ & \times\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_3)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_1)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4) \end{aligned} \tag{2.90}$$

$$\begin{aligned} + & \frac{\beta^2}{2} \sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma=e_\beta+e_\delta\}} f_\beta(e_\alpha-\mu)\left[1-f_\beta(e_\beta-\mu)\right] f_\beta(e_\gamma-\mu)\left[1-f_\beta(e_\delta-\mu)\right] \\ & \times\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_3)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_1)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4). \end{aligned} \tag{2.91}$$

Summing I_1 and I_2 we see that the terms (2.86) and (2.90) cancel out.

Let's treat the remaining terms, by proceeding to the change of the summation indices $(\alpha,\gamma)\leftrightarrow(\beta,\delta)$ in (2.89), and replacing $e_\beta+e_\delta$ by $e_\alpha+e_\gamma$ in (2.91). We find

$$
\begin{aligned}
I \;=\; & \sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{\beta}{(e_\alpha+e_\gamma-e_\beta-e_\delta)}\left[1-f_\beta(e_\alpha-\mu)\right] \\
& \qquad \times f_\beta(e_\beta-\mu)\left[1-f_\beta(e_\gamma-\mu)\right]f_\beta(e_\delta-\mu) \\
& \qquad \times\Big(\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_3)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_1)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4) \\
& \qquad +\psi^\star_\alpha(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_3)\psi^\star_\beta(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi^\star_\gamma(\boldsymbol{x}_1)\psi_\gamma(\boldsymbol{x}_4)\psi^\star_\delta(\boldsymbol{x}_4)\psi_\delta(\boldsymbol{x}_1)\Big) \\
& +\beta^2\sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma=e_\beta+e_\delta\}}\left[1-f_\beta(e_\alpha-\mu)\right]f_\beta(e_\beta-\mu)\left[1-f_\beta(e_\gamma-\mu)\right]f_\beta(e_\delta-\mu) \\
& \qquad \times\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_3)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_1)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4).
\end{aligned}
\tag{2.92}
$$

Taking the zero temperature limit (using (2.54) and (2.58)) we find

$$
\begin{aligned}
I \;=\; & \sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{\beta}{(e_\alpha+e_\gamma-e_\beta-e_\delta)}\theta(e_\alpha-\mu) \\
& \qquad \times\theta(\mu-e_\beta)\theta(e_\gamma-\mu)\theta(\mu-e_\delta) \\
& \qquad \times\Big(\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_3)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_1)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4) \\
& \qquad +\psi^\star_\alpha(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_3)\psi^\star_\beta(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi^\star_\gamma(\boldsymbol{x}_1)\psi_\gamma(\boldsymbol{x}_4)\psi^\star_\delta(\boldsymbol{x}_4)\psi_\delta(\boldsymbol{x}_1)\Big) \\
& +\beta^2\sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma=e_\beta+e_\delta\}}\theta(e_\alpha-\mu)\theta(\mu-e_\beta)\theta(e_\gamma-\mu)\theta(\mu-e_\delta)\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2) \\
& \qquad \times\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_3)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_1)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4).
\end{aligned}
\tag{2.93}
$$

In order to use a continuous description of the energy, we introduce the density of states

$$
\rho^\sigma(e;\boldsymbol{x},\boldsymbol{y}) \doteq \sum_\alpha \delta(e-e_\alpha)\psi^\star_\alpha(\boldsymbol{x})\psi_\alpha(\boldsymbol{y}). \tag{2.94}
$$

An expression of this density of states will be obtained as a function of the self-consistent potential in the semiclassical limit.

Introducing the density of states into the expression for I, using the indices

$(\alpha,\beta,\gamma,\delta)\mapsto(e_1,e_2,e_3,e_4)$, we find

$$\begin{aligned} I &= \beta\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\frac{1}{(e_1+e_3-e_2-e_4)} \\ &\quad\times\Big(\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_2,\boldsymbol{x}_3)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_1)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4) \\ &\quad+\rho^\sigma(e_1,\boldsymbol{x}_2,\boldsymbol{x}_3)\rho^\sigma(e_2,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_3,\boldsymbol{x}_1,\boldsymbol{x}_4)\rho^\sigma(e_4,\boldsymbol{x}_4,\boldsymbol{x}_1)\Big) \\ &\quad+\beta^2\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\delta(e_1+e_3-e_2-e_4) \\ &\quad\times\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_2,\boldsymbol{x}_3)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_1)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4). \end{aligned} \tag{2.95}$$

The second term of (2.95) is zero, because $e_1+e_3>2\mu$ while $e_2+e_4<2\mu$, the constraint $e_1+e_3=e_2+e_4$ is therefore never satisfied.

Introducing the result (2.95) in (2.81) we find a contribution to the pressure P_3 which is, using (2.78)

$$\begin{aligned} P_3^2 &= \frac{s^2}{4N^2}\int\prod_{i=1}^4 \mathrm{d}^d\boldsymbol{x}_i\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\frac{1}{(e_1+e_3-e_2-e_4)} \\ &\quad\times\Big(\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_2,\boldsymbol{x}_3)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_1)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4) \\ &\quad+\rho^\sigma(e_1,\boldsymbol{x}_2,\boldsymbol{x}_3)\rho^\sigma(e_2,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_3,\boldsymbol{x}_1,\boldsymbol{x}_4)\rho^\sigma(e_4,\boldsymbol{x}_4,\boldsymbol{x}_1)\Big) \\ &\quad\times V(\boldsymbol{x}_1,\boldsymbol{x}_2)V(\boldsymbol{x}_3,\boldsymbol{x}_4). \end{aligned} \tag{2.96}$$

For the second term we proceed to the change of the integration variables $(\boldsymbol{x}_1,\boldsymbol{x}_2)\leftrightarrow(\boldsymbol{x}_4,\boldsymbol{x}_3)$ and use the symmetry of the potential V to finally obtain

$$\begin{aligned} P_3^2 &= \frac{s^2}{2N^2}\int\prod_{i=1}^4 \mathrm{d}^d\boldsymbol{x}_i\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\frac{1}{(e_1+e_3-e_2-e_4)} \\ &\quad\times\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_2,\boldsymbol{x}_3)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_1)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4) \\ &\quad\times V(\boldsymbol{x}_1,\boldsymbol{x}_2)V(\boldsymbol{x}_3,\boldsymbol{x}_4). \end{aligned} \tag{2.97}$$

2.3.4 P_4

The last term we need to evaluate will be calculated using Wick's theorem. The reference measure will be $(V^{-1}-\frac{\Gamma}{N})$. However, as we are interested in calculations up to the order of N^{-2}, we will not consider the contribution arising from the term $\frac{\Gamma}{N}$. Therefore, the measure term we will consider is V^{-1}.

Using a cumulant expansion we find, from (2.69):

$$Q_4 = \left\langle e^{-\frac{s}{4N^2}\mathrm{Tr}(G\theta)^4+\mathcal{O}(N^{-3})}\right\rangle_{\theta,\left(V^{-1}-\frac{\Gamma}{N}\right)} = e^{-\frac{s}{4N^2}\left\langle\mathrm{Tr}(G\theta)^4\right\rangle_{\theta,V^{-1}}+\mathcal{O}(N^{-3})}. \tag{2.98}$$

This expression leads to the pressure

$$P_4 = -\lim_{\beta\to\infty}\frac{s}{4\beta N^2}\left\langle\mathrm{Tr}(G\theta)^4\right\rangle_{\theta,V^{-1}} + \mathcal{O}(N^{-3}). \tag{2.99}$$

We therefore have to evaluate

$$\begin{aligned}\left\langle\mathrm{Tr}(G\theta)^4\right\rangle_{\theta,V^{-1}}=&\Bigg\langle\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\mathrm{d}t_i G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)G(\boldsymbol{x}_2,t_2,\boldsymbol{x}_3,t_3)G(\boldsymbol{x}_3,t_3,\boldsymbol{x}_4,t_4)\\&\qquad\times G(\boldsymbol{x}_4,t_4,\boldsymbol{x}_1,t_1)\theta(\boldsymbol{x}_1,t_1)\theta(\boldsymbol{x}_2,t_2)\theta(\boldsymbol{x}_3,t_3)\theta(\boldsymbol{x}_4,t_4)\Bigg\rangle_{\theta,V^{-1}}\\=&\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\mathrm{d}t_i G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)G(\boldsymbol{x}_2,t_2,\boldsymbol{x}_3,t_3)G(\boldsymbol{x}_3,t_3,\boldsymbol{x}_4,t_4)\\&\times G(\boldsymbol{x}_4,t_4,\boldsymbol{x}_1,t_1)\left\langle\theta(\boldsymbol{x}_1,t_1)\theta(\boldsymbol{x}_2,t_2)\theta(\boldsymbol{x}_3,t_3)\theta(\boldsymbol{x}_4,t_4)\right\rangle_{\theta,V^{-1}}.\end{aligned} \tag{2.100}$$

Let's establish the Wick's theorem's result we need. We introduce the generating functional and use a usual equality (the fact that the Fourier transform of a gaussian is a gaussian)

$$\left\langle e^{(j|\theta)}\right\rangle_{\theta,V^{-1}} = e^{\frac{1}{2}(j|V|j)}, \tag{2.101}$$

take its functional derivative with respect to $j(\boldsymbol{x}_1,t_1), j(\boldsymbol{x}_2,t_2), j(\boldsymbol{x}_3,t_3), j(\boldsymbol{x}_4,t_4)$, and evaluate at $j=0$. We find

$$\begin{aligned}&\left\langle\theta(\boldsymbol{x}_1,t_1)\theta(\boldsymbol{x}_2,t_2)\theta(\boldsymbol{x}_3,t_3)\theta(\boldsymbol{x}_4,t_4)\right\rangle_{\theta,V^{-1}}\\&\qquad= +V(\boldsymbol{x}_1,\boldsymbol{x}_2)\delta(t_1-t_2)V(\boldsymbol{x}_3,\boldsymbol{x}_4)\delta(t_3-t_4)\\&\qquad\quad +V(\boldsymbol{x}_1,\boldsymbol{x}_3)\delta(t_1-t_3)V(\boldsymbol{x}_2,\boldsymbol{x}_4)\delta(t_2-t_4)\\&\qquad\quad +V(\boldsymbol{x}_1,\boldsymbol{x}_4)\delta(t_1-t_4)V(\boldsymbol{x}_2,\boldsymbol{x}_3)\delta(t_2-t_3).\end{aligned} \tag{2.102}$$

We can introduce this result in (2.100) to find

$$\begin{aligned}\left\langle \mathrm{Tr}(G\theta)^4\right\rangle_{\theta,V^{-1}} &= \int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\mathrm{d}t_i G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)G(\boldsymbol{x}_2,t_2,\boldsymbol{x}_3,t_3)\\ &\qquad\times G(\boldsymbol{x}_3,t_3,\boldsymbol{x}_4,t_4)G(\boldsymbol{x}_4,t_4,\boldsymbol{x}_1,t_1)\\ &\quad\times\Big(V(\boldsymbol{x}_1,\boldsymbol{x}_2)\delta(t_1-t_2)V(\boldsymbol{x}_3,\boldsymbol{x}_4)\delta(t_3-t_4)\\ &\quad+V(\boldsymbol{x}_1,\boldsymbol{x}_3)\delta(t_1-t_3)V(\boldsymbol{x}_2,\boldsymbol{x}_4)\delta(t_2-t_4)\\ &\quad+V(\boldsymbol{x}_1,\boldsymbol{x}_4)\delta(t_1-t_4)V(\boldsymbol{x}_2,\boldsymbol{x}_3)\delta(t_2-t_3)\Big)\end{aligned} \tag{2.103}$$

$$\begin{aligned}&= \int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\mathrm{d}t_1\mathrm{d}t_2 G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_1)G(\boldsymbol{x}_2,t_1,\boldsymbol{x}_3,t_2)\\ &\qquad\times G(\boldsymbol{x}_3,t_2,\boldsymbol{x}_4,t_2)G(\boldsymbol{x}_4,t_2,\boldsymbol{x}_1,t_1)\\ &\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_2)V(\boldsymbol{x}_3,\boldsymbol{x}_4)\\ &+\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\mathrm{d}t_1\mathrm{d}t_2 G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)G(\boldsymbol{x}_2,t_2,\boldsymbol{x}_3,t_1)\\ &\qquad\times G(\boldsymbol{x}_3,t_1,\boldsymbol{x}_4,t_2)G(\boldsymbol{x}_4,t_2,\boldsymbol{x}_1,t_1)\\ &\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_3)V(\boldsymbol{x}_2,\boldsymbol{x}_4)\\ &+\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\mathrm{d}t_1\mathrm{d}t_2 G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)G(\boldsymbol{x}_2,t_2,\boldsymbol{x}_3,t_2)\\ &\qquad\times G(\boldsymbol{x}_3,t_2,\boldsymbol{x}_4,t_1)G(\boldsymbol{x}_4,t_1,\boldsymbol{x}_1,t_1)\\ &\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_4)V(\boldsymbol{x}_2,\boldsymbol{x}_3).\end{aligned} \tag{2.104}$$

The third term is equal to the first one, which can be seen by proceeding to the permutation of the integration variables: $(\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{x}_3,\boldsymbol{x}_4)\mapsto(\boldsymbol{x}_2,\boldsymbol{x}_3,\boldsymbol{x}_4,\boldsymbol{x}_1)$, and using the symmetry of V. We find

$$\begin{aligned}\left\langle \mathrm{Tr}(G\theta)^4\right\rangle_{\theta,V^{-1}} &= 2\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\mathrm{d}t_1\mathrm{d}t_2 G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_1)G(\boldsymbol{x}_2,t_1,\boldsymbol{x}_3,t_2)\\ &\qquad\times G(\boldsymbol{x}_3,t_2,\boldsymbol{x}_4,t_2)G(\boldsymbol{x}_4,t_2,\boldsymbol{x}_1,t_1)\\ &\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_2)V(\boldsymbol{x}_3,\boldsymbol{x}_4)\\ &+\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\mathrm{d}t_1\mathrm{d}t_2 G(\boldsymbol{x}_1,t_1,\boldsymbol{x}_2,t_2)G(\boldsymbol{x}_2,t_2,\boldsymbol{x}_3,t_1)\\ &\qquad\times G(\boldsymbol{x}_3,t_1,\boldsymbol{x}_4,t_2)G(\boldsymbol{x}_4,t_2,\boldsymbol{x}_1,t_1)\\ &\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_3)V(\boldsymbol{x}_2,\boldsymbol{x}_4).\end{aligned} \tag{2.105}$$

We will evaluate these two terms separately. Remembering that when evaluated at same times the propagator is time-independent, we have to calculate

$$J^1 \doteq \int_0^\beta \mathrm{d}t_1 \int_0^\beta \mathrm{d}t_2 G(\boldsymbol{x}_2, t_1, \boldsymbol{x}_3, t_2) G(\boldsymbol{x}_4, t_2, \boldsymbol{x}_1, t_1) \tag{2.106}$$

and

$$J^2 \doteq \int_0^\beta \mathrm{d}t_1 \int_0^\beta \mathrm{d}t_2 G(\boldsymbol{x}_1, t_1, \boldsymbol{x}_2, t_2) G(\boldsymbol{x}_2, t_2, \boldsymbol{x}_3, t_1) G(\boldsymbol{x}_3, t_1, \boldsymbol{x}_4, t_2) G(\boldsymbol{x}_4, t_2, \boldsymbol{x}_1, t_1). \tag{2.107}$$

Let's start with the determination of J^1. In the same way as previously, we replace the propagator by its expression (2.47), and integrate over the imaginary times, separating the contributions for $t_1 > t_2$ and $t_1 < t_2$. Let's calculate

$$\begin{aligned}
J^1 &= \int_0^\beta \mathrm{d}t_1 \int_0^\beta \mathrm{d}t_2 G(\boldsymbol{x}_2, t_1, \boldsymbol{x}_3, t_2) G(\boldsymbol{x}_4, t_2, \boldsymbol{x}_1, t_1) \\
&= \int_0^\beta \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 G(\boldsymbol{x}_2, t_1, \boldsymbol{x}_3, t_2) G(\boldsymbol{x}_4, t_2, \boldsymbol{x}_1, t_1) \\
&\quad + \int_0^\beta \mathrm{d}t_1 \int_{t_1}^\beta \mathrm{d}t_2 G(\boldsymbol{x}_2, t_1, \boldsymbol{x}_3, t_2) G(\boldsymbol{x}_4, t_2, \boldsymbol{x}_1, t_1) \\
&\doteq J_1^1 + J_2^1,
\end{aligned} \tag{2.108}$$

with

$$\begin{aligned}
J_1^1 &= -\sum_{\alpha,\beta} \int_0^\beta \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 e^{-(e_\alpha - e_\beta)(t_1 - t_2)} \left[1 - f_\beta(e_\alpha - \mu)\right] f_\beta(e_\beta - \mu) \\
&\qquad \times \psi_\alpha^\star(\boldsymbol{x}_3) \psi_\alpha(\boldsymbol{x}_2) \psi_\beta^\star(\boldsymbol{x}_1) \psi_\beta(\boldsymbol{x}_4).
\end{aligned} \tag{2.109}$$

We have to separate the terms $e_\alpha \neq e_\beta$ and $e_\alpha = e_\beta$.

Using the result (2.84) we find

$$\begin{aligned}
J_1^1 = &- \sum_{\{\alpha,\beta | e_\alpha \neq e_\beta\}} \frac{\beta}{(e_\alpha - e_\beta)} \left[1 - f_\beta(e_\alpha - \mu)\right] f_\beta(e_\beta - \mu) \\
&\qquad \times \psi_\alpha^\star(\boldsymbol{x}_3) \psi_\alpha(\boldsymbol{x}_2) \psi_\beta^\star(\boldsymbol{x}_1) \psi_\beta(\boldsymbol{x}_4) && (2.110) \\
&- \sum_{\{\alpha,\beta | e_\alpha \neq e_\beta\}} \frac{\left(e^{\beta(e_\beta - \mu)} - e^{\beta(e_\alpha - \mu)}\right)}{(e_\alpha - e_\beta)^2} f_\beta(e_\alpha - \mu) f_\beta(e_\beta - \mu) \\
&\qquad \times \psi_\alpha^\star(\boldsymbol{x}_3) \psi_\alpha(\boldsymbol{x}_2) \psi_\beta^\star(\boldsymbol{x}_1) \psi_\beta(\boldsymbol{x}_4) && (2.111) \\
&- \frac{\beta^2}{2} \sum_{\{\alpha,\beta | e_\alpha = e_\beta\}} \left[1 - f_\beta(e_\alpha - \mu)\right] f_\beta(e_\beta - \mu) \psi_\alpha^\star(\boldsymbol{x}_3) \psi_\alpha(\boldsymbol{x}_2) \psi_\beta^\star(\boldsymbol{x}_1) \psi_\beta(\boldsymbol{x}_4).
\end{aligned}$$

(2.112)

We evaluate J_2^1 in the same way. Using the result (2.88) we find

$$
\begin{aligned}
J_2^1 = & \sum_{\{\alpha,\beta|e_\alpha\neq e_\beta\}} \frac{\beta}{(e_\alpha - e_\beta)} f_\beta(e_\alpha-\mu)\left[1-f_\beta(e_\beta-\mu)\right] \\
& \qquad \times\psi_\alpha^\star(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi_\beta^\star(\boldsymbol{x}_1)\psi_\beta(\boldsymbol{x}_4) && (2.113) \\
& - \sum_{\{\alpha,\beta|e_\alpha\neq e_\beta\}} \frac{\left(e^{\beta(e_\alpha-\mu)}-e^{\beta(e_\beta-\mu)}\right)}{(e_\alpha-e_\beta)^2} f_\beta(e_\alpha-\mu) f_\beta(e_\beta-\mu) \\
& \qquad \times\psi_\alpha^\star(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi_\beta^\star(\boldsymbol{x}_1)\psi_\beta(\boldsymbol{x}_4) && (2.114) \\
& -\frac{\beta^2}{2}\sum_{\{\alpha,\beta|e_\alpha=e_\beta\}} f_\beta(e_\alpha-\mu)\left[1-f_\beta(e_\beta-\mu)\right]\psi_\alpha^\star(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi_\beta^\star(\boldsymbol{x}_1)\psi_\beta(\boldsymbol{x}_4). && (2.115)
\end{aligned}
$$

Summing J_1^1 and J_2^1 we see that the term (2.111) and (2.114) cancel out.

Let's consider the remaining terms, by proceeding to the change of the summation indices $\alpha \leftrightarrow \beta$ in (2.113), and replacing e_β by e_α in (2.115). We find

$$
\begin{aligned}
J^1 \quad = \quad & -\sum_{\{\alpha,\beta|e_\alpha\neq e_\beta\}} \frac{\beta}{(e_\alpha-e_\beta)}\left[1-f_\beta(e_\alpha-\mu)\right] f_\beta(e_\beta-\mu) \\
& \times\left(\psi_\alpha^\star(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi_\beta^\star(\boldsymbol{x}_1)\psi_\beta(\boldsymbol{x}_4)+\psi_\alpha^\star(\boldsymbol{x}_1)\psi_\alpha(\boldsymbol{x}_4)\psi_\beta^\star(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\right) \\
& -\beta^2\sum_{\{\alpha,\beta|e_\alpha=e_\beta\}}\left[1-f_\beta(e_\alpha-\mu)\right] f_\beta(e_\beta-\mu)\psi_\alpha^\star(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi_\beta^\star(\boldsymbol{x}_1)\psi_\beta(\boldsymbol{x}_4). \qquad (2.116)
\end{aligned}
$$

Taking the zero temperature limit (using (2.54) and (2.58)) we find

$$
\begin{aligned}
J^1 \quad = \quad & -\sum_{\{\alpha,\beta|e_\alpha\neq e_\beta\}} \frac{\beta}{(e_\alpha-e_\beta)}\theta(e_\alpha-\mu)\theta(\mu-e_\beta) \\
& \times\left(\psi_\alpha^\star(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi_\beta^\star(\boldsymbol{x}_1)\psi_\beta(\boldsymbol{x}_4)+\psi_\alpha^\star(\boldsymbol{x}_1)\psi_\alpha(\boldsymbol{x}_4)\psi_\beta^\star(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\right) \\
& -\beta^2\sum_{\{\alpha,\beta|e_\alpha=e_\beta\}}\theta(e_\alpha-\mu)\theta(\mu-e_\beta)\psi_\alpha^\star(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi_\beta^\star(\boldsymbol{x}_1)\psi_\beta(\boldsymbol{x}_4). \qquad (2.117)
\end{aligned}
$$

Introducing the density of states (2.94), and using the indices $(\alpha,\beta)\mapsto(e_1,e_2)$ for the continuous description of the energy, we find

$$
\begin{aligned}
J^1 \quad = \quad & -\beta\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\frac{1}{(e_1-e_2)}\Big(\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_1,\boldsymbol{x}_4) \\
& \qquad +\rho^\sigma(e_1,\boldsymbol{x}_1,\boldsymbol{x}_4)\rho^\sigma(e_2,\boldsymbol{x}_3,\boldsymbol{x}_2)\Big) \\
& -\beta^2\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\delta(e_1-e_2)\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_1,\boldsymbol{x}_4). \qquad (2.118)
\end{aligned}
$$

The second term of (2.118) is zero, because $e_1 > \mu$ while $e_2 < \mu$, the constraint $e_1 = e_2$ is therefore never satisfied.

Introducing the result (2.118) in (2.105), and using (2.50), we find a contribution to the pressure P_4 which is, using (2.99)

$$\begin{aligned} P_4^1 \;=\; & \frac{s}{2N^2} \int \prod_{i=1}^{4} \mathrm{d}^d \boldsymbol{x}_i \int_{\mu}^{\infty} \mathrm{d}e_1 \int_{0}^{\mu} \mathrm{d}e_2 \frac{1}{(e_1 - e_2)} \\ & \times \left(\rho^{\sigma}(e_1, \boldsymbol{x}_3, \boldsymbol{x}_2) \rho^{\sigma}(e_2, \boldsymbol{x}_1, \boldsymbol{x}_4) + \rho^{\sigma}(e_1, \boldsymbol{x}_1, \boldsymbol{x}_4) \rho^{\sigma}(e_2, \boldsymbol{x}_3, \boldsymbol{x}_2) \right) \\ & \times \rho^{\sigma}(\boldsymbol{x}_1, \boldsymbol{x}_2) \rho^{\sigma}(\boldsymbol{x}_3, \boldsymbol{x}_4) V(\boldsymbol{x}_1, \boldsymbol{x}_2) V(\boldsymbol{x}_3, \boldsymbol{x}_4). \end{aligned} \tag{2.119}$$

For the second term we proceed to the change of the integration variables $(\boldsymbol{x}_1, \boldsymbol{x}_4) \leftrightarrow (\boldsymbol{x}_3, \boldsymbol{x}_2)$ to finally obtain

$$\begin{aligned} P_4^1 \;=\; & \frac{s}{N^2} \int \prod_{i=1}^{4} \mathrm{d}^d \boldsymbol{x}_i \int_{\mu}^{\infty} \mathrm{d}e_1 \int_{0}^{\mu} \mathrm{d}e_2 \frac{1}{(e_1 - e_2)} \rho^{\sigma}(e_1, \boldsymbol{x}_3, \boldsymbol{x}_2) \rho^{\sigma}(e_2, \boldsymbol{x}_1, \boldsymbol{x}_4) \\ & \times \rho^{\sigma}(\boldsymbol{x}_1, \boldsymbol{x}_2) \rho^{\sigma}(\boldsymbol{x}_3, \boldsymbol{x}_4) V(\boldsymbol{x}_1, \boldsymbol{x}_2) V(\boldsymbol{x}_3, \boldsymbol{x}_4). \end{aligned} \tag{2.120}$$

We still have to determine J^2. We replace the propagator by its expression (2.47), and integrate over the imaginary times, separating the contributions for $t_1 > t_2$ and $t_1 < t_2$.

We have

$$\begin{aligned} J^2 &= \int_0^{\beta} \mathrm{d}t_1 \int_0^{\beta} \mathrm{d}t_2 G(\boldsymbol{x}_1, t_1, \boldsymbol{x}_2, t_2) G(\boldsymbol{x}_2, t_2, \boldsymbol{x}_3, t_1) G(\boldsymbol{x}_3, t_1, \boldsymbol{x}_4, t_2) G(\boldsymbol{x}_4, t_2, \boldsymbol{x}_1, t_1) \\ &= \int_0^{\beta} \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 G(\boldsymbol{x}_1, t_1, \boldsymbol{x}_2, t_2) G(\boldsymbol{x}_2, t_2, \boldsymbol{x}_3, t_1) G(\boldsymbol{x}_3, t_1, \boldsymbol{x}_4, t_2) G(\boldsymbol{x}_4, t_2, \boldsymbol{x}_1, t_1) \\ &\quad + \int_0^{\beta} \mathrm{d}t_1 \int_{t_1}^{\beta} \mathrm{d}t_2 G(\boldsymbol{x}_1, t_1, \boldsymbol{x}_2, t_2) G(\boldsymbol{x}_2, t_2, \boldsymbol{x}_3, t_1) G(\boldsymbol{x}_3, t_1, \boldsymbol{x}_4, t_2) G(\boldsymbol{x}_4, t_2, \boldsymbol{x}_1, t_1) \\ &\doteq J_1^2 + J_2^2, \end{aligned} \tag{2.121}$$

with

$$\begin{aligned} J_1^2 \;=\; & \sum_{\alpha,\beta,\gamma,\delta} \int_0^{\beta} \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 e^{-(e_\alpha + e_\gamma - e_\beta - e_\delta)(t_1 - t_2)} \left[1 - f_\beta(e_\alpha - \mu) \right] f_\beta(e_\beta - \mu) \\ & \times \left[1 - f_\beta(e_\gamma - \mu) \right] f_\beta(e_\delta - \mu) \psi_\alpha^{\star}(\boldsymbol{x}_2) \psi_\alpha(\boldsymbol{x}_1) \\ & \times \psi_\beta^{\star}(\boldsymbol{x}_3) \psi_\beta(\boldsymbol{x}_2) \psi_\gamma^{\star}(\boldsymbol{x}_4) \psi_\gamma(\boldsymbol{x}_3) \psi_\delta^{\star}(\boldsymbol{x}_1) \psi_\delta(\boldsymbol{x}_4). \end{aligned} \tag{2.122}$$

We have to separate the terms $e_\alpha + e_\gamma \neq e_\beta + e_\delta$ and $e_\alpha + e_\gamma = e_\beta + e_\delta$.

Using the result (2.84) we find

$$\begin{aligned}
J_1^2 = & \sum_{\{\alpha,\beta,\gamma,\delta | e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{\beta}{(e_\alpha+e_\gamma-e_\beta-e_\delta)} \left[1-f_\beta(e_\alpha-\mu)\right] f_\beta(e_\beta-\mu) \\
& \times \left[1-f_\beta(e_\gamma-\mu)\right] f_\beta(e_\delta-\mu) \psi_\alpha^\star(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1) \\
& \times \psi_\beta^\star(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi_\gamma^\star(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_3)\psi_\delta^\star(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4)
\end{aligned} \tag{2.123}$$

$$\begin{aligned}
& + \sum_{\{\alpha,\beta,\gamma,\delta | e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{e^{\beta(e_\beta+e_\delta-2\mu)}-e^{\beta(e_\alpha+e_\gamma-2\mu)}}{(e_\alpha+e_\gamma-e_\beta-e_\delta)^2} f_\beta(e_\alpha-\mu) f_\beta(e_\beta-\mu) \\
& \times f_\beta(e_\gamma-\mu) f_\beta(e_\delta-\mu) \psi_\alpha^\star(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1) \\
& \times \psi_\beta^\star(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi_\gamma^\star(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_3)\psi_\delta^\star(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4)
\end{aligned} \tag{2.124}$$

$$\begin{aligned}
& + \frac{\beta^2}{2} \sum_{\{\alpha,\beta,\gamma,\delta | e_\alpha+e_\gamma= e_\beta+e_\delta\}} \left[1-f_\beta(e_\alpha-\mu)\right] f_\beta(e_\beta-\mu) \left[1-f_\beta(e_\gamma-\mu)\right] \\
& \times f_\beta(e_\delta-\mu) \psi_\alpha^\star(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1) \\
& \times \psi_\beta^\star(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi_\gamma^\star(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_3)\psi_\delta^\star(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4).
\end{aligned} \tag{2.125}$$

We evaluate J_2^2 in the same manner. Using the result (2.88) we find

$$\begin{aligned}
J_2^2 = & \sum_{\{\alpha,\beta,\gamma,\delta | e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{-\beta}{(e_\alpha+e_\gamma-e_\beta-e_\delta)} f_\beta(e_\alpha-\mu) \left[1-f_\beta(e_\beta-\mu)\right] \\
& \times f_\beta(e_\gamma-\mu) \left[1-f_\beta(e_\delta-\mu)\right] \psi_\alpha^\star(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1) \\
& \times \psi_\beta^\star(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi_\gamma^\star(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_3)\psi_\delta^\star(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4)
\end{aligned} \tag{2.126}$$

$$\begin{aligned}
& + \sum_{\{\alpha,\beta,\gamma,\delta | e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{e^{\beta(e_\alpha+e_\gamma-2\mu)}-e^{\beta(e_\beta+e_\delta-2\mu)}}{(e_\alpha+e_\gamma-e_\beta-e_\delta)^2} f_\beta(e_\alpha-\mu) f_\beta(e_\beta-\mu) \\
& \times f_\beta(e_\gamma-\mu) f_\beta(e_\delta-\mu) \psi_\alpha^\star(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1) \\
& \times \psi_\beta^\star(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi_\gamma^\star(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_3)\psi_\delta^\star(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4)
\end{aligned} \tag{2.127}$$

$$\begin{aligned}
& + \frac{\beta^2}{2} \sum_{\{\alpha,\beta,\gamma,\delta | e_\alpha+e_\gamma= e_\beta+e_\delta\}} f_\beta(e_\alpha-\mu) \left[1-f_\beta(e_\beta-\mu)\right] f_\beta(e_\gamma-\mu) \\
& \times \left[1-f_\beta(e_\delta-\mu)\right] \psi_\alpha^\star(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1) \\
& \times \psi_\beta^\star(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi_\gamma^\star(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_3)\psi_\delta^\star(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4).
\end{aligned} \tag{2.128}$$

Summing J_1^2 and J_2^2 we see that the term (2.124) and (2.127) cancel out.

Let's consider the remaining terms, by proceeding to the change of the summation indices $(\alpha,\gamma) \leftrightarrow (\beta,\delta)$ in (2.126), and replacing $e_\beta+e_\delta$ by $e_\alpha+e_\gamma$ in

(2.128). We find

$$\begin{aligned}
J^2 &= \sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{\beta}{(e_\alpha+e_\gamma-e_\beta-e_\delta)}\left[1-f_\beta(e_\alpha-\mu)\right] \\
&\qquad\qquad \times f_\beta(e_\beta-\mu)\left[1-f_\beta(e_\gamma-\mu)\right]f_\beta(e_\delta-\mu) \\
&\qquad \times\Big(\psi^\star_\alpha(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1)\psi^\star_\beta(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_3)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4) \\
&\qquad\quad +\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_1)\psi^\star_\gamma(\boldsymbol{x}_1)\psi_\gamma(\boldsymbol{x}_4)\psi^\star_\delta(\boldsymbol{x}_4)\psi_\delta(\boldsymbol{x}_3)\Big) \\
&\quad +\beta^2\sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma=e_\beta+e_\delta\}}\left[1-f_\beta(e_\alpha-\mu)\right]f_\beta(e_\beta-\mu)\left[1-f_\beta(e_\gamma-\mu)\right]f_\beta(e_\delta-\mu) \\
&\qquad\quad \times\psi^\star_\alpha(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1)\psi^\star_\beta(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_3)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4).
\end{aligned} \tag{2.129}$$

Taking the zero temperature limit (using (2.54) and (2.58)) we find

$$\begin{aligned}
J^2 &= \sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma\neq e_\beta+e_\delta\}} \frac{\beta}{(e_\alpha+e_\gamma-e_\beta-e_\delta)}\theta(e_\alpha-\mu) \\
&\qquad\qquad \times\theta(\mu-e_\beta)\theta(e_\gamma-\mu)\theta(\mu-e_\delta) \\
&\qquad \times\Big(\psi^\star_\alpha(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1)\psi^\star_\beta(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_3)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4) \\
&\qquad\quad +\psi^\star_\alpha(\boldsymbol{x}_3)\psi_\alpha(\boldsymbol{x}_2)\psi^\star_\beta(\boldsymbol{x}_2)\psi_\beta(\boldsymbol{x}_1)\psi^\star_\gamma(\boldsymbol{x}_1)\psi_\gamma(\boldsymbol{x}_4)\psi^\star_\delta(\boldsymbol{x}_4)\psi_\delta(\boldsymbol{x}_3)\Big) \\
&\quad +\beta^2\sum_{\{\alpha,\beta,\gamma,\delta|e_\alpha+e_\gamma=e_\beta+e_\delta\}}\theta(e_\alpha-\mu)\theta(\mu-e_\beta)\theta(e_\gamma-\mu)\theta(\mu-e_\delta) \\
&\qquad\quad \times\psi^\star_\alpha(\boldsymbol{x}_2)\psi_\alpha(\boldsymbol{x}_1)\psi^\star_\beta(\boldsymbol{x}_3)\psi_\beta(\boldsymbol{x}_2)\psi^\star_\gamma(\boldsymbol{x}_4)\psi_\gamma(\boldsymbol{x}_3)\psi^\star_\delta(\boldsymbol{x}_1)\psi_\delta(\boldsymbol{x}_4).
\end{aligned} \tag{2.130}$$

Introducing the density of states (2.94), and using the indices $(\alpha,\beta,\gamma,\delta)\mapsto(e_1,e_2,e_3,e_4)$ for the continuous description of the energy, we find

$$\begin{aligned}
J^2 &= \beta\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\frac{1}{(e_1+e_3-e_2-e_4)} \\
&\qquad \times\Big(\rho^\sigma(e_1,\boldsymbol{x}_2,\boldsymbol{x}_1)\rho^\sigma(e_2,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_3)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4) \\
&\qquad\quad +\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_2,\boldsymbol{x}_1)\rho^\sigma(e_3,\boldsymbol{x}_1,\boldsymbol{x}_4)\rho^\sigma(e_4,\boldsymbol{x}_4,\boldsymbol{x}_3)\Big)
\end{aligned} \tag{2.131}$$

$$\begin{aligned}
&+\beta^2\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\delta(e_1+e_3-e_2-e_4) \\
&\qquad \times\rho^\sigma(e_1,\boldsymbol{x}_2,\boldsymbol{x}_1)\rho^\sigma(e_2,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_3)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4).
\end{aligned} \tag{2.132}$$

The second term of (2.132) is zero, because $e_1+e_3>2\mu$ while $e_2+e_4<2\mu$, the constraint $e_1+e_3=e_2+e_4$ is therefore never satisfied.

Introducing the result (2.132) in (2.105) we find a contribution to the pressure P_4 which is, using (2.99)

$$\begin{aligned}
P_4^2 \;=\; & -\frac{s}{4N^2}\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\frac{1}{(e_1+e_3-e_2-e_4)}\\
&\times\Big(\rho^\sigma(e_1,\boldsymbol{x}_2,\boldsymbol{x}_1)\rho^\sigma(e_2,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_3)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4)\\
&+\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_2,\boldsymbol{x}_1)\rho^\sigma(e_3,\boldsymbol{x}_1,\boldsymbol{x}_4)\rho^\sigma(e_4,\boldsymbol{x}_4,\boldsymbol{x}_3)\Big)\\
&\times V(\boldsymbol{x}_1,\boldsymbol{x}_3)V(\boldsymbol{x}_2,\boldsymbol{x}_4).
\end{aligned} \tag{2.133}$$

For the second term we proceed to the change of the integration variables $(\boldsymbol{x}_1,\boldsymbol{x}_2,\boldsymbol{x}_3,\boldsymbol{x}_4)\mapsto(\boldsymbol{x}_2,\boldsymbol{x}_3,\boldsymbol{x}_4,\boldsymbol{x}_1)$, and $e_1\leftrightarrow e_3$ to finally obtain

$$\begin{aligned}
P_4^2 \;=\; & -\frac{s}{2N^2}\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\frac{1}{(e_1+e_3-e_2-e_4)}\\
&\times\rho^\sigma(e_1,\boldsymbol{x}_2,\boldsymbol{x}_1)\rho^\sigma(e_2,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_3)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4)\\
&\times V(\boldsymbol{x}_1,\boldsymbol{x}_3)V(\boldsymbol{x}_2,\boldsymbol{x}_4).
\end{aligned} \tag{2.134}$$

2.3.5 Total pressure

The total ground state pressure, up to the order N^{-2}, is

$$P=p_0+p_1N^{-1}+p_2N^{-2}+\mathcal{O}(N^{-3})+\mu N, \tag{2.135}$$

where

$$\begin{aligned}
p_0 &= -s\sum_{i=1}^{N/s}e_i+\frac{1}{2N}\int \mathrm{d}^d\boldsymbol{x}\int \mathrm{d}^d\boldsymbol{y}V(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y}),\\
p_1 &= \frac{1}{2s}\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}^d\boldsymbol{y}V(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{y},\boldsymbol{x}),
\end{aligned} \tag{2.136}$$

$$
\begin{aligned}
p_2 &= \frac{s^2}{2}\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\frac{1}{(e_1+e_3-e_2-e_4)}\\
&\qquad\times\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_2,\boldsymbol{x}_3)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_1)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4)\\
&\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_2)V(\boldsymbol{x}_3,\boldsymbol{x}_4) \qquad (2.137)\\
&+s\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\frac{1}{(e_1-e_2)}\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_1,\boldsymbol{x}_4)\\
&\qquad\times\rho^\sigma(\boldsymbol{x}_1,\boldsymbol{x}_2)\rho^\sigma(\boldsymbol{x}_3,\boldsymbol{x}_4)V(\boldsymbol{x}_1,\boldsymbol{x}_2)V(\boldsymbol{x}_3,\boldsymbol{x}_4) \qquad (2.138)\\
&-\frac{s}{2}\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\frac{1}{(e_1+e_3-e_2-e_4)}\\
&\qquad\times\rho^\sigma(e_1,\boldsymbol{x}_2,\boldsymbol{x}_1)\rho^\sigma(e_2,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_3)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4)\\
&\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_3)V(\boldsymbol{x}_2,\boldsymbol{x}_4) \qquad (2.139)
\end{aligned}
$$

2.4 Ground state energy

The ground state energy is immediately obtained from the ground state pressure using equation (2.3). We find

$$E(N) = e_0 + e_1N^{-1} + e_2N^{-2} + \mathcal{O}(N^{-3}), \tag{2.140}$$

where

$$
\begin{aligned}
e_0 &= s\sum_{i=1}^{N/s} e_i - \frac{1}{2N}\int \mathrm{d}^d\boldsymbol{x}\int \mathrm{d}^d\boldsymbol{y}V(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{x})\rho(\boldsymbol{y}),\\
e_1 &= -\frac{1}{2s}\int \mathrm{d}^d\boldsymbol{x}\mathrm{d}^d\boldsymbol{y}V(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{y},\boldsymbol{x}),\\
e_2 &= -\frac{s^2}{2}\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\frac{1}{(e_1+e_3-e_2-e_4)}\\
&\qquad\times\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_2,\boldsymbol{x}_3)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_1)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4)\\
&\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_2)V(\boldsymbol{x}_3,\boldsymbol{x}_4)\\
&-s\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\frac{1}{(e_1-e_2)}\rho^\sigma(e_1,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_2,\boldsymbol{x}_1,\boldsymbol{x}_4)\\
&\qquad\times\rho^\sigma(\boldsymbol{x}_1,\boldsymbol{x}_2)\rho^\sigma(\boldsymbol{x}_3,\boldsymbol{x}_4)V(\boldsymbol{x}_1,\boldsymbol{x}_2)V(\boldsymbol{x}_3,\boldsymbol{x}_4)\\
&+\frac{s}{2}\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\int_\mu^\infty \mathrm{d}e_1\int_0^\mu \mathrm{d}e_2\int_\mu^\infty \mathrm{d}e_3\int_0^\mu \mathrm{d}e_4\frac{1}{(e_1+e_3-e_2-e_4)}\\
&\qquad\times\rho^\sigma(e_1,\boldsymbol{x}_2,\boldsymbol{x}_1)\rho^\sigma(e_2,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_3)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4)\\
&\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_3)V(\boldsymbol{x}_2,\boldsymbol{x}_4).
\end{aligned} \tag{2.141}
$$

2.5 Ground state pressure in the semiclassical limit

We have obtained an expression of the ground state energy of a system of N fermions. To extract explicit results from this expression we work in the large N limit. This allows us to work in the frame of semiclassical physics and obtain explicit expressions for the sum of the N first eigenvalues, as well as for the electron density (solution of the self-consistent equation). These expressions are specific to the dimension of the system considered and have to be treated separately for the two- and three-dimensional cases. They also depend on the external potential, which is why we will treat in detail some particular cases later (see the case of quantum dots in part II).

It is possible to use the semiclassical values of the densities of states (2.94) to compute the corrections p_2. Let's note that this density of states depend on the semiclassical density, which is the solution of the self-consistent equation and depends therefore on the specific dimension and external potential of the problem. But we will see that these terms are actually independent of this density. This result implies the universality of these corrections.

2.5.1 Semiclassical density of states

Before evaluating the different terms of p_2 we simplify them by using the relation

$$\frac{1}{\alpha} = \int_0^\infty \mathrm{d}t e^{-\alpha t}, \quad \alpha > 0 \tag{2.142}$$

in order to separate the variables e_1, e_2, e_3 and e_4.

We will therefore have to evaluate semiclassically

$$\begin{aligned} \rho^\sigma(\boldsymbol{x}, \boldsymbol{x}+\epsilon\boldsymbol{r}) &= \frac{1}{(2\pi\epsilon)^d}\int \mathrm{d}^d\boldsymbol{k} e^{i\boldsymbol{k}\boldsymbol{r}}\theta(\mu-(\boldsymbol{k}^2+V(\boldsymbol{x}))), \\ \rho^\sigma(e; \boldsymbol{x}, \boldsymbol{x}+\epsilon\boldsymbol{r}) &= \frac{1}{(2\pi\epsilon)^d}\int \mathrm{d}^d\boldsymbol{k} e^{i\boldsymbol{k}\boldsymbol{r}}\delta(e-(\boldsymbol{k}^2+V(\boldsymbol{x}))), \end{aligned} \tag{2.143}$$

which leads to

$$\begin{aligned} \int_0^\mu \mathrm{d}e e^{te}\rho^\sigma(e; \boldsymbol{x}, \boldsymbol{x}+\epsilon\boldsymbol{r}) &= \frac{1}{(2\pi\epsilon)^d}\int \mathrm{d}^d\boldsymbol{k} e^{i\boldsymbol{k}\boldsymbol{r}} e^{t(\boldsymbol{k}^2+V(\boldsymbol{x}))}\theta((\mu-V(\boldsymbol{x}))-\boldsymbol{k}^2), \\ \int_\mu^\infty \mathrm{d}e e^{-te}\rho^\sigma(e; \boldsymbol{x}, \boldsymbol{x}+\epsilon\boldsymbol{r}) &= \frac{1}{(2\pi\epsilon)^d}\int \mathrm{d}^d\boldsymbol{k} e^{i\boldsymbol{k}\boldsymbol{r}} e^{-t(\boldsymbol{k}^2+V(\boldsymbol{x}))}\theta(\boldsymbol{k}^2-(\mu-V(\boldsymbol{x}))). \end{aligned} \tag{2.144}$$

These objects can now be introduced in p_2 to obtain explicit semiclassical expressions of the corrections to the pressure.

Let's note that all these objects are non zero only if evaluated for positions separated by a length of the order of ϵ, which will be used later.

In our applications we will also use the Fourier representation of the electron-electron interaction to take advantage of its translation invariance ($V(\boldsymbol{x}_i, \boldsymbol{x}_j) = V(|\boldsymbol{x}_i - \boldsymbol{x}_j|)$.

We have

$$V(\boldsymbol{x}) = \frac{1}{(2\pi)^d} \int \mathrm{d}^d\boldsymbol{k} e^{i\boldsymbol{k}\boldsymbol{x}} \hat{V}(\boldsymbol{k}) \quad \Rightarrow \quad \hat{V}(\boldsymbol{k}) = \int \mathrm{d}^d\boldsymbol{x} e^{-i\boldsymbol{k}\boldsymbol{x}} V(\boldsymbol{x}). \tag{2.145}$$

We will only consider the 3-dimensional electron-electron interaction $V(\boldsymbol{x}) = \frac{1}{|\boldsymbol{x}|}$:

$$V(\boldsymbol{x}) = \frac{1}{|\boldsymbol{x}|} \quad \Rightarrow \quad \hat{V}(\boldsymbol{k}) = \frac{S_d}{|\boldsymbol{k}|^{d-1}}, \quad \left\{ \begin{array}{lcl} S_2 & = & 2\pi, \\ S_3 & = & 4\pi. \end{array} \right. \tag{2.146}$$

Another equality we will use in the computations is an integral representation of the delta function

$$\int \mathrm{d}^d\boldsymbol{x} e^{i\boldsymbol{k}\boldsymbol{x}} = (2\pi)^d \delta(\boldsymbol{x}). \tag{2.147}$$

2.5.2 Semiclassical correction p_2

Let's evaluate the first term (2.137) of p_2, corresponding to the renormalisation term. Using (2.144), as well as proceeding to the change of variables

$$\begin{array}{lcl} \boldsymbol{x}_2 & \mapsto & \boldsymbol{r}_2, \quad \epsilon\boldsymbol{r}_2 = \boldsymbol{x}_2 - \boldsymbol{x}_1, \quad \epsilon^d \mathrm{d}^d\boldsymbol{r}_2 = \mathrm{d}^d\boldsymbol{x}_2, \\ \boldsymbol{x}_3 & \mapsto & \boldsymbol{r}_3, \quad \epsilon\boldsymbol{r}_3 = \boldsymbol{x}_3 - \epsilon\boldsymbol{r}_2 - \epsilon\boldsymbol{r}_1, \quad \epsilon^d \mathrm{d}^d\boldsymbol{r}_3 = \mathrm{d}^d\boldsymbol{x}_3, \\ \boldsymbol{x}_4 & \mapsto & \boldsymbol{r}_4, \quad \epsilon\boldsymbol{r}_4 = \boldsymbol{x}_4 - \boldsymbol{x}_1, \quad \epsilon^d \mathrm{d}^d\boldsymbol{r}_4 = \mathrm{d}^d\boldsymbol{x}_4, \end{array} \tag{2.148}$$

this term becomes

$$\begin{aligned} p_2^1 \;=\; & \frac{s^2}{2} \int \prod_{i=1}^{4} \mathrm{d}^d\boldsymbol{x}_i \int_\mu^\infty \mathrm{d}e_1 \int_0^\mu \mathrm{d}e_2 \int_\mu^\infty \mathrm{d}e_3 \int_0^\mu \mathrm{d}e_4 \frac{1}{(e_1 + e_3 - e_2 - e_4)} \\ & \times \rho^\sigma(e_1, \boldsymbol{x}_3, \boldsymbol{x}_2) \rho^\sigma(e_2, \boldsymbol{x}_2, \boldsymbol{x}_3) \rho^\sigma(e_3, \boldsymbol{x}_4, \boldsymbol{x}_1) \rho^\sigma(e_4, \boldsymbol{x}_1, \boldsymbol{x}_4) \\ & \times V(\boldsymbol{x}_1, \boldsymbol{x}_2) V(\boldsymbol{x}_3, \boldsymbol{x}_4) \end{aligned}$$

$$\begin{aligned}
&= \frac{s^2}{2}\epsilon^{3d}\int_0^\infty \mathrm{d}t \int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4 \\
&\qquad\qquad \times\int_\mu^\infty \mathrm{d}e_1 e^{-te_1}\rho^\sigma(e_1;\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2+\epsilon\boldsymbol{r}_3,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2) \\
&\qquad\qquad \times\int_0^\mu \mathrm{d}e_2 e^{te_2}\rho^\sigma(e_2;\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2+\epsilon\boldsymbol{r}_3) \\
&\qquad \times\int_\mu^\infty \mathrm{d}e_3 e^{-te_3}\rho^\sigma(e_3;\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4,\boldsymbol{x}_1)\int_0^\mu \mathrm{d}e_4 e^{te_4}\rho^\sigma(e_4;\boldsymbol{x}_1,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4) \\
&\qquad\qquad \times V(\boldsymbol{x}_1,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2)V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2+\epsilon\boldsymbol{r}_3,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4) \\
&= \frac{s^2}{2}\frac{\epsilon^{-d}}{(2\pi)^{4d}}\int_0^\infty \mathrm{d}t \int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4 \int\prod_{i=1}^4 \mathrm{d}^d\boldsymbol{k}_i \\
&\qquad \times e^{-t(\boldsymbol{k}_1^2+V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2+\epsilon\boldsymbol{r}_3))}e^{t(\boldsymbol{k}_2^2+V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2))}e^{-t(\boldsymbol{k}_3^2+V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4))}e^{t(\boldsymbol{k}_4^2+V(\boldsymbol{x}_1))} \\
&\qquad \times e^{i[\boldsymbol{r}_3(\boldsymbol{k}_2-\boldsymbol{k}_1)+\boldsymbol{r}_4(\boldsymbol{k}_4-\boldsymbol{k}_3)]}V(\boldsymbol{x}_1,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2)V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2+\epsilon\boldsymbol{r}_3,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4) \\
&\qquad \times\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2+\epsilon\boldsymbol{r}_3)))\theta((\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2))-\boldsymbol{k}_2^2) \\
&\qquad \times\theta(\boldsymbol{k}_3^2-(\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2).
\end{aligned} \tag{2.149}$$

At this stage we take the semiclassical limit. In this limit we know that the density matrix $\rho(e_k,\boldsymbol{x}_i,\boldsymbol{x}_j)$ is non zero only if $|\boldsymbol{x}_j-\boldsymbol{x}_i|\simeq\epsilon$ (more exactly, the decrease is exponential). This implies that $\boldsymbol{r}_3$ and $\boldsymbol{r}_4$ are of the order of 1, and therefore $\boldsymbol{x}_i+\epsilon\boldsymbol{r}_j\simeq\boldsymbol{x}_i,\ j=3,4$. The treatment of $\boldsymbol{r}_2$ is more delicate: the decrease is not exponential in this case, as $\boldsymbol{x}_1$ are $\boldsymbol{x}_2$ are not separated by a density matrix, but by the electronic interaction.

Using moreover the translation invariance of V ($V(\boldsymbol{x}_i,\boldsymbol{x}_j)=V(|\boldsymbol{x}_i-\boldsymbol{x}_j|)$), this term becomes

$$\begin{aligned}
p_2^1 &= \frac{s^2}{2}\frac{\epsilon^{-d}}{(2\pi)^{4d}}\int_0^\infty \mathrm{d}t \int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4 \int\prod_{i=1}^4 \mathrm{d}^d\boldsymbol{k}_i e^{-t(\boldsymbol{k}_1^2-\boldsymbol{k}_2^2+\boldsymbol{k}_3^2-\boldsymbol{k}_4^2)} \\
&\qquad \times e^{i[\boldsymbol{r}_3(\boldsymbol{k}_2-\boldsymbol{k}_1)+\boldsymbol{r}_4(\boldsymbol{k}_4-\boldsymbol{k}_3)]}V(\epsilon\boldsymbol{r}_2)V(\epsilon\boldsymbol{r}_4-\epsilon\boldsymbol{r}_3-\epsilon\boldsymbol{r}_2) \\
&\qquad \times\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2)))\theta((\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2))-\boldsymbol{k}_2^2) \\
&\qquad \times\theta(\boldsymbol{k}_3^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2).
\end{aligned} \tag{2.150}$$

Let's introduce the Fourier transform (2.145) of V, use the scaling property $V(\epsilon\boldsymbol{r})=\frac{1}{\epsilon}V(\boldsymbol{r})$, and integrate over $\boldsymbol{r}_3,\boldsymbol{r}_4$ using the delta function (2.147):

$$\begin{aligned}
p_2^1 &= \frac{s^2}{2}\frac{\epsilon^{-(d+2)}}{(2\pi)^{6d}}\int_0^\infty \mathrm{d}t \int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4 \int\prod_{i=1}^4 \mathrm{d}^d\boldsymbol{k}_i\mathrm{d}^d\boldsymbol{q}_1\mathrm{d}^d\boldsymbol{q}_2\hat{V}(\boldsymbol{q}_1)\hat{V}(\boldsymbol{q}_2) \\
&\qquad \times e^{-t(\boldsymbol{k}_1^2-\boldsymbol{k}_2^2+\boldsymbol{k}_3^2-\boldsymbol{k}_4^2)}e^{i[\boldsymbol{r}_2(\boldsymbol{q}_1-\boldsymbol{q}_2)+\boldsymbol{r}_3(\boldsymbol{k}_2-\boldsymbol{k}_1-\boldsymbol{q}_2)+\boldsymbol{r}_4(\boldsymbol{k}_4-\boldsymbol{k}_3+\boldsymbol{q}_2)]}
\end{aligned}$$

$$
\begin{aligned}
&\times\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2)))\theta((\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2))-\boldsymbol{k}_2^2)\\
&\times\theta(\boldsymbol{k}_3^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2).\\
= &\frac{s^2}{2}\frac{\epsilon^{-(d+2)}}{(2\pi)^{4d}}\int_0^\infty \mathrm{d}t\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\int\prod_{i=1}^4 \mathrm{d}^d\boldsymbol{k}_i\mathrm{d}^d\boldsymbol{q}_1\mathrm{d}^d\boldsymbol{q}_2\hat{V}(\boldsymbol{q}_1)\hat{V}(\boldsymbol{q}_2)\\
&\times e^{-t(\boldsymbol{k}_1^2-\boldsymbol{k}_2^2+\boldsymbol{k}_3^2-\boldsymbol{k}_4^2)}e^{i\boldsymbol{r}_2(\boldsymbol{q}_1-\boldsymbol{q}_2)}\delta(\boldsymbol{k}_2-\boldsymbol{k}_1-\boldsymbol{q}_2)\delta(\boldsymbol{k}_4-\boldsymbol{k}_3+\boldsymbol{q}_2)\\
&\times\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2)))\theta((\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2))-\boldsymbol{k}_2^2)\\
&\times\theta(\boldsymbol{k}_3^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2).
\end{aligned}
\tag{2.151}
$$

We make use of the delta functions to integrate over $\boldsymbol{k}_1, \boldsymbol{k}_3$, and we integrate over t:

$$
\begin{aligned}
p_2^1 = &\frac{s^2}{4}\frac{\epsilon^{-(d+2)}}{(2\pi)^{4d}}\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\int \mathrm{d}^d\boldsymbol{k}_2\mathrm{d}^d\boldsymbol{k}_4\mathrm{d}^d\boldsymbol{q}_1\mathrm{d}^d\boldsymbol{q}_2\hat{V}(\boldsymbol{q}_1)\hat{V}(\boldsymbol{q}_2)\\
&\times\frac{e^{i\boldsymbol{r}_2(\boldsymbol{q}_1-\boldsymbol{q}_2)}}{\boldsymbol{q}_2^2+\boldsymbol{q}_2(\boldsymbol{k}_4-\boldsymbol{k}_2)}\theta((\boldsymbol{k}_2-\boldsymbol{q}_2)^2-(\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2)))\\
&\times\theta((\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2))-\boldsymbol{k}_2^2)\theta((\boldsymbol{k}_4+\boldsymbol{q}_2)^2-(\mu-V(\boldsymbol{x}_1)))\\
&\times\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2).
\end{aligned}
\tag{2.152}
$$

We used the result

$$
\boldsymbol{k}_1^2-\boldsymbol{k}_2^2+\boldsymbol{k}_3^2-\boldsymbol{k}_4^2 = 2[\boldsymbol{q}_2^2+\boldsymbol{q}_2(\boldsymbol{k}_4-\boldsymbol{k}_2)]. \tag{2.153}
$$

This result remains to be understood. In particular one may be tempted to neglect the terms $\epsilon\boldsymbol{r}_2$ in the integral, to obtain a delta function when integrating over $\boldsymbol{r}_2$. As we will see in further developments, this leads to the same term as in the jellium model, for which a lot of research was performed. In doing so, we find, introducing the delta function (2.147):

$$
\begin{aligned}
p_2^1 = &\frac{s^2}{4}\frac{\epsilon^{-(d+2)}}{(2\pi)^{4d}}\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\int \mathrm{d}^d\boldsymbol{k}_2\mathrm{d}^d\boldsymbol{k}_4\mathrm{d}^d\boldsymbol{q}_1\mathrm{d}^d\boldsymbol{q}_2\hat{V}(\boldsymbol{q}_1)\hat{V}(\boldsymbol{q}_2)\\
&\times\frac{e^{i\boldsymbol{r}_2(\boldsymbol{q}_1-\boldsymbol{q}_2)}}{\boldsymbol{q}_2^2+\boldsymbol{q}_2(\boldsymbol{k}_4-\boldsymbol{k}_2)}\theta((\boldsymbol{k}_2-\boldsymbol{q}_2)^2-(\mu-V(\boldsymbol{x}_1)))\\
&\times\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_2^2)\theta((\boldsymbol{k}_4+\boldsymbol{q}_2)^2-(\mu-V(\boldsymbol{x}_1)))\\
&\times\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2)
\end{aligned}
$$

$$\begin{aligned} =\ & \frac{s^2}{4}\frac{\epsilon^{-(d+2)}}{(2\pi)^{3d}}\int \mathrm{d}^d\boldsymbol{x}_1\int \mathrm{d}^d\boldsymbol{k}_2\mathrm{d}^d\boldsymbol{k}_4\mathrm{d}^d\boldsymbol{q}_1\mathrm{d}^d\boldsymbol{q}_2\hat{V}(\boldsymbol{q}_1)\hat{V}(\boldsymbol{q}_2)\\ & \times\frac{\delta(\boldsymbol{q}_1-\boldsymbol{q}_2)}{\boldsymbol{q}_2^2+\boldsymbol{q}_2(\boldsymbol{k}_4-\boldsymbol{k}_2)}\theta((\boldsymbol{k}_2-\boldsymbol{q}_2)^2-(\mu-V(\boldsymbol{x}_1)))\\ & \times\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_2^2)\theta((\boldsymbol{k}_4+\boldsymbol{q}_2)^2-(\mu-V(\boldsymbol{x}_1)))\\ & \times\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2). \end{aligned} \tag{2.154}$$

The delta function is used to integrate over $\boldsymbol{q}_1$, and we use the symmetry of $\hat{V}$. Writing $\boldsymbol{q}_2=\boldsymbol{q}$ we find

$$\begin{aligned} p_2^1 =\ & \frac{s^2}{4}\frac{\epsilon^{-(d+2)}}{(2\pi)^{3d}}\int \mathrm{d}^d\boldsymbol{x}_1\int \mathrm{d}^d\boldsymbol{k}_2\mathrm{d}^d\boldsymbol{k}_4\mathrm{d}^d\boldsymbol{q}\hat{V}(\boldsymbol{q})\hat{V}(\boldsymbol{q})\\ & \times\frac{1}{\boldsymbol{q}^2+\boldsymbol{q}(\boldsymbol{k}_4-\boldsymbol{k}_2)}\theta((\boldsymbol{k}_2-\boldsymbol{q})^2-(\mu-V(\boldsymbol{x}_1)))\\ & \times\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_2^2)\theta((\boldsymbol{k}_4+\boldsymbol{q})^2-(\mu-V(\boldsymbol{x}_1)))\\ & \times\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2). \end{aligned} \tag{2.155}$$

Using the expression (2.146) for the Fourier transform of the potential, we find

$$\begin{aligned} p_2^1 =\ & \frac{s^2}{4}\frac{S_d^2}{\epsilon^{(d+2)}(2\pi)^{3d}}\int \mathrm{d}^d\boldsymbol{x}_1\int \mathrm{d}^d\boldsymbol{k}_2\mathrm{d}^d\boldsymbol{k}_4\mathrm{d}^d\boldsymbol{q}\frac{1}{\boldsymbol{q}^{2(d-1)}}\frac{1}{\boldsymbol{q}^2+\boldsymbol{q}(\boldsymbol{k}_4-\boldsymbol{k}_2)}\\ & \times\theta((\boldsymbol{k}_2-\boldsymbol{q})^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_2^2)\\ & \times\theta((\boldsymbol{k}_4+\boldsymbol{q})^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2). \end{aligned} \tag{2.156}$$

We can separate the integration over $\boldsymbol{x}_1$ from the other variables by the change of variables

$$\begin{aligned} \boldsymbol{k}_2 &\mapsto \boldsymbol{k}_2', & \sqrt{\mu-V(\boldsymbol{x})}\boldsymbol{k}_2' &= \boldsymbol{k}_2, & \mathrm{d}^d\boldsymbol{k}_2 &= (\mu-V(\boldsymbol{x}))^{\frac{d}{2}}\,\mathrm{d}^d\boldsymbol{k}_2',\\ \boldsymbol{k}_4 &\mapsto \boldsymbol{k}_4', & \sqrt{\mu-V(\boldsymbol{x})}\boldsymbol{k}_4' &= \boldsymbol{k}_4, & \mathrm{d}^d\boldsymbol{k}_4 &= (\mu-V(\boldsymbol{x}))^{\frac{d}{2}}\,\mathrm{d}^d\boldsymbol{k}_4',\\ \boldsymbol{q} &\mapsto \boldsymbol{q}', & \sqrt{\mu-V(\boldsymbol{x})}\boldsymbol{q}' &= \boldsymbol{q}, & \mathrm{d}^d\boldsymbol{q} &= (\mu-V(\boldsymbol{x}))^{\frac{d}{2}}\,\mathrm{d}^d\boldsymbol{q}'. \end{aligned} \tag{2.157}$$

With this change of variables the contribution to the pressure becomes

$$\begin{aligned} p_2^1 =\ & \underbrace{\frac{s^2}{4}\frac{S_d^2}{\epsilon^{(d+2)}(2\pi)^{3d}}\int \mathrm{d}^d\boldsymbol{x}(\mu-V(\boldsymbol{x}))^{\frac{d}{2}}}_{\doteq C}\int \mathrm{d}^d\boldsymbol{k}_2\mathrm{d}^d\boldsymbol{k}_4\mathrm{d}^d\boldsymbol{q}\frac{1}{\boldsymbol{q}^{2(d-1)}}\\ & \times\frac{1}{\boldsymbol{q}^2+\boldsymbol{q}(\boldsymbol{k}_4-\boldsymbol{k}_2)}\theta((\boldsymbol{k}_2-\boldsymbol{q})^2-1)\theta(1-\boldsymbol{k}_2^2)\\ & \times\theta((\boldsymbol{k}_4+\boldsymbol{q})^2-1)\theta(1-\boldsymbol{k}_4^2). \end{aligned} \tag{2.158}$$

The entire N-dependence of this term is contained in part C. It can be established by replacing $(\mu - V(\boldsymbol{x}))$ by the density, using the lowest order relation between $(\mu - V(\boldsymbol{x}))$ and $\rho(\boldsymbol{x})$. This relation can be obtained by integrating over $\boldsymbol{k}$ in (2.143), with $\boldsymbol{r} = 0$:

$$\begin{aligned}\rho(\boldsymbol{x}) = s\rho^\sigma(\boldsymbol{x}) &= \frac{s}{(2\pi\epsilon)^d}\int \mathrm{d}^d\boldsymbol{k}\theta(\mu - (\boldsymbol{k}^2 + V(\boldsymbol{x})))\\ &= \frac{sS_d}{(2\pi\epsilon)^d}\int_0^{\sqrt{\mu - V(\boldsymbol{x})}} \mathrm{d}k k^{(d-1)}\\ &= \frac{sS_d}{(2\pi\epsilon)^d d}(\mu - V(\boldsymbol{x}))^{\frac{d}{2}}. \end{aligned} \tag{2.159}$$

We have therefore

$$\begin{aligned} C &= \frac{s}{4}\frac{S_d d}{\epsilon^2(2\pi)^{2d}}\underbrace{\int \mathrm{d}^d\boldsymbol{x}\rho(\boldsymbol{x})}_{=N} = \frac{s}{4}\frac{S_d d}{(2\pi)^{2d}}\frac{N}{\epsilon^2}\\ &= \frac{s}{2}\frac{S_d d}{(2\pi)^{2d}}N^{1+\frac{2}{d}} = \begin{cases} \frac{1}{4\pi^3}N^2 & , \quad d = 2,\\ \frac{3}{16\pi^5}N^{\frac{5}{3}} & , \quad d = 3, \end{cases} \end{aligned} \tag{2.160}$$

and p_2^1 becomes

$$p_2^1 = N^{1+\frac{2}{d}}\frac{s}{2}\frac{S_d d}{(2\pi)^{2d}}\int_\Lambda \mathrm{d}^d\boldsymbol{k}\mathrm{d}^d\boldsymbol{k}'\mathrm{d}^d\boldsymbol{q}\frac{1}{\boldsymbol{q}^{2(d-1)}}\frac{1}{\boldsymbol{q}^2 + \boldsymbol{q}(\boldsymbol{k}' - \boldsymbol{k})}, \tag{2.161}$$

where the integration domain Λ is such that

$$|\boldsymbol{k} - \boldsymbol{q}| > 1 \quad |\boldsymbol{k}' - \boldsymbol{q}| > 1, \quad |\boldsymbol{k}| < 1, \quad |\boldsymbol{k}'| < 1. \tag{2.162}$$

When returning to the energy, and proceed to the inverse scaling of the energy, the final expression we have to integrate corresponds to that of the jellium model. This is why this integral was already studied (in (Gell-Mann and Brueckner, 1957)) for three-dimensional systems. It is divergent, and an infinite number of selected terms (the "ring diagrams") has to be taken into account to obtain a finite contribution, which is computed using the Random Phase Approximation. Our problem is however different from the jellium model: the density is not uniform, and is not infinitely extended. This is why we believe that our term may not be divergent. We believe that the approximations that led us to this result are too strong.

Let's evaluate the second term (2.138) of p_2. Using (2.143), and (2.144), as well as proceeding to the change of variables

$$\begin{aligned} \boldsymbol{x}_2 &\mapsto \boldsymbol{r}_2, \quad \epsilon\boldsymbol{r}_2 = \boldsymbol{x}_2 - \boldsymbol{x}_1, \quad \epsilon^d\mathrm{d}^d\boldsymbol{r}_2 = \mathrm{d}^d\boldsymbol{x}_2,\\ \boldsymbol{x}_3 &\mapsto \boldsymbol{r}_3, \quad \epsilon\boldsymbol{r}_3 = \boldsymbol{x}_3 - \boldsymbol{x}_1, \quad \epsilon^d\mathrm{d}^d\boldsymbol{r}_3 = \mathrm{d}^d\boldsymbol{x}_3,\\ \boldsymbol{x}_4 &\mapsto \boldsymbol{r}_4, \quad \epsilon\boldsymbol{r}_4 = \boldsymbol{x}_4 - \boldsymbol{x}_1, \quad \epsilon^d\mathrm{d}^d\boldsymbol{r}_4 = \mathrm{d}^d\boldsymbol{x}_4, \end{aligned} \tag{2.163}$$

this term becomes

$$\begin{aligned}
p_2^2 &= s\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i\int_{\mu}^{\infty}\mathrm{d}e_1\int_0^{\mu}\mathrm{d}e_2\frac{1}{(e_1-e_2)}\rho^{\sigma}(e_1;\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^{\sigma}(e_2;\boldsymbol{x}_1,\boldsymbol{x}_4)\\
&\qquad\times\rho^{\sigma}(\boldsymbol{x}_1,\boldsymbol{x}_2)\rho^{\sigma}(\boldsymbol{x}_3,\boldsymbol{x}_4)V(\boldsymbol{x}_1,\boldsymbol{x}_2)V(\boldsymbol{x}_3,\boldsymbol{x}_4)\\
&= \epsilon^{3d}s\int_0^{\infty}\mathrm{d}t\int\mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4\int_{\mu}^{\infty}\mathrm{d}e_1e^{-te_1}\rho^{\sigma}(e_1;\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2)\\
&\quad\times\int_0^{\mu}\mathrm{d}e_2e^{te_2}\rho^{\sigma}(e_2;\boldsymbol{x}_1,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4)\rho^{\sigma}(\boldsymbol{x}_1,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2)\rho^{\sigma}(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4)\\
&\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2)V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4)\\
&= \frac{\epsilon^{-d}s}{(2\pi)^{4d}}\int_0^{\infty}\mathrm{d}t\int\mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{k}_i\\
&\qquad\times e^{-t(\boldsymbol{k}_1^2+V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3))}e^{t(\boldsymbol{k}_2^2+V(\boldsymbol{x}_1))}e^{i[\boldsymbol{r}_2(\boldsymbol{k}_1+\boldsymbol{k}_3)-\boldsymbol{r}_3(\boldsymbol{k}_1+\boldsymbol{k}_4)+\boldsymbol{r}_4(\boldsymbol{k}_2+\boldsymbol{k}_4)]}\\
&\qquad\times\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_2^2)\\
&\qquad\times\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_3^2)\theta((\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3))-\boldsymbol{k}_4^2)\\
&\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2)V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4).
\end{aligned}\tag{2.164}$$

Taking the semiclassical limit $\epsilon \ll 1$, which implies $\boldsymbol{x}_i+\epsilon\boldsymbol{r}_j\simeq\boldsymbol{x}_i$, we find, using the translation invariance of V ($V(\boldsymbol{x}_1,\boldsymbol{x}_2)=V(|\boldsymbol{x}_1-\boldsymbol{x}_2|)$),

$$\begin{aligned}
p_2^2 &= \frac{\epsilon^{-d}s}{(2\pi)^{4d}}\int_0^{\infty}\mathrm{d}t\int\mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{k}_ie^{-t(\boldsymbol{k}_1^2-\boldsymbol{k}_2^2)}\\
&\qquad\times e^{i[\boldsymbol{r}_2(\boldsymbol{k}_1+\boldsymbol{k}_3)-\boldsymbol{r}_3(\boldsymbol{k}_1+\boldsymbol{k}_4)+\boldsymbol{r}_4(\boldsymbol{k}_2+\boldsymbol{k}_4)]}V(\epsilon\boldsymbol{r}_2)V(\epsilon|\boldsymbol{r}_3-\boldsymbol{r}_4|)\\
&\qquad\times\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_2^2)\\
&\qquad\times\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_3^2)\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2).
\end{aligned}\tag{2.165}$$

Let's introduce the Fourier transform (2.145) of V, use the scaling property $V(\epsilon\boldsymbol{r})=\frac{1}{\epsilon}V(\boldsymbol{r})$, and integrate over $\boldsymbol{r}_2,\boldsymbol{r}_3,\boldsymbol{r}_4$ using the delta functions (2.147):

$$\begin{aligned}
p_2^2 &= \frac{\epsilon^{-(d+2)}s}{(2\pi)^{6d}}\int_0^{\infty}\mathrm{d}t\int\mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4\int\prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{k}_i\mathrm{d}^d\boldsymbol{q}_1\mathrm{d}^d\boldsymbol{q}_2e^{-t(\boldsymbol{k}_1^2-\boldsymbol{k}_2^2)}\\
&\qquad\times e^{i[\boldsymbol{r}_2(\boldsymbol{k}_1+\boldsymbol{k}_3+\boldsymbol{q}_1)-\boldsymbol{r}_3(\boldsymbol{k}_1+\boldsymbol{k}_4+\boldsymbol{q}_2)+\boldsymbol{r}_4(\boldsymbol{k}_2+\boldsymbol{k}_4+\boldsymbol{q}_2)]}\hat{V}(\boldsymbol{q}_1)\hat{V}(\boldsymbol{q}_2)\\
&\qquad\times\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_2^2)\\
&\qquad\times\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_3^2)\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2)
\end{aligned}$$

$$
\begin{aligned}
&= \frac{\epsilon^{-(d+2)}s}{(2\pi)^{3d}} \int_0^\infty \mathrm{d}t \int \mathrm{d}^d\boldsymbol{x}_1 \int \prod_{i=1}^{4} \mathrm{d}^d\boldsymbol{k}_i \mathrm{d}^d\boldsymbol{q}_1 \mathrm{d}^d\boldsymbol{q}_2 e^{-t(\boldsymbol{k}_1^2-\boldsymbol{k}_2^2)} \hat{V}(\boldsymbol{q}_1)\hat{V}(\boldsymbol{q}_2) \\
&\quad \times \delta(\boldsymbol{k}_1+\boldsymbol{k}_3+\boldsymbol{q}_1) \underbrace{\delta(\boldsymbol{k}_1+\boldsymbol{k}_4+\boldsymbol{q}_2)\delta(\boldsymbol{k}_2+\boldsymbol{k}_4+\boldsymbol{q}_2)}_{=\delta(\boldsymbol{k}_1+\boldsymbol{k}_4+\boldsymbol{q}_2)\delta(\boldsymbol{k}_1+\boldsymbol{k}_2)} \theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1))) \\
&\quad \times \theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_2^2)\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_3^2)\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2).
\end{aligned}
\tag{2.166}
$$

We integrate over $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{k}_2$, and use the parity of $\hat{V}$ to find

$$
\begin{aligned}
p_2^2 &= \frac{\epsilon^{-(d+2)}s}{(2\pi)^{3d}} \int_0^\infty \mathrm{d}t \int \mathrm{d}^d\boldsymbol{x}_1 \int \mathrm{d}^d\boldsymbol{k}_1 \mathrm{d}^d\boldsymbol{k}_3 \mathrm{d}^d\boldsymbol{k}_4 \hat{V}(\boldsymbol{k}_1+\boldsymbol{k}_3)\hat{V}(\boldsymbol{k}_1+\boldsymbol{k}_4) \\
&\quad \times \underbrace{\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_1^2)}_{=0} \\
&\quad \times \theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_3^2)\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2) \\
&= 0.
\end{aligned}
\tag{2.167}
$$

This contribution therefore vanishes in the semiclassical limit.

Let’s evaluate the third term (2.139) of p_2. Using (2.143), and (2.144), as well as proceeding to the change of variables

$$
\begin{aligned}
\boldsymbol{x}_2 &\mapsto \boldsymbol{r}_2, & \epsilon\boldsymbol{r}_2 &= \boldsymbol{x}_2-\boldsymbol{x}_1, & \epsilon^d\mathrm{d}^d\boldsymbol{r}_2 &= \mathrm{d}^d\boldsymbol{x}_2, \\
\boldsymbol{x}_3 &\mapsto \boldsymbol{r}_3, & \epsilon\boldsymbol{r}_3 &= \boldsymbol{x}_3-\boldsymbol{x}_1, & \epsilon^d\mathrm{d}^d\boldsymbol{r}_3 &= \mathrm{d}^d\boldsymbol{x}_3, \\
\boldsymbol{x}_4 &\mapsto \boldsymbol{r}_4, & \epsilon\boldsymbol{r}_4 &= \boldsymbol{x}_4-\boldsymbol{x}_1, & \epsilon^d\mathrm{d}^d\boldsymbol{r}_4 &= \mathrm{d}^d\boldsymbol{x}_4,
\end{aligned}
\tag{2.168}
$$

this term becomes

$$
\begin{aligned}
p_2^3 &= -\frac{s}{2}\int \prod_{i=1}^{4}\mathrm{d}^d\boldsymbol{x}_i \int_\mu^\infty \mathrm{d}e_1 \int_0^\mu \mathrm{d}e_2 \int_\mu^\infty \mathrm{d}e_3 \int_0^\mu \mathrm{d}e_4 \frac{1}{(e_1+e_3-e_2-e_4)} \\
&\quad \times \rho^\sigma(e_1,\boldsymbol{x}_2,\boldsymbol{x}_1)\rho^\sigma(e_2,\boldsymbol{x}_3,\boldsymbol{x}_2)\rho^\sigma(e_3,\boldsymbol{x}_4,\boldsymbol{x}_3)\rho^\sigma(e_4,\boldsymbol{x}_1,\boldsymbol{x}_4) \\
&\quad \times V(\boldsymbol{x}_1,\boldsymbol{x}_3)V(\boldsymbol{x}_2,\boldsymbol{x}_4) \\
&= -\frac{\epsilon^{3d}s}{2}\int_0^\infty \mathrm{d}t \int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4 \int_\mu^\infty \mathrm{d}e_1 e^{-te_1}\rho^\sigma(e_1;\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2,\boldsymbol{x}_1) \\
&\quad \times \int_0^\mu \mathrm{d}e_2 e^{te_2}\rho^\sigma(e_2;\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2) \int_\mu^\infty \mathrm{d}e_3 e^{-te_3}\rho^\sigma(e_3;\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3) \\
&\quad \times \int_0^\mu \mathrm{d}e_4 e^{te_4}\rho^\sigma(e_4;\boldsymbol{x}_1,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4)V(\boldsymbol{x}_1,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3)V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4)
\end{aligned}
$$

$$\begin{aligned}
&= -\frac{s}{2}\frac{\epsilon^{-d}}{(2\pi)^{4d}}\int_0^\infty \mathrm{d}t\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4\int\prod_{i=1}^4\mathrm{d}^d\boldsymbol{k}_i \\
&\qquad\times e^{-t(\boldsymbol{k}_1^2+V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2))}e^{t(\boldsymbol{k}_2^2+V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3))}e^{-t(\boldsymbol{k}_3^2+V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4))}e^{t(\boldsymbol{k}_4^2+V(\boldsymbol{x}_1))} \\
&\qquad\times e^{i[\boldsymbol{r}_2(-\boldsymbol{k}_1+\boldsymbol{k}_2)+\boldsymbol{r}_3(-\boldsymbol{k}_2+\boldsymbol{k}_3)+\boldsymbol{r}_4(-\boldsymbol{k}_3+\boldsymbol{k}_4)]} \\
&\qquad\times V(\boldsymbol{x}_1,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3)V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2,\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4) \\
&\qquad\times\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_2)))\theta((\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_3))-\boldsymbol{k}_2^2) \\
&\qquad\times\theta(\boldsymbol{k}_3^2-(\mu-V(\boldsymbol{x}_1+\epsilon\boldsymbol{r}_4)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_1^2).
\end{aligned} \tag{2.169}$$

Taking the semiclassical limit $\epsilon \ll 1$, which implies $\boldsymbol{x}_i+\epsilon\boldsymbol{r}_j \simeq \boldsymbol{x}_i$, and using the symmetry of V, we find

$$\begin{aligned}
p_2^3 &= -\frac{s}{2}\frac{\epsilon^{-d}}{(2\pi)^{4d}}\int_0^\infty \mathrm{d}t\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4\int\prod_{i=1}^4\mathrm{d}^d\boldsymbol{k}_iV(\epsilon|\boldsymbol{r}_3|)V(\epsilon|\boldsymbol{r}_4-\boldsymbol{r}_2|) \\
&\qquad\times e^{-t(\boldsymbol{k}_1^2-\boldsymbol{k}_2^2+\boldsymbol{k}_3^2-\boldsymbol{k}_4^2)}e^{i[\boldsymbol{r}_2(-\boldsymbol{k}_1+\boldsymbol{k}_2)+\boldsymbol{r}_3(-\boldsymbol{k}_2+\boldsymbol{k}_3)+\boldsymbol{r}_4(-\boldsymbol{k}_3+\boldsymbol{k}_4)]} \\
&\qquad\times\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_2^2) \\
&\qquad\times\theta(\boldsymbol{k}_3^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2).
\end{aligned} \tag{2.170}$$

Let's introduce the Fourier transform (2.145) of V, use the scaling property $V(\epsilon\boldsymbol{r})=\frac{1}{\epsilon}V(\boldsymbol{r})$, and integrate over $\boldsymbol{r}_2,\boldsymbol{r}_3,\boldsymbol{r}_4$ using the delta functions (2.147):

$$\begin{aligned}
p_2^3 &= -\frac{s}{2}\frac{\epsilon^{-(d+2)}}{(2\pi)^{6d}}\int_0^\infty \mathrm{d}t\int \mathrm{d}^d\boldsymbol{x}_1\mathrm{d}^d\boldsymbol{r}_2\mathrm{d}^d\boldsymbol{r}_3\mathrm{d}^d\boldsymbol{r}_4\int\prod_{i=1}^4\mathrm{d}^d\boldsymbol{k}_i\mathrm{d}^d\boldsymbol{q}_1\mathrm{d}^d\boldsymbol{q}_2\hat{V}(\boldsymbol{q}_1)\hat{V}(\boldsymbol{q}_2) \\
&\qquad\times e^{-t(\boldsymbol{k}_1^2-\boldsymbol{k}_2^2+\boldsymbol{k}_3^2-\boldsymbol{k}_4^2)}e^{i[\boldsymbol{r}_2(-\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{q}_2)+\boldsymbol{r}_3(-\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{q}_1)+\boldsymbol{r}_4(-\boldsymbol{k}_3+\boldsymbol{k}_4+\boldsymbol{q}_2)]} \\
&\qquad\times\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_2^2) \\
&\qquad\times\theta(\boldsymbol{k}_3^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2) \\
&= -\frac{s}{2}\frac{\epsilon^{-(d+2)}}{(2\pi)^{3d}}\int_0^\infty \mathrm{d}t\int \mathrm{d}^d\boldsymbol{x}_1\int\prod_{i=1}^4\mathrm{d}^d\boldsymbol{k}_i\mathrm{d}^d\boldsymbol{q}_1\mathrm{d}^d\boldsymbol{q}_2e^{-t(\boldsymbol{k}_1^2-\boldsymbol{k}_2^2+\boldsymbol{k}_3^2-\boldsymbol{k}_4^2)}\hat{V}(\boldsymbol{q}_1)\hat{V}(\boldsymbol{q}_2) \\
&\qquad\times\delta(-\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{q}_2)\delta(-\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{q}_1)\delta(-\boldsymbol{k}_3+\boldsymbol{k}_4+\boldsymbol{q}_2) \\
&\qquad\times\theta(\boldsymbol{k}_1^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_2^2) \\
&\qquad\times\theta(\boldsymbol{k}_3^2-(\mu-V(\boldsymbol{x}_1)))\theta((\mu-V(\boldsymbol{x}_1))-\boldsymbol{k}_4^2).
\end{aligned} \tag{2.171}$$

We integrate over $6d$ variables in Fourier space, and there are $3d$ delta functions. We will therefore have $3d$ variables left.

We have

$$\delta(-\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{q}_2)\delta(-\boldsymbol{k}_3+\boldsymbol{k}_4+\boldsymbol{q}_2)=\delta(\boldsymbol{q}_2+\boldsymbol{k}_1-\boldsymbol{k}_2)\delta(-\boldsymbol{k}_1+\boldsymbol{k}_2-\boldsymbol{k}_3+\boldsymbol{k}_4). \tag{2.172}$$

We integrate over $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{k}_4$ and proceed to the change of variables

$$(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{k}_3) \mapsto (\boldsymbol{k}, \boldsymbol{q}_+, \boldsymbol{q}_-), \tag{2.173}$$

$$\begin{aligned} \boldsymbol{k} &= \frac{\boldsymbol{k}_1 + \boldsymbol{k}_3}{2}, \\ \boldsymbol{q}_- &= \boldsymbol{k}_2 - \frac{\boldsymbol{k}_1 + \boldsymbol{k}_3}{2}, \\ \boldsymbol{q}_+ &= \frac{-\boldsymbol{k}_1 + \boldsymbol{k}_3}{2}, \end{aligned} \tag{2.174}$$

$$\mathrm{d}^d\boldsymbol{k}_1 \mathrm{d}^d\boldsymbol{k}_2 \mathrm{d}^d\boldsymbol{k}_3 = 2^d \mathrm{d}^d\boldsymbol{k} \mathrm{d}^d\boldsymbol{q}_+ \mathrm{d}^d\boldsymbol{q}_-. \tag{2.175}$$

The old variables become

$$\begin{aligned} \boldsymbol{k}_1 &= \boldsymbol{k} - \boldsymbol{q}_+, \\ \boldsymbol{k}_3 &= \boldsymbol{k} + \boldsymbol{q}_+, \\ \boldsymbol{k}_2 &= \boldsymbol{k} + \boldsymbol{q}_-, \\ \boldsymbol{k}_4 &= \boldsymbol{k}_1 - \boldsymbol{k}_2 + \boldsymbol{k}_3 = \boldsymbol{k} - \boldsymbol{q}_-, \\ \boldsymbol{q}_1 &= \boldsymbol{k}_2 - \boldsymbol{k}_3 = \boldsymbol{q}_- - \boldsymbol{q}_+, \\ \boldsymbol{q}_2 &= -\boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{q}_+ + \boldsymbol{q}_-. \end{aligned} \tag{2.176}$$

We establish

$$\boldsymbol{k}_1^2 + \boldsymbol{k}_3^2 - \boldsymbol{k}_2^2 - \boldsymbol{k}_4^2 = 2(\boldsymbol{q}_+^2 - \boldsymbol{q}_-^2). \tag{2.177}$$

The contribution to the pressure becomes

$$\begin{aligned} p_2^3 = {} & -2^{(d-1)} \frac{\epsilon^{-(d+2)} s}{(2\pi)^{3d}} \int_0^\infty \mathrm{d}t \int \mathrm{d}^d\boldsymbol{x} \int \mathrm{d}^d\boldsymbol{k} \mathrm{d}^d\boldsymbol{q}_+ \mathrm{d}^d\boldsymbol{q}_- e^{-2t(\boldsymbol{q}_+^2 - \boldsymbol{q}_-^2)} \\ & \times \hat{V}(\boldsymbol{q}_- - \boldsymbol{q}_+) \hat{V}(\boldsymbol{q}_+ + \boldsymbol{q}_-) \\ & \times \theta((\boldsymbol{k} - \boldsymbol{q}_+)^2 - (\mu - V(\boldsymbol{x}))) \theta((\mu - V(\boldsymbol{x})) - (\boldsymbol{k} + \boldsymbol{q}_-)^2) \\ & \times \theta((\boldsymbol{k} + \boldsymbol{q}_+)^2 - (\mu - V(\boldsymbol{x}))) \theta((\mu - V(\boldsymbol{x})) - (\boldsymbol{k} - \boldsymbol{q}_-)^2). \end{aligned} \tag{2.178}$$

Integrating over t, and replacing $\hat{V}$ by its value (2.146), we find

$$\begin{aligned} p_2^3 = {} & -2^{(d-2)} \frac{\epsilon^{-(d+2)} S_d^2 s}{(2\pi)^{3d}} \int \mathrm{d}^d\boldsymbol{x} \mathrm{d}^d\boldsymbol{q}_+ \mathrm{d}^d\boldsymbol{q}_- \frac{1}{(\boldsymbol{q}_+^2 - \boldsymbol{q}_-^2)} \\ & \times \frac{1}{((\boldsymbol{q}_+^2 + \boldsymbol{q}_-^2)^2 - 4(\boldsymbol{q}_+ \boldsymbol{q}_-)^2)^{\frac{(d-1)}{2}}} \\ & \times \int \mathrm{d}^d\boldsymbol{k} \theta((\boldsymbol{k} - \boldsymbol{q}_+)^2 - (\mu - V(\boldsymbol{x}))) \theta((\mu - V(\boldsymbol{x})) - (\boldsymbol{k} + \boldsymbol{q}_-)^2) \\ & \times \theta((\boldsymbol{k} + \boldsymbol{q}_+)^2 - (\mu - V(\boldsymbol{x}))) \theta((\mu - V(\boldsymbol{x})) - (\boldsymbol{k} - \boldsymbol{q}_-)^2), \end{aligned} \tag{2.179}$$

where we used the equality

$$(\boldsymbol{q}_+ - \boldsymbol{q}_-)^2(\boldsymbol{q}_+ + \boldsymbol{q}_-)^2 = (\boldsymbol{q}_+^2 + \boldsymbol{q}_-^2)^2 - 4(\boldsymbol{q}_+\boldsymbol{q}_-)^2. \tag{2.180}$$

We can separate the integration over $\boldsymbol{x}$ and $\boldsymbol{k}, \boldsymbol{q}_+, \boldsymbol{q}_-$ by the change of variables

$$\begin{array}{lll} \boldsymbol{k} & \mapsto & \boldsymbol{k}', \quad \sqrt{\mu - V(\boldsymbol{x})}\boldsymbol{k}' = \boldsymbol{k}, \quad \mathrm{d}^d\boldsymbol{k} = (\mu - V(\boldsymbol{x}))^{\frac{d}{2}}\,\mathrm{d}^d\boldsymbol{k}', \\ \boldsymbol{q}_+ & \mapsto & \boldsymbol{q}'_+, \quad \sqrt{\mu - V(\boldsymbol{x})}\boldsymbol{q}'_+ = \boldsymbol{q}_+, \quad \mathrm{d}^d\boldsymbol{q}_+ = (\mu - V(\boldsymbol{x}))^{\frac{d}{2}}\,\mathrm{d}^d\boldsymbol{q}'_+, \\ \boldsymbol{q}_- & \mapsto & \boldsymbol{q}'_-, \quad \sqrt{\mu - V(\boldsymbol{x})}\boldsymbol{q}'_- = \boldsymbol{q}_-, \quad \mathrm{d}^d\boldsymbol{q}_- = (\mu - V(\boldsymbol{x}))^{\frac{d}{2}}\,\mathrm{d}^d\boldsymbol{q}'_-. \end{array} \tag{2.181}$$

With this change of variables the contribution to the pressure becomes

$$\begin{aligned} p_2^3 &= -2^{(d-2)}\frac{\epsilon^{-(d+2)}S_d^2 s}{(2\pi)^{3d}}\int \mathrm{d}^d\boldsymbol{x}(\mu - V(\boldsymbol{x}))^{\frac{d}{2}}\int \mathrm{d}^d\boldsymbol{q}_+\mathrm{d}^d\boldsymbol{q}_-\frac{1}{(\boldsymbol{q}_+^2 - \boldsymbol{q}_-^2)} \\ &\qquad \times\frac{1}{((\boldsymbol{q}_+^2 + \boldsymbol{q}_-^2)^2 - 4(\boldsymbol{q}_+\boldsymbol{q}_-)^2)^{\frac{(d-1)}{2}}} \\ &\qquad \times\int \mathrm{d}^d\boldsymbol{k}\theta((\boldsymbol{k} - \boldsymbol{q}_+)^2 - 1)\theta(1 - (\boldsymbol{k} + \boldsymbol{q}_-)^2) \\ &\qquad \times\theta((\boldsymbol{k} + \boldsymbol{q}_+)^2 - 1)\theta(1 - (\boldsymbol{k} - \boldsymbol{q}_-)^2) \\ &\doteq \underbrace{-2^{(d-2)}\frac{\epsilon^{-(d+2)}S_d^2 s}{(2\pi)^{3d}}\int \mathrm{d}^d\boldsymbol{x}(\mu - V(\boldsymbol{x}))^{\frac{d}{2}}}_{\doteq C'}\int \mathrm{d}^d\boldsymbol{q}_+\mathrm{d}^d\boldsymbol{q}_-\frac{1}{(\boldsymbol{q}_+^2 - \boldsymbol{q}_-^2)} \\ &\qquad \times\frac{1}{((\boldsymbol{q}_+^2 + \boldsymbol{q}_-^2)^2 - 4(\boldsymbol{q}_+\boldsymbol{q}_-)^2)^{\frac{(d-1)}{2}}}f_d(q_+, q_-, \boldsymbol{q}_+\boldsymbol{q}_-). \end{aligned} \tag{2.182}$$

The function f_d has a geometrical interpretation: it corresponds to the surface contained in two hyperspheres of radius one and of center $\pm\boldsymbol{q}_-$, minus their intersection with hyperspheres of radius one and of center $\pm\boldsymbol{q}_+$.

The entire N-dependence of this term is contained in part C'. Its N-dependence can be established by replacing $(\mu - V(\boldsymbol{x}))$ by the density, using the relation (2.159). We find

$$\begin{aligned} C' &= \frac{2^{(d-2)}S_d d}{\epsilon^2(2\pi)^{2d}}\underbrace{\int \mathrm{d}^d\boldsymbol{x}\rho(\boldsymbol{x})}_{=N} = \frac{2^{(d-2)}S_d d}{(2\pi)^{2d}}\frac{N}{\epsilon^2} \\ &= \frac{2^{(d-1)}S_d d}{(2\pi)^{2d}}N^{1+\frac{2}{d}} = \begin{cases} \frac{1}{2\pi^3}N^2 & , \quad d = 2, \\ \frac{3}{4\pi^5}N^{\frac{5}{3}} & , \quad d = 3, \end{cases} \end{aligned} \tag{2.183}$$

and p_2^3 becomes

$$p_2^3 = -N^{1+\frac{2}{d}}\frac{2^{(d-1)}S_d d}{(2\pi)^{2d}}\int \mathrm{d}^d\boldsymbol{q}_+\mathrm{d}^d\boldsymbol{q}_-\frac{1}{(\boldsymbol{q}_+^2 - \boldsymbol{q}_-^2)}\frac{f_d(q_+, q_-, \boldsymbol{q}_+\boldsymbol{q}_-)}{((\boldsymbol{q}_+^2 + \boldsymbol{q}_-^2)^2 - 4(\boldsymbol{q}_+\boldsymbol{q}_-)^2)^{\frac{(d-1)}{2}}}. \tag{2.184}$$

2.5.3 Total semiclassical pressure

The ground state pressure in the semiclassical limit is therefore

$$P = p_0^{SC} + p_1^{SC} N^{-1} + p_2^{SC} N^{-2} + \mathcal{O}(N^{-3}) + \mu N, \tag{2.185}$$

where

$$\begin{aligned}
p_0^{SC} &= -s \sum_{i=1}^{N/s} e_i^{SC} + \frac{1}{2N} \int \mathrm{d}^d \boldsymbol{x} \mathrm{d}^d \boldsymbol{y} V(\boldsymbol{x}, \boldsymbol{y}) \rho^{SC}(\boldsymbol{x}) \rho^{SC}(\boldsymbol{y}), \\
p_1^{SC} &= \frac{1}{2s} \int \mathrm{d}^d \boldsymbol{x} \mathrm{d}^d \boldsymbol{y} V(\boldsymbol{x}, \boldsymbol{y}) \rho^{SC}(\boldsymbol{x}, \boldsymbol{y}) \rho^{SC}(\boldsymbol{y}, \boldsymbol{x}), \\
p_2^{SC} &= p_2^1 - N^{1+\frac{2}{d}} \frac{2^{(d-1)} S_d d}{(2\pi)^{2d}} \int \mathrm{d}^d \boldsymbol{q}_+ \mathrm{d}^d \boldsymbol{q}_- \frac{1}{(\boldsymbol{q}_+^2 - \boldsymbol{q}_-^2)} \\
&\qquad \times \frac{f_d(q_+, q_-, \boldsymbol{q}_+ \boldsymbol{q}_-)}{((\boldsymbol{q}_+^2 + \boldsymbol{q}_-^2)^2 - 4(\boldsymbol{q}_+ \boldsymbol{q}_-)^2)^{\frac{(d-1)}{2}}}.
\end{aligned} \tag{2.186}$$

The eigenvalues e_i are evaluated semiclassically, as well as the self-consistent density and potential, evaluated with the use of the self-consistent equation (2.63). This will be done in detail for the quantum dots later (see part II).

2.6 Semiclassical energy

The semiclassical energy is immediately obtained from the semiclassical pressure using equality (2.3). We find

$$E = e_0^{SC} + e_1^{SC} N^{-1} + e_2^{SC} N^{-2} + \mathcal{O}(N^{-3}), \tag{2.187}$$

where

$$\begin{aligned}
e_0^{SC} &= s \sum_{i=1}^{N/s} e_i^{SC} - \frac{1}{2N} \int \mathrm{d}^d \boldsymbol{x} \mathrm{d}^d \boldsymbol{y} V(\boldsymbol{x}, \boldsymbol{y}) \rho^{SC}(\boldsymbol{x}) \rho^{SC}(\boldsymbol{y}), \\
e_1^{SC} &= -\frac{1}{2s} \int \mathrm{d}^d \boldsymbol{x} \mathrm{d}^d \boldsymbol{y} V(\boldsymbol{x}, \boldsymbol{y}) \rho^{SC}(\boldsymbol{x}, \boldsymbol{y}) \rho^{SC}(\boldsymbol{y}, \boldsymbol{x}), \\
e_2^{SC} &= e_2^1 + N^{1+\frac{2}{d}} \frac{2^{(d-1)} S_d d}{(2\pi)^{2d}} \int \mathrm{d}^d \boldsymbol{q}_+ \mathrm{d}^d \boldsymbol{q}_- \frac{1}{(\boldsymbol{q}_+^2 - \boldsymbol{q}_-^2)} \\
&\qquad \times \frac{f_d(q_+, q_-, \boldsymbol{q}_+ \boldsymbol{q}_-)}{((\boldsymbol{q}_+^2 + \boldsymbol{q}_-^2)^2 - 4(\boldsymbol{q}_+ \boldsymbol{q}_-)^2)^{\frac{(d-1)}{2}}},
\end{aligned} \tag{2.188}$$

where $e_2^1 = -p_2^1$.

Let's proceed to a discussion of this result. The lowest order term, e_0^{SC}, corresponds to the Hartree energy: it consists of the sum of the N lowest eigenvalues of a single particle system, submitted to a potential obtained with the self-consistent equation (2.63), plus an additional term, the opposite of the self-energy of the electrons. The interpretation is the following: it consists of approximating the system by a system of independent particles, respecting the Fermi-Dirac statistics by filling the N lowest energy eigenstates of a single-particle hamiltonian. In this system, the self-energy of the electrons is counted twice, and this is why the second term of e_0^{SC} corresponds to the opposite of this self-energy, and therefore cancels the term in excess. The Hartree energy can be expanded in the semiclassical regime, to obtain an expansion around a small parameter, given by an inverse power of N. This was done by Englert and Schwinger (1985b) for the atom, and we do it in chapter 5 for the quantum dot, with a more detailed study of the sum of the eigenvalues in chapter 6.

The first order term, e_1^{SC}, corresponds to the exchange energy. This result is equal to that we obtain in the semiclassical Hartree development, as is done in chapter 5.

The sum of these two first terms correspond to semiclassical Hartree-Fock results.

The second order term, e_2^{SC}, corresponds to the first correction beyond the semiclassical Hartree-Fock model. It is the lowest order of the correlation energy, and this is why it is particularly interesting.

Let's evaluate the orders in N of these terms. To proceed to these evaluations, we need to know the orders $e_i = \mathcal{O}(1)$, $\rho = \mathcal{O}(N)$. Moreover, the density matrix is such that $\rho(\boldsymbol{x}, \boldsymbol{y}) \neq 0$ only if $|\boldsymbol{y} - \boldsymbol{x}| \simeq \epsilon$. Changes of variable will be performed to establish the order of the terms we computed. We are interested in the order of magnitude of the physical energy, which is obtained from E by the inverse of the scaling (2.10): $\hat{E} = N^{2-\frac{2}{d}} E$. Moreover, the small parameter is $\epsilon \simeq N^{-\frac{1}{d}}$.

The order of $\sum_{i=1}^{N} e_i$ is N (as it consists of a sum of N terms of the order of 1). It provides a contribution of $N^{3-\frac{2}{d}}$ to the ground state energy, which is $N^{\frac{7}{3}}$ for $d = 3$ dimensions, and N^2 for $d = 2$ dimensions. To compute the self-energy of the electrons, we use $\rho = \mathcal{O}(N)$ to obtain a term of the order of N. Proceeding to the inverse scaling we find that its contribution to the ground state energy is $N^{3-\frac{2}{d}}$, which is the same as the sum of the eigenvalues. These orders in N are well-known results.

In the case of quantum dots, let's note that there is a second parameter, in addition to N, which has to be taken into account. It is the strength of the confining potential, κ, which fixes the length scale. This is why a more comprehensive treatment has to be done, with a scaling depending on this parameter. This is done in chapter 5 for a parabolic quantum dot, where we find that the Thomas-Fermi energy is of the order of $\frac{N^2}{L_\star}$, where $L_\star = \mathcal{O}(\kappa^{-\frac{1}{3}})$, and leads finally to an asymptotic energy of the order of $N^{\frac{3}{2}}$ (depending however on how we model the confining potential, as discussed in chapter 4).

To establish the order of the exchange energy, e_1^{SC}, we proceed to the change of variable $\boldsymbol{y} \mapsto \boldsymbol{r}$, $\epsilon \boldsymbol{r} = \boldsymbol{y}$. This implies $\mathrm{d}^d \boldsymbol{y} = \epsilon^d \mathrm{d}^d \boldsymbol{r}$ and $V(\epsilon \boldsymbol{r}) = \mathcal{O}(\epsilon^{-1})$. The energy is therefore of the order of $N^{-1} e_1^{SC} \simeq N \epsilon^{d-1} = N^{\frac{1}{d}}$. The contribution to the ground state energy is therefore $N^{2-\frac{2}{d}+\frac{1}{d}} = N^{2-\frac{1}{d}}$. It is
$N^{\frac{5}{3}}$ in $d=3$ dimensions, and $N^{\frac{3}{2}}$ in $d=2$ dimensions.

In the case of a parabolic quantum dot, we find that the exchange energy is of the order of $\frac{N^{\frac{3}{2}}}{L_\star} \simeq N$.

We made explicit the order of one part of e_2^{SC}. We find $N^{-2} e_2^{SC} = \mathcal{O}(N^{-1+\frac{2}{d}})$, its contribution to the ground state being therefore $N^{2-\frac{2}{d}} N^{-1+\frac{2}{d}} = N$. The order of the other part of e_2^{SC} still has to be determined.

The order of this correction is independent of the dimension of the system. In the case of atoms, there are more important corrections to the ground state energy arising from the semiclassical Hartree-Fock development (of the order of $N^{\frac{4}{3}}$), which corresponds to corrections to e_0^{SC}. These corrections are therefore contained in our developments, but are out of reach analytically. It is therefore not necessary to take this term into account for the computation of the ground state energy of atoms. But is it useless to compute this term? No. The term we compute is the main term of the correlation energy. There are numerical simulations, with very high accuracy, computed in the Hartree-Fock model, that is without correlations. The correlation energy can therefore be isolated, by subtracting the numerical Hartree-Fock results to the experimental energy. We obtain this way the correlation energy, and our results can be compared to experimental data.

This result deserves a comment: as written in Lieb (1976), in the Thomas-Fermi approximation, the electrons of the outer region of the atom are not considered. If the theory is applied to molecules, this implies the no-binding theorem (due to Teller (1962)), which states that the Thomas-Fermi energy is unstable under the decomposition of a big molecule into any smaller ones. Moreover, Lieb (1976) writes that the binding energy is of the order of N, which is precisely the order of the correction we computed. This correction corresponds to the first term including correlation effects. These terms may therefore correspond to the binding energy. The application of our formalism to molecules may answer this question.

In the case of quantum dots, as we will see later, this correction has to be taken into account for the computation of the ground state energy for consistency. As said earlier, we have to proceed to a scaling of the length, which depends on an external parameter, as will be done in chapter 5. By proceeding to this scaling we find that this correction is (in this case, too) of the order of N, independent of the new length scale, for the parabolic quantum dot.

One part of the energy e_2^{SC} will be computed in chapter 3, for the two- and three-dimensional cases, to obtain quantitative results.

We computed the first and second orders of the perturbative expansion of the ground state energy. While we do not compute higher orders corrections, there is no conceptual difficulty in doing so.

Chapter 3

Semiclassical atoms – correlation energy

Contents

The objective of this chapter is to compute new corrections to the ground state energy of quantum dots and large atoms, a term including correlation effects.

In chapter 2 we developed a new approach to compute, with a systematic expansion around a small parameter, the ground state energy of a many-fermion system. We apply this method to the problem of the quantum dot and the atom in this chapter.

The semiclassical Hartree-Fock approach was already applied to atoms (Englert, 1988), this is why we focus on the new corrections. We compute one term of the corrections, which is, as established in chapter 2, universal and depends on the dimension of the system only. To compute this new contribution to quantum dots and atoms, we compute this term for the two- and three-dimensional problems, which reduces to the computation of multiple integrals, computed numerically.

The expression we have to compute is written in equation (2.188). The expression in the d-dimensional case is

$$\hat{E}_2^{SC} = N \frac{2^{(d-1)} S_d d}{(2\pi)^{2d}} \underbrace{\int \mathrm{d}^d \boldsymbol{q}_+ \mathrm{d}^d \boldsymbol{q}_- \frac{1}{(\boldsymbol{q}_+^2 - \boldsymbol{q}_-^2)} \frac{f_d(q_+, q_-, \boldsymbol{q}_+ \boldsymbol{q}_-)}{((\boldsymbol{q}_+^2 + \boldsymbol{q}_-^2)^2 - 4(\boldsymbol{q}_+ \boldsymbol{q}_-)^2)^{\frac{(d-1)}{2}}}}_{\doteq \Delta_d}, \quad (3.1)$$

where the function f_d is defined by

$$\begin{aligned} f_d(q_+, q_-, \boldsymbol{q}_+\boldsymbol{q}_-) &= \int \mathrm{d}^d\boldsymbol{k}\theta((\boldsymbol{k}-\boldsymbol{q}_+)^2-1)\theta(1-(\boldsymbol{k}+\boldsymbol{q}_-)^2) \\ &\quad \times\theta((\boldsymbol{k}+\boldsymbol{q}_+)^2-1)\theta(1-(\boldsymbol{k}-\boldsymbol{q}_-)^2) \\ &= \int \mathrm{d}^d\boldsymbol{k}\theta(\boldsymbol{k}^2+\boldsymbol{q}_+^2-2|\boldsymbol{k}\boldsymbol{q}_+|-1)\theta(1-\boldsymbol{k}^2-\boldsymbol{q}_-^2-2|\boldsymbol{k}\boldsymbol{q}_-|). \end{aligned} \tag{3.2}$$

To compute this integral numerically, we simplify it to the maximum. Let's separate the integration variables in the radial and angular parts:

$$\begin{aligned} &\boldsymbol{q}_\pm = q_\pm\hat{\boldsymbol{e}}_\pm,\ |\hat{\boldsymbol{e}}_\pm| = 1,\ \boldsymbol{k} = k\hat{\boldsymbol{e}}, |\hat{\boldsymbol{e}}| = 1 \\ \Rightarrow\quad &\mathrm{d}^d\boldsymbol{q}_\pm = q_\pm^{(d-1)}\mathrm{d}q_\pm\mathrm{d}\hat{\boldsymbol{e}}_\pm,\ \mathrm{d}^d\boldsymbol{k} = k^{(d-1)}\mathrm{d}k\mathrm{d}\hat{\boldsymbol{e}}. \end{aligned} \tag{3.3}$$

We obtain

$$\begin{aligned} \Delta_d &= \int \mathrm{d}q_+\mathrm{d}q_-\mathrm{d}\hat{\boldsymbol{e}}_+\mathrm{d}\hat{\boldsymbol{e}}_-\frac{q_+^{d-1}q_-^{d-1}}{(q_+^2-q_-^2)}\frac{1}{((q_+^2+q_-^2)^2-4(q_+q_-\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-)^2)^{\frac{(d-1)}{2}}} \\ &\quad\times\int \mathrm{d}kk^{d-1}\mathrm{d}\hat{\boldsymbol{e}}\theta(k^2+q_+^2-2kq_+|\hat{\boldsymbol{e}}\hat{\boldsymbol{e}}_+|-1)\theta(1-k^2-q_-^2-2kq_-|\hat{\boldsymbol{e}}\hat{\boldsymbol{e}}_-|). \end{aligned} \tag{3.4}$$

There is an invariance under the variation of $\hat{\boldsymbol{e}}$, which is why we integrate over these variables, and fix $\hat{\boldsymbol{e}} = \hat{\boldsymbol{e}}_n$, the n^{th} direction. The integration provides a factor S_d.

Moreover we perform the change of variables

$$(q_+, q_-) \mapsto (x, \alpha), \quad q_+ = kx\cos\frac{\alpha}{2},\ q_- = kx\sin\frac{\alpha}{2},\ \mathrm{d}q_+\mathrm{d}q_- = \frac{k^2x}{2}\mathrm{d}x\mathrm{d}\alpha. \tag{3.5}$$

The integration limits are $x \in [0, \infty[,\ \alpha \in [0, \pi]$. Using usual trigonometric relations we find, after computation,

$$\begin{aligned} \Delta_d &= \frac{S_d}{2^d}\int\frac{\mathrm{d}x}{x}\mathrm{d}\alpha\frac{\sin^{(d-1)}\alpha}{\cos\alpha}\int\mathrm{d}\hat{\boldsymbol{e}}_+\mathrm{d}\hat{\boldsymbol{e}}_-\frac{1}{\left(1-\sin^2\alpha(\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-)^2\right)^{\frac{(d-1)}{2}}} \\ &\quad\times\int\mathrm{d}kk^{(d-1)}\theta(A_+-\frac{1}{k^2})\theta(\frac{1}{k^2}-A_-), \end{aligned} \tag{3.6}$$

where

$$\left\{\begin{aligned} A_+ &= 1+x^2\cos^2\tfrac{\alpha}{2}-2x\cos\tfrac{\alpha}{2}|e_+^n|, \\ A_- &= 1+x^2\sin^2\tfrac{\alpha}{2}+2x\sin\tfrac{\alpha}{2}|e_-^n|. \end{aligned}\right. \tag{3.7}$$

The integration over k can be performed, proceeding to the change of variable $k \mapsto y = \frac{1}{k^2}$, we find

$$\begin{aligned}\int \mathrm{d}k k^{(d-1)} \theta(A_+ - \frac{1}{k^2})\theta(\frac{1}{k^2} - A_-) &= \theta(A_+ - A_-)\frac{1}{2}\int_{A_-}^{A_+} \mathrm{d}y y^{-(1+\frac{d}{2})} \\ &= \theta(A_+ - A_-)\frac{1}{d}\left[A_-^{-\frac{d}{2}} - A_+^{-\frac{d}{2}}\right]. \quad (3.8)\end{aligned}$$

The condition $\theta(A_+ - A_-)$ is

$$A_+ - A_- = x^2 \cos\alpha - 2x(\cos\frac{\alpha}{2}|e_+^n| + \sin\frac{\alpha}{2}|e_-^n|) \geq 0 \quad (3.9)$$

and can be written as

$$x \geq 2\frac{\cos\frac{\alpha}{2}|e_+^n| + \sin\frac{\alpha}{2}|e_-^n|}{\cos\alpha} \doteq x_0 \geq 0. \quad (3.10)$$

The numerator of the expression above is always positive ($\alpha \in [0,\pi]$), while the denominator is negative for $\frac{\pi}{2} < \alpha < \pi$. This implies a new condition on the integration domain of α, which becomes $\alpha \in [0, \frac{\pi}{2}]$. The condition applies also to the integration over x. Returning to (3.6) we find

$$\begin{aligned}\Delta_d &= \frac{S_d}{2^d d}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \frac{\sin^{(d-1)}\alpha}{\cos\alpha}\int \mathrm{d}\hat{\boldsymbol{e}}_+ \mathrm{d}\hat{\boldsymbol{e}}_- \frac{1}{\left(1 - \sin^2\alpha(\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-)^2\right)^{\frac{(d-1)}{2}}} \\ &\quad \times \int_{x_0}^{\infty} \frac{\mathrm{d}x}{x}\left[A_-^{-\frac{d}{2}} - A_+^{-\frac{d}{2}}\right]. \quad (3.11)\end{aligned}$$

Let's mention that x_0 is positive for any values of α, e_+^n, e_-^n in the range of integration.

This expression can be further simplified. For the integration over x, let's consider separately the contributions of A_- and A_+, and write, for simplicity, $s_\pm \doteq |e_\pm^n|$. We write $A_\pm$ by completing the square of the expression:

$$\left\{\begin{array}{lcl} A_+ &=& 1 + x^2\cos^2\frac{\alpha}{2} - 2x\cos\frac{\alpha}{2}s_+ = 1 - s_+^2 + (x\cos\frac{\alpha}{2} - s_+)^2, \\ A_- &=& 1 + x^2\sin^2\frac{\alpha}{2} + 2x\sin\frac{\alpha}{2}s_- = 1 - s_-^2 + (x\sin\frac{\alpha}{2} + s_-)^2. \end{array}\right. \quad (3.12)$$

To compute the first contribution we have to evaluate

$$\int \frac{\mathrm{d}x}{x}\frac{\theta(A_+ - A_-)}{A_-^{\frac{d}{2}}} = \int \frac{\mathrm{d}x}{x}\frac{\theta(x\cos\alpha - 2(\cos\frac{\alpha}{2}s_+ + \sin\frac{\alpha}{2}s_-))}{\left(1 - s_-^2 + (x\sin\frac{\alpha}{2} + s_-)^2\right)^{\frac{d}{2}}}. \quad (3.13)$$

Proceeding to the change of variable $x \mapsto x\sin\frac{\alpha}{2}$, and using trigonometric relations, we find

$$\begin{aligned}\int \frac{\mathrm{d}x}{x}\frac{\theta((x+s_-)\cos\alpha-(\sin\alpha s_+ + s_-))}{(1-s_-^2+(x+s_-)^2)^{\frac{d}{2}}} \\ = \int \frac{\mathrm{d}x}{(x-s_-)}\frac{\theta(x\cos\alpha-(\sin\alpha s_+ + s_-))}{(1-s_-^2+x^2)^{\frac{d}{2}}},\end{aligned} \tag{3.14}$$

where we proceeded to the change of variable $x \mapsto x + s_-$. The contribution to Δ_d is therefore

$$\begin{aligned}\Delta_d^- &= \frac{S_d}{2^d d}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha\frac{\sin^{(d-1)}\alpha}{\cos\alpha}\int \mathrm{d}\hat{\boldsymbol{e}}_+\mathrm{d}\hat{\boldsymbol{e}}_-\frac{1}{\left(1-\sin^2\alpha(\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-)^2\right)^{\frac{(d-1)}{2}}} \\ &\quad \times\int \frac{\mathrm{d}x}{(x-s_-)}\frac{\theta(x\cos\alpha-(\sin\alpha s_+ + s_-))}{(1-s_-^2+x^2)^{\frac{d}{2}}}.\end{aligned} \tag{3.15}$$

To compute the second contribution we have to evaluate

$$\int \frac{\mathrm{d}x}{x}\frac{\theta(A_+-A_-)}{A_+^{\frac{d}{2}}} = \int \frac{\mathrm{d}x}{x}\frac{\theta(x\cos\alpha-2(\cos\frac{\alpha}{2}s_+ + \sin\frac{\alpha}{2}s_-))}{\left(1-s_+^2+(x\cos\frac{\alpha}{2}-s_+)^2\right)^{\frac{d}{2}}}. \tag{3.16}$$

Proceeding to the change of variable $x \mapsto x\cos\frac{\alpha}{2}$, and using trigonometric relations, we find

$$\begin{aligned}\int \frac{\mathrm{d}x}{x}\frac{\theta((x-s_+)\cos\alpha-(s_+ + \sin\alpha s_-))}{(1-s_+^2+(x-s_+)^2)^{\frac{d}{2}}} \\ = \int \frac{\mathrm{d}x}{(x+s_+)}\frac{\theta(x\cos\alpha-(s_+ + \sin\alpha s_-))}{(1-s_+^2+x^2)^{\frac{d}{2}}},\end{aligned} \tag{3.17}$$

where we proceeded to the change of variable $x \mapsto x - s_+$. When introduced in Δ_d, the symmetry allows the exchange of the variables $s_+ \leftrightarrow s_-$. The contribution to Δ_d is therefore

$$\begin{aligned}\Delta_d^+ &= -\frac{S_d}{2^d d}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha\frac{\sin^{(d-1)}\alpha}{\cos\alpha}\int \mathrm{d}\hat{\boldsymbol{e}}_+\mathrm{d}\hat{\boldsymbol{e}}_-\frac{1}{\left(1-\sin^2\alpha(\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-)^2\right)^{\frac{(d-1)}{2}}} \\ &\quad \times\int \frac{\mathrm{d}x}{(x+s_-)}\frac{\theta(x\cos\alpha-(s_- + \sin\alpha s_+))}{(1-s_-^2+x^2)^{\frac{d}{2}}}.\end{aligned} \tag{3.18}$$

Combining (3.15) and (3.18) we find

$$\begin{aligned}\Delta_d &= \frac{S_d}{2^d d}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \frac{\sin^{(d-1)}\alpha}{\cos\alpha}\int \mathrm{d}\hat{\boldsymbol{e}}_+ \mathrm{d}\hat{\boldsymbol{e}}_- \frac{1}{\left(1-\sin^2\alpha(\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-)^2\right)^{\frac{(d-1)}{2}}} \\ &\quad\times\int \mathrm{d}x \frac{\theta(x\cos\alpha - (\sin\alpha s_+ + s_-))}{(1-s_-^2+x^2)^{\frac{d}{2}}}\left[\frac{1}{x-s_-}-\frac{1}{x+s_-}\right]. \end{aligned} \tag{3.19}$$

Introducing this result in (3.1) we find

$$\begin{aligned}\hat{E}_2^{SC} &= N\frac{S_d^2}{2(2\pi)^{2d}}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \frac{\sin^{(d-1)}\alpha}{\cos\alpha}\int \mathrm{d}\hat{\boldsymbol{e}}_+ \mathrm{d}\hat{\boldsymbol{e}}_- \frac{1}{\left(1-\sin^2\alpha(\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-)^2\right)^{\frac{(d-1)}{2}}} \\ &\quad\times\int \mathrm{d}x \frac{\theta(x\cos\alpha - (\sin\alpha s_+ + s_-))}{(1-s_-^2+x^2)^{\frac{d}{2}}}\left[\frac{1}{x-s_-}-\frac{1}{x+s_-}\right]. \end{aligned} \tag{3.20}$$

From now we work in the specific $d = 2$ and $d = 3$ dimensions.

3.1 Universal correction in $d = 2$ dimensions

As mentioned in chapter 2, the term we compute is universal and only dependent on the dimension of the problem. Let's compute the correction for a two-dimensional system, in order to apply it to quantum dots in part II.

In this case, the angular integration is

$$\hat{\boldsymbol{e}}_\pm = (\sin\phi_\pm, \cos\phi_\pm), \quad \mathrm{d}\hat{\boldsymbol{e}}_\pm = \mathrm{d}\phi_\pm, \quad \phi_\pm \in [-\pi, \pi]. \tag{3.21}$$

The correction to the energy becomes

$$\begin{aligned}\hat{E}_2^{SC} &= \frac{N}{2(2\pi)^2}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \frac{\sin\alpha}{\cos\alpha}\int_{-\pi}^{\pi}\mathrm{d}\phi_+\int_{-\pi}^{\pi}\mathrm{d}\phi_- \frac{1}{\left(1-\sin^2\alpha\cos^2(\phi_+-\phi_-)\right)^{\frac{1}{2}}} \\ &\quad\times\int \mathrm{d}x \frac{\theta(x\cos\alpha - (\sin\alpha|\cos\phi_+| + |\cos\phi_-|))}{(1-\cos^2\phi_- + x^2)} \\ &\quad\times\left[\frac{1}{x-|\cos\phi_-|}-\frac{1}{x+|\cos\phi_-|}\right]. \end{aligned} \tag{3.22}$$

Before developing this expression, let's note that the symmetries with regards to (ϕ_+, ϕ_-) imply that the integration over $\phi_\pm \in [-\pi, \pi]$ is equal to four times the integration over $\phi_\pm \in [-\frac{\pi}{2}, \frac{\pi}{2}]$. These new integration limits allow us to drop the absolute values ($\cos\phi_\pm \geq 0$). We therefore have to evaluate, using moreover $1-\cos^2\phi_- = \sin^2\phi_-$:

$$\begin{aligned}\hat{E}_2^{SC} &= \frac{N}{2\pi^2}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \tan\alpha \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}\phi_+ \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}\phi_- \frac{1}{\left(1-\sin^2\alpha\cos^2(\phi_+-\phi_-)\right)^{\frac{1}{2}}} \\ &\qquad\times \int \mathrm{d}x \frac{\theta(x\cos\alpha - (\sin\alpha\cos\phi_+ + \cos\phi_-))}{\left(\sin^2\phi_- + x^2\right)} \\ &\qquad\qquad\times \left[\frac{1}{x-\cos\phi_-} - \frac{1}{x+\cos\phi_-}\right].\end{aligned} \tag{3.23}$$

Let's integrate over x. The integration is

$$\begin{aligned}&\int \mathrm{d}x \frac{\theta(x\cos\alpha - (\sin\alpha\cos\phi_+ + \cos\phi_-))}{\left(x^2+\sin^2\phi_-\right)}\left[\frac{1}{x-\cos\phi_-} - \frac{1}{x+\cos\phi_-}\right] \\ &\qquad = \int_{x_0}^{\infty} \mathrm{d}x \frac{1}{\left(x^2+\sin^2\phi_-\right)}\left[\frac{1}{x-\cos\phi_-} - \frac{1}{x+\cos\phi_-}\right] \\ &\qquad = 2\cos\phi_- \int_{x_0}^{\infty} \mathrm{d}x \frac{1}{\left(x^2+\sin^2\phi_-\right)}\frac{1}{\left(x^2-\cos^2\phi_-\right)} \\ &\qquad = 2\cos\phi_- \left[\int_{x_0}^{\infty} \mathrm{d}x \frac{1}{\left(x^2-\cos^2\phi_-\right)} - \int_{x_0}^{\infty} \mathrm{d}x \frac{1}{\left(x^2+\sin^2\phi_-\right)}\right],\end{aligned} \tag{3.24}$$

where we redefined $x_0 = \frac{\sin\alpha\cos\phi_+ + \cos\phi_-}{\cos\alpha}$. This lower integration limit is larger than $\cos\phi_-$, the first integrand being therefore not divergent. We treat separately these two integrations.

The first one is

$$2\cos\phi_- \int_{x_0}^{\infty} \frac{\mathrm{d}x}{\left(x^2-\cos^2\phi_-\right)} = \ln\frac{(x_0+\cos\phi_-)}{(x_0-\cos\phi_-)}. \tag{3.25}$$

Replacing x_0 by its value, and using trigonometric properties, this term becomes

$$-\ln\tan\frac{\alpha}{2} - \ln\frac{(\cos\frac{\alpha}{2}\cos\phi_+ + \sin\frac{\alpha}{2}\cos\phi_-)}{(\sin\frac{\alpha}{2}\cos\phi_+ + \cos\frac{\alpha}{2}\cos\phi_-)}. \tag{3.26}$$

The second term is antisymmetric under the exchange $\phi_+ \leftrightarrow \phi_-$, while the rest of (3.23) is symmetric, as well as the integration limits. This means that this term will not contribute, and will be neglected from now.

The second integration is

$$\begin{aligned} 2\cos\phi_- \int_{x_0}^{\infty} \frac{\mathrm{d}x}{(x^2+\sin^2\phi_-)} &= 2\frac{\cos\phi_-}{|\sin\phi_-|}\int_{\frac{x_0}{|\sin\phi_-|}}^{\infty}\frac{\mathrm{d}x}{(x^2+1)} \\ &= 2\frac{\cos\phi_-}{|\sin\phi_-|}\left[\frac{\pi}{2}-\arctan\frac{x_0}{|\sin\phi_-|}\right] \\ &= \frac{2}{|\tan\phi_-|}\left[\frac{\pi}{2}-\arctan\frac{(\sin\alpha\cos\phi_+ + \cos\phi_-)}{\cos\alpha|\sin\phi_-|}\right], \end{aligned} \tag{3.27}$$

where we proceeded to the change of variable $x \mapsto x|\sin\phi_-|$.

The correction (3.23) to the energy is therefore

$$\begin{aligned} \hat{E}_2^{SC} &= \frac{N}{2\pi^2}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \tan\alpha \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}\phi_+ \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}\phi_- \frac{1}{\left(1-\sin^2\alpha\cos^2(\phi_+-\phi_-)\right)^{\frac{1}{2}}} \\ &\quad \times \left[-\ln\tan\frac{\alpha}{2} - \frac{2}{|\tan\phi_-|}\left[\frac{\pi}{2}-\arctan\frac{(\sin\alpha\cos\phi_+ + \cos\phi_-)}{\cos\alpha|\sin\phi_-|}\right]\right] \\ &\quad \doteq \hat{E}_{2a}^{SC} + \hat{E}_{2b}^{SC}. \end{aligned} \tag{3.28}$$

For the first term, we can integrate over ϕ_+ and ϕ_- to obtain

$$\begin{aligned} \hat{E}_{2a}^{SC} &= -\frac{N}{2\pi^2}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \tan\alpha \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}\phi_+ \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}\phi_- \frac{\ln\tan\frac{\alpha}{2}}{\left(1-\sin^2\alpha\cos^2(\phi_+-\phi_-)\right)^{\frac{1}{2}}} \\ &= -\frac{N}{2\pi}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \tan\alpha \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}\phi_+ \frac{\ln\tan\frac{\alpha}{2}}{\left(1-\sin^2\alpha\cos^2\phi_+\right)^{\frac{1}{2}}} \\ &= -\frac{N}{\pi}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \tan\alpha \ln\tan\frac{\alpha}{2} K(\sin^2\alpha), \end{aligned} \tag{3.29}$$

where we used the result

$$\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \mathrm{d}\theta \frac{1}{\sqrt{x-\cos^2\theta}} = 2\frac{K\left(\frac{1}{x}\right)}{\sqrt{x}}. \tag{3.30}$$

The integral is computed numerically with Mathematica. We extract the asymptotic behaviour at the integration limits and compute them analytically, the rest being computed numerically. We find

$$\hat{E}_{2a}^{SC} = +\frac{N}{\pi}2.8776 = 0.9160N. \tag{3.31}$$

For the second term, the symmetries in the variables (ϕ_+, ϕ_-) are such that the integration over $\phi_- \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ is twice the integration over $\phi_- \in [0, \frac{\pi}{2}]$. We separate the integration on $\phi_+ < 0$, and on $\phi_+ > 0$. We use Matlab to integrate numerically and find

$$\begin{aligned}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \int_{-\frac{\pi}{2}}^{0} \mathrm{d}\phi_+ \int_0^{\frac{\pi}{2}} \mathrm{d}\phi_- \frac{\tan\alpha}{\tan\phi_-} &\frac{1}{\left(1 - \sin^2\alpha\cos^2(\phi_+ - \phi_-)\right)^{\frac{1}{2}}} \\ &\times \left[\frac{\pi}{2} - \arctan\frac{(\sin\alpha\cos\phi_+ + \cos\phi_-)}{\cos\alpha\sin\phi_-}\right] \\ &= 1.5201, \end{aligned} \tag{3.32}$$

and

$$\begin{aligned}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \int_0^{\frac{\pi}{2}} \mathrm{d}\phi_+ \int_0^{\frac{\pi}{2}} \mathrm{d}\phi_- \frac{\tan\alpha}{\tan\phi_-} &\frac{1}{\left(1 - \sin^2\alpha\cos^2(\phi_+ - \phi_-)\right)^{\frac{1}{2}}} \\ &\times \left[\frac{\pi}{2} - \arctan\frac{(\sin\alpha\cos\phi_+ + \cos\phi_-)}{\cos\alpha\sin\phi_-}\right] \\ &= 2.4357. \end{aligned} \tag{3.33}$$

This leads to

$$\hat{E}_{2b}^{SC} = -\frac{2N}{\pi^2} 3.9558 = -0.8016N. \tag{3.34}$$

The whole contribution to the energy is therefore

$$\hat{E}_2^{SC} = 0.1144N. \tag{3.35}$$

After having done these computations, a bibliographical research led us to note that this integral appears in the problem of the two-dimensional jellium model at high density: the correlation energy of a uniform high density electron gas, with a positive background, was computed first in three dimensions by Gell-Mann and Brueckner (1957). The two-dimensional analog term was computed in (Isihara and Ioriatti, 1980). The result is the same as ours.

3.2 Universal correction in $d = 3$ dimensions

Let's compute the correction for a three-dimensional system, in order to apply this result to the atoms.

In this case, the angular integration is

$$\begin{aligned}\hat{\boldsymbol{e}}_\pm = (\cos\phi_\pm \sin\theta_\pm, \sin\phi_\pm \sin\theta_\pm, \cos\theta_\pm), \quad \mathrm{d}\hat{\boldsymbol{e}}_\pm = \sin\theta_\pm \mathrm{d}\phi_\pm \mathrm{d}\theta_\pm, \\ \phi_\pm \in [-\pi, \pi], \quad \theta_\pm \in [0, \pi]. \end{aligned} \tag{3.36}$$

The correction to the energy becomes

$$\begin{aligned}
\hat{E}_2^{SC} &= \frac{N}{2^3\pi^4}\int_0^{\frac{\pi}{2}}\mathrm{d}\alpha\frac{\sin^2\alpha}{\cos\alpha}\int_0^{\pi}\mathrm{d}\theta_+\int_0^{\pi}\mathrm{d}\theta_-\int_{-\pi}^{\pi}\mathrm{d}\phi_+\int_{-\pi}^{\pi}\mathrm{d}\phi_-\frac{\sin\theta_+\sin\theta_-}{\left(1-\sin^2\alpha(\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-)^2\right)} \\
&\qquad\times\int\mathrm{d}x\frac{\theta(x\cos\alpha-(\sin\alpha|\cos\theta_+|+|\cos\theta_-|))}{(1-\cos^2\theta_-+x^2)^{\frac{3}{2}}} \\
&\qquad\times\left[\frac{1}{x-|\cos\theta_-|}-\frac{1}{x+|\cos\theta_-|}\right], \\
&= \frac{N}{(2\pi)^4}\int_0^{\frac{\pi}{2}}\mathrm{d}\alpha\frac{\sin^2\alpha}{\cos\alpha}\int_0^{\pi}\mathrm{d}\theta_+\int_0^{\pi}\mathrm{d}\theta_-\int_{-\pi}^{\pi}\mathrm{d}\phi_+\int_{-\pi}^{\pi}\mathrm{d}\phi_-\sin\theta_+\sin\theta_- \\
&\qquad\times\left(\frac{1}{(1-\sin\alpha(\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-))}+\frac{1}{(1+\sin\alpha(\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-))}\right) \\
&\qquad\times\int\mathrm{d}x\frac{\theta(x\cos\alpha-(\sin\alpha|\cos\theta_+|+|\cos\theta_-|))}{(1-\cos^2\theta_-+x^2)^{\frac{3}{2}}} \\
&\qquad\times\left[\frac{1}{x-|\cos\theta_-|}-\frac{1}{x+|\cos\theta_-|}\right].
\end{aligned} \tag{3.37}$$

Let's replace the scalar product by

$$\begin{aligned}
\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_- &= (\cos\phi_+\cos\phi_-+\sin\phi_+\sin\phi_-)\sin\theta_+\sin\theta_-+\cos\theta_+\cos\theta_- \\
&= \cos(\phi_+-\phi_-)\sin\theta_+\sin\theta_-+\cos\theta_+\cos\theta_-
\end{aligned} \tag{3.38}$$

and integrate over the variables $\phi_\pm$. We proceed to the change of variables $\phi_+ \mapsto \phi = \phi_+ - \phi_-$, make use of the periodicity of the cosine, implying that the integration bounds do not depend on ϕ_-. Its integration is therefore trivial and provides 2π. The parity of the cosine implies moreover that the integration over $\phi \in [-\pi, \pi]$ is equal to twice the integration over $\phi \in [0, \pi]$. The integrations over ϕ are of the form

$$\int_0^{\pi}\mathrm{d}\phi\frac{1}{(A_- - B\cos\phi)},\quad \int_0^{\pi}\mathrm{d}\phi\frac{1}{(A_+ + B\cos\phi)}, \tag{3.39}$$

with $A_\pm = 1 \pm \sin\alpha\cos\theta_+\cos\theta_-$, and $B = \sin\alpha\sin\theta_+\sin\theta_-$. The conditions $A_\pm > B$ are satisfied, and the integrations therefore yield

$$\frac{\pi}{\sqrt{A_\pm^2 - B^2}}. \tag{3.40}$$

Using this formula we obtain, after computation,

$$\int_{-\pi}^{\pi} \mathrm{d}\phi_+ \int_{-\pi}^{\pi} \mathrm{d}\phi_- \left(\frac{1}{(1-\sin\alpha(\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-))} + \frac{1}{(1+\sin\alpha(\hat{\boldsymbol{e}}_+\hat{\boldsymbol{e}}_-))} \right)$$
$$= (2\pi)^2 \left[\frac{1}{\left(1-2\sin\alpha\cos\theta_+\cos\theta_- - \sin^2\alpha(1-\cos^2\theta_+ - \cos^2\theta_-)\right)^{\frac{1}{2}}} + \frac{1}{\left(1+2\sin\alpha\cos\theta_+\cos\theta_- - \sin^2\alpha(1-\cos^2\theta_+ - \cos^2\theta_-)\right)^{\frac{1}{2}}} \right]. \tag{3.41}$$

This expression is invariant under the change $\cos\theta_+ \mapsto -\cos\theta_+$, as well as $\cos\theta_- \mapsto -\cos\theta_-$. This means that it depends on their absolute value only. The integrand in (3.37) therefore depends on the absolute value of $\cos\theta_\pm$ only. The integral over $\theta_+ \in [0,\pi]$, $\theta_- \in [0,\pi]$ is therefore equal to 4 times the same integral over $\theta_+ \in [0,\frac{\pi}{2}]$, $\theta_- \in [0,\frac{\pi}{2}]$. In this interval the absolute values can be dropped, the values being always positive.

We proceed to the change of variables $\theta_\pm \mapsto s_\pm = \cos\theta_\pm$, $\sin\theta_\pm \mathrm{d}\theta_\pm = \mathrm{d}s_\pm$. With these new variables, and using (3.41), the energy (3.37) becomes

$$\begin{aligned} \hat{E}_2^{SC} &= \frac{N}{\pi^2} \int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \frac{\sin^2\alpha}{\cos\alpha} \int_0^1 \mathrm{d}s_+ \int_0^1 \mathrm{d}s_- g(\alpha,s_+,s_-) \\ &\quad \times \int \mathrm{d}x \frac{\theta(x\cos\alpha - (\sin\alpha s_+ + s_-))}{(1-s_-^2+x^2)^{\frac{3}{2}}} \left[\frac{1}{x-s_-} - \frac{1}{x+s_-} \right], \end{aligned} \tag{3.42}$$

where

$$\begin{aligned} g(\alpha,s_+,s_-) &\doteq \frac{1}{\left(1-2\sin\alpha s_+ s_- - \sin^2\alpha(1-s_+^2-s_-^2)\right)^{\frac{1}{2}}} \\ &\quad + \frac{1}{\left(1+2\sin\alpha s_+ s_- - \sin^2\alpha(1-s_+^2-s_-^2)\right)^{\frac{1}{2}}}. \end{aligned} \tag{3.43}$$

Let's integrate over x, from $x_0 \doteq \frac{\sin\alpha s_+ + s_-}{\cos\alpha}$ to infinity. This integration yields

$$\begin{aligned} h(\alpha,s_+,s_-) &\doteq \int_{x_0}^{\infty} \mathrm{d}x \frac{1}{(1-s_-^2+x^2)^{\frac{3}{2}}} \left[\frac{1}{x-s_-} - \frac{1}{x+s_-} \right] \\ &= 2s_- \int_{x_0}^{\infty} \mathrm{d}x \frac{1}{(1-s_-^2+x^2)^{\frac{3}{2}}} \frac{1}{(x^2-s_-^2)} \end{aligned}$$

$$
\begin{aligned}
&= \frac{2s_-}{1-s_-^2}\left[\frac{x_0}{\sqrt{1-s_-^2+x_0^2}} - 1\right] \\
&+ \left[\ln\left(\frac{1-s_-}{1+s_-}\right) + \ln\left(\frac{x_0+s_-}{x_0-s_-}\right)\right. \\
&\quad \left. + \ln\left(\frac{1-s_-^2+s_-x_0+\sqrt{1-s_-^2+x_0^2}}{1-s_-^2-s_-x_0+\sqrt{1-s_-^2+x_0^2}}\right)\right].
\end{aligned} \tag{3.44}
$$

The integral has been reduced to the following

$$\hat{E}_2^{SC} = \frac{N}{\pi^2}\int_0^{\frac{\pi}{2}} \mathrm{d}\alpha \int_0^1 \mathrm{d}s_+ \int_0^1 \mathrm{d}s_- \frac{\sin^2\alpha}{\cos\alpha} g(\alpha, s_+, s_-) h(\alpha, s_+, s_-). \tag{3.45}$$

and is evaluated numerically. This numerical integration shows no difficulty (there are no convergence problems), and is evaluated using Matlab. We find, in Hartree

$$\hat{E}_2^{SC} = \frac{N}{\pi^2} 0.23864 = 0.024179N. \tag{3.46}$$

After having done these computations, a bibliographical research led us to note that this integral appears in the problem of the jellium model at high density: the correlation energy of a uniform high density electron gas, with a positive background, was computed first by Gell-Mann and Brueckner (1957). They find that one contribution to this energy is the same as that we computed, and this integral was solved analytically by Onsager et al. (1966). They find, in Hartree

$$\hat{E}_2^{SC} = \left(\frac{1}{6}\ln(2) - \frac{3}{4\pi^2}\zeta(3)\right) N = 0.024179N. \tag{3.47}$$

We can understand the fact that our results are the same as those found for the jellium model in the following way: due to the semiclassical regime, only local values are in play. This means that, around $\boldsymbol{x}$, the system behaves as if it were uniform, with a "local chemical potential" $(\mu - V(\boldsymbol{x}))$. The integration over $\boldsymbol{x}$ then provides the factor N. This discussion holds for the two-dimensional case, too.

At this stage, it is interesting to compare qualitatively this result to experimental data. The first point to mention is that this contribution to the correlation energy is positive and should be overcompensated by the other contribution: the true ground state energy is less than the Hartree-Fock energy (which is an approximation providing an energy larger than the true energy, as explained in chapter 5). The correlation energy has therefore to be negative.

Experimental results can be found in (Clementi, 1963a,b; Chakravorty et al., 1993), but only up to $N = 18$ electrons, for which our theory is not justified (we work in the large N-limit). The experimental ground state energy is the sum of all the ionization potentials. Hartree-Fock energy is subtracted to it, which provides the correlation energy. This data is corrected by taking into account the effects due to the nuclear motion, Breit and Dirac relativistic corrections, finite nuclear radius corrections, and quantum electrodynamical corrections (the Lamb shift). Results for the neutral atom are presented in Figure 1. It is difficult to state if it behaves as $N^{\frac{4}{3}}$ (as many people think) or as N. If it behaved as N, a linear interpolation of this data provides, in Hartree

$$-E_{corr} \simeq 0.043N. \tag{3.48}$$

Our results have therefore the right order of magnitude, but let's recall that our theory is justified in the large N-limit only.

Let's finally note that numerical efforts are made to compute the correlation energy. A numerical method which shows analogies with our work is the Moller-Plesset perturbative approach (see for example (Helgaker et al., 2000)). It consists of proceeding beyond a self-consistent Hartree-Fock approach, up to a given order. Another self-consistent approach, known as the GW approximation, and developed in (Hedin, 1965), consists of computing the self-energy of the electrons. This approach was applied to the electron gas (Holm and Barth, 1998; Garcia-Gonzalez and Godby, 2001), to atoms (Dahlen and Barth, 2004), and to molecules (Dahlen et al., 2005). The interest of this approach is that it could be used for systems with many particles, unlike other computation approaches which can be used for systems with few particles only. It is considered by the authors of these computations as a possible alternative to density functional theory.

One of the main differences between these two methods is that the GW approach makes use of resummation of graphs. A comparison between these two approaches is done in (Holleboom and Snijders, 1990).

Part II

Quantum dots

Chapter 4

Introduction

Contents

The objective of this chapter is to describe quantum dots, to describe and discuss their modeling, and to present existing results on the computation of the ground state energy.

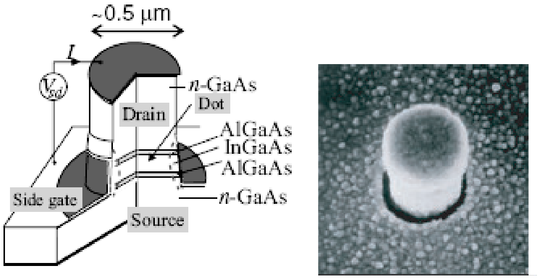
After having developed a technique for the computation of the ground state energy of many-fermion systems in chapter 2, we apply it to quantum dots. This is why we describe in detail what a quantum dot is, then develop the semiclassical Hartree-Fock model in chapter 5 and apply it to quantum dots. As this model does not include energy oscillations, they are treated separately by another development in chapter 6. To use the expressions obtained this way, we have to solve the self-consistent equation, which is done in chapter 7, before we use the result in chapter 8 to obtain the semiclassical energy, which we compare to experimental results.

4.1 Quantum dot description

The technology of solid state physics allows the creation of quantum wells: electrons are constrained in a plane, which induces the quantization of energy levels in the third direction. It is possible to constrain the electrons in one further dimension, leading to one-dimensional objects called quantum wires. Constraining the electrons in the third dimension leads to a zero-dimensional object which is called a quantum dot, or an artificial atom.

There are different kinds of quantum dots, which have to be treated theoretically in different ways. We will describe two types of dots to which our calculations can apply.

The first kind of quantum dot is called a vertical quantum dot. It consists of growing a succession of very thin layers on a wafer. Let's describe the dots obtained by Tarucha's group as an example. As shown in Figure 4.1 (from (Kouwenhoven et al., 2001)), the dot is on a *GaAs* layer, which acts as a source of electrons. On it there is a thin layer of *AlGaAs*, then the dot, which is a layer of $In_{0.05}Ga_{0.95}As$, then a thin layer of *AlGaAs*, and finally a large layer of *GaAs*, acting as a drain. A voltage difference is created between the source and the drain. The *AlGaAs* layers act as barriers to constrain the electrons in the dot. They act here as insulators: the bandgap of *AlGaAs* is bigger than the bandgap of *InGaAs*, the electrons in the dot therefore feel this gap as an (almost) infinite potential. Moreover these layers are thin enough that a current can be established by tunneling. The current established this way is vertical to the dot, which is why these quantum dots are called vertical quantum dots. These dots can have different shapes: circular, triangular, square. The dots which are best adapted to our work are circular quantum dots.



(a) (b)

Figure 4.1: *Schematic representation of a vertical quantum dot (a) and electron micrograph of the dot (b).*

The second kind of quantum dots we will describe is called a lateral quantum dot. We consider the dots constructed by Marcus's group, used for example in (Folk et al., 1996). It consists of using a quantum well, by wrapping a *GaAs* layer by two *AlGaAs* layers. Electrons can then move "freely" (they actually have an effective mass) in the *GaAs* layer and therefore form a two-dimensional electron gas. With lithographic techniques, electrostatic gates are patterned on this system, and this constrains the electrons in a small region of the quantum well. A schematic picture is shown in Figure 4.2 (from (Alhassid, 2000)). To feed the dot with electrons, the potential is modified to bring electrons from the source, and the electrons can move to the drain (see figure). The current established this way is lateral to the dot, which is why this kind of dots is called lateral quantum dots.

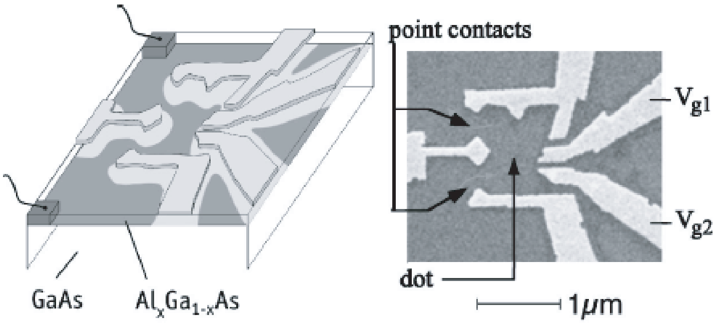


Figure 4.2: *Schematic representation and picture of a lateral quantum dot.*

A measurement technique of the energy of quantum dots will be described later in this chapter.

4.2 The model

The problem consists of studying properties of a quantum dot containing N electrons. The typical sizes ($10 - 1000 nm$) of these systems are such that the study has to be done in the theoretical framework of quantum mechanics (further considerations will allow us to work in the semiclassical regime).

As explained in the preceding section, the quantum dots we consider are a set of electrons evolving in a very thin layer of a semiconductor. The electron is described by a wave function which is the product of a wave function depending on the two dimensions of the plane, x and y, and a wave function depending on z. The z-direction presents an excitation energy which is about ten times larger than the excitation energy of the $x - y$ plane. The experimental results we will use to compare to our theoretical results are such that the wave function in the z-direction is always in its ground state (see (Kouwenhoven et al., 2001)), which justifies a two-dimensional model. But if a larger number of electrons were considered, the excitations in the z-direction would have to be taken into account.

The electrons are not evolving in the vacuum, but in a semiconductor. Solid state physics theory teaches us that an electron evolving in a semiconductor (that is a periodic potential for the electron) has a dispersion relation which is different from the one in the vacuum ($\epsilon(\boldsymbol{k}) = \frac{\hbar^2 \boldsymbol{k}^2}{2m}$). The dispersion relation takes place on bands in the Brillouin zone, and a semiconductor is such that the bands are either completely filled or completely empty (at zero temperature, which is what we will consider). An electron in excess (which is the situation of the electron we introduce in the system) therefore occupies a state in a new band, which presents a quadratic profile for $|\boldsymbol{k}| \approx 0$, different from that in the vacuum. This quadratic profile allows the definition of an effective mass $m_\star$: $\epsilon(\boldsymbol{k}) = \frac{\hbar^2 \boldsymbol{k}^2}{2m_\star} + \mathcal{O}(\boldsymbol{k}^4)$. According to Li (2000), in the case of $In_{0.05}Ga_{0.95}As$ (which the quantum dot we will consider is made of), this effective mass is $m_\star \approx 0.064m$, where m is the mass of an electron.

The electronic interaction is also influenced by the fact that the electrons are not in a vacuum. The electron-electron interaction in matter is

$$V(\boldsymbol{x}_i, \boldsymbol{x}_j) = \frac{e^2}{\epsilon |\boldsymbol{x}_i - \boldsymbol{x}_j|} = \frac{e_\star^2}{|\boldsymbol{x}_i - \boldsymbol{x}_j|}, \tag{4.1}$$

where $e = \frac{q}{\sqrt{4\pi}}$, with q the electronic charge (expressed in the MKSA units), and ϵ is the dielectric constant of the environment. This constant can be viewed as a modification of the electron charge due to the semiconductor. According to Li (2000), in the case of $In_{0.05}Ga_{0.95}As$, this constant is $e_\star \approx 0.283e$. The environment also has other effects on the electronic interaction: since the background consists of positive and negative charges (globally neutral, however), there is a screening effect, which implies that the real long distance potential is lower than the usual electronic interaction. Moreover, the electrons are expanded in the z-direction, which means that the real short distance potential is lower than the usual electronic interaction. All this was modeled by McEuen et al. (1992) by a potential of the kind

$$V(\boldsymbol{x}_i, \boldsymbol{x}_j) = e_\star^2 \left(\frac{1}{(|\boldsymbol{x}_i - \boldsymbol{x}_j|^2 + \delta_+^2)^{\frac{1}{2}}} - \frac{1}{(|\boldsymbol{x}_i - \boldsymbol{x}_j|^2 + \delta_-^2)^{\frac{1}{2}}} \right), \tag{4.2}$$

where $\delta_- > \delta_+ > 0$. In the review (Reimann, 2002), Reimann writes that this difference in the electron-electron interaction is the main effect due to the third dimension of the system. In our problem, however, we consider the usual electron-electron interaction (4.1), with the influence of the background in the interaction constant only. The fact that we have a two-dimensional system with a three-dimensional electronic interaction has a very deep consequence for our developments: we cannot make use of the Poisson equation to make the self-consistent equation a differential equation, instead of an integral one, as will be established later.

In order to be able to model our system we still have to define a confinement potential. It may depend on the kind of quantum dot we consider. The lateral quantum dots, whose confinement potential is established with electrodes, can have almost any kind of confinement. In particular they can have a parabolic confinement $V_{ext}(\boldsymbol{x}) = \frac{1}{2}k\boldsymbol{x}^2$, where the confinement strength can be set experimentally. The other kind of quantum dots, the vertical quantum dots, can have different shapes, as already discussed. In the case of circular dots, a parabolic confinement potential seems to be a good model: many numerical simulations using this model are in very good agreement with experimental results. Moreover, some typical effects, like the shell structure, correspond to the effects observed in a quantum dot with parabolic confinement. Hence a quantum dot with few electrons is well modeled with a parabolic confinement. But with this model, the density increases with the number of electrons, which is not observed in experiments, where the density is more or less constant. The model has to be modified to a constant density model, which is obtained by making the confinement strength N-dependent. The mean density is $\rho \simeq \frac{N}{R^2}$, where R is the radius of the dot. We will establish in chapter 7 that, at lowest order, this radius is $R \simeq \left(\frac{N}{k}\right)^{\frac{1}{3}}$. The mean density is therefore $\rho \simeq N^{\frac{1}{3}}k^{\frac{2}{3}}$. For this density to be independent of N, we have to impose $k = \frac{k'}{N^{\frac{1}{2}}}$. This is the model proposed in (Koskinen et al., 1997), and is the model we will use.

Let's note that a sophisticated numerical work done by Bednarek et al. (2003), which takes into account the whole system (the electrons and the dot), leads to a confinement constant which is almost independent of N. However, these simulations were done for a low number of electrons only.

Square-shaped quantum dots are also sometimes modeled as systems with circular symmetry, with a parabolic confinement potential. This is due to numerical simulations done by Kumar et al. (1990), which show that the effective potential is close to a circular potential, even for a few number of electrons. As we are looking for very weak effects such as energy oscillations (which are different for systems with radial symmetry or not), we will not use experimental results obtained with square-shaped quantum dots.

Our model is now complete, having defined the effective dimension of the system, an effective mass for the kinetic energy term, an interaction and a confinement potential. The hamiltonian of the system is, writing it with a tilde

$$\tilde{H} = -\frac{\hbar^2}{2m_\star}\sum_{i=1}^{N}\tilde{\Delta}_i + \sum_{i=1}^{N}\tilde{V}_{ext}(\tilde{\boldsymbol{x}}_i) + \frac{1}{2}\sum_{i,j=1,i\neq j}^{N}\frac{e_\star^2}{|\tilde{\boldsymbol{x}}_i - \tilde{\boldsymbol{x}}_j|}. \tag{4.3}$$

This hamiltonian is written in the (arbitrary) MKSA units. It is however more comfortable to work in modified atomic units. We proceed in the same way as for the atom. The energy unit is the modified Hartree

$$E_\star = \frac{m_\star e_\star^4}{\hbar^2} \approx 6.39 \cdot 10^{-3}E_0 \approx 11.2meV, \tag{4.4}$$

and the length unit is the modified Bohr radius

$$a_\star = \frac{\hbar^2}{m_\star e_\star^2} \approx 194 a_0 \approx 10.3nm. \tag{4.5}$$

The energy unit can be expressed in terms of the length unit

$$E_\star = \frac{e_\star^2}{a_\star}. \tag{4.6}$$

The new variables are, writing them with a hat:

$$\hat{H} = \frac{\tilde{H}}{E_\star}, \quad \hat{\boldsymbol{x}} = \frac{\tilde{\boldsymbol{x}}}{a_\star}, \quad \frac{\partial^k}{\partial \hat{x}^k} = a_\star^k \frac{\partial^k}{\partial \tilde{x}^k}. \tag{4.7}$$

The hamiltonian has now the very simple form

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N} \hat{\Delta}_i + \sum_{i=1}^{N} \hat{V}_{ext}(\hat{\boldsymbol{x}}_i) + \frac{1}{2}\sum_{i,j=1, i\neq j}^{N} \frac{1}{|\hat{\boldsymbol{x}}_i - \hat{\boldsymbol{x}}_j|}, \tag{4.8}$$

where we defined $\hat{V}_{ext}(\hat{\boldsymbol{x}}) = \frac{\tilde{V}_{ext}(a_\star \hat{\boldsymbol{x}})}{E_\star}$.

Let's note that the modified atomic units, which are the natural units of $In_{0.05}Ga_{0.95}As$ quantum dots, are very different than for atoms (whose natural units are the atomic units).

Let's finally note that the size of the quantum dot, expressed in the modified Bohr radius, will be very large (as computations will show later). This means that the quantum effects (which are present at sizes of the order of the modified Bohr radius) will be weak, and this is one argument for working in the semiclassical regime. Stronger arguments, based on the number of electrons only, will be developed later, when we will proceed to a new scaling depending on N.

4.3 A basic model: the harmonic oscillator

By analogy with the case of the atom, where the shell structure, and consequently the periodic table of the elements, is well reproduced by the energy levels of the hydrogen atom, we proceed the same way for the quantum dots, by developing the basic two-dimensional harmonic oscillator. This corresponds to the case where the electron-electron interaction is neglected.

The energy levels of the two-dimensional harmonic oscillator are easily obtained by separating it into two one-dimensional harmonic oscillators. We can proceed in another way, in order to make use of the radial symmetry, by expressing the problem in polar coordinates. An exact development can be found, for example, in (Schwinger, 2001). It leads to the following energy levels:

$$E_{n_\rho, m} = \sqrt{k}\left(2n_\rho + |m| + 1\right), \quad n_\rho = 0, 1, 2, \ldots, \quad m = 0, \pm 1, \pm 2, \ldots \tag{4.9}$$

n_ρ and m are the radial and quantum numbers respectively.

There are degenerate states, and it is these degenerate states that form the shells.

An interesting result we can derive from this simple model is the number of electrons a shell contains. The first shell contains 2 electrons ($(n, m) = (0, 0)$, with the spin degeneracy), the second shell contains 4 electrons ($(n, m) = (0, \pm 1)$, with the spin degeneracy). The n^{th} shell has $n_n = 2n$ electrons, which means that the shell fillings occur at

$$N_n = 2\sum_{k=1}^{n} k = n(n+1). \tag{4.10}$$

We will establish later that the energy oscillations are a quasi-periodic function of $\sqrt{N}$. We will moreover establish that this function is dominated by a single periodic function of $\sqrt{N}$, of period 1.0376, and with peaks occuring at about 0.5, 1.5, 2.5, and so on. These values are represented, in our harmonic oscillator model, by shell fillings. These are listed in table 4.1.

n	N_n	$\sqrt{N_n}$
1	2	1.41
2	6	2.45
3	12	3.46
4	20	4.47
5	30	5.48
6	42	6.48
7	56	7.48
8	72	8.49
9	90	9.49
10	110	10.49

Table 4.1: *Shell fillings, their corresponding number of electrons N, and the square root of N.*

There is a remarkable periodicity in the filled shells, in very good agreement with the results we develop in chapter 8 with a more realistic model.

The shells are characterized by the fact that all the electrons of a shell have a given energy, the electrons of the n^{th} shell having an energy of $n\sqrt{k}$. This fact corresponds to what is called a degeneracy. It is moreover possible to characterize a shell in another way: let's compute the quadratic mean distance of a particle in a state (n, m) from the center, which is

$$\langle r^2 \rangle - \underbrace{\langle r \rangle^2}_{0} = \langle \psi_{n,m} | r^2 | \psi_{n,m} \rangle. \tag{4.11}$$

The wave function of this state is:

$$\psi_{n_\rho,m}(r,\theta) = k^{\frac{1}{4}} \frac{e^{im\theta}}{\sqrt{2\pi}} \sqrt{\frac{n_\rho!}{(n_\rho + |m|)!}} e^{-\frac{1}{2}\frac{\sqrt{k}}{2}r^2} \left(\sqrt{\frac{\sqrt{k}}{2}}r\right)^{|m|} L_{n_\rho}^{|m|}\left(\frac{\sqrt{k}}{2}r^2\right). \quad (4.12)$$

The angular part plays no role, and its integration in (4.11) provides a factor of 2π. Introducing (4.12) in (4.11), we find, after computation

$$\langle r^2 \rangle = \frac{4}{\sqrt{k}} \frac{n!}{(n+|m|)!} \int_0^\infty \mathrm{d}r r^{3+2|m|} e^{-r^2} \left(L_n^{|m|}(r^2)\right)^2 = \frac{2}{\sqrt{k}}(2n + |m| + 1). \quad (4.13)$$

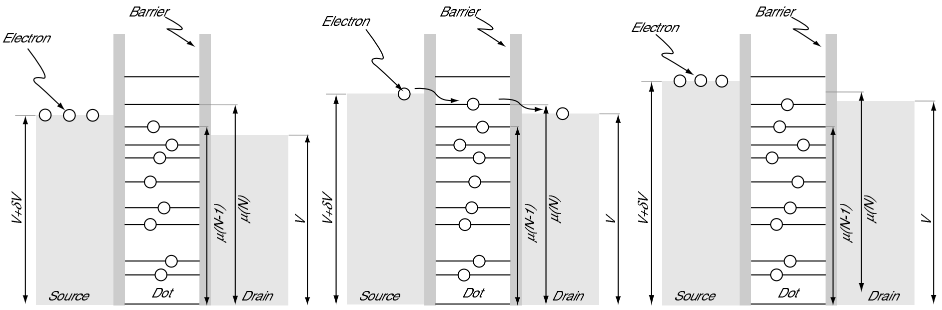
Unsurprisingly, we find that the more energy the state has, the higher its quadratic mean distance is. The electrons belonging to the same shell are therefore at the same mean distance from the center, and this is a way to characterize a shell. Within this shell picture, we could introduce an electron-electron interaction between the electrons of the different shells, and obtain this way an approximation of the ground state energy. This is what Englert (1988) did for the hydrogen atom. He obtained a surprisingly good approximation of the ground state energy of the atom.

We may ask if the energy oscillations we observe are related to the shell fillings. As noted by Englert (1988), in the case of the atom, and more generally for three-dimensional systems, two quantum numbers characterize the shells, and it is therefore difficult to observe a structure in these oscillations. Conversely, for a quantum dot, and in general for two-dimensional systems, the energy is characterized by a single quantum number (for the hamonic oscillator, the energy depends on the single quantum number $(2n_\rho + |m|)$). The study of two-dimensional systems presents the advantage to answer whether the energy oscillations are related to shell fillings or not. If it is, the oscillations must be such that their peaks occur at shell fillings. And as mentioned above, our computations show that the oscillations are dominated by one term of period $1.0376\sqrt{N}$, and with peaks in very good agreement with those obtained in Table 4.1. This shows a link between energy oscillations and shell fillings, which can be observed in two-dimensional systems only.

4.4 Experimental methods

To compare the results provided by these theoretical models to experimental ones we need a method to proceed to the measures we are interested in, which is in our case, the ground state energy. We describe one of these methods (which was used to measure the results we use), because we think it may be part of the discussion of our results.

This method makes use of Coulomb blockade. The dot is fed by a source of electrons, and electrons can leave the dot to a drain. A voltage difference between the source and the drain can establish a current in the dot. This dot can be coupled strongly or weakly to the source and to the drain. The first case corresponds to open quantum dots, the second one to closed quantum dots. As we are interested in isolated quantum dots, this is best approached with a closed one. A schematic of this system is shown in Figure 4.3.



(a) (b) (c)

Figure 4.3: *Schematic representation of a quantum dot. In (a), there are $(N-1)$ electrons; in (b), a tunneling current is established; in (c), there are N electrons.*

The source is on the left and the drain on the right of the dot. The barriers represent the potential needed for the electrons to tunnel from one system to another. The higher they are the less the systems are coupled. The potential $V+\delta V$ of the source is slightly higher than the potential V of the drain. The dot is characterized by energy levels $\mu(N)$. At low temperature, if $\delta V < (\mu(N)-\mu(N-1))$, the variation of the potential V will modify the number of electrons in the dot, one by one. If there are $(N-1)$ electrons in the dot, and if $V+\delta V < \mu(N)$, there is no electron transfer. If $V+\delta V > \mu(N) > V$, an electric current arises, and if $\mu(N) < V$ this electric current stops. We therefore observe electric current peaks at given values of the potential, as shown by experimental results of Meirav et al. (1990) in Figure 4.4.

With an increasing temperature the widths of these peaks will increase and they will progressively vanish, until the signal becomes continuous, as shown on the same figure.

These experimental results provide the chemical potential $\mu(N)$. From the chemical potential we can easily obtain the total energy of the system, which is $E(N)=\sum_{k=1}^{N}\mu(k)$. More detailed explanations can be found in the reviews of Ashoori (1996) and Reimann (2002).

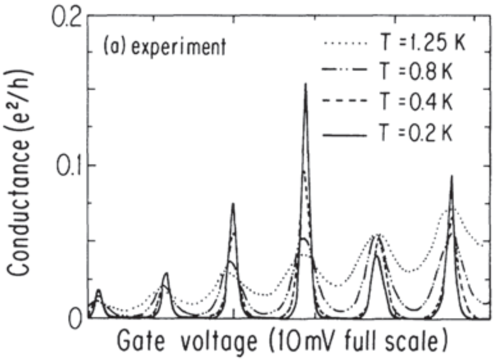


Figure 4.4: *Coulomb Blockade peaks, and their temperature dependence.*

4.5 Experimental results

The experimental results we need for comparison are the ground state energy as a function of N, for many electrons. The results which are the most relevant to our work are, to our knowledge, those from Tarucha, which can be found in (Kouwenhoven et al., 2001). They are reproduced in Figure 4.5. Results were obtained for circular vertical quantum dots. They show results for up to 41 electrons, and these results are presented as the function $\Delta_2(N)$, where $\Delta_2(N) = \mu(N+1) - \mu(N)$.

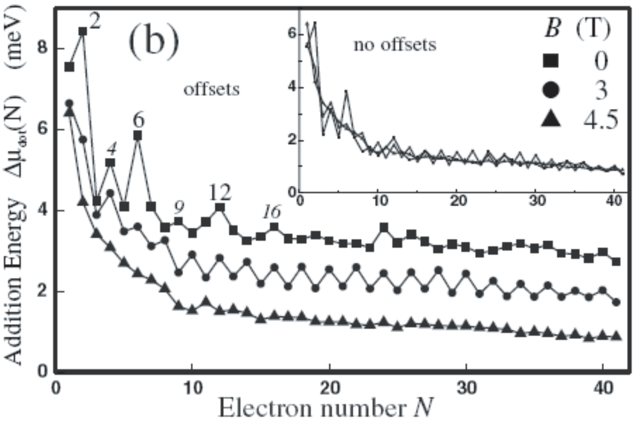


Figure 4.5: *Addition energy as a function of the number of electrons.*

From these values we deduce the chemical potential $\mu(N)$, from which we deduce the ground state energy $E(N)$. The results we obtain are shown in Figure 4.6.

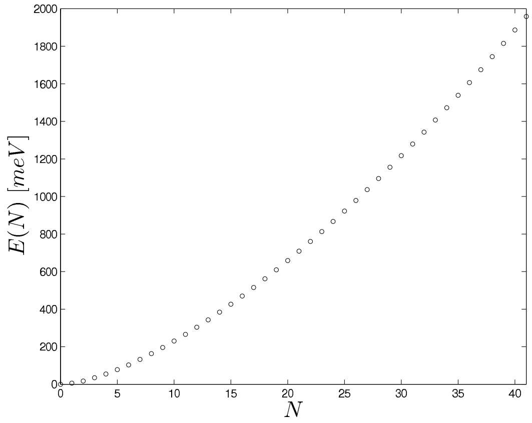


Figure 4.6: *Experimental ground state energy as a function of the number of electrons* N*.*

As will be established later (see chapter 8), the asymptotic behaviour of the ground state energy is given by $E \sim N^{\frac{5}{3}}k^{\frac{1}{3}} = N^{\frac{3}{2}}k'^{\frac{1}{3}}$, where $k' = \frac{k}{\sqrt{N}}$ is a constant, as explained earlier in this chapter.

In order to compare our results to experimental results, we need to know the numerical value of the confinement strength, k'. It is obtained in the following way: we know that in the limit $N \to \infty$, the energy divided by $N^{\frac{3}{2}}$ tends to a constant, which is $1.06k'^{\frac{1}{3}}$, as established in our developments. In these developments we also establish that $\frac{E(N)}{N^{\frac{3}{2}}}$ can be expanded as a polynomial of $N^{-\frac{1}{2}}$. This is why we represent $\frac{E(N)}{N^{\frac{3}{2}}}$ as a function of $N^{-\frac{1}{2}}$ in Figure 4.7, and proceed to a polynomial fitting. The 0^{th} order of this polynomial corresponds to $\lim_{N^{-\frac{1}{2}} \to 0} \frac{E(N)}{N^{\frac{3}{2}}}$. We find 7.7 meV. Dividing it by 11.2 meV (which is the energy unit of this dot, a modified Hartree), and equating it to $1.06k'^{\frac{1}{3}}$, we find

$$k' = 0.27 \tag{4.14}$$

in the modified atomic units.

4.6 Theoretical results – asymptotic limit

A rigorous study of the asymptotic limit of the ground state energy of quantum dots with many electrons was done by Lieb et al. (1995). They studied the dot in a perpendicular magnetic field B and found three distinct regimes. We will restrict our discussion to the $B = 0$ regime. They prove that the ground state energy is a functional of the density, the density being solution of a self-consistent

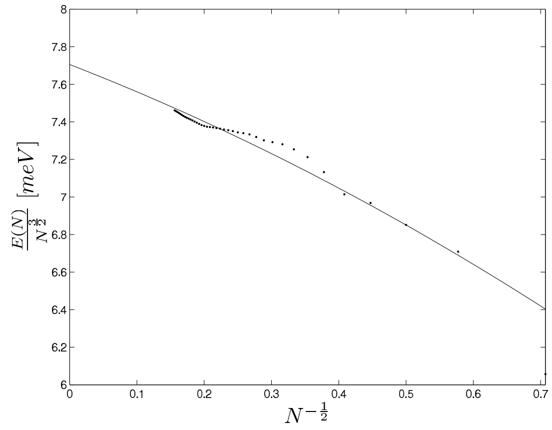


Figure 4.7: *Experimental ground state energy divided by* $N^{\frac{3}{2}}$*, as a function of* $N^{-\frac{1}{2}}$*, for* $N = 2$ *to* 41*, compared to a polynomial fitting.*

equation. This result is expressed in the following theorem. Let

$$\mathcal{E}^{TF}[\rho, V_{ext}] = \frac{\pi}{2} \int \mathrm{d}^2\boldsymbol{x} \rho^2(\boldsymbol{x}) + \int \mathrm{d}^2\boldsymbol{x} \rho(\boldsymbol{x}) V_{ext}(\boldsymbol{x}) + \frac{1}{2} \int \mathrm{d}^2\boldsymbol{x} \int \mathrm{d}^2\boldsymbol{y} \frac{\rho(\boldsymbol{x})\rho(\boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|} \tag{4.15}$$

be the Thomas-Fermi energy functional. Then there exists one unique density ρ^{TF} which minimizes the energy functional under the constraint $\int \mathrm{d}^2\boldsymbol{x}\rho(\boldsymbol{x}) = N$, whose energy is $E^{TF}(N, V_{ext})$. For an external potential of the order of N ($V_{ext}(\boldsymbol{x}) = N v_{ext}(\boldsymbol{x})$), this minimal energy is related to the quantum energy $E^Q(N, B, V_{ext})$ by

$$\lim_{N\to\infty} \frac{E^Q(N, B, V_{ext})}{E^{TF}(N, V_{ext})} = 1, \qquad \text{if} \quad \frac{B}{N} \longrightarrow 0. \tag{4.16}$$

Let

$$\mathcal{E}^{C}[\rho, V_{ext}] = \int \mathrm{d}^2\boldsymbol{x} \rho(\boldsymbol{x}) V_{ext}(\boldsymbol{x}) + \frac{1}{2} \int \mathrm{d}^2\boldsymbol{x} \int \mathrm{d}^2\boldsymbol{y} \frac{\rho(\boldsymbol{x})\rho(\boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|} \tag{4.17}$$

be the classical energy functional. Then there exists one unique density ρ^C which minimizes the energy functional under the constraint $\int \mathrm{d}^2\boldsymbol{x}\rho(\boldsymbol{x}) = N$, whose energy is $E^C(N, V_{ext})$. For an external potential of the order of k ($V_{ext}(\boldsymbol{x}) = k v_{ext}(\boldsymbol{x})$, v_{ext} being of the order of 1), and for a homogeneous external potential ($V_{ext}(\lambda\boldsymbol{x}) = \lambda^s V_{ext}(\boldsymbol{x})$, $s \geq 1$), this minimal energy is related to the quantum energy $E^Q(N, B, V_{ext})$ by

$$\lim_{N\to\infty} \frac{E^Q(N, 0, V_{ext})}{E^{C}(N, V_{ext})} = 1, \qquad \text{if} \quad \frac{k}{N} \longrightarrow 0. \tag{4.18}$$

This last asymptotic limit corresponds to the case where the kinetic energy is negligible compared to the other energies. The situation $\kappa \doteq \frac{k}{N} \ll 1$ is often observed experimentally, and the asymptotic limit is therefore a good starting point for theoretical developments (and this is what we used in our calculations). Let's finally note that all these limits converge uniformly, which allows a perturbative treatment (for $N \gg 1,\ \kappa \ll 1$).

A perturbative treatment also applies to the case of a small perpendicular magnetic field ($B \ll 1$), which will not be studied in this thesis.

Shikin et al. (1991) were, to our knowledge, the first to find a solution for the asymptotic limit $\kappa \to 0$, in the case of a parabolic confining potential. They found a solution to the self-consistent equation (where μ is the chemical potential)

$$\frac{1}{2}N\kappa\boldsymbol{x}^2 + \int \mathrm{d}^d\boldsymbol{y}\,\frac{\rho(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|} = \mu. \tag{4.19}$$

obtaining the self-consistent density. It is

$$\rho^C(\boldsymbol{x}) = \frac{3}{2\pi}\frac{N}{R^2}\sqrt{1-\frac{\boldsymbol{x}^2}{R^2}}, \quad R = \left(\frac{3\pi}{4\kappa}\right)^{\frac{1}{3}}, \quad \mu = \left(\frac{3\pi}{4}\right)^{\frac{2}{3}} N\kappa^{\frac{1}{3}}. \tag{4.20}$$

Introducing it in the energy functional one easily finds the ground state energy:

$$E^C = \frac{3}{5}\left(\frac{3\pi}{4}\right)^{\frac{2}{3}} N^2\kappa^{\frac{1}{3}}. \tag{4.21}$$

An exact solution of the general self-consistent equation (including the kinetic energy) does not exist, to our knowledge.

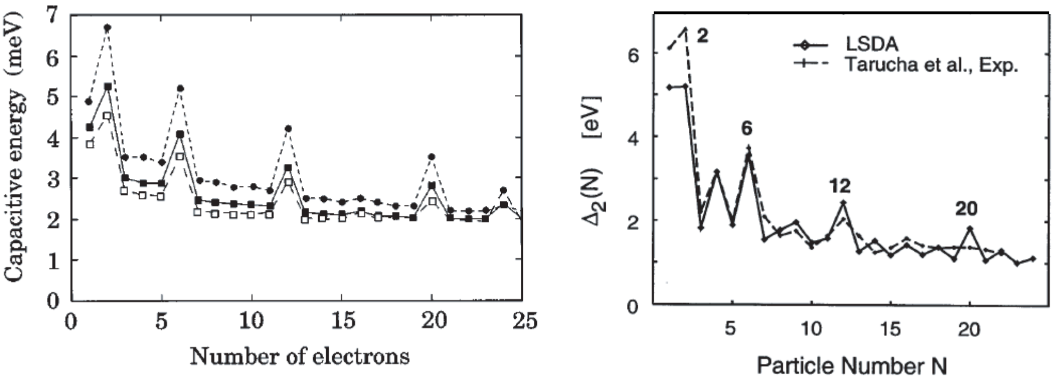
To obtain exact results, research was done by replacing the three-dimensional electron-electron interaction by the two-dimensional one, that is $V(\boldsymbol{x}) = -\ln|\boldsymbol{x}|$. This allows the use of the Poisson equation, which simplifies the problem. This was done by Sinha et al. (2000) and independently by Pino (1998). They obtained the asymptotic ground state energy for a number of electrons tending to infinity. Corrections to this asymptotic limit were obtained by Dalessi and Kunz (2003) in a master thesis. This approach is interesting because everything can be treated analytically, but it presents more an academic interest than a physical one, due to the fact that the electron-electron interaction is not the real one.

4.7 Theoretical results – energy oscillations

Not only the main (and smooth) asymptotic energy has been studied until now. Research has been done on the oscillatory behaviour of the energy, in very different ways, and using sometimes a different language. We proceed to a short description of the main approaches we found in the literature.

Considerable numerical effort was done to understand the electronic structure of quantum dots. We will specifically discuss the research done to obtain the addition spectrum, which corresponds experimentally to the Coulomb blockade peak spacings. The spacing between the $(N-1)^{th}$ and the N^{th} peaks is, in our language, simply $(\mu(N) - \mu(N-1))$. There are many experimental results, see for example Tarucha's results (Tarucha et al., 1996). They show "magic numbers" for 2, 6, 12 and 20 electrons, corresponding to filled shells of a two-dimensional harmonic oscillator, as shown in Figure 4.5.

We mention two numerical results obtained by modeling the dot as a two-dimensional system with a harmonic confining potential, for up to 25-30 electrons. The first was obtained by Macucci et al. (1997), using a self-consistent potential approach, and including the exchange and correlation effects. The results are shown in Figure 4.8(a). The second was obtained by Reimann et al. (1999), using Spin Density Functional Theory. Their results are very similar to the experimental ones, reproducing the "magic numbers" perfectly. Results are shown in Figure 4.8(b). Numerical results were also obtained for up to 400 electrons by Jiang et al. (2003b,a); they were interested in the statistical behaviour of the peak spacings, which is discussed below.



(a) Addition energy as a function of the number of electrons, obtained by self-consistent calculations, for a dot with a radius of $90nm$, and with a parabolic confinement of strength $\hbar\omega = 4meV$ (solid dots), $3meV$ (solid squares), and $2.5meV$ (empty squares).

(b) Addition energy as a function of the number of electrons, obtained with SDFT calculations (solid line), compared to Tarucha's results.

Figure 4.8: *Addition energy as a function of N.*

As explained previously, one method to measure the ground state energy consists of using the Coulomb Blockade. The distribution of the peak spacings was extensively studied, both experimentally and theoretically. A chaotic behaviour is expected due to the impurities and irregularities of the dot, and a simple model of independent particles with constant interaction leads to an RMT model and the (normalized) peak spacing distribution is the Wigner surmise. However, the experimental results do not agree with RMT predictions: the fluctuations are considerably larger than expected, and the distribution is gaussian. Similar results were obtained for GaAs dots by Sivan et al. (1996), an extensive study was done by Patel et al. (1998), and finally Simmel et al. (1997) obtained the same results for silicon dots. The distribution of (normalized) Coulomb blockade peak spacings is shown in Figure 4.9, the figure is from Patel et al. (1998).

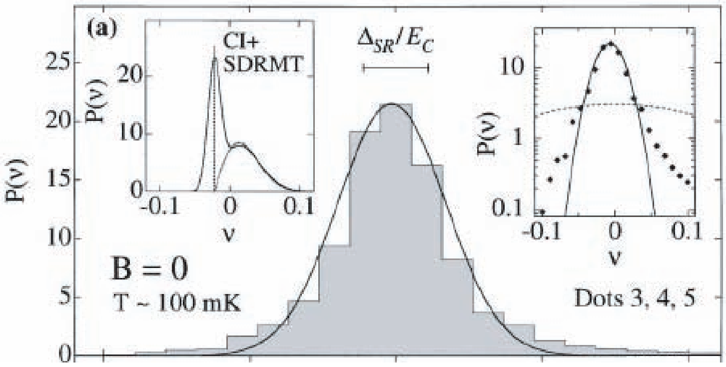


Figure 4.9: *Normalized Coulomb blockade peak spacings distribution (bars), obtained with* ~ 4300 *peaks, and from 3 different devices. The solid curve corresponds to a gaussian shape.*

The mismatching with theoretical predictions was explained by the fact that the electron density is too high, the electronic interaction therefore has to be taken into account beyond the constant interaction approach. The gaussian distribution was confirmed by Hartree-Fock calculations for random hamiltonians with an interaction term by Levit and Orgad (1999), Walker et al. (1999), and Cohen et al. (1999). A theoretical model including (random) interactions studied by Alhassid et al. (2000) models a crossover from a Wigner surmise distribution at low density, to a gaussian distribution at high density.

But is it justified to consider a chaotic quantum dot? An extensive numerical work was done by Jiang et al. (2003b,a), where they used refined numerical techniques (in the framework of Spin Density Functional Theory) to compute the ground state energy of a quantum dot, with symmetric and chaotic confinement potentials, for dots containing up to 400 electrons. As shown in Figure 4.10, they found, in both symmetric and chaotic potentials, that the peak-spacing distribution has an almost gaussian shape. They distinguish the cases N odd and N even, and observe differences. Moreover the symmetric case has a broader distribution than the chaotic one. But there seems to be no clear answer whether the experimental dots have a symmetric confining potential or not.

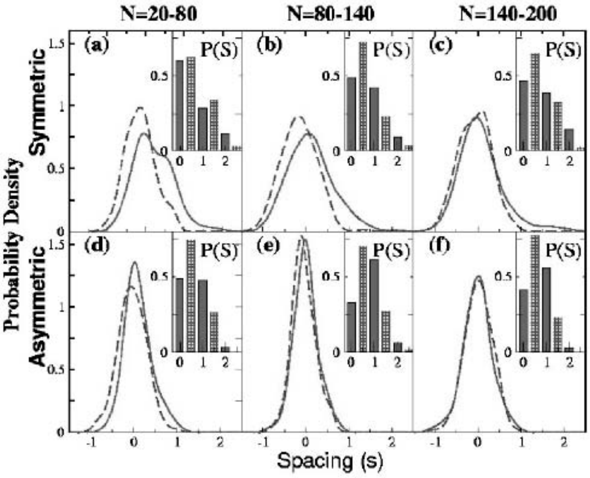
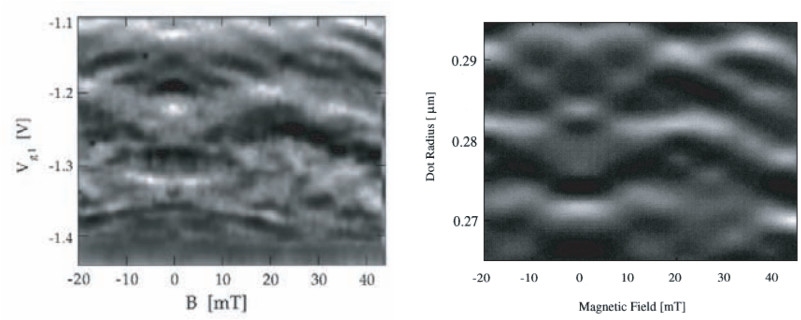


Figure 4.10: Distributions of normalized peak spacing for even (solid) and odd (dashed) N, for a symmetric, and an asymmetric potential, obtained with density functional calculations.

The energy oscillations are also treated in another work, done by Reimann et al. (1996). They consider a dot with a fixed number of electrons (about 1000), submitted to a magnetic field, and whose radius can be varied by modifying the external electrostatic potential. In this case the two parameters are the radius and the magnetic field. They measured the conductance, which shows clearly an oscillatory behaviour. This is explained by the variation of the density of states (at the Fermi surface) as a function of the radius and the magnetic field. This density of states can be easily related to the ground state energy (by integrating two times over the density of states, as will be done in chapter 6). The theoretical approach used to explain these experimental oscillations is done in the framework of semiclassical physics, using the periodic orbit theory. They consider the cases of a circular billiard (high density, the self-consistent potential does not depend on the confinement) and of a harmonic oscillator (low density, the self-consistent potential is the confining potential, the other electrons do not modify it). As shown in Figure 4.11, the high-density model is qualitatively similar to the experimental results, which confirms both the existence of these oscillations, and that the self-consistent potential is, in good approximation, that of a circular billiard.



(a) (b)

Figure 4.11: *Oscillations of the density at the Fermi surface, as a function of the magnetic field and the radius of the dot. (a) is the experimental result, (b) is obtained using the periodic orbit theory for a circular billiard.*

Chapter 5

Semiclassical Hartree-Fock development

Contents

The objective of this chapter is to develop the semiclassical approach and apply it to the problem of a quantum dot.

In chapter 2 we developed a new approach for the treatment of many-fermion systems. At lowest orders we established that the semiclassical Hartree-Fock approach was correct. We therefore develop this approach to obtain the ground state energy of quantum dots. As this approach does not contain energy oscillations, we use another approach in chapter 6 to obtain them. Moreover this approach needs the solution of a self-consistent equation, which is done in chapter 7, before the self-consistent potential obtained this way is used in chapter 8 to obtain the ground state energy of quantum dots.

In this chapter, we proceed first by a description of the Hartree-Fock approach, then proceed to a relevant scaling, to justify the use of a semiclassical approach. We then develop the semiclassical Hartree-Fock theory; we compute the density matrix in this theory, proceed to an inverse Laplace transform, and proceed to some integrations to obtain the semiclassical density, and from it the integrated density of states, to finally derive the Hartree energy. The Hartree-Fock energy is obtained by adding perturbatively the lowest order of the exchange energy. The energy is obtained as a functional of a potential, solution of a self-consistent equation.

5.1 Hartree-Fock

The semiclassical Hartree-Fock development is very general and this is why we will work in arbitrary dimension d, except when the specific dimension is mentioned. We will eventually discuss the particular cases $d = 3$, and $d = 2$ in more detail.

The hamiltonian we consider is given in equation (2.7) with the three-dimensional electron-electron interaction. For the quantum dots problem, it corresponds to the hamiltonian (4.8), which is the hamiltonian expressed in the modified atomic units. It is

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hat{\Delta}_i}{2} + \sum_{i=1}^{N} \hat{V}_{ext}(\hat{\boldsymbol{x}}_i) + \frac{1}{2} \sum_{i,j=1,i\neq j}^{N} \frac{1}{|\hat{\boldsymbol{x}}_i - \hat{\boldsymbol{x}}_j|}. \tag{5.1}$$

Let's consider the ground state $|\hat{\Psi}_0\rangle$. We approximate it as a product of one-particle wave functions, taking into account the Fermi-Dirac statistics (we will write it as an equality and call the new wave function the ground state):

$$\langle \hat{\boldsymbol{x}}_1, \ldots, \hat{\boldsymbol{x}}_N | \hat{\Psi}_0 \rangle = \frac{1}{\sqrt{N!}} \sum_{\pi \in Perm(N)} (-1)^{\pi} \hat{\psi}_{\pi(1)}(\hat{\boldsymbol{x}}_1) \hat{\psi}_{\pi(2)}(\hat{\boldsymbol{x}}_2) \ldots \hat{\psi}_{\pi(N)}(\hat{\boldsymbol{x}}_N). \tag{5.2}$$

The one-particle wave functions have to be determined such that the ground state energy $\hat{E}_0$ (which is the quantity that interests us) is best approximated by the energy of the new wave function.

To derive such a condition we know that the hamiltonian (5.1) is self-adjoint and hence, by the spectral theorem, its eigenfunctions $\{|\hat{\Psi}_k\rangle\}_{k\geq 0}$ provide a basis for N-particle wave functions. Any N-particle wave function $|\hat{\Phi}\rangle$ can therefore be written as

$$|\hat{\Phi}\rangle = \sum_{k\geq 0} c_k |\hat{\Psi}_k\rangle, \tag{5.3}$$

with the normalization condition $\sum_{k=0}^{\infty} |c_k|^2 = 1$.

The energy of this state $|\hat{\Phi}\rangle$ is therefore

$$\langle\hat{\Phi}|\hat{H}|\hat{\Phi}\rangle = \sum_{k,k'} c_k^\star c_{k'} \langle\hat{\Psi}_k| \underbrace{\hat{H}|\hat{\Psi}_{k'}\rangle}_{=\hat{E}_{k'}|\hat{\Psi}_{k'}\rangle} = \sum_{k,k'} c_k^\star c_{k'} \hat{E}_{k'} \underbrace{\langle\hat{\Psi}_k|\hat{\Psi}_{k'}\rangle}_{=\delta_{k,k'}} = \sum_k |c_k|^2 \hat{E}_k \geq \hat{E}_0. \tag{5.4}$$

The ground state energy is therefore best approached by minimizing the energy we obtain with the Ansatz (5.2).

We now need an intuitive approach to build the one-particle functions. The Fermi-Dirac statistics implies that these functions have to be orthogonal (they are even orthonormal): $\langle\hat{\psi}_i|\hat{\psi}_j\rangle = \delta_{i,j}$. This is why we build them from a one-particle operator $\hat{H} = -\frac{\hat{\Delta}}{2} + \hat{V}$, by considering the N first eigenfunctions and eigenvalues of this operator:

$$\left(-\frac{\hat{\Delta}}{2} + \hat{V}(\hat{\boldsymbol{x}})\right)\hat{\psi}_i(\hat{\boldsymbol{x}}) = \hat{e}_i\hat{\psi}_i(\hat{\boldsymbol{x}}). \tag{5.5}$$

With this procedure, the wave functions are now functionals of the potential $\hat{V}$. The ground state energy is therefore a functional of this potential, and the minimization condition becomes a minimization with regards to this "parameter" $\hat{V}$.

Let's rewrite the ground state energy with this potential $\hat{V}$.

$$\begin{aligned}
\hat{E}_0 &= \langle\hat{\Psi}_0|\hat{H}|\hat{\Psi}_0\rangle \\
&= \langle\hat{\Psi}_0| - \frac{1}{2}\sum_{i=1}^{N}\hat{\Delta}_i + \sum_{i=1}^{N}\hat{V}(\hat{\boldsymbol{x}}_i)|\hat{\Psi}_0\rangle \\
&\quad + \langle\hat{\Psi}_0|\sum_{i=1}^{N}\hat{V}_{ext}(\hat{\boldsymbol{x}}_i) + \frac{1}{2}\sum_{i,j=1,i\neq j}^{N}\frac{1}{|\hat{\boldsymbol{x}}_i - \hat{\boldsymbol{x}}_j|} - \sum_{i=1}^{N}\hat{V}(\hat{\boldsymbol{x}}_i)|\hat{\Psi}_0\rangle \\
&= \sum_{i=1}^{N}\hat{e}_i + \int \mathrm{d}^d\hat{\boldsymbol{x}}\left(\hat{V}_{ext}(\hat{\boldsymbol{x}}) - \hat{V}(\hat{\boldsymbol{x}})\right)\underbrace{\sum_{i=1}^{N}\hat{\psi}_i^\star(\hat{\boldsymbol{x}})\hat{\psi}_i(\hat{\boldsymbol{x}})}_{=\hat{\rho}(\boldsymbol{x})} \\
&\quad + \frac{1}{2}\int \mathrm{d}^d\hat{\boldsymbol{x}}\int \mathrm{d}^d\hat{\boldsymbol{y}}\frac{1}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|}\sum_{i,j=1,i\neq j}^{N}\hat{\psi}_i^\star(\hat{\boldsymbol{x}})\hat{\psi}_j^\star(\hat{\boldsymbol{y}})\left(\hat{\psi}_i(\hat{\boldsymbol{x}})\hat{\psi}_j(\hat{\boldsymbol{y}}) - \hat{\psi}_i(\hat{\boldsymbol{y}})\hat{\psi}_j(\hat{\boldsymbol{x}})\right) \\
&= \sum_{i=1}^{N}\hat{e}_i + \int \mathrm{d}^d\hat{\boldsymbol{x}}\left(\hat{V}_{ext}(\hat{\boldsymbol{x}}) + \frac{1}{2}\int \mathrm{d}^d\hat{\boldsymbol{y}}\frac{\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|} - \hat{V}(\hat{\boldsymbol{x}})\right)\hat{\rho}(\hat{\boldsymbol{x}}) \\
&\quad - \frac{1}{2}\int \mathrm{d}^d\hat{\boldsymbol{x}}\int \mathrm{d}^d\hat{\boldsymbol{y}}\frac{1}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|}\sum_{i,j=1,i\neq j}^{N}\hat{\psi}_i^\star(\hat{\boldsymbol{x}})\hat{\psi}_j^\star(\hat{\boldsymbol{y}})\hat{\psi}_i(\hat{\boldsymbol{x}})\hat{\psi}_j(\hat{\boldsymbol{y}}).
\end{aligned} \tag{5.6}$$

Using the definition $\hat{\rho}(\hat{\boldsymbol{x}},\hat{\boldsymbol{y}}) = \sum_{i=1}^{N} \hat{\psi}_i^\star(\hat{\boldsymbol{y}})\hat{\psi}_i(\hat{\boldsymbol{x}})$ we can write the ground state energy as

$$\begin{aligned}\hat{E}_0 &= \sum_{i=1}^{N} \hat{e}_i + \int \mathrm{d}^d\hat{\boldsymbol{x}} \left(\hat{V}_{ext}(\hat{\boldsymbol{x}}) + \frac{1}{2}\int \mathrm{d}^d\hat{\boldsymbol{y}} \frac{\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|} - \hat{V}(\hat{\boldsymbol{x}})\right)\hat{\rho}(\hat{\boldsymbol{x}}) \\ &\quad -\frac{1}{2}\int \mathrm{d}^d\hat{\boldsymbol{x}} \int \mathrm{d}^d\hat{\boldsymbol{y}} \frac{1}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|}\hat{\rho}(\hat{\boldsymbol{y}},\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{x}},\hat{\boldsymbol{y}}). \end{aligned} \tag{5.7}$$

We have to minimize this energy, with regards to the potential $\hat{V}$. To proceed we neglect the exchange term. It will be established *a posteriori* that, for $N \gg 1$, this approximation is valid. The energy is then

$$\hat{E}_0 = \sum_{i=1}^{N} \hat{e}_i + \int \mathrm{d}^d\hat{\boldsymbol{x}} \left(\hat{V}_{ext}(\hat{\boldsymbol{x}}) + \frac{1}{2}\int \mathrm{d}^d\hat{\boldsymbol{y}} \frac{\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|} - \hat{V}(\hat{\boldsymbol{x}})\right)\hat{\rho}(\hat{\boldsymbol{x}}). \tag{5.8}$$

To minimize this functional, let's look how the first term is modified by the change $\hat{V} \mapsto \hat{V} + \delta\hat{V}$. For this let's consider it changes as $\hat{\psi}_i \mapsto \hat{\psi}_i + \delta\hat{\psi}_i$, $\hat{e}_i \mapsto \hat{e}_i + \delta\hat{e}_i$. To establish it let's compute (without writing the $\hat{\boldsymbol{x}}$ dependence)

$$\begin{aligned}\hat{e}_i + \delta\hat{e}_i &= \int \mathrm{d}^d\hat{\boldsymbol{x}} \left(\hat{\psi}_i^\star + \delta\hat{\psi}_i^\star\right)(\hat{e}_i + \delta\hat{e}_i)\left(\hat{\psi}_i + \delta\hat{\psi}_i\right) \\ &= \int \mathrm{d}^d\hat{\boldsymbol{x}} \left(\hat{\psi}_i^\star + \delta\hat{\psi}_i^\star\right)\left(-\frac{\hat{\Delta}}{2} + \hat{V} + \delta\hat{V}\right)\left(\hat{\psi}_i + \delta\hat{\psi}_i\right) \\ &= \hat{e}_i + \int \mathrm{d}^d\hat{\boldsymbol{x}}\hat{\psi}_i^\star\delta\hat{V}\hat{\psi}_i + \hat{e}_i\int \mathrm{d}^d\hat{\boldsymbol{x}}\left(\hat{\psi}_i^\star\delta\hat{\psi}_i + \delta\hat{\psi}_i^\star\hat{\psi}_i\right) \\ &\quad +\mathcal{O}(\delta\hat{\psi}_i^\star\delta\hat{\psi}_i, \delta\hat{\psi}_i^\star\delta\hat{e}_i, \delta\hat{e}_i\delta\hat{\psi}_i). \end{aligned} \tag{5.9}$$

The last term is of the order of $\mathcal{O}(\delta\hat{\psi}_i^\star\delta\hat{\psi}_i)$, because of the normalization condition:

$$1 = \int \mathrm{d}^d\hat{\boldsymbol{x}}(\hat{\psi}_i^\star + \delta\hat{\psi}_i^\star)(\hat{\psi}_i + \delta\hat{\psi}_i) = 1 + \int \mathrm{d}^d\hat{\boldsymbol{x}}(\delta\hat{\psi}_i^\star\hat{\psi}_i + \hat{\psi}_i^\star\delta\hat{\psi}_i + \delta\hat{\psi}_i^\star\delta\hat{\psi}_i), \tag{5.10}$$

hence

$$\int \mathrm{d}^d\hat{\boldsymbol{x}}(\delta\hat{\psi}_i^\star\hat{\psi}_i + \hat{\psi}_i^\star\delta\hat{\psi}_i) = -\int \mathrm{d}^d\hat{\boldsymbol{x}}\delta\hat{\psi}_i^\star\delta\hat{\psi}_i. \tag{5.11}$$

We finally obtain the result

$$\delta\hat{e}_i = \int \mathrm{d}^d\hat{\boldsymbol{x}}\delta\hat{V}(\hat{\boldsymbol{x}})\hat{\psi}_i^\star(\hat{\boldsymbol{x}})\hat{\psi}_i(\hat{\boldsymbol{x}}). \tag{5.12}$$

Summing over the N first eigenvalues we find

$$\delta\left(\sum_{i=1}^{N}\hat{e}_i\right) = \sum_{i=1}^{N}\delta\hat{e}_i = \int \mathrm{d}^d\hat{\boldsymbol{x}}\delta\hat{V}(\hat{\boldsymbol{x}})\sum_{i=1}^{N}\hat{\psi}_i^\star(\hat{\boldsymbol{x}})\hat{\psi}_i(\hat{\boldsymbol{x}}) = \int \mathrm{d}^d\hat{\boldsymbol{x}}\delta\hat{V}(\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{x}}). \tag{5.13}$$

We have to determine how the other terms of (5.8) are modified by a change of $\hat{V}$. We define $\delta\hat{\rho}$ such that $\hat{V} \mapsto \hat{V} + \delta\hat{V}$ implies $\hat{\rho} \mapsto \hat{\rho} + \delta\hat{\rho}$. The last terms of the ground state energy become

$$\begin{aligned}
&\delta\left(\int \mathrm{d}^d\hat{\boldsymbol{x}} \left(\hat{V}_{ext}(\hat{\boldsymbol{x}}) + \frac{1}{2}\int \mathrm{d}^d\hat{\boldsymbol{y}} \frac{\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|} - \hat{V}(\hat{\boldsymbol{x}})\right)\hat{\rho}(\hat{\boldsymbol{x}})\right) \\
&\quad = -\int \mathrm{d}^d\hat{\boldsymbol{x}}\delta\hat{V}(\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{x}}) + \int \mathrm{d}^d\hat{\boldsymbol{x}}\left(\hat{V}_{ext}(\hat{\boldsymbol{x}}) - \hat{V}(\hat{\boldsymbol{x}})\right)\delta\hat{\rho}(\hat{\boldsymbol{x}}) + \int \mathrm{d}^d\hat{\boldsymbol{y}} \frac{\delta\hat{\rho}(\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|} \\
&\quad = -\int \mathrm{d}^d\hat{\boldsymbol{x}}\delta\hat{V}(\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{x}}) + \int \mathrm{d}^d\hat{\boldsymbol{x}}\left(\hat{V}_{ext}(\hat{\boldsymbol{x}}) + \int \mathrm{d}^d\hat{\boldsymbol{y}} \frac{\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|} - \hat{V}(\hat{\boldsymbol{x}})\right)\delta\hat{\rho}(\hat{\boldsymbol{x}}).
\end{aligned} \tag{5.14}$$

Summing (5.13) and (5.14) we find

$$\delta\hat{E}_0 = \int \mathrm{d}^d\hat{\boldsymbol{x}}\left(\hat{V}_{ext}(\hat{\boldsymbol{x}}) + \int \mathrm{d}^d\hat{\boldsymbol{y}} \frac{\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|} - \hat{V}(\hat{\boldsymbol{x}})\right)\delta\hat{\rho}(\hat{\boldsymbol{x}}). \tag{5.15}$$

Hence the ground state energy $\hat{E}_0$ is minimized with regards to the potential $\hat{V}$ if $\delta\hat{E}_0 = 0$. This condition is satisfied for any (small) modification of $\hat{V}$ if the potential is

$$\hat{V}(\hat{\boldsymbol{x}}) = \hat{V}_{ext}(\hat{\boldsymbol{x}}) + \int \mathrm{d}^d\hat{\boldsymbol{y}} \frac{\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|}. \tag{5.16}$$

This result is not surprising. It provides a potential which corresponds to the mean-field potential: the particles feel the external potential and the mean electron-electron interaction produced by the other particles.

This relation is not enough: the density $\hat{\rho}$ has to be related to the potential. This is done through the relation (5.5), which we are unable to use analytically. Instead we will use a semiclassical approximation which will be valid for $N \gg 1$. Let's note that the relation (5.5) could easily be used numerically.

We can now return to the ground state energy (5.7) (including now the exchange energy):

$$\hat{E}_0 = \sum_{i=1}^{N} \hat{e}_i - \frac{1}{2}\int \mathrm{d}^d\hat{\boldsymbol{x}} \int \mathrm{d}^d\hat{\boldsymbol{y}} \frac{\hat{\rho}(\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|} - \frac{1}{2}\int \mathrm{d}^d\hat{\boldsymbol{x}} \int \mathrm{d}^d\hat{\boldsymbol{y}} \frac{\hat{\rho}(\hat{\boldsymbol{x}},\hat{\boldsymbol{y}})\hat{\rho}(\hat{\boldsymbol{y}},\hat{\boldsymbol{x}})}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|}. \tag{5.17}$$

This formulation of the ground state energy can have a physical interpretation: the first term contains the electron-electron interaction counted twice, one time for each electron. Hence we have to subtract it, which explains the second term.

This theory can be generalized to a theory which includes the exchange term for the determination of the self-consistent potential $\hat{V}$. It is however more difficult to give a physical interpretation of such a potential. The equation for the eigenfunctions $\hat{\psi}_i$ and eigenvalues $\hat{e}_i$ is obtained by minimizing the ground state energy, taking into account the orthonormal constraints of the wave functions, by means of Lagrange parameters. After diagonalization these parameters correspond to the eigenvalues of a Schrödinger equation, and play the same role as the eigenvalues established previously. Detailed developments can be found in (Martin and Rothen, 2004). The equation we obtain is

$$\left(-\frac{\hat{\Delta}}{2}+\hat{V}_{ext}(\hat{\boldsymbol{x}})+\int \mathrm{d}^d\hat{\boldsymbol{y}}\frac{\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|}\right)\hat{\psi}_i(\hat{\boldsymbol{x}})-\int \mathrm{d}^d\hat{\boldsymbol{y}}\frac{\hat{\rho}(\hat{\boldsymbol{x}},\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|}\hat{\psi}_i(\hat{\boldsymbol{y}})=\hat{e}_i\hat{\psi}_i(\hat{\boldsymbol{x}}). \tag{5.18}$$

The total energy becomes

$$\hat{E}_0=\sum_{i=1}^{N}\hat{e}_i-\frac{1}{2}\left(\int \mathrm{d}^d\hat{\boldsymbol{x}}\int \mathrm{d}^d\hat{\boldsymbol{y}}\frac{\hat{\rho}(\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|}-\int \mathrm{d}^d\hat{\boldsymbol{x}}\int \mathrm{d}^d\hat{\boldsymbol{y}}\frac{\hat{\rho}(\hat{\boldsymbol{x}},\hat{\boldsymbol{y}})\hat{\rho}(\hat{\boldsymbol{y}},\hat{\boldsymbol{x}})}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|}\right). \tag{5.19}$$

We observe that the sign of the exchange energy has changed between formulas (5.17) and (5.19). This is explained by the fact that, in the first case, the sum $\sum_{i=1}^{N}\hat{e}_i$ does not take into account the exchange energy. In the second case this term includes twice the exchange energy, this is why we have to subtract it from the total energy.

5.1.1 Scaling

From the formula for the ground state energy, we want to extract the N dependence as well as identify which quantities are small, in order to identify which asymptotic limit to study.

We already changed the units of our problem. We chose the modified atomic units, which allowed us to write the ground state energy in an elegant way. However these units are not necessarily the natural ones of the system. In the problem of quantum dots, there is a parameter, independent of N, the strength of the confining potential. This is why we have to take it into account when proceeding to a scaling, as it will have an influence on the size of the system, and therefore on its typical length scale. The scaling will be therefore slightly different from that we performed in the general study of chapter 2.

Let's proceed to a scaling of the length, $\hat{\boldsymbol{x}}\mapsto\frac{\hat{\boldsymbol{x}}}{L_\star}$, where $L_\star$ is a characteristic length of the system, whose N dependence will be established *a posteriori*. The length is denoted by a star to remind us that it is expressed in modified atomic units.

The new wave functions will still be normalized to 1 but the new density ρ is defined such that it is of the order of $\mathcal{O}(1)$, in order to quickly identify the orders of the final expression of the energy (in chapter 2 the density was normalized to

N, but there is no fundamental difference):

$$\hat{\boldsymbol{x}} \mapsto \boldsymbol{x} = \frac{\hat{\boldsymbol{x}}}{L_\star}, \quad \mathrm{d}^d\boldsymbol{x} = L_\star^{-d}\mathrm{d}^d\hat{\boldsymbol{x}}, \quad \frac{\partial^k}{\partial x_i^k} = L_\star^k \frac{\partial^k}{\partial \hat{x}_i^k}. \tag{5.20}$$

We have then

$$1 = \int \mathrm{d}^d\hat{\boldsymbol{x}} \hat{\psi}_i^\star(\hat{\boldsymbol{x}})\hat{\psi}_i(\hat{\boldsymbol{x}}) = L_\star^d \int \mathrm{d}^d\boldsymbol{x} \hat{\psi}_i^\star(L_\star\boldsymbol{x})\hat{\psi}_i(L_\star\boldsymbol{x}). \tag{5.21}$$

In order to have normalized wave functions we impose

$$\int \mathrm{d}^d\boldsymbol{x} \psi_i^\star(\boldsymbol{x})\psi_i(\boldsymbol{x}) = 1. \tag{5.22}$$

From (5.21), the functions ψ_i are therefore

$$\psi_i(\boldsymbol{x}) = L_\star^{\frac{d}{2}} \hat{\psi}_i(L_\star\boldsymbol{x}). \tag{5.23}$$

The densities are defined as

$$\rho(\boldsymbol{x},\boldsymbol{y}) = \frac{1}{N}\sum_{i=1}^N \psi_i^\star(\boldsymbol{y})\psi_i(\boldsymbol{x}), \tag{5.24}$$

$$\rho(\boldsymbol{x}) = \frac{1}{N}\sum_{i=1}^N \psi_i^\star(\boldsymbol{x})\psi_i(\boldsymbol{x}). \tag{5.25}$$

With this scaling, and the division by N, equation (5.18) becomes

$$\left(-\frac{1}{2NL_\star^2}\Delta + \frac{\hat{V}_{ext}(L_\star\boldsymbol{x})}{N} + \frac{1}{L_\star}\int \mathrm{d}^d\boldsymbol{y}\frac{\rho(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\right)\psi_i(\boldsymbol{x}) \\ -\frac{1}{L_\star}\int \mathrm{d}^d\boldsymbol{y}\frac{\rho(\boldsymbol{x},\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\psi_i(\boldsymbol{y}) = \frac{\hat{e}_i}{N}\psi_i(\boldsymbol{x}). \tag{5.26}$$

Multiplying it by $L_\star$ we finally obtain

$$\left(-\frac{1}{2NL_\star}\Delta + \frac{\hat{V}_{ext}(L_\star\boldsymbol{x})}{\frac{N}{L_\star}} + \int \mathrm{d}^d\boldsymbol{y}\frac{\rho(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\right)\psi_i(\boldsymbol{x}) \\ -\int \mathrm{d}^d\boldsymbol{y}\frac{\rho(\boldsymbol{x},\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\psi_i(\boldsymbol{y}) = \frac{\hat{e}_i}{\frac{N}{L_\star}}\psi_i(\boldsymbol{x}). \tag{5.27}$$

Let's define $\epsilon^2 = \frac{1}{2NL_\star}$, $e_i = \frac{\hat{e}_i}{\frac{N}{L_\star}}$, and $V_{ext}(\boldsymbol{x}) = \frac{\hat{V}_{ext}(L_\star\boldsymbol{x})}{\frac{N}{L_\star}}$. The equation we look at is now

$$\left(-\epsilon^2\Delta + V_{ext}(\boldsymbol{x}) + \int \mathrm{d}^d\boldsymbol{y}\frac{\rho(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\right)\psi_i(\boldsymbol{x}) - \int \mathrm{d}^d\boldsymbol{y}\frac{\rho(\boldsymbol{x},\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\psi_i(\boldsymbol{y}) = e_i\psi_i(\boldsymbol{x}). \tag{5.28}$$

Let's write the ground state energy (5.17) in terms of these new variables. We find

$$\hat{E}_0 = \frac{N}{L_\star}\sum_{i=1}^{N} e_i - \frac{N^2}{2L_\star}\int \mathrm{d}^d\boldsymbol{x}\int \mathrm{d}^d\boldsymbol{y}\frac{(\rho(\boldsymbol{x})\rho(\boldsymbol{y}) + \rho(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{y},\boldsymbol{x}))}{|\boldsymbol{x}-\boldsymbol{y}|}. \tag{5.29}$$

5.1.2 Chemical potential versus electron number

In our developments it will be more convenient to work with the chemical potential μ instead of the number of electrons N (which are thermodynamically conjugated), which means that we will change from the canonical to the grand canonical ensemble. This chemical potential is defined as the energy such that the energy levels e_i are filled until this value.

Moreover we take into account a degeneracy factor s, which is the degeneracy due to the spin of the electron: $s = 2$. We conserve this letter throughout the computations, and replace s by its number at the end of the computations. This degeneracy is not contained in our hamiltonian, this is why we have to add it.

The relation between N and μ is given by

$$N(\mu) = s\sum_{i=1}^{\infty}\theta(\mu - e_i), \tag{5.30}$$

where θ is the Heaviside step function.

This immediately defines the chemical potential μ as a function of the number of electrons N, by the implicit equation

$$N = N(\mu). \tag{5.31}$$

We can also write the energy

$$s\sum_{i=1}^{N} e_i = s\sum_{i=1}^{\infty} e_i\theta(\mu - e_i) \tag{5.32}$$

as well as the electron density

$$\rho(\boldsymbol{x},\boldsymbol{y}) = \frac{s}{N}\sum_{i=1}^{N}\psi_i^\star(\boldsymbol{y})\psi_i(\boldsymbol{x}) = \frac{s}{N}\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{y})\psi_i(\boldsymbol{x})\theta(\mu - e_i), \tag{5.33}$$

$$\rho(\boldsymbol{x}) = \frac{s}{N}\sum_{i=1}^{N}\psi_i^\star(\boldsymbol{x})\psi_i(\boldsymbol{x}) = \frac{s}{N}\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{x})\psi_i(\boldsymbol{x})\theta(\mu - e_i). \tag{5.34}$$

At this stage we introduce the density $\rho(e;\boldsymbol{x},\boldsymbol{y})$, whose importance will become clear later. It is defined by

$$\rho(e;\boldsymbol{x},\boldsymbol{y}) = s\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{y})\psi_i(\boldsymbol{x})\delta(e - e_i), \tag{5.35}$$

$$\rho(e;\boldsymbol{x}) = s\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{x})\psi_i(\boldsymbol{x})\delta(e-e_i). \tag{5.36}$$

$\rho(\boldsymbol{x},\boldsymbol{y})$ and $\rho(\boldsymbol{x})$ can be related to $\rho(e;\boldsymbol{x},\boldsymbol{y})$ and $\rho(e;\boldsymbol{x})$ respectively:

$$\begin{aligned}\rho(\boldsymbol{x},\boldsymbol{y}) &= \frac{s}{N}\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{y})\psi_i(\boldsymbol{x})\theta(\mu-e_i)\\ &= \frac{1}{N}\int^{\mu}\mathrm{d}e\ s\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{y})\psi_i(\boldsymbol{x})\delta(e-e_i)\\ &= \frac{1}{N}\int^{\mu}\mathrm{d}e\rho(e;\boldsymbol{x},\boldsymbol{y}),\end{aligned} \tag{5.37}$$

$$\begin{aligned}\rho(\boldsymbol{x}) &= \frac{s}{N}\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{x})\psi_i(\boldsymbol{x})\theta(\mu-e_i)\\ &= \frac{1}{N}\int^{\mu}\mathrm{d}e\ s\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{x})\psi_i(\boldsymbol{x})\delta(e-e_i)\\ &= \frac{1}{N}\int^{\mu}\mathrm{d}e\rho(e;\boldsymbol{x}).\end{aligned} \tag{5.38}$$

The energy can be formulated with the density of states $\rho(e)$ and the integrated density of states $N(e)$, which are very usual objects in quantum chaos, and which are defined by

$$\rho(e) = s\sum_{i=1}^{\infty}\delta(e-e_i),\quad N(e) = s\sum_{i=1}^{\infty}\theta(e-e_i)\quad\Rightarrow\quad \rho(e) = \frac{\mathrm{d}}{\mathrm{d}e}N(e). \tag{5.39}$$

The density of states can be obtained from the density $\rho(e;\boldsymbol{x})$, using the normalization of the wave functions $\int \mathrm{d}^d\boldsymbol{x}\psi_i^\star(\boldsymbol{x})\psi_i(\boldsymbol{x}) = 1$:

$$\rho(e) = s\sum_{i=1}^{\infty}\delta(e-e_i) = \int \mathrm{d}^d\boldsymbol{x}\ s\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{x})\psi_i(\boldsymbol{x})\delta(e-e_i) = \int \mathrm{d}^d\boldsymbol{x}\rho(e;\boldsymbol{x}), \tag{5.40}$$

while the integrated density of states can be obtained from the density $\rho(\boldsymbol{x})$:

$$N(\mu) = s\sum_{i=1}^{\infty}\theta(\mu-e_i) = \int \mathrm{d}^d\boldsymbol{x}\ s\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{x})\psi_i(\boldsymbol{x})\theta(\mu-e_i) = N\int \mathrm{d}^d\boldsymbol{x}\rho(\boldsymbol{x}). \tag{5.41}$$

The energy (5.32) can then be written as

$$\begin{aligned}
s\sum_{i=1}^{\infty} e_i\theta(\mu - e_i) &= \int^{\infty} \mathrm{d}e\theta(\mu - e)e\, \underbrace{s\sum_{i=1}^{\infty} \delta(e - e_i)}_{=\rho(e)} = \int^{\mu} \mathrm{d}ee\rho(e) \\
&= \int^{\mu} \mathrm{d}ee\frac{\mathrm{d}}{\mathrm{d}e}N(e) = eN(e)|^{\mu} - \int^{\mu} \mathrm{d}eN(e) \\
&= \mu N - \int^{\mu} \mathrm{d}eN(e), \qquad (5.42)
\end{aligned}$$

where we proceeded to an integration by parts.

5.1.3 Ground state energy

With this formalism, the ground state energy (5.29) can be written

$$\hat{E}_0 = \frac{N^2}{L_\star}\left(\mu - \frac{1}{N}\int^{\mu} \mathrm{d}eN(e) - \frac{1}{2}\int \mathrm{d}^d\boldsymbol{x}\int \mathrm{d}^d\boldsymbol{y}\frac{(\rho(\boldsymbol{x})\rho(\boldsymbol{y}) + \rho(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{y},\boldsymbol{x}))}{|\boldsymbol{x}-\boldsymbol{y}|}\right). \tag{5.43}$$

Having extracted the N and $L_\star$ dependencies, let's simplify the problem by considering only the energy $E_0 = \frac{L_\star}{N^2}\hat{E}_0$:

$$E_0 = \mu - \frac{1}{N}\int^{\mu} \mathrm{d}eN(e) - \frac{1}{2}\int \mathrm{d}^d\boldsymbol{x}\int \mathrm{d}^d\boldsymbol{y}\frac{(\rho(\boldsymbol{x})\rho(\boldsymbol{y}) + \rho(\boldsymbol{x},\boldsymbol{y})\rho(\boldsymbol{y},\boldsymbol{x}))}{|\boldsymbol{x}-\boldsymbol{y}|}. \tag{5.44}$$

The self-consistent potential in these new variables, defining it as $V(\boldsymbol{x}) = \frac{L_\star}{N}\hat{V}(L_\star\boldsymbol{x})$, where we defined $\hat{V}$ in (5.16), is given by

$$V(\boldsymbol{x}) = V_{ext}(\boldsymbol{x}) + \int \mathrm{d}^d\boldsymbol{y}\frac{\rho(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}. \tag{5.45}$$

It is now necessary to proceed to some discussion. Throughout this development we have considered that the external potential divided by N is of the order of $\mathcal{O}(1)$, which is not the case in quantum dots, since this potential is an external condition and does not necessarily depend on N. However this study is more general and we will consider at the end the case where the external potential divided by N is small. More precisely, the potential will depend on a parameter, let's say k, and we will consider the limit $\kappa \doteq \frac{k}{N} \ll 1$. This limit will be considered independently of the limit $N \gg 1$. The factor κ depends on the strength of the external potential, but also on N. It is representative of the electron density in the dot. The ground state energy has a uniform convergence in the limit $\kappa \to 0$, as shown in (Lieb et al., 1995). Let's note that instead of κ we will consider $L_\star$ as a parameter of the system, which is directly related to the density of the system, as we will see below, and which, in the specific case of homogeneous potentials, will be related to k explicitly in the asymptotic limit.

Let's add a comment about the small parameter ϵ. This parameter plays the role of the usual $\frac{\hbar^2}{2m}$ in quantum mechanics. Very powerful tools were developed to study the asymptotic behaviour when this parameter is small. But small compared to what? This parameter is not dimensionless, it therefore has to be compared to other physical values, which are characteristic of the physical system. Then "$\hbar$ small" means $\hbar \ll S$, where S is the biggest action of the system ($\hbar$ has the dimensions of an action). This regime is called the semiclassical limit, because the limit $\hbar \to 0$ corresponds asymptotically to classical physics.

In our case we proceeded to a scaling, and the equation we obtained is dimensionless. In particular the parameter ϵ is dimensionless ($L_\star = \frac{L}{a_\star}$ has no dimension). Let's recall that ϵ is defined by

$$\epsilon^2 = \frac{1}{2}\frac{1}{NL_\star}. \tag{5.46}$$

This parameter is characterized by two independent ones: N and $L_\star$. The length $L_\star$ contains information about the density of the system, which is proportional to $\frac{N}{L_\star^2}$. If $L_\star \gg N^{\frac{1}{2}}$ the system is diluted, hence it is not surprising that we are working in the semiclassical regime. Conversely, if $L_\star \ll N^{\frac{1}{2}}$, the density is high. In this case it is not obvious whether the semiclassical regime is valid or not: there is a competition between the two parameters $L_\star$ and N. Looking at (5.46) we see that the condition on $L_\star$ in order to work in the semiclassical regime is $L_\star \gg \frac{1}{N}$.

The low density semiclassical regime is therefore given by

$$L_\star \gg N^{\frac{1}{2}}, \tag{5.47}$$

while the high density semiclassical regime is given by

$$\frac{1}{N} \ll L_\star \ll N^{\frac{1}{2}}. \tag{5.48}$$

The lower bound corresponds to the semiclassical regime limit, while the upper bound corresponds to the high density regime limit.

On what does $L_\star$ depend? It depends, first, on the number of electrons N, but also on another parameter of the system, the strength of the external potential. This can be physically understood by the fact that if the confinement potential is strong, the electrons will be confined in a small region and the density will be high. In our developments we will consider two parameters, N and $L_\star$ independently.

How large is $L_\star$? In order to give numerical values of this length, we will develop the semiclassical limit of this problem, and determine, from this, its N dependence in the different regimes. Moreover a particular case of physical interest, the parabolic confinement, will be considered, and experimental estimations of the confinement potential strength will be discussed, which will allow us to obtain an estimation of the length $L_\star$. After this discussion we will see that the experimental conditions are such that the semiclassical limit can be used.

At this stage we can already discuss qualitatively the length scale in the case of a homogeneous potential of degree p, that is such that $k\hat{V}_{ext}(\lambda\hat{\boldsymbol{x}}) = k\lambda^p\hat{V}_{ext}(\hat{\boldsymbol{x}})$, where k represents the strength of the potential. We want that in equation (5.28), all the terms are of the order of $\mathcal{O}(1)$, except the parameter ϵ. We already extracted the $L_\star$ dependence of the electron-electron interaction, we still have to impose that the external potential is of the order of $\mathcal{O}(1)$, which will impose a condition on the length scale. Returning to the initial definition of the external potential, we find (working in the modified atomic units)

$$kV_{ext}(\boldsymbol{x}) = \frac{kL_\star}{N}\hat{V}_{ext}(L_\star\boldsymbol{x}) = \frac{kL_\star^{(p+1)}}{N}\hat{V}_{ext}(\boldsymbol{x}) = \mathcal{O}(1). \tag{5.49}$$

Hence the length scale is defined by $k\frac{L_\star^{(p+1)}}{N} \simeq 1$, therefore

$$L_\star \simeq \left(\frac{N}{k}\right)^{\frac{1}{(p+1)}}. \tag{5.50}$$

In the specific case of the two-dimensional harmonic potential $\hat{V}_{ext}(\hat{\boldsymbol{x}}) = \frac{1}{2}k\hat{\boldsymbol{x}}^2$ we find

$$L_\star \simeq \left(\frac{N}{k}\right)^{\frac{1}{3}}. \tag{5.51}$$

From this result we can determine the asymptotic limit of the ground state energy (5.43) with regards to N:

$$\hat{E}_0 \simeq \frac{N^2}{L_\star} \simeq N^{\frac{5}{3}}k^{\frac{1}{3}}. \tag{5.52}$$

In some cases (as will be the case for the experimental data we will use), the strength "constant" depends on N; we have typically $k = \frac{k'}{\sqrt{N}}$, which leads to the asymptotic energy

$$\hat{E}_0 \simeq \frac{N^2}{L_\star} \simeq N^2\frac{k'^{\frac{1}{3}}}{N^{\frac{1}{2}}} = N^{\frac{3}{2}}k'^{\frac{1}{3}}. \tag{5.53}$$

We may ask if it is possible to measure experimentally the ground state energy of a quantum dot. Actually it is. We discussed the experimental results in chapter 4.

5.2 Semiclassical Hartree-Fock

Our starting point in this section will be the self-consistent equation (5.45).

In order to obtain an equation for V, the density ρ has to be related to the potential V. This will be done in the semiclassical regime, using equation (5.28) (and neglecting the exchange term):

$$\left(-\epsilon^2\Delta + V(\boldsymbol{x})\right)\psi_i(\boldsymbol{x}) = e_i\psi_i(\boldsymbol{x}), \tag{5.54}$$

and we will work in the semiclassical limit

$$\epsilon \ll 1. \tag{5.55}$$

This equation will allow us to write $\rho[V]$ as an asymptotic expansion in powers of ϵ^2, where ρ is defined by equation (5.34).

We will also compute the density $\rho(\boldsymbol{x},\boldsymbol{y})$, which will allow us to compute the exchange energy. This density has been defined in (5.33).

We cannot proceed to an asymptotic expansion of the density in powers of ϵ^2. We have to consider the expansion of the density matrix, from which we will compute the density $\rho(\boldsymbol{x},\boldsymbol{y})$. This density matrix is

$$e^{-\beta H}(\boldsymbol{x},\boldsymbol{y}) = \langle\boldsymbol{x}|e^{-\beta H}|\boldsymbol{y}\rangle, \tag{5.56}$$

which can be easily computed in the framework of semiclassical physics, in an asymptotic expansion in powers of ϵ.

Let's see how these two objects are related (taking into account the spin degeneracy s):

$$\begin{aligned} e^{-\beta H}(\boldsymbol{x},\boldsymbol{y}) &= \langle\boldsymbol{x}|s\sum_{i=1}^{\infty} e^{-\beta e_i}|\psi_i\rangle\langle\psi_i|\boldsymbol{y}\rangle = s\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{y})\psi_i(\boldsymbol{x})e^{-\beta e_i} \\ &= \int^{\infty} \mathrm{d}e\ s\sum_{i=1}^{\infty}\psi_i^\star(\boldsymbol{y})\psi_i(\boldsymbol{x})\delta(e-e_i)e^{-\beta e} = \int^{\infty} \mathrm{d}e\rho(e;\boldsymbol{x},\boldsymbol{y})e^{-\beta e}, \end{aligned} \tag{5.57}$$

where the last equality comes from the definition (5.35). Let's note that $\rho(e;\boldsymbol{x},\boldsymbol{y})$ is a distribution, not a usual function.

The density is then obtained from $\rho(e;\boldsymbol{x},\boldsymbol{y})$ by equality (5.37).

From equation (5.57) we see that $\rho(e;\boldsymbol{x},\boldsymbol{y})$ is the inverse Laplace transform of the density matrix $e^{-\beta H}(\boldsymbol{x},\boldsymbol{y})$. Hence, we can obtain $\rho(\boldsymbol{x},\boldsymbol{y})$ by computing $e^{-\beta H}(\boldsymbol{x},\boldsymbol{y})$ semiclassically, applying the inverse Laplace transform to obtain $\rho(e;\boldsymbol{x},\boldsymbol{y})$, then integrating over e and dividing by N to obtain $\rho(\boldsymbol{x},\boldsymbol{y})$.

5.2.1 Density matrix

The density matrix will be computed at lowest order in ϵ using functional integration. We will discuss our approach as in the real time case (the density matrix corresponds to the propagator $e^{-\frac{i}{\hbar}Ht}$), and compute it directly in the imaginary time. The semiclassical approach is much more intuitive in real time.

We will consider the trajectory of a classical free particle from $\boldsymbol{x}$ at time 0 to $\boldsymbol{y}$ at time 1. This trajectory is given by

$$\boldsymbol{x}_{cl}(t) = (1-t)\boldsymbol{x} + t\boldsymbol{y}. \tag{5.58}$$

The quantum effects, which consist of quantum fluctuations around the classical path, are computed exactly. We find, writing $H_0 = -\epsilon^2\Delta$, and considering the spin degeneracy s:

$$e^{-\beta H_0}(\boldsymbol{x},\boldsymbol{y}) = s\langle \boldsymbol{x}|e^{\beta\epsilon^2\Delta}|\boldsymbol{y}\rangle = s\left(\frac{1}{4\pi\beta\epsilon^2}\right)^{\frac{d}{2}} e^{-\frac{1}{4\beta\epsilon^2}(\boldsymbol{y}-\boldsymbol{x})^2}, \tag{5.59}$$

which is a well-known result (see for example (Kleinert, 2004)).

In the semiclassical limit, which in our case is the limit $\epsilon \ll 1$, the potential is treated perturbatively around the classical trajectory of the free particle, using the cumulant expansion with a gaussian measure arising from the quantum fluctuations. Normalizing the imaginary time to 1 we find (writing $\boldsymbol{x}(t) = \boldsymbol{x}_{cl}(t)+\delta\boldsymbol{x}(t)$, and introducing $\delta\boldsymbol{y}(t) = \frac{\delta\boldsymbol{x}(t)}{\epsilon\sqrt{2\beta}}$):

$$\begin{aligned}
e^{-\beta H}(\boldsymbol{x},\boldsymbol{y}) &= s\langle \boldsymbol{x}|e^{\beta\epsilon^2\Delta-\beta V(\boldsymbol{x})}|\boldsymbol{y}\rangle \\
&= s\int_{\boldsymbol{x}(0)=\boldsymbol{x},\boldsymbol{x}(1)=\boldsymbol{y}} \mathcal{D}\boldsymbol{x} e^{-\int_0^1 \mathrm{d}t\left(\frac{1}{2}\frac{\dot{\boldsymbol{x}}^2(t)}{2\beta\epsilon^2}+\beta V(\boldsymbol{x}(t))\right)} \\
&= s\left(\frac{1}{4\pi\beta\epsilon^2}\right)^{\frac{d}{2}} e^{-\frac{1}{4\beta\epsilon^2}(\boldsymbol{y}-\boldsymbol{x})^2} \\
&\quad\times\frac{\int_{\delta\boldsymbol{x}(0)=\delta\boldsymbol{x}(1)=0}\mathcal{D}\delta\boldsymbol{x} e^{-\int_0^1 \mathrm{d}t\left(\frac{1}{2}\frac{\delta\dot{\boldsymbol{x}}^2(t)}{2\beta\epsilon^2}+\beta V(\boldsymbol{x}_{cl}(t)+\delta\boldsymbol{x}(t))\right)}}{\int_{\delta\boldsymbol{x}(0)=\delta\boldsymbol{x}(1)=0}\mathcal{D}\delta\boldsymbol{x} e^{-\int_0^1 \mathrm{d}t\frac{1}{2}\frac{\delta\dot{\boldsymbol{x}}^2(t)}{2\beta\epsilon^2}}} \\
&= s\left(\frac{1}{4\pi\beta\epsilon^2}\right)^{\frac{d}{2}} e^{-\frac{1}{4\beta\epsilon^2}(\boldsymbol{y}-\boldsymbol{x})^2} \\
&\quad\times\frac{\int_{\delta\boldsymbol{y}(0)=\delta\boldsymbol{y}(1)=0}\mathcal{D}\delta\boldsymbol{y} e^{-\int_0^1 \mathrm{d}t\left(\frac{1}{2}\delta\dot{\boldsymbol{y}}^2(t)+\beta V(\boldsymbol{x}_{cl}(t)+\epsilon\sqrt{2\beta}\delta\boldsymbol{y}(t))\right)}}{\int_{\delta\boldsymbol{y}(0)=\delta\boldsymbol{y}(1)=0}\mathcal{D}\delta\boldsymbol{y} e^{-\int_0^1 \mathrm{d}t\frac{1}{2}\delta\dot{\boldsymbol{y}}^2(t)}} \\
&= s\left(\frac{1}{4\pi\beta\epsilon^2}\right)^{\frac{d}{2}} e^{-\frac{1}{4\beta\epsilon^2}(\boldsymbol{y}-\boldsymbol{x})^2}\left\langle e^{-\beta\int_0^1 \mathrm{d}t V(\boldsymbol{x}_{cl}(t)+\epsilon\sqrt{2\beta}\delta\boldsymbol{y}(t))}\right\rangle_0.
\end{aligned} \tag{5.60}$$

The measure is a gaussian measure, arising from the normalized quantum fluctuations. It is defined by

$$\langle \delta y_i(t)\rangle_0 = 0; \qquad \langle \delta y_i(t)\delta y_j(t')\rangle_0 = \left\{\begin{array}{lcl} \delta_{i,j}t(1-t') & , & t<t', \\ \delta_{i,j}t'(1-t) & , & t>t'. \end{array}\right.$$

This result can be obtained easily when returning to the discrete version of the functional integral. Another approach to obtain this result, working in the continuum, is to invert the operator $-\Delta(t,t') = -\delta(t-t')\frac{\partial^2}{\partial t^2}$, which means having to find $G(t',t'')$ such that

$$-\int_0^1 \mathrm{d}t' \Delta(t,t') G(t',t'') = \delta(t-t''). \tag{5.61}$$

Using the definition of $\Delta(t,t')$ we find

$$\ddot{G}(t',t'') = -\delta(t'-t''), \tag{5.62}$$

where the dot refers to a derivation with respect to the first variable (t'). Integrating over t' from 0 to t we obtain

$$\int_0^t \mathrm{d}t' \ddot{G}(t',t'') = \dot{G}(t,t'') - \dot{G}(0,t'') = -\int_0^t \mathrm{d}t' \delta(t'-t'') = -\theta(t-t''). \tag{5.63}$$

Integrating again over t', from 0 to t, and reminding that $G(0,t) = G(1,t) = 0$ (the boundary conditions are fixed), we find

$$\begin{aligned}\int_0^t \mathrm{d}t' \dot{G}(t',t'') &= G(t,t'') - G(0,t'') = G(t,t'') \\ &= \int_0^t \mathrm{d}t' \dot{G}(0,t'') - \int_0^t \mathrm{d}t' \theta(t'-t'') \\ &= s\dot{G}(0,t'') - (t-t'')\theta(t-t''). \end{aligned} \tag{5.64}$$

$\dot{G}(0,t'')$ is computed with the boundary condition:

$$0 = G(1,t'') = \dot{G}(0,t'') - (1-t'') \Rightarrow \dot{G}(0,t'') = (1-t''). \tag{5.65}$$

We finally obtain

$$G(t,t') = \begin{cases} t(1-t') & , \quad t < t', \\ t'(1-t) & , \quad t > t'. \end{cases}$$

To compute (5.60) we perform an expansion in powers of $\epsilon\sqrt{2\beta}$ and proceed to a cumulant expansion:

$$\langle e^{A_1} \rangle_0 = e^{\langle A_1 \rangle_0 + \frac{1}{2}\left(\langle A_1^2 \rangle_0 - \langle A_1 \rangle_0^2\right) + \cdots}. \tag{5.66}$$

We obtain

$$
\begin{aligned}
-\beta\int_0^1 \mathrm{d}tV\left(\boldsymbol{x}_{cl}(t)+\epsilon\sqrt{2\beta}\delta\boldsymbol{y}(t)\right) \quad = \quad & -\beta\int_0^1 \mathrm{d}t\Bigg(V(\boldsymbol{x}_{cl}(t)) \\
& +\epsilon\sqrt{2\beta}\sum_{i=1}^{d}\frac{\partial}{\partial x_i}V(\boldsymbol{x}_{cl}(t))\delta y_i(t) \\
& +\frac{1}{2}2\beta\epsilon^2\sum_{i,j=1}^{d}\frac{\partial^2}{\partial x_i\partial x_j}V(\boldsymbol{x}_{cl}(t))\delta y_i(t)\delta y_j(t)\Bigg) \\
& +\mathcal{O}(\epsilon^3), \qquad (5.67)
\end{aligned}
$$

which implies

$$
\begin{aligned}
&\left\langle -\beta\int_0^1 \mathrm{d}tV\left(\boldsymbol{x}_{cl}(t)+\epsilon\sqrt{2\beta}\delta\boldsymbol{y}(t)\right)\right\rangle_0 \\
&\qquad = -\beta\int_0^1 \mathrm{d}t\left(V(\boldsymbol{x}_{cl}(t))+\beta\epsilon^2\Delta V(\boldsymbol{x}_{cl}(t))t(1-t)\right)+\mathcal{O}(\epsilon^4)
\end{aligned}
\qquad (5.68)
$$

and

$$
\begin{aligned}
&\frac{1}{2}\Bigg(\left\langle\left(-\beta\int_0^1 \mathrm{d}tV\left(\boldsymbol{x}_{cl}(t)+\epsilon\sqrt{2\beta}\delta\boldsymbol{y}(t)\right)\right)^2\right\rangle_0 \\
&\quad -\left\langle -\beta\int_0^1 \mathrm{d}tV\left(\boldsymbol{x}_{cl}(t)+\epsilon\sqrt{2\beta}\delta\boldsymbol{y}(t)\right)\right\rangle_0^2\Bigg) \\
&\qquad = 2\beta^3\epsilon^2\int_0^1 \mathrm{d}t\int_0^t \mathrm{d}t'\nabla V(\boldsymbol{x}_{cl}(t))\cdot\nabla V(\boldsymbol{x}_{cl}(t'))t'(1-t)+\mathcal{O}(\epsilon^4).
\end{aligned}
\qquad (5.69)
$$

The final result for the density matrix is then

$$
\begin{aligned}
e^{-\beta H}(\boldsymbol{x},\boldsymbol{y}) \quad = \quad & s\left(\frac{1}{4\pi\beta\epsilon^2}\right)^{\frac{d}{2}} e^{-\frac{1}{4\beta\epsilon^2}(\boldsymbol{y}-\boldsymbol{x})^2} e^{-\beta\int_0^1 \mathrm{d}tV(\boldsymbol{x}_{cl}(t))} \\
& \times\exp\Big(-\beta^2\epsilon^2\int_0^1 \mathrm{d}t\Delta V(\boldsymbol{x}_{cl}(t))t(1-t)\Big) \\
& \times\exp\Big(2\beta^3\epsilon^2\int_0^1 \mathrm{d}t\int_0^t \mathrm{d}t'\nabla V(\boldsymbol{x}_{cl}(t))\cdot\nabla V(\boldsymbol{x}_{cl}(t'))t'(1-t)\Big) \\
& +\mathcal{O}(\epsilon^4). \qquad (5.70)
\end{aligned}
$$

5.2.2 Semiclassical density $\rho_0(\boldsymbol{x},\boldsymbol{y})$

Let's proceed to some discussion about this result. The factor $e^{-\frac{(\boldsymbol{y}-\boldsymbol{x})^2}{4\beta\epsilon^2}}$ implies that the density matrix vanishes if $|\boldsymbol{y}-\boldsymbol{x}| \gg \epsilon$. Let's define $\boldsymbol{r}$ such that $\boldsymbol{y}=\boldsymbol{x}+\epsilon\boldsymbol{r}$ and compute $e^{-\beta H}(\boldsymbol{x},\boldsymbol{x}+\epsilon\boldsymbol{r})$, for $\epsilon \ll 1$, at lowest order in ϵ:

$$\epsilon^d \left(e^{-\beta H}\right)_0 (\boldsymbol{x},\boldsymbol{x}+\epsilon\boldsymbol{r}) = s\left(\frac{1}{4\pi\beta}\right)^{\frac{d}{2}} e^{-\frac{\boldsymbol{r}^2}{4\beta}} e^{-\beta V(\boldsymbol{x})}, \tag{5.71}$$

where we used the fact that the classical trajectory is $\boldsymbol{x}_{cl}(t)=\boldsymbol{x}+t\epsilon\boldsymbol{r} \overset{\epsilon\to 0}{\to} \boldsymbol{x}$.

Using the gaussian relation

$$\int \mathrm{d}p_i e^{-\beta p_i^2 + i r_i p_i} = \sqrt{\frac{\pi}{\beta}}\, e^{-\frac{r_i^2}{4\beta}} \tag{5.72}$$

the density matrix (5.71) becomes

$$\left(e^{-\beta H}\right)_0 (\boldsymbol{x},\boldsymbol{x}+\epsilon\boldsymbol{r}) = \frac{1}{\epsilon^d}\frac{s}{(2\pi)^d}\int \mathrm{d}^d\boldsymbol{p} e^{-\beta\boldsymbol{p}^2 + i\boldsymbol{r}\cdot\boldsymbol{p} - \beta V(\boldsymbol{x})}. \tag{5.73}$$

In order to compute the density $\rho(e;\boldsymbol{x},\boldsymbol{y})$ at lowest order, related to the density matrix by equation (5.57), we write

$$\begin{aligned} \left(e^{-\beta H}\right)_0 (\boldsymbol{x},\boldsymbol{x}+\epsilon\boldsymbol{r}) &= \int^{\infty} \mathrm{d}e \rho_0(e;\boldsymbol{x},\boldsymbol{x}+\epsilon\boldsymbol{r}) e^{-\beta e} \\ &= \frac{1}{\epsilon^d}\frac{s}{(2\pi)^d}\int^{\infty}\mathrm{d}e\int \mathrm{d}^d\boldsymbol{p} e^{-\beta e + i\boldsymbol{r}\cdot\boldsymbol{p}}\delta(e-(\boldsymbol{p}^2+V(\boldsymbol{x}))). \end{aligned} \tag{5.74}$$

The density $\rho(e;\boldsymbol{x},\boldsymbol{x}+\epsilon\boldsymbol{r})$ at lowest order in ϵ is then

$$\rho_0(e;\boldsymbol{x},\boldsymbol{x}+\epsilon\boldsymbol{r}) = \frac{1}{\epsilon^d}\frac{s}{(2\pi)^d}\int \mathrm{d}^d\boldsymbol{p} e^{i\boldsymbol{r}\cdot\boldsymbol{p}}\delta(e-(\boldsymbol{p}^2+V(\boldsymbol{x}))). \tag{5.75}$$

We will rewrite the integral over $\boldsymbol{p}$ by writing it in hyperspherical coordinates, and perform the integration over $p=|\boldsymbol{p}|$ using the delta function. The hyperspherical measure is $\mathrm{d}^d\boldsymbol{p} = p^{(d-1)}\sin^{(d-2)}\theta_{(d-1)}\sin^{(d-3)}\theta_{(d-2)}\ldots\sin\theta_2\theta_1\ \mathrm{d}p\mathrm{d}\theta_{(d-1)}\cdots\mathrm{d}\theta_1$, and the basis is chosen such that the scalar product is $\boldsymbol{r}\cdot\boldsymbol{p} = rp\cos\theta_{(d-1)}$. Integration over the angles $\theta_{(d-2)},\ldots,\theta_1$ can be performed and we obtain $S_{(d-1)} = \frac{2\pi^{\frac{(d-1)}{2}}}{\Gamma\left(\frac{(d-1)}{2}\right)}$, where $S_{(d-1)}$ is the surface of a $(d-2)$-dimensional hypersphere of radius 1. This result can be found in (Gradshteyn et al., 2000).

Using the result

$$\delta(e-p^2-V(\boldsymbol{x})) = \begin{cases} \frac{1}{2\sqrt{e-V(\boldsymbol{x})}}\delta(p-\sqrt{e-V(\boldsymbol{x})}), & \text{if} \quad e > V(\boldsymbol{x}), \\ 0, & \text{if} \quad e < V(\boldsymbol{x}), \end{cases}$$

the density matrix is written, if $e > V(\boldsymbol{x})$,

$$\begin{aligned}
\rho_0(e;\boldsymbol{x},\boldsymbol{x}+\epsilon\boldsymbol{r}) &= s\frac{S_{(d-1)}}{\epsilon^d}\frac{1}{(2\pi)^d}\frac{1}{2\sqrt{e-V(\boldsymbol{x})}}\int_0^\pi \mathrm{d}\theta\int_0^\infty \mathrm{d}pp^{(d-1)}\sin^{(d-2)}\theta \\
&\qquad\times\delta(p-\sqrt{e-V(\boldsymbol{x})})e^{irp\cos\theta} \\
&= s\frac{S_{(d-1)}}{\epsilon^d}\frac{1}{(2\pi)^d}\frac{1}{2}(e-V(\boldsymbol{x}))^{\frac{(d-2)}{2}} \\
&\qquad\times\int_0^\pi \mathrm{d}\theta\sin^{(d-2)}\theta e^{ir\sqrt{e-V(\boldsymbol{x})}\cos\theta}.
\end{aligned} \tag{5.76}$$

Using the integral representation of the Bessel function (Gradshteyn et al., 2000)

$$J_\nu(x) = \frac{\left(\frac{x}{2}\right)^\nu}{\pi^{\frac{1}{2}}\Gamma(\nu+\frac{1}{2})}\int_0^\pi e^{ix\cos\theta}\sin^{(2\nu)}\theta\mathrm{d}\theta, \tag{5.77}$$

and introducing this result in (5.76) with $\nu = \frac{(d-2)}{2}$, and $x = r\sqrt{e-V(\boldsymbol{x})}$ we obtain, after some computation:

$$\rho_0(e;\boldsymbol{x},\boldsymbol{x}+\epsilon\boldsymbol{r}) = \frac{s}{2}\left(\frac{\sqrt{e-V(\boldsymbol{x})}}{r}\right)^{\frac{(d-2)}{2}}\frac{1}{(2\pi)^{\frac{d}{2}}}\frac{1}{\epsilon^d}J_{\frac{(d-2)}{2}}\left(r\sqrt{e-V(\boldsymbol{x})}\right). \tag{5.78}$$

If $e < V(\boldsymbol{x})$ the density matrix is 0.

To obtain the density we still have to integrate $\rho(e;\boldsymbol{x},\boldsymbol{y})$ over e, from formula (5.37). To proceed let's note that $\rho(e;\boldsymbol{x},\boldsymbol{y})$ is zero if $e < V(\boldsymbol{x})$. The integration is then performed from $V(\boldsymbol{x})$ to μ:

$$\begin{aligned}
\rho_0(\boldsymbol{x},\boldsymbol{x}+\epsilon\boldsymbol{r}) &= \frac{1}{N}\int_0^\mu \mathrm{d}e\rho_0(e;\boldsymbol{x},\boldsymbol{x}+\epsilon\boldsymbol{r}) \\
&= \frac{1}{2}\frac{1}{r^{\frac{(d-2)}{2}}}\frac{s}{(2\pi)^{\frac{d}{2}}}\frac{1}{N\epsilon^d}\int_{V(\boldsymbol{x})}^\mu \mathrm{d}e\left(\sqrt{e-V(\boldsymbol{x})}\right)^{\frac{(d-2)}{2}} \\
&\qquad\times J_{\frac{(d-2)}{2}}\left(r\sqrt{e-V(\boldsymbol{x})}\right) \\
&= \frac{1}{2}\frac{1}{r^{\frac{(d-2)}{2}}}\frac{s}{(2\pi)^{\frac{d}{2}}}\frac{1}{N\epsilon^d}\int_0^{\mu-V(\boldsymbol{x})}\mathrm{d}e'\left(\sqrt{e'}\right)^{\frac{(d-2)}{2}}J_{\frac{(d-2)}{2}}\left(r\sqrt{e'}\right) \\
&= \frac{1}{r^d}\frac{s}{(2\pi)^{\frac{d}{2}}}\frac{1}{N\epsilon^d}\int_0^{r\sqrt{\mu-V(\boldsymbol{x})}}\mathrm{d}yy^{\frac{d}{2}}J_{\frac{(d-2)}{2}}(y) \\
&= \frac{1}{r^d}\frac{s}{(2\pi)^{\frac{d}{2}}}\frac{1}{N\epsilon^d}\left(r\sqrt{\mu-V(\boldsymbol{x})}\right)^{\frac{d}{2}}J_{\frac{d}{2}}\left(r\sqrt{\mu-V(\boldsymbol{x})}\right) \\
&= \frac{1}{r^{\frac{d}{2}}}\frac{s}{(2\pi)^{\frac{d}{2}}}\frac{1}{N\epsilon^d}\left(\sqrt{\mu-V(\boldsymbol{x})}\right)^{\frac{d}{2}}J_{\frac{d}{2}}\left(r\sqrt{\mu-V(\boldsymbol{x})}\right),
\end{aligned} \tag{5.79}$$

where we performed the changes of variables $e \mapsto e' = e - V(\boldsymbol{x})$ and $e' \mapsto y = r\sqrt{e'}$. We used the equality (Gradshteyn et al., 2000)

$$\int_0^{x_0} \mathrm{d}x x^{(1+n)} J_n(x) = x^{(1+n)} J_{1+n}(x). \tag{5.80}$$

5.2.3 Semiclassical density $\rho(e; \boldsymbol{x})$ in $d = 2$ dimensions

We will now focus on the case we are most interested in, the two-dimensional one. Although a general treatment in arbitrary dimension d is possible, it cannot always be treated uniformly, we would therefore have to consider some cases separately, which is not useful for our work. We will keep however the arbitrary dimension d in our computations when they can be performed uniformly for any dimension.

The density $\rho(\boldsymbol{x})$ is related to the density matrix: it corresponds to its diagonal part:

$$\rho(\boldsymbol{x}) = \rho(\boldsymbol{x}, \boldsymbol{x}). \tag{5.81}$$

It is much simpler to compute than the density matrix, because the classical path is $\boldsymbol{x}_{cl}(t) = \boldsymbol{x}$, it is independent of the imaginary time t. Hence we will be able to integrate explicitly over t the terms in (5.70).

Let's compute $e^{-\beta H}(\boldsymbol{x}, \boldsymbol{x})$ explicitly. From expression (5.70) we find

$$\begin{aligned}
e^{-\beta H}(\boldsymbol{x}, \boldsymbol{x}) &= s\left(\frac{1}{4\pi\beta\epsilon^2}\right)^{\frac{d}{2}} \exp\left(-\beta\int_0^1 \mathrm{d}t V(\boldsymbol{x})\right) \\
&\qquad \times \exp\left(-\beta^2\epsilon^2 \Delta V(\boldsymbol{x}) \int_0^1 \mathrm{d}t t(1-t)\right) \\
&\qquad \times \exp\left(+2\beta^3\epsilon^2 \left(\nabla V(\boldsymbol{x})\right)^2 \int_0^1 \mathrm{d}t \int_0^t \mathrm{d}t' t'(1-t)\right) \\
&\qquad \times \exp\left(\mathcal{O}(\epsilon^4)\right) \\
&= s\left(\frac{1}{4\pi\beta\epsilon^2}\right)^{\frac{d}{2}} \exp\left(-\beta V(\boldsymbol{x}) - \frac{\beta^2\epsilon^2}{6}\Delta V(\boldsymbol{x})\right) \\
&\qquad \times \exp\left(+\frac{\beta^3\epsilon^2}{12}\left(\nabla V(\boldsymbol{x})\right)^2 + \mathcal{O}(\epsilon^4)\right) \\
&= s\left(\frac{1}{4\pi\beta\epsilon^2}\right)^{\frac{d}{2}} e^{-\beta V(\boldsymbol{x})}\left(1 - \frac{\beta^2\epsilon^2}{6}\Delta V(\boldsymbol{x})\right. \\
&\qquad \left. + \frac{\beta^3\epsilon^2}{12}\left(\nabla V(\boldsymbol{x})\right)^2 + \mathcal{O}(\epsilon^4)\right) \\
&= \left(e^{-\beta H}\right)_0 (\boldsymbol{x}, \boldsymbol{x}) + \epsilon^2 \left(e^{-\beta H}\right)_1 (\boldsymbol{x}, \boldsymbol{x}) + \mathcal{O}(\epsilon^4).
\end{aligned} \tag{5.82}$$

where we used $\int_0^1 \mathrm{d}t t(1-t) = \frac{1}{6}$ and $\int_0^1 \mathrm{d}t \int_0^t \mathrm{d}t' t'(1-t) = \frac{1}{24}$.

To compute the density $\rho(\boldsymbol{x})$, we introduce $\rho(e;\boldsymbol{x})$, which is related to the density by equation (5.38). $\rho(e;\boldsymbol{x})$ is itself related to the density matrix by relation (5.57).

We expand the density matrix in powers of ϵ^2, as well as the density $\rho(e;\boldsymbol{x})$:

$$\begin{aligned}\left(e^{-\beta H}\right)_0 (\boldsymbol{x},\boldsymbol{x}) + \epsilon^2 \left(e^{-\beta H}\right)_1 (\boldsymbol{x},\boldsymbol{x}) + \mathcal{O}(\epsilon^4) \\ = \int^{\infty} \mathrm{d}e \left(\rho_0(e;\boldsymbol{x}) + \epsilon^2 \rho_1(e;\boldsymbol{x})\right) e^{-\beta e} + \mathcal{O}(\epsilon^4).\end{aligned} \tag{5.83}$$

We will define $\rho_0(e;\boldsymbol{x})$ as the inverse Laplace transform of $\left(e^{-\beta H}\right)_0 (\boldsymbol{x},\boldsymbol{x})$, and $\rho_1(e;\boldsymbol{x})$ as the inverse Laplace transform of $\left(e^{-\beta H}\right)_1 (\boldsymbol{x},\boldsymbol{x})$. This implies that we suppose that the ϵ expansion and the Laplace transform are commutative.

Lowest order

Let's compute the first term explicitly:

$$\begin{aligned}\left(e^{-\beta H}\right)_0 (\boldsymbol{x},\boldsymbol{x}) &= s\left(\frac{1}{4\pi\beta\epsilon^2}\right)^{\frac{d}{2}} e^{-\beta V(\boldsymbol{x})} = \frac{s}{(2\pi)^d \epsilon^d} \int \mathrm{d}^d\boldsymbol{p} e^{-\beta(\boldsymbol{p}^2 + V(\boldsymbol{x}))} \\ &= \frac{s}{(2\pi)^d \epsilon^d} \int_0^{\infty} \mathrm{d}e \int \mathrm{d}^d\boldsymbol{p} \delta(e - (\boldsymbol{p}^2 + V(\boldsymbol{x}))) e^{-\beta e},\end{aligned} \tag{5.84}$$

where we used the gaussian identity $\int \mathrm{d}^d\boldsymbol{p} e^{-\beta \boldsymbol{p}^2} = \left(\frac{\pi}{\beta}\right)^{\frac{d}{2}}$.

The density at lowest order is then

$$\begin{aligned}\rho_0(e;\boldsymbol{x}) &= \frac{s}{(2\pi)^d \epsilon^d} \int \mathrm{d}^d\boldsymbol{p} \delta(e - (\boldsymbol{p}^2 + V(\boldsymbol{x}))) \\ &= \frac{1}{2} \frac{s}{(2\pi)^d \epsilon^d} \frac{1}{\sqrt{e - V(\boldsymbol{x})}} S_d \int_0^{\infty} \mathrm{d}p p^{(d-1)} \delta(p - \sqrt{e - V(\boldsymbol{x})}) \\ &= \frac{s}{2} \frac{S_d}{(2\pi)^d \epsilon^d} \left(\sqrt{e - V(\boldsymbol{x})}\right)_+^{(d-2)} \\ &= \frac{\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \frac{s}{(2\pi)^d \epsilon^d} \left(\sqrt{e - V(\boldsymbol{x})}\right)_+^{(d-2)},\end{aligned} \tag{5.85}$$

where we integrated over the angular part of $\boldsymbol{p}$, making the factor $S_d = \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)}$ appear, integrating then over p.

The case $d = 2$ seems special. However this formula is also valid in this case, as can be seen by replacing d by 2. We obtain (with $\Gamma(1) = 1$)

$$\rho_0(e;\boldsymbol{x}) = \frac{s}{4\pi\epsilon^2} \theta(e - V(\boldsymbol{x})). \tag{5.86}$$

First correction

First term Let's now consider the higher corrections to the density. We first consider the term

$$-\frac{s}{6}\left(\frac{1}{4\pi\epsilon^2}\right)^{\frac{d}{2}} e^{-\beta V(\boldsymbol{x})}\beta^{\left(2-\frac{d}{2}\right)}\Delta V(\boldsymbol{x}). \tag{5.87}$$

Here the approach will depend on the dimension d. Let's consider the two-dimensional one.

This term is written

$$\begin{aligned} -\frac{s}{24\pi}\frac{1}{\epsilon^2}e^{-\beta V(\boldsymbol{x})}\beta\Delta V(\boldsymbol{x}) &= \frac{s}{24\pi}\frac{1}{\epsilon^2}\left(\frac{\partial}{\partial V}e^{-\beta V(\boldsymbol{x})}\right)\Delta V(\boldsymbol{x}) \\ &= \frac{s}{24\pi}\frac{1}{\epsilon^2}\int_0^{\infty}\mathrm{d}e\left(\frac{\partial}{\partial V}\delta(e-V(\boldsymbol{x}))\right)\Delta V(\boldsymbol{x})e^{-\beta e}. \end{aligned} \tag{5.88}$$

The contribution to the density is then

$$\frac{s}{24\pi}\frac{1}{\epsilon^2}\left(\frac{\partial}{\partial V}\delta(e-V(\boldsymbol{x}))\right)\Delta V(\boldsymbol{x}). \tag{5.89}$$

Second term Let's now consider the second term of the first correction. It is

$$\frac{s}{12}\left(\frac{1}{4\pi\epsilon^2}\right)^{\frac{d}{2}} e^{-\beta V(\boldsymbol{x})}\beta^{3-\frac{d}{2}}\left(\nabla V(\boldsymbol{x})\right)^2. \tag{5.90}$$

As previously, the approach will depend on the dimension. This is why we only compute the two-dimensional case. We write the term as follows:

$$\begin{aligned} &\frac{s}{12}\left(\frac{1}{4\pi\epsilon^2}\right)e^{-\beta V(\boldsymbol{x})}\beta^2\left(\nabla V(\boldsymbol{x})\right)^2 \\ &\qquad = \frac{s}{48\pi}\frac{1}{\epsilon^2}\left(\frac{\partial^2}{\partial V^2}e^{-\beta V(\boldsymbol{x})}\right)\left(\nabla V(\boldsymbol{x})\right)^2 \\ &\qquad = \frac{s}{48\pi}\frac{1}{\epsilon^2}\int_0^{\infty}\mathrm{d}e\left(\frac{\partial^2}{\partial V^2}\delta(e-V(\boldsymbol{x}))\right)\left(\nabla V(\boldsymbol{x})\right)^2 e^{-\beta e}. \end{aligned} \tag{5.91}$$

The contribution to the density is then

$$\frac{s}{48\pi}\frac{1}{\epsilon^2}\left(\frac{\partial^2}{\partial V^2}\delta(e-V(\boldsymbol{x}))\right)\left(\nabla V(\boldsymbol{x})\right)^2. \tag{5.92}$$

Final expression

In two dimensions the density $\rho(e;\boldsymbol{x})$ at order $\mathcal{O}(\epsilon^2)$ is, from equations (5.86), (5.89) and (5.92):

$$\rho(e;\boldsymbol{x}) = \rho_0(e;\boldsymbol{x}) + \epsilon^2\rho_1(e;\boldsymbol{x}) + \mathcal{O}(\epsilon^4), \tag{5.93}$$

where

$$\rho_0(e;\boldsymbol{x}) = \frac{s}{4\pi\epsilon^2}\theta(e - V(\boldsymbol{x})), \tag{5.94}$$

$$\begin{aligned}\rho_1(e;\boldsymbol{x}) \quad &= \quad \frac{s}{4\pi\epsilon^2}\left(\frac{1}{6}\left(\frac{\partial}{\partial V}\delta(e - V(\boldsymbol{x}))\right)\Delta V(\boldsymbol{x})\right. \\ &\qquad \left. + \frac{s}{12}\left(\frac{\partial^2}{\partial V^2}\delta(e - V(\boldsymbol{x}))\right)(\nabla V(\boldsymbol{x}))^2\right).\end{aligned} \tag{5.95}$$

5.2.4 Semiclassical density $\rho(\boldsymbol{x})$ in $d = 2$ dimensions

The semiclassical density $\rho(\boldsymbol{x})$ is obtained from $\rho(e;\boldsymbol{x})$ by equation (5.38).

We integrate each term of the expansion above separately and obtain

$$\rho(\boldsymbol{x}) = \rho_0(\boldsymbol{x}) + \epsilon^2\rho_1(\boldsymbol{x}) + \mathcal{O}(\epsilon^4), \tag{5.96}$$

where $\rho_0(\boldsymbol{x}) = \frac{1}{N}\int^\mu \mathrm{d}e\rho_0(e;\boldsymbol{x})$, and $\rho_1(\boldsymbol{x}) = \frac{1}{N}\int^\mu \mathrm{d}e\rho_1(e;\boldsymbol{x})$.

Lowest order

The lowest order is easily computed:

$$\rho_0(\boldsymbol{x}) = \frac{s}{4\pi N\epsilon^2}\int^\mu \mathrm{d}e\theta(e - V(\boldsymbol{x})) = \frac{s}{4\pi N\epsilon^2}(\mu - V(\boldsymbol{x}))_+. \tag{5.97}$$

Let's compute the lowest order of the density $\rho(\boldsymbol{x})$ in arbitrary dimension d, which will be necessary for the computation of the lowest order of the exchange energy, which will be done later in this chapter. From equation (5.85), we integrate over e, and divide by N to obtain

$$\rho_0(\boldsymbol{x}) = \frac{sS_d}{(2\pi)^d\epsilon^d N}\int^\mu \mathrm{d}e\,(e - V(\boldsymbol{x}))_+^{\frac{d}{2}-1} = \frac{sS_d}{(2\pi)^d\epsilon^d Nd}\,(\mu - V(\boldsymbol{x}))_+^{\frac{d}{2}}. \tag{5.98}$$

Unsurprisingly, we find the same result as in equation (2.159), except the normalization to 1 instead of N.

First order

Using the equalities $\frac{\partial}{\partial V}\delta(e-V(\boldsymbol{x})) = -\frac{\partial}{\partial e}\delta(e-V(\boldsymbol{x}))$ and $\delta(e-V(\boldsymbol{x})) = \frac{\partial}{\partial e}\theta(e-V(\boldsymbol{x}))$, the first order correction is

$$\begin{aligned}
\rho_1(\boldsymbol{x}) &= \frac{s}{4\pi N\epsilon^2}\int^{\mu} \mathrm{d}e\Bigg(\frac{1}{6}\left(\frac{\partial}{\partial V}\delta(e-V(\boldsymbol{x}))\right)\Delta V(\boldsymbol{x}) \\
&\qquad +\frac{1}{12}\left(\frac{\partial^2}{\partial V^2}\delta(e-V(\boldsymbol{x}))\right)\left(\nabla V(\boldsymbol{x})\right)^2\Bigg) \\
&= \frac{s}{4\pi N\epsilon^2}\int^{\mu} \mathrm{d}e\Bigg(-\frac{1}{6}\left(\frac{\partial}{\partial e}\delta(e-V(\boldsymbol{x}))\right)\Delta V(\boldsymbol{x}) \\
&\qquad +\frac{1}{12}\frac{\partial^2}{\partial e^2}\delta(e-V(\boldsymbol{x}))\left(\nabla V(\boldsymbol{x})\right)^2\Bigg) \\
&= \frac{s}{4\pi N\epsilon^2}\left(-\frac{1}{6}\delta(\mu-V(\boldsymbol{x}))\Delta V(\boldsymbol{x}) + \frac{1}{12}\frac{\partial}{\partial\mu}\delta(\mu-V(\boldsymbol{x}))\left(\nabla V(\boldsymbol{x})\right)^2\right) \\
&= \frac{s}{4\pi N\epsilon^2}\frac{\partial}{\partial\mu}\left(-\frac{1}{6}\theta(\mu-V(\boldsymbol{x}))\Delta V(\boldsymbol{x}) + \frac{1}{12}\delta(\mu-V(\boldsymbol{x}))\left(\nabla V(\boldsymbol{x})\right)^2\right).
\end{aligned} \tag{5.99}$$

Keeping in mind that we will perform the integration over $\boldsymbol{x}$ in order to obtain the integrated density of states, let's rewrite the second part of this expression:

$$\begin{aligned}
\frac{\partial}{\partial\mu}\delta(\mu-V(\boldsymbol{x}))\left(\nabla V(\boldsymbol{x})\right)^2 &= -\frac{\partial}{\partial\mu}\frac{\partial}{\partial V}\left(\theta(\mu-V(\boldsymbol{x}))\right)\nabla V(\boldsymbol{x})\cdot\nabla V(\boldsymbol{x}) \\
&= -\frac{\partial}{\partial\mu}\nabla\theta(\mu-V(\boldsymbol{x}))\cdot\nabla V(\boldsymbol{x}) \\
&= -\frac{\partial}{\partial\mu}\Big\{\mathrm{div}\left(\theta(\mu-V(\boldsymbol{x}))\nabla V(\boldsymbol{x})\right) \\
&\qquad -\theta(\mu-V(\boldsymbol{x}))\Delta V(\boldsymbol{x})\Big\}.
\end{aligned} \tag{5.100}$$

where we used the identity $\nabla f\cdot\nabla g = \mathrm{div}(f\nabla g) - f\Delta g$.

The first correction to the density becomes

$$\begin{aligned}
\rho_1(\boldsymbol{x}) &= \frac{s}{4\pi N\epsilon^2}\frac{\partial}{\partial\mu}\Bigg(-\frac{1}{6}\theta(\mu-V(\boldsymbol{x}))\Delta V(\boldsymbol{x}) \\
&\qquad -\frac{1}{12}\left\{\mathrm{div}\left(\theta(\mu-V(\boldsymbol{x}))\nabla V(\boldsymbol{x})\right) - \theta(\mu-V(\boldsymbol{x}))\Delta V(\boldsymbol{x})\right\}\Bigg) \\
&= -\frac{s}{48\pi N\epsilon^2}\frac{\partial}{\partial\mu}\left\{\theta(\mu-V(\boldsymbol{x}))\Delta V(\boldsymbol{x}) + \mathrm{div}\left(\theta(\mu-V(\boldsymbol{x}))\nabla V(\boldsymbol{x})\right)\right\}.
\end{aligned} \tag{5.101}$$

Final expression

The final expression for the density is

$$\rho(\boldsymbol{x}) = \rho_0(\boldsymbol{x}) + \epsilon^2 \rho_1(\boldsymbol{x}) + \mathcal{O}(\epsilon^4), \tag{5.102}$$

where

$$\rho_0(\boldsymbol{x}) = \frac{s}{4\pi N \epsilon^2} (\mu - V(\boldsymbol{x}))_+ \tag{5.103}$$

and

$$\rho_1(\boldsymbol{x}) = -\frac{s}{48\pi N \epsilon^2} \frac{\partial}{\partial \mu} \left\{ \theta(\mu - V(\boldsymbol{x})) \Delta V(\boldsymbol{x}) + \operatorname{div}\left(\theta(\mu - V(\boldsymbol{x})) \nabla V(\boldsymbol{x}) \right) \right\}. \tag{5.104}$$

Let's note that μ also depends on ϵ. This dependence and its consequences will be discussed in the part concerning the self-consistent equation.

5.2.5 Semiclassical integrated density of states in $d = 2$ dimensions

From equation (5.41) the integrated density of states is

$$N(e) = N \int \mathrm{d}^2\boldsymbol{x} \rho(\boldsymbol{x}), \tag{5.105}$$

where the μ dependence has become an e dependence. As in the previous cases we integrate each term separately, obtaining an expansion of the integrated density of states in powers of ϵ^2:

$$N(e) = N_0(e) + \epsilon^2 N_1(e) + \mathcal{O}(\epsilon^4), \tag{5.106}$$

where

$$N_0(e) = N \int \mathrm{d}^2\boldsymbol{x} \rho_0(\boldsymbol{x}), \tag{5.107}$$

$$N_1(e) = N \int \mathrm{d}^2\boldsymbol{x} \rho_1(\boldsymbol{x}). \tag{5.108}$$

Lowest order

We find immediately

$$N_0(e) = N \int \mathrm{d}^2\boldsymbol{x} \rho_0(\boldsymbol{x}) = \frac{s}{4\pi\epsilon^2} \int \mathrm{d}^2\boldsymbol{x} (e - V(\boldsymbol{x}))_+. \tag{5.109}$$

First correction

Using the divergence theorem and the boundary conditions we find

$$\begin{aligned}\int_{\mathbb{R}^2} \mathrm{d}^2\boldsymbol{x}\,(\mathrm{div}\,(\theta(e-V(\boldsymbol{x}))\nabla V(\boldsymbol{x}))) &= \int_{\Omega} \mathrm{d}^2\boldsymbol{x}\,(\mathrm{div}\,(\theta(e-V(\boldsymbol{x}))\nabla V(\boldsymbol{x}))) \\ &= \int_{\partial\Omega} \mathrm{d}\sigma\cdot(\theta(e-V(\boldsymbol{x}))\nabla V(\boldsymbol{x})) \\ &= 0, \qquad (5.110)\end{aligned}$$

where $\Omega = \mathbb{R}^3$. We consider the function $\theta(e - V(\boldsymbol{x}))\nabla V(\boldsymbol{x})$ as a distribution, we "smoothen" it, and it becomes zero at infinity.

The first correction is then

$$\begin{aligned}N_1(e) = N\int \mathrm{d}^2\boldsymbol{x}\rho_1(\boldsymbol{x}) &= -\frac{s}{48\pi\epsilon^2}\int \mathrm{d}^2\boldsymbol{x}\frac{\partial}{\partial e}\theta(e-V(\boldsymbol{x}))\Delta V(\boldsymbol{x}) \\ &= -\frac{s}{48\pi\epsilon^2}\int \mathrm{d}^2\boldsymbol{x}\delta(e-V(\boldsymbol{x}))\Delta V(\boldsymbol{x}). \qquad (5.111)\end{aligned}$$

Final expression

The integrated density of states is therefore

$$N(e) = N_0(e) + \epsilon^2 N_1(e) + \mathcal{O}(\epsilon^4), \qquad (5.112)$$

where

$$N_0(e) = \frac{s}{4\pi\epsilon^2}\int \mathrm{d}^2\boldsymbol{x}(e-V(\boldsymbol{x}))_+, \qquad (5.113)$$

and

$$N_1(e) = -\frac{s}{48\pi\epsilon^2}\int \mathrm{d}^2\boldsymbol{x}\delta(e-V(\boldsymbol{x}))\Delta V(\boldsymbol{x}). \qquad (5.114)$$

5.2.6 Semiclassical self-consistent equation

We can now return to the self-consistent equation (5.45) to replace the density $\rho(\boldsymbol{x})$ by its semiclassical expression, which is expressed in terms of the potential V. Before doing this, let's expand V in powers of ϵ^2:

$$V(\boldsymbol{x}) = V_0(\boldsymbol{x}) + \epsilon^2 V_1(\boldsymbol{x}) + \mathcal{O}(\epsilon^4). \qquad (5.115)$$

To write the density $\rho(\boldsymbol{x})$ in powers of ϵ^2 we will also need the chemical potential, which we expand in powers of ϵ^2:

$$\mu = \mu_0 + \epsilon^2\mu_1 + \mathcal{O}(\epsilon^4). \qquad (5.116)$$

It is defined as a function of N by the implicit equation (5.31). To obtain an equation for each term of the expansion (5.116) we use the expansion (5.112) of $N(\mu)$. Let's write the V dependence of $N(\mu)$ as $N^V(\mu)$.

From equation (5.113) we see that N_0 depends on V and μ only by $(\mu - V)$. We write this dependence as $N_0^{(\mu-V)}$. Moreover the dependence of N_0 is such that

$$N_0^{(\mu-V)} = N_0^{(\mu_0-V_0)} + \epsilon^2 N_0^{(\mu_1-V_1)} + \mathcal{O}(\epsilon^4). \tag{5.117}$$

Further computations show that the modification of the integration domain (when $(\mu - V)$ changes from $(\mu_0 - V_0)$ to $(\mu_0 - V_0) + \epsilon^2(\mu_1 - V_1)$) modifies N_0 of an order $\mathcal{O}(\epsilon^4)$.

Hence the function $N(\mu)$ is expanded as follows (returning to the initial notations):

$$N = N(\mu) = N_0^{V_0}(\mu_0) + \epsilon^2 \left(N_0^{V_1}(\mu_1) + N_1^{V_0}(\mu_0)\right) + \mathcal{O}(\epsilon^4). \tag{5.118}$$

The lowest order defines μ_0:

$$N = N_0^{V_0}(\mu_0) \tag{5.119}$$

and the first order defines μ_1, as a function of μ_0:

$$N_0^{V_1}(\mu_1) = -N_1^{V_0}(\mu_0). \tag{5.120}$$

Let's now write the μ and V dependencies of $\rho(\boldsymbol{x})$ as $\rho^{V,\mu}(\boldsymbol{x})$. From (5.103) we see that $\rho_0(\boldsymbol{x})$ depends on V and μ only by $(\mu - V)$, which we write as $\rho_0^{(\mu-V)}(\boldsymbol{x})$. Moreover the dependence of $\rho_0(\boldsymbol{x})$ is such that

$$\rho_0^{(\mu-V)}(\boldsymbol{x}) = \rho_0^{(\mu_0-V_0)}(\boldsymbol{x}) + \epsilon^2 \rho_0^{(\mu_1-V_1)}(\boldsymbol{x}) + \mathcal{O}(\epsilon^4). \tag{5.121}$$

Further computations show that the modification of the integration domain (when $(\mu - V)$ changes from $(\mu_0 - V_0)$ to $(\mu_0 - V_0) + \epsilon^2(\mu_1 - V_1)$) modifies ρ_0 by an order $\mathcal{O}(\epsilon^4)$.

Hence the function ρ is expanded as follows (returning to the initial notations):

$$\rho^{V,\mu}(\boldsymbol{x}) = \rho_0^{V_0,\mu_0}(\boldsymbol{x}) + \epsilon^2 \left(\rho_0^{V_1,\mu_1}(\boldsymbol{x}) + \rho_1^{V_0,\mu_0}(\boldsymbol{x})\right) + \mathcal{O}(\epsilon^4). \tag{5.122}$$

Let's note that the normalization condition is now

$$\int \mathrm{d}^2\boldsymbol{x}\, \rho_0^{V_0,\mu_0}(\boldsymbol{x}) = 1. \tag{5.123}$$

Having extracted the ϵ^2 dependencies of $\rho(\boldsymbol{x})$ we can write the self-consistent equation (5.45):

$$\begin{aligned} &V_0(\boldsymbol{x}) + \epsilon^2 V_1(\boldsymbol{x}) + \mathcal{O}(\epsilon^4) \\ &\quad = V_{ext}(\boldsymbol{x}) + \int \mathrm{d}^2\boldsymbol{y} \frac{\left(\rho_0^{V_0,\mu_0}(\boldsymbol{y}) + \epsilon^2 \left(\rho_0^{V_1,\mu_1}(\boldsymbol{y}) + \rho_1^{V_0,\mu_0}(\boldsymbol{y})\right)\right)}{|\boldsymbol{x} - \boldsymbol{y}|} + \mathcal{O}(\epsilon^4). \end{aligned} \tag{5.124}$$

Hence at lowest order we find

$$V_0(\boldsymbol{x}) = V_{ext}(\boldsymbol{x}) + \int \mathrm{d}^2\boldsymbol{y} \frac{\rho_0^{V_0,\mu_0}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}, \tag{5.125}$$

and at first order

$$V_1(\boldsymbol{x}) = \int \mathrm{d}^2\boldsymbol{y} \frac{\left(\rho_0^{V_1,\mu_1}(\boldsymbol{y}) + \rho_1^{V_0,\mu_0}(\boldsymbol{y})\right)}{|\boldsymbol{x}-\boldsymbol{y}|}. \tag{5.126}$$

Writing $\rho^{V,\mu}$ explicitly using equation (5.102) we find

$$V_0(\boldsymbol{x}) = V_{ext}(\boldsymbol{x}) + \frac{s}{4\pi N\epsilon^2} \int \mathrm{d}^2\boldsymbol{y} \frac{(\mu_0 - V_0(\boldsymbol{y}))_+}{|\boldsymbol{x}-\boldsymbol{y}|} \tag{5.127}$$

and

$$V_1(\boldsymbol{x}) = \frac{s}{4\pi N\epsilon^2} \int \mathrm{d}^2\boldsymbol{y} \frac{\left((\mu_1 - V_1(\boldsymbol{y})) - \frac{1}{12}\delta(\mu_0 - V_0(\boldsymbol{y}))\Delta V_0(\boldsymbol{y})\right)}{|\boldsymbol{x}-\boldsymbol{y}|}. \tag{5.128}$$

5.2.7 Hartree energy

We now have all we need to compute the Hartree energy. It corresponds to the smooth part of the ground state energy of the dot, neglecting (for the moment) the exchange energy. We compute the energy E_0, given by equation (5.44).

As for the previous quantities we expand the energy in powers of ϵ^2:

$$E_0 = E_{00} + \epsilon^2 E_{01} + \mathcal{O}(\epsilon^4). \tag{5.129}$$

To do this we have to extract the ϵ^2 dependence of $\int^\mu \mathrm{d}eN(e)$. Looking explicitly at the expansion of $N(e)$ in (5.112), we write:

$$\begin{aligned}
\int^\mu \mathrm{d}eN(e) &= \int^\mu \mathrm{d}e(N_0^V(e) + \epsilon^2 N_1^V(e)) + \mathcal{O}(\epsilon^4) \\
&= \frac{1}{2}\frac{s}{4\pi\epsilon^2}\int \mathrm{d}^2\boldsymbol{x}\,(\mu - V(\boldsymbol{x}))_+^2 + \epsilon^2 \int^\mu \mathrm{d}eN_1^V(e) + \mathcal{O}(\epsilon^4) \\
&= \frac{1}{2}\frac{s}{4\pi\epsilon^2}\int \mathrm{d}^2\boldsymbol{x}\left(\mu_0 - V_0(\boldsymbol{x}) + \epsilon^2\left(\mu_1 - V_1(\boldsymbol{x})\right) + \mathcal{O}(\epsilon^4)\right)_+^2 \\
&\qquad + \epsilon^2 \int^\mu \mathrm{d}eN_1^{V_0}(e) + \mathcal{O}(\epsilon^4)
\end{aligned}$$

$$\begin{aligned} &= \frac{1}{2}\frac{s}{4\pi\epsilon^2}\int \mathrm{d}^2\boldsymbol{x}\left(\mu_0 - V_0(\boldsymbol{x})\right)_+^2 \\ &\qquad +\epsilon^2\left(\frac{s}{4\pi\epsilon^2}\int \mathrm{d}^2\boldsymbol{x}\left(\mu_0 - V_0(\boldsymbol{x})\right)_+\left(\mu_1 - V_1(\boldsymbol{x})\right)_+ \right. \\ &\qquad\qquad \left. + \int^{\mu_0} \mathrm{d}eN_1^{V_0}(e)\right) + \mathcal{O}(\epsilon^4) \\ &= \int^{\mu_0} \mathrm{d}eN_0^{V_0}(e) + \epsilon^2\left(\frac{s}{4\pi\epsilon^2}\int \mathrm{d}^2\boldsymbol{x}\left(\mu_0 - V_0(\boldsymbol{x})\right)_+\left(\mu_1 - V_1(\boldsymbol{x})\right)_+ \right. \\ &\qquad\qquad \left. + \int^{\mu_0} \mathrm{d}eN_1^{V_0}(e)\right) + \mathcal{O}(\epsilon^4). \end{aligned} \tag{5.130}$$

We have

$$E_{00} = \mu_0 - \frac{1}{N}\int^{\mu_0} \mathrm{d}eN_0^{V_0}(e) - \frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{y}\frac{\rho_0^{V_0,\mu_0}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}, \tag{5.131}$$

and

$$\begin{aligned} E_{01} &= \mu_1 - \frac{s}{4\pi\epsilon^2 N}\int \mathrm{d}^2\boldsymbol{x}\left(\mu_0 - V_0(\boldsymbol{x})\right)_+\left(\mu_1 - V_1(\boldsymbol{x})\right)_+ - \frac{1}{N}\int^{\mu_0} \mathrm{d}eN_1^{V_0}(e) \\ &\quad - \int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{y}\frac{\rho_0^{V_0,\mu_0}(\boldsymbol{x})\left(\rho_0^{V_1,\mu_1}(\boldsymbol{y}) + \rho_1^{V_0,\mu_0}(\boldsymbol{y})\right)}{|\boldsymbol{x}-\boldsymbol{y}|}. \end{aligned} \tag{5.132}$$

Lowest order

We want to compute

$$E_{00} = \mu_0 - \frac{1}{N}\int^{\mu_0} \mathrm{d}eN_0^{V_0}(e) - \frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{y}\frac{\rho_0^{V_0,\mu_0}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}. \tag{5.133}$$

Returning to the definition (5.113) of N_0 and the relation (5.103) between V_0 and $\rho_0^{V_0,\mu_0}$ we establish

$$\begin{aligned} \frac{1}{N}\int^{\mu_0} \mathrm{d}eN_0^{V_0}(e) &= \frac{s}{4\pi\epsilon^2 N}\int^{\mu_0} \mathrm{d}e\int \mathrm{d}^2\boldsymbol{x}\left(e - V_0(\boldsymbol{x})\right)_+ \\ &= \frac{1}{2}\frac{s}{4\pi\epsilon^2 N}\int \mathrm{d}^2\boldsymbol{x}\left(\mu_0 - V_0(\boldsymbol{x})\right)_+^2 \\ &= \frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\rho_0^{V_0,\mu_0}(\boldsymbol{x})\left(\mu_0 - V_0(\boldsymbol{x})\right)_+. \end{aligned} \tag{5.134}$$

Using the equality (5.125) we can write

$$\frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{y}\frac{\rho_0^{V_0,\mu_0}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|} = \frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\rho_0^{V_0,\mu_0}(\boldsymbol{x})\left(V_0(\boldsymbol{x}) - V_{ext}(\boldsymbol{x})\right). \tag{5.135}$$

Introducing (5.134) and (5.135) in (5.133), and using the normalization $\int \mathrm{d}^2\boldsymbol{x}\rho_0^{V_0,\mu_0}(\boldsymbol{x}) = 1$, we find

$$E_{00} = \frac{1}{2}\left(\mu_0 + \int \mathrm{d}^2\boldsymbol{x} V_{ext}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{x})\right). \tag{5.136}$$

First order

Let's compute

$$\begin{aligned} E_{01} &= \mu_1 - \frac{s}{4\pi\epsilon^2 N}\int \mathrm{d}^2\boldsymbol{x}\,(\mu_0 - V_0(\boldsymbol{x}))_+ (\mu_1 - V_1(\boldsymbol{x}))_+ - \frac{1}{N}\int^{\mu_0} \mathrm{d}e N_1^{V_0}(e) \\ &\quad - \int \mathrm{d}^2\boldsymbol{x} \int \mathrm{d}^2\boldsymbol{y} \frac{\rho_0^{V_0,\mu_0}(\boldsymbol{x})\left(\rho_0^{V_1,\mu_1}(\boldsymbol{y}) + \rho_1^{V_0,\mu_0}(\boldsymbol{y})\right)}{|\boldsymbol{x}-\boldsymbol{y}|}. \end{aligned} \tag{5.137}$$

From (5.113) and (5.103) we have

$$-\frac{s}{4\pi\epsilon^2 N}\int \mathrm{d}^2\boldsymbol{x}\,(\mu_0 - V_0(\boldsymbol{x}))_+ (\mu_1 - V_1(\boldsymbol{x}))_+ = -\int \mathrm{d}^2\boldsymbol{x}\rho_0^{V_0,\mu_0}(\mu_1 - V_1(\boldsymbol{x}))_+ . \tag{5.138}$$

From (5.114) we have

$$\begin{aligned} -\frac{1}{N}\int^{\mu_0} \mathrm{d}e N_1^{V_0}(e) &= \frac{s}{48\pi\epsilon^2 N}\int^{\mu_0} \mathrm{d}e \int \mathrm{d}^2\boldsymbol{x}\delta(e - V_0(\boldsymbol{x}))\Delta V_0(\boldsymbol{x}) \\ &= \frac{s}{48\pi\epsilon^2 N}\int \mathrm{d}^2\boldsymbol{x}\Delta V_0(\boldsymbol{x})\theta(\mu_0 - V_0(\boldsymbol{x})). \end{aligned} \tag{5.139}$$

Using equation (5.126) and the normalization $\int \mathrm{d}^2\boldsymbol{x}\rho_0^{V_0,\mu_0}(\boldsymbol{x}) = 1$ we obtain

$$\begin{aligned} \mu_1 - \int \mathrm{d}^2\boldsymbol{x} \int \mathrm{d}^2\boldsymbol{y} \frac{\rho_0^{V_0,\mu_0}(\boldsymbol{x})\left(\rho_0^{V_1,\mu_1}(\boldsymbol{y}) + \rho_1^{V_0,\mu_0}(\boldsymbol{y})\right)}{|\boldsymbol{x}-\boldsymbol{y}|} \\ = \int \mathrm{d}^2\boldsymbol{x}\rho_0^{V_0,\mu_0}(\boldsymbol{x})(\mu_1 - V_1(\boldsymbol{x})). \end{aligned} \tag{5.140}$$

This term is exactly cancelled by the term (5.138). The first order term is finally

$$E_{01} = \frac{s}{48\pi\epsilon^2 N}\int \mathrm{d}^2\boldsymbol{x}\Delta V_0(\boldsymbol{x})\theta(\mu_0 - V_0(\boldsymbol{x})). \tag{5.141}$$

Final expression

Returning to the energy $\hat{E}_0$ defined by equation (5.43), we find

$$\hat{E}_0 = \hat{E}_{00} + \epsilon^2\hat{E}_{01} + \mathcal{O}(\epsilon^4), \tag{5.142}$$

where

$$\hat{E}_{00} = \frac{N^2}{L_\star}\frac{1}{2}\left(\mu_0 + \int \mathrm{d}^2\boldsymbol{x} V_{ext}(\boldsymbol{x})\rho_0(\boldsymbol{x})\right), \tag{5.143}$$

and

$$\begin{aligned}\hat{E}_{01} &= \frac{N^2}{L_\star}\frac{s}{48\pi\epsilon^2 N}\int \mathrm{d}^2\boldsymbol{x}\Delta V_0(\boldsymbol{x})\theta(\mu_0 - V_0(\boldsymbol{x})) \\ &= \frac{N^2}{12\pi}\int \mathrm{d}^2\boldsymbol{x}\Delta V_0(\boldsymbol{x})\theta(\mu_0 - V_0(\boldsymbol{x})),\end{aligned} \tag{5.144}$$

where we used the definition (5.46) of ϵ^2, as well as the numerical value of $s = 2$.

The first term is of the order of $\mathcal{O}(\frac{N^2}{L_\star})$, and the second is $\mathcal{O}(\frac{N}{L_\star})$.

Let's add some comments about this result. Concerning technical aspects, it is very important to notice that this result depends on V_0 only, and not on V_1. It remarkably simplifies the calculation of this energy: the self-consistent equation has to be solved at lowest order only, that is with equation (5.127). We will not have to solve equation (5.128). In our computations, this is due to the fact that two terms (whose origin is different) cancel out.

Let's come back to the quantum dot with a homogeneous external potential of degree p. The length $L_\star$ is given by (5.50), which means that the first term is of order $\mathcal{O}(N^{\frac{2p+1}{p+1}})$ and the second $\mathcal{O}(N^{\frac{p}{p+1}})$.

In the particular case of the parabolic external potential ($p = 2$) the first term is of the order of $\mathcal{O}(N^{\frac{5}{3}})$, the second $\mathcal{O}(N^{\frac{2}{3}})$.

In the case where the confinement strength depends on N ($k = \frac{k'}{N^{\frac{1}{2}}}$), the first term is of the order of $\mathcal{O}(N^{\frac{3}{2}})$, the second $\mathcal{O}(N^{\frac{1}{2}})$.

Equivalence with Thomas-Fermi energy

The ground state energy of quantum dots, for a number of electrons tending to infinity, is the Thomas-Fermi energy, as shown in (Lieb et al., 1995). It is, in $d = 2$ dimensions,

$$E^{TF} = \frac{\pi}{2}\int \mathrm{d}^2\boldsymbol{x}\rho^2(\boldsymbol{x}) + \int \mathrm{d}^2\boldsymbol{x} V_{ext}(\boldsymbol{x})\rho(\boldsymbol{x}) + \frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{y}\frac{\rho(\boldsymbol{x})\rho(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}, \tag{5.145}$$

where ρ is solution to the extremization equation:

$$V(\boldsymbol{x}) = V_{ext}(\boldsymbol{x}) + \int \mathrm{d}^2\boldsymbol{y}\frac{\rho(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}, \qquad \rho(\boldsymbol{x}) = \frac{L_\star}{\pi}(\mu - V(\boldsymbol{x})). \tag{5.146}$$

This self-consistent equation is exactly the same as (5.125), with the semiclassical density (5.103).

Let's show that the lowest order of the Hartree energy we computed at (5.142) is the Thomas-Fermi energy. Starting from expression (5.143) using the self-consistent equation (5.125), the semiclassical density (5.103) and the normalization condition $\int \mathrm{d}^2\boldsymbol{x}\rho_0^{V_0,\mu_0}(\boldsymbol{x}) = 1$, we find (without noting N and $L_\star$):

$$
\begin{aligned}
&\frac{1}{2}\left(\mu_0 + \int \mathrm{d}^2\boldsymbol{x} V_{ext}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{x})\right)\\
&\qquad = \frac{1}{2}\left(\mu_0 - \int \mathrm{d}^2\boldsymbol{x} V_{ext}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{x})\right) + \int \mathrm{d}^2\boldsymbol{x} V_{ext}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{x})\\
&\qquad = \frac{\mu_0}{2} - \frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\left(V_0(\boldsymbol{x}) - \int \mathrm{d}^2\boldsymbol{y}\frac{\rho_0^{V_0,\mu_0}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\right)\rho_0^{V_0,\mu_0}(\boldsymbol{x})\\
&\qquad\qquad + \int \mathrm{d}^2\boldsymbol{x} V_{ext}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{x})\\
&\qquad = \frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\left(\mu_0 - V_0(\boldsymbol{x})\right)\rho_0^{V_0,\mu_0}(\boldsymbol{x}) + \int \mathrm{d}^2\boldsymbol{x} V_{ext}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{x})\\
&\qquad\qquad + \frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{y}\frac{\rho_0^{V_0,\mu_0}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\\
&\qquad = \frac{\pi}{2}\frac{1}{L_\star}\int \mathrm{d}^2\boldsymbol{x}\left(\rho_0^{V_0,\mu_0}(\boldsymbol{x})\right)^2 + \int \mathrm{d}^2\boldsymbol{x} V_{ext}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{x})\\
&\qquad\qquad + \frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{y}\frac{\rho_0^{V_0,\mu_0}(\boldsymbol{x})\rho_0^{V_0,\mu_0}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}.
\end{aligned}
\tag{5.147}
$$

The first term is the kinetic energy, the second one is the confinement energy, the last one is the electron-electron interaction. This result shows that for an harmonic external potential, when $L_\star \simeq N^{\frac{1}{3}}$, the kinetic energy is of the order of $N^{\frac{4}{3}}$, while the other terms are of the order of $N^{\frac{5}{3}}$. If the confinement strength is $k = \frac{k'}{N^{\frac{1}{2}}}$, $L_\star \simeq N^{\frac{1}{2}}$, and the kinetic energy is of the order of N, while the other terms are of the order of $N^{\frac{3}{2}}$.

5.2.8 Exchange energy

The exchange energy, computed from the density matrix, in any dimension d, is given by equation (5.44). It is

$$
E_0^{ex} = -\frac{1}{2}\int \mathrm{d}^d\boldsymbol{x}\int \mathrm{d}^d\boldsymbol{y}\frac{\rho_0^2(\boldsymbol{x},\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}. \tag{5.148}
$$

In fact, in view of the density defined in equation (5.33), where the spin degeneracy was already taken into account, we have to modify this formula. The correct formula is derived as follows. Introducing the spin, the exchange energy is

$$
-\frac{1}{2}\sum_{\alpha,\beta}\int \mathrm{d}^d\boldsymbol{x}\int \mathrm{d}^d\boldsymbol{y}\sum_{\sigma,\sigma'}\frac{\psi_\alpha^\star(\boldsymbol{x},\sigma)\psi_\beta^\star(\boldsymbol{y},\sigma')\psi_\beta(\boldsymbol{x},\sigma)\psi_\alpha(\boldsymbol{y},\sigma')}{|\boldsymbol{x}-\boldsymbol{y}|}. \tag{5.149}
$$

The wave function is characterized by two numbers, $\alpha = (i, \mu)$, where μ is the spin index, which takes s values. The wave function is

$$\psi_\alpha(\boldsymbol{x}, \sigma) = \psi_i(\boldsymbol{x})\delta_{\mu,\sigma}. \tag{5.150}$$

Introducing this function in the exchange energy, we obtain

$$\begin{aligned}
-\frac{1}{2}\sum_{i,j}\int \mathrm{d}^d\boldsymbol{x}\int \mathrm{d}^d\boldsymbol{y}\frac{\psi_i^\star(\boldsymbol{x})\psi_j^\star(\boldsymbol{y})\psi_j(\boldsymbol{x})\psi_i(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}&\underbrace{\sum_{\mu,\nu}\sum_{\sigma,\sigma'}\delta_{\mu,\sigma}\delta_{\nu,\sigma'}\delta_{\nu,\sigma}\delta_{\mu,\sigma'}}_{=s} \\
&= -\frac{1}{2s}\int \mathrm{d}^d\boldsymbol{x}\int \mathrm{d}^d\boldsymbol{y}\frac{\rho_0^2(\boldsymbol{x},\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|},
\end{aligned} \tag{5.151}$$

where we introduced the density (5.33).

Using the result (5.79) and performing the change of variables $\boldsymbol{y} \mapsto \boldsymbol{r}$ such that $\boldsymbol{y} = \boldsymbol{x} + \epsilon\boldsymbol{r}$:

$$\begin{aligned}
E_0^{ex} &= -\frac{1}{2s}\int \mathrm{d}^d\boldsymbol{x}\int \mathrm{d}^d\boldsymbol{y}\frac{\rho_0^2(\boldsymbol{x},\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|} \\
&= -\frac{1}{2}\frac{s}{(2\pi)^d}\frac{1}{N^2\epsilon^{d+1}}\int \mathrm{d}^d\boldsymbol{x}\int \mathrm{d}^d\boldsymbol{r}\frac{\left(\sqrt{\mu - V(\boldsymbol{x})}\right)^d J_{\frac{d}{2}}^2\left(r\sqrt{\mu - V(\boldsymbol{x})}\right)}{r^{d+1}} \\
&= -\frac{1}{2}\frac{s}{(2\pi)^d}\frac{1}{N^2\epsilon^{d+1}}S_d\int \mathrm{d}^d\boldsymbol{x}\int_0^\infty \mathrm{d}r\frac{\left(\sqrt{\mu - V(\boldsymbol{x})}\right)^d J_{\frac{d}{2}}^2\left(r\sqrt{\mu - V(\boldsymbol{x})}\right)}{r^2} \\
&= -\frac{1}{2}\frac{s}{(2\pi)^d}\frac{1}{N^2\epsilon^{d+1}}S_d\int \mathrm{d}^d\boldsymbol{x}\left(\sqrt{\mu - V(\boldsymbol{x})}\right)^{d+1}\underbrace{\int_0^\infty \mathrm{d}y\frac{J_{\frac{d}{2}}^2(y)}{y^2}}_{=\frac{1}{\pi}\frac{4}{(d^2-1)}} \\
&= -\frac{1}{2}\frac{s}{(2\pi)^d}\frac{1}{N^2\epsilon^{d+1}}S_d\frac{1}{\pi}\frac{4}{(d^2-1)}\int \mathrm{d}^d\boldsymbol{x}\left(\sqrt{\mu - V(\boldsymbol{x})}\right)_+^{d+1}
\end{aligned} \tag{5.152}$$

where we integrated over the angular part of $\boldsymbol{r}$, and performed the change of variable $r \mapsto y = r\sqrt{\mu - V(\boldsymbol{x})}$.

To extract the N dependence of this energy, let's express the lowest order of this exchange energy in term of the density (which allows a better control of the N dependence, because we know that ρ is of the order of $\mathcal{O}(1)$, by construction). Using equality (5.98) for arbitrary dimension d, the exchange energy becomes, after computation

$$E_0^{ex} = -N^{(\frac{1}{d}-1)}\frac{4s^{-\frac{1}{d}}d^{(1+\frac{1}{d})}}{S_d^{\frac{1}{d}}(d^2-1)}\int \mathrm{d}^d\boldsymbol{x}\rho_0^{(1+\frac{1}{d})}(\boldsymbol{x}), \tag{5.153}$$

The exchange energy of the initial problem $\hat{E}_0^{ex}$ is then

$$\hat{E}_0^{ex} = -\frac{N^{1+\frac{1}{d}}}{L_\star}\frac{4s^{-\frac{1}{d}}d^{(1+\frac{1}{d})}}{S_d^{\frac{1}{d}}(d^2-1)}\int \mathrm{d}^d\boldsymbol{x}\rho_0^{(1+\frac{1}{d})}(\boldsymbol{x}). \tag{5.154}$$

Let's explicitly compute the numerical constant for the two and three dimensional cases. We find

$$d=2 \quad : \quad \hat{E}_0^{ex} = -\frac{N^{\frac{3}{2}}}{L_\star}\frac{2^3}{3\pi^{\frac{1}{2}}s^{\frac{1}{2}}}\int \mathrm{d}^2\boldsymbol{x}\rho_0^{\frac{3}{2}}(\boldsymbol{x}) \tag{5.155}$$

$$d=3 \quad : \quad \hat{E}_0^{ex} = -\frac{N^{\frac{4}{3}}}{L_\star}\frac{3^{\frac{4}{3}}}{2^{\frac{5}{3}}\pi^{\frac{1}{3}}s^{\frac{1}{3}}}\int \mathrm{d}^3\boldsymbol{x}\rho_0^{\frac{4}{3}}(\boldsymbol{x}). \tag{5.156}$$

For the two-dimensional case, the exchange energy is of the order of $N^{\frac{3}{2}}$, which is less than for the direct energy, which is of the order of N^2. This implies that the fact of neglecting the exchange term in the self-consistent equation (5.28) is justified *a posteriori*. Taking this term into account would lead to corrections of higher order than those in which we are interested.

Let's now discuss the case of the homogeneous potential of degree s with strength k, for which the length scale is $L_\star \simeq \left(\frac{N}{k}\right)^{\frac{1}{s+1}}$. For the d dimensional case the N dependence of the exchange energy is $E_0^{ex} \simeq N^{\frac{1}{d}+\frac{s}{(s+1)}}$.

In particular the case of the quantum dot ($d = 2$) with harmonic potential ($s = 2$) provides $E_0^{ex} \simeq N^{\frac{7}{6}}$, which less than the direct energy (which is of the order of $\mathcal{O}(N^{\frac{5}{3}})$). In the case where the confinement strength is $k = \frac{k'}{N^{\frac{1}{2}}}$, the length scale is $L_\star \simeq N^{\frac{1}{2}}$, and the exchange energy is therefore of the order of $\mathcal{O}(N)$.

In the case of the atom, the typical length scale is of the order $L_\star \simeq N^{-\frac{1}{3}}$, as was established with scalings in chapter 2. The exchange energy is therefore of the order $N^{\frac{5}{3}}$, which is exactly what other authors, for example Englert (1988), find. To confirm our result, we see that the numerical constant is correct, as compared to Englert's results.

Chapter 6

Semiclassical energy of a two-dimensional system

Contents

The objective of this chapter is to obtain the semiclassical energy of a two-dimensional system of independent particles, submitted to a monotonous growing potential with radial symmetry. We are especially interested in the lowest order energy oscillations.

In chapter 5 we obtained the ground state energy of the Hartree-Fock approach. It is given by a functional of the self-consistent potential. However, with this procedure we lose some information: as can be established with a careful analysis of our approximations, the resolution of the energy is of the order of $\hbar = \epsilon$. This implies that we lose information on the details of the energy. Is this loss important? Actually the effects we miss are weak, but they present a great interest, because they are oscillating terms, which can be related to the stability of these systems of fermions. Moreover with these oscillations we can distinguish integrable from chaotic systems, the oscillations being more important in the first case. A detailed study of energy oscillations in both chaotic and integrable systems can be found in (Brack and Bhaduri, 1997).

These reasons lead us to adopt another, more systematic approach, within the semiclassical framework: we consider a two-dimensional system of N independent particles, submitted to a monotonous growing potential V with radial symmetry, and compute the ground state energy, which is the sum of the N first eigenvalues. This general formula will be used by replacing this potential by the self-consistent potential at the end (done in chapter 8, the self-consistent potential being itself computed by solving the self-consistent equation in chapter 7). Moreover, the smooth part we obtain with this approach allows the verification of the results obtained in chapter 5.

In this chapter we start by using the radial symmetry to write the problem in the action-angle variables, before proceeding to a WKB quantization of the actions. We proceed beyond this quantization, using the work of Feffermann and Seco (1992). Having obtained this quantization, we compute the integrated density of states using the Poisson sum formula, and from this, the ground state energy of this system of independent fermions. The energy consists of a smooth contribution (which can be related to the results obtained in chapter 5), and oscillating terms, which are related to the classical dynamics of a particle in the potential. These expressions are functionals of the potential.

In all the developments, we write ϵ instead of $\hbar$, as the small parameter is obtained after a scaling, and does not have the physical meaning of $\hbar$.

6.1 Computation of the integrated density of states

6.1.1 Quantization condition

WKB quantization

Let's consider a two-dimensional system of independent particles in an isotropic monotonous growing potential V. Such a system is classically integrable. We can therefore proceed to the well-known semiclassical quantization.

The classical one particle hamiltonian of the system is

$$H(\boldsymbol{p},\boldsymbol{q}) = \boldsymbol{p}^2 + V(|\boldsymbol{q}|). \tag{6.1}$$

A canonical transformation $(\boldsymbol{p},\boldsymbol{q}) \mapsto (\boldsymbol{\phi},\boldsymbol{I})$ leads to the angle-action variables and the hamiltonian takes the form

$$H(\boldsymbol{p}(\boldsymbol{\phi},\boldsymbol{I}),\boldsymbol{q}(\boldsymbol{\phi},\boldsymbol{I})) = H(\boldsymbol{I}), \tag{6.2}$$

where $H(\boldsymbol{I}) = e$ is defined by

$$I_1 = \frac{1}{\pi}\int_{r_1(e,I_2)}^{r_2(e,I_2)} \mathrm{d}r \sqrt{e - V(r) - \frac{I_2^2}{r^2}} \doteq s_0(e,I_2), \tag{6.3}$$

where r_1, r_2 are the classically turning points.

The equations of motion are given by

$$\left\{\begin{array}{lllll} \dot{\phi}_i & = & \frac{\partial}{\partial I_i}H(\boldsymbol{I}) = \omega_i(\boldsymbol{I}) & \Rightarrow & \phi_i(t) = \omega_i t + \phi_i(0), \quad i = 1,2 \\ \dot{I}_i & = & -\frac{\partial}{\partial \phi_i}H(\boldsymbol{I}) = 0 & \Rightarrow & I_i(t) = cst, \quad i = 1,2. \end{array}\right.$$

The motion is developing on a torus in phase space, the variables $\boldsymbol{I}$ being constants of the motion. ω_1 and ω_2 are the frequencies. If $\frac{\omega_2}{\omega_1}$ is rational, the motion is periodic.

The semiclassical quantization, justified by the WKB approximation (at lowest order in ϵ), is in our case

$$\left\{\begin{array}{lll} I_1 & \mapsto \epsilon(n+\frac{1}{2}), & n \in \mathbb{N}, \\ I_2 & \mapsto \epsilon m, & m \in \mathbb{Z}. \end{array}\right.$$

The semiclassically quantized energy levels are therefore defined by

$$e_{n,m} \doteq H(\epsilon(n+\frac{1}{2}), \epsilon m). \tag{6.4}$$

The term $\frac{1}{2}$ appears for the radial quantum number. For the angular quantum number, there is no correction term, conversely to the three-dimensional case, where the Langer correction appears.

Beyond WKB

The approach we presented is the intuitive semiclassical approach and is called WKB quantization (and more generally, for an arbitrary number of degrees of freedom, EBK quantization). This quantization corresponds to the lowest order of an expansion for ϵ small, where the general quantization formula is written as

$$\epsilon(n+\frac{1}{2}) = s(e,\epsilon m) = s_0(e,\epsilon m) + \epsilon^2 s_1(e,\epsilon m) + \mathcal{O}(\epsilon^4). \tag{6.5}$$

Let's note that the quantization of the angular momentum is exact, not just semiclassical.

To obtain this quantization condition, there is an approach which provides WKB at lowest order. It was developed by Dunham (1932) and Bender et al. (1977) for a one-dimensional problem, and an explicit formal formula on the real axis is given by Robnik and Salasnich (1997). In this approach, the wave function is written as $\psi(x) = \exp\left\{\frac{i}{\epsilon}\sum_{i=0}^{\infty}\epsilon^i\sigma_i(x)\right\}$. We consider analytic continuity $x \in \mathbb{C}$. The n^{th} eigenfunction of the operator H is such that the real axis has n zeroes x_i ($\psi_n(x_i) = 0$). Hence by considering a contour around these zeroes in the complex plane, the residue theorem provides the quantization. It yields recursion relations on the functions σ_i. For a one-dimensional system, it provides the following formal quantization condition:

$$\begin{aligned}\epsilon\left(n+\frac{1}{2}\right) &= \frac{1}{\pi}\int \mathrm{d}r\,(e-V(r))^{\frac{1}{2}} - \frac{\epsilon^2}{32\pi}\int \mathrm{d}r\left(\frac{\partial V(r)}{\partial r}\right)^2 (e-V(r))^{-\frac{5}{2}} + \mathcal{O}(\epsilon^4)\\ &= \frac{1}{\pi}\int \mathrm{d}r\,(e-V(r))^{\frac{1}{2}} + \frac{\epsilon^2}{48\pi}\int \mathrm{d}r\left(\frac{\partial^2 V(r)}{\partial r^2}\right)(e-V(r))^{-\frac{3}{2}} + \mathcal{O}(\epsilon^4),\end{aligned} \tag{6.6}$$

where we proceeded to a formal integration by parts. The integration is performed between the classical turning points r_1 and r_2. From now on it will be the case if not otherwise specified.

This quantization is formal: the second term of the right hand side of equation (6.6) is divergent. An exact formula was given by Feffermann and Seco (1992), who simply remove the divergent term. The quantization is given by the following theorem:

$$\epsilon(n+\frac{1}{2}) = \phi(e_n) + \epsilon^2\psi(e_n) + o(\epsilon^2), \tag{6.7}$$

where

$$\phi(e) \doteq \frac{1}{\pi}\int_{r_1}^{r_2} \mathrm{d}r\,(e-V(r))^{\frac{1}{2}} \tag{6.8}$$

is the usual WKB quantization, and

$$\psi(e) \doteq \frac{1}{48\pi}\lim_{\delta\to 0_+}\left[\int\limits_{e-V>\delta} \mathrm{d}r V''(r)\,(e-V(r))^{-\frac{3}{2}} - q(e)\delta^{-\frac{1}{2}}\right], \tag{6.9}$$

where

$$q(e) \doteq \frac{2V''(r_2(e))}{V'(r_2(e))} - \frac{2V''(r_1(e))}{V'(r_1(e))}. \tag{6.10}$$

This correction is

$$\psi(e) = -\frac{2}{48\pi} \lim_{\delta\to 0_+} \frac{\partial}{\partial e} \int\limits_{e-V>\delta} \mathrm{d}r V''(r)\left(e - V(r)\right)^{-\frac{1}{2}}. \tag{6.11}$$

To establish this result, let's compute the derivative of the integral above (where the integration limits are the turning points $r_i,\ i = 1,2$):

$$\begin{aligned}\frac{\partial}{\partial e}\int_{r_1(e-\delta)}^{r_2(e-\delta)} \mathrm{d}r V''\left(e-V\right)^{-\frac{1}{2}} &= r_{2e}(e-\delta)\frac{V''(r_2(e-\delta))}{\left(e - V(r_2(e-\delta))\right)^{\frac{1}{2}}}\\ &\quad - r_{1e}(e-\delta)\frac{V''(r_1(e-\delta))}{\left(e - V(r_1(e-\delta))\right)^{\frac{1}{2}}}\\ &\quad -\frac{1}{2}\int\limits_{e-V>\delta}\mathrm{d}r\frac{V''(r)}{\left(e-V(r)\right)^{\frac{3}{2}}},\end{aligned} \tag{6.12}$$

where $r_{ie},\ i = 1,2$, is the derivative of r_i with respect to e. $r_i(e)$ is defined by $e - V(r_i) = 0$, that is $r_i(e) = V^{-1}(e)$, therefore, $r_{ie}(e) = \frac{1}{V'(r_i(e))}$. Introducing it into equation (6.12), and using the definition of r_i (which is $e - V(r_i(e-\delta)) = \delta$), we find (working with $\delta \ll 1$)

$$\begin{aligned}\frac{\partial}{\partial e}\int_{r_1(e-\delta)}^{r_2(e-\delta)} \mathrm{d}r V''\left(e-V\right)^{-\frac{1}{2}} &= \delta^{-\frac{1}{2}}\frac{V''(r_2(e))}{V'(r_2(e))} - \delta^{-\frac{1}{2}}\frac{V''(r_1(e))}{V'(r_1(e))}\\ &\quad -\frac{1}{2}\int\limits_{e-V>\delta}\mathrm{d}r\frac{V''(r)}{\left(e-V(r)\right)^{\frac{3}{2}}}.\end{aligned} \tag{6.13}$$

This way we obtain the function ψ, the second quantizaton term. The boundary terms correspond to the divergence terms given in the quantization theorem.

To apply this theorem to our two-dimensional system we have to simplify the problem we consider. Let's use the radial symmetry to transform it into a one-dimensional problem.

In this problem we have two conserved quantities, the energy $H = -\epsilon^2\Delta + V(|\boldsymbol{q}|) = -\epsilon^2\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right) + V(r)$ and the square of the angular momentum L^2, where $L = -i\epsilon\frac{\partial}{\partial\theta}$, because $[H, L^2] = 0$. We have used the usual polar coordinates (r,θ) defined by $(q_1, q_2) = (r\cos\theta, r\sin\theta)$.

Using the fact that L^2 is a constant of the motion, we rewrite the wave function: $\psi(\boldsymbol{x}) = \varphi(r)e^{im\theta}$, $m = 0, \pm1, \pm2, \ldots$. This way, it is an eigenfunction of L^2. The Schrödinger equation $\left(-\epsilon^2\Delta + V(|\boldsymbol{x}|)\right)\psi(\boldsymbol{x}) = e\psi(\boldsymbol{x})$ becomes

$$\left(-\epsilon^2\frac{\partial^2}{\partial r^2} - \frac{\epsilon^2}{r}\frac{\partial}{\partial r} + \frac{\epsilon^2 m^2}{r^2} + V(r)\right)\varphi(r) = e\varphi(r), \tag{6.14}$$

with $\int_0^\infty \mathrm{d}r r|\varphi(r)|^2 = \frac{1}{2\pi}$. The problem has been reduced to one dimension. However, we cannot use equation (6.6) to quantize, because the structure of the equation is not the same. We solve it by defining $\phi(r) \doteq \sqrt{r}\varphi(r)$. The equation becomes

$$-\epsilon^2 \frac{\partial^2}{\partial r^2}\phi(r) + \left(\frac{\epsilon^2(m^2-\frac{1}{4})}{r^2} + V(r)\right)\phi(r) = e\phi(r), \tag{6.15}$$

with $\int \mathrm{d}r|\phi(r)|^2 = \frac{1}{2\pi}$. Let's divide this equation by ϵ^2, and redefine $\epsilon^{-2}V(r) \mapsto V(r)$, as well as $\epsilon^{-2}e \mapsto e$. This is equivalent to considering $\epsilon = 1$.

Can we apply Feffermann's quantization condition? We have made our problem a one-dimensional one, but the variable r is defined on $\mathbb{R}_+$, which makes the theorem impossible to apply. If $m^2 > 0$, there will be a centrifugal barrier and the wave function will be zero for $r < 0$. But a problem remains for $m^2 = 0$. To avoid it, and apply the quantization theorem, we proceed to the change of variable $r \mapsto x,\ r = e^{\alpha x},\ \alpha > 0$. The condition $r \in [0, \infty]$ becomes $x \in [-\infty, \infty]$. The parameter α will be determined *a posteriori*. Moreover, we define a new wave function $\psi(x) \doteq e^{-\beta x}\phi(e^{\alpha x})$, where β will be determined *a posteriori* as well.

To write Schrödinger's equation (6.15) in these new variables, let's compute

$$\frac{\partial^2}{\partial r^2}\phi(r) = \frac{e^{(\beta-2\alpha)x}}{\alpha^2}\left[\psi''(x) + (2\beta-\alpha)\psi'(x) + (\beta^2-\alpha\beta)\psi(x)\right]. \tag{6.16}$$

In order to have a one-dimensional Scrödinger-like equation, we have to eliminate the first derivative, which leads to the following condition on the parameters

$$2\beta = \alpha. \tag{6.17}$$

We find

$$\frac{\partial^2}{\partial r^2}\phi(r) = e^{-3\beta x}\left[\frac{\psi''(x)}{4\beta^2} - \frac{\psi(x)}{4}\right], \tag{6.18}$$

and equation (6.15) becomes (with $\epsilon = 1$, and writing $m = \lambda$):

$$-e^{-3\beta x}\left[\frac{\psi''(x)}{4\beta^2} - \frac{\psi(x)}{4}\right] + e^{-3\beta x}\left[\lambda^2\psi(x) - \frac{\psi(x)}{4}\right] + e^{\beta x}\left[V(e^{2\beta x}) - e\right]\psi(x) = 0. \tag{6.19}$$

Multiplying by $e^{3\beta x}$ we find

$$-\frac{\psi''(x)}{4\beta^2} + e^{4\beta x}\left[V(e^{2\beta x}) - e\right]\psi(x) = -\lambda^2\psi(x). \tag{6.20}$$

The normalization of the wave function is, using the normalization of the function ϕ,

$$\int \mathrm{d}x\psi^2(x) = \frac{1}{2\beta}\int \frac{\mathrm{d}r}{r^2}\phi^2(r). \tag{6.21}$$

Is this function square integrable, that is, is this integration finite? In the limit $r \to \infty$, there will be no divergence (the function ϕ is square integrable, therefore $\frac{\phi}{r^2}$ is decreasing rapidly. In the limit $r \to 0$, we know that ϕ decreases exponentially due to the centrifugal barrier, and therefore decreases faster than r^{-2}. The wave function ψ is therefore a square integrable function and Feffermann's theorem can be used.

We have some liberty to set the constant β. Let's set $\beta = \frac{1}{2}$. Equation (6.20) becomes

$$-\psi''(x) + f(x)\psi(x) = -\lambda^2\psi(x), \tag{6.22}$$

where $f(x) \doteq e^{2x}\left(V(e^x) - e\right) \doteq -W(e^x)$.

We have transformed our problem into a new one. We want to determine the quantization condition of the problem given by equation (6.22). In this new problem, the role of the energy is played by $-\lambda^2$, the square angular momentum, while the real energy plays the role of a parameter. The potential of this new problem is $f(x)$.

Which values can these parameters take ? The square angular momentum is limited in the range $\lambda^2 \in [0, (\lambda^e)^2]$, where λ^e is the maximal classical value the angular momentum can have, at a fixed energy e. The energy is itself limited by $e \in [V_0, \infty]$, where $V_0 = V(0)$ is the lowest value the classical energy can have.

We can now apply Feffermann's quantization condition (6.7) to this new problem. At lowest order we find

$$\begin{aligned}
\phi(-\lambda^2) &= \frac{1}{\pi}\int\limits_{f<-\lambda^2} \mathrm{d}x \left(-\lambda^2 - f(x)\right)^{\frac{1}{2}} \\
&= \frac{1}{\pi}\int_{r_1}^{r_2} \frac{\mathrm{d}r}{r}\left(-\lambda^2 - r^2(V(r) - e)\right)^{\frac{1}{2}} \\
&= \frac{1}{\pi}\int_{r_1}^{r_2} \mathrm{d}r \left(e - V(r) - \frac{\lambda^2}{r^2}\right)^{\frac{1}{2}},
\end{aligned} \tag{6.23}$$

where we expressed this condition in the old variables. Let's note that this first order term corresponds exactly to the WKB quantization described earlier in this chapter. It also corresponds to the first order quantization of the "naive" approach given in equation (6.6).

The second term is

$$\psi(-\lambda^2) = \frac{1}{48\pi}\lim_{\delta\to 0_+}\left[\int\limits_{-\lambda^2-f>\delta} \mathrm{d}x \frac{f''(x)}{\left(-\lambda^2 - f(x)\right)^{\frac{3}{2}}} - q(-\lambda^2)\delta^{-\frac{1}{2}}\right], \tag{6.24}$$

where

$$q(-\lambda^2) = \frac{2f''(x_2(-\lambda^2))}{f'(x_2(-\lambda^2))} - \frac{2f''(x_1(-\lambda^2))}{f'(x_1(-\lambda^2))}. \tag{6.25}$$

Let's express this quantization in the old variables. Using the result

$$f''(x) = r^4 V''(r) + 5r^3 V'(r) - 4r^2(e - V(r)), \tag{6.26}$$

the second quantization term becomes

$$\psi(-\lambda^2) = \frac{1}{48\pi} \lim_{\delta\to 0_+} \left[\int\limits_{r^2(e-V)-\lambda^2>\delta} \frac{\mathrm{d}r}{r} \frac{\left(rV''(r) + 5V'(r) - 4\frac{(e-V(r))}{r}\right)}{\left(e - V(r) - \frac{\lambda^2}{r^2}\right)^{\frac{3}{2}}} - q(-\lambda^2)\delta^{-\frac{1}{2}} \right]. \tag{6.27}$$

To make use of this equation, let's anticipate the next sections and look at what we are interested in. We want to compute the integrated density of states, and later the energy of the system. Only the lowest order contribution of this term has to be considered for consistency. As explained later in this chapter, it is given by

$$\begin{aligned} N_1(e) &= \int_{-\lambda^e}^{\lambda^e} \mathrm{d}\lambda \psi(-\lambda^2) \doteq N_1^a(e) + N_1^b(e) \\ &= \frac{1}{48\pi} \lim_{\delta\to 0_+} \left[\int_{-\lambda^e}^{\lambda^e} \mathrm{d}\lambda \int\limits_{-\lambda^2 - f>\delta} \mathrm{d}x \frac{f''(x)}{(-\lambda^2 - f(x)^2)^{\frac{3}{2}}} - \int_{-\lambda^e}^{\lambda^e} \mathrm{d}\lambda q(-\lambda^2)\delta^{-\frac{1}{2}} \right]. \end{aligned} \tag{6.28}$$

Let's evaluate the first term of (6.28). We commute the integration over λ and x to find (using the fact that $f = -W < 0$)

$$\begin{aligned} \int \mathrm{d}x f''(x) \int\limits_{\lambda^2<(-f-\delta)} \mathrm{d}\lambda \frac{1}{(-f(x) - \lambda^2)^{\frac{3}{2}}} \\ &= -\int \mathrm{d}x \frac{W''(x)}{W(x)^{\frac{3}{2}}} \int_{-\sqrt{W-\delta}}^{\sqrt{W-\delta}} \mathrm{d}\lambda \frac{1}{\left(1 - \frac{\lambda^2}{W(x)}\right)^{\frac{3}{2}}} \\ &= -\int \mathrm{d}x \frac{W''(x)}{W(x)} \underbrace{\int_{-1+\alpha}^{1-\alpha} \mathrm{d}y \frac{1}{(1-y^2)^{\frac{3}{2}}}}_{\frac{\sqrt{2}}{\sqrt{\alpha}} + \mathcal{O}(\alpha)} \\ &= -\sqrt{2} \int \mathrm{d}x \frac{W''(x)}{\sqrt{\alpha} W(x)} + \mathcal{O}(\alpha) \\ &= -\frac{2}{\sqrt{\delta}} \int\limits_{W>\delta} \mathrm{d}x \frac{W''(x)}{\sqrt{W(x)}} + \mathcal{O}(\delta), \end{aligned} \tag{6.29}$$

where we performed the change of variable $\lambda \mapsto y = \frac{\lambda}{\sqrt{W(x)}}$, and defined $\alpha \doteq \frac{\delta}{2W(x)}$.

It leads to the contribution to the integrated density of states

$$N_1^a(e) = -\frac{1}{48\pi}\lim_{\delta\to 0_+}\frac{2}{\sqrt{\delta}}\left[\int\limits_{W>\delta} \mathrm{d}x \frac{W''(x)}{\sqrt{W(x)}} + \mathcal{O}(\delta)\right]. \tag{6.30}$$

To evaluate the second term of (6.28), let's compute

$$2\int_{-\lambda^e}^{\lambda^e} \mathrm{d}\lambda \frac{W''(x_2(-\lambda^2))}{W'(x_2(-\lambda^2))} = 4\int_0^{\lambda^e} \mathrm{d}\lambda \frac{W''(x_2(-\lambda^2))}{W'(x_2(-\lambda^2))}, \tag{6.31}$$

where we used the symmetry of the integrand (depending on λ^2 only). To perform this integration we need to know the meaning of $x_2(-\lambda^2)$: it corresponds to the classical turning point for a given angular momentum λ. Therefore, this turning point is a monotonous decreasing function of λ, we can therefore perform a change of variable $\lambda \mapsto x_2$. This relation is defined by

$$\lambda = \sqrt{W(x_2)} \quad \Rightarrow \quad \mathrm{d}\lambda = \frac{1}{2}\frac{W'(x_2)}{\sqrt{W(x_2)}}\mathrm{d}x_2, \tag{6.32}$$

The integration (6.31) becomes

$$-2\int_{x_{max}}^{x_2(0)} \mathrm{d}x_2 \frac{W''(x_2)}{\sqrt{W(x_2)}}. \tag{6.33}$$

The integration is performed from the minimum value of x_2 (defined by $W(x_2) = (\lambda^e)^2$) to its minimum value (defined by $W(x_2) = 0$) (explaining a change in the sign of the integral).

The integration

$$2\int_{-\lambda^e}^{\lambda^e} \mathrm{d}\lambda \frac{W''(x_1(-\lambda^2))}{W'(x_1(-\lambda^2))} = 4\int_0^{\lambda^e} \mathrm{d}\lambda \frac{W''(x_1(-\lambda^2))}{W'(x_1(-\lambda^2))} \tag{6.34}$$

is treated exactly the same way: we perform the change of variables

$$\lambda = \sqrt{W(x_1)} \quad \Rightarrow \quad \mathrm{d}\lambda = \frac{1}{2}\frac{W'(x_1)}{\sqrt{W(x_1)}}\mathrm{d}x_1, \tag{6.35}$$

yielding the result

$$2\int_{x_1(0)}^{x_{max}} \mathrm{d}x_1 \frac{W''(x_1)}{\sqrt{W(x_1)}}. \tag{6.36}$$

The integration is performed from the minimum value of x_1 (defined by $W(x_1) = 0$) to its maximum value (defined by $W(x_1) = (\lambda^e)^2$).

Using (6.33) and (6.36) we find, from (6.28), that $N_1^b(e)$ is

$$N_1^b(e) = \frac{1}{48\pi} \lim_{\delta \to 0_+} \frac{2}{\sqrt{\delta}} \int\limits_{W>0} \mathrm{d}x \frac{W''(x)}{\sqrt{W(x)}}. \tag{6.37}$$

We can now compute the total contribution to the density of states $N_1(e)$, which is

$$N_1(e) = \frac{1}{48\pi} \lim_{\delta \to 0_+} \frac{2}{\sqrt{\delta}} \int\limits_{0<W<\delta} \mathrm{d}x \frac{W''(x)}{\sqrt{W(x)}}. \tag{6.38}$$

We have to make this expression explicit to see that there is a contribution of the order of 1 in δ to this term. Let's introduce the value (6.26) of f'' to integrate

$$-\int\limits_{0<r^2(e-V)<\delta} \mathrm{d}r \frac{r^3 V''(r) + 5r^2 V'(r) - 4r(e - V(r))}{\sqrt{r^2(e - V(r))}}. \tag{6.39}$$

We can rewrite the numerator of the integrand as

$$r^2 \Delta V(r) + 2r^2 V'(r) - 2\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2(e - V(r))\right), \tag{6.40}$$

where we used $\Delta V(r) = V'(r) + rV''(r)$ and $\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2(e - V(r))\right) = 2r(e - V(r)) - r^2 V'(r)$. This integral can be decomposed in two parts: the first concerns the region $r \sim r_1$, the second one concerns the region $r \sim r_2$.

Let's study the first part. The first contribution is

$$-\int_{r_1}^{r_1+\alpha} \mathrm{d}r \frac{r^2 \Delta V(r)}{\sqrt{r^2(e - V(r))}}. \tag{6.41}$$

r_1 is defined by $r_1^2(e - V(r_1)) = 0 \;\Rightarrow\; r_1 = 0$, α is small. We proceed to the change of variable

$$y = r^2 \quad \Rightarrow \quad \mathrm{d}y = 2r\mathrm{d}r, \tag{6.42}$$

which leads to

$$-\frac{1}{2}\int_0^{\frac{\delta}{(e-V(r_1))}} \mathrm{d}y \frac{\Delta V(r_1)}{\sqrt{(e - V(r_1))}} = -\frac{\delta}{2}\frac{\Delta V(r_1)}{(e - V(r_1))^{\frac{3}{2}}} \xrightarrow{\delta \to 0} 0. \tag{6.43}$$

For $\delta \ll 1$, we replaced $\Delta V(r)$ by $\Delta V(r_1)$, because its y-dependence is weak. Therefore this term does not contribute to the integrated density of states.

The second contribution is, proceeding to the same change of variable as above,

$$-2\int_{r_1}^{r_1+\alpha} \mathrm{d}r \frac{r^2 V'(r)}{\sqrt{r^2(e - V(r))}} = -\int\limits_0^{\frac{\delta}{(e-V(r_1))}} \mathrm{d}y \frac{V'(r_1)}{\sqrt{(e - V(r_1))}} = -\delta \frac{V'(r_1)}{(e - V(r_1))^{\frac{3}{2}}} \xrightarrow{\delta \to 0} 0. \tag{6.44}$$

This term does not contribute either.

The third contribution is

$$2\int_{r_1}^{r_1+\alpha} \mathrm{d}r \frac{\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2(e-V(r))\right)}{\sqrt{r^2(e-V(r))}} = 2\int_0^\delta \frac{\mathrm{d}y}{\sqrt{y}} = 4\sqrt{\delta}, \tag{6.45}$$

where we proceeded to the change of variable $y = r^2(e - V(r))$.

Let's now study the second part of (6.39), that is the integration in the region $r \sim r_2$.

The first contribution is

$$-\int_{r_2-\alpha}^{r_2} \mathrm{d}r \frac{r^2 \Delta V(r)}{\sqrt{r^2(e-V(r))}} = -\int_{r_2-\alpha}^{r_2} \mathrm{d}r r \frac{\Delta V(r)}{\sqrt{(e-V(r))}}. \tag{6.46}$$

We proceed to the change of variable

$$y = e - V(r) \quad \Rightarrow \quad \mathrm{d}y = -V'(r)\mathrm{d}r \tag{6.47}$$

to find (the y-dependence of $\frac{r\Delta V(r)}{V'(r)}$ is weak, we replace it by $\frac{r_2 \Delta V(r_2)}{V'(r_2)}$ for $\delta \ll 1$)

$$-\int_0^\delta \frac{\mathrm{d}y}{\sqrt{y}} \frac{r_2 \Delta V(r_2)}{V'(r_2)} = -2\sqrt{\delta}\frac{r_2 \Delta V(r_2)}{V'(r_2)}. \tag{6.48}$$

The second contribution is

$$-2\int_{r_2-\alpha}^{r_2} \mathrm{d}r \frac{r^2 V'(r)}{\sqrt{r^2(e-V(r))}} = -2\int_{r_2-\alpha}^{r_2} \mathrm{d}r \frac{r V'(r)}{\sqrt{e-V(r)}}. \tag{6.49}$$

We proceed to the same change of variable as above and find

$$-2\int_0^{\frac{\delta}{r_2^2}} \frac{\mathrm{d}y}{\sqrt{y}} r_2 = -4\sqrt{\delta}. \tag{6.50}$$

The third contribution is

$$2\int_{r_2-\alpha}^{r_2} \mathrm{d}r \frac{\frac{\mathrm{d}}{\mathrm{d}r}(r^2(e-V(r)))}{\sqrt{r^2(e-V(r))}} = -2\int_0^\delta \frac{\mathrm{d}y}{\sqrt{y}} = -4\sqrt{\delta}, \tag{6.51}$$

where we proceeded to the change of variable $y = r^2(e - V(r))$.

Grouping all these terms, the integrated density of states is

$$N_1(e) = \frac{1}{48}\left[4 - 8 - 2\frac{r_2 \Delta V(r_2)}{V'(r_2)}\right] = -\frac{1}{12} - \frac{1}{24}\frac{r_2 \Delta V(r_2)}{V'(r_2)}. \tag{6.52}$$

The second part can be written as

$$-\frac{1}{48\pi}\int \mathrm{d}^2\boldsymbol{x} \Delta V(r) \delta(e - V(r)). \tag{6.53}$$

This is established as follows:

$$\begin{aligned}
-\frac{1}{48\pi}\int \mathrm{d}^2\boldsymbol{x}\Delta V(r)\delta(e-V(r)) &= -\frac{1}{24}\int_0^\infty \mathrm{d}rr\Delta V(r)\frac{\delta(r-r_2)}{V'(r_2)} \\
&= -\frac{1}{24}\frac{r_2\Delta V(r_2)}{V'(r_2)}. \qquad (6.54)
\end{aligned}$$

The energy we obtain from (6.52) is (as will be explained later)

$$E_1(\mu) = \int^\mu \mathrm{d}eN_1(e) = -\frac{1}{48\pi}\int \mathrm{d}^2\boldsymbol{x}\Delta V(\boldsymbol{x})\theta(\mu - V(r)) - \frac{\mu}{12}. \qquad (6.55)$$

6.1.2 Integrated density of states

We are interested in computing the integrated density of states

$$N(e) = s\sum_{n=0}^{\infty}\sum_{m=-\infty}^{\infty}\theta(e-e_{n,m}), \qquad (6.56)$$

where we included the spin degeneracy $s = 2$, which will be replaced by its numerical value at the end.

A similar development was done by Berry and Tabor (1977), who computed the integrated density of states of an integrable system in d dimensions with this approach.

From now on the sum will be denoted by $\sum_{n,m}$.

An equivalent way of writing (6.56) is:

$$N(e) = s\sum_{n,m}\theta(s(e,\epsilon m) - \epsilon(n+\frac{1}{2})). \qquad (6.57)$$

Formula (6.57) is the starting point of our calculations. We will proceed to an ϵ expansion, extracting the smooth parts as well as the oscillating parts of the integrated density of states.

It is easily seen from (6.3) that, at lowest order in ϵ, e is a monotonous growing function of I_2, for all I_1. Moreover I_1 is a monotonous decreasing (resp. increasing) function of I_2, for $I_2 > 0$ (resp. $I_2 < 0$), and for all e. This allows us to give a geometrical interpretation of the integrated density of states (6.57): it is the number of points $(n,m) \in \mathbb{N}\times\mathbb{Z}$ contained in the contour $H(I_1,I_2) = e$, as shown in Figure 6.1. Let's mention that an analogy can be made with Gauss's circle problem, a problem in number theory consisting of counting the number of points on the lattice $\mathbb{Z}^2$ enclosed by a large circle. This problem is still open. It was proven that, for a circle of radius R, this number behaves as $N \simeq CR^\alpha$, where $\frac{1}{2} < \alpha \leq \frac{46}{73}$. The higher bound is due to Huxley (1990), and has been improved continuously since Gauss's work.

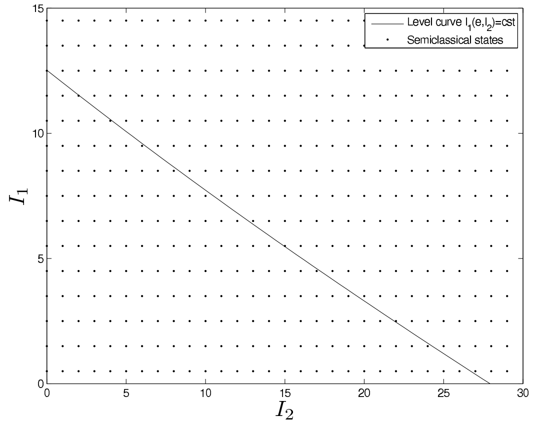


Figure 6.1: *Representation of semiclassical states in the I_1, I_2 plane. The integrated density of states corresponds to the number of points enclosed in the energy level curve. The level curve is that of the self-consistent potential of a quantum dot (see chapter 8).*

To proceed from formula (6.57), we will replace the sums by integrations using the Poisson sum formula, which is

$$\sum_{m=-\infty}^{\infty} \exp\{2\pi i m x\} = \sum_{p=-\infty}^{\infty} \delta(x-p). \tag{6.58}$$

We get

$$\begin{aligned} N(e) &= s\sum_{n=0}^{\infty}\sum_{m=-\infty}^{\infty} \theta(s(e,\epsilon m) - \epsilon(n+\frac{1}{2})) \\ &= s\int_{-\infty}^{\infty} \mathrm{d}x \int_{0}^{\infty} \mathrm{d}\nu \sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} \delta(m-x)\delta(n+\frac{1}{2}-\nu)\theta(s(e,\epsilon x)-\epsilon\nu) \\ &= s\int_{-\infty}^{\infty} \mathrm{d}x \int_{0}^{\infty} \mathrm{d}\nu \sum_{k=-\infty}^{\infty}\sum_{j=-\infty}^{\infty} (-1)^j \exp\left\{2\pi i[kx+j\nu]\right\}\theta(s(e,\epsilon x)-\epsilon\nu) \\ &= \frac{s}{\epsilon^2}\int_{-\infty}^{\infty} \mathrm{d}x \int_{0}^{\infty} \mathrm{d}\nu \sum_{k=-\infty}^{\infty}\sum_{j=-\infty}^{\infty} (-1)^j \exp\left\{\frac{2\pi i}{\epsilon}[kx+j\nu]\right\}\theta(s(e,x)-\nu), \end{aligned} \tag{6.59}$$

where we have used the equality $e^{-i\pi} = -1$. We integrate ν from 0. Other possible choices are between $-\frac{1}{2}+\epsilon$ and $\frac{1}{2}-\epsilon$, $\epsilon < 1$. The last equality is obtained through a change of variables.

We finally obtain the expression

$$N(e) = \frac{s}{\epsilon^2} \int_{-\lambda^e}^{\lambda^e} \mathrm{d}x \int_0^{s(e,x)} \mathrm{d}\nu \sum_{k=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} (-1)^j \exp\left\{ \frac{2\pi i}{\epsilon}[kx + j\nu] \right\}, \tag{6.60}$$

where λ^e is defined by $s(e, \lambda^e) = 0,\ \lambda^e > 0$.

We will compute the main contributions to the integrated density of states by considering the different terms of the sum (6.60).

6.1.3 Thomas-Fermi model

The contribution of the term $j = 0, k = 0$ of the sum (6.60) consists of neglecting the quantization of the action variables, considered in this case as continuum variables. Unsurprisingly, we get the main contribution to the smooth part of the integrated density of states, which is the Thomas-Fermi term, by considering the lowest order term of $s(e,x)$ only, which is $s_0(e,x) = \frac{1}{\pi}\int \mathrm{d}r \left(e - V(r) - \frac{x^2}{r^2}\right)^{\frac{1}{2}}$:

$$\begin{aligned} N_0(e) &= \frac{s}{\epsilon^2} \int_{-\lambda^e}^{\lambda^e} \mathrm{d}x \int_0^{s_0(e,x)} \mathrm{d}\nu \\ &= \frac{s}{\epsilon^2} \int_{-\lambda^e}^{\lambda^e} \mathrm{d}x \ s_0(e,x) \\ &= \frac{s}{\pi\epsilon^2} \int_{-\lambda^e}^{\lambda^e} \mathrm{d}x \int_{r_1}^{r_2} \mathrm{d}r \sqrt{e - V(r) - \frac{x^2}{r^2}}. \end{aligned} \tag{6.61}$$

Let's compute this term. The integration is performed on the domain where the integrand is positive. Let's define

$$(f(x))_+ \doteq \begin{cases} f(x), & \text{if } f(x) > 0, \\ 0, & \text{if } f(x) \le 0. \end{cases}$$

$N_0(e)$ becomes

$$\begin{aligned} N_0(e) &= \frac{s}{\pi\epsilon^2} \int_{\mathbb{R}} \mathrm{d}x \int_{\mathbb{R}_+} \mathrm{d}r \sqrt{\left(e - V(r) - \frac{x^2}{r^2}\right)_+} \\ &= \frac{2s}{\pi\epsilon^2} \int_{\mathbb{R}_+} \mathrm{d}x \int_{\mathbb{R}_+} \mathrm{d}r \sqrt{\left(e - V(r) - \frac{x^2}{r^2}\right)_+} \\ &= \frac{2s}{\pi\epsilon^2} \int_{\mathbb{R}_+} \mathrm{d}r \int_{\mathbb{R}_+} \mathrm{d}x \sqrt{\left(e - V(r) - \frac{x^2}{r^2}\right)_+} \end{aligned}$$

$$\begin{aligned}
&= \frac{2s}{\pi\epsilon^2}\int_{\mathbb{R}_+}\frac{\mathrm{d}r}{r}\int_0^{r^2(e-V(r))_+}\mathrm{d}x\sqrt{(r^2(e-V(r))-x^2)} \\
&= \frac{2s}{\pi\epsilon^2}\int_{\mathbb{R}_+}\frac{\mathrm{d}r}{r}r^2(e-V(r))_+\underbrace{\int_0^1\mathrm{d}x\sqrt{(1-x^2)}}_{=\frac{\pi}{4}} \\
&= \frac{s}{2\epsilon^2}\int_{\mathbb{R}_+}r\mathrm{d}r(e-V(r))_+ \\
&= \frac{s}{4\pi\epsilon^2}\int_{\mathbb{R}^2}\mathrm{d}^2\boldsymbol{x}(e-V(|\boldsymbol{x}|))_+. \qquad (6.62)
\end{aligned}$$

This result is the same as the one obtained in the semiclassical Hartree-Fock approach in chapter 5, it confirms therefore the result we obtained.

6.1.4 First correction to WKB quantization

The first correction to WKB quantization leads to a correction to the integrated density of states which was already computed in section 6.1.1, where the result was given in equation (6.52). Adding the spin factor s we find

$$N_1(e) = -\frac{s}{48\pi}\int\mathrm{d}^2\boldsymbol{x}\Delta V(r)\delta(e-V(r)) - \frac{s}{12}. \qquad (6.63)$$

This result is the same as the one obtained in the semiclassical Hartree-Fock approach in chapter 5.

6.1.5 l-quantized Thomas-Fermi model

From now on, we will consider the function s at lowest order in ϵ only (that is s_0). Higher orders will not be necessary for our computations. For simplicity we write this lowest order s.

To proceed further with expression (6.60), we consider all the terms $j = 0, k \neq 0$. The physical meaning is that we quantize the variable x, which is the angular momentum, but not the radial quantum number. This is why this model is usually called the lTF model. It will provide oscillating terms, which is why we write its contribution to the integrated density of states N^I_{osc}:

$$\begin{aligned}
N^I_{osc}(e) &= \frac{s}{\epsilon^2}\int_{-\lambda^e}^{\lambda^e}\mathrm{d}x\int_0^{s(e,x)}\mathrm{d}\nu\sum_{k\neq 0}\exp\left\{\frac{2\pi i}{\epsilon}kx\right\} \\
&= \frac{s}{\epsilon^2}\sum_{k\neq 0}\int_{-\lambda^e}^{\lambda^e}\mathrm{d}x\ s(e,x)\exp\left\{\frac{2\pi i}{\epsilon}kx\right\} \\
&= \frac{2s}{\epsilon^2}\sum_{k=1}^{\infty}\int_{-\lambda^e}^{\lambda^e}\mathrm{d}x\ s(e,x)\cos\left\{\frac{2\pi}{\epsilon}kx\right\}
\end{aligned}$$

$$= \frac{4s}{\epsilon^2} \sum_{k=1}^{\infty} \int_0^{\lambda^e} \mathrm{d}x \; s(e,x) \cos\left\{ \frac{2\pi}{\epsilon} kx \right\}. \tag{6.64}$$

To extract the terms of lowest order in ϵ we integrate two times by parts this expression:

$$\begin{aligned}
\int_0^{\lambda^e} \mathrm{d}x \; s(e,x) \cos\left(\frac{2\pi}{\epsilon} kx \right) &= \frac{\epsilon}{2\pi k} \underbrace{s(e,\lambda^e)}_{=0 \text{ (see definition of } \lambda^e)} \sin\left(\frac{2\pi}{\epsilon} k\lambda^e \right) \\
&\quad - \frac{\epsilon}{2\pi k} \int_0^{\lambda^e} \mathrm{d}x \; s_x(e,x) \sin\left(\frac{2\pi}{\epsilon} kx \right) \\
&= - \frac{\epsilon}{2\pi k} \int_0^{\lambda^e} \mathrm{d}x \; s_x(e,x) \sin\left(\frac{2\pi}{\epsilon} kx \right) \\
&= \frac{\epsilon^2}{(2\pi)^2 k^2} \left(s_x(e,\lambda^e) \cos\left(\frac{2\pi}{\epsilon} k\lambda^e \right) - s_x(e,0) \right) \\
&\quad - \frac{\epsilon^2}{(2\pi)^2 k^2} \int_0^{\lambda^e} \mathrm{d}x \; s_{xx}(e,x) \cos\left(\frac{2\pi}{\epsilon} kx \right) \\
&= \frac{\epsilon^2}{(2\pi)^2 k^2} s_x(e,\lambda^e) \cos\left(\frac{2\pi}{\epsilon} k\lambda^e \right) - \frac{\epsilon^2}{(2\pi)^2 k^2} s_x(e,0) \\
&\quad + o(\epsilon^2),
\end{aligned} \tag{6.65}$$

where $s_x(e,x) \doteq \frac{\partial s(e,x)}{\partial x}$.

To establish that the rest is of the order of $o(\epsilon^2)$, further calculations show that

$$\int_0^{\lambda^e} \mathrm{d}x |s_{xx}(e,x)| < \infty. \tag{6.66}$$

Hence, by the Riemann-Lebesgue lemma (if a function is integrable, its Fourier transform is zero when evaluated at infinity),

$$\lim_{\epsilon \to 0} \int_0^{\lambda^e} \mathrm{d}x s_{xx}(e,x) \cos\left(\frac{2\pi}{\epsilon} kx \right) = 0, \tag{6.67}$$

that is

$$\int_0^{\lambda^e} \mathrm{d}x s_{xx}(e,x) \cos\left(\frac{2\pi}{\epsilon} kx \right) = \mathcal{O}(\epsilon^\delta), \;\; \delta > 0. \tag{6.68}$$

The rest is therefore of the order of $\mathcal{O}(\epsilon^{2+\delta}), \delta > 0$, that is $o(\epsilon^2)$. The Riemann-Lebesgue lemma will be used several times to prove that the remaining terms are tending to 0.

Therefore we get, for the lTF contribution to the integrated density of states

$$N^I_{osc}(e) \;\; = \;\; \frac{s}{\pi^2} \sum_{k=1}^{\infty} s_x(e,\lambda^e) \frac{\cos\left(\frac{2\pi}{\epsilon} k\lambda^e\right)}{k^2} - \frac{s}{\pi^2} s_x(e,0) \underbrace{\sum_{k=1}^{\infty} \frac{1}{k^2}}_{=\pi^2/6} + o(1)$$

$$\begin{aligned}
&= \frac{s}{\pi^2}\sum_{k=1}^{\infty} s_x(e,\lambda^e)\frac{\cos\left(\frac{2\pi}{\epsilon}k\lambda^e\right)}{k^2} - \frac{s}{6}s_x(e,0) + o(1) \\
&= \frac{s}{\pi^2}\sum_{k=1}^{\infty} s_x(e,\lambda^e)\frac{\cos\left(\frac{2\pi}{\epsilon}k\lambda^e\right)}{k^2} + \frac{s}{12} + o(1), \qquad (6.69)
\end{aligned}$$

where the last equality comes from the fact that $s_x(e,0) = -\frac{1}{2}$ for a very general class of potentials (the condition is that the potential must be $\mathcal{C}^1$ at $r = 0$), see annex 6.3.1.

The term $\frac{s}{12}$ will cancel the constant term arising from the smooth correction to WKB in equation (6.63).

These terms can be interpreted in terms of Fourier series. It seems natural to interpret the λ oscillations (6.69) in terms of the function $\langle x\rangle \doteq x - \frac{1}{2} - [x]$, where $[x]$ is the largest integer smaller than x. This comes from the fact that the N^I_{osc} term is a correction of the "smoothed" integrated density of states. These corrections should naturally be described by a function of $\langle x\rangle$.

Let's write the Fourier series of $\langle x\rangle$:

$$\langle x\rangle = \sum_{k=1}^{\infty} c_k \sin(2\pi k x), \qquad (6.70)$$

where $c_k \doteq \frac{1}{N_k}\int_0^1 \mathrm{d}x\, x \sin(2\pi k x) = -\frac{1}{N_k}\frac{1}{2\pi k}$. The factor N_k is the normalization of the function $\sin(2\pi k x)$: $N_k \doteq \int_0^1 \mathrm{d}x \sin^2(2\pi k x) = \frac{1}{2}$. We finally find

$$\langle x\rangle = -\sum_{k=1}^{\infty} \frac{1}{\pi k}\sin(2\pi k x), \qquad (6.71)$$

where the equality is valid almost everywhere in x.

Let's integrate $\langle x\rangle$:

$$\int_0^x \mathrm{d}x'\langle x'\rangle = \frac{1}{2}\sum_{k=1}^{\infty}\frac{1}{(\pi k)^2}\cos(2\pi k x) - \frac{1}{12}, \qquad (6.72)$$

valid for $x \in \mathbb{R}$ (*a.e.* x), not only in the interval $[0,1]$.

Identifying (6.69) and (6.72) we can rewrite the l-quantized integrated density of states in terms of $\langle x\rangle$:

$$N^I_{osc}(e) = 2s s_x(e,\lambda^e)\int_0^{\frac{\lambda^e}{\epsilon}} \mathrm{d}x'\langle x'\rangle + s\frac{(s_x(e,\lambda^e) - s_x(e,0))}{6} + o(1). \qquad (6.73)$$

6.1.6 Complete model

The last terms we have not considered until now in the sums (6.60) are those of the type $j \neq 0, k \in \mathbb{Z}$. The contribution to the integrated density of states will be oscillating terms, we write it N^{II}_{osc}.

We compute these terms:

$$\begin{aligned}
N^{II}_{osc}(e) &= \frac{s}{\epsilon^2}\int_{-\lambda^e}^{\lambda^e} \mathrm{d}x \int_0^{s(e,x)} \mathrm{d}\nu \sum_{j\neq 0}\sum_{k=-\infty}^{\infty} (-1)^j \exp\left\{\frac{2\pi i}{\epsilon}[kx + j\nu]\right\} \\
&= \frac{2s}{\epsilon^2}\int_{-\lambda^e}^{\lambda^e} \mathrm{d}x \int_0^{s(e,x)} \mathrm{d}\nu \Re\left\{\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty} (-1)^j \exp\left\{\frac{2\pi i}{\epsilon}[kx + j\nu]\right\}\right\} \\
&= \frac{2s}{\epsilon^2}\int_{-\lambda^e}^{\lambda^e} \mathrm{d}x \Re\left\{\int_0^{s(e,x)} \mathrm{d}\nu \sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty} (-1)^j \exp\left\{\frac{2\pi i}{\epsilon}[kx + j\nu]\right\}\right\} \\
&= \frac{s}{\pi\epsilon}\int_{-\lambda^e}^{\lambda^e} \mathrm{d}x \Re\left\{\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty} \frac{(-1)^j}{ij}\left\{\exp\left\{\frac{2\pi i}{\epsilon}[kx + js(e,x)]\right\}\right.\right. \\
&\qquad\qquad\qquad\qquad\left.\left. - \exp\left\{\frac{2\pi i}{\epsilon}kx\right\}\right\}\right\} \\
&= \frac{s}{\pi\epsilon}\int_{-\lambda^e}^{\lambda^e} \mathrm{d}x \left\{\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty} \frac{(-1)^j}{j}\left\{\sin\left\{\frac{2\pi}{\epsilon}[kx + js(e,x)]\right\}\right.\right. \\
&\qquad\qquad\qquad\qquad\left.\left. - \sin\left\{\frac{2\pi}{\epsilon}kx\right\}\right\}\right\} \\
&= \frac{s}{\pi\epsilon}\int_{-\lambda^e}^{\lambda^e} \mathrm{d}x \left\{\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty} \frac{(-1)^j}{j}\left\{\sin\left\{\frac{2\pi}{\epsilon}[kx + js(e,x)]\right\}\right\}\right\} \\
&= \frac{2s}{\pi\epsilon}\int_0^{\lambda^e} \mathrm{d}x \left\{\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty} \frac{(-1)^j}{j}\left\{\sin\left\{\frac{2\pi}{\epsilon}[kx + js(e,x)]\right\}\right\}\right\}. \qquad (6.74)
\end{aligned}$$

To establish the second equality we compute these sums:

$$\begin{aligned}
\sum_{j\neq 0}\sum_{k=-\infty}^{\infty} \exp\left\{\frac{2\pi i}{\epsilon}[kx + j\nu]\right\} &= 2\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty} \exp\left\{\frac{2\pi i}{\epsilon}kx\right\}\cos\left\{\frac{2\pi}{\epsilon}j\nu\right\} \\
&= 2\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty} \cos\left\{\frac{2\pi}{\epsilon}kx\right\}\cos\left\{\frac{2\pi}{\epsilon}j\nu\right\}.
\end{aligned} \qquad (6.75)$$

$$
\begin{aligned}
&\Re\left\{\sum_{j\neq 0}\sum_{k=-\infty}^{\infty}\exp\left\{\frac{2\pi i}{\epsilon}[kx+j\nu]\right\}\right\} \\
&\qquad\qquad\qquad = \Re\left\{\sum_{j\neq 0}\sum_{k=-\infty}^{\infty}\exp\left\{\frac{2\pi i}{\epsilon}kx\right\}\exp\left\{\frac{2\pi i}{\epsilon}j\nu\right\}\right\} \\
&\qquad\qquad\qquad = \sum_{j\neq 0}\sum_{k=-\infty}^{\infty}\cos\left\{\frac{2\pi}{\epsilon}kx\right\}\cos\left\{\frac{2\pi}{\epsilon}j\nu\right\} \\
&\qquad\qquad\qquad = 2\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty}\cos\left\{\frac{2\pi}{\epsilon}kx\right\}\cos\left\{\frac{2\pi}{\epsilon}j\nu\right\}, \qquad (6.76)
\end{aligned}
$$

where we have used the fact that sin is an odd function, so that $\sum_{k=-\infty}^{\infty}\sin(kx) = 0$.

We have to compute terms of the type

$$\frac{2s}{\pi\epsilon}\int_0^{\lambda^e}\mathrm{d}x\frac{(-1)^j}{j}\sin\left\{\frac{2\pi}{\epsilon}[kx+js(e,x)]\right\}. \tag{6.77}$$

For convenience, let's define the action

$$A(x,e;k,j) \doteq kx + js(e,x) \tag{6.78}$$

and the function $x^\star(e,k,j)$, solution of the equation

$$\frac{\partial A(x^\star,e;k,j)}{\partial x} = k + js_x(e,x^\star) = 0, \tag{6.79}$$

hence

$$s_x(e,x^\star) = -\frac{k}{j}, \quad k\in\mathbb{Z}, j\in\mathbb{N}^\star. \tag{6.80}$$

The equation (6.80) will not have a solution for all triples (e,k,j).

To perform the computation of (6.77) we will distinguish four families of triples:

1. $x^\star(e,k,j) \in]0,\lambda^e[$,
2. $x^\star(e,k,j) = 0$,
3. $x^\star(e,k,j) = \lambda^e$,
4. $x^\star(e,k,j)$ does not exist.

In the first three cases, the dominating contributions will arise from a stationary phase approximation. For consistency, we will have to proceed beyond this approximation by integrations by parts. In the last case, there will be no stationary phase approximation and we will extract the dominating contributions by integrations by parts only.

Let's study these contributions separately. From now on we will not write the dependencies of the functions in the variables e,k,j.

1. $x^\star \in]0, \lambda^e[$

The term we compute is

$$\begin{aligned} \int_0^{\lambda^e} \mathrm{d}x \sin\left\{\frac{2\pi}{\epsilon} A(x)\right\} &= \Im\left\{\int_0^{\lambda^e} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon} A(x)\right\}\right\} \\ &= \Im\left\{\int_0^{x^\star-\delta} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon} A(x)\right\}\right\} \qquad (6.81) \\ &\quad +\Im\left\{\int_{x^\star-\delta}^{x^\star+\delta} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon} A(x)\right\}\right\} \qquad (6.82) \\ &\quad +\Im\left\{\int_{x^\star+\delta}^{\lambda^e} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon} A(x)\right\}\right\}, \qquad (6.83) \end{aligned}$$

where $\delta \ll 1$.

We extract the asymptotic behaviour of the first term (6.81) by integration by parts:

$$\begin{aligned} \int_0^{x^\star-\delta} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon} A(x)\right\} &= \int_0^{x^\star-\delta} \mathrm{d}x \frac{1}{A_x(x)} \left\{A_x(x) \exp\left\{\frac{2\pi i}{\epsilon} A(x)\right\}\right\} \\ &= \frac{\epsilon}{2\pi i} \left\{\frac{\exp\left\{\frac{2\pi i}{\epsilon} A(x^\star-\delta)\right\}}{A_x(x^\star-\delta)} - \frac{\exp\left\{\frac{2\pi i}{\epsilon} A(0)\right\}}{A_x(0)}\right\} \\ &\quad +o(\epsilon). \qquad (6.84) \end{aligned}$$

The rest is of the order of $o(\epsilon)$: it is

$$\begin{aligned} &\frac{\epsilon}{2\pi i} \int_0^{x^\star-\delta} \mathrm{d}x \frac{A_{xx}(x)}{A_x^2(x)} \exp\left\{\frac{2\pi i}{\epsilon} A(x)\right\} \\ = &\frac{\epsilon}{2\pi i} \int_{A(0)}^{A(x^\star-\delta)} \mathrm{d}y \frac{A_{xx}(x(y))}{A_x^3(x(y))} \exp\left\{\frac{2\pi i}{\epsilon} y\right\}, \qquad (6.85) \end{aligned}$$

where we proceeded to the change of variable $y = A(x)$, $\mathrm{d}y = A_x(x)\mathrm{d}x$ (the function A is invertible on the specified domain, because we consider functions with one extremum only, reached at $x = x^\star$).

The rest is then of the order of $o(\epsilon)$ because further computations show that

$$\int_{A(0)}^{A(x^\star-\delta)} \mathrm{d}y \left|\frac{A_{xx}(x(y))}{A_x^3(x(y))}\right| = \int_0^{x^\star-\delta} \mathrm{d}x \left|\frac{A_{xx}(x)}{A_x^2(x)}\right| < \infty, \qquad (6.86)$$

and the Riemann-Lebesgue lemma leads to the conclusion.

For the second term (6.82) we introduce the stationary phase approximation

$$
\begin{aligned}
&\int_{x^\star-\delta}^{x^\star+\delta} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon}A(x)\right\} \\
&\qquad = \int_{-\delta}^{+\delta} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon}A(x^\star+\delta)\right\} \\
&\qquad \simeq \exp\left\{\frac{2\pi i}{\epsilon}A(x^\star)\right\} \int_{-\delta}^{+\delta} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon}\frac{\sigma|A_{xx}(x^\star)|}{2}x^2\right\} \\
&\qquad = \exp\left\{\frac{2\pi i}{\epsilon}A(x^\star)\right\} \sqrt{\frac{\epsilon}{2\pi}\frac{2}{\sigma|A_{xx}(x^\star)|}} \int_{-\sqrt{\frac{2\pi}{\epsilon}\frac{\sigma|A_{xx}(x^\star)|}{2}}\delta}^{+\sqrt{\frac{2\pi}{\epsilon}\frac{\sigma|A_{xx}(x^\star)|}{2}}\delta} \mathrm{d}y \exp\left\{iy^2\right\} \\
&\qquad = \exp\left\{\frac{2\pi i}{\epsilon}A(x^\star)\right\} \sqrt{\frac{\epsilon}{2\pi}\frac{2}{\sigma|A_{xx}(x^\star)|}} \int_{-\infty}^{\infty} \mathrm{d}y \exp\left\{iy^2\right\} \\
&\qquad\quad - \exp\left\{\frac{2\pi i}{\epsilon}A(x^\star)\right\} \sqrt{\frac{\epsilon}{2\pi}\frac{2}{\sigma|A_{xx}(x^\star)|}} \int_{-\infty}^{-\sqrt{\frac{2\pi}{\epsilon}\frac{\sigma|A_{xx}(x^\star)|}{2}}\delta} \mathrm{d}y \exp\left\{iy^2\right\} \\
&\qquad\quad - \exp\left\{\frac{2\pi i}{\epsilon}A(x^\star)\right\} \sqrt{\frac{\epsilon}{2\pi}\frac{2}{\sigma|A_{xx}(x^\star)|}} \int_{+\sqrt{\frac{2\pi}{\epsilon}\frac{\sigma|A_{xx}(x^\star)|}{2}}\delta}^{\infty} \mathrm{d}y \exp\left\{iy^2\right\} \\
&\qquad\quad +o(\epsilon) \\
&\qquad = \exp\left\{\frac{2\pi i}{\epsilon}A(x^\star)\right\} \sqrt{\frac{\epsilon}{2\pi(-i)}\frac{2\pi}{\sigma|A_{xx}(x^\star)|}} \\
&\qquad\quad - \exp\left\{\frac{2\pi i}{\epsilon}A(x^\star)\right\} \sqrt{\frac{\epsilon}{2\pi}\frac{2}{\sigma|A_{xx}(x^\star)|}} \\
&\qquad\qquad\qquad \times \int_{-\infty}^{-\sqrt{\frac{2\pi}{\epsilon}\frac{\sigma|A_{xx}(x^\star)|}{2}}\delta} \mathrm{d}y \frac{1}{2iy}\left\{2iy \exp\left\{iy^2\right\}\right\} \\
&\qquad\quad - \exp\left\{\frac{2\pi i}{\epsilon}A(x^\star)\right\} \sqrt{\frac{\epsilon}{2\pi}\frac{2}{\sigma|A_{xx}(x^\star)|}} \\
&\qquad\qquad\qquad \times \int_{+\sqrt{\frac{2\pi}{\epsilon}\frac{\sigma|A_{xx}(x^\star)|}{2}}\delta}^{\infty} \mathrm{d}y \frac{1}{2iy}\left\{2iy \exp\left\{iy^2\right\}\right\} \\
&\qquad\quad +o(\epsilon) \\
&\qquad = \sqrt{\frac{\epsilon}{2\pi}\frac{2\pi}{|A_{xx}(x^\star)|}} \exp\left\{\frac{2\pi i}{\epsilon}A(x^\star) + i\frac{\sigma\pi}{4}\right\} \\
&\qquad\quad + \exp\left\{\frac{2\pi i}{\epsilon}A(x^\star)\right\} \frac{\epsilon}{2\pi i}\frac{2}{\sigma|A_{xx}(x^\star)|\delta} \exp\left\{i\frac{2\pi}{\epsilon}\frac{\sigma|A_{xx}(x^\star)|}{2}\delta^2\right\} \\
&\qquad\quad +o(\epsilon),
\end{aligned}
\tag{6.87}
$$

where $\sigma = \text{sign}A_{xx}(x^\star)$. The rest if of the order of $o(\epsilon)$. One of these terms is (the other is treated in the same way)

$$\begin{aligned}
&-\exp\left\{\frac{2\pi i}{\epsilon}A(x^\star)\right\}\sqrt{\frac{\epsilon}{2\pi}\frac{2}{\sigma|A_{xx}(x^\star)|}}\int_{\sqrt{\frac{2\pi}{\epsilon}\frac{\sigma|A_{xx}(x^\star)|}{2}}\delta}^{\infty}\mathrm{d}y\frac{\exp\{iy^2\}}{2iy^2}\\
&\qquad = -\epsilon\exp\left\{\frac{2\pi i}{\epsilon}A(x^\star)\right\}\sqrt{\frac{1}{2\pi}\frac{2}{\sigma|A_{xx}(x^\star)|}}\int_{2\pi\frac{\sigma|A_{xx}(x^\star)|}{2}\delta^2}^{\infty}\mathrm{d}x\frac{\exp\left\{i\frac{x}{\epsilon}\right\}}{4ix^{\frac{3}{2}}},
\end{aligned} \tag{6.88}$$

where we used the change of variable $x = \epsilon y^2$. Then, using the Riemann-Lebesgue lemma and the result

$$\int_{2\pi\frac{\sigma|A_{xx}(x^\star)|}{2}\delta^2}^{\infty}\frac{\mathrm{d}x}{x^{\frac{3}{2}}} < \infty, \tag{6.89}$$

we can conclude.

The third term (6.83) is computed in the same way than the first one. We find

$$\begin{aligned}
\int_{x^\star+\delta}^{\lambda^e}\mathrm{d}x\exp\left\{\frac{2\pi i}{\epsilon}A(x)\right\} &= \frac{\epsilon}{2\pi i}\left\{\frac{\exp\left\{\frac{2\pi i}{\epsilon}A(\lambda^e)\right\}}{A_x(\lambda^e)} - \frac{\exp\left\{\frac{2\pi i}{\epsilon}A(x^\star+\delta)\right\}}{A_x(x^\star+\delta)}\right\}\\
&\quad +o(\epsilon).
\end{aligned} \tag{6.90}$$

We use again the Riemann-Lebesgue lemma and the result

$$\int_{x^\star+\delta}^{\lambda^e}\mathrm{d}x\left|\frac{A_{xx}(x)}{A_x^2(x)}\right| < \infty \tag{6.91}$$

to establish the order of the rest.

Combining these terms, and taking into account the fact that, for δ small, we have $A(x^\star \pm \delta) = A(x^\star) \pm A_x(x^\star)\delta + \frac{1}{2}A_{xx}(x^\star)\delta^2 = A(x^\star) + \frac{1}{2}A_{xx}(x^\star)\delta^2$ and $A_x(x^\star \pm \delta) = A_x(x^\star) \pm A_{xx}(x^\star)\delta = \pm A_{xx}(x^\star)\delta$, we get as a final result

$$\begin{aligned}
\int_0^{\lambda^e}\mathrm{d}x\exp\left\{\frac{2\pi i}{\epsilon}A(x)\right\} &= \sqrt{\frac{\epsilon}{2\pi}\frac{2\pi}{|A_{xx}(x^\star)|}}\exp\left\{\frac{2\pi i}{\epsilon}A(x^\star) + i\frac{\sigma\pi}{4}\right\}\\
&\quad -\frac{\epsilon}{2\pi i}\frac{\exp\left\{\frac{2\pi i}{\epsilon}A(0)\right\}}{A_x(0)}\\
&\quad +\frac{\epsilon}{2\pi i}\frac{\exp\left\{\frac{2\pi i}{\epsilon}A(\lambda^e)\right\}}{A_x(\lambda^e)}\\
&\quad +o(\epsilon).
\end{aligned} \tag{6.92}$$

Only the imaginary part of this expression contributes to the integrated density of states. We obtain

$$\begin{aligned}\int_0^{\lambda^e} \mathrm{d}x \sin\left\{\frac{2\pi}{\epsilon}A(x)\right\} &= \sqrt{\frac{\epsilon}{2\pi}}\sqrt{\frac{2\pi}{j|s_{xx}(e,x^\star)|}}\sin\left\{\frac{2\pi}{\epsilon}[kx^\star + js(e,x^\star)] + \frac{\sigma\pi}{4}\right\} \\ &\quad -\frac{\epsilon}{2\pi}\frac{\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\}}{(k+js_x(e,\lambda^e))} \\ &\quad +\frac{\epsilon}{2\pi}\frac{\cos\left\{\frac{2\pi}{\epsilon}s(e,0)\right\}}{(k+js_x(e,0))} \\ &\quad +o(\epsilon). \end{aligned} \tag{6.93}$$

Let's note that the stationary points exist only if there is a solution $x^\star \in [0,\lambda^e]$. The function $s(e,x)$ is decreasing with respect to x. Its slope $s_x(e,x)$ is therefore negative, and the equation (6.80) may have a solution only in the case $k \in \mathbb{N}$.

The main oscillating contributions to the integrated density of states arise from the stationary points. They can be interpreted in terms of periodic orbits. The function $s(e,I_2)$ is the level curve of energy $H(I_1,I_2)$ in the (I_1,I_2) plane. Its derivative $s_x(e,I_2)$ is tangent to this level curve. Hence the variation of energy is perpendicular to this vector: $\mathrm{d}H(I_1,I_2) \perp s_x(e,I_2)$, as shown in Figure 6.2. The slope of $\mathrm{d}H(I_1,I_2) = \frac{\partial H(I_1,I_2)}{\partial I_1}\mathrm{d}I_1 + \frac{\partial H(I_1,I_2)}{\partial I_2}\mathrm{d}I_2 = \omega_1(I_1,I_2)\mathrm{d}I_1 + \omega_2(I_1,I_2)\mathrm{d}I_2$ is given by $\frac{\omega_1(I_1,I_2)}{\omega_2(I_1,I_2)}$, where ω_1 and ω_2 are the frequencies of the angle variables on the torus. The fact that the contributions to the integrated density of states arise from terms for which $-s_x(e,x^\star) \in \mathbb{Q}$ implies $\frac{\omega_1(I_1,I_2)}{\omega_2(I_1,I_2)} \in \mathbb{Q}$, which consists of periodic orbits. Let's write the main contribution of the stationary points to the

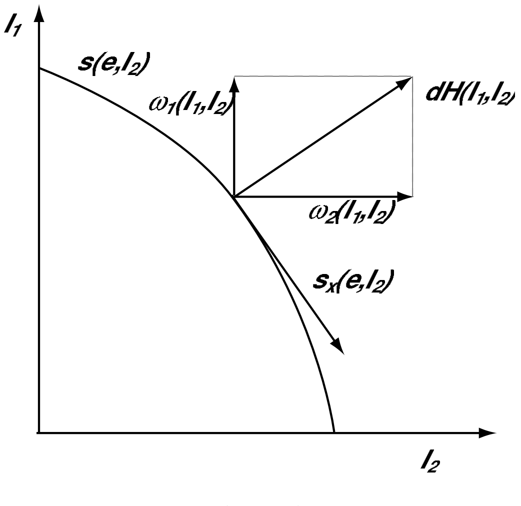


Figure 6.2: *The vector* $\mathrm{d}H(I_1,I_2)$ *is perpendicular to the tangent* $s_x(e,I_2)$*. The rationality of* s_x *implies the rationality of the frequencies ratio, given by the slope of the vector* $\mathrm{d}H(I_1,I_2)$*.*

integrated density of states:

$$N^{IIa}_{osc}(e) = \frac{2s}{\pi\sqrt{\epsilon}} \sum_{k,j}{}' \frac{(-1)^j}{j^{\frac{3}{2}}} \frac{\sin\left\{\frac{2\pi}{\epsilon}[kx^\star + js(e,x^\star)] + \sigma\frac{\pi}{4}\right\}}{\sqrt{|s_{xx}(e,x^\star)|}}, \tag{6.94}$$

where the sum runs over the pairs (k,j) such that $x^\star(e,k,j) \in]0,\lambda^e[$. Let's note that this sum will depend on the energy e. This implies that $N^{IIa}_{osc}(e)$ is not a continuous function of e.

Observing that all the pairs (nk,nj), $n \in \mathbb{N}^\star$ provide the same stationary point $x^\star(e,k,j)$, and that $A(x^\star,e;nk,nj) = nA(x^\star,e;k,j)$, we finally find

$$N^{IIa}_{osc}(e) = \frac{2s}{\pi\sqrt{\epsilon}} \sum_{n=1}^{\infty} \sum_{\{k,j|\,\gcd(k,j)=1\}}{}' \frac{(-1)^{nj}}{n^{\frac{3}{2}} j^{\frac{3}{2}}} \frac{\sin\left\{\frac{2\pi}{\epsilon}n[kx^\star + js(e,x^\star)] + \sigma\frac{\pi}{4}\right\}}{\sqrt{|s_{xx}(e,x^\star)|}}, \tag{6.95}$$

where the sum is the same as previously, but such that the greatest common divisor is $\gcd(k,j) = 1$.

2. $x^\star(e,k,j) = 0$

This case is treated in a similar way as the previous one.

The final result is

$$\begin{aligned}
\int_0^{\lambda^e} \mathrm{d}x \sin\left\{\frac{2\pi}{\epsilon}A(x)\right\} &= \Im\left\{\int_0^{\lambda^e} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon}A(x)\right\}\right\} \\
&= \Im\left\{\int_0^{\delta} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon}A(x)\right\}\right\} \\
&\quad + \Im\left\{\int_\delta^{\lambda^e} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon}A(x)\right\}\right\} \\
&= \frac{1}{2}\sqrt{\frac{\epsilon}{2\pi}}\sqrt{\frac{2\pi}{j|s_{xx}(e,0)|}} \sin\left\{\frac{2\pi}{\epsilon}js(e,0) + \sigma\frac{\pi}{4}\right\} \\
&\quad - \frac{\epsilon}{2\pi}\frac{\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\}}{(k + js_x(e,\lambda^e))} + o(\epsilon).
\end{aligned} \tag{6.96}$$

The order of the rest can be established using the Riemann-Lebesgue lemma.

The family of triples (e,k,j) which are of this type is easy to determine. They are defined by (6.80). Moreover we establish (see annex 6.3.1) that $s_x(e,0) = -\frac{1}{2}$, for a very general class of potentials (the only condition is that the potential has to be $\mathcal{C}^1$ at $r = 0$). This implies that the condition is

$$2k = j, \tag{6.97}$$

which is independent of e, and the main contribution to the integrated density of states is

$$\begin{aligned} N_{osc}^{IIb}(e) &= \frac{s}{\pi\sqrt{\epsilon}}\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty}\bigg|_{x^\star=0}\frac{(-1)^j}{j^{\frac{3}{2}}}\frac{\sin\left\{\frac{2\pi}{\epsilon}js(e,0)+\sigma\frac{\pi}{4}\right\}}{\sqrt{|s_{xx}(e,0)|}} \\ &= \frac{s}{\pi\sqrt{\epsilon}}\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty}\delta_{2k,j}\frac{(-1)^j}{j^{\frac{3}{2}}}\frac{\sin\left\{\frac{2\pi}{\epsilon}js(e,0)+\sigma\frac{\pi}{4}\right\}}{\sqrt{|s_{xx}(e,0)|}} \\ &= \frac{s}{\pi\sqrt{\epsilon}}\sum_{k=1}^{\infty}\frac{(-1)^{(2k)}}{(2k)^{\frac{3}{2}}}\frac{\sin\left\{\frac{2\pi}{\epsilon}(2k)s(e,0)+\sigma\frac{\pi}{4}\right\}}{\sqrt{|s_{xx}(e,0)|}} \\ &= \frac{s}{\pi\sqrt{8\epsilon}}\sum_{n=1}^{\infty}\frac{1}{n^{\frac{3}{2}}}\frac{\sin\left\{\frac{4\pi}{\epsilon}ns(e,0)+\sigma\frac{\pi}{4}\right\}}{\sqrt{|s_{xx}(e,0)|}}. \end{aligned} \tag{6.98}$$

3. $x^\star(e,k,j)=\lambda^e$

This case is treated in the same way than the previous cases again. We obtain

$$\begin{aligned} \int_0^{\lambda^e}\mathrm{d}x\sin\left\{\frac{2\pi}{\epsilon}A(x)\right\} &= \Im\left\{\int_0^{\lambda^e}\mathrm{d}x\exp\left\{\frac{2\pi i}{\epsilon}A(x)\right\}\right\} \\ &= \Im\left\{\int_0^{\lambda^e-\delta}\mathrm{d}x\exp\left\{\frac{2\pi i}{\epsilon}A(x)\right\}\right\} \\ &\quad+\Im\left\{\int_{\lambda^e-\delta}^{\lambda^e}\mathrm{d}x\exp\left\{\frac{2\pi i}{\epsilon}A(x)\right\}\right\} \\ &= \frac{1}{2}\sqrt{\frac{\epsilon}{2\pi}}\sqrt{\frac{2\pi}{j|s_{xx}(e,\lambda^e)|}}\sin\left\{\frac{2\pi}{\epsilon}k\lambda^e+\sigma\frac{\pi}{4}\right\} \\ &\quad+\frac{\epsilon}{2\pi}\frac{\cos\left\{\frac{2\pi}{\epsilon}js(e,0)\right\}}{(k+js_x(e,0))}+o(\epsilon). \end{aligned} \tag{6.99}$$

The rest is again estimated using the Riemann-Lebesgue lemma.

The triples (e,k,j) for which this situation occurs are very rare.

The main contribution from this term to the sum (6.74) will be

$$N_{osc}^{IIc}(e) = \frac{1}{\pi\sqrt{\epsilon}}\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty}\bigg|_{x^\star=\lambda^e}\frac{(-1)^j}{j^{\frac{3}{2}}}\frac{1}{\sqrt{|s_{xx}(e,\lambda^e)|}}\sin\left\{\frac{2\pi}{\epsilon}k\lambda^e+\sigma\frac{\pi}{4}\right\}. \tag{6.100}$$

4. $x^\star$ does not exist

In this case we can perform integrations by parts:

$$\begin{aligned}
\int_0^{\lambda^e} \mathrm{d}x \sin\left\{\frac{2\pi}{\epsilon}A(x)\right\} &= \Im\left\{\int_0^{\lambda^e} \mathrm{d}x \exp\left\{\frac{2\pi i}{\epsilon}A(x)\right\}\right\} \\
&= \Im\left\{\int_0^{\lambda^e} \mathrm{d}x \frac{1}{A_x(x)}\left\{A_x(x)\exp\left\{\frac{2\pi i}{\epsilon}A(x)\right\}\right\}\right\} \\
&= \Im\frac{\epsilon}{2\pi i}\left\{\frac{1}{A_x(\lambda^e)}\exp\left\{\frac{2\pi i}{\epsilon}A(\lambda^e)\right\}\right. \\
&\qquad\left. -\frac{1}{A_x(0)}\exp\left\{\frac{2\pi i}{\epsilon}A(0)\right\}\right\} + o(\epsilon) \\
&= -\frac{\epsilon}{2\pi}\frac{\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\}}{(k+js_x(e,\lambda^e))} + \frac{\epsilon}{2\pi}\frac{\cos\left\{\frac{2\pi}{\epsilon}js(e,0)\right\}}{(k+js_x(e,0))} + o(\epsilon),
\end{aligned} \tag{6.101}$$

the rest being estimated using the Riemann-Lebesgue lemma.

Complete expression

We can now combine these four types of terms to give an explicit formula for the sum (6.74):

$$N_{osc}^{II}(e) = N_{osc}^{IIa}(e) + N_{osc}^{IIb}(e) + N_{osc}^{IIc}(e) + N_{osc}^{IId}(e) + N_{osc}^{IIe}(e), \tag{6.102}$$

where $N_{osc}^{IIa}(e)$ is given by (6.95), $N_{osc}^{IIb}(e)$ by (6.98), $N_{osc}^{IIc}(e)$ by (6.100), and

$$\begin{aligned}
N_{osc}^{IId}(e) &= -\frac{s}{\pi^2}\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty}\Bigg|_{x^\star\neq\lambda^e} \frac{(-1)^j}{j\,(k+js_x(e,\lambda^e))}\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\} \\
&= -\frac{s}{\pi^2}\underbrace{\sum_{j=1}^{\infty}\frac{(-1)^j}{j^2}}_{=\frac{-\pi^2}{12}}\frac{1}{s_x(e,\lambda^e)} \\
&\quad -\frac{s}{\pi^2}\sum_{j=1}^{\infty}\sum_{k\neq 0}\Bigg|_{x^\star\neq\lambda^e} \frac{(-1)^j}{j\,(k+js_x(e,\lambda^e))}\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\} \\
&= \frac{s}{12}\frac{1}{s_x(e,\lambda^e)} - \frac{s}{\pi^2}\sum_{j=1}^{\infty}\sum_{k\neq 0}\Bigg|_{x^\star\neq\lambda^e} \frac{(-1)^j}{j\,(k+js_x(e,\lambda^e))}\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\}.
\end{aligned} \tag{6.103}$$

$$\begin{aligned} N^{IIe}_{osc}(e) &= \frac{s}{\pi^2}\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty}\Bigg|_{x^\star\neq 0} \frac{(-1)^j}{j\left(k+js_x(e,0)\right)}\cos\left\{\frac{2\pi}{\epsilon}js(e,0)\right\} \\ &= \frac{2s}{\pi^2}\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty}\Bigg|_{j\neq 2k} \frac{(-1)^j}{j\left(2k-j\right)}\cos\left\{\frac{2\pi}{\epsilon}js(e,0)\right\}. \end{aligned} \tag{6.104}$$

To establish the last equality we used the result $s_x(e,0) = -\frac{1}{2}$, as computed in annex 6.3.1, valid for a very general class of potentials (which have to be $\mathcal{C}^1$ at $r=0$).

6.1.7 λ oscillations

The oscillations of frequency $\frac{\lambda^e}{\epsilon}$ will be referred to as the λ oscillations, following Englert's notations in (Englert, 1988). They are composed of a part of N^I_{osc}, N^{IIc}_{osc}, and the oscillating part of N^{IId}_{osc}. In this section we will combine these terms in a different way. For energies e such that $s_x(e,\lambda^e)\notin\mathbb{Q}$, which is the most probable case (the set of energies for which s_x is rational is of measure zero), we group N^I_{osc} and N^{IId}_{osc} to get, for the contribution of the order of ϵ^0, using the fact that $\frac{\cos(kx)}{k^2}$ is an even function of k,

$$\begin{aligned} N^{II}_{\lambda}(e) &= \frac{s}{\pi^2}\sum_{k\neq 0}\left\{\frac{s_x(e,\lambda^e)}{2k^2}-\sum_{j=1}^{\infty}\frac{(-1)^j}{j\left(k+js_x(e,\lambda^e)\right)}\right\}\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\} \\ &= \frac{s}{\pi^2}\sum_{k\neq 0}\frac{1}{k}\left\{\frac{s_x(e,\lambda^e)}{2k}-\sum_{j=1}^{\infty}\frac{(-1)^j k}{j\left(k+js_x(e,\lambda^e)\right)}\right\}\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\} \\ &= \frac{s}{\pi^2}\sum_{k\neq 0}\frac{1}{k}\left\{\frac{s_x(e,\lambda^e)}{2k}-\sum_{j=1}^{\infty}(-1)^j\left\{\frac{1}{j}-\frac{1}{\frac{k}{s_x(e,\lambda^e)}+j}\right\}\right\}\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\}, \end{aligned} \tag{6.105}$$

where we used the equality

$$\frac{k}{j(k+js_x(e,\lambda^e))}=\frac{1}{j}-\frac{1}{\frac{k}{s_x(e,\lambda^e)}+j}. \tag{6.106}$$

The term

$$-\frac{s}{\pi^2}\sum_{k\neq 0}\frac{1}{k}\sum_{j=1}^{\infty}(-1)^j\frac{1}{j}\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\}=0 \tag{6.107}$$

is odd in the variable k. Hence, by summing over $k\neq 0$, we find that this sum is 0.

The term

$$\frac{s}{\pi^2}\sum_{k\neq 0}\frac{1}{k}\sum_{j=1}^{\infty}(-1)^j\frac{1}{\frac{k}{s_x(e,\lambda^e)}+j}\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\} \tag{6.108}$$

is of the kind $\gamma(k,j)=\beta(k,j)f(k)$, such that $\beta(k,j)=-\beta(-k,-j)$, and $f(k)$ is odd. Hence $\beta(k,j)f(k)=\beta(-k,-j)f(-k)$. The consequence is that

$$\begin{aligned}\sum_{k\neq 0}\sum_{j>0}\gamma(k,j) &= \sum_{k<0}\sum_{j>0}\gamma(k,j)+\sum_{k>0}\sum_{j>0}\gamma(k,j)\\ &= \frac{1}{2}\sum_{k<0}\sum_{j>0}\{\gamma(k,j)+\gamma(-k,-j)\}\\ &\quad +\frac{1}{2}\sum_{k>0}\sum_{j>0}\{\gamma(k,j)+\gamma(-k,-j)\}\\ &= \frac{1}{2}\sum_{k<0}\sum_{j>0}\gamma(k,j)+\frac{1}{2}\sum_{k>0}\sum_{j<0}+\gamma(k,j)\\ &\quad +\frac{1}{2}\sum_{k>0}\sum_{j>0}\gamma(k,j)+\frac{1}{2}\sum_{k<0}\sum_{j<0}\gamma(k,j)\\ &= \frac{1}{2}\sum_{k\neq 0}\sum_{j\neq 0}\gamma(k,j).\end{aligned} \tag{6.109}$$

Using the result

$$\sum_{j=-\infty}^{\infty}\frac{(-1)^j}{x-\pi j}=\frac{1}{\sin(x)}\Rightarrow\sum_{j\neq 0}\frac{(-1)^j}{x-\pi j}=\frac{1}{\sin(x)}-\frac{1}{x}, \tag{6.110}$$

we establish

$$\begin{aligned}&\frac{s}{\pi^2}\sum_{k\neq 0}\frac{1}{k}\sum_{j=1}^{\infty}(-1)^j\frac{1}{\frac{k}{s_x(e,\lambda^e)}+j}\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\}\\ &\qquad =\frac{s}{2\pi}\sum_{k\neq 0}\left\{\frac{\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\}}{k\sin\left(\frac{\pi k}{s_x(e,\lambda^e)}\right)}-\frac{s_x(e,\lambda^e)}{\pi k^2}\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\}\right\}.\end{aligned} \tag{6.111}$$

Introducing (6.107) and (6.111) in (6.105) we find

$$N_\lambda^{II}(e)=\frac{s}{2\pi}\sum_{k\neq 0}\frac{1}{k}\frac{\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\}}{\sin\left(\frac{\pi k}{s_x(e,\lambda^e)}\right)}. \tag{6.112}$$

The slope $s_x(e,x)$ is negative. Therefore we can finally write

$$N_\lambda^{II}(e)=-\frac{s}{2\pi}\sum_{k\neq 0}\frac{1}{k}\frac{\cos\left\{\frac{2\pi}{\epsilon}k\lambda^e\right\}}{\sin\left(\frac{\pi k}{|s_x(e,\lambda^e)|}\right)}. \tag{6.113}$$

6.1.8 ν oscillations

The oscillations of frequency $\frac{s(e,0)}{\epsilon}$ will be referred to as the ν oscillations, following Englert's notations in (Englert, 1988). They are composed of the contributions $N^{IIb}_{osc}(e)$, and $N^{IIe}_{osc}(e)$.

Let's explicitly compute the term $N^{IIe}_{osc}(e)$. We note that the sum over k is divergent. To avoid this divergence we will sum in the following order: $\lim_{N\to\infty}\sum_{k=-N}^{N} f(k)$, and separate the terms j even and j odd.

For notational convenience let's write the terms of the sum N^{IIe}_{osc} as $f(j, 2k-j)$. The sum we have to compute is

$$\begin{aligned}
\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty}\Big|_{j\neq 2k} f(j,2k-j) &= \sum_{j=1}^{\infty}\sum_{k\neq j} f(2j,2k-2j) \\
&\quad + \sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty} f(2j-1,2k-2j+1) \\
&\overset{m=k-j}{=} \sum_{j=1}^{\infty}\sum_{m\neq 0} f(2j,2m) \\
&\quad + \sum_{j=1}^{\infty}\sum_{m=-\infty}^{\infty} f(2j-1,2m+1). \qquad (6.114)
\end{aligned}$$

The function $f(2j, 2m)$ is odd in the variable m. Hence the first sum gives 0.

The second sum is:

$$\begin{aligned}
\sum_{m=-\infty}^{\infty} f(2j-1,2m+1) &= f(2j-1,1) \\
&\quad + \sum_{m=1}^{\infty}\Big(f(2j-1,2m+1)+f(2j-1,-2m+1)\Big). \qquad (6.115)
\end{aligned}$$

The dependence in the second variable is $f(x,y) = \frac{g(x)}{y}$. Hence

$$\begin{aligned}
f(2j-1,1) &+ \sum_{m=1}^{\infty}\left(f(2j-1,2m+1)+f(2j-1,-2m+1)\right) \\
&= g(2j-1) + 2g(2j-1)\underbrace{\sum_{m=1}^{\infty}\frac{1}{(1-4m^2)}}_{=-\frac{1}{2}} \\
&= g(2j-1) - g(2j-1) \\
&= 0. \qquad (6.116)
\end{aligned}$$

We have established $N_{osc}^{IIe}(e) = 0$.

The ν oscillations are therefore only given by N_{osc}^{IIb}:

$$N_\nu(e) = \frac{s}{\pi\sqrt{8\epsilon}} \sum_{n=1}^{\infty} \frac{1}{n^{\frac{3}{2}}} \frac{\sin\left\{\frac{4\pi}{\epsilon} n s(e,0) + \sigma\frac{\pi}{4}\right\}}{\sqrt{|s_{xx}(e,0)|}}. \tag{6.117}$$

6.1.9 Integrated density of states

The integrated density of states, computed up to the order ϵ^0, is

$$N(e) = N_0(e) + N_1(e) + N_{stat}(e) + N_\lambda(e) + N_\nu(e) + o(\epsilon^0), \tag{6.118}$$

where the smooth contribution is

$$\begin{aligned} N_0(e) + N_1(e) &= \frac{s}{4\pi\epsilon^2} \int_{\mathbb{R}^2} \mathrm{d}^2\boldsymbol{x}(e - V(|\boldsymbol{x}|))_+ \\ &\quad - \frac{s}{48\pi} \int \mathrm{d}^2\boldsymbol{x} \Delta V(r) \delta(e - V(r)) \\ &\quad + \frac{s}{12 s_x(e, \lambda^e)}, \end{aligned} \tag{6.119}$$

where the terms come from the N_0, N_1, N_{osc}^{I} and N_{osc}^{II} parts of $N(e)$.

The terms from the stationary phase approximation are given by N_{osc}^{IIa}:

$$N_{stat}(e) = \frac{2s}{\pi\sqrt{\epsilon}} \sum_{\{k,j|\, \mathrm{gcd}(k,j)=1\}}{}' \frac{(-1)^{nj}}{n^{\frac{3}{2}} j^{\frac{3}{2}}} \frac{\sin\left\{\frac{2\pi}{\epsilon} n[kx^\star + js(e,x^\star)] + \sigma\frac{\pi}{4}\right\}}{\sqrt{|s_{xx}(e,x^\star)|}} \tag{6.120}$$

The λ oscillations are given by N_{osc}^{IIc} and N_λ^{II}:

$$\begin{aligned} N_\lambda(e) &= -\frac{s}{\pi\sqrt{\epsilon}} \sum_{j=1}^{\infty} \sum_{k=-\infty}^{\infty} \Bigg|_{x^\star = \lambda^e} \frac{(-1)^j}{j^{\frac{3}{2}}} \frac{\sin\left\{\frac{2\pi}{\epsilon} k\lambda^e + \sigma\frac{\pi}{4}\right\}}{\sqrt{|s_{xx}(e,\lambda^e)|}} \\ &\quad - \frac{s}{2\pi} \sum_{k\neq 0} \frac{1}{k} \frac{\cos\left\{\frac{2\pi}{\epsilon} k\lambda^e\right\}}{\sin\left(\frac{\pi k}{|s_x(e,\lambda^e)|}\right)}. \end{aligned} \tag{6.121}$$

The ν oscillations are given by N_{osc}^{IIb} only:

$$N_\nu(e) = \frac{s}{\pi\sqrt{8\epsilon}} \sum_{n=1}^{\infty} \frac{1}{n^{\frac{3}{2}}} \frac{\sin\left\{\frac{4\pi}{\epsilon} n s(e,0) + \sigma\frac{\pi}{4}\right\}}{\sqrt{|s_{xx}(e,0)|}}. \tag{6.122}$$

6.2 Computation of the energy of the system

As it was established previously, one part of the ground state energy is derived from the integrated density of states, and is given by

$$E(\mu) = \int^{\mu} \mathrm{d}e N(e) = \int_{V_0}^{\mu} \mathrm{d}e N(e). \tag{6.123}$$

$V_0 \doteq V(0)$ is the smallest value the chemical potential can have: it is the smallest value of the energy, corresponding to a kinetic energy of 0, and the smallest possible potential energy (the potential is a monotonous growing function of r, its smallest value is at $r = 0$).

This integration over e implies some technical difficulties, which can be avoided if we first integrate over e, then over x. This is what we will do to compute this term.

The term to compute is established in the same way than for $N(e)$ in formula (6.60). We have to compute

$$\begin{aligned} E(\mu) &= \frac{s}{\epsilon^2} \sum_{k=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \int_{V_0}^{\mu} \mathrm{d}e \int_{-\lambda^e}^{\lambda^e} \mathrm{d}x \int_0^{s(e,x)} \mathrm{d}\nu (-1)^j \exp\left\{\frac{2\pi i}{\epsilon} kx\right\} \exp\left\{\frac{2\pi i}{\epsilon} j\nu\right\} \\ &= \frac{2s}{\epsilon^2} \sum_{k=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \int_0^{\lambda^\mu} \mathrm{d}x \int_{e^x}^{\mu} \mathrm{d}e \int_0^{s(e,x)} \mathrm{d}\nu (-1)^j \exp\left\{\frac{2\pi i}{\epsilon} kx\right\} \exp\left\{\frac{2\pi i}{\epsilon} j\nu\right\}, \end{aligned} \tag{6.124}$$

where e^x is a function of x defined by $s(e^x, x) = 0$. The factor 2 comes from the fact that we integrate only over the positive values of x.

6.2.1 Thomas-Fermi model

The Thomas-Fermi term, which corresponds to the $k = 0, j = 0$ term, is obtained from (6.62), which we integrate over e. There is no convergence problem, we obtain

$$E_0(\mu) = \int_{V_0}^{\mu} \mathrm{d}e N_{TF}(e) = \frac{s}{8\pi\epsilon^2} \int_{\mathbb{R}^2} \mathrm{d}^2\boldsymbol{x} (\mu - V(|\boldsymbol{x}|))_+^2. \tag{6.125}$$

6.2.2 First correction to WKB quantization

The first correction to WKB arising from the quantization condition was already computed at (6.55). Adding the spin factor we find

$$E_1(\mu) = -\frac{s}{48\pi} \int \mathrm{d}^2\boldsymbol{x} \Delta V(r) \theta(\mu - V(r)) + \frac{s\mu}{12}. \tag{6.126}$$

6.2.3 l-quantized Thomas-Fermi model

To compute the contribution from the lTF model, which arises from the terms $j=0, k \neq 0$ from the sum (6.124), we first integrate over e:

$$\begin{aligned} E^I_{osc}(\mu) &= \frac{2s}{\epsilon^2}\sum_{k\neq 0}\int_0^{\lambda^\mu} \mathrm{d}x \int_{e^x}^{\mu} \mathrm{d}e \; s(e,x)\exp\left\{\frac{2\pi i}{\epsilon}kx\right\} \\ &= \frac{2s}{\epsilon^2}\sum_{k\neq 0}\int_0^{\lambda^\mu} \mathrm{d}x S(\mu,x)\cos\left\{\frac{2\pi}{\epsilon}kx\right\}, \end{aligned} \tag{6.127}$$

where

$$S(\mu,x) \doteq \int^{\mu} \mathrm{d}e s(e,x) = \frac{2}{3\pi}\int \mathrm{d}r\left(\mu - V(r) - \frac{x^2}{r^2}\right)^{\frac{3}{2}}. \tag{6.128}$$

We have used the equality $\sum_{k\neq 0}\sin\{\frac{2\pi}{\epsilon}kx\} = 0$, because the sine function is odd, and $S(e^x,x)=0$.

We extract the terms of lowest order in ϵ by integrating by parts:

$$\begin{aligned} &\int_0^{\lambda^\mu} \mathrm{d}x S(\mu,x)\cos\left\{\frac{2\pi}{\epsilon}kx\right\} \\ &= \frac{\epsilon}{2\pi k}S(\mu,x)\sin\left\{\frac{2\pi}{\epsilon}kx\right\}\Bigg|_{x=0}^{x=\lambda^\mu} - \frac{\epsilon}{2\pi k}\int_0^{\lambda^\mu}\mathrm{d}x S_x(\mu,x)\sin\left\{\frac{2\pi}{\epsilon}kx\right\} \\ &= -\frac{\epsilon}{2\pi k}\int_0^{\lambda^\mu}\mathrm{d}x S_x(\mu,x)\sin\left\{\frac{2\pi}{\epsilon}kx\right\} \\ &= \underbrace{\frac{\epsilon^2}{(2\pi k)^2}S_x(\mu,\lambda^\mu)\cos\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}}_{=0} - \frac{\epsilon^2}{(2\pi k)^2}S_x(\mu,0) \\ &\quad - \frac{\epsilon^2}{(2\pi k)^2}\int_0^{\lambda^\mu}\mathrm{d}x S_{xx}(\mu,x)\cos\left\{\frac{2\pi}{\epsilon}kx\right\} \\ &= -\frac{\epsilon^2}{(2\pi k)^2}\underbrace{S_x(\mu,0)}_{=-\frac{\mu}{2}} - \frac{\epsilon^3}{(2\pi k)^3}S_{xx}(\mu,\lambda^\mu)\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\} + o(\epsilon^3). \end{aligned} \tag{6.129}$$

We used the results $S(\mu,\lambda^\mu)=0$, and $S(\mu,0)<\infty$ to establish the second equality. The result $S_x(\mu,\lambda^\mu)=0$ is also obvious. The result $\lim_{x\to 0}S_x(\mu,x) = -\frac{\mu}{2}$ is established in the annex 6.3.2. We also used the result $S_{xx}(\mu,0)<\infty$.

The order of the rest is estimated using the Riemann-Lebesgue lemma and using

$$\int \mathrm{d}x\,|S_{xxx}(\mu,x)| < \infty. \tag{6.130}$$

The lTF contribution to the energy is finally

$$\begin{aligned} E^{I}_{osc}(\mu) &= \sum_{k\neq 0} \frac{s\mu}{(2\pi k)^2} - \sum_{k\neq 0} \frac{s\epsilon}{4(\pi k)^3} S_{xx}(\mu,\lambda^{\mu}) \sin\left\{\frac{2\pi}{\epsilon}k\lambda^{\mu}\right\} + o(\epsilon) \\ &= \frac{s\mu}{12} - \sum_{k=1}^{\infty} \frac{s\epsilon}{2(\pi k)^3} S_{xx}(\mu,\lambda^{\mu}) \sin\left\{\frac{2\pi}{\epsilon}k\lambda^{\mu}\right\} + o(\epsilon), \end{aligned} \tag{6.131}$$

where we used the equality $\sum_{k=1}^{\infty}\frac{1}{k^2}=\frac{\pi^2}{6}$, and the fact that the function $\frac{\sin(k)}{k^3}$ is even.

The term $\frac{s\mu}{12}$ will cancel the constant term arising from the smooth correction to WKB in equation (6.126).

Let's note that this result can be obtained by integrating (6.69) over e, and proceeding to integrations by parts. We obtain

$$E^{I}_{osc}(\mu) = \frac{s\mu}{12} + \sum_{k=1}^{\infty} \frac{s\epsilon}{2(\pi k)^3} \frac{s_x(\mu,\lambda^{\mu})}{\lambda^{\mu}_{e}} \sin\left\{\frac{2\pi}{\epsilon}k\lambda^{\mu}\right\} + o(\epsilon). \tag{6.132}$$

Some calculations provide the result:

$$S_{xx}(\mu,\lambda^{\mu}) = -\frac{s_x(\mu,\lambda^{\mu})}{\lambda^{\mu}_{e}} = \frac{2W_{\star}}{r_{\star}^3}\sqrt{\frac{2}{|W''_{\star}|}}, \tag{6.133}$$

where $W(r) \doteq r^2(\mu - V(r))$, and $r_{\star}$ is defined by $W'(r_{\star}) = 0$, and $W_{\star} \doteq W(r_{\star})$, $W''_{\star} \doteq W''(r_{\star})$.

To obtain these results, we calculate the functions in this way: $f(x^e, e) = \lim_{x\to x^e} f(x,e)$, and $f(x, e^x) = \lim_{e\to e^x} f(x,e)$.

6.2.4 Complete model

We still have to compute the energy arising from the other terms, those with $j \neq 0, k \in \mathbb{Z}$. This expression is obtained in the same way than for the integrated density of states, we find

$$\begin{aligned} E^{II}_{osc}(\mu) &= \frac{2s}{\epsilon^2}\sum_{j\neq 0}\sum_{k=-\infty}^{\infty}\int_0^{\lambda^{\mu}}\mathrm{d}x\int_{e^x}^{\mu}\mathrm{d}e\int_0^{s(e,x)}\mathrm{d}\nu(-1)^j \exp\left\{\frac{2\pi i}{\epsilon}kx\right\}\exp\left\{\frac{2\pi i}{\epsilon}j\nu\right\} \\ &= \frac{s}{\pi i\epsilon}\sum_{j\neq 0}\sum_{k=-\infty}^{\infty}\int_0^{\lambda^{\mu}}\mathrm{d}x\frac{(-1)^j}{j}\exp\left\{\frac{2\pi i}{\epsilon}kx\right\}\int_{e^x}^{\mu}\mathrm{d}e \exp\left\{\frac{2\pi i}{\epsilon}js(e,x)\right\}. \end{aligned} \tag{6.134}$$

To proceed further we integrate by parts over e:

$$\begin{aligned}
&\int_{e^x}^{\mu} \mathrm{d}e \frac{1}{s_e(e,x)} s_e(e,x) \exp\left\{\frac{2\pi i}{\epsilon} j s(e,x)\right\} \\
&\qquad = \frac{\epsilon}{2\pi j i} \frac{\exp\left\{\frac{2\pi i}{\epsilon} j s(\mu,x)\right\}}{s_e(\mu,x)} - \frac{\epsilon}{2\pi j i} \frac{\exp\left\{\frac{2\pi i}{\epsilon} j s(e^x,x)\right\}}{s_e(e^x,x)} \\
&\qquad\quad + \frac{\epsilon}{2\pi j i} \int_{e^x}^{\mu} \mathrm{d}e \frac{s_{ee}(e,x)}{s_e^2(e,x)} \exp\left\{\frac{2\pi i}{\epsilon} j s(e,x)\right\} \\
&\qquad = \frac{\epsilon}{2\pi j i} \frac{\exp\left\{\frac{2\pi i}{\epsilon} j s(\mu,x)\right\}}{s_e(\mu,x)} - \frac{\epsilon}{2\pi j i} \frac{1}{s_e(e^x,x)} + o(\epsilon),
\end{aligned} \tag{6.135}$$

where we used the fact that $s(e^x, x) = 0$, and (using the Riemann-Lebesgue lemma)

$$\int_{e^x}^{\mu} \mathrm{d}e \left| \frac{s_{ee}(e,x)}{s_e^2(e,x)} \right| < \infty \tag{6.136}$$

to establish the order of the rest.

The complete expression is then

$$\begin{aligned}
E_{osc}^{II}(\mu) &= -\frac{s}{2\pi^2} \sum_{j\neq 0} \sum_{k=-\infty}^{\infty} \int_0^{\lambda\mu} \mathrm{d}x \frac{(-1)^j}{j^2} \left(\frac{\exp\left\{\frac{2\pi i}{\epsilon}[kx + j s(\mu,x)]\right\}}{s_e(\mu,x)} \right. \\
&\qquad \left. - \frac{\exp\left\{\frac{2\pi i}{\epsilon} kx\right\}}{s_e(e^x,x)} \right) \\
&= -\frac{s}{\pi^2} \Re \left\{ \sum_{j=1}^{\infty} \sum_{k=-\infty}^{\infty} \int_0^{\lambda\mu} \mathrm{d}x \frac{(-1)^j}{j^2} \left(\frac{\exp\left\{\frac{2\pi i}{\epsilon}[kx + j s(\mu,x)]\right\}}{s_e(\mu,x)} \right. \right. \\
&\qquad \left. \left. - \frac{\exp\left\{\frac{2\pi i}{\epsilon} kx\right\}}{s_e(e^x,x)} \right) \right\} \\
&= -\frac{s}{\pi^2} \sum_{j=1}^{\infty} \sum_{k=-\infty}^{\infty} \int_0^{\lambda\mu} \mathrm{d}x \frac{(-1)^j}{j^2} \frac{\cos\left\{\frac{2\pi}{\epsilon}[kx + j s(\mu,x)]\right\}}{s_e(\mu,x)} \\
&\quad + \frac{s}{\pi^2} \sum_{j=1}^{\infty} \sum_{k=-\infty}^{\infty} \int_0^{\lambda\mu} \mathrm{d}x \frac{(-1)^j}{j^2} \frac{\cos\left\{\frac{2\pi}{\epsilon} kx\right\}}{s_e(e^x,x)}
\end{aligned}$$

$$\begin{aligned}
= & -\frac{s}{\pi^2}\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty}\int_0^{\lambda^\mu}\mathrm{d}x\frac{(-1)^j}{j^2}\frac{\cos\left\{\frac{2\pi}{\epsilon}[kx+js(\mu,x)]\right\}}{s_e(\mu,x)} \\
& +\frac{s}{\pi^2}\sum_{j=1}^{\infty}\sum_{k\neq 0}\int_0^{\lambda^\mu}\mathrm{d}x\frac{(-1)^j}{j^2}\frac{\cos\left\{\frac{2\pi}{\epsilon}kx\right\}}{s_e(e^x,x)} \\
& -\frac{s}{12}\int_0^{\lambda^\mu}\mathrm{d}x\frac{1}{s_e(e^x,x)},
\end{aligned} \tag{6.137}$$

where we used formulas equivalent to (6.75), (6.76), and $\sum_{j=1}^{\infty}\frac{(-1)^j}{j^2}=-\frac{\pi^2}{12}$.

We can now perform the integration over x. Let's consider the two terms separately. The first one is computed exactly in the same way than in the computation of the integrated density of states. The dominating contribution is given by a stationary phase, for the pairs (k,j) such that $x^\star(\mu,k,j)\in[0,\lambda^\mu]$, where $x^\star(\mu,k,j)$ is defined by

$$s_x(\mu,x^\star)=-\frac{k}{j}. \tag{6.138}$$

If $x^\star(\mu,k,j)=0$, we obtain ν oscillations. If $x^\star(\mu,k,j)\in]0,\lambda^\mu[$, we obtain normal oscillations. If $x^\star(\mu,k,j)=\lambda^\mu$, we obtain λ oscillations.

If the point $x^\star(\mu,k,j)$ does not exist for a pair (k,j), we calculate the energy by integrations by parts only. Hence we have to consider four families of pairs (k,j), and proceed exactly in the same way than for the computation of the integrated density of states.

We obtain four different types of terms. By analogy with the results (6.93), (6.96), (6.99), and (6.101), we find

$$E_{osc}^{IIa}(\mu)=-\frac{s\sqrt{\epsilon}}{\pi^2}{\sum_{k,j}}'\frac{(-1)^j}{j^{\frac{5}{2}}}\frac{\cos\left\{\frac{2\pi}{\epsilon}[kx^\star+js(\mu,x^\star)]+\frac{\sigma\pi}{4}\right\}}{s_e(\mu,x^\star)\sqrt{|s_{xx}(\mu,x^\star)|}}, \tag{6.139}$$

where the sum runs over all the pairs (k,j) such that $x^\star(\mu,k,j)\in]0,\lambda^\mu[$.

$$E_{osc}^{IIb}(\mu)=-\frac{s\sqrt{\epsilon}}{8\sqrt{2}\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^{\frac{5}{2}}}\frac{\cos\left\{\frac{4\pi}{\epsilon}[ns(\mu,0)]+\frac{\sigma\pi}{4}\right\}}{s_e(\mu,0)\sqrt{|s_{xx}(\mu,0)|}}. \tag{6.140}$$

We proceeded to the sum over the saddle points which are equal to 0. In this case, we have $s_x(\mu,0)=-\frac{1}{2}$, which provides the relation $2k=j$, which was used to obtain this result.

$$E_{osc}^{IIc}(\mu)=-\frac{s\sqrt{\epsilon}}{2\pi^2}\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty}\Bigg|_{x^\star=\lambda^\mu}\frac{(-1)^j}{j^{\frac{5}{2}}}\frac{\cos\left\{\frac{2\pi}{\epsilon}k\lambda^\mu+\frac{\sigma\pi}{4}\right\}}{s_e(\mu,\lambda^\mu)\sqrt{|s_{xx}(\mu,\lambda^\mu)|}}. \tag{6.141}$$

The sum runs over the pairs (k,j) such that $k=-js_e(\mu,\lambda^\mu)$. This means that if $s_e(\mu,\lambda^\mu)$ is irrational this sum is zero.

The first contribution beyond the saddle-point approximation is zero:

$$\begin{aligned} E^{IIe}_{osc}(\mu) &= \frac{s\epsilon}{2\pi^3} \sum_{j=1}^{\infty} \sum_{k=-\infty}^{\infty} \Bigg|_{j\neq 2k} \frac{(-1)^j}{j^2} \frac{\sin\left\{\frac{2\pi}{\epsilon} j s(\mu,0)\right\}}{s_e(\mu,0)[k+js_x(\mu,0)]} \\ &= \frac{s\epsilon}{\pi^3} \sum_{j=1}^{\infty} \sum_{k=-\infty}^{\infty} \Bigg|_{j\neq 2k} \frac{(-1)^j}{j^2} \frac{\sin\left\{\frac{2\pi}{\epsilon} j s(\mu,0)\right\}}{s_e(\mu,0)(2k-j)} \\ &= 0, \end{aligned} \tag{6.142}$$

for the same reason than the reason why $N^{IIe}_{osc} = 0$.

The second contribution beyond the saddle-point approximation is

$$\begin{aligned} E^{IId}_{osc}(\mu) &= -\frac{s\epsilon}{2\pi} \frac{1}{\pi^2} \sum_{j=1}^{\infty} \sum_{k=-\infty}^{\infty} \Bigg|_{k\neq -s_x(\mu,\lambda^\mu)j} \frac{(-1)^j}{j^2} \frac{\sin\left\{\frac{2\pi}{\epsilon} k\lambda^\mu\right\}}{s_e(\mu,\lambda^\mu)[k+js_x(\mu,\lambda^\mu)]} \\ &= -\frac{s\epsilon}{2\pi} \frac{1}{\pi^2} \sum_{j=1}^{\infty} \sum_{k\neq 0} \Bigg|_{k\neq -s_x(\mu,\lambda^\mu)j} \frac{(-1)^j}{j^2} \frac{\sin\left\{\frac{2\pi}{\epsilon} k\lambda^\mu\right\}}{s_e(\mu,\lambda^\mu)[k+js_x(\mu,\lambda^\mu)]}. \end{aligned} \tag{6.143}$$

If $s_x(\mu,\lambda^\mu)$ is irrational, the sum has no restriction. The term $k=0$ is not oscillatory. This term is however 0, because it is multiplied by $\sin(0)$.

We still have to compute the second term of the expression (6.137). We integrate over x by parts

$$\int_0^{\lambda^\mu} \mathrm{d}x \frac{\cos\left\{\frac{2\pi}{\epsilon} kx\right\}}{s_e(e^x,x)} = \frac{\epsilon}{2\pi k} \frac{\sin\left\{\frac{2\pi}{\epsilon} k\lambda^\mu\right\}}{s_e(\mu,\lambda^\mu)} + o(\epsilon) \tag{6.144}$$

to obtain

$$+\frac{s}{\pi^2} \sum_{j=1}^{\infty} \sum_{k\neq 0} \int_0^{\lambda^\mu} \mathrm{d}x \frac{(-1)^j}{j^2} \frac{\cos\left\{\frac{2\pi}{\epsilon} kx\right\}}{s_e(e^x,x)} = \frac{s\epsilon}{2\pi^3} \sum_{j=1}^{\infty} \sum_{k\neq 0} \frac{(-1)^j}{j^2} \frac{\sin\left\{\frac{2\pi}{\epsilon} k\lambda^\mu\right\}}{k\ s_e(\mu,\lambda^\mu)}. \tag{6.145}$$

Summing this term with (6.143) we obtain

$$\begin{aligned} &-\frac{s\epsilon}{2\pi^3} \sum_{j=1}^{\infty} \sum_{k\neq 0} \frac{(-1)^j}{j^2} \left(\frac{1}{s_e(\mu,\lambda^\mu)[k+js_x(\mu,\lambda^\mu)]} - \frac{1}{k\ s_e(\mu,\lambda^\mu)} \right) \sin\left\{\frac{2\pi}{\epsilon} k\lambda^\mu\right\} \\ &\qquad = -\frac{s\epsilon}{2\pi^3} \sum_{j=1}^{\infty} \sum_{k\neq 0} \frac{(-1)^j}{j^2} \frac{1}{s_e(\mu,\lambda^\mu)} \frac{-js_x(\mu,\lambda^\mu)}{k(k+js_x(\mu,\lambda^\mu))} \sin\left\{\frac{2\pi}{\epsilon} k\lambda^\mu\right\} \\ &\qquad = -\frac{s\epsilon}{2\pi^3} \sum_{j=1}^{\infty} \sum_{k\neq 0} \frac{(-1)^j}{j} \frac{1}{k\lambda^\mu_e(k+js_x(\mu,\lambda^\mu))} \sin\left\{\frac{2\pi}{\epsilon} k\lambda^\mu\right\}. \end{aligned} \tag{6.146}$$

We used the following result:

$$s_e(\mu, \lambda^\mu) = -\lambda^\mu_e s_x(\mu, \lambda^\mu), \tag{6.147}$$

which comes from the condition (which is the definition of λ^μ)

$$s(e, \lambda^e) = 0 \ \forall e \ \Rightarrow \frac{\mathrm{d}}{\mathrm{d}e} s(e, \lambda^e) = s_e(e, \lambda^e) + \lambda^e_e s_x(e, \lambda^e) = 0. \tag{6.148}$$

The result is exactly the result we would obtain if we integrated the second term of (6.103). This means that the integration over x and e is commutative.

The third term of (6.137) is the same as the one which arises from the integration over e of the first term of (6.103):

$$-\frac{1}{12}\int_0^{\lambda^\mu} \mathrm{d}x \frac{1}{s_e(e^x, x)} = -\frac{1}{12}\int_{V_0}^{\mu} \mathrm{d}e \frac{\lambda^e}{s_e(e, \lambda^e_e)} = \frac{1}{12}\int_{V_0}^{\mu} \mathrm{d}e \frac{1}{s_x(e, \lambda^e)}, \tag{6.149}$$

where we performed the change of variable $x \mapsto e = e^x \Rightarrow x = \lambda^e$, $\lambda^e_e \mathrm{d}e = \mathrm{d}x$ and used the equality (6.148).

6.2.5 λ oscillations

The λ oscillations can be grouped, in the same way as was done for the integrated density of states. To do it, let's use the equality

$$\frac{(-1)^j}{kj(k + js_x(e, \lambda^e))} = \frac{(-1)^j}{k^2}\left(\frac{1}{j} - \frac{s_x(e, \lambda^e)}{(k + js_x(e, \lambda^e))}\right), \tag{6.150}$$

and

$$\sum_{k \neq 0} \frac{1}{k^2} \sin\left\{\frac{2\pi}{\epsilon} k\lambda^e\right\} = 0, \tag{6.151}$$

because this function is odd in the variable k.

This allows us to rewrite the sum (6.146) as

$$\begin{aligned} &-\frac{s\epsilon}{2\pi^3}\frac{1}{\lambda^\mu_e}\sum_{j=1}^{\infty}\sum_{k \neq 0}\frac{(-1)^j}{j}\frac{1}{k(k + js_x(\mu, \lambda^\mu))}\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\} \\ &\qquad = \frac{s\epsilon}{2\pi^3}\frac{s_x(\mu, \lambda^\mu)}{\lambda^\mu_e}\sum_{j=1}^{\infty}\sum_{k \neq 0}\frac{(-1)^j}{k^2}\frac{1}{(k + js_x(\mu, \lambda^\mu))}\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}. \end{aligned} \tag{6.152}$$

We will now sum this contribution with that arising from the lTF model (6.132):

$$\begin{aligned}
&\frac{s\epsilon}{2\pi^3}\frac{s_x(\mu,\lambda^\mu)}{\lambda_e^\mu}\sum_{k\neq 0}\left[\frac{1}{2k^3}+\sum_{j=1}^{\infty}\frac{(-1)^j}{k^2}\frac{1}{(k+js_x(\mu,\lambda^\mu))}\right]\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}\\
&\quad=\frac{s\epsilon}{2\pi^3}\frac{s_x(\mu,\lambda^\mu)}{\lambda_e^\mu}\sum_{k\neq 0}\frac{1}{k^2}\left[\frac{1}{2k}+\sum_{j=1}^{\infty}\frac{(-1)^j}{(k+js_x(\mu,\lambda^\mu))}\right]\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}\\
&\quad=\frac{s\epsilon}{4\pi^3}\frac{s_x(\mu,\lambda^\mu)}{\lambda_e^\mu}\sum_{k\neq 0}\frac{1}{k^2}\left[\frac{1}{k}+\sum_{j\neq 0}\frac{(-1)^j}{(k+js_x(\mu,\lambda^\mu))}\right]\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}\\
&\quad=\frac{s\epsilon}{4\pi^3}\frac{s_x(\mu,\lambda^\mu)}{\lambda_e^\mu}\sum_{k\neq 0}\frac{1}{k^2}\sum_{j=-\infty}^{\infty}\frac{(-1)^j}{(k+js_x(\mu,\lambda^\mu))}\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}\\
&\quad=\frac{s\epsilon}{4\pi^3}\frac{s_x(\mu,\lambda^\mu)}{\lambda_e^\mu}\sum_{k\neq 0}\frac{1}{k^2}\frac{\pi}{s_x(\mu,\lambda^\mu)}\sum_{j=-\infty}^{\infty}\frac{(-1)^j}{\left(\frac{\pi k}{s_x(\mu,\lambda^\mu)}+\pi j\right)}\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}\\
&\quad=\frac{s\epsilon}{4\pi^2}\frac{1}{\lambda_e^\mu}\sum_{k\neq 0}\frac{1}{k^2}\frac{\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}}{\sin\left\{\pi\frac{k}{s_x(\mu,\lambda^\mu)}\right\}}\\
&\quad=-\frac{s\epsilon}{4\pi^2}\frac{1}{\lambda_e^\mu}\sum_{k\neq 0}\frac{1}{k^2}\frac{\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}}{\sin\left\{\frac{\pi k}{|s_x(\mu,\lambda^\mu)|}\right\}},
\end{aligned}\tag{6.153}$$

where we used the equality

$$\sum_{j=-\infty}^{\infty}\frac{(-1)^j}{(x+\pi j)}=\frac{1}{\sin(x)}.\tag{6.154}$$

This result can be obtained by integrating directly over e the integrated density of states N_λ (6.113), proceeding by integrations by parts.

The result can be written explicitly, using the results

$$s_x(\mu,\lambda^\mu)=-\frac{1}{r_\star}\sqrt{\frac{2W_\star}{W''_\star}}\tag{6.155}$$

and

$$\lambda_e^\mu=\frac{r_\star^2}{2\sqrt{W_\star}}.\tag{6.156}$$

We obtain

$$E_\lambda(\mu)=-\frac{s\epsilon}{2\pi^2}\frac{\sqrt{W_\star}}{r_\star^2}\sum_{k\neq 0}\frac{1}{k^2}\frac{\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}}{\sin\left\{\frac{\pi k r_\star\sqrt{W''_\star}}{\sqrt{2W_\star}}\right\}}.\tag{6.157}$$

The complete λ oscillations are therefore, from E_{osc}^{IIc} and E_{osc}^{IId}:

$$\begin{aligned} E_\lambda(\mu) &= -\frac{s\sqrt{\epsilon}}{2\pi^2}\sum_{j=1}^{\infty}\sum_{k=-\infty}^{\infty}\Bigg|_{x^\star=\lambda^\mu}\frac{(-1)^j}{j^{\frac{5}{2}}}\frac{\cos\left\{\frac{2\pi}{\epsilon}k\lambda^\mu+\frac{\sigma\pi}{4}\right\}}{s_e(\mu,\lambda^\mu)\sqrt{|s_{xx}(\mu,\lambda^\mu)|}} \\ &\quad -\frac{s\epsilon}{2\pi^2}\frac{\sqrt{W_\star}}{r_\star^2}\sum_{k\neq 0}\frac{1}{k^2}\frac{\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}}{\sin\left\{\frac{\pi k r_\star\sqrt{W_\star''}}{\sqrt{2W_\star}}\right\}}. \end{aligned} \tag{6.158}$$

6.2.6 ν oscillations

The ν oscillations are only given by the stationary phase terms, E_{osc}^{IIb}. They are

$$E_\nu(\mu) = -\frac{s\sqrt{\epsilon}}{8\sqrt{2}\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^{\frac{5}{2}}}\frac{\cos\left\{\frac{4\pi}{\epsilon}[ns(\mu,0)]+\frac{\sigma\pi}{4}\right\}}{s_e(\mu,0)\sqrt{|s_{xx}(\mu,0)|}}. \tag{6.159}$$

6.2.7 Energy oscillations

The complete energy is given by

$$E(\mu) = E_0(\mu) + E_1(\mu) + E_{stat}(\mu) + E_\lambda(\mu) + E_\nu(\mu), \tag{6.160}$$

where

$$\left\{\begin{array}{lcl} E_0(\mu)+E_1(\mu) & = & \frac{s}{8\pi\epsilon^2}\int_{\mathbb{R}^2}\mathrm{d}^2\boldsymbol{x}(\mu-V(|\boldsymbol{x}|))_+^2 - \frac{s}{48\pi}\int\mathrm{d}^2\boldsymbol{x}\Delta V(r)\theta(\mu-V(r)) \\ & & +\frac{s}{12}\int_0^\mu\mathrm{d}e\frac{1}{s_x(e,\lambda^e)}, \\ E_{stat}(\mu) & = & -\frac{s\sqrt{\epsilon}}{\pi^2}\sum_{k,j}{}' \frac{(-1)^j}{j^{\frac{5}{2}}}\frac{\cos\left\{\frac{2\pi}{\epsilon}[kx^\star+js(\mu,x^\star)]+\frac{\sigma\pi}{4}\right\}}{s_e(\mu,x^\star)\sqrt{|s_{xx}(\mu,x^\star)|}}, \\ E_\lambda(\mu) & = & -\frac{s\epsilon}{2\pi^2}\frac{\sqrt{W_\star}}{r_\star^2}\sum_{k\neq 0}\frac{1}{k^2}\frac{\sin\left\{\frac{2\pi}{\epsilon}k\lambda^\mu\right\}}{\sin\left\{\frac{\pi k r_\star\sqrt{W_\star''}}{\sqrt{2W_\star}}\right\}}, \\ E_\nu(\mu) & = & -\frac{s\sqrt{\epsilon}}{8\sqrt{2}\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^{\frac{5}{2}}}\frac{\cos\left\{\frac{4\pi}{\epsilon}[ns(\mu,0)]+\frac{\sigma\pi}{4}\right\}}{s_e(\mu,0)\sqrt{|s_{xx}(\mu,0)|}}. \end{array}\right. \tag{6.161}$$

We supposed that λ^μ is irrational, which implies that there are no λ oscillations of the order $\sqrt{\epsilon}$. For quantum dots (see chapter 8), it is the case. It is an interesting question to know whether this is the case in any system or not.

6.3 Annex

6.3.1 Computation of $\lim_{x\to 0} s_x(e,x)$

From the definition (6.3) of s, we establish that its derivative with respect to x is

$$\begin{aligned} s_x(e,x) &= -\frac{x}{\pi}\int_{r_1(e,x)}^{r_2(e,x)} \frac{\mathrm{d}r}{r^2}\frac{1}{\sqrt{e-V(r)-\frac{x^2}{r^2}}} \\ &\quad +\frac{r_{2x}(e,x)}{\pi}\sqrt{e-V(r_2(e,x))-\frac{x^2}{r_2^2(e,x)}} \\ &\quad -\frac{r_{1x}(e,x)}{\pi}\sqrt{e-V(r_1(e,x))-\frac{x^2}{r_1^2(e,x)}}, \end{aligned} \tag{6.162}$$

where $r_{ix},\ i=1,2$, is the derivative of r_i with respect to x.

The two last terms are zero: $e-V(r_i(e,x))-\frac{x^2}{r_i^2(e,x)}=0,\ i=1,2$, is the definition of r_i.

The function is therefore

$$\begin{aligned} s_x(e,x) &= -\frac{x}{\pi}\int_{r_1(e,x)}^{r_2(e,x)} \frac{\mathrm{d}r}{r^2}\frac{1}{\sqrt{e-V(r)-\frac{x^2}{r^2}}} \\ &= -\frac{x}{\pi}\int_{r_1(e,x)}^{r_2(e,x)} \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2\left(e-V(r)\right)-x^2}}. \end{aligned} \tag{6.163}$$

In the limit $x \longrightarrow 0$, the lower bound of the integral tends to 0, which implies that the integrand (the term $\frac{1}{r}$) diverges. We have to determine how it diverges, and will see that it compensates the prefactor x in the expression of s_x.

We separate the integral in two terms:

$$\begin{aligned} \int_{r_1(e,x)}^{r_2(e,x)} \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2\left(e-V(r)\right)-x^2}} &= \int_{r_1(e,x)}^{r_0} \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2\left(e-V(r)\right)-x^2}} \\ &\quad +\int_{r_0}^{r_2(e,x)} \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2\left(e-V(r)\right)-x^2}}, \end{aligned} \tag{6.164}$$

where $r_0 \ll 1$ is such that the potential V can be expanded in a Taylor series in the first term: $V(r)=V_0+V_0'r+\frac{1}{2}V_0''r^2+\mathcal{O}(r^3)$. The second term is finite and will therefore be cancelled by the prefactor x in the limit $x \longrightarrow 0$. Let's focus on the first term:

$$\begin{aligned}\int_{r_1(e,x)}^{r_0} \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2\left(e-V(r)\right)-x^2}} &\simeq \int_{r_1(e,x)}^{r_0} \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2\left(e-V_0\right)-x^2}}\\ &= \frac{1}{x}\int_1^{\frac{\alpha}{x}} \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2-1}}\\ &\xrightarrow{x\to 0} \frac{1}{x}\underbrace{\int_1^{\infty} \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2-1}}}_{=\frac{\pi}{2}} = \frac{1}{x}\frac{\pi}{2}, \qquad (6.165)\end{aligned}$$

where we proceeded to the change of variable $r \mapsto r' = \frac{r\sqrt{e-V_0}}{x}$.

Returning to the expression (6.163) of s_x we find

$$\lim_{x\to 0} s_x(e,x) = -\frac{1}{2}. \qquad (6.166)$$

This result is universal, it does not depend on the nature of the potential, whose condition is only to be $\mathcal{C}^1$ at $r=0$.

6.3.2 Computation of $\lim_{x\to 0} S_x(e,x)$

From the definition (6.128) of S, we establish that its derivative with respect to x is

$$\begin{aligned}S_x(e,x) &= -\frac{2x}{\pi}\int_{r_1(e,x)}^{r_2(e,x)} \frac{\mathrm{d}r}{r^2}\sqrt{e-V(r)-\frac{x^2}{r^2}}\\ &+\frac{2r_{2x}(e,x)}{3\pi}\left(e-V(r_2(e,x))-\frac{x^2}{r_2^2(e,x)}\right)^{\frac{3}{2}}\\ &-\frac{2r_{1x}(e,x)}{3\pi}\left(e-V(r_1(e,x))-\frac{x^2}{r_1^2(e,x)}\right)^{\frac{3}{2}}, \qquad (6.167)\end{aligned}$$

where $r_{ix},\ i=1,2$, is the derivative of r_i with respect to x.

The two last terms are zero: $e-V(r_i(e,x))-\frac{x^2}{r_i^2(e,x)} = 0,\ i=1,2$, is the definition of r_i.

The function is therefore

$$\begin{aligned}S_x(e,x) &= -\frac{2x}{\pi}\int_{r_1(e,x)}^{r_2(e,x)} \frac{\mathrm{d}r}{r^2}\sqrt{e-V(r)-\frac{x^2}{r^2}}\\ &= -\frac{2x}{\pi}\int_{r_1(e,x)}^{r_2(e,x)} \frac{\mathrm{d}r}{r^3}\sqrt{r^2\left(e-V(r)\right)-x^2}. \qquad (6.168)\end{aligned}$$

In the limit $x\longrightarrow 0$, the lower bound of the integral tends to 0, which implies that the integrand (the term $\frac{1}{r^3}$) diverges. We have to determine how it diverges, and will see that it compensates the prefactor x in the expression of S_x.

We separate the integral in two terms:

$$\begin{aligned}\int_{r_1(e,x)}^{r_2(e,x)} \frac{\mathrm{d}r}{r^3}\sqrt{r^2\left(e-V(r)\right)-x^2} &= \int_{r_1(e,x)}^{r_0} \frac{\mathrm{d}r}{r^3}\sqrt{r^2\left(e-V(r)\right)-x^2} \\ &\quad + \int_{r_0}^{r_2(e,x)} \frac{\mathrm{d}r}{r^3}\sqrt{r^2\left(e-V(r)\right)-x^2},\end{aligned} \tag{6.169}$$

where $r_0 \ll 1$ is such that the potential V can be expanded in a Taylor series in the first term: $V(r) = V_0 + V_0' r + \frac{1}{2}V_0'' r^2 + \mathcal{O}(r^3)$. The second term is finite and will therefore be cancelled by the prefactor x in the limit $x \to 0$. Let's focus on the first term:

$$\begin{aligned}\int_{r_1(e,x)}^{r_0} \frac{\mathrm{d}r}{r^3}\sqrt{r^2\left(e-V(r)\right)-x^2} &\simeq \int_{r_1(e,x)}^{r_0} \frac{\mathrm{d}r}{r^3}\sqrt{r^2\left(e-V_0\right)-x^2} \\ &= \frac{(e-V_0)}{x}\int_1^{\frac{\alpha}{x}} \frac{\mathrm{d}r}{r^3}\sqrt{r^2-1} \\ &\xrightarrow{x\to 0} \frac{(e-V_0)}{x}\underbrace{\int_1^{\infty} \frac{\mathrm{d}r}{r^3}\frac{1}{\sqrt{r^2-1}}}_{=\frac{\pi}{4}} \\ &= \frac{(e-V_0)}{x}\frac{\pi}{4},\end{aligned} \tag{6.170}$$

where we proceeded to the change of variable $r \mapsto r' = \frac{r\sqrt{e-V_0}}{x}$.

Returning to the expression (6.168) of S_x we find

$$\lim_{x\to 0} S_x(e,x) = -\frac{(e-V_0)}{2}. \tag{6.171}$$

This result is universal, it does not depend on the nature of the potential, whose condition is only to be $\mathcal{C}^1$ at $r=0$.

Chapter 7

Analytical and numerical study of the self-consistent equation

Contents

The objective of this chapter is to obtain a solution of the self-consistent equation of a quantum dot, in order to introduce the self-consistent potential in the formulas of the ground state energy.

In chapter 5 we established formulas for the computation of the ground state energy of many-fermion systems. We obtained these results in the semiclassical Hartree-Fock framework, which was justified by the developments of chapter 2.

As our technique does not provide the oscillating terms, these were computed in chapter 6 in the specific two-dimensional case. All these formulas are functionals of a potential, the self-consistent potential. This self-consistent potential is solution of the self-consistent equation (5.45). As established in the developments of chapter 5, only the lowest order of this equation (5.125) has to be solved, so as to obtain results at the desired order in our small parameters.

In this chapter we start by establishing the self-consistent equation of our specific problem, a two-dimensional system with a parabolic confinement ($V^{ext}(x) = \frac{1}{2}\kappa x^2$). We are interested in having a solution for realistic experimental situations, for which $\kappa \ll 1$. There exists an analytical solution in the asymptotic limit $\kappa \to 0$. This limit motivates us to define a new basis of functions, in which the energy to minimize becomes a quadratic form, plus a linear term. We then use this new approach analytically and establish the already known limit $\kappa \to 0$, as well as a new limit $\kappa \to \infty$ (of no relevance for experimental work). Based on these limits, we use this new basis analytically by solving the problem in a restricted vector space, that is by considering a few basis elements instead of the complete basis. Unfortunately we face some difficulties: it is hard to do analytical developments for a large number of basis elements, and – even worse – the series are asymptotics: they diverge, very quickly if we consider only 5 basis elements. To verify these analytical developments, we proceed to numerical computations, in this new basis, on a bigger number of basis elements. We conclude that these analytical results have insufficient precision, which is why we finally solve the problem by doing numerical simulations. As we need functional relations, we have to proceed to many numerical simulations, and proceed to a polynomial fitting. We look for the optimal compromise between speed and precision, this is why we first calibrate our program. We finally obtain the energy and chemical potential of the system, as well as the density, and the radius of the dot. They are obtained as polynomial functions of $\kappa^{\frac{1}{3}}$. These results will be used in chapter 8, where we will make use of the formulas developed earlier.

7.1 Self-consistent equation

As derived in chapter 5, the self-consistent equation is, in terms of the density $\hat{\rho}$:

$$\pi\hat{\rho}(\hat{\boldsymbol{x}}) + \frac{1}{2}k\hat{\boldsymbol{x}}^2 + \int \mathrm{d}^2\hat{\boldsymbol{y}}\frac{\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|} = \hat{\mu}. \tag{7.1}$$

We restrict to the two-dimensional case. This equation corresponds to the minimization of the functional energy (which is the Thomas-Fermi energy)

$$\hat{E}^{TF}[\hat{\rho}] = \frac{\pi}{2}\int \mathrm{d}^2\hat{\boldsymbol{x}}\hat{\rho}^2(\hat{\boldsymbol{x}}) + \int \mathrm{d}^2\hat{\boldsymbol{x}}\frac{1}{2}k\hat{\boldsymbol{x}}^2\hat{\rho}(\hat{\boldsymbol{x}}) + \frac{1}{2}\int \mathrm{d}^2\hat{\boldsymbol{x}}\int \mathrm{d}^2\hat{\boldsymbol{y}}\frac{\hat{\rho}(\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|}, \tag{7.2}$$

with the normalization constraint

$$\int \mathrm{d}^2\hat{\boldsymbol{x}}\hat{\rho}(\hat{\boldsymbol{x}}) = N, \tag{7.3}$$

and the constraint of positivity

$$\hat{\rho}(\hat{\boldsymbol{x}}) \geq 0. \tag{7.4}$$

For simplicity, we normalize the density to 1, and introduce the parameter $\kappa \doteq \frac{k}{N}$. The Thomas-Fermi energy becomes

$$\frac{\hat{E}^{TF}[\hat{\rho}_1]}{N^2} = \frac{\pi}{2}\int \mathrm{d}^2\hat{\boldsymbol{x}}\hat{\rho}_1^2(\hat{\boldsymbol{x}}) + \int \mathrm{d}^2\hat{\boldsymbol{x}}\frac{1}{2}\kappa\hat{\boldsymbol{x}}^2\hat{\rho}_1(\hat{\boldsymbol{x}}) + \frac{1}{2}\int \mathrm{d}^2\hat{\boldsymbol{x}}\int \mathrm{d}^2\hat{\boldsymbol{y}}\frac{\hat{\rho}_1(\hat{\boldsymbol{x}})\hat{\rho}_1(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}|}. \tag{7.5}$$

If we consider a solution with radial symmetry $\hat{\rho}_1(\hat{x})$, the energy becomes, introducing $E^{TF} \doteq \frac{\hat{E}^{TF}}{N^2}$:

$$\begin{aligned} E^{TF}[\hat{\rho}_1] &= \pi^2\int \mathrm{d}\hat{x}\hat{x}\hat{\rho}_1^2(\hat{x}) + \pi\kappa\int \mathrm{d}\hat{x}\hat{x}^3\hat{\rho}_1(\hat{x}) \\ &\quad +\pi\int \mathrm{d}\hat{x}\int \mathrm{d}\hat{y}\int_0^{2\pi} \mathrm{d}\theta\frac{\hat{x}\hat{y}\hat{\rho}_1(\hat{x})\hat{\rho}_1(\hat{y})}{\sqrt{\hat{x}^2 + \hat{y}^2 - 2\hat{x}\hat{y}\cos\theta}}, \end{aligned} \tag{7.6}$$

where we used the equality $|\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}| = \sqrt{(\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}}) \cdot (\hat{\boldsymbol{x}} - \hat{\boldsymbol{y}})} = \sqrt{\hat{\boldsymbol{x}}^2 + \hat{\boldsymbol{y}}^2 - 2\hat{\boldsymbol{x}} \cdot \hat{\boldsymbol{y}}} = \sqrt{\hat{x}^2 + \hat{y}^2 - 2\hat{x}\hat{y}\cos\theta}$, where θ is the angle between $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$.

It was proven that by considering a function with radial symmetry $\hat{\rho}_1(\hat{x})$, there exists a unique solution to this problem (Lieb et al., 1995). A solution was found in the asymptotic limit $\kappa \longrightarrow 0$ (Shikin et al., 1991). It is

$$\hat{\rho}_1(\hat{x}) = \frac{3}{2\pi R^2}\sqrt{1 - \frac{\hat{x}^2}{R^2}}, \quad R = \left(\frac{3\pi}{4\kappa}\right)^{\frac{1}{3}}. \tag{7.7}$$

It is proven in (Lieb et al., 1995) that the support of $\hat{\rho}_1$ is compact, that is there exists a radius $R > 0$ such that $\hat{\rho}_1(\hat{x}) = 0, \hat{x} \geq R$. It is therefore appropriate to proceed to a scaling, which preserves the normalization condition:

$$\begin{aligned} \hat{x} &\mapsto x = \frac{\hat{x}}{R}, \\ \hat{\rho}_1(\hat{x}) &\mapsto \rho(x) = R^2\hat{\rho}_1(\hat{x}) = R^2\hat{\rho}_1(Rx). \end{aligned} \tag{7.8}$$

The last equality implies $1 = \int \mathrm{d}^2\boldsymbol{x}\rho(x)$.

In these new variables the problem consists of finding a positive function ρ in the interval $[0, 1]$, with $\rho(1) = 0$, and a radius R, which minimize the functional

$$\begin{aligned} E[\rho, R] &= \frac{\pi^2}{R^2}\int_0^1 \mathrm{d}x x\rho^2(x) + R^2\pi\kappa\int_0^1 \mathrm{d}x x^3\rho(x) \\ &\quad +\frac{\pi}{R}\int_0^1 \mathrm{d}x\int_0^1 \mathrm{d}y\int_0^{2\pi} \mathrm{d}\theta\frac{xy\rho(x)\rho(y)}{\sqrt{x^2 + y^2 - 2xy\cos\theta}}. \end{aligned} \tag{7.9}$$

7.1.1 New basis

Experimental results indicate that we always work in the regime $\kappa \ll 1$ (McEuen et al., 1992), (Zhitenev et al., 1997), (Kouwenhoven et al., 2001). Hence, by continuity (the convergence $\kappa \to 0$ is uniform, (Lieb et al., 1995)), the solution is close to the solution obtained in the limit $\kappa \to 0$. This is why we introduce a basis for the functions in the interval $[0,1]$, defined by $\varphi_n(x) \doteq (1-x^2)^{\frac{n}{2}}, n \geq 1$, and suppose that we can consider a small number of basis elements (and that the precision will be sufficient).

Proposition 1
$\{\varphi_n\}_{n\geq 1}$ is a basis of $\{f : [0,1] \to \mathbb{R} | f(1) = 0\}$

Proof 1
Let's define the change of variable $x \mapsto y = \arcsin(x)$ and define $\psi_n(y) \doteq \varphi_n(x(y)) = \left(1-\sin^2(y)\right)^{\frac{n}{2}} = \cos^n(y)$. Let's proceed to another change of variable $y \mapsto z = \cos(y)$ and define $\phi_n(z) \doteq \psi_n(y(z)) = z^n$. The condition $\varphi_n(1) = 0$ becomes $\phi_n(0) = 0$. It is a well-known result that $\{\phi_n\}_{n\geq 1}$ is a basis of the set of functions $\{f : [0,1] \to \mathbb{R} | f(0) = 0\}$, which concludes the proof.

Let's note that this basis is not orthonormal. The nature of our problem (a two-dimensional one) is such that the natural scalar product is $\langle f|g\rangle \doteq 2\pi \int_0^1 \mathrm{d}x x f(x) g(x)$, whose corresponding norm is $\|f\| \doteq \sqrt{2\pi \int_0^1 \mathrm{d}x x f^2(x)}$, which we will use later. The scalar product between the basis elements is $\langle \varphi_n|\varphi_m\rangle = \frac{2\pi}{2+n+m}$. The Hilbert space we consider is therefore

$$\mathcal{H} \doteq L^2([0,1], 2\pi x \mathrm{d}x). \tag{7.10}$$

A function $\rho : [0,1] \to \mathbb{R}$, with $\rho(1) = 0$, can be written as

$$\rho(x) = \sum_{n\geq 1} c_n \varphi_n(x). \tag{7.11}$$

The energy and the constraint have now to be expressed in this basis. The first term of (7.9), which is the kinetic energy, becomes

$$\begin{aligned} T &\doteq \frac{t}{R^2} \\ &= \frac{\pi^2}{R^2} \int_0^1 \mathrm{d}x x \rho^2(x) \\ &= \frac{\pi^2}{R^2} \sum_{n,m\geq 1} c_n c_m \int_0^1 \mathrm{d}x x \varphi_n(x) \varphi_m(x) \end{aligned}$$

$$\begin{aligned}
&= \frac{\pi^2}{R^2}\sum_{n,m\geq 1} c_n c_m \underbrace{\int_0^1 \mathrm{d}x x(1-x^2)^{\frac{(n+m)}{2}}}_{=\frac{1}{(2+n+m)}} \\
&= \frac{\pi^2}{R^2}\sum_{n,m\geq 1} \frac{c_n c_m}{2+n+m} \\
&\doteq \frac{1}{R^2}\sum_{n,m\geq 1} t_{nm} c_n c_m \\
&\doteq \sum_{n,m\geq 1} T_{nm} c_n c_m. \qquad (7.12)
\end{aligned}$$

The second term of (7.9), the confining potential, becomes

$$\begin{aligned}
V^{ext} &\doteq R^2 v^{ext} \\
&= R^2\pi\kappa \int_0^1 \mathrm{d}x x^3 \rho(x) \\
&= R^2\pi\kappa \sum_{n\geq 1} c_n \int_0^1 \mathrm{d}x x^3 \varphi_n(x) \\
&= R^2\pi\kappa \sum_{n\geq 1} c_n \int_0^1 \mathrm{d}x x^3 \varphi_n(x) \\
&= R^2\pi\kappa \sum_{n\geq 1} c_n \underbrace{\int_0^1 \mathrm{d}x x^3 (1-x^2)^{\frac{n}{2}}}_{=\frac{2}{(2+n)(4+n)}} \\
&= R^2 2\pi\kappa \sum_{n\geq 1} \frac{c_n}{(2+n)(4+n)} \\
&\doteq R^2 \sum_{n\geq 1} v_n^{ext} c_n \\
&\doteq \sum_{n\geq 1} V_n^{ext} c_n. \qquad (7.13)
\end{aligned}$$

The last term of (7.9), the electrostatic interaction V, needs some more developments. Let's use the following integral representation of $\frac{1}{|\boldsymbol{x}-\boldsymbol{y}|}$:

$$\frac{1}{|\boldsymbol{x}-\boldsymbol{y}|} = \int_0^\infty \mathrm{d}k J_0(k|\boldsymbol{x}-\boldsymbol{y}|). \qquad (7.14)$$

This result is obtained by expressing the Fourier transform of the function $\frac{1}{|\boldsymbol{x}|}$ (which is a function of $|\boldsymbol{k}|$ only):

$$\begin{aligned} f(|\boldsymbol{k}|) &= \int \mathrm{d}^2\boldsymbol{x}\frac{e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}}{|\boldsymbol{x}|} \\ &= \int_0^\infty \mathrm{d}x \underbrace{\int_0^{2\pi} \mathrm{d}\theta e^{-ikx\cos\theta}}_{2\pi J_0(kx)} \\ &= \underbrace{2\pi\int_0^\infty \mathrm{d}x J_0(kx)}_{\frac{1}{|k|}} = \frac{2\pi}{|k|}. \end{aligned} \tag{7.15}$$

The function $\frac{1}{|\boldsymbol{x}|}$ can be expressed as

$$\begin{aligned} \frac{1}{|\boldsymbol{x}|} &= \frac{1}{(2\pi)^2}\int \mathrm{d}^2\boldsymbol{k}\frac{2\pi}{|\boldsymbol{k}|}e^{i\boldsymbol{k}\cdot\boldsymbol{x}} \\ &= \frac{1}{2\pi}\int_0^\infty \mathrm{d}k \underbrace{\int_0^{2\pi} \mathrm{d}\theta e^{ikx\cos\theta}}_{=2\pi J_0(kx)} \\ &= \int_0^\infty \mathrm{d}k J_0(kx). \end{aligned} \tag{7.16}$$

We use the equality (Gradshteyn et al., 2000)

$$\begin{aligned} J_0(k|\boldsymbol{x}-\boldsymbol{y}|) &= J_0(k\sqrt{x^2+y^2-2xy\cos\theta}) \\ &= J_0(kx)J_0(ky) + 2\sum_{l=1}^{\infty} J_l(kx)J_l(ky)\cos(l\theta) \end{aligned} \tag{7.17}$$

to proceed further.

Returning to the electrostatic interaction (7.9) we find

$$\begin{aligned} V &= \frac{1}{2R}\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{y}\frac{\rho(x)\rho(y)}{|\boldsymbol{x}-\boldsymbol{y}|} \\ &= \frac{1}{2R}\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{y}\int_0^\infty \mathrm{d}k\rho(x)\rho(y)J_0(k|\boldsymbol{x}-\boldsymbol{y}|) \\ &= \frac{\pi}{R}\int_0^1 \mathrm{d}x\int_0^1 \mathrm{d}y\int_0^{2\pi} \mathrm{d}\theta\int_0^\infty \mathrm{d}kxy\rho(x)\rho(y)J_0(k\sqrt{x^2+y^2-2xy\cos\theta}) \end{aligned}$$

$$
\begin{aligned}
&= \frac{\pi}{R}\int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y \int_0^{2\pi} \mathrm{d}\theta \int_0^\infty \mathrm{d}k xy\rho(x)\rho(y) \\
&\quad \times \left(J_0(kx)J_0(ky) + 2\sum_{l=1}^{\infty} J_l(kx)J_l(ky)\cos(l\theta) \right) \\
&= \frac{2\pi^2}{R}\int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y \int_0^\infty \mathrm{d}k xy\rho(x)\rho(y)J_0(kx)J_0(ky). \qquad (7.18)
\end{aligned}
$$

The other terms vanish when integrating over the angle θ.

Let's note that the expression (7.18) shows that $V[\rho]$ is positive definite (even for functions which are not positive):

$$
\begin{aligned}
V &= \frac{2\pi^2}{R}\int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y \int_0^\infty \mathrm{d}k xy\rho(x)\rho(y)J_0(kx)J_0(ky) \\
&= \frac{2\pi^2}{R}\int_0^\infty \mathrm{d}k \left(\int_0^1 \mathrm{d}x x\rho(x)J_0(kx) \right)^2 \geq 0. \qquad (7.19)
\end{aligned}
$$

To express this energy in the chosen basis we have to compute

$$
\begin{aligned}
V_{nm} &= \frac{2\pi^2}{R}\int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y \int_0^\infty \mathrm{d}k xy(1-x^2)^{\frac{n}{2}}(1-y^2)^{\frac{m}{2}} J_0(kx)J_0(ky) \\
&= \frac{2\pi^2}{R} 2^{\frac{n}{2}}\Gamma\left(\frac{n}{2}+1\right)\int_0^1 \mathrm{d}y \int_0^\infty \mathrm{d}k y(1-y^2)^{\frac{m}{2}} \frac{J_{\frac{n}{2}+1}(k)J_0(ky)}{k^{\frac{n}{2}+1}} \\
&= \frac{\pi^2}{R}\frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{n}{2}+1\right)}{\Gamma\left(\frac{n}{2}+\frac{3}{2}\right)}\int_0^1 \mathrm{d}y y(1-y^2)^{\frac{m}{2}} F\left(\frac{1}{2}, -\frac{n}{2}-\frac{1}{2}, 1, y^2\right) \\
&= \frac{\pi^{\frac{5}{2}}}{2R}\frac{\Gamma\left(\frac{n}{2}+1\right)\Gamma\left(\frac{m}{2}+1\right)\Gamma\left(\frac{n}{2}+\frac{m}{2}+2\right)}{\Gamma\left(\frac{n}{2}+\frac{3}{2}\right)\Gamma\left(\frac{m}{2}+\frac{3}{2}\right)\Gamma\left(\frac{n}{2}+\frac{m}{2}+\frac{5}{2}\right)}. \qquad (7.20)
\end{aligned}
$$

To establish this result we first integrated over x, using the equality (Gradshteyn et al., 2000)

$$
\int_0^1 \mathrm{d}x x(1-x^2)^\mu J_0(kx) = \frac{2^\mu \Gamma(\mu+1)J_{\mu+1}(k)}{k^{\mu+1}}. \qquad (7.21)
$$

Then we integrated over k, using (Gradshteyn et al., 2000)

$$
\int_0^\infty \mathrm{d}k \frac{J_0(ky)J_{\mu+1}(k)}{k^{\mu+1}} = \frac{1}{2^{\mu+1}}\frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\mu+\frac{3}{2}\right)} F\left(\frac{1}{2}, -\mu-\frac{1}{2}, 1, y^2\right). \qquad (7.22)
$$

Finally we integrated over y, proceeding to the change of variable $x = y^2$, and using the result (Gradshteyn et al., 2000)

$$\begin{aligned}
\int_0^1 \mathrm{d}yy(1-y^2)^\nu F\left(\frac{1}{2}, -\mu-\frac{1}{2}, 1, y^2\right) \\
&= \frac{1}{2}\int_0^1 \mathrm{d}x(1-x)^\nu F\left(\frac{1}{2}, -\mu-\frac{1}{2}, 1, x\right) \\
&= \frac{1}{2}\frac{\Gamma(1)\Gamma(\nu+1)\Gamma(\mu+\nu+2)}{\Gamma\left(\nu+\frac{3}{2}\right)\Gamma\left(\mu+\nu+\frac{5}{2}\right)}. \qquad (7.23)
\end{aligned}$$

Using $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$ and $\Gamma(1) = 1$, we find the result (7.20).

The electrostatic potential is therefore, in the chosen basis, for $\rho(x) = \sum_{n\geq 1} c_n\varphi_n(x)$, expressed as (using (7.20))

$$\begin{aligned}
V &\doteq \frac{v}{R} \\
&= \frac{\pi}{R}\int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y \int_0^{2\pi} \mathrm{d}\theta \frac{xy\rho(x)\rho(y)}{\sqrt{x^2+y^2-2xy\cos\theta}} \\
&= \sum_{n,m\geq 1} c_n c_m \frac{\pi}{R}\int_0^1 \mathrm{d}x \int_0^1 \mathrm{d}y \int_0^{2\pi} \mathrm{d}\theta \frac{xy(1-x^2)^{\frac{n}{2}}(1-y^2)^{\frac{m}{2}}}{\sqrt{x^2+y^2-2xy\cos\theta}} \\
&= \frac{1}{R}\sum_{n,m\geq 1} \frac{\pi^{\frac{5}{2}}}{2}\frac{\Gamma\left(\frac{n}{2}+1\right)\Gamma\left(\frac{m}{2}+1\right)\Gamma\left(\frac{n}{2}+\frac{m}{2}+2\right)}{\Gamma\left(\frac{n}{2}+\frac{3}{2}\right)\Gamma\left(\frac{m}{2}+\frac{3}{2}\right)\Gamma\left(\frac{n}{2}+\frac{m}{2}+\frac{5}{2}\right)} c_n c_m \\
&\doteq \frac{1}{R}\sum_{n,m\geq 1} v_{nm} c_n c_m \\
&\doteq \sum_{n,m\geq 1} V_{nm} c_n c_m. \qquad (7.24)
\end{aligned}$$

The constraint (7.3) becomes, in the chosen basis, for $\rho(x) = \sum_{n\geq 1} c_n\varphi_n(x)$:

$$2\pi\int_0^1 \mathrm{d}xx\rho(x) = 2\pi\sum_{n\geq 1} c_n \int_0^1 \mathrm{d}xx(1-x^2)^{\frac{n}{2}} = 2\pi\sum_{n\geq 1}\frac{c_n}{2+n} \doteq \sum_{n\geq 1} k_n c_n = 1. \qquad (7.25)$$

We obtain a constraint which we call an affine constraint: we can write a coefficient as an affine function of the others. The result is not surprising: the constraint is already affine in the initial problem, and the change of basis is linear.

7.1.2 Existence and uniqueness of a solution

The existence and uniqueness of a solution was proven in (Lieb et al., 1995). However, in order to have a better understanding of our approach, it is useful to prove it in our basis. In this case the problem consists of finding a solution $(\{c_n\}_{n\geq 1}, R) \doteq (\underline{c}, R)$ which minimizes the function

$$E(\underline{c}, R) = \frac{1}{R^2} \sum_{n,m\geq 1} t_{nm} c_n c_m + R^2 \sum_{n\geq 1} v_n^{ext} c_n + \frac{1}{R} \sum_{n,m\geq 1} v_{nm} c_n c_m \tag{7.26}$$

under the affine constraint

$$\sum_{n\geq 1} k_n c_n = 1. \tag{7.27}$$

This can be written using the Lagrange multiplier μ: we have to minimize the function $F(\underline{c}, R, \mu)$ defined by

$$\begin{aligned} F(\underline{c}, R, \mu) \quad = \quad & \frac{1}{R^2} \sum_{n,m\geq 1} t_{nm} c_n c_m + R^2 \sum_{n\geq 1} v_n^{ext} c_n \\ & + \frac{1}{R} \sum_{n,m\geq 1} v_{nm} c_n c_m - \mu \left(\sum_{n\geq 1} k_n c_n - 1 \right). \end{aligned} \tag{7.28}$$

The Lagrange multiplier μ has the physical meaning of the chemical potential.

To prove the existence and uniqueness of a solution to this problem we will minimize $E(\underline{c}, R)$ with regards to $\underline{c}$ only, including the constraint condition. We will show the uniqueness of a solution $\underline{c}^\star(R)$, for R fixed. To prove the existence and uniqueness of a solution we have to prove the existence of a unique global minimum of the function $E(\underline{c}^\star(R), R)$ which is a function of one variable, R. This will lead to $R^\star$. Unfortunately we could not prove this point, but there is numerical evidence for this, as we will illustrate later with numerical simulations.

To show the uniqueness of $\underline{c}^\star(R)$, let's note that the energy is given by a quadratic form of $\underline{c}$, plus a linear term in $\underline{c}$. Let's write it as

$$E(\underline{c}) = \frac{1}{2} \sum_{n,m\geq 1} g_{nm} c_n c_m + \sum_{n\geq 1} V_n^{ext} c_n. \tag{7.29}$$

If the quadratic form is invertible, let's proceed to the change of variable

$$\gamma_n = c_n + \sum_{m\geq 1} g^{-1}_{nm} V_m^{ext}. \tag{7.30}$$

The energy becomes

$$E(\underline{\gamma}) = \frac{1}{2} \sum_{n,m\geq 1} g_{nm} \gamma_n \gamma_m - \frac{1}{2} \sum_{n,m\geq 1} g^{-1}_{nm} V_m^{ext} V_n^{ext}. \tag{7.31}$$

Hence, if the quadratic term of the energy g is positive definite, the energy will be a paraboloid with regards to $\underline{c}$, centered at $\underline{\gamma}^\star$, defined by $\gamma_n^\star = -\sum_{m\geq 1} g^{-1}_{nm} V_m^{ext}$. Moreover the paraboloid is shifted by an energy $-\frac{1}{2} \sum_{n,m\geq 1} g^{-1}_{nm} V_m^{ext} V_n^{ext}$.

Let's prove that $\frac{1}{2} g = \frac{t}{R^2} + \frac{v}{R}$ is positive definite.

Proposition 2
The kinetic energy t is a positive definite quadratic form.

Proof 2
The kinetic energy (7.12) has the integral representation

$$t_{nm} = \frac{\pi^2}{2+n+m} = \pi^2 \int_0^\infty \mathrm{d}t e^{-(2+n+m)t}. \tag{7.32}$$

For any $\underline{c}$, the kinetic energy can be written

$$\begin{aligned} t &= \sum_{n,m\geq 1} t_{nm} c_n c_m = \pi^2 \sum_{n,m\geq 1} \int_0^\infty \mathrm{d}t e^{-(2+n+m)t} c_n c_m \\ &= \int_0^\infty \mathrm{d}t e^{-2t} \left(\pi \sum_{n\geq 1} e^{-nt} c_n\right)^2 \geq 0 \quad \forall \underline{c} \neq \underline{0}. \end{aligned} \tag{7.33}$$

Proposition 3
The electrostatic energy v is a positive definite quadratic form.

Proof 3
Let's use the formula (Gradshteyn et al., 2000)

$$\frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu+\nu)} = \int_0^1 \mathrm{d}t t^{\mu-1}(1-t)^{\nu-1}, \tag{7.34}$$

which is equal to the beta function, in order to separate n and m in the electrostatic energy (7.24):

$$\frac{\Gamma\left(\frac{n}{2}+\frac{m}{2}+2\right)}{\Gamma\left(\frac{n}{2}+\frac{m}{2}+\frac{5}{2}\right)} = \frac{1}{\pi^{\frac{1}{2}}} \frac{\Gamma\left(\frac{1}{2}\right)\Gamma\left(\frac{n}{2}+\frac{m}{2}+2\right)}{\Gamma\left(\frac{n}{2}+\frac{m}{2}+\frac{5}{2}\right)} = \frac{1}{\pi^{\frac{1}{2}}} \int_0^1 \mathrm{d}t t^{\left(\frac{n}{2}+\frac{m}{2}+1\right)}(1-t)^{-\frac{1}{2}}. \tag{7.35}$$

For any $\underline{c}$, the electrostatic energy can be written

$$\begin{aligned} v &= \sum_{n,m\geq 1} \frac{\pi^{\frac{5}{2}}}{2} \frac{\Gamma\left(\frac{n}{2}+1\right)\Gamma\left(\frac{m}{2}+1\right)\Gamma\left(\frac{n}{2}+\frac{m}{2}+2\right)}{\Gamma\left(\frac{n}{2}+\frac{3}{2}\right)\Gamma\left(\frac{m}{2}+\frac{3}{2}\right)\Gamma\left(\frac{n}{2}+\frac{m}{2}+\frac{5}{2}\right)} c_n c_m \\ &= \int_0^1 \mathrm{d}t t(1-t)^{-\frac{1}{2}} \frac{\pi^2}{2} \left(\sum_{n\geq 1} \frac{\Gamma\left(\frac{n}{2}+1\right)}{\Gamma\left(\frac{n}{2}+\frac{3}{2}\right)} t^{\frac{n}{2}} c_n\right)^2 \geq 0 \quad \forall \underline{c} \neq \underline{0}. \end{aligned} \tag{7.36}$$

The sum of two positive definite quadratic forms is trivially a positive definite quadratic form. Hence:

Corollary 1
The quadratic form $\frac{1}{2}g = \frac{t}{R^2} + \frac{v}{R}$ is positive definite.

Let's note that the vector space is of infinite dimension and requires therefore a more careful study. A more detailed study shows that 0 is an accumulation point of the spectrum. Does this imply that g is not positive definite? No, because the operator g does not act on any vector, it acts on functions normalized to 1. These functions are in particular square integrable, which means that the coefficients $\{c_n\}_{n\geq 1}$ are decreasing at a certain speed ($c_n \sim n^{-\frac{1}{2}}, n \gg 1$).The speed at which the eigenvalues of g tend to 0 is slow enough in order that g is invertible on the considered space of functions.

Proposition 4
For fixed R, there exists one unique solution $\underline{c}^{\star}(R)$ which minimizes the energy (7.26) with regards to $\underline{c}$, under the constraint (7.27).

Proof 4
This result can be seen immediately in Figure 7.1, but let's prove it.

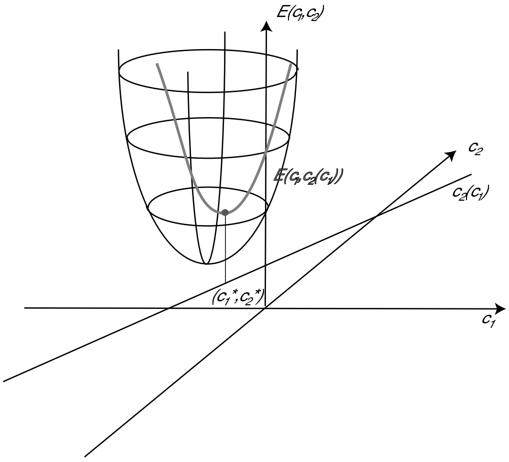


Figure 7.1: *Minimum of the energy under the constraint.*

The function we have to minimize is given at (7.28). In the notations introduced in (7.29) it becomes

$$F(\underline{c}, \mu) = \frac{1}{2} \sum_{n,m\geq 1} g_{nm} c_n c_m + \sum_{n\geq 1} V_n^{ext} c_n - \mu \left(\sum_{n\geq 1} k_n c_n - 1 \right). \tag{7.37}$$

It has to be minimized with regards to $\underline{c}$ and μ. Proceeding to the change of variables (7.30), the constraint remains affine:

$$\sum_{n\geq 1} k_n c_n - 1 = \sum_{n\geq 1} k_n (\gamma_n - \sum_{m\geq 1} g_{nm}^{-1} V_m^{ext}) - 1 \doteq \sum_{n\geq 1} k_n \gamma_n - \alpha. \tag{7.38}$$

In these new variables the function F becomes

$$F(\underline{\gamma},\mu)=\frac{1}{2}\sum_{n,m\geq 1} g_{nm}\gamma_n\gamma_m-\frac{1}{2}\sum_{n,m\geq 1} g^{-1}_{nm}V^{ext}_m V^{ext}_n-\mu\left(\sum_{n\geq 1}k_n\gamma_n-\alpha\right). \tag{7.39}$$

This function has a quadratic and a linear term in $\underline{\gamma}$. We proceed again to a change of variables to eliminate the linear term. Let's define

$$\lambda_n=\gamma_n-\mu\sum_{m\geq 1} g^{-1}_{nm}k_m. \tag{7.40}$$

The function F becomes

$$F(\underline{\lambda},\mu)=\frac{1}{2}\sum_{n,m\geq 1} g_{nm}\lambda_n\lambda_m-\frac{1}{2}\sum_{n,m\geq 1} g^{-1}_{nm}V^{ext}_m V^{ext}_n-\frac{\mu^2}{2}\sum_{n,m\geq 1} g^{-1}_{nm}k_n k_m+\mu\alpha. \tag{7.41}$$

The Lagrange multiplier has been separated from the other variables. The extremization with regards to the initial variables $(\underline{c},\mu)$ is equivalent to the extremization with regards to the new variables $(\underline{\lambda},\mu)$. g is positive definite, hence the extremization with regards to $\underline{\lambda}$ provides the solution $\underline{\lambda}^\star=\underline{0}$. The extremization with regards to μ provides the equation for μ (using the definition (7.38) of α):

$$\frac{\partial F(\underline{\lambda},\mu)}{\partial\mu}=-\mu\sum_{n,m\geq 1} g^{-1}_{nm}k_n k_m+\alpha=0 \quad\Rightarrow\quad \mu=\frac{1+\sum_{n,m\geq 1} g^{-1}_{nm}k_n V^{ext}_m}{\sum_{n,m\geq 1} g^{-1}_{nm}k_n k_m}. \tag{7.42}$$

We computed explicitly the solution which extremizes the function F, and found it to be unique, which concludes the demonstration.

Let's note that we can give the solution to the extremization problem explicitly in terms of the initial variables. These are

$$\begin{aligned} c^\star_n &= \gamma^\star_n-\sum_{m\geq 1} g^{-1}_{nm}V^{ext}_m=\underbrace{\lambda^\star_n}_{0}+\mu\sum_{m\geq 1} g^{-1}_{nm}k_m-\sum_{m\geq 1} g^{-1}_{nm}V^{ext}_m \\ &= \mu\sum_{m\geq 1} g^{-1}_{nm}k_m-\sum_{m\geq 1} g^{-1}_{nm}V^{ext}_m \\ &= \frac{1+\sum_{p,m\geq 1} g^{-1}_{pm}k_p V^{ext}_m}{\sum_{p,m\geq 1} g^{-1}_{pm}k_p k_n}\sum_{m\geq 1} g^{-1}_{nm}k_m-\sum_{m\geq 1} g^{-1}_{nm}V^{ext}_m. \end{aligned} \tag{7.43}$$

Let's note however that to have an explicit result from this formula we have to invert the matrix g which is numerically not obvious. We will not proceed this way for the numerical computations.

We were unable to prove the uniqueness of a radius $R^\star$ which minimizes $E(\underline{c}^\star(R),R)$. Numerical simulations, however, show strong evidence for this, as can be seen on Figure 7.2, which is the result of a simulation with $N=5$, $\epsilon=10^{-4}$, and $\kappa=0.0625$ in the modified atomic units. R is not a variable, it is fixed in these simulations (see the numerical part, section 7.3, for explanation).

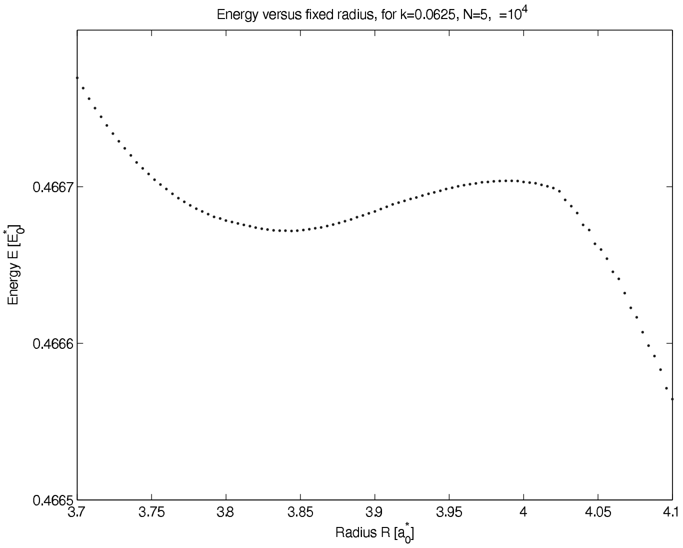


Figure 7.2: *Energy versus fixed radius. The energy $E(\underline{c}^\star(R), R)$ has one unique minimum, at $R^\star$. It is a local minimum of E. The configurations $(\underline{c}, R)$ which have an energy smaller than $E(\underline{c}^\star(R^\star), R^\star)$ are such that the corresponding density ρ is not positive everywhere.*

7.2 Analytical approach

This new description of the problem leads to a new analytical approach. First we derive the result obtained by Shikin (Shikin et al., 1991) in the asymptotic limit $\kappa \to 0$. We find the result $\rho = c_1\varphi_1$. A new asymptotic limit, $\kappa \to \infty$ is established, too, and we find $\rho = c_2\varphi_2$. These asymptotic limits lead us to approximate the solution by $\rho = c_1(\kappa)\varphi_1$ (resp. $\rho = c_2(\kappa)\varphi_2$) in the asymptotic limit $\kappa \to 0$ (resp. $\kappa \to \infty$). Mathematically this means that we look for a solution in the restricted vector space E_1 (resp. E_2) spanned by φ_1 (resp. φ_2). This leads to analytical approximations of the radius R, the energy E and the chemical potential μ, for $\kappa \ll 1$ (resp. $\kappa \gg 1$), but provides no information about the shape of the density. This is why we proceed to a better approximation: we consider a solution $\rho = c_1(\kappa)\varphi_1 + c_2(\kappa)\varphi_2$. Mathematically this means that we look for a solution in the restricted vector space $E_1 \times E_2$. Comparison with numerical results are done in section 7.4. We even go beyond this approximation and span ρ on the first three basis elements, and eventually on the first five basis elements. We will see however that in these two cases the series are strongly divergent and cannot be used for further computations.

7.2.1 Asymptotic limit $\kappa \to 0$

The uniqueness of a solution was proven in (Lieb et al., 1995). In the limit $\kappa \to 0$ this solution was established in (Shikin et al., 1991) and is of the type $\rho = c_1\varphi_1$. Let's establish this result with our approach, looking for a solution defined by

$$\rho = c_1\varphi_1. \tag{7.44}$$

If one finds a solution, it is, by uniqueness, the right solution.

The constraint (7.27) fixes the coefficient c_1:

$$c_1 = \frac{3}{2\pi}. \tag{7.45}$$

Introducing (7.44) in the energy (7.26) and using (7.45) we find

$$\begin{aligned} E(c_1, R) &= \frac{\pi^2}{4}\frac{1}{R^2}c_1^2 + \frac{2\pi\kappa}{15}R^2 c_1 + \frac{2\pi^3}{15}\frac{1}{R}c_1^2 \\ &= \frac{9}{16}\frac{1}{R^2} + \frac{\kappa}{5}R^2 + \frac{3\pi}{10}\frac{1}{R}. \end{aligned} \tag{7.46}$$

Extremizing with regards to R we find

$$\frac{\mathrm{d}E(c_1, R)}{\mathrm{d}R} = -\frac{9}{8}\frac{1}{R^3} + \frac{2\kappa}{5}R - \frac{3\pi}{10}\frac{1}{R^2} = 0. \tag{7.47}$$

Multiplying by R^3 we find the extremization equation

$$-\frac{9}{8} + \frac{2\kappa}{5}R^4 - \frac{3\pi}{10}R = 0, \tag{7.48}$$

which consists of finding the roots of a polynomial of the fourth order, which can be done analytically. We are however interested in the asymptotic limit $\kappa \to 0$, and in this limit there are two ways to solve this equation: we can consider that R is of the order of 1, which implies that the second term of the equation is negligible. This would imply that the confining energy is negligible compared to the others and would lead to a free gas of fermions, for which the radius R would tend to infinity. It would therefore not be of the order of 1, which leads to a contradiction. We have to reject this solution. Another possibility is that R is of the order of $\kappa^{-\frac{1}{3}}$. In this case the first term is negligible: the kinetic energy is therefore negligible compared to the other energies. This leads to the result

$$\frac{2\kappa}{5}R^4 - \frac{3\pi}{10}R = 0 \quad \Rightarrow \quad R = \left(\frac{3\pi}{4\kappa}\right)^{\frac{1}{3}}. \tag{7.49}$$

We reject the solution $R = 0$ (which would have implied division by 0 in the developments).

Now we have to prove that it is the solution of our problem in the asymptotic limit. In this limit the kinetic energy can be neglected and we have to minimize (7.28)

$$F(\underline{c}, R, \mu) = R^2 \sum_{n\geq 1} v_n^{ext} c_n + \frac{1}{R} \sum_{n,m\geq 1} v_{nm} c_n c_m - \mu \left(\sum_{n\geq 1} k_n c_n - 1 \right), \tag{7.50}$$

which leads to the equations

$$\frac{\partial F}{\partial c_n} = 0, \tag{7.51}$$

hence

$$R^2 \frac{2\pi\kappa}{(2+n)(4+n)} + \frac{1}{R} \frac{3\pi^2}{4} \frac{\Gamma\left(\frac{n}{2}+1\right)\Gamma\left(\frac{n}{2}+\frac{5}{2}\right)}{\Gamma\left(\frac{n}{2}+\frac{3}{2}\right)\Gamma\left(\frac{n}{2}+3\right)} = \frac{2\pi}{(2+n)}\mu, \tag{7.52}$$

where we used $\Gamma\left(\frac{3}{2}\right) = \frac{\pi^{\frac{1}{2}}}{2}$ and $\Gamma(2) = 1$.

This equality has to be satisfied for all n. The equation for $n = 1$ provides the value of the chemical potential (using the value established at (7.49) for R)

$$\mu = \left(\frac{3\pi}{4}\right)^{\frac{2}{3}} \kappa^{\frac{1}{3}}. \tag{7.53}$$

We still have to show that the equations (7.52) are satisfied for $n \neq 1$. Introducing the radius R (7.49) and the chemical potential μ (7.53) we find

$$\frac{1}{(2+n)(4+n)} + \frac{1}{2} \frac{\Gamma\left(\frac{n}{2}+1\right)}{\Gamma\left(\frac{n}{2}+\frac{3}{2}\right)} \frac{\Gamma\left(\frac{n}{2}+\frac{5}{2}\right)}{\Gamma\left(\frac{n}{2}+3\right)} - \frac{1}{(2+n)} = 0. \tag{7.54}$$

We have to distinguish the cases n even and n odd, and use formulas (Gradshteyn et al., 2000), for μ an integer:

$$\Gamma(\mu) = (\mu-1)!, \qquad \Gamma\left(\mu + \frac{1}{2}\right) = \frac{\pi^{\frac{1}{2}}}{2^\mu}(2\mu-1)!!. \tag{7.55}$$

In both cases this leads to

$$\frac{1}{2} \frac{\Gamma\left(\frac{n}{2}+1\right)}{\Gamma\left(\frac{n}{2}+\frac{3}{2}\right)} \frac{\Gamma\left(\frac{n}{2}+\frac{5}{2}\right)}{\Gamma\left(\frac{n}{2}+3\right)} = \frac{(n+3)}{(n+4)(n+2)}, \tag{7.56}$$

which implies immediately that (7.54) is satisfied for all n.

The solution $\rho(x) = \frac{3}{2\pi}\sqrt{1-x^2}$, $R = \left(\frac{3\pi}{4\kappa}\right)^{\frac{1}{3}}$ is therefore the solution to the extremization problem in the asymptotic limit $\kappa \to 0$.

Our approach allows a simple computation of the energy, which is (still neglecting the kinetic energy)

$$E = \frac{3}{5}\left(\frac{3\pi}{4}\right)^{\frac{2}{3}} \kappa^{\frac{1}{3}}. \tag{7.57}$$

7.2.2 Asymptotic limit $\kappa \to \infty$

This asymptotic limit can be understood in the following way: the confining energy is very strong, hence the self-consistent potential tends to the confining potential. This self-consistent potential is related to the density by the equality

$$\hat{\rho}(\hat{x}) = \frac{1}{\pi}\left(\hat{\mu} - \hat{V}(\hat{x})\right) \to \frac{1}{\pi}\left(\hat{\mu} - \frac{1}{2}\kappa\hat{x}^2\right). \tag{7.58}$$

In the normalized variables the only way to satisfy such a relation is $\rho(x) = \frac{2}{\pi}\left(1-x^2\right)$, because ρ has to satisfy the condition $\rho(1) = 0$ and the normalization condition (7.3).

The density is therefore given by $\rho = c_2\varphi_2$. Let's check this result by considering a function

$$\rho = c_2\varphi_2. \tag{7.59}$$

The constraint implies

$$c_2 = \frac{2}{\pi}. \tag{7.60}$$

Introducing (7.59) in the energy (7.26) and using (7.60) we find

$$\begin{aligned} E(c_2, R) &= \frac{\pi^2}{6}\frac{1}{R^2}c_2^2 + \frac{\pi\kappa}{12}R^2c_2 + \frac{256\pi}{315}\frac{1}{R}c_2^2 \\ &= \frac{2}{3}\frac{1}{R^2} + \frac{\kappa}{6}R^2 + \frac{1024}{315\pi}\frac{1}{R}. \end{aligned} \tag{7.61}$$

Extremizing with regards to R we find

$$\frac{\mathrm{d}E(c_2,R)}{\mathrm{d}R} = -\frac{4}{3}\frac{1}{R^3} + \frac{\kappa}{3}R - \frac{1024}{315\pi}\frac{1}{R^2} = 0. \tag{7.62}$$

Multiplying by R^3 we find the extremization equation

$$-\frac{4}{3} + \frac{\kappa}{3}R^4 - \frac{1024}{315\pi}R^2 = 0. \tag{7.63}$$

Solving this equation consists of finding the roots of a polynomial of the second order (replacing R by $x = R^2$), which is easily computed. However, in the asymptotic limit $\kappa \to \infty$ there are two ways to solve this equation: we could consider R of the order of $\kappa^{-\frac{1}{2}}$. In this case the second and third terms would be negligible (of the order of κ^{-1}) compared to the first one (of the order of 1), which has to be rejected: the confining potential cannot be neglected, otherwise the electron gas would be free and the radius would tend to infinity. The other solution is to consider a radius of the order of $\kappa^{-\frac{1}{4}}$. The third term is negligible compared to the others, which means that the electrostatic energy is negligible. This leads to the result

$$-\frac{4}{3} + \frac{\kappa}{3}R^4 = 0 \quad \Rightarrow \quad R = \frac{2^{\frac{1}{2}}}{\kappa^{\frac{1}{4}}}. \tag{7.64}$$

Now we have to prove that it is the solution of our problem in the asymptotic limit. In this limit the electrostatic energy can be neglected and we have to minimize (7.28)

$$F(\underline{c}, R, \mu) = \frac{1}{R^2} \sum_{n,m\geq 1} t_{nm} c_n c_m + R^2 \sum_{n\geq 1} v_n^{ext} c_n - \mu \left(\sum_{n\geq 1} k_n c_n - 1 \right), \tag{7.65}$$

which leads to the equations

$$\frac{\partial F}{\partial c_n} = 0, \tag{7.66}$$

hence

$$\frac{1}{R^2} \frac{4\pi}{(4+n)} + R^2 \frac{2\pi\kappa}{(2+n)(4+n)} = \frac{2\pi}{(2+n)} \mu. \tag{7.67}$$

This equality has to be satisfied for all n. The equation for $n = 2$ provides the value of the chemical potential (using the value established at (7.64) for R):

$$\mu = \kappa^{\frac{1}{2}}. \tag{7.68}$$

We still have to show that the equations (7.67) are satisfied for $n \neq 2$. Introducing the radius R (7.64) and the chemical potential μ (7.68) we find

$$\frac{1}{(4+n)} + \frac{2}{(2+n)(4+n)} - \frac{1}{(2+n)} = 0, \tag{7.69}$$

which is clearly satisfied for all n.

The solution $\rho(x) = \frac{2}{\pi}\left(1 - x^2\right)$, $R = \frac{2^{\frac{1}{2}}}{\kappa^{\frac{1}{4}}}$ is therefore the solution to the extremization problem in the asymptotic limit $\kappa \to \infty$.

Our approach allows a simple computation of the energy, which is (still neglecting the kinetic energy)

$$E = \frac{2}{3} \kappa^{\frac{1}{2}}. \tag{7.70}$$

Let's return now to equation (7.58), and proceed to the scaling of the length and the density, using the radius established at (7.64). The chemical potential scales trivially:

$$\rho(x) = R^2 \hat{\rho}(Rx) = \frac{2}{\pi}(1 - x^2). \tag{7.71}$$

We find exactly the same solution, which confirms that our solution expresses nothing else but the fact that, in the limit $\kappa \to \infty$, the self-consistent potential is the confining potential.

7.2.3 Restriction to E_1, for $\kappa \ll 1$

In order to find a solution close to the exact one, for $\kappa \ll 1$, we restrict the space of functions to E_1, and look for a solution in this subspace which minimizes the energy. This provides no information about the shape of the density, but on the radius of the dot, on its energy and chemical potential. The solution is

$$\rho = c_1 \varphi_1. \tag{7.72}$$

The constant c_1 is fixed by the constraint and is $c_1 = \frac{3}{2\pi}$. The development is similar than in section 7.2.1, except that we take into account the kinetic energy. The extremization equation is (7.48)

$$-\frac{9}{8} + \frac{2\kappa}{5} R^4 - \frac{3\pi}{10} R = 0. \tag{7.73}$$

The exact solution was computed with Mathematica. Only one root is real, and its series expansion around $\kappa = 0$, at first order in $\kappa^{\frac{1}{3}}$, is

$$R = \left(\frac{3\pi}{4\kappa}\right)^{\frac{1}{3}} + \frac{5}{4\pi} + \mathcal{O}(\kappa^{\frac{1}{3}}) = 1.33067\kappa^{-\frac{1}{3}} + 0.39789 + \mathcal{O}(\kappa^{\frac{1}{3}}). \tag{7.74}$$

The energy is, from (7.46), using the radius (7.74):

$$\begin{aligned} E &= \frac{9}{16}\frac{1}{R^2} + \frac{\kappa}{5} R^2 + \frac{3\pi}{10}\frac{1}{R} \\ &= \frac{3}{5}\left(\frac{3\pi}{4}\right)^{\frac{2}{3}} \kappa^{\frac{1}{3}} + \left(\frac{3}{4}\right)^{\frac{4}{3}} \frac{1}{\pi^{\frac{2}{3}}} \kappa^{\frac{2}{3}} + \mathcal{O}(\kappa) \\ &= 1.06241\kappa^{\frac{1}{3}} + 0.31767\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa). \end{aligned} \tag{7.75}$$

The chemical potential is computed using the extremization equation

$$\frac{\partial F}{\partial c_1} = 0, \tag{7.76}$$

which is (without neglecting the kinetic energy)

$$\frac{3\pi}{2}\frac{1}{R^2} + \frac{2\pi\kappa}{15} R^2 + \frac{2\pi^2}{5}\frac{1}{R} = \mu \frac{2\pi}{3}. \tag{7.77}$$

This leads to the result

$$\begin{aligned} \mu &= \left(\frac{3\pi}{4}\right)^{\frac{2}{3}} \kappa^{\frac{1}{3}} + \frac{5}{2}\left(\frac{3}{4}\right) \frac{1}{\pi^{\frac{2}{3}}} \kappa^{\frac{2}{3}} + \mathcal{O}(\kappa) \\ &= 1.77068\kappa^{\frac{1}{3}} + 1.05891\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa). \end{aligned} \tag{7.78}$$

Let's note that the extremization equations with regards to the other coefficients c_n, $n \neq 1$ are not satisfied, because the solution is not exact.

7.2.4 Restriction to E_2, for $\kappa \gg 1$

In order to find a solution close to the exact one, for $\kappa \gg 1$, we restrict the subspace of functions to E_2, and look for a solution in this space which minimizes the energy. This provides no information about the shape of the density, but on the radius of the dot, on its energy and chemical potential. The solution is

$$\rho = c_2 \varphi_2. \tag{7.79}$$

The constant c_2 is fixed by the constraint and is $c_2 = \frac{2}{\pi}$. The development is similar than in section 7.2.2, except that we take into account the electrostatic energy. The extremization equation is (7.63)

$$-\frac{4}{3} + \frac{\kappa}{3} R^4 - \frac{1024}{315\pi} R^2 = 0. \tag{7.80}$$

The exact solution was computed with Mathematica. Only one root is real and positive, and its series expansion around $\kappa^{-1} = 0$, at first order in $\kappa^{-\frac{1}{4}}$, is

$$R = 2^{\frac{1}{2}} \kappa^{-\frac{1}{4}} + \frac{128\ 2^{\frac{1}{2}}}{105\pi} \kappa^{-\frac{3}{4}} + \mathcal{O}(\kappa^{-\frac{5}{4}}) = 1.41421 \kappa^{-\frac{1}{4}} + 0.54876 \kappa^{-\frac{3}{4}} + \mathcal{O}(\kappa^{-\frac{5}{4}}). \tag{7.81}$$

The energy is, from (7.61), using the radius (7.81):

$$\begin{aligned} E &= \frac{2}{3} \frac{1}{R^2} + \frac{\kappa}{6} R^2 + \frac{1024}{315\pi} \frac{1}{R} \\ &= \frac{2}{3} \kappa^{\frac{1}{2}} + \frac{512\ 2^{\frac{1}{2}}}{315\pi} \kappa^{\frac{1}{4}} + \mathcal{O}(\kappa^{-\frac{1}{4}}) \\ &= 0.66667 \kappa^{\frac{1}{2}} + 0.73169 \kappa^{\frac{1}{4}} + \mathcal{O}(\kappa^{-\frac{1}{4}}). \end{aligned} \tag{7.82}$$

The chemical potential is computed using the extemalization equation

$$\frac{\partial F}{\partial c_2} = 0, \tag{7.83}$$

which is (without neglecting the kinetic energy)

$$\frac{1}{R^2} \frac{\pi}{3} + R^2 \frac{\pi\kappa}{12} + \frac{1}{R} \frac{1024}{315\pi} = \frac{\pi}{2} \mu. \tag{7.84}$$

This leads to the result

$$\begin{aligned} \mu &= \frac{2}{3} \kappa^{\frac{1}{2}} + \frac{1024\ 2^{\frac{1}{2}}}{315\pi^2} \kappa^{\frac{1}{4}} + \mathcal{O}(\kappa^{-\frac{1}{4}}) \\ &= 0.66667 \kappa^{\frac{1}{4}} + 0.46581 \kappa^{\frac{1}{4}} + \mathcal{O}(\kappa^{-\frac{1}{4}}). \end{aligned} \tag{7.85}$$

Let's note that the extremization equations with regards to the other coefficients c_n, $n \neq 2$ are not satisfied, because the solution is not exact.

7.2.5 Restriction to $E_1 \times E_2$, for $\kappa \ll 1$

In order to get more information about the solution for $\kappa \ll 1$, mainly on the shape of the density, we restrict the space of solutions to $E_1 \times E_2$. This approach is motivated by the fact that the solution has to be close to $\frac{3}{2\pi}\varphi_1$, which is exact in the limit $\kappa \to 0$. Moreover, the fact that the exact solution is $\frac{2}{\pi}\varphi_2$ in the limit $\kappa \to \infty$ motivates the choice of the two basis elements φ_1 and φ_2, which span $E_1 \times E_2$. The error is not controlled, which is why our results will be compared to numerical ones later.

To find an exact solution in this subspace $E_1 \times E_2$, we have to find the roots of a polynomial of degree 9, which is not possible analytically. This is why we solve it perturbatively at first order in $\kappa^{\frac{1}{3}}$. The solution is written $\rho = c_1\varphi_1 + c_2\varphi_2$, and we compute $c_1, c_2, R, E, \mu,$. Computations are done with Mathematica and we present the procedure.

The energy we have to minimize is (7.26)

$$\begin{aligned} E(c_1, c_2, R) \;=\; & \frac{1}{R^2}\left(\frac{\pi^2}{4}c_1^2 + \frac{2\pi^2}{5}c_1c_2 + \frac{\pi^2}{6}c_2^2\right) \\ & + R^2\left(\frac{2\pi\kappa}{15}c_1 + \frac{\pi\kappa}{12}c_2\right) \\ & + \frac{1}{R}\left(\frac{2\pi}{15}c_1^2 + \frac{5\pi^3}{24}c_1c_2 + \frac{256\pi}{315}c_2^2\right). \end{aligned} \tag{7.86}$$

The constraint (7.27) gives $c_2(c_1)$:

$$\frac{2\pi}{3}c_1 + \frac{\pi}{2}c_2 = 1 \quad \Rightarrow \quad c_2(c_1) = \frac{2}{\pi} - \frac{4}{3}c_1. \tag{7.87}$$

Introducing (7.87) in (7.86), we obtain after some coputations

$$\begin{aligned} E(c_1, c_2(c_1), R) \;\doteq\; & E(c_1, R) \\ = \; & \left(\frac{7\pi^2}{540}\frac{1}{R^2} + \frac{4096\pi}{2835}\frac{1}{R} - \frac{13\pi^3}{90}\frac{1}{R}\right)c_1^2 \\ & + \left(-\frac{4\pi}{45}\frac{1}{R^2} + \frac{\pi\kappa}{45}R^2 + \left(\frac{5\pi^2}{12} - \frac{4096}{945}\right)\frac{1}{R}\right)c_1 \\ & + \left(\frac{2}{3}\frac{1}{R^2} + \frac{\kappa}{6}R^2 + \frac{1024}{315\pi}\frac{1}{R}\right). \end{aligned} \tag{7.88}$$

The extremization equation with regards to the variable c_1 provides the relation $c_1(R)$:

$$\frac{\mathrm{d}E(c_1, R)}{\mathrm{d}c_1} = 0 \;\Rightarrow\; c_1(R) = \frac{\left(\frac{4\pi}{45}\frac{1}{R^2} - \frac{\pi\kappa}{45}R^2 + \left(-\frac{5\pi^2}{12} + \frac{4096}{945}\right)\frac{1}{R}\right)}{\left(\frac{7\pi^2}{270}\frac{1}{R^2} + \frac{8192\pi}{2835}\frac{1}{R} - \frac{13\pi^3}{45}\frac{1}{R}\right)}, \tag{7.89}$$

which can be simplified to

$$c_1(R) = \frac{-1008\pi - 49152R + 4725\pi^2 R + 252\kappa\pi R^4}{-294\pi^2 - 32768\pi R + 3276\pi^3 R}. \tag{7.90}$$

Long computations provide the energy as a function of R only

$$E(c_1(R), R) \doteq E(R) = \frac{P_1(R)}{P_2(R)}, \tag{7.91}$$

where $P_1(R)$ and $P_2(R)$ are polynomials of degree 8 and 3 respectively:

$$\begin{aligned}
P_1(R) &= -6048\pi + (70560\pi^2 - 737280)R \\
&\quad +(39375\pi^3 - 393216\pi)R^2 \\
&\quad -2856\pi\kappa R^4 + (26040\pi^2\kappa - 262144\kappa)R^5 \\
&\quad +112\pi\kappa^2 R^8, \\
P_2(R) &= -11760\pi R^2 + (131040\pi^2 - 1310720)R^3.
\end{aligned} \tag{7.92}$$

This energy has to be minimized with regards to this variable. The extremization equation is, after computation

$$\frac{\mathrm{d}E(R)}{\mathrm{d}R} = \frac{P_3(R)}{P_4(R)} \doteq 0, \tag{7.93}$$

where $P_3(R)$ and $P_4(R)$ are polynomials of degree 9 and 5 respectively:

$$\begin{aligned}
P_3(R) &= -889056\pi^2 + (-202825728\pi + 20046096\pi^3)R \\
&\quad +(-12079595520 + 2363719680\pi^2 - 115577280\pi^4)R^2 \\
&\quad +(-3221225472\pi + 644603904\pi^3 - 32248125\pi^5)R^3 \\
&\quad +419831\pi^2\kappa R^4 + (81199104\pi\kappa - 8080884\pi^3\kappa)R^5 \\
&\quad +(4294967296\kappa - 856031232\pi^2\kappa + 42653520\pi^4\kappa)R^6 \\
&\quad -49392\pi^2\kappa^2 R^8 + (458640\pi^3\kappa^2 - 4587520\pi\kappa^2)R^9, \\
P_4(R) &= 864360\pi^2 R^3 + (192675840\pi - 19262880\pi^3)R^4 \\
&\quad +(10737418240 - 2146959360\pi^2 + 107321760\pi^4)R^5.
\end{aligned} \tag{7.94}$$

The extremization equation reduces therefore to

$$P_3(R) = 0, \tag{7.95}$$

whose results are roots of a polynomial of degree 9, which cannot be solved analytically. We proceed to an expansion for $\kappa \ll 1$, reminding that the solution is of the order $R = \mathcal{O}(\kappa^{-\frac{1}{3}})$ in the limit $\kappa \to 0$. Writing

$$R = R_{-1}\kappa^{-\frac{1}{3}} + R_0 + \mathcal{O}(\kappa^{\frac{1}{3}}) \tag{7.96}$$

and

$$P_3(R) = a_0 + a_1 R + a_2 R^2 + a_3 R^3 + a_5 \kappa R^5 + a_6 \kappa R^6 + a_8 \kappa^2 R^8 + a_9 \kappa^2 R^9 = 0, \quad (7.97)$$

and introducing (7.96) in (7.97), we find, at first orders in $\kappa^{-\frac{1}{3}}$:

$$\begin{aligned} & a_3 R_{-1}^3 + a_6 R_{-1}^6 + a_9 R_{-1}^9 = 0 \Rightarrow R_{-1} = \left(\frac{3\pi}{4}\right)^{\frac{1}{3}}, \\ & a_2 R_{-1}^2 + 3a_3 R_{-1}^2 R_0 + 6a_6 R_{-1}^5 R_0 + a_8 R_{-1}^8 + 9a_9 R_{-1}^8 R_0 = 0 \\ & \quad \Rightarrow R_0 = \frac{81920 - 8253\pi^2}{65536\pi - 6615\pi^3}. \end{aligned} \quad (7.98)$$

We find two real positive solutions for R_0. One corresponds to the minimum we are looking for, the other one to a local maximum of $E(R)$. R_0 is obtained by substituting R_{-1} in the equation.

The final result is therefore

$$\begin{aligned} R &= \left(\frac{3\pi}{4}\right)^{\frac{1}{3}} \kappa^{-\frac{1}{3}} + \frac{81920 - 8253\pi^2}{65536\pi - 6615\pi^3} + \mathcal{O}(\kappa^{\frac{1}{3}}) \\ &= 1.33067\kappa^{-\frac{1}{3}} + 0.59695 + \mathcal{O}(\kappa^{\frac{1}{3}}). \end{aligned} \quad (7.99)$$

Returning to (7.90) the coefficient c_1 becomes

$$\begin{aligned} c_1 &= \frac{3}{2\pi} + \frac{189\ 3^{\frac{2}{3}}}{(2\pi)^{\frac{1}{3}}(6615\pi^2 - 65536)} \kappa^{\frac{1}{3}} + \mathcal{O}(\kappa^{\frac{2}{3}}) \\ &= 0.47747 - 0.85712\kappa^{\frac{1}{3}} + \mathcal{O}(\kappa^{\frac{2}{3}}), \end{aligned} \quad (7.100)$$

while the constraint (7.87) provides c_2

$$\begin{aligned} c_2 &= \frac{126\ 6^{\frac{2}{3}}}{\pi^{\frac{1}{3}}(65536 - 6615\pi^2)} \kappa^{\frac{1}{3}} + \mathcal{O}(\kappa^{\frac{2}{3}}) \\ &= 1.14282\kappa^{\frac{1}{3}} + \mathcal{O}(\kappa^{\frac{2}{3}}). \end{aligned} \quad (7.101)$$

The energy is obtained with (7.91) and we find

$$\begin{aligned} E &= \frac{3(3\pi)^{\frac{2}{3}}}{10\ 2^{\frac{1}{3}}} \kappa^{\frac{1}{3}} + \frac{3}{4} \frac{3^{\frac{1}{3}}}{(2\pi)^{\frac{2}{3}}} \kappa^{\frac{2}{3}} + \mathcal{O}(\kappa) \\ &= 1.06241\kappa^{\frac{1}{3}} + 0.31767\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa). \end{aligned} \quad (7.102)$$

The chemical potential is computed using the extremization equation

$$\frac{\partial F}{\partial c_1} = 0. \quad (7.103)$$

The equation $\frac{\partial F}{\partial c_2} = 0$ would lead to the same result in our perturbative treatment. This equation is

$$\frac{\pi^2}{2}\frac{1}{R^2}c_1 + \frac{2\pi^2}{5}\frac{1}{R^2}c_2 + \frac{2\pi\kappa}{15}R^2 + \frac{4\pi^3}{15}\frac{1}{R}c_1 + \frac{5\pi^3}{24}\frac{1}{R}c_2 = \mu\frac{2\pi}{3}. \tag{7.104}$$

Using (7.87) and (7.90) we express the chemical potential as a function of R:

$$\mu(R) = \frac{P_5(R)}{P_6(R)}, \tag{7.105}$$

where $P_5(R)$ and $P_6(R)$ are polynomials of degree 5 and 3 respectively:

$$\begin{aligned} P_5(R) &= -6048\pi + (-737280 + 70560\pi^2)R \\ &\quad +(-393216\pi + 39375\pi^3)R^2 - 1428\pi\kappa R^4 \\ &\quad +(-131072\kappa + 13020\pi^2\kappa)R^5, \\ P_6(R) &= -5880\pi R^2 + (-655360 + 65520\pi^2)R^3. \end{aligned} \tag{7.106}$$

Replacing R by its value (7.99) we find

$$\begin{aligned} \mu &= \left(\frac{3\pi}{4}\right)^{\frac{2}{3}}\kappa^{\frac{1}{3}} + \frac{3^{\frac{1}{3}}}{(2\pi)^{\frac{2}{3}}}\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa) \\ &= 1.77068\kappa^{\frac{1}{3}} + 0.42357\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa). \end{aligned} \tag{7.107}$$

Another approach, which can be easily generalized to $N > 2$, consists of using formula (7.43) to obtain $c^\star(R)$. Let's note that we have to invert g, which is done with Mathematica. To obtain the radius we have to solve the equation

$$\frac{\mathrm{d}E(c^\star(R), R)}{\mathrm{d}R} = 0, \tag{7.108}$$

where the energy is given at equation (7.26). It leads to the evaluation of the roots of a polynomial (of order 9, 11, 13 and 15 for $N = 2, 3, 4$ and 5 respectively). In each case, in the limit $\kappa \to 0$, there are two real positive solutions and we keep the solution which corresponds to a minimum of $E(c^\star(R), R)$.

For the case $N = 2$ we obtain exactly the same result as above, the advantage is that this approach allows for a better control of the expansions. We generalized the previous result to a perturbative expansion of order 3. The result is

$$R(\kappa) = 1.33067\kappa^{-\frac{1}{3}} + 0.59695 - 0.61552\kappa^{\frac{1}{3}} + 0.14827\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa). \tag{7.109}$$

The coefficients $\underline{c}$ become

$$\left\{ \begin{aligned} c_1(\kappa) &= 0.47746 - 0.85712\kappa^{\frac{1}{3}} + 1.99747\kappa^{\frac{2}{3}} - 5.08758\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}), \\ c_2(\kappa) &= 1.14282\kappa^{\frac{1}{3}} - 2.66329\kappa^{\frac{2}{3}} + 6.78344\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}), \end{aligned} \right.$$

while the energy and the chemical potential are

$$\begin{aligned} E(\kappa) &= 1.06241\kappa^{\frac{1}{3}} + 0.31767\kappa^{\frac{2}{3}} - 0.10449\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}), \\ \mu(\kappa) &= 1.77068\kappa^{\frac{1}{3}} + 0.42357\kappa^{\frac{2}{3}} - 0.10449\kappa + 0.06519\kappa^{\frac{4}{3}} + \mathcal{O}(\kappa^{\frac{5}{3}}). \end{aligned} \tag{7.110}$$

All these numbers have an analytical expression, which is however too long to be written here.

Is this approach a good one? We can see that the perturbative expansion of the physical values (radius, energy, chemical potential) have coefficients which are decreasing fast, and it is reasonable to think that the expansion is convergent (in fact it is, because the convergence for $\kappa \to 0$ is uniform (Lieb et al., 1995)). Conversely to the coefficients $\underline{c}$, whose perturbative expansion coefficients are strongly increasing: the series is divergent and has to be interpreted as an asymptotic series. An explanation is that our approach has no physical meaning, and we have no information about its convergence with regards to κ, for $\kappa \to 0$. This approach should be avoided, but we will check if the results are in agreement with a reference solution anyway (which is obtained by numerical simulations, see section 7.3). This is done in section 7.4.

We proceeded to the same computations for $N = 3$. The perturbative expansion in powers of $\kappa^{\frac{1}{3}}$ leads unfortunately to a solution which is not physical: we find a solution $\underline{c}$ for which $\rho(x)$ is negative for some $x \in [0, 1]$. Moreover the coefficients of the perturbative expansion are strongly increasing and the density does not have a realistic shape at all. These coefficients are

$$\left\{ \begin{aligned} c_1(\kappa) &= 0.47746 - 2.95522\kappa^{\frac{1}{3}} + 15.37408\kappa^{\frac{2}{3}} - 77.09687\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}), \\ c_2(\kappa) &= 6.70975\kappa^{\frac{1}{3}} - 38.86535\kappa^{\frac{2}{3}} + 203.65683\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}), \\ c_3(\kappa) &= -3.46182\kappa^{\frac{1}{3}} + 22.95823\kappa^{\frac{2}{3}} - 126.07627\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}). \end{aligned} \right. \tag{7.111}$$

The radius is

$$R(\kappa) = 1.33067\kappa^{-\frac{1}{3}} + 0.73966 - 1.31194\kappa^{\frac{1}{3}} + 4.39461\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa), \tag{7.112}$$

the energy and chemical potential are

$$\begin{aligned} E(\kappa) &= 1.06241\kappa^{\frac{1}{3}} + 0.31767\kappa^{\frac{2}{3}} - 0.10692\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}), \\ \mu(\kappa) &= 1.77068\kappa^{\frac{1}{3}} + 0.42357\kappa^{\frac{2}{3}} - 0.10692\kappa + 0.08148\kappa^{\frac{4}{3}} + \mathcal{O}(\kappa^{\frac{5}{3}}). \end{aligned} \tag{7.113}$$

We also studied in detail the case $N = 5$, and the same discussion holds. The increase of the coefficients of the expansion is even worse, and we couldn't proceed beyond the order 2. These coefficients are

$$\begin{cases} c_1(\kappa) &= 0.47746 - 13.6144\kappa^{\frac{1}{3}} - 2.00819 \cdot 10^{20}\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa), \\ c_2(\kappa) &= 66.5609\kappa^{\frac{1}{3}} + 1.80427 \cdot 10^{17}\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa), \\ c_3(\kappa) &= -125.834\kappa^{\frac{1}{3}} + 8.34655 \cdot 10^{20}\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa), \\ c_4(\kappa) &= 108.642\kappa^{\frac{1}{3}} - 4.36091 \cdot 10^{16}\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa), \\ c_5(\kappa) &= -35.2962\kappa^{\frac{1}{3}} - 3.99756 \cdot 10^{20}\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa). \end{cases} \tag{7.114}$$

The radius is

$$R(\kappa) = 1.33067\kappa^{-\frac{1}{3}} + 0.94956 - 4.33755\kappa^{\frac{1}{3}} + \mathcal{O}(\kappa^{\frac{2}{3}}). \tag{7.115}$$

We didn't compute the energy and chemical potential from these results which are clearly a divergent series.

It seems that for $N > 2$, for the description of the density with the coefficients $\underline{c}$ and the radius R, an expansion around $\kappa = 0$ is not adapted: the series is an asymptotic one and is clearly divergent. However, the functions $\underline{c}(\kappa)$ exist (and are finite for all κ) and we want to approximate them by a polynomial function of $\kappa^{\frac{1}{3}}$.

The asymptotic series appear in numerous physical situations, a typical one arising from the existence of solitons (or equivalently instantons): it can imply a small effect (of the order of $\mathcal{O}(e^{-\frac{1}{T}})$, $T \ll 1$), which can however not be treated by a perturbative expansion, because the function $e^{-\frac{1}{T}}$ is not analytic. This is why different techniques have been developed to handle these series, mainly resummation techniques.

For example we can proceed to a Padé resummation: we replace the desired function by a rational function $\frac{\sum_{i=0}^{M} a_i x^i}{1+\sum_{j=1}^{N} b_i x^j}$, whose coefficients are determined by making its perturbative expansion match the divergent perturbative expansion until the order $M+N$. This provides $(M+N+1)$ equations from which we obtain the coefficients $\{a_i\}_{i=0}^{M}$ and $\{b_i\}_{i=1}^{N}$. Then we can proceed to an expansion of this new rational function to obtain an expansion of the desired function, which is not divergent this time. The results are often in very good agreement with the desired function. This technique is very useful if we proceed to an expansion of a higher order than what we do: we have to provide at least 2 coefficients of the expansion, and we want to proceed until the order 2! Hence this technique is of no use for us.

We need another approach to get a functional relation $\underline{c}(\kappa)$, which is done in section 7.5: using the numerical results for $N = 5$ we proceed to a polynomial fitting of $\underline{c}(\kappa)$ of order 2 in powers of $\kappa^{\frac{1}{3}}$.

7.3 Numerical approach

7.3.1 Optimization algorithm

We adopt a numerical approach to obtain a solution of the self-consistent equation (7.1), which is equivalent to minimizing Thomas-Fermi energy given by formula (7.26) in our basis, under the constraint (7.27). Instead of solving numerically (7.1) we use an optimization algorithm, which consists of determining the solution which minimizes the energy $E(\underline{c}, R)$ with regards to the variables $(\underline{c}, R)$, under the constraint (7.27). In this language, E is the energy-cost function. It depends on an infinite number of variables. However, for evident reasons we have to restrict ourselves to a finite number of basis elements N for the description of the function ρ, hence the energy $E(R \doteq c_0, c_1, \ldots, c_N)$ is a function of $(N+1)$ variables. It is numerically simple to include the constraint, which is why we do it from the beginning. The energy becomes $E(c_0, \ldots, c_N(c_1, \ldots, c_{N-1}))$ and is a function of N variables. Based on the asymptotic limit $\kappa \to 0$, we work with the energy-cost function $e \doteq \frac{E}{\kappa^{\frac{1}{3}}}$, and with the variable $r \doteq R\kappa^{\frac{1}{3}}$. This allows dealing with numbers of the order 1 and we therefore have a better numerical stability.

The asymptotic limits provide the solution $\rho = \frac{3}{2\pi}\varphi_1$ in the limit $\kappa \to 0$ and $\rho = \frac{2}{\pi}\varphi_2$ in the limit $\kappa \to \infty$, this is why we make the conjecture that we can work with a small number of basis elements, $N = \mathcal{O}(1)$. This result will be established numerically.

Our work is based on (Bonnans et al., 2003). A great number of algorithms exists to compute the optimal solution, but the main idea is very often the same: we start from an initial condition $c^0 \doteq (c_0^0, \ldots, c_{N-1}^0)$, look for the negative steepest direction $-\nabla E(c_0^0, \ldots, c_{N-1}^0)$, and modify $c_i^0 \mapsto c_i^1$ such that the minimum is reached along this direction. This consists of defining $E(t) \doteq E(c^0 - t\nabla E(c^0))$ and determining the minimum of $E(t)$, reached at $t = t_{min}^0$. We define then $c^1 \doteq c^0 - t_{min}^0 \nabla E(c^0)$, and proceed in the same way with this new starting point. We proceed iteratively until we reach the minimum of the energy-cost function, which is considered attained when the steepest slope is less than a threshold ϵ. The algorithm is very simple, and many variations exist to accelerate the convergence, which is not necessary in our case: as we have a small number of variables only, the speed of convergence is not crucial.

7.3.2 Program description

Numerical simulations were done with Fortran 90, with the Salford compiler. The algorithm is based on the previous discussion.

The function ρ is square integrable, $\int \mathrm{d}^2\boldsymbol{x}\rho^2(\boldsymbol{x}) < \infty$, which means, in terms of the coefficients $\underline{c}$: $2\pi \sum_{n,m\geq 1} \frac{c_n c_m}{2+n+m} < \infty$. Hence, $c_n \to 0$, $n \to \infty$. In the asymptotic limit we establish $c_n \sim n^{-\frac{1}{2}}$, which decreases slowly. To accelerate decrease, we "normalize" the basis elements φ_n, replacing them by $\psi_n \doteq \sqrt{2+2n}\varphi_n$. The density becomes $\rho = \sum_{n\geq 1} c_n\varphi_n = \sum_{n\geq 1} a_n\psi_n$, where $a_n = \frac{c_n}{\sqrt{2+2n}}$. The new basis is not orthonormal but the norms of the basis elements are now independent of n:

$$\langle\psi_n|\psi_m\rangle = \frac{2\pi\sqrt{2+2n}\sqrt{2+2m}}{2+n+m} = \frac{4\pi\sqrt{1+n}\sqrt{1+m}}{\left(\sqrt{1+n}-\sqrt{1+m}\right)^2 + 2\sqrt{1+m}\sqrt{1+n}}, \tag{7.116}$$

which implies in particular

$$\|\psi_n\| = \sqrt{2\pi}. \tag{7.117}$$

The decreasing of a_n is faster in the asymptotic limit $n \to \infty$ ($a_n \sim n^{-1}$). This is why this description is best adapted for the numerical computations, and we use it instead of the non "normalized" basis.

The threshold ϵ has to be determined carefully. The energy-cost function is given by a positive definite quadratic form (called $\frac{1}{2}g$ previously), but a careful analysis of it shows that its eigenvalues can be very small. For example, for $N = 5$ and $\kappa = 0.0625$, the smallest eigenvalue is of the order of 10^{-7}. Hence the solution we find can be "far" (in the $\mathbb{R}^N$ sense, that is with the euclidean distance $\left(\sum_{n=1}^{N} c_n^2\right)^{\frac{1}{2}}$) from the exact solution. If λ is the smallest eigenvalue, after some iterations, the solution "falls" in the valley given by the eigenvector direction $\underline{e}_\lambda$, and stays at a distance d from the exact solution. The energy is $E(d) = E^\star + \frac{1}{2}\lambda d^2$, where $E^\star$ is the minimal energy. Hence the absolute value of the slope in the direction $\underline{e}_\lambda$ (that is the slope in the direction of the solution $\underline{c}^\star$) is $\frac{\mathrm{d}E(d)}{\mathrm{d}d} = \lambda d$. The algorithm stops once the slope ϵ is reached, which means $\epsilon = \lambda d \Rightarrow d = \frac{\epsilon}{\lambda}$. Therefore, if we choose $\epsilon = 10^{-5}, N = 5, \kappa = 0.0625$, we have $d = \mathcal{O}(10^2)$! However, the distance d is not the relevant distance to measure the difference between two solutions $\underline{c}$ and $\underline{c}'$, as we will see later. From these considerations we decided to work with a double precision.

We start the procedure with the initial condition $c_1^0 = \frac{3}{2\pi}$, $c_i^0 = 0$, $i = 2, \ldots, 5$, as the solution, for $\kappa \ll 1$, is close to this value.

7.3.3 Numerical tests

In order to validate our program and to determine which value of the parameters N and ϵ provide a sufficient precision, we proceed to different tests.

First we test the program in the asymptotic limits $\kappa \ll 1$ and $\kappa \gg 1$, for which we obtain the same results than the analytical ones.

We compute results for fixed κ (we choose $\kappa = 1.0$ and $\kappa = 0.0625$, which corresponds to $\hbar\omega = 3meV$, in modified atomic units), and for $N = 2, 3, \ldots, 10$, $\epsilon = 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}$. Another set of tests are done for $N = 2, 3, \ldots, 20$, $\epsilon =$

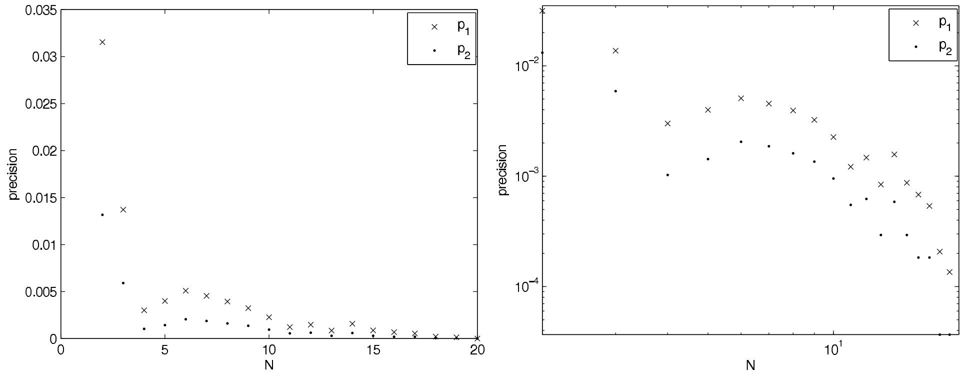
10^{-4}. We compare the results to a reference solution (ρ^{ref}, R^{ref}). This reference solution is that which has the highest N and the smallest ϵ of the set of computations.

We characterize the precision of the solution $(\underline{c}, R)$ with two parameters, p_1 and p_2, defined as follows:

$$\begin{aligned} p_1 &= \frac{\|\rho-\rho^{ref}\|}{\|\rho^{ref}\|} = \left(\frac{\sum_{n,m\geq 1} \frac{(c_n c_m + c_n^{ref} c_m^{ref} - 2 c_n c_m^{ref})}{(2+n+m)}}{\sum_{n,m\geq 1} \frac{c_n^{ref} c_m^{ref}}{(2+n+m)}} \right)^{\frac{1}{2}}, \\ p_2 &= \frac{|R-R^{ref}|}{|R^{ref}|}. \end{aligned}$$

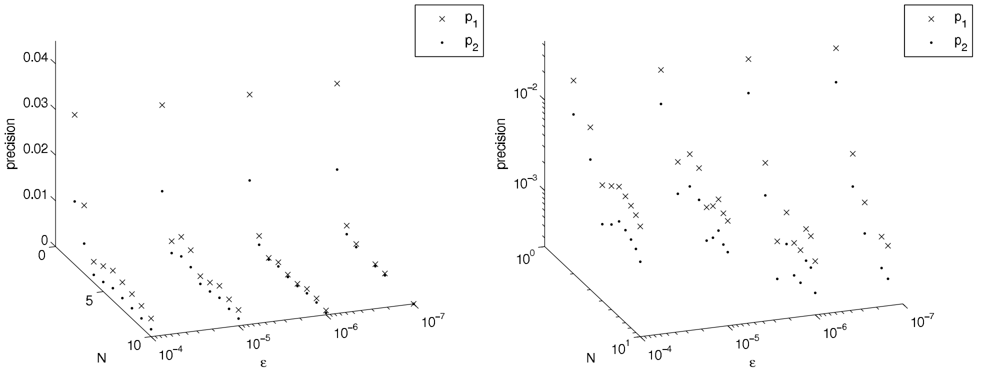
The results are shown in Figures 7.3 and 7.4 for $\kappa = 1.0$, and in Figures 7.5 and 7.6 for $\kappa = 0.0625$.

These results show that the precision is in each case less than a few percent, and becomes rapidly less than 10^{-2}. This is why we restrict to $N = 5$ and $\epsilon = 10^{-6}$: the precision is sufficient (for $\kappa = 1.0$ we find $p_1 = 1.62 \cdot 10^{-3}$, $p_2 = 7.30 \cdot 10^{-4}$, and for $\kappa = 0.0625$ we find $p_1 = 3.66 \cdot 10^{-3}$, $p_2 = 1.52 \cdot 10^{-3}$).



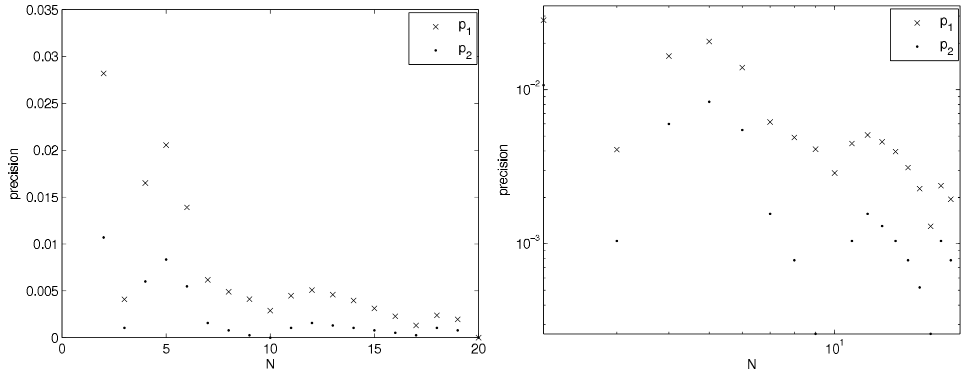
(a) (b)

Figure 7.3: *Precision p_1, p_2 versus N, for $\epsilon = 10^{-4}$, on a linear (left) and logarithmic (right) scale, for $\kappa = 1.0$.*



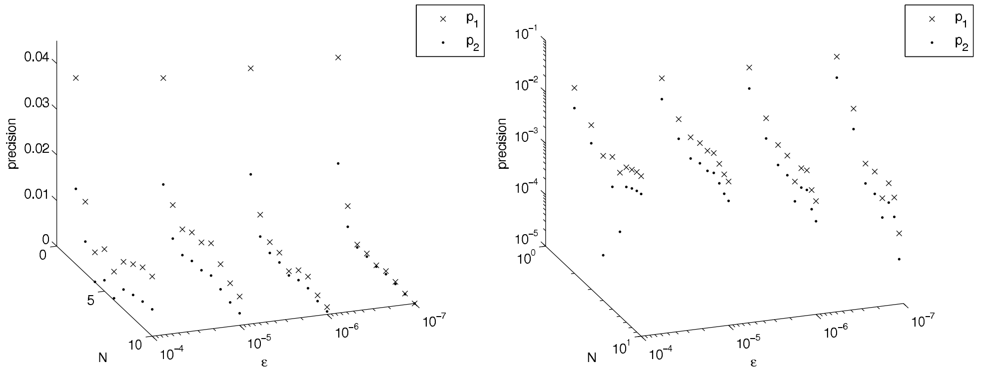
(a) (b)

Figure 7.4: *Precision p_1, p_2 versus N and ϵ, on a linear (left) and logarithmic (right) scale, for $\kappa = 1.0$.*



(a) (b)

Figure 7.5: *Precision* p_1, p_2 *versus* N, *for* $\epsilon = 10^{-4}$, *on a linear (left) and logarithmic (right) scale, for* $\kappa = 0.0625$.



(a) (b)

Figure 7.6: *Precision* p_1, p_2 *versus* N *and* ϵ, *on a linear (left) and logarithmic (right) scale, for* $\kappa = 0.0625$.

7.4 Verification of the analytical approximations

Our analytical approximations correspond to the first terms of a divergent series, hence there is no reason why our results should be close to the exact solution. This is why we compare it to a reference solution, which is chosen to be the numerical simulation with $N = 5,\ \epsilon = 10^{-6}$, which is a solution with enough precision (see section 7.3.3).

Another reason which implies the necessity to verify the results is that we do not have a control on the analytical approximations. We have a control through the parameter κ, but we work on a restricted subspace $E_1 \times E_2$, and this approximation is not controllable (the control parameter would be N).

Experimental conditions are such that $\kappa \ll 1$. For example, the results in (Kouwenhoven et al., 2001) are modeled with $\kappa = \frac{k'}{N_e^{\frac{3}{2}}}$, where k' is a constant and is $k' = 0.27$ in our units, and N_e is the number of electrons, as established in chapter 4. The small parameter we use in our developments is $p = \kappa^{\frac{1}{3}} = \frac{0.65}{N_e^{\frac{1}{2}}}$, which is not that small, and this is another reason why our results have to be verified. However, let's note that we work with large N_e, which makes this parameter smaller. For example, for $N_e = 30$, this parameter is $p = 0.12$.

We obtain a functional relation $R(\kappa)$. The density is also obtained as a function of κ through the coefficients $c_i(\kappa),\ i = 1, 2$.

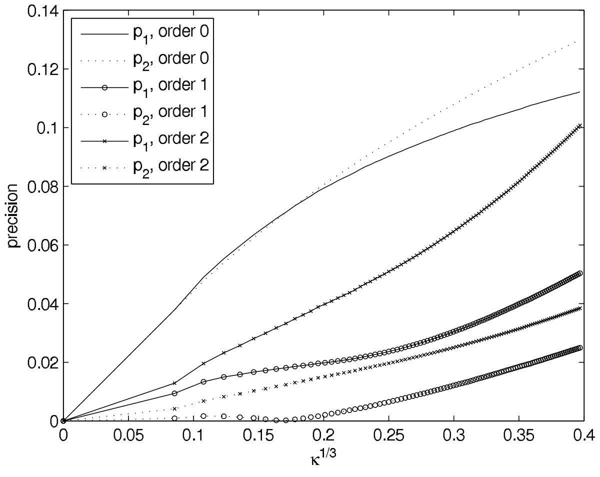


Figure 7.7: *Precision* p_1, p_2 *versus* $p = \kappa^{\frac{1}{3}}$ *for the analytical approximations of orders* $0, 1, 2$ *and* 3. *The reference solution is the numerical simulation, obtained with* $N = 5, \epsilon = 10^{-6}$.

The analytical approximation is compared to the numerical reference solution quantitatively: we compute the precision p_1 and p_2 as a function of κ, for κ between 0.0 and 0.0625. We do it for all orders from 0 to 3. We show it as a function of $p = \kappa^{\frac{1}{3}}$ at Figure 7.7. Unsurprisingly, the two precision parameters are increasing with p. The development at order 0 is the worst case, and we can see, for $p \ll 1$, that p_1 and p_2 are linear with regards to p. Surprisingly, the best approximation, for values of κ smaller than $\kappa = 0.0625$, is that of order 1, for both p_1 and p_2. Let's note that the precision, for $\kappa = 0.0625$, is $p_1 = 0.050$, which is too high, and the precision $p_2 = 0.025$ is less but still important. The difference comes from the fact that p_1 provides information on the precision of the shape of the density. We developed it on two basis elements only, which implies that this shape cannot be precisely approximated.

Our analytical results are therefore not precise enough and we need another approach to obtain an expansion of the solution of the self-consistent equation (that is $\underline{c}$ and R) in powers of $\kappa^{\frac{1}{3}}$. The approach we adopt is more pragmatic and consists of fitting the numerical solution for the coefficients $\{c_i\}_{i=1}^{N}$ as well as R by a polynomial of order two in $p = \kappa^{\frac{1}{3}}$. We do it for $N = 5$.

7.5 Polynomial fitting

To obtain the density as an expansion in powers of $p = \kappa^{\frac{1}{3}}$ we proceed to a polynomial fitting of order 3 of the numerical results as a function of p. As mentioned previously, the solution in the space $\{c_i\}$ can be far from the real solution (in the $\mathbb{R}^N$ sense), and this is why we increase the precision to the highest level, by fixing the threshold at $\epsilon = 10^{-8}$, in which case numerical computations are long.

We do the simulations for 100 values of p, uniformly distributed between 0 and 0.5. Due to the very small threshold, the results are precise enough and show a regular curve, which allow us to do a polynomial fitting. We obtain numerical functions $\{c_i(\kappa)\}_{i=1}^{5}$, which we approximate with a polynomial fitting.

To fit the coefficients $\{c_i\}_{i=1}^{5}$ with a polynomial of order 3 of p we use the method of least squares: for each coefficient $\{c_i\}_{i=1}^{4}$ we define a polynomial $c_i^{fit}(p) \doteq a_i^0 + a_i^1 p + a_i^2 p^2 + a_i^3 p^3$. The numerical function $c_i(p)$ is defined by M values c_i^j corresponding to the points p_j ($M = 100$ in our case). We minimize the function

$$f(a_i^0, a_i^1, a_i^2, a_i^3) \doteq \sum_{j=1}^{M} \left(c_i^j - c_i^{fit}(p_j) \right)^2 \tag{7.118}$$

with regards to its variables $a_i^j, i = 0, 1, 2, 3$. It provides 4 equations from which we compute the coefficients of the polynomial. In our problem, we know the values of $c_i(p = 0)$ from the asymptotic limit $\kappa \to 0$. They are $c_1(0) = \frac{3}{2\pi} = 0.4775$, $c_i(0) = 0$, $i = 2, 3, 4$, which are constraints and fix the parameters a_i^0. The last coefficient c_5 is defined as a polynomial such that the constraint (7.27) is satisfied at each order. It is in very good agreement with a polynomial fitting c_5^{fit} obtained with the procedure explained above.

This method provides the following results:

$$\left\{\begin{array}{lcl} c_1(\kappa) & = & 0.4775 - 0.9344\kappa^{\frac{1}{3}} + 1.6326\kappa^{\frac{2}{3}} - 1.1788\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}), \\ c_2(\kappa) & = & 0.6107\kappa^{\frac{1}{3}} - 1.0730\kappa^{\frac{2}{3}} + 0.7500\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}), \\ c_3(\kappa) & = & 1.0926\kappa^{\frac{1}{3}} - 2.0541\kappa^{\frac{2}{3}} + 1.5380\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}), \\ c_4(\kappa) & = & 0.7770\kappa^{\frac{1}{3}} - 1.5356\kappa^{\frac{2}{3}} + 1.1935\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}), \\ c_5(\kappa) & = & -1.3246\kappa^{\frac{1}{3}} + 2.7356\kappa^{\frac{2}{3}} - 2.1076\kappa + \mathcal{O}(\kappa^{\frac{4}{3}}). \end{array}\right. \tag{7.119}$$

These polynomial fittings are superposed to the numerical solution in Figure 7.8.

To fit the radius R we proceed to a polynomial fitting of order 2 of $r = R\kappa^{\frac{1}{3}}$ as a function of p, again with the method of least squares. The constraint is $\lim_{\kappa\to 0} R(\kappa)\kappa^{\frac{1}{3}} = \left(\frac{3\pi}{4}\right)^{\frac{1}{3}} = 1.3307$, which is the asymptotic limit $\kappa \to 0$. We obtain

$$R(\kappa)\kappa^{\frac{1}{3}} = 1.3307 + 0.5885\kappa^{\frac{1}{3}} - 0.3081\kappa^{\frac{2}{3}} + \mathcal{O}(\kappa). \tag{7.120}$$

This polynomial fitting is superposed to the numerical solution in Figure 7.9.

What do the results look like? To have an idea of the shape of the density $\rho(x)$ obtained with this fitting, we compare it to the reference numerical solution for 2 values of κ: 0.001 and 0.125. They are shown in Figure 7.10. They are in very good agreement with the reference solution in both cases.

Let's proceed to a quantitative analysis of the precision of the fitting. We do it by computing the precision parameters p_1 and p_2 as functions of $\kappa^{\frac{1}{3}}$. Results are shown in Figure 7.11

p_1 and p_2 present oscillations as a function of $\kappa^{\frac{1}{3}}$, but with a very low amplitude: the values are of the order of a thousandth, which means that the precision is very high.

The solution we obtained with the polynomial fitting can therefore be used for further computations and be considered as a solution of the self-consistent equation, its precision being sufficient in the domain of the parameter κ which we will use.

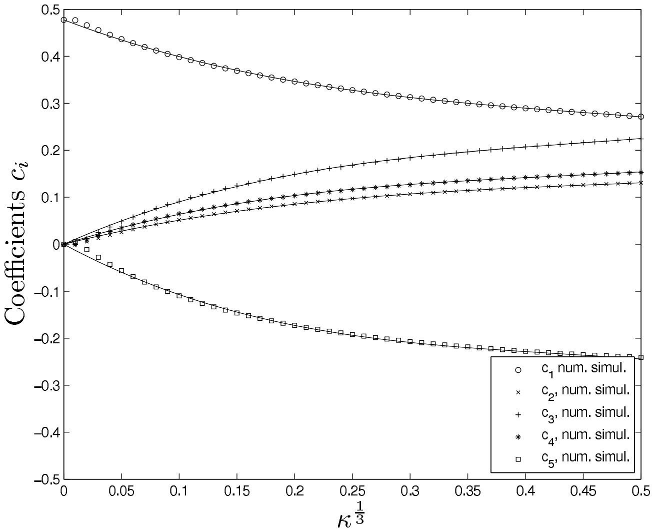


Figure 7.8: *Numerical results ($N = 5, \epsilon = 10^{-8}$) and polynomial fitting of the coefficients $\{c_i\}_{i=1}^{5}$ versus $\kappa^{\frac{1}{3}}$. The polynomial fittings are represented by solid lines.*

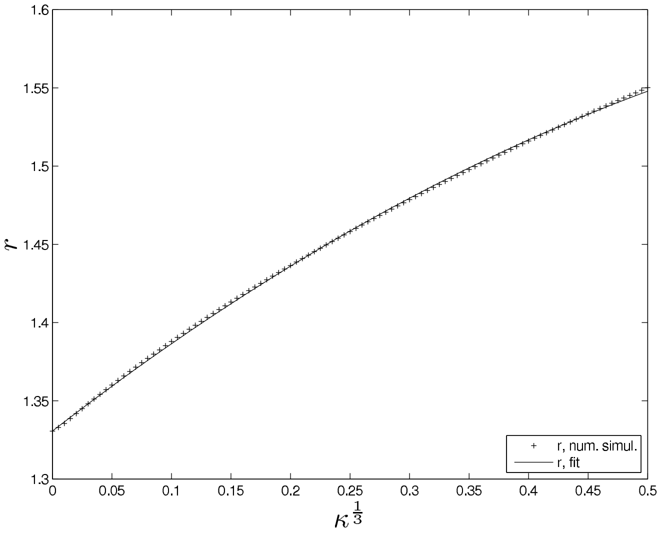
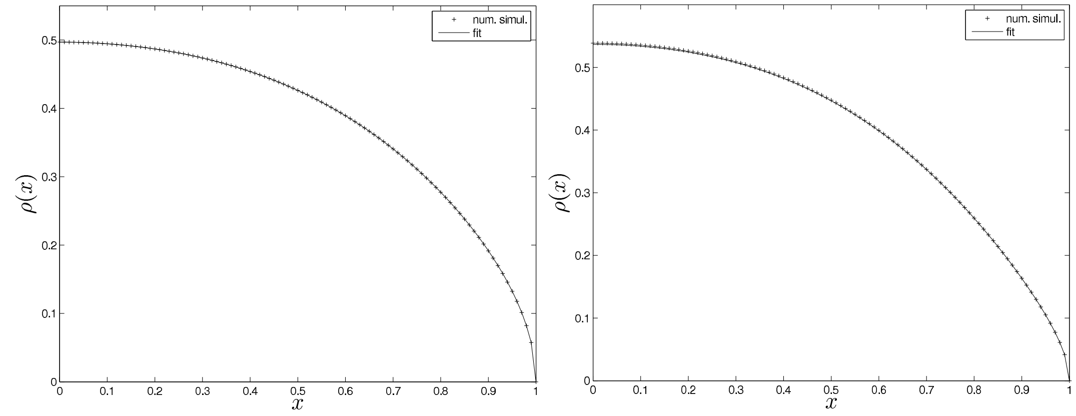


Figure 7.9: *Numerical results ($N = 5, \epsilon = 10^{-8}$) and polynomial fitting of $r = R(\kappa)\kappa^{\frac{1}{3}}$ versus $\kappa^{\frac{1}{3}}$.*



(a)

(b)

Figure 7.10: *Scaled density $\rho(x)$, for the numerical solution ($N = 5, \epsilon = 10^{-8}$) and for the polynomial fitting, for $\kappa = 0.001$ and $\kappa = 0.125$.*

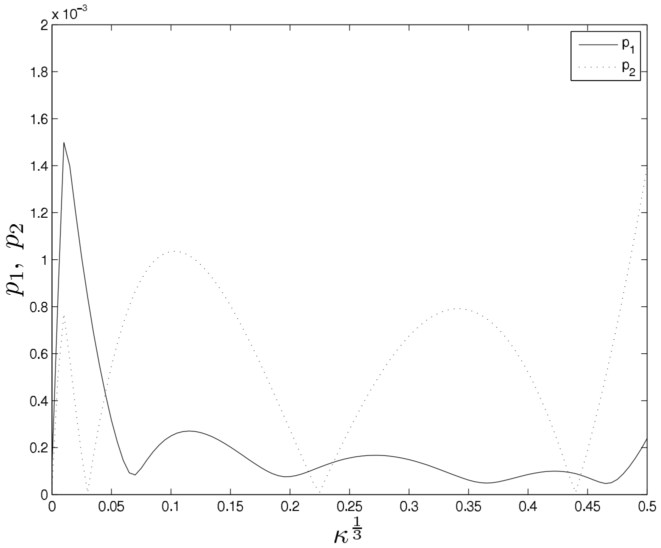


Figure 7.11: *Precision of the polynomial fitting, compared to numerical simulations ($N = 5, \epsilon = 10^{-8}$).*

Chapter 8

Smooth and oscillating energy

Contents

The objective of this chapter is to obtain an explicit expression of the smooth and oscillating parts of the ground state energy of a quantum dot.

In chapter 5 we established formulas for the computation of the ground state energy of many-fermion systems. We obtained these results in the semiclassical Hartree-Fock framework, which was justified by the developments of chapter 2.

As our technique does not provide the oscillating terms, these were computed at chapter 6 in the specific two-dimensional case. All these formulas are functionals of a potential, the self-consistent potential, which was computed numerically in chapter 7. We still have to introduce this solution in the formulas, which is what we do in this chapter.

We first compute the smooth contribution to the ground state energy. We use the density obtained by the self-consistent equation in chapter 7 (it is equivalent to consider the self-consistent density or the self-consistent potential) to first compute the lowest order contribution to the energy, given by Thomas-Fermi energy, as established in chapter 5, and proceed to an expansion in powers of $p \doteq \kappa^{\frac{1}{3}}$. The next term is treated using the lowest order part of the self-consistent potential, for which we have an analytical expression. We then compute the exchange energy, introducing the self-consistent potential in the formula obtained in chapter 5, and proceed to an expansion in powers of p.

Next we compute the energy oscillations. To simplify the problem we scale the expressions. We study some relevant properties of the periodic orbits, and identify which ones have to be considered. We observe that only one family of periodic orbits has to be considered, the other ones being negligible. Having obtained the energy oscillations, we return to the non scaled system to obtain the final oscillations.

8.1 Smooth terms

8.1.1 Thomas-Fermi energy

We established that the dominant contribution to the energy is the Hartree energy, and we established that it is equivalent to Thomas-Fermi energy, which is better adapted to our needs. It is

$$\hat{E}_{00} = \frac{N^2}{L_\star}\left(\frac{\pi}{2}\frac{1}{L_\star}\int \mathrm{d}^2\hat{\boldsymbol{x}}\hat{\rho}^2(\hat{\boldsymbol{x}}) + \int \mathrm{d}^2\hat{\boldsymbol{x}}\hat{V}_{ext}(\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{x}}) + \frac{1}{2}\int \mathrm{d}^2\hat{\boldsymbol{x}}\int \mathrm{d}^2\hat{\boldsymbol{y}}\frac{\hat{\rho}(\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|}\right). \tag{8.1}$$

The length $L_\star$ was introduced to identify the importance of the length. We can however choose it as we want. For convenience we will fix it to $L_\star = 1$: the length scale is the Bohr radius. Hence the energy becomes

$$\begin{aligned}\hat{E}_{00} &= N^2\left(\frac{\pi}{2}\int \mathrm{d}^2\hat{\boldsymbol{x}}\hat{\rho}^2(\hat{\boldsymbol{x}}) + \int \mathrm{d}^2\hat{\boldsymbol{x}}\hat{V}_{ext}(\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{x}}) + \frac{1}{2}\int \mathrm{d}^2\hat{\boldsymbol{x}}\int \mathrm{d}^2\hat{\boldsymbol{y}}\frac{\hat{\rho}(\hat{\boldsymbol{x}})\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|}\right)\\ &= \frac{N^2}{R}\left(\frac{\pi}{2}\frac{1}{R}\int \mathrm{d}^2\boldsymbol{x}\rho^2(\boldsymbol{x}) + \int \mathrm{d}^2\boldsymbol{x}V_{ext}(\boldsymbol{x})\rho(\boldsymbol{x}) + \frac{1}{2}\int \mathrm{d}^2\boldsymbol{x}\int \mathrm{d}^2\boldsymbol{y}\frac{\rho(\boldsymbol{x})\rho(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\right),\end{aligned} \tag{8.2}$$

where $\rho(\boldsymbol{x}) = R^2\hat{\rho}(R\boldsymbol{x})$ is the normalized density, as defined by a scaling in chapter 7.

It is simple to express this energy in terms of the parametrization we used to compute numerically the solution of the self-consistent equation (we solved the self-consistent equation for the density ρ, which is equivalent to solving it for the potential V). Writing the normalized density in the basis $\{\varphi_n\}_{n\geq 1}$, $\varphi_n(x) \doteq (1-x^2)^{\frac{n}{2}}$:

$$\rho(x) = \sum_{n\geq 1} c_n\varphi_n(x), \tag{8.3}$$

the energy becomes

$$\hat{E}_{00} = N^2E_{00} = N^2\left(\frac{1}{R^2}\sum_{n,m\geq 1} t_{nm}c_nc_m + R^2\kappa\sum_{n\geq 1} v_n^{ext}c_n + \frac{1}{R}\sum_{n,m\geq 1} v_{nm}c_nc_m\right), \tag{8.4}$$

where t, v^{ext}, and v were established in chapter 7.

Numerically, we restricted the number of basis elements to 5 and proceeded to a polynomial fitting in powers of $p \doteq \kappa^{\frac{1}{3}}$, to obtain

$$\left\{\begin{array}{rcl} c_n(p) &=& c_{n0} + c_{n1}p + c_{n2}p^2 + c_{n3}p^3 + \mathcal{O}(p^4), \quad n = 1,\ldots 5, \\ R(p) &=& R_{-1}p^{-1} + R_0 + R_1p + \mathcal{O}(p^2). \end{array}\right. \tag{8.5}$$

The lowest order terms, determined analytically in the asymptotic limit, are

$$\left\{\begin{array}{rcl} c_{10} &=& \frac{3}{2\pi}, \\ c_{n0} &=& 0, \; n \neq 1, \\ R_{-1} &=& \left(\frac{3\pi}{4}\right)^{\frac{1}{3}}. \end{array}\right. \tag{8.6}$$

The energy becomes

$$\begin{aligned} \hat{E}_{00} \;=\; N^2\Bigg[& \frac{1}{\left(\sum_{i=-1}^{1} R_ip^i\right)^2}\sum_{n,m=1}^{5} t_{nm}\left(\sum_{i=0}^{2} c_{ni}p^i\right)\left(\sum_{j=0}^{2} c_{mj}p^j\right) \\ & + \left(\sum_{i=-1}^{1} R_ip^i\right)^2 p^3\sum_{n=1}^{5} v_n^{ext}\left(\sum_{i=0}^{2} c_{ni}p^i\right) \\ & + \frac{1}{\left(\sum_{i=-1}^{1} R_ip^i\right)}\sum_{n,m=1}^{5} v_{nm}\left(\sum_{i=0}^{2} c_{ni}p^i\right)\left(\sum_{j=0}^{2} c_{mj}p^j\right) + \mathcal{O}(p^3)\Bigg]. \end{aligned} \tag{8.7}$$

From this formula we can proceed to an expansion of the energy in powers of p (remembering that $c_{n0} = 0, \; n \neq 1$):

$$\hat{E}_{00} = N^2\left(e_1p + e_2p^2 + e_3p^3 + e_4p^4 + \mathcal{O}(p^5)\right), \tag{8.8}$$

where long calculations provide

$$\begin{aligned}
e_1 &= \frac{2\pi^3}{15}\frac{c_{10}^2}{R_{-1}} + \frac{2\pi}{15}c_{10}R_{-1}^2,\\
e_2 &= \frac{\pi^2}{4}\frac{c_{10}^2}{R_{-1}^2} - \frac{2\pi^3}{15}\frac{c_{10}^2 R_0}{R_{-1}^2} + \frac{4\pi}{15}c_{10}R_0R_{-1}\\
&\quad + \frac{\pi}{3}R_{-1}^2\left[\frac{2}{5}c_{11} + \frac{1}{4}c_{21} + \frac{6}{35}c_{31} + \frac{1}{8}c_{41} + \frac{2}{21}c_{51}\right]\\
&\quad + \frac{\pi^3}{3}\frac{c_{10}}{R_{-1}}\left[\frac{4}{5}c_{11} + \frac{5}{8}c_{21} + \frac{18}{35}c_{31} + \frac{7}{16}c_{41} + \frac{8}{21}c_{51}\right],\\
e_3 &= -\frac{\pi^2}{2}\frac{c_{10}^2 R_0}{R_{-1}^3} + \frac{2\pi^3}{15}\frac{c_{10}^2 R_0^2}{R_{-1}^3} - \frac{2\pi^3}{15}\frac{c_{10}^2 R_1}{R_{-1}^2}\\
&\quad + \frac{\pi^2}{R_{-1}^2}c_{10}\left[\frac{1}{2}c_{11} + \frac{2}{5}c_{21} + \frac{1}{3}c_{31} + \frac{2}{7}c_{41} + \frac{1}{4}c_{51}\right]\\
&\quad - \pi^3\frac{c_{10}R_0}{R_{-1}^2}\left[\frac{4}{15}c_{11} + \frac{5}{24}c_{21} + \frac{6}{35}c_{31} + \frac{7}{48}c_{41} + \frac{8}{63}c_{51}\right]\\
&\quad + \pi^3\frac{c_{10}}{R_{-1}}\left[\frac{4}{15}c_{12} + \frac{5}{24}c_{22} + \frac{6}{35}c_{32} + \frac{7}{48}c_{42} + \frac{8}{63}c_{52}\right]\\
&\quad + \frac{2\pi}{15}c_{10}R_0^2 + \frac{4\pi}{15}c_{10}R_{-1}R_1\\
&\quad + \pi\frac{1}{R_{-1}}\left[\frac{2\pi^2}{15}c_{11}^2 + \frac{256}{315}c_{21}^2 + \frac{2\pi^2}{35}c_{31}^2 + \frac{65536}{155925}c_{41}^2 + \frac{100\pi^2}{3003}c_{51}^2\right]\\
&\quad + \pi\frac{1}{R_{-1}}\left[\frac{5\pi^2}{24}c_{11}c_{21} + \frac{6\pi^2}{35}c_{11}c_{31} + \frac{7\pi^2}{48}c_{11}c_{41} + \frac{8\pi^2}{63}c_{11}c_{51} + \frac{35\pi^2}{256}c_{21}c_{31}\right.\\
&\quad \left. + \frac{16384}{14175}c_{21}c_{41} + \frac{105\pi^2}{1024}c_{21}c_{51} + \frac{63\pi^2}{640}c_{31}c_{41} + \frac{20\pi^2}{231}c_{31}c_{51} + \frac{77\pi^2}{1024}c_{41}c_{51}\right]\\
&\quad + \pi R_0R_{-1}\left[\frac{4}{15}c_{11} + \frac{1}{6}c_{21} + \frac{4}{35}c_{31} + \frac{1}{12}c_{41} + \frac{4}{63}c_{51}\right]\\
&\quad + \pi R_{-1}^2\left[\frac{2}{15}c_{12} + \frac{1}{12}c_{22} + \frac{2}{35}c_{32} + \frac{1}{24}c_{42} + \frac{2}{63}c_{52}\right]. \qquad (8.9)
\end{aligned}$$

The analytical formula of e_4 is very long (but its computation presents no technical difficulty), we do not write it here.

We can now introduce the value of c_{10} and R_{-1} given by (8.6) to obtain

$$\begin{aligned}
e_1 &= \frac{3^{\frac{5}{3}}\pi^{\frac{2}{3}}}{2^{\frac{4}{3}}5},\\
e_2 &= \frac{3^{\frac{4}{3}}}{2^{\frac{8}{3}}\pi^{\frac{2}{3}}} + \frac{\pi^{\frac{5}{3}}}{2^{\frac{1}{3}}3^{\frac{1}{3}}}c_{11} + \frac{3^{\frac{2}{3}}\pi^{\frac{5}{3}}}{2^{\frac{7}{3}}}c_{21} + \frac{3^{\frac{2}{3}}\pi^{\frac{5}{3}}}{2^{\frac{1}{3}}5}c_{31} + \frac{\pi^{\frac{5}{3}}}{2^{\frac{4}{3}}3^{\frac{1}{3}}}c_{41} + \frac{3^{\frac{2}{3}}\pi^{\frac{5}{3}}}{2^{\frac{1}{3}}7}c_{51},
\end{aligned}$$

$$\begin{aligned}
e_3 \;=\;& -\frac{3}{2\pi}R_0 + \frac{3}{5}R_0^2 + \left(\frac{3^{\frac{1}{3}}\pi^{\frac{1}{3}}}{2^{\frac{2}{3}}} - \frac{2^{\frac{4}{3}}\pi^{\frac{4}{3}}}{3^{\frac{2}{3}}5}R_0\right)c_{11} \\
&+\left(\frac{2^{\frac{4}{3}}3^{\frac{1}{3}}\pi^{\frac{1}{3}}}{5} - \frac{3^{\frac{1}{3}}\pi^{\frac{4}{3}}}{2^{\frac{8}{3}}}R_0\right)c_{21} + \left(\frac{2^{\frac{1}{3}}\pi^{\frac{1}{3}}}{3^{\frac{2}{3}}} - \frac{2^{\frac{7}{3}}3^{\frac{1}{3}}\pi^{\frac{4}{3}}}{5\cdot 7}R_0\right)c_{31} \\
&+\left(\frac{2^{\frac{4}{3}}3^{\frac{1}{3}}\pi^{\frac{1}{3}}}{7} - \frac{5\pi^{\frac{4}{3}}}{2^{\frac{11}{3}}3^{\frac{2}{3}}}R_0\right)c_{41} + \left(\frac{3^{\frac{1}{3}}\pi^{\frac{1}{3}}}{2^{\frac{5}{3}}} - \frac{2^{\frac{4}{3}}\pi^{\frac{4}{3}}}{3^{\frac{2}{3}}7}R_0\right)c_{51} \\
&+\frac{\pi^{\frac{5}{3}}}{2^{\frac{1}{3}}3^{\frac{1}{3}}}c_{12} + \frac{3^{\frac{2}{3}}\pi^{\frac{5}{3}}}{2^{\frac{7}{3}}}c_{22} + \frac{3^{\frac{2}{3}}\pi^{\frac{5}{3}}}{2^{\frac{1}{3}}5}c_{32} + \frac{\pi^{\frac{5}{3}}}{2^{\frac{4}{3}}3^{\frac{1}{3}}}c_{42} + \frac{3^{\frac{2}{3}}\pi^{\frac{5}{3}}}{2^{\frac{1}{3}}7}c_{52} \\
&+\frac{2^{\frac{2}{3}}\pi^{\frac{2}{3}}}{3^{\frac{1}{3}}}\left[\frac{2\pi^2}{15}c_{11}^2 + \frac{256}{315}c_{21}^2 + \frac{2\pi^2}{35}c_{31}^2 + \frac{65536}{155925}c_{41}^2 + \frac{100\pi^2}{3003}c_{51}^2\right] \\
&+\frac{2^{\frac{2}{3}}\pi^{\frac{2}{3}}}{3^{\frac{1}{3}}}\left[\frac{5\pi^2}{24}c_{11}c_{21} + \frac{6\pi^2}{35}c_{11}c_{31} + \frac{7\pi^2}{48}c_{11}c_{41} + \frac{8\pi^2}{63}c_{11}c_{51} + \frac{35\pi^2}{256}c_{21}c_{31}\right. \\
&\left.+\frac{16384}{14175}c_{21}c_{41} + \frac{105\pi^2}{1024}c_{21}c_{51} + \frac{63\pi^2}{640}c_{31}c_{41} + \frac{20\pi^2}{231}c_{31}c_{51} + \frac{77\pi^2}{1024}c_{41}c_{51}\right].
\end{aligned} \tag{8.10}$$

We find analytically the asymptotic limit $\kappa \to 0$:

$$\hat{E}_{00} \sim \frac{3^{\frac{5}{3}}\pi^{\frac{2}{3}}}{2^{\frac{4}{3}}5}N^2\kappa^{\frac{1}{3}} = 1.0624N^2\kappa^{\frac{1}{3}}. \tag{8.11}$$

Introducing now the numerical value of the other coefficients, and adding the fourth order term e_4, we find

$$\hat{E}_{00} = N^2\big[1.0624\kappa^{\frac{1}{3}} + 0.3177\kappa^{\frac{2}{3}} - 0.1074\kappa^{\frac{3}{3}} + 0.0977\kappa^{\frac{4}{3}} + \mathcal{O}(\kappa^{\frac{5}{3}})\big]. \tag{8.12}$$

The numbers e_i show a decrease as i increases, which is an indicator of the convergence of this series.

8.1.2 First corrections to Thomas-Fermi

We need to go beyond Thomas-Fermi energy for consistency (it will become evident later). Let's note that if we use the general formulas developed previously, that is, writing with the initial variables,

$$\begin{aligned}
\hat{E}_{01} &= \frac{N}{24\pi}\int \mathrm{d}^2\hat{\boldsymbol{x}}\hat{\Delta}\hat{V}(\hat{\boldsymbol{x}})\theta(\hat{\mu} - \hat{V}(\hat{\boldsymbol{x}})) \\
&= \frac{N}{24\pi}\int_\Omega \mathrm{d}^2\hat{\boldsymbol{x}}\hat{\nabla}\cdot\hat{\nabla}\hat{V}(\hat{\boldsymbol{x}}) \\
&= \frac{N}{24\pi}\int_{\partial\Omega} \mathrm{d}\hat{\sigma}\cdot\hat{\nabla}\hat{V}(\hat{\boldsymbol{x}}) \\
&= \frac{N}{12}\,\hat{V}'(\hat{r})\Big|_{\hat{r}=R}.
\end{aligned} \tag{8.13}$$

We therefore have to compute $\hat{V}'(R)$. If we naively take the first derivative of the self-consistent potential at $\hat{r} = R$, it diverges. Is this divergence a real divergence? No, it arises from the non commutativity of the limit $\kappa \to 0$, and the derivative with respect to $\hat{r}$.

To compute $\hat{V}'(R)$ we will return to the self-consistent equation, which defines $\hat{V}$, and proceed the following way: we start by evaluating

$$\hat{\nabla}\hat{V}(\hat{r}) = \hat{\boldsymbol{e}}_{\hat{r}}\hat{V}'(\hat{r}) + \hat{\boldsymbol{e}}_{\hat{\theta}}\frac{1}{\hat{r}}\underbrace{\frac{\partial}{\partial\hat{\theta}}\hat{V}(\hat{r})}_{=0} \quad \Rightarrow \quad \hat{\boldsymbol{e}}_{\hat{r}}\cdot\hat{\nabla}\hat{V}(\hat{r}) = \hat{V}'(\hat{r}). \tag{8.14}$$

As we want to evaluate $\hat{V}'(R)$, we will evaluate $\hat{\boldsymbol{e}}_{\hat{r}}\cdot\hat{\nabla}\hat{V}(\hat{\boldsymbol{x}})$ at $\hat{\boldsymbol{x}} = R\hat{\boldsymbol{e}}_1$ to simplify the problem, to have $\hat{\boldsymbol{e}}_1 = \hat{\boldsymbol{e}}_{\hat{r}}$.

The self-consistent equation is

$$\hat{V}(\hat{\boldsymbol{x}}) = \frac{1}{2}\kappa\hat{\boldsymbol{x}}^2 + \int \mathrm{d}^2\hat{\boldsymbol{y}}\frac{\hat{\rho}(\hat{\boldsymbol{y}})}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|}. \tag{8.15}$$

Taking the gradient we find

$$\begin{aligned}\hat{\nabla}_{\hat{\boldsymbol{x}}}\hat{V}(\hat{\boldsymbol{x}}) &= \kappa\hat{\boldsymbol{x}} + \int \mathrm{d}^2\hat{\boldsymbol{y}}\hat{\rho}(\hat{\boldsymbol{y}})\frac{(\hat{\boldsymbol{y}}-\hat{\boldsymbol{x}})}{|\hat{\boldsymbol{x}}-\hat{\boldsymbol{y}}|^3}\\ &= \kappa\hat{\boldsymbol{x}} + \int \mathrm{d}^2\hat{\boldsymbol{y}}\hat{\rho}(\hat{\boldsymbol{y}}+\hat{\boldsymbol{x}})\frac{\hat{\boldsymbol{y}}}{|\hat{\boldsymbol{y}}|^3},\end{aligned} \tag{8.16}$$

where we proceeded to the change of variables $\hat{\boldsymbol{y}} \mapsto \hat{\boldsymbol{y}}-\hat{\boldsymbol{x}}$. As explained previously, we take $\hat{\boldsymbol{x}} = R\hat{\boldsymbol{e}}_1$, and project this equation on $\hat{\boldsymbol{e}}_1$ to obtain, with the change of variable $\hat{y} \mapsto y = \frac{\hat{y}}{R}$,

$$\begin{aligned}\hat{V}'(R) &= \kappa R + \int \mathrm{d}^2\boldsymbol{y}\hat{\rho}\left(R\sqrt{(y_1+1)^2+y_2^2}\right)\frac{y_1}{|\boldsymbol{y}^3|}\\ &= \kappa R + \int \mathrm{d}\theta\cos\theta\int \mathrm{d}y\hat{\rho}\left(R\sqrt{1+2y\cos\theta+y^2}\right),\end{aligned} \tag{8.17}$$

where we introduced the polar coordinates. The integration limits are such that $\rho(r) = 0,\ r > R$. This condition is (the variables being, of course, limited by $y > 0,\ \theta \in [0, 2\pi]$),

$$y < -2\cos\theta. \tag{8.18}$$

This implies $\cos\theta < 0$, which restricts $\theta \in [\frac{\pi}{2}, \frac{3\pi}{2}]$. A second condition is $1 + 2y\cos\theta + y^2 > 0$, but this is always satisfied for $y > 0$.

Let's note that, in view of this result, which we can write as (using the fact that $\hat{\rho}(R) = 0$):

$$\hat{V}'(R) = \kappa R + \int \mathrm{d}\theta\cos\theta\int \mathrm{d}y\left[\hat{\rho}\left(R\sqrt{1+2y\cos\theta+y^2}\right) - \hat{\rho}(R)\right], \tag{8.19}$$

we can conclude that if $\hat{\rho}(R-\epsilon)-\hat{\rho}(R)\sim\epsilon^{\alpha},\ \alpha>0$, this term will be finite, and the correction to the energy will be finite.

We can now compute the integral in (8.17). Using the density

$$\hat{\rho}(Rx)=\frac{3}{2\pi}\frac{1}{R^2}\sqrt{1-x^2}, \tag{8.20}$$

we find

$$\begin{aligned}\frac{3}{2\pi}\frac{1}{R^2}\int_{\frac{\pi}{2}}^{\frac{3\pi}{2}}\mathrm{d}\theta\cos\theta\int_0^{-2\cos\theta}\frac{\mathrm{d}y}{y}\sqrt{-y^2-2y\cos\theta}&\\ &=-\frac{3}{2\pi}\frac{1}{R^2}2\underbrace{\int_{\frac{\pi}{2}}^{\frac{3\pi}{2}}\mathrm{d}\theta\cos^2\theta}_{=\frac{\pi}{2}}\underbrace{\int_0^1\mathrm{d}z\sqrt{-1+\frac{1}{z}}}_{=\frac{\pi}{2}}\\ &=-\frac{3\pi}{4}\frac{1}{R^2},\end{aligned} \tag{8.21}$$

where we proceeded to the change of variable $y\mapsto z=-\frac{y}{2\cos\theta}$.

Let's return to equation (8.17):

$$V'(R)=\kappa R-\frac{3\pi}{4}\frac{1}{R^2}. \tag{8.22}$$

As established previously, the radius R is given by

$$R=\left(\frac{3\pi}{4\kappa}\right)^{\frac{1}{3}}, \tag{8.23}$$

the derivative of V is therefore

$$V'(R)=\kappa\left(\frac{3\pi}{4\kappa}\right)^{\frac{1}{3}}-\frac{3\pi}{4}\left(\frac{4\kappa}{3\pi}\right)^{\frac{2}{3}}=0. \tag{8.24}$$

Surprisingly, we find that this contribution is zero. Moreover, this energy would have been of the order of $Np^2=\mathcal{O}(1)$. There is therefore no need to compute the hypothetical corrections to this energy, as they would be of an order in N too low for our interest.

8.2 Exchange energy

Let's now consider the exchange energy. In equation (5.155) we found the result

$$\begin{aligned}\hat{E}_0^{ex}&=-N^{\frac{3}{2}}\frac{4\sqrt{2}}{3\sqrt{\pi}}\int\mathrm{d}^2\hat{\boldsymbol{x}}\hat{\rho}^{\frac{3}{2}}(\hat{\boldsymbol{x}})\\ &=-\frac{N^{\frac{3}{2}}}{R}\frac{4\sqrt{2}}{3\sqrt{\pi}}\int\mathrm{d}^2\boldsymbol{x}\rho^{\frac{3}{2}}(\boldsymbol{x})\end{aligned} \tag{8.25}$$

$$= -\frac{N^{\frac{3}{2}}}{R}\frac{4\sqrt{2}}{3\sqrt{\pi}}2\pi\int_0^1 \mathrm{d}rr\left(\sum_{n\geq 1} c_n\varphi_n(r)\right)^{\frac{3}{2}}. \tag{8.26}$$

Considering the expansion of the density in powers of p, and remembering that $c_{n0} = 0,\ n \neq 1$, we find

$$\begin{aligned}
&\int_0^1 \mathrm{d}rr\left(\sum_{n\geq 1} c_n\varphi_n(r)\right)^{\frac{3}{2}}\\
&= c_{10}^{\frac{3}{2}}\int_0^1 \mathrm{d}rr\varphi_1^{\frac{3}{2}}(r)\left(1+p\sum_{n\geq 1}\frac{c_{n1}}{c_{10}}\frac{\varphi_n(r)}{\varphi_1(r)}+p^2\sum_{n\geq 1}\frac{c_{n2}}{c_{10}}\frac{\varphi_n(r)}{\varphi_1(r)}+\mathcal{O}(p^3)\right)^{\frac{3}{2}}\\
&= c_{10}^{\frac{3}{2}}\int_0^1 \mathrm{d}rr\varphi_1^{\frac{3}{2}}\left(1+\frac{3}{2}p\sum_{n\geq 1}\frac{c_{n1}}{c_{10}}\frac{\varphi_n}{\varphi_1}\right.\\
&\qquad\left.+p^2\left(\frac{3}{8}\sum_{n,m\geq 1}\frac{c_{n1}c_{m1}}{c_{10}^2}\frac{\varphi_n\varphi_m}{\varphi_1^2}+\frac{3}{2}\sum_{n\geq 1}\frac{c_{n2}}{c_{10}}\frac{\varphi_n}{\varphi_1}\right)+\mathcal{O}(p^3)\right)\\
&= c_{10}^{\frac{3}{2}}\int_0^1 \mathrm{d}rr(1-r^2)^{\frac{3}{4}}+p\frac{3}{2}c_{10}^{\frac{1}{2}}\sum_{n\geq 1}c_{n1}\int_0^1 \mathrm{d}rr(1-r^2)^{\frac{n}{2}+\frac{1}{4}}\\
&\qquad+p^2\left(\frac{3}{8}c_{10}^{-\frac{1}{2}}\sum_{n,m\geq 1}c_{n1}c_{m1}\int_0^1 \mathrm{d}rr(1-r^2)^{\frac{n}{2}+\frac{m}{2}-\frac{1}{4}}\right.\\
&\qquad\left.+\frac{3}{2}c_{10}^{\frac{1}{2}}\sum_{n\geq 1}c_{n2}\int_0^1 \mathrm{d}rr(1-r^2)^{\frac{n}{2}+\frac{1}{4}}\right)+\mathcal{O}(p^3).
\end{aligned} \tag{8.27}$$

Using the result

$$\int_0^1 \mathrm{d}rr(1-r^2)^k = \frac{1}{2k+2}, \tag{8.28}$$

we finally obtain

$$\begin{aligned}
\int_0^1 \mathrm{d}rr\left(\sum_{n\geq 1} c_n\varphi_n(r)\right)^{\frac{3}{2}} &= \frac{2}{7}c_{10}^{\frac{3}{2}}+3c_{10}^{\frac{1}{2}}\sum_{n\geq 1}\frac{c_{n1}}{5+2n}p\\
&+\left(\frac{3}{4}c_{10}^{-\frac{1}{2}}\sum_{n,m\geq 1}\frac{c_{n1}c_{m1}}{3+2n+2m}+3c_{10}^{\frac{1}{2}}\sum_{n\geq 1}\frac{c_{n2}}{5+2n}\right)p^2\\
&+\mathcal{O}(p^3).
\end{aligned} \tag{8.29}$$

To obtain the expansion of the exchange energy we still have to proceed to the expansion of $\frac{1}{R}$:

$$\frac{1}{R} = \frac{p}{R_{-1}}\left(1-\frac{R_0}{R_{-1}}p+\left(\frac{R_0^2}{R_{-1}^2}-\frac{R_1}{R_{-1}}\right)p^2\right)+\mathcal{O}(p^3). \tag{8.30}$$

Combining these two expansions we finally write the expansion of the exchange energy

$$\begin{aligned}
\hat{E}_0^{ex} &= -N^{\frac{3}{2}}p\frac{8\sqrt{2\pi}}{3}\frac{1}{R_{-1}}\left[\frac{2}{7}c_{10}^{\frac{3}{2}}+p\left\{3c_{10}^{\frac{1}{2}}\sum_{n,m\geq 1}\frac{c_{n1}}{5+2n}-\frac{2}{7}c_{10}^{\frac{3}{2}}\frac{R_0}{R_{-1}}\right\}\right.\\
&\quad +p^2\left\{\frac{2}{7}c_{10}^{\frac{3}{2}}\left(\frac{R_0^2}{R_{-1}^2}-\frac{R_1}{R_{-1}}\right)-3\frac{R_0}{R_{-1}}c_{10}^{\frac{1}{2}}\sum_{n\geq 1}\frac{c_{n1}}{5+2n}\right.\\
&\quad \left.\left.+\left(\frac{3}{4}c_{10}^{-\frac{1}{2}}\sum_{n,m\geq 1}\frac{c_{n1}c_{m1}}{3+2n+2m}+3c_{10}^{\frac{1}{2}}\sum_{n\geq 1}\frac{c_{n2}}{5+2n}\right)\right\}\right]\\
&\quad +\mathcal{O}(p^4).
\end{aligned}\tag{8.31}$$

Expanding this expression we find

$$\hat{E}_0^{ex} = N^{\frac{3}{2}}\left(e_1^{ex}p+e_2^{ex}p^2+e_3^{ex}p^3+\mathcal{O}(p^4)\right),\tag{8.32}$$

where long calculations provide

$$\begin{aligned}
e_1^{ex} &= -\sqrt{2\pi}\frac{16}{21}\frac{c_{10}^{\frac{3}{2}}}{R_{-1}},\\
e_2^{ex} &= \sqrt{2\pi}\left\{-\frac{8c_{10}^{\frac{1}{2}}}{R_{-1}}\left(\frac{1}{7}c_{11}+\frac{1}{9}c_{21}+\frac{1}{11}c_{31}+\frac{1}{13}c_{41}+\frac{1}{15}c_{51}\right)+\frac{16}{21}\frac{c_{10}^{\frac{3}{2}}R_0}{R_{-1}^2}\right\},\\
e_3^{ex} &= +\sqrt{2\pi}\left\{\frac{8c_{10}^{\frac{1}{2}}R_0}{R_{-1}^2}\left(\frac{1}{7}c_{11}+\frac{1}{9}c_{21}+\frac{1}{11}c_{31}+\frac{1}{13}c_{41}+\frac{1}{15}c_{51}\right)\right.\\
&\quad -\frac{2c_{10}^{\frac{1}{2}}}{R_{-1}}\left(\frac{1}{7}c_{12}+\frac{1}{9}c_{22}+\frac{1}{11}c_{32}+\frac{1}{13}c_{42}+\frac{1}{15}c_{52}\right)\\
&\quad -\frac{2}{c_{10}^{\frac{1}{2}}R_{-1}}\left(\frac{1}{7}c_{11}^2+\frac{1}{11}c_{21}^2+\frac{1}{15}c_{31}^2+\frac{1}{19}c_{41}^2+\frac{1}{23}c_{51}^2\right)\\
&\quad -\frac{4}{c_{10}^{\frac{1}{2}}R_{-1}}\left(+\frac{1}{9}c_{11}c_{21}+\frac{1}{11}c_{11}c_{31}+\frac{1}{13}c_{11}c_{41}+\frac{1}{15}c_{11}c_{51}+\frac{1}{13}c_{21}c_{31}\right.\\
&\quad \left.+\frac{1}{15}c_{21}c_{41}+\frac{1}{17}c_{21}c_{51}+\frac{1}{17}c_{31}c_{41}+\frac{1}{19}c_{31}c_{51}+\frac{1}{21}c_{41}c_{51}\right)\\
&\quad \left.-\frac{16}{21}\frac{R_0^2c_{10}^{\frac{3}{2}}}{R_{-1}^3}\right\}.
\end{aligned}\tag{8.33}$$

Let's finally replace c_{10} and R_{-1} by their value given at (8.6):

$$e_1^{ex} = -\frac{2^{\frac{11}{3}}3^{\frac{1}{6}}}{7\pi^{\frac{4}{3}}},$$

$$\begin{aligned}
e_2^{ex} &= -\frac{2^{\frac{11}{3}}3^{\frac{1}{6}}}{\pi^{\frac{1}{3}}}\Big(\frac{1}{7}c_{11}+\frac{1}{9}c_{21}+\frac{1}{11}c_{31}+\frac{1}{13}c_{41}+\frac{1}{15}c_{51}\Big)+\frac{2^{\frac{13}{3}}}{3^{\frac{1}{6}}7\pi^{\frac{5}{3}}}R_0,\\
e_3^{ex} &= \frac{2^{\frac{13}{3}}}{3^{\frac{1}{6}}\pi^{\frac{2}{3}}}R_0\Big(\frac{1}{7}c_{11}+\frac{1}{9}c_{21}+\frac{1}{11}c_{31}+\frac{1}{13}c_{41}+\frac{1}{15}c_{51}\Big)\\
&\quad -\frac{2^{\frac{11}{3}}3^{\frac{1}{6}}}{\pi^{\frac{1}{3}}}\Big(\frac{1}{7}c_{12}+\frac{1}{9}c_{22}+\frac{1}{11}c_{32}+\frac{1}{13}c_{42}+\frac{1}{15}c_{52}\Big)\\
&\quad -\frac{2^{\frac{8}{3}}\pi^{\frac{2}{3}}}{3^{\frac{5}{6}}}\Big(\frac{1}{7}c_{11}^2+\frac{1}{11}c_{21}^2+\frac{1}{15}c_{31}^2+\frac{1}{19}c_{41}^2+\frac{1}{23}c_{51}^2\Big)\\
&\quad -\frac{2^{\frac{11}{3}}\pi^{\frac{2}{3}}}{3^{\frac{5}{6}}}\Big(+\frac{1}{9}c_{11}c_{21}+\frac{1}{11}c_{11}c_{31}+\frac{1}{13}c_{11}c_{41}+\frac{1}{15}c_{11}c_{51}+\frac{1}{13}c_{21}c_{31}\\
&\quad +\frac{1}{15}c_{21}c_{41}+\frac{1}{17}c_{21}c_{51}+\frac{1}{17}c_{31}c_{41}+\frac{1}{19}c_{31}c_{51}+\frac{1}{21}c_{41}c_{51}\Big)\\
&\quad -\frac{2^5}{3^{\frac{1}{2}}7\pi^2}R_0^2. \qquad (8.34)
\end{aligned}$$

We find analytically the asymptotic limit $\kappa \to 0$:

$$\hat{E}_0^{ex} \sim -\frac{2^{\frac{11}{3}}3^{\frac{1}{6}}}{7\pi^{\frac{4}{3}}}N^{\frac{3}{2}}\kappa^{\frac{1}{3}} = -0.4735N^{\frac{3}{2}}\kappa^{\frac{1}{3}}. \qquad (8.35)$$

Replacing the other variables by their numerical values established in chapter 7, we find

$$\hat{E}_0^{ex} = N^{\frac{3}{2}}\big[-0.4735\kappa^{\frac{1}{3}}+0.1319\kappa^{\frac{2}{3}}-0.1195\kappa^{\frac{3}{3}}+\mathcal{O}(\kappa^{\frac{4}{3}})\big]. \qquad (8.36)$$

We observe that the dominant term has the largest numerical prefactor.

8.3 Oscillating terms

Let's now focus on the oscillating terms. In order to determine them, we will have to calculate different functions of interest. They will be calculated analytically when possible, otherwise numerically (the numerical computations show no difficulty; they will be computed with Mathematica).

As developed in chapter 6, the oscillating terms require the knowledge of the function

$$s(e,x) = \frac{1}{\pi}\int_{r_1(e,x)}^{r_2(e,x)} \mathrm{d}r\sqrt{e - V(r) - \frac{x^2}{r^2}}, \qquad (8.37)$$

and s_e, the first derivative of s with respect to e, as well as s_{xx}, the second derivative of s with respect to x.

In our problem, V is the self-consistent potential. The contribution of the oscillating terms to the total energy of the system is very low, which is why we are only interested in its main contribution. Hence we will only consider the lowest order of the self-consistent potential, which will considerably simplify this study. e is the energy, x the angular momentum, and $r_i,\ i = 1, 2$ are the turning points.

Moreover the main oscillating terms consist of a sum over the periodic orbits of the classical dynamics of a particle in the self-consistent potential. We have to determine which orbits will contribute to the oscillating terms, and which ones will be negligible. For this we will need to know s_x, the first derivative of s with respect to x.

8.3.1 Scaling

In order to simplify the study of the function $s(e, x)$, let's proceed to relevant scalings. As previously we will consider $L_\star = 1$. At lowest order, the density and chemical potential are

$$\hat{\rho}(\hat{r}) = \frac{3}{2\pi}\frac{1}{R^2}\sqrt{1 - \frac{\hat{r}^2}{R^2}}, \quad R = \left(\frac{3\pi}{4\kappa}\right)^{\frac{1}{3}}, \quad \hat{\mu} = \left(\frac{3\pi}{4}\right)^{\frac{2}{3}}\kappa^{\frac{1}{3}}. \tag{8.38}$$

Hence, at lowest order, the self-consistent potential is

$$\hat{V}(\hat{r}) = \hat{\mu} - \pi\hat{\rho}(\hat{r}) = \hat{\mu} - \frac{3}{2}\frac{1}{R^2}\sqrt{1 - \frac{\hat{r}^2}{R^2}}. \tag{8.39}$$

The energy and chemical potential are always grouped, this is why we define the variable $\hat{\epsilon} \doteq (\hat{e} - \hat{\mu})$.

The function s becomes

$$\begin{aligned}
\hat{s}(\hat{\epsilon}, \hat{x}) &= \frac{1}{\pi}\int_{r_1(\hat{\epsilon},\hat{x})}^{r_2(\hat{\epsilon},\hat{x})} \mathrm{d}\hat{r}\sqrt{\hat{\epsilon} + \frac{3}{2}\frac{1}{R^2}\sqrt{1 - \frac{\hat{r}^2}{R^2}} - \frac{\hat{x}^2}{\hat{r}^2}} \\
&= \frac{1}{\pi}R\int_{\frac{r_1(\hat{\epsilon},\hat{x})}{R}}^{\frac{r_2(\hat{\epsilon},\hat{x})}{R}} \mathrm{d}r\sqrt{\hat{\epsilon} + \frac{3}{2}\frac{1}{R^2}\sqrt{1 - r^2} - \frac{\hat{x}^2}{R^2 r^2}} \\
&= \frac{1}{\pi}\int_{\frac{r_1(\hat{\epsilon},\hat{x})}{R}}^{\frac{r_2(\hat{\epsilon},\hat{x})}{R}} \mathrm{d}r\sqrt{R^2\hat{\epsilon} + \frac{3}{2}\sqrt{1 - r^2} - \frac{\hat{x}^2}{r^2}} \\
&= \frac{1}{\pi}\int_{r_1(\epsilon',x')}^{r_2(\epsilon',x')} \mathrm{d}r\sqrt{\epsilon' + \frac{3}{2}\sqrt{1 - r^2} - \frac{x'^2}{r^2}} \\
&= s'(\epsilon', x'),
\end{aligned} \tag{8.40}$$

where we proceeded to the change of variable $\hat{r} \mapsto r = \frac{\hat{r}}{R}$, and defined $\epsilon' \doteq R^2\hat{\epsilon}$, and $x' \doteq \hat{x}$. For notational simplicity, the turning points are noted with the same symbol.

We can still simplify this expression for further calculations. Let's write

$$\begin{aligned}\sqrt{\epsilon' + \frac{3}{2}\sqrt{1-r^2} - \frac{x'^2}{r^2}} &= \sqrt{\frac{3}{2}}\sqrt{\frac{2}{3}\epsilon' + \sqrt{1-r^2} - \frac{2}{3}\frac{x'^2}{r^2}} \\ &= \sqrt{\frac{3}{2}}\sqrt{\epsilon + \sqrt{1-r^2} - \frac{x^2}{r^2}}, \end{aligned} \tag{8.41}$$

where we defined $\epsilon \doteq \frac{2}{3}\epsilon'$, and $x \doteq \sqrt{\frac{2}{3}}x'$. We will study the function

$$s(\epsilon, x) \doteq \sqrt{\frac{2}{3}}s'\left(\frac{3}{2}\epsilon, \sqrt{\frac{3}{2}}x\right) = \frac{1}{\pi}\int_{r_1(\epsilon,x)}^{r_2(\epsilon,x)} \mathrm{d}r \sqrt{\epsilon + \sqrt{1-r^2} - \frac{x^2}{r^2}}. \tag{8.42}$$

The study of the function $s(\epsilon, x)$ will provide results for the function $\hat{s}$. This function is easily interpreted: we study the classical dynamics of a particle evolving in a potential $V(r) = -\sqrt{1-r^2}$, with energy ϵ, and angular momentum x. For the derivation of some results it will be useful to use this physical interpretation.

A case whose importance will become clear later (it will provide the main oscillating contribution) is the case $\hat{e} = \hat{\mu}$, that is $\epsilon = 0$. We will focus on this case, for which some analytical calculations are possible.

8.3.2 Turning points

In order to calculate all we need for the determination of the oscillating terms, we have to determine the turning points $r_i(\epsilon, x)$, $i = 1, 2$. These turning points are defined by

$$\epsilon + \sqrt{1 - r_i^2} - \frac{x^2}{r_i^2} = 0. \tag{8.43}$$

This equation can be rewritten as

$$-r_i^6 + (1-\epsilon^2)r_i^4 + 2\epsilon x^2 r_i^2 - x^4 = 0. \tag{8.44}$$

r_i appears at even powers only. Defining $p_i \doteq r_i^2$, we have to determine the roots of a polynomial of the third order, which is possible analytically. We did it with Mathematica. Two out of six roots are real and nonnegative, these are r_1 and r_2. The result is a very long formula and there is no need to write it down here. In Figure 8.1 we show r_1 and r_2 as functions of x, for different values of ϵ.

8.3.3 r_{max}, λ_{max}

Other functions of interest are the radius r_{max}, and the angular momentum λ_{max}. The radius is the one for which, at fixed energy ϵ, the angular momentum takes the maximum value λ_{max} the system can have. The radius r_{max} can be obtained

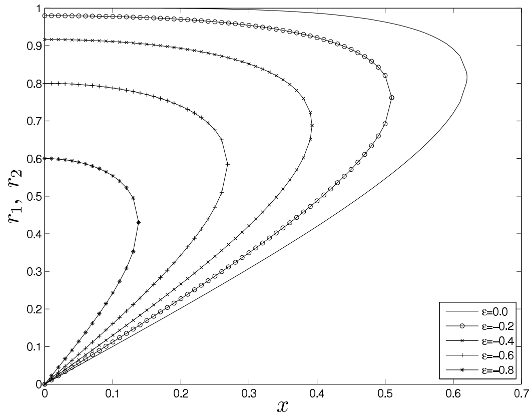


Figure 8.1: *Turning points as a function of x, for different values of ϵ.*

by maximizing $x(r_1)$ (or equivalently $x(r_2)$). We maximize $x^2(r_i)$ instead, which is easier to obtain. Let's recall that r_i is defined by equation (8.43), hence

$$r_i^2\left(\epsilon+\sqrt{1-r_i^2}\right)=x^2. \tag{8.45}$$

Taking the derivative of equation (8.45) with respect to r_i, we obtain the solution r_{max}. The final equation is

$$9r^4+4(\epsilon^2-3)r^2+4(1-\epsilon^2)=0, \tag{8.46}$$

for which there are two nonnegative solutions. One solution increases when ϵ increases, the other one decreases. If the energy increases, the maximal radius increases, too. This is why the physical solution is the first one, and is

$$r_{max}(\epsilon)=\frac{\sqrt{2}}{3}\sqrt{3-\epsilon^2-\epsilon\sqrt{3+\epsilon^2}}. \tag{8.47}$$

The maximum angular momentum is directly obtained, introducing r_{max} in equation (8.45):

$$\lambda_{max}(\epsilon)=\frac{\sqrt{2}}{3}\sqrt{\left(3-\epsilon^2-\epsilon\sqrt{3+\epsilon^2}\right)\left(\epsilon+\sqrt{1-\frac{2}{9}\left(3-\epsilon^2-\epsilon\sqrt{3+\epsilon^2}\right)}\right)}. \tag{8.48}$$

This function is represented in Figure 8.2. It shows a weak curvature. Applying these results to the case $\epsilon=0$ we find the very simple results

$$\left\{\begin{array}{lclcl} r_{max}(0) & = & \sqrt{\frac{2}{3}} & = & 0.8165, \\ \lambda_{max}(0) & = & \frac{\sqrt{2}}{3^{\frac{3}{4}}} & = & 0.6204. \end{array}\right. \tag{8.49}$$

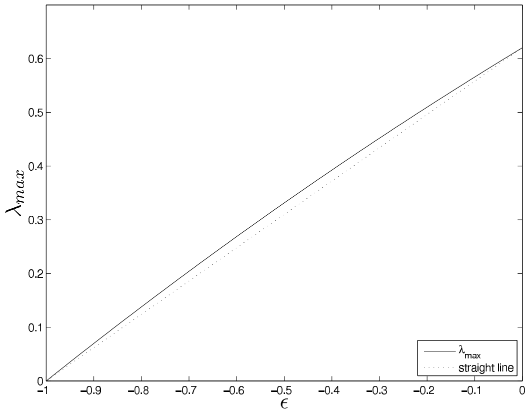


Figure 8.2: *Maximal angular momentum as a function of ϵ, compared to a straight line.*

Unsurprisingly we also find

$$\lambda_{max}(-1) = 0. \tag{8.50}$$

If there is no energy in the system ($\epsilon = -1$ is the lowest energy the system can have), the particle has no movement and its angular momentum can only be zero.

8.3.4 $s(\epsilon, x)$

Let's evaluate the function $s(\epsilon, x)$, defined in equation (8.42). It is clear that the limit $\epsilon \longrightarrow 0$ converges uniformly. Moreover we see graphically (see Figure 8.3) that the limit $x \longrightarrow 0$ converges uniformly, too. The integral is the square root of the area, which varies uniformly as $x \longrightarrow 0$. Hence we can evaluate s analytically as $\epsilon = 0,\ x = 0$. We find

$$s(0,0) = \frac{1}{\pi}\int_0^1 \mathrm{d}r \left(1 - r^2\right)^{\frac{1}{4}} = \frac{1}{6\sqrt{\pi}}\frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)} = 0.2782. \tag{8.51}$$

We were unable to evaluate analytically all other cases. In Figure 8.4 we show the function $s(\epsilon, x)$ as a function of x, for different values of ϵ. The curvature of these functions is weak.

Let's note that this figure shows the level curves of the energy, as a function of the two actions. We can proceed to an analogy with the case of the atom. The shell structure of the atoms is usually modeled by the energy levels of the hydrogen atom, which corresponds to the picture of independent electrons, evolving in the confining potential produced by the nucleus. The same picture can be used in the case of quantum dots. This case is modeled as independent electrons evolving in the harmonic confining potential (see chapter 4, where we describe some properties related to the shell structure of this model). Its semiclassical states are given by the quantization of the actions. In this case the level curves are straight

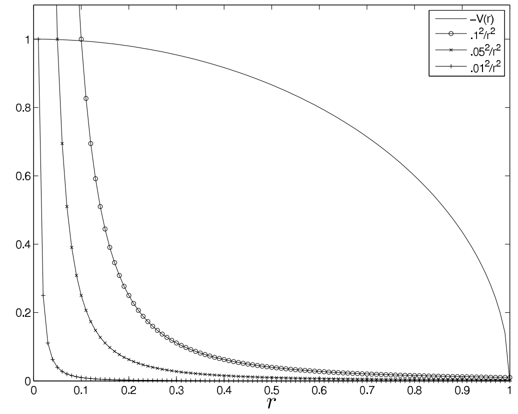


Figure 8.3: *$s(\epsilon, x)$ is the square root of the enclosed area. It converges uniformly in the limit $x \to 0$.*

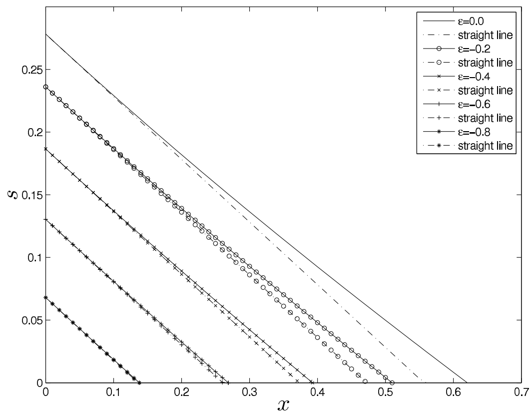


Figure 8.4: *Level curves of ϵ as a function of x and s, compared to straight lines.*

lines, with slope $-\frac{1}{2}$. Many levels are degenerated. Our work is more precise, and this degeneracy disappears. Our calculations are then predictive: it shows in which order the states are filled. These results could be tested experimentally.

8.3.5 $s_x(\epsilon, x)$

Let's study the first derivative of s with respect to x, which will be useful to determine which periodic orbits we will have to consider. This function is

$$s_x(\epsilon, x) \;=\; -\frac{x}{\pi}\int_{r_1(\epsilon,x)}^{r_2(\epsilon,x)} \frac{\mathrm{d}r}{r^2}\frac{1}{\sqrt{\epsilon+\sqrt{1-r^2}-\frac{x^2}{r^2}}}$$

$$
\begin{aligned}
&+\frac{r_{2x}(\epsilon,x)}{\pi}\sqrt{\epsilon+\sqrt{1-r_2^2(\epsilon,x)}-\frac{x^2}{r_2^2(\epsilon,x)}}\\
&-\frac{r_{1x}(\epsilon,x)}{\pi}\sqrt{\epsilon+\sqrt{1-r_1^2(\epsilon,x)}-\frac{x^2}{r_1^2(\epsilon,x)}},
\end{aligned}
\tag{8.52}
$$

where $r_{ix},\ i=1,2$, is the derivative of r_i with respect to x.

The two last terms are zero: $\epsilon+\sqrt{1-r_i^2(\epsilon,x)}-\frac{x^2}{r_i^2(\epsilon,x)}=0,\ i=1,2$, is the definition of r_i. Hence, even if r_{ix} diverges for both $i=1,2$ in the limit $x\longrightarrow\lambda_{max}$, they are multiplied by 0, and their product is zero.

The function is therefore

$$
\begin{aligned}
s_x(\epsilon,x) &= -\frac{x}{\pi}\int_{r_1(\epsilon,x)}^{r_2(\epsilon,x)}\frac{\mathrm{d}r}{r^2}\frac{1}{\sqrt{\epsilon+\sqrt{1-r^2}-\frac{x^2}{r^2}}}\\
&= -\frac{x}{\pi}\int_{r_1(\epsilon,x)}^{r_2(\epsilon,x)}\frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2\left(\epsilon+\sqrt{1-r^2}\right)-x^2}}\\
&= -\frac{x}{\pi}\int_{r_1(\epsilon,x)}^{r_2(\epsilon,x)}\frac{\mathrm{d}r}{r}\frac{1}{\sqrt{W(r)-x^2}},
\end{aligned}
\tag{8.53}
$$

where we defined $W(r)\doteq r^2\left(\epsilon+\sqrt{1-r^2}\right)$.

We want to study this function. First of all, we will verify that this function is not divergent. Then we will extract all analytical information we are able to obtain, that is the limits $\lim_{x\to 0}s_x(\epsilon,x)$ and $\lim_{x\to\lambda_{max}}s_x(\epsilon,x)$. The complete function will be computed numerically.

From equation (8.53) we see that the integrand diverges at the integration limits. But does this imply that the integral is divergent? To answer this question, let's look how this integrand diverges as $r\longrightarrow r_i$. Let's define $r\doteq r_i+\delta$. Proceeding to an expansion for δ small, we find

$$
W(r)-x^2=\underbrace{r_i^2\left(\epsilon+\sqrt{1-r_i^2}\right)-x^2}_{=0}+\delta W'(r_i).
\tag{8.54}
$$

Hence the integrand behaviour near r_i is of the order of $\frac{1}{\sqrt{\delta}}$, which means that the hypothetical divergence behaves as $\int\frac{\mathrm{d}\delta}{\sqrt{\delta}}\sim\sqrt{\delta}$, and is therefore finite. If $W'(r_i)=0$ this result is not true. This case arises when $r_1=r_2=r_{max}$ and will be studied in detail later. Another singularity may arise from the term $\frac{1}{r}$ of the integrand, that is when $r_1\to 0$, which happens when $x\to 0$. This case will also be studied in detail later.

Let's focus on the limit $x\longrightarrow 0$. This case was already studied while we developed formulas for the oscillating terms in chapter 6. The general result (applying to any "smooth" potential) was

$$\lim_{x\to 0} s_x(\epsilon, x) = -\frac{1}{2}. \tag{8.55}$$

The divergence appearing in the integrand (from the $\frac{1}{r}$ term) compensates the prefactor x to provide a finite limit.

Another interesting limit is the limit $x \to \lambda_{max}$. We proceed to an expansion around r_{max}, writing $r = r_{max} + y$, to find

$$W(r) - x^2 \cong \underbrace{\lambda_{max}^2 - x^2}_{\doteq\delta\ll 1} - \frac{|W''_{max}|}{2} y^2. \tag{8.56}$$

Introducing it into the integral (8.53) we find

$$\begin{aligned}
-\frac{x}{\pi}\int_{r_1}^{r_2}\frac{\mathrm{d}r}{r}\frac{1}{\sqrt{W(r)-x^2}} &= -\frac{x}{\pi}\int_{-\sqrt{\frac{2\delta}{|W''_{max}|}}}^{+\sqrt{\frac{2\delta}{|W''_{max}|}}}\frac{\mathrm{d}y}{(r_{max}+y)}\frac{1}{\sqrt{\delta-\frac{|W''_{max}|}{2}y^2}} \\
&= -\frac{x}{\pi}\frac{1}{r_{max}}\sqrt{\frac{2}{|W''_{max}|}}\underbrace{\int_{-1}^{+1}\frac{\mathrm{d}\lambda}{\sqrt{1-\lambda^2}}}_{=\pi} \\
&= -\frac{x}{r_{max}}\sqrt{\frac{2}{|W''_{max}|}}, \qquad (8.57)
\end{aligned}$$

where we proceeded to the change of variable $y \mapsto \lambda \doteq \sqrt{\frac{|W''_{max}|}{2\delta}}y$.

There is no convergence problem, we can take the limit $x \to \lambda_{max}$ to find

$$\lim_{x\to\lambda_{max}} s_x(\epsilon, x) = -\sqrt{2}\frac{\lambda_{max}}{r_{max}\sqrt{|W''_{max}|}}. \tag{8.58}$$

$\lambda_{max}(\epsilon)$ and $r_{max}(\epsilon)$ were established previously at equations (8.47) and (8.48). The function W is, by definition, $W(r) = r^2(e - V(r))$. The second derivative of W is

$$W''(r) = 2(e - V) - 4rV' - r^2V''. \tag{8.59}$$

Evaluating it for $r = r_{max}$ and multiplying by r_{max}^2, elementary calculations provide

$$\begin{aligned}
r_{max}^2 W''(r_{max}) &= r_{max}\underbrace{\left(2r_{max}(e-V) - r_{max}^2V'\right)}_{=W'(r_{max})=0} - 3r_{max}^3V' - r_{max}^4V'' \\
&= -3r_{max}^3V' - r_{max}^4V'', \qquad (8.60)
\end{aligned}$$

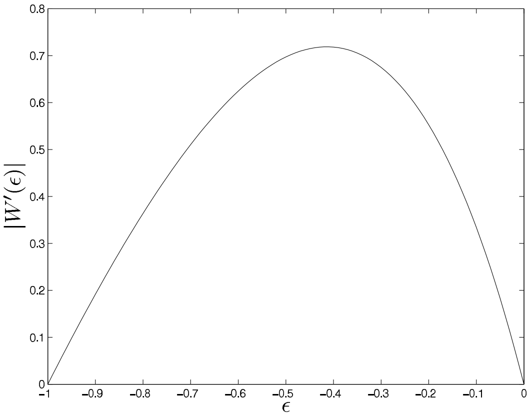


Figure 8.5: *Absolute value of the second derivative of* W*, as a function of* ϵ*.*

therefore

$$r_{max}^2|W_{max}''| = 3r_{max}^3 V'(r_{max}) + r_{max}^4 V''(r_{max}). \tag{8.61}$$

It is easily evaluated and is shown in Figure 8.5

In the particular case $\epsilon \longrightarrow 0$, using the results (8.49) and (8.61), we find

$$\lim_{\epsilon \longrightarrow 0} \lim_{x \longrightarrow \lambda_{max}(\epsilon)} s_x(\epsilon, x) = -\frac{1}{\sqrt{6}} = -0.4082. \tag{8.62}$$

Finally, we have to compute the complete function s_x. This is done numerically. To deal with the numerical divergence at the integration limits we integrate from $r_1+\delta$ to $r_2-\delta$, and consider δ small enough so that it has no influence. The function s_x is represented as a function of x, for different values of ϵ, in Figure 8.6.

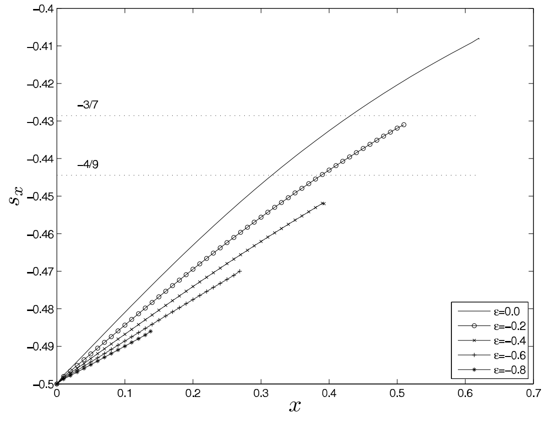


Figure 8.6: *First derivative of* s *with respect to* x*, for different values of* x*.*

8.3.6 Periodic orbits

In our previous developments, we characterized the periodic orbits with two natural numbers, k and j. The periodic orbits are such that

$$s_x(\epsilon, x^\star(\epsilon)) = -\frac{k}{j}, \tag{8.63}$$

which is a condition that defines $x^\star(\epsilon)$.

This condition expresses the fact that the ratio of the two classical actions of a periodic orbit is a rational number.

The amplitude of the energy oscillations is multiplied by $\frac{1}{j^{\frac{5}{2}}}$. This amplitude is multiplied by other terms, which have, however, a weak dependence on j and k. As a function of j and k, it is therefore dominated by the term $\frac{1}{j^{\frac{5}{2}}}$, which implies that the orbits with a large value of j can be neglected. It is not surprising that only a few orbits have to be considered: if it were not the case, the sum would diverge.

Let's focus on the case $\epsilon = 0$, as the energy oscillations only depend on this case. As we can see in Figure 8.6, the periodic orbits must be such that

$$\frac{k}{j} \in \left[\frac{1}{\sqrt{6}}, \frac{1}{2}\right] = [0.4082, 0.5000]\,. \tag{8.64}$$

Hence the orbits allowed are

$$(k:j) = (1:2),\ (2:4),\ (3:6),\ (3:7),\ (4:8),\ (4:9),\ (5:10),\ \ldots \tag{8.65}$$

These orbits can be grouped in families of periodic orbits, defined by $\frac{k}{j} = \text{cst}$. The orbits involved consist of only three families!

We still have to determine the relative order of magnitude of the oscillating terms generated by these orbits. The first one is of the order of $\frac{1}{2^{\frac{5}{2}}}$. Hence the relative order of magnitude of the other ones is $\left(\frac{2}{j}\right)^{\frac{5}{2}}$. We find

$$\left(\frac{j}{2}\right)^{\frac{5}{2}} = \begin{cases} 5.66 & , \quad j = 4, \\ 15.59 & , \quad j = 6, \\ 22.92 & , \quad j = 7, \\ 32.00 & , \quad j = 8, \\ 42.96 & , \quad j = 9, \\ 55.90 & , \quad j = 10, \\ \ldots & \end{cases}$$

The energy corresponding to the orbit with $j = 6$ is already an order of magnitude higher than the energy corresponding to the orbit with $j = 2$. Hence it seems that only one family of periodic orbits (actually only the first two terms) will have to be considered. To complete our study we will include the orbits $(k:j) = (3:7),\ (4:9)$ in our final results.

To proceed further we have to determine $x^\star(0)$, corresponding to the different orbits. We easily find

$$x^\star_{(1:2)}(0) = x^\star_{(2:4)}(0) = x^\star_{(3:6)}(0) = x^\star_{(4:8)}(0) = x^\star_{(5:10)}(0) = \lambda_{max}(0) = \frac{\sqrt{2}}{3^{\frac{3}{4}}} = 0.6204. \tag{8.66}$$

For the other periodic orbits ($\frac{3}{7} = 0.4286$, $\frac{4}{9} = 0.4444$) we find numerically

$$x^\star_{(3:7)}(0) = 0.4318; \quad x^\star_{(4:9)}(0) = 0.3163, \tag{8.67}$$

as can be seen in Figure 8.6.

From these results, let's note that when summing over the orbits of a given family, the first term will provide the amplitude, the others will influence (almost) only the shape of the oscillations.

Let's finally note that $\lambda_{max}(0) \notin \mathbb{Q}$, which means that some of the oscillating terms calculated will be zero (see chapter 6).

The case $\epsilon \neq 0$ is necessary for the computations of the integrated density of states. From our results we can see that if the energy ϵ decreases, the number of periodic orbits diminishes. This is not surprising: some periodic orbits need energy, and if the available energy is unsufficient, the orbit cannot be realized. Let's determine for which energy the orbits disappear (as well as its corresponding oscillating term). This is obtained by inverting the function $\lambda_{max}(\epsilon)$, which is done graphically with means of Figure 8.2. We have $x^\star_{(3:7)} = \lambda_{max}(\epsilon_{(3:7)}),\ x^\star_{(4:9)} = \lambda_{max}(\epsilon_{(4:9)})$. We obtain

$$\begin{aligned} &\epsilon_{(1:2)} = \epsilon_{(2:4)} = \epsilon_{(3:6)} = \epsilon_{(4:8)} = \epsilon_{(5:10)} = -1; \\ &\epsilon_{(3:7)} = -0.3399; \quad \epsilon_{(4:9)} = -0.3130. \end{aligned} \tag{8.68}$$

There will be no discontinuity in the integrated density of states at these energies. This discontinuity only appears because of our description and is not intrinsic to the problem.

8.3.7 $s_\epsilon(\epsilon, x)$

The amplitude of the energy oscillations depends on the derivative of s with respect to ϵ. It is

$$s_\epsilon(\epsilon, x) = \frac{1}{2\pi} \int_{r_1(\epsilon,x)}^{r_2(\epsilon,x)} \mathrm{d}r \frac{1}{\sqrt{\epsilon + \sqrt{1 - r^2} - \frac{x^2}{r^2}}}$$

$$
\begin{aligned}
&+\frac{r_{2\epsilon}(\epsilon,x)}{\pi}\sqrt{\epsilon+\sqrt{1-r_2^2(\epsilon,x)}-\frac{x^2}{r_2^2(\epsilon,x)}} \\
&-\frac{r_{1\epsilon}(\epsilon,x)}{\pi}\sqrt{\epsilon+\sqrt{1-r_1^2(\epsilon,x)}-\frac{x^2}{r_1^2(\epsilon,x)}},
\end{aligned}
\tag{8.69}
$$

where $r_{i\epsilon},\ i=1,2$, is the derivative of r_i with respect to ϵ.

The two last terms are zero: $\epsilon+\sqrt{1-r_i^2(\epsilon,x)}-\frac{x^2}{r_i^2(\epsilon,x)}=0,\ i=1,2$, is the definition of r_i. Hence, even if $r_{i\epsilon}$ diverges for both $i=1,2$, in the limit $x\longrightarrow\lambda_{max}$, they are multiplied by 0, and their product is zero.

The function is therefore

$$
\begin{aligned}
s_\epsilon(\epsilon,x) &= \frac{1}{2\pi}\int_{r_1(\epsilon,x)}^{r_2(\epsilon,x)}\mathrm{d}r\frac{1}{\sqrt{\epsilon+\sqrt{1-r^2}-\frac{x^2}{r^2}}} \\
&= \frac{1}{2\pi}\int_{r_1(\epsilon,x)}^{r_2(\epsilon,x)}\mathrm{d}r\frac{r}{\sqrt{r^2\left(\epsilon+\sqrt{1-r^2}\right)-x^2}} \\
&= \frac{1}{2\pi}\int_{r_1(\epsilon,x)}^{r_2(\epsilon,x)}\mathrm{d}r\frac{r}{\sqrt{W(r)-x^2}},
\end{aligned}
\tag{8.70}
$$

where W was defined previously ($W(r)=r^2\left(\epsilon+\sqrt{1-r^2}\right)$).

We want to study this function. First of all we will verify if this function is not divergent. Then we will extract all analytical information we are able to obtain, that is the limits $\lim_{x\to 0}s_\epsilon(\epsilon,x)$ and $\lim_{x\to\lambda_{max}}s_\epsilon(\epsilon,x)$. The complete function will be computed numerically.

From equation (8.70) we see that the integrand diverges at the integration limits. But does this imply that the integral is divergent? To answer this question, let's look at how this integrand diverges as $r\longrightarrow r_i$. Let's define $r\doteq r_i+\delta$. Proceeding to an expansion for δ small, we find (see equation (8.54))

$$
W(r)-x^2=\delta W'(r_i). \tag{8.71}
$$

Hence the integrand behaviour near r_i is of the order of $\frac{1}{\sqrt{\delta}}$, which means that the hypothetical divergence behaves as $\int\frac{\mathrm{d}\delta}{\sqrt{\delta}}\sim\sqrt{\delta}$, and is therefore finite. If $W'(r_i)=0$ this result is not true. This case arises when $r_1=r_2=r_{max}$ and will be studied in detail later. Clearly, no singularity arises from the term r of the integrand.

Let's focus on the limit $x\longrightarrow 0$. The integrand is an integrable function, hence, by Lebesgue's theorem, the integral and the limit can be commuted and we find

$$
\lim_{x\to 0}s_\epsilon(\epsilon,x)=\frac{1}{2\pi}\int_0^1\mathrm{d}r\frac{1}{\sqrt{\epsilon+\sqrt{1-r^2}}}. \tag{8.72}
$$

We cannot solve this integral analytically, except in the case $\epsilon = 0$ (in which case the integrand is also an integrable function, and the limit and the integral can be commuted), where we find

$$\lim_{\epsilon \to 0} \lim_{x \to 0} s_\epsilon(\epsilon, x) = \frac{1}{2\pi} \int_0^1 \frac{1}{(1-r^2)^{\frac{1}{4}}} = \frac{1}{\sqrt{\pi}} \frac{\Gamma\left(\frac{3}{4}\right)}{\Gamma\left(\frac{1}{4}\right)} = 0.5991. \tag{8.73}$$

Another interesting limit is the limit $x \to \lambda_{max}$. We proceed to an expansion around r_{max}, writing $r = r_{max} + y$, to find

$$W(r) - x^2 \cong \underbrace{\lambda_{max}^2 - x^2}_{\doteq \delta \ll 1} - \frac{|W''_{max}|}{2} y^2. \tag{8.74}$$

Introducing it into the integral (8.70) we find

$$\begin{aligned}
\frac{1}{2\pi} \int_{r_1}^{r_2} \mathrm{d}r \frac{r}{\sqrt{W(r) - x^2}} &= \frac{1}{2\pi} \int_{-\sqrt{\frac{2\delta}{|W''_{max}|}}}^{+\sqrt{\frac{2\delta}{|W''_{max}|}}} \mathrm{d}y \frac{(r_{max} + y)}{\sqrt{\delta - \frac{|W''_{max}|}{2} y^2}} \\
&= \frac{r_{max}}{2\pi} \sqrt{\frac{2}{|W''_{max}|}} \underbrace{\int_{-1}^{+1} \frac{\mathrm{d}\lambda}{\sqrt{1 - \lambda^2}}}_{=\pi} \\
&= \frac{r_{max}}{\sqrt{2}} \frac{1}{\sqrt{|W''_{max}|}},
\end{aligned} \tag{8.75}$$

where we proceeded to the change of variable $y \mapsto \lambda \doteq \sqrt{\frac{|W''_{max}|}{2\delta}} y$.

There is no convergence problem, we can take the limit $x \to \lambda_{max}$ to find

$$\lim_{x \to \lambda_{max}} s_\epsilon(\epsilon, x) = \frac{r_{max}}{\sqrt{2|W''_{max}|}}. \tag{8.76}$$

$r_{max}(\epsilon)$ was established previously in equation (8.47). The second derivative of W was already calculated in equation (8.59).

In the particular case $\epsilon \to 0$, using the results (8.49) and (8.61), we find

$$\lim_{\epsilon \to 0} \lim_{x \to \lambda_{max}(\epsilon)} s_\epsilon(\epsilon, x) = \frac{1}{2} \frac{1}{3^{\frac{3}{4}}} = 0.2193. \tag{8.77}$$

Finally we have to compute the function for an arbitrary energy ϵ. It is done numerically. To deal with the numerical divergence at the integration limits we integrate from $r_1 + \delta$ to $r_2 - \delta$, and consider δ small enough that it has no influence. The function s_ϵ is represented as a function of x, for different values of ϵ, in Figure 8.7.

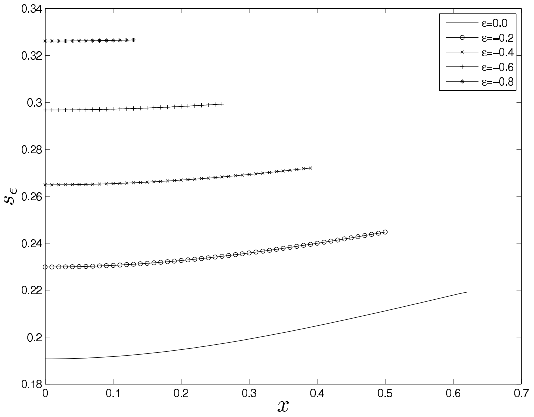


Figure 8.7: *First derivative of s with respect to ϵ, for different values of ϵ.*

8.3.8 $s_{xx}(\epsilon, x)$

The amplitude of the energy oscillations depends on the second derivative of s with respect to x. We have to compute the derivative of s_x (established in equation (8.53)) with respect to x:

$$\begin{aligned} s_{xx}(\epsilon, x) &= -\frac{1}{\pi}\int_{r_1(\epsilon,x)}^{r_2(\epsilon,x)} \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{W(r)-x^2}} \\ &\quad -\frac{x^2}{\pi}\int_{r_1(\epsilon,x)}^{r_2(\epsilon,x)} \frac{\mathrm{d}r}{r}\frac{1}{\left(W(r)-x^2\right)^{\frac{3}{2}}} \\ &\quad -\frac{x}{\pi}\frac{r_{2x}(\epsilon,x)}{r_2(\epsilon,x)\sqrt{W(r_2(\epsilon,x))-x^2}} \\ &\quad +\frac{x}{\pi}\frac{r_{1x}(\epsilon,x)}{r_1(\epsilon,x)\sqrt{W(r_1(\epsilon,x))-x^2}}. \end{aligned} \tag{8.78}$$

Except the first term, all the terms diverge! However, the whole expression (s_{xx}) does not. The divergence arises from the separation we did during the calculations.

Let's note that, except in the limits $x \to 0$ and $x \to \lambda_{max}(\epsilon)$, we cannot calculate analytically s_{xx}. To deal numerically with the divergences we introduce a cut-off: we replace r_1 by $(r_1 + \delta)$ and r_2 by $(r_2 - \delta)$, choosing δ small enough that it has no influence on the result.

As explained before we can calculate the limit $x \to 0$. To avoid the divergences, and see that they cancel out, we could consider a cut-off. We would integrate from $r_1(\epsilon, x + \delta)$ to $r_2(\epsilon, x + \delta)$, and, at the end, take the limit $\delta \to 0$. This way the $\frac{1}{\sqrt{\delta}}$ divergences would cancel, as well as the $\frac{1}{x}$ divergence (in the limit $x \to 0$).

The way we proceed is different: the derivative of the self-consistent potential, at $r = 0$, is 0. Hence we know that $s_x(\epsilon, x) = -\frac{1}{2} + \mathcal{O}(x)$ (see chapter 6). We therefore have to find a way to determine the first order in x of $s_x(0, x)$, which corresponds to $\lim_{x\to 0} s_{xx}(0, x)$. For this let's recall that s_x is

$$s_x(0,x) = -\frac{x}{\pi}\int_{r_1(0,x)}^{r_2(0,x)} \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2\sqrt{1-r^2}-x^2}}. \tag{8.79}$$

To determine the limit $x \to 0$ we replaced the integrand by

$$\frac{1}{\sqrt{r^2\sqrt{1-r^2}-x^2}} \longrightarrow \frac{1}{\sqrt{r^2-x^2}}, \tag{8.80}$$

which can be easily integrated in the limit $x \ll 1$ (introducing the cut-off $r_2 = 1$):

$$\begin{aligned} -\frac{x}{\pi}\int_x^1 \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2-x^2}} &= -\frac{1}{\pi}\int_1^{\frac{1}{x}} \frac{\mathrm{d}r}{r}\frac{1}{\sqrt{r^2-1}} \\ &= -\frac{1}{\pi}\arccos(x) \\ &= -\frac{1}{2} + \frac{x}{\pi} + \mathcal{O}(x^3). \end{aligned} \tag{8.81}$$

The first part of the first order correction to s_x is then $\frac{1}{\pi}$. However, this correction does not arise from the real integrand, but from its asymptotic corresponding function. To this correction we have to add

$$\begin{aligned} &\lim_{x\to 0}\frac{1}{x}\left(-\frac{x}{\pi}\int_{r_1(0,x)}^{r_2(0,x)}\frac{\mathrm{d}r}{r}\left(\frac{1}{\sqrt{r^2\sqrt{1-r^2}-x^2}}-\frac{1}{\sqrt{r^2-x^2}}\right)\right) \\ &\lim_{x\to 0}\left(-\frac{1}{\pi}\int_{r_1(0,x)}^{r_2(0,x)}\frac{\mathrm{d}r}{r}\left(\frac{1}{\sqrt{r^2\sqrt{1-r^2}-x^2}}-\frac{1}{\sqrt{r^2-x^2}}\right)\right). \end{aligned} \tag{8.82}$$

Let's note that we can take the lower integration limit 0: the divergences arising from the integrand cancel out.

Rearranging the integrand we find

$$\begin{aligned} \lim_{x\to 0}\Bigg(-\frac{1}{\pi}\int_{r_1(0,x)}^{r_2(0,x)}\frac{\mathrm{d}r}{r}\Bigg[&\frac{(r^2-x^2)\sqrt{r^2\sqrt{1-r^2}-x^2}(r^2\sqrt{1-r^2}+x^2)}{(r^4(1-r^2)-x^2)(r^2-x^2)} \\ &-\frac{(r^4(1-r^2)-x^2)\sqrt{r^2-x^2}}{(r^4(1-r^2)-x^2)(r^2-x^2)}\Bigg]\Bigg). \end{aligned} \tag{8.83}$$

Taking the limit $x \to 0$ we obtain

$$-\frac{1}{\pi}\int_0^1 \frac{\mathrm{d}r}{r^2}\left(\frac{1}{(1-r^2)^{\frac{1}{4}}}-1\right) = -\frac{1}{\pi} + \frac{\sqrt{2\pi}}{\Gamma^2\left(\frac{1}{4}\right)}. \tag{8.84}$$

Summing (8.81) and (8.84) we find

$$\lim_{x\to 0} s_{xx}(0,x) = \frac{\sqrt{2\pi}}{\Gamma^2\left(\frac{1}{4}\right)} = 0.19069. \tag{8.85}$$

We compute the whole function $s_{xx}(\epsilon, x)$ numerically. Due to the numerical instability we cannot compute it in the limits $x \ll 1$ and $x \lesssim \lambda_{max}(\epsilon)$. In Figure 8.8 we show $s_{xx}(\epsilon, x)$ as a function of x, for different values of ϵ.

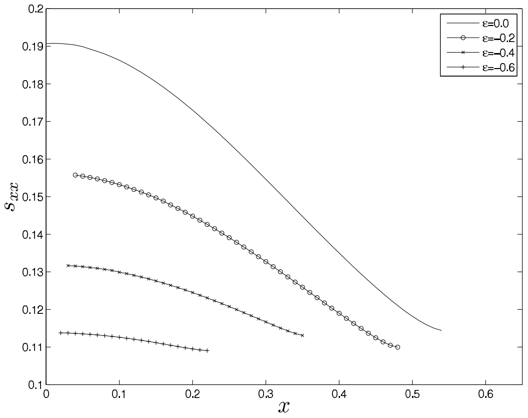


Figure 8.8: *Second derivative of s with respect to x, for different values of ϵ.*

8.3.9 Inverse scaling

We established results for the scaled problem. To apply them to our problem, we still have to proceed to an inverse scaling.

We need to calculate $\hat{s}$. Using the scaling relations we find

$$\hat{s}(\hat{e}, \hat{x}) = \sqrt{\frac{3}{2}} s \left(\frac{2}{3} R^2 (\hat{e} - \mu), \sqrt{\frac{2}{3}} \hat{x} \right). \tag{8.86}$$

We need to calculate $\hat{s}_{\hat{x}}$. Using the scaling relations we find

$$\hat{s}_{\hat{x}}(\hat{e}, \hat{x}) = \sqrt{\frac{3}{2}} s_{\hat{x}} \left(\frac{2}{3} R^2 (\hat{e} - \mu), \sqrt{\frac{2}{3}} \hat{x} \right) = s_x \left(\frac{2}{3} R^2 (\hat{e} - \mu), \sqrt{\frac{2}{3}} \hat{x} \right). \tag{8.87}$$

The scaling of s is exactly compensated by the scaling of x. This means that the relevant periodic orbits are exactly the same in the original system as in the scaled system. The discussion held previously is still valid here.

We need to calculate $\hat{s}_{\hat{e}}$. Using the scaling relations we find

$$\hat{s}_{\hat{e}}(\hat{e},\hat{x}) = \sqrt{\frac{3}{2}} s_{\hat{e}} \left(\frac{2}{3} R^2 (\hat{e}-\mu), \sqrt{\frac{2}{3}}\hat{x} \right) = \sqrt{\frac{2}{3}} R^2 s_{\epsilon} \left(\frac{2}{3} R^2 (\hat{e}-\mu), \sqrt{\frac{2}{3}}\hat{x} \right). \tag{8.88}$$

We also need to calculate $\hat{s}_{\hat{x}\hat{x}}$. Using the scaling relations we find

$$\hat{s}_{\hat{x}\hat{x}}(\hat{e},\hat{x}) = \sqrt{\frac{3}{2}} s_{\hat{x}\hat{x}} \left(\frac{2}{3} R^2 (\hat{e}-\mu), \sqrt{\frac{2}{3}}\hat{x} \right) = \sqrt{\frac{2}{3}} s_{xx} \left(\frac{2}{3} R^2 (\hat{e}-\mu), \sqrt{\frac{2}{3}}\hat{x} \right). \tag{8.89}$$

8.3.10 Energy oscillations

We have calculated all we need to obtain an analytical formula for the main energy oscillations. Let's recall (see chapter 6) that the formula is given by

$$E_{osc} = -\frac{2\sqrt{\epsilon}}{\pi^2} \sum_{k,j}{}' \frac{(-1)^j}{j^{\frac{5}{2}}} \frac{\cos\left\{ \frac{2\pi}{\epsilon}[kx^\star + js(\mu,x^\star)] + \frac{\sigma\pi}{4} \right\}}{s_e(\mu,x^\star)\sqrt{|s_{xx}(\mu,x^\star)|}}, \tag{8.90}$$

where the sum is performed over all the periodic orbits of the classical dynamics in the self-consistent potential.

For the orbits which contribute most to the oscillations (those corresponding to $(k:j)=(1:2)$), we obtained a special result, the amplitude being divided by 2 (the value of x was at the lower limit of its integration domain, implying that only half of the saddle-point integration had to be taken into account). These contributions were called the ν oscillations.

In this case we find $x^\star = 0$, and therefore

$$\begin{cases} \hat{s}(\mu,0) & = & \sqrt{\frac{3}{2\pi}\frac{1}{6}\frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)}} \\ \hat{s}_{\hat{e}}(\mu,0) & = & \sqrt{\frac{2}{3}}\frac{1}{\sqrt{\pi}}\frac{\Gamma\left(\frac{3}{4}\right)}{\Gamma\left(\frac{1}{4}\right)} R^2 = \frac{3^{\frac{1}{6}}\pi^{\frac{1}{6}}}{2^{\frac{5}{6}}}\frac{\Gamma\left(\frac{3}{4}\right)}{\Gamma\left(\frac{1}{4}\right)}\kappa^{-\frac{2}{3}} \\ \hat{s}_{\hat{x}\hat{x}}(\mu,0) & = & \sqrt{\frac{2}{3}}\frac{\sqrt{2\pi}}{\Gamma^2\left(\frac{1}{4}\right)}. \end{cases}$$

Replacing in formula (8.90) we find

$$\begin{aligned} E_{osc}^{(1:2)} &= -\sqrt{\epsilon}\frac{3^{\frac{1}{12}}\kappa^{\frac{2}{3}}}{2^{\frac{13}{6}}\pi^{\frac{29}{12}}}\frac{\Gamma^2\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)} \cos\left(\frac{2\pi}{\epsilon}\frac{1}{\sqrt{6\pi}}\frac{\Gamma\left(\frac{1}{4}\right)}{\Gamma\left(\frac{3}{4}\right)} + \frac{\pi}{4} \right) \\ &= -0.1647\sqrt{\epsilon}\kappa^{\frac{2}{3}} \cos\left(0.6815\frac{2\pi}{\epsilon} + \frac{\pi}{4} \right) \\ &= -0.1385\frac{\kappa^{\frac{2}{3}}}{N^{\frac{1}{4}}} \cos\left(0.9637 \cdot 2\pi\sqrt{N} + \frac{\pi}{4} \right), \end{aligned} \tag{8.91}$$

where we used $\epsilon = \frac{1}{\sqrt{2}}\frac{1}{\sqrt{N}}$.

Let's consider the other terms of the same family of periodic orbits, in order to provide to the oscillations its shape:

$$\sum_{n\geq 1} E_{osc}^{(n:2n)} = -0.1385\frac{\kappa^{\frac{2}{3}}}{N^{\frac{1}{4}}}\sum_{n=1}^{\infty}\frac{1}{n^{\frac{5}{2}}}\cos\left(0.9637\cdot 2\pi n\sqrt{N}+\frac{\pi}{4}\right). \tag{8.92}$$

The result is an oscillating function of $\sqrt{N}$, of period $\frac{1}{0.9637} = 1.0376$.

Similar to previous work, we have to multiply this energy by N to obtain the real energy. We also use $\kappa = \frac{k'}{N^{\frac{3}{2}}}$, according to our model described in chapter 4, to find

$$\sum_{n\geq 1} \hat{E}_{osc}^{(n:2n)} = -0.1385\frac{k'^{\frac{2}{3}}}{N^{\frac{1}{4}}}\sum_{n=1}^{\infty}\frac{1}{n^{\frac{5}{2}}}\cos\left(0.9637\cdot 2\pi n\sqrt{N}+\frac{\pi}{4}\right). \tag{8.93}$$

Let's now add the two next terms, which will be small compared to the main one. We find numerically

$$\left\{\begin{array}{lcl} x^{\star}_{(3:7)} & = & 0.4318 \\ \hat{x}^{\star}_{(3:7)} & = & 0.5288 \\ \hat{s}(\mu,\hat{x}^{\star}_{(3:7)}) & = & 0.0965 \\ \hat{s}_{\hat{e}}(\mu,\hat{x}^{\star}_{(3:7)}) & = & 0.1689R^2 = 0.2990\kappa^{-\frac{2}{3}} \\ \hat{s}_{\hat{x}\hat{x}}(\mu,\hat{x}^{\star}_{(3:7)}) & = & 0.1035. \end{array}\right.$$

This leads to the energy contribution

$$\begin{aligned} E_{osc}^{(3:7)} &= 0.01625\sqrt{\epsilon}\kappa^{\frac{2}{3}}\cos\left\{2.2619\frac{2\pi}{\epsilon}+\frac{\pi}{4}\right\} \\ &= 0.01367\frac{\kappa^{\frac{2}{3}}}{N^{\frac{1}{4}}}\cos\left\{3.1988\cdot 2\pi\sqrt{N}+\frac{\pi}{4}\right\}. \end{aligned} \tag{8.94}$$

The inclusion of the whole family of the corresponding periodic orbits provides

$$\sum_{n\geq 1} E_{osc}^{(3n:7n)} = -0.01367\frac{\kappa^{\frac{2}{3}}}{N^{\frac{1}{4}}}\sum_{n\geq 1}\frac{(-1)^n}{n^{\frac{5}{2}}}\cos\left\{3.1988\cdot 2\pi n\sqrt{N}+\frac{\pi}{4}\right\}. \tag{8.95}$$

The real energy is obtained by multiplying by N. We also use $\kappa = \frac{k'}{N^{\frac{3}{2}}}$ to obtain

$$\sum_{n\geq 1} \hat{E}_{osc}^{(3n:7n)} = -0.01367\frac{k'^{\frac{2}{3}}}{N^{\frac{1}{4}}}\sum_{n\geq 1}\frac{(-1)^n}{n^{\frac{5}{2}}}\cos\left\{3.1988\cdot 2\pi n\sqrt{N}+\frac{\pi}{4}\right\}. \tag{8.96}$$

The next correction is given by

$$\begin{cases} x^\star_{(4:9)} & = \;\; 0.3163 \\ \hat{x}^\star_{(4:9)} & = \;\; 0.3874 \\ \hat{s}(\mu, \hat{x}^\star_{(4:9)}) & = \;\; 0.1582 \\ \hat{s}_{\hat{e}}(\mu, \hat{x}^\star_{(4:9)}) & = \;\; 0.1633 R^2 = 0.2892 \kappa^{-\frac{2}{3}} \\ \hat{s}_{\hat{x}\hat{x}}(\mu, \hat{x}^\star_{(4:9)}) & = \;\; 0.1225. \end{cases}$$

This leads to the energy contribution

$$\begin{aligned} E^{(4:9)}_{osc} &= 0.0082 \sqrt{\epsilon} \kappa^{\frac{2}{3}} \cos\left\{ 2.9734 \frac{2\pi}{\epsilon} + \frac{\pi}{4} \right\} \\ &= 0.0069 \frac{\kappa^{\frac{2}{3}}}{N^{\frac{1}{4}}} \cos\left\{ 4.2050 \cdot 2\pi \sqrt{N} + \frac{\pi}{4} \right\}. \end{aligned} \tag{8.97}$$

The inclusion of the whole family of the corresponding periodic orbits provides

$$\sum_{n \geq 1} E^{(4n:9n)}_{osc} = -0.0069 \frac{\kappa^{\frac{2}{3}}}{N^{\frac{1}{4}}} \sum_{n \geq 1} \frac{(-1)^n}{n^{\frac{5}{2}}} \cos\left\{ 4.2050 \cdot 2\pi n \sqrt{N} + \frac{\pi}{4} \right\}. \tag{8.98}$$

The real energy is obtained by multiplying by N. We make use of $\kappa = \frac{k'}{N^{\frac{3}{2}}}$ to obtain

$$\sum_{n \geq 1} \hat{E}^{(4n:9n)}_{osc} = -0.0069 \frac{k'^{\frac{2}{3}}}{N^{\frac{1}{4}}} \sum_{n \geq 1} \frac{(-1)^n}{n^{\frac{5}{2}}} \cos\left\{ 4.2050 \cdot 2\pi n \sqrt{N} + \frac{\pi}{4} \right\}. \tag{8.99}$$

As was already mentioned, the contribution arising from the other terms are small compared to the main contribution. It is represented in Figure 8.9, where the energy oscillations of the three most contributing families of orbits are shown, as well as their sum. This figure confirms the fact that mainly one family of orbits contributes to the energy oscillations.

We still have to calculate the λ oscillations. They should be less important than the other terms. The general formula is (see chapter 6):

$$E^{\lambda}_{osc} = -\frac{\epsilon}{2\pi^2} \frac{1}{\hat{\lambda}_{max,\hat{e}}(\mu)} \sum_{k \geq 1} \frac{1}{k^2} \frac{\sin\left\{ \frac{2\pi}{\epsilon} k \hat{\lambda}_{max}(\mu) \right\}}{\sin\left\{ \frac{\pi k}{|\hat{s}_{\hat{x}}(\mu, \hat{\lambda}_{max}(\mu))} \right\}}. \tag{8.100}$$

We find

$$\begin{cases} \hat{\lambda}_{max,\hat{e}}(\mu) & = \;\; \sqrt{\frac{2}{3}} R^2 \lambda_{max,\epsilon}(0) = \frac{1}{3^{\frac{3}{4}}} R^2 = \frac{\pi^{\frac{2}{3}}}{2^{\frac{4}{3}} 3^{\frac{1}{12}}} \kappa^{-\frac{2}{3}} \\ \hat{\lambda}_{max}(\mu) & = \;\; \sqrt{\frac{3}{2}} \lambda_{max}(0) = \frac{1}{3^{\frac{1}{4}}} \\ \hat{s}_{\hat{x}}(\mu, \hat{\lambda}_{max}(\mu)) & = \;\; s_x(0, \lambda_{max}(0)) = -\frac{1}{\sqrt{6}}. \end{cases}$$

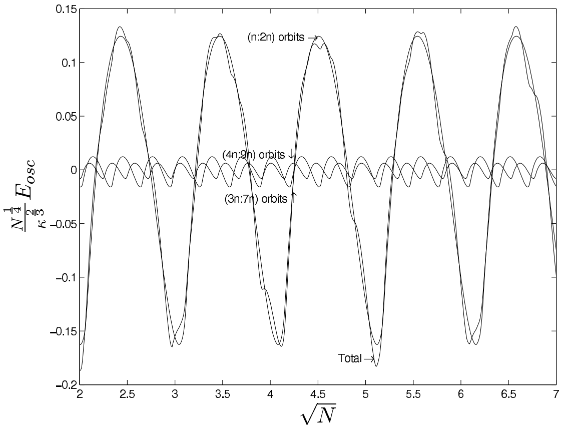


Figure 8.9: *Normalized main energy oscillations as a function of $\sqrt{N}$.*

Introducing these values in expression (8.100) we find

$$
\begin{aligned}
E_{osc}^{\lambda} &= -\epsilon \frac{3^{\frac{3}{4}}}{2\pi^2} \frac{1}{R^2} \sum_{k\geq 1} \frac{1}{k^2} \frac{\sin\left\{\frac{2\pi}{\epsilon} \frac{k}{3^{\frac{1}{4}}}\right\}}{\sin\left\{\pi k \sqrt{6}\right\}} \\
&= -\epsilon \frac{2^{\frac{1}{3}} 3^{\frac{1}{12}}}{\pi^{\frac{8}{3}}} \kappa^{\frac{2}{3}} \sum_{k\geq 1} \frac{1}{k^2} \frac{\sin\left\{\frac{2\pi}{\epsilon} \frac{k}{3^{\frac{1}{4}}}\right\}}{\sin\left\{\pi k \sqrt{6}\right\}} \\
&= -0.0461 \frac{\kappa^{\frac{2}{3}}}{\sqrt{N}} \sum_{k\geq 1} \frac{1}{k^2} \frac{\sin\left\{1.0746 k 2\pi \sqrt{N}\right\}}{\sin\left\{0.4082 k\pi\right\}}. \qquad (8.101)
\end{aligned}
$$

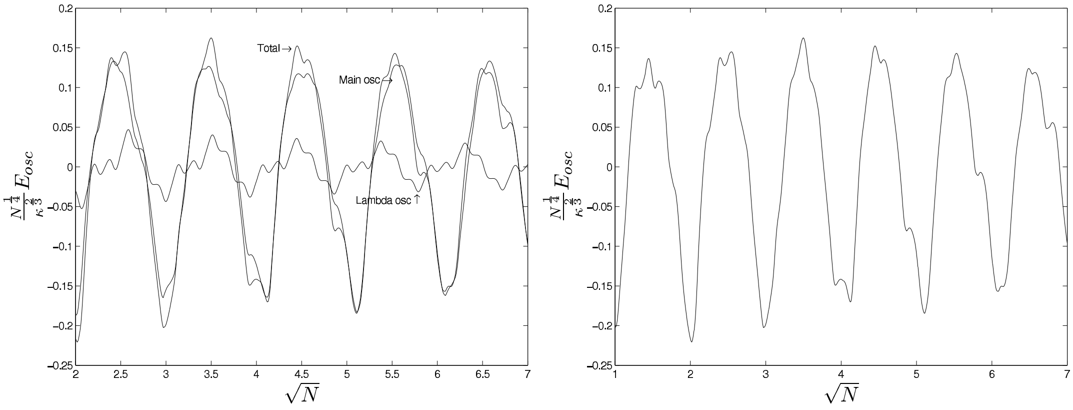
The real energy is obtained by multiplying by N. We also make use of $\kappa = \frac{k'}{N^{\frac{3}{2}}}$ to find

$$
\hat{E}_{osc}^{\lambda} = -0.0461 \frac{k'^{\frac{2}{3}}}{\sqrt{N}} \sum_{k\geq 1} \frac{1}{k^2} \frac{\sin\left\{1.0746 k 2\pi \sqrt{N}\right\}}{\sin\left\{0.4082 k\pi\right\}}. \qquad (8.102)
$$

A plot of this function is shown in Figure 8.10, superposed with the other contributions to the energy oscillations. This contribution is decreasing compared to the others (the relative decrease is $\sim \frac{1}{N^{\frac{1}{4}}}$). We also show the sum of all these contributions, and a separate plot with the total energy oscillations only.

Let's replace k by its experimental value. In comparison with Tarucha's results (see chapter 4), we find that the constant k' is estimated as $k' = 0.205$ in our units. To express the final energy in meV we have to multiply the energy by $E_\star = 11.2 meV$. The final result is

$$
\hat{E}_{osc} = \sum_{n\geq 1} \left(\hat{E}_{osc}^{(n:2n)} + \hat{E}_{osc}^{(3n:7n)} + \hat{E}_{osc}^{(4n:9n)} \right) + \hat{E}_{osc}^{\lambda} \qquad (8.103)
$$



(a) (b)

Figure 8.10: *Total energy oscillations.*

and is shown in Figure 8.11.

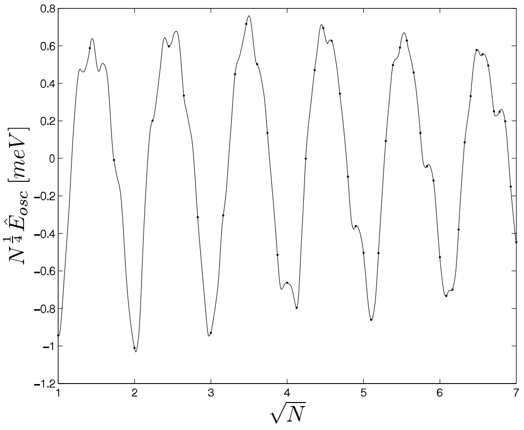


Figure 8.11: *Total energy oscillations expressed in meV.*

8.4 Comparison with experimental results

Our results can be compared to experimental results (Tarucha's results presented in the introduction – chapter 4).

We start by comparing the classical energy, which is the only analytical result we can obtain. It is plotted in Figure 8.12.

We observe a difference between the classical energy and the experimental one. The two curves however seem to be in good agreement qualitatively, which

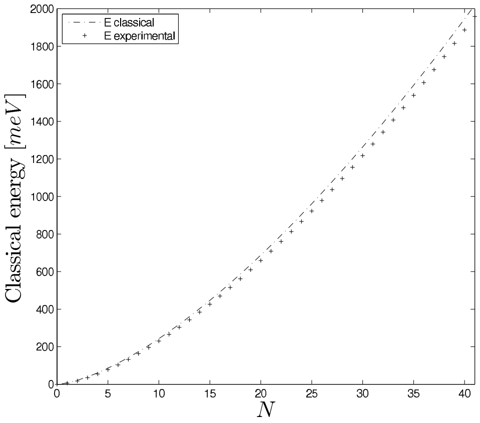


Figure 8.12: *Classical energy compared to experimental energy.*

confirms the relevance of the model we used.

We can still improve this analytical result by adding the exchange energy of this model, which is the lowest order exchange energy. It can also be computed analytically. It is plotted in Figure 8.13.

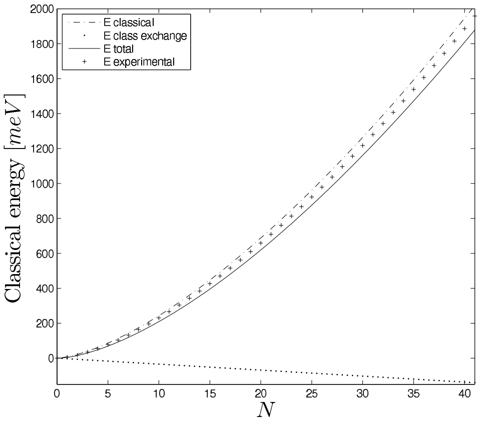


Figure 8.13: *Classical energy (with the exchange term) compared to experimental energy.*

Let's plot the total energy, obtained with numerical simulations. It corresponds to Hartree energy, or Thomas-Fermi energy (which is equivalent in this case). It is plotted in Figure 8.14.

Surprisingly, the total energy is worse than the classical energy, when compared to the experimental results. However, the difference is small.

Let's note that there is no quantum correction: as established in the developments, this correction is zero.

To improve the results, let's add the exchange energy to Hartree energy. The

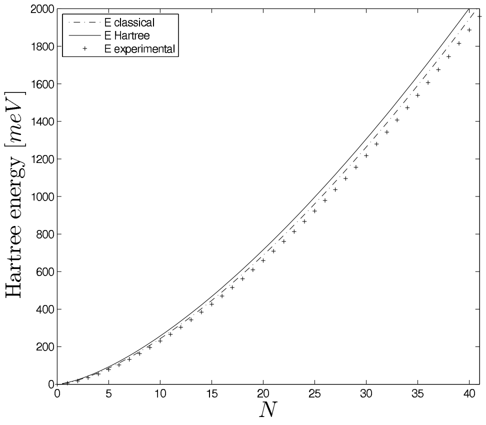


Figure 8.14: *Hartree energy compared to experimental energy.*

result is plotted in Figure 8.15 and leads to Hartree-Fock energy.

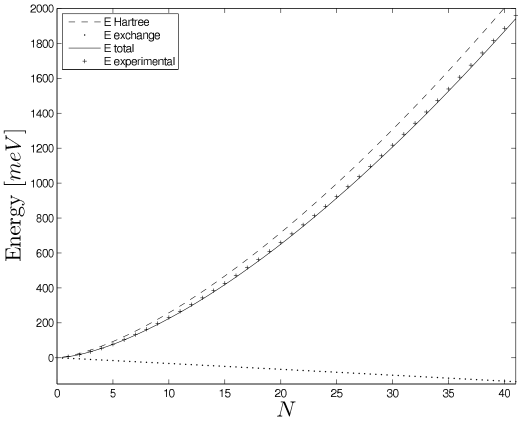


Figure 8.15: *Theoretical energy compared to experimental energy.*

There is a remarkable similarity between the theoretical and experimental curves. To evaluate quantitatively these results, we compute the relative error as a function of N, defined as

$$Error(N) \doteq \frac{|E_{exp}(N) - E_{th}(N)|}{|E_{exp}(N)|}. \tag{8.104}$$

This error is plotted in Figure 8.16 as a function of $\sqrt{N}$.

The relative error is more than 5% for $N = 2$. However, let's recall that our theory is justified for $N \gg 1$. From $\sqrt{N} = 5$, the relative error is stabilized at about 1%. It is low enough to validate our theory.

There is, however, a weak effect we want to observe in this comparison between experimental and theoretical results: the energy oscillations. Let's estimate

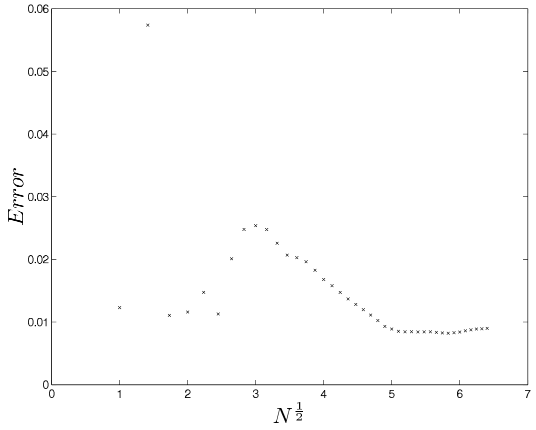
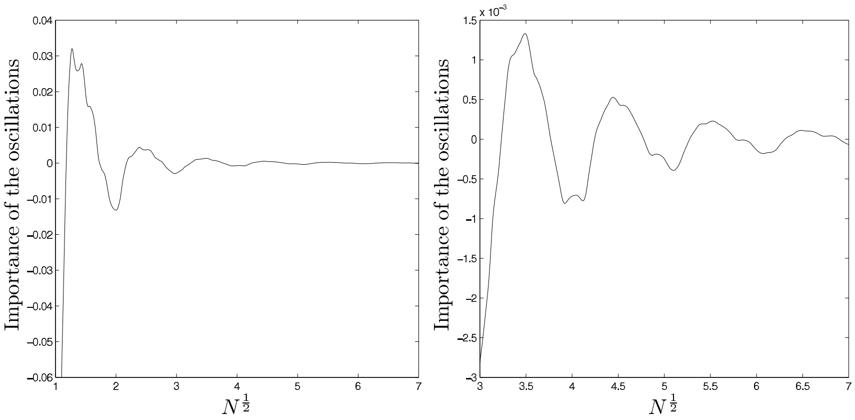


Figure 8.16: *Relative error of the energy as a function of* $\sqrt{N}$.

the relative importance of these oscillations. We plot the theoretical energy oscillations, divided by the smooth energy. It is shown in Figure 8.17.



(a) (b)

Figure 8.17: *Relative importance of the oscillations.*

The relative importance of the energy oscillations is, from $\sqrt{N} = 3$, of the order of 10^{-3}. This is a very weak effect, which is very difficult to observe. We established above that the precision of our results is of the order 10^{-2}, which makes it impossible to observe the oscillations.

Let's look however at the difference of the experimental energy, and the theoretical energy (which plays the role of the "smooth" energy), multiplied by $N^{\frac{1}{4}}$, in order to compare with the theoretical energy oscillations from Figure 8.11. In Figure 8.18 we represent $(E_{exp} - E_{smooth})N^{\frac{1}{4}}$ as a function of $N^{\frac{1}{2}}$.

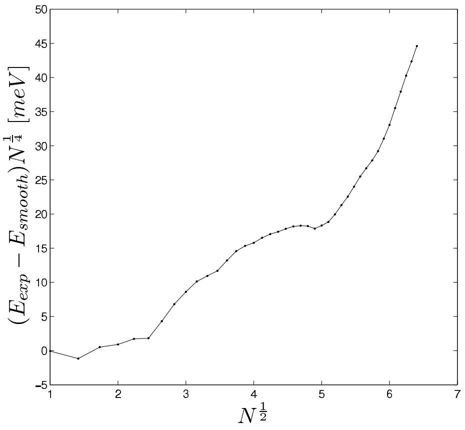


Figure 8.18: *Normalized experimental oscillations.*

As already mentioned, the oscillations, if they exist, are hidden by other effects, which have to be discussed. There are no clear oscillations in this figure.

8.5 Discussion of the results

Before explaining the potential reasons of the difference between our results and experimental results, let's mention the high sensitivity of the experimental oscillations with regards to the experimental parameter k': a slight change in this parameter has an important effect on the experimental oscillations: by changing this parameter of a few percent only, the curve of Figure 8.18 can go up or down. Moreover, it is impossible to set the value of this parameter with a sufficient precision. It is not surprising that the energy oscillations are so sensitive: it is a very weak effect and is therefore naturally sensitive to any change of the parameters.

The theory we developed is valid for $N \gg 1$, and we were able to compare our results with experimental results for up to 41 electrons only.

The ground state energy we computed is in good agreement with the experimental values, the relative error being a few percent only. This relative error seems to be stabilized at about 1% from $\sqrt{N} = 5$. Even if the theoretical energy is in good agreement with experimental results, it is still insufficient (of an order of magnitude) to observe the experimental oscillations, and it needs therefore an explanation.

The most plausible explanation comes from the approximations we made by defining the model. We used a model with a density independent of N, by fixing the confining strength to be N-dependent. Reimann (2002) mentions that this model is a good one for quantum dots with a large number of electrons. One of the main consequences of such a model is that the asymptotic limit of the ground state energy behaves as $N^{\frac{3}{2}}$. Moreover, following our developments, the energy divided by $N^{\frac{3}{2}}$ can be expanded in powers of $\delta \doteq N^{-\frac{1}{2}}$. This function is therefore a smooth function of δ. A look at Figure 4.7 shows that this experimental function is not smooth: there is a large oscillation around a smooth curve. However, the smaller δ is, the straighter the curve seems to be. From $\delta < 0.2$, the experimental curve seems to be smooth. This confirms that the constant density model is adapted for $N \gg 1$, but not for N small. We think that this approximation is the main reason explaining the errors between our results and the experimental results.

Another approximation we did is to model the confining potential as a parabolic potential. This is however what most researchers do, and this model leads to numerical results in very good agreement with the experiments.

One approximation we did is to consider a two-dimensional problem. In real systems, the effective electrons-electron interaction is slightly modified at small and large distances, which could have consequences on the results. Another effect of the third dimension is that electrons could be in excited states in the z-direction. However, as we considered a number of electrons smaller than 41, we are not concerned with this, as it was established by Kouwenhoven et al. (2001).

In our model we considered the approximation of effective mass. This approximation is valid for $k \approx 0$. To estimate the maximal value $\boldsymbol{k}_F$ of our system, let's use a qualitative argument. We simplify by modeling the system as N independent particles in a square of radius $R = \left(\frac{3\pi}{4\kappa}\right)^{\frac{1}{3}}$ (the radius of the dot). The states are quantized as $\boldsymbol{k}_n = \frac{2\pi\boldsymbol{n}}{R} \Rightarrow \boldsymbol{k}_n^2 = \frac{4\pi^2\boldsymbol{n}^2}{R^2}$. For $N \gg 1$, the number of electrons is given by the surface in the reciprocal lattice: $N \approx \pi\boldsymbol{n}_F^2$, where $\boldsymbol{n}_F$ is the Fermi surface. From this we conclude that the Fermi wave vector is

$$k_F \approx \frac{2\pi n_F}{R} \approx \frac{2^{\frac{5}{3}}\pi^{\frac{1}{6}}}{3^{\frac{1}{3}}} k'^{\frac{1}{3}} = 1.72 a_\star^{-1} = 0.167 nm^{-1}. \qquad (8.105)$$

The maximal value k_F is independent of N and is small enough to validate the effective mass approximation in our problem.

Our model was developed in a non relativistic theory. Englert (1988) observes that relativistic effects are crucial in the case of the atoms. In the case of quantum dots, Jacak et al. (1997) compute the spin-orbit interaction, and conclude that it has to be taken into account for N large.

We cannot observe clearly the energy oscillations experimentally, but for a small number of electrons, there is a strong evidence of shell filling for $N = 2, 6, 12, 20, \ldots$ However, as mentioned in (Kouwenhoven et al., 2001), the existence and amplitude of these peaks depend strongly on the dot considered. Moreover, compared to numerical simulations (Reimann et al., 1999), these peaks are smaller than what the theory predicts. It may be explained by a loss of the radial symmetry: energy oscillations are weaker in chaotic systems.

The error is too important to compare the experimental oscillations to the theoretical ones. We can however proceed to a qualitative discussion of these oscillations. As written in table 4.1, in the harmonic oscillator model, the shells are filled at values which are in very good agreement with the peaks of the theoretical energy oscillations. This is an argument to confirm our results.

To compare our theoretical energy oscillations to experimental results, we need results with a larger number of electrons. In this case however, we would reach the limits of our model: the third dimension of the dot could not be neglected, and spin-orbit interactions should be considered, too. Moreover, as written in (Kouwenhoven et al., 2001), the experimental oscillations seem to disappear for N larger.

Conclusion and outlook

In this thesis, we introduced and investigated a functional integration approach for the treatment of many-fermion systems. For systems with a large number of particles, a systematic expansion is possible, and leads to the semiclassical Hartree energy at lowest order, the first order being the exchange energy. This approach therefore justifies the Hartree-Fock theory, which is widely used for the treatment of the many-fermion problem. The terms beyond the Hartree-Fock approach correspond to the correlation energy, which we developed at lowest order.

The Hartree-Fock theory was applied to the atoms in (Englert, 1988). With the method we developed, we computed the correlation energy of atoms at lowest order.

This method could be applied to other systems of fermions. One case of interest is molecules: a system with several nuclei could be investigated, in order to compute its correlation energy. This correlation energy could be responsible for the existence of molecules (which is excluded in the Thomas-Fermi approach by Teller's no binding theorem).

We concentrated our application of the method to quantum dots. We computed the ground state energy of these systems, that is the Hartree-Fock energy, the energy oscillations, and the correlation energy. A comparison to experimental results showed that the smooth part of the energy is in good agreement, but that the energy oscillations are too weak to be compared to experimental ones.

The computation of the Hartree energy required the solving of a self-consistent equation. To solve this equation and obtain the self-consistent potential, we introduced a new basis of functions which yielded the known asymptotic results in a simple form. This basis could serve as a starting point for further calculations.

The computation of the energy oscillations led us to the development of a formula for the energy of independent particles in two dimensions, confined with a monotonous growing potential with radial symmetry. This formula is general and could serve for other computations.

We observe that in two-dimensional systems, the correlation energy is – relatively to the dominant energy – more important than in three-dimensional systems. It would be interesting to know if this result has physical consequences.

We also observe that in two-dimensional systems, the energy oscillations are mainly dominated by one term, conversely to three-dimensional systems, where the superposition of functions with incommensurable frequencies leads to apparently random energy oscillations. It is believed that these oscillations are related to the shell structure, and the comparison of the energy oscillations we obtained to the shell fillings of a two-dimensional harmonic oscillator confirms it. This link between shell structure and energy oscillations could certainly be observed experimentally in two-dimensional systems.

To be able to compare the energy oscillations to experimental results, a study of the "second derivative" of $E(N)$, $\Delta_2(N) = E(N+1) - 2E(N) + E(N-1)$ could be done. The energy oscillations – relatively to the total energy – would be much more important, and should therefore be observable. Moreover, a statistical study of $\Delta_2(N)$ could be done and compared to existing results – both experimental and theoretical (a certain number of models were proposed).

The method we developed could be applied to chaotic quantum dots, like quantum dots with a magnetic field, or quantum dots with a confining potential without radial symmetry. Both have been realized experimentally. In the latter case, the first step would be to solve the self-consistent equation – which would be solved numerically. This would answer whether the self-consistent potential has a radial symmetry or not, and under which conditions on the confining potential. For chaotic systems, there would be differences for the treatment of the energy oscillations. The Gutzwiller trace formula could be used, and it would not be necessary to proceed to a detailed calculation, as was made in this thesis for quantum dots with radial symmetry.

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Curriculum vitae

I was born on September 28th, 1978, in Lausanne (Switzerland). I did my secondary education at the Gymnase du Bugnon in Lausanne and obtained a certificate of secondary studies in 1997, with orientation science.

The same year I started studies in physics at the Swiss Federal Institute of Technology (EPFL). I obtained the EPF Physics Engineer degree in 2002, after having completed my master thesis. This thesis, entitled *Statistical mechanics of topological defects in the bidimensional Heisenberg model*, was undertaken at the Institute of Theoretical Physics under the supervision of Prof. Hervé Kunz.

Since 2002, I have been working as a research assistant at the Institute of Theoretical Physics, under the supervision of Prof. Hervé Kunz. My research topic has been semiclassical atoms and quantum dots. I was involved in many teaching activities: I worked as a teaching assistant for the courses of general relativity, non linear phenomena and chaos, and mathematical physics (Prof. Kunz), and statistical physics (Prof. Martin). I also worked as an expert for exams of linear algebra (Prof. Thévenaz), mathematical physics (Prof. Savona), and cosmology (Prof. Chapochnikov). I was the teaching assistants' representative in the teaching commission .