EVOLUTION OF OPEN MANY-ELECTRON SYSTEMS: FROM A QUANTUM STATISTICAL DESCRIPTION TOWARDS THE SEMI-CLASSICAL BOLTZMANN EQUATION

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It was once believed, by many speculative scientists that there might be dozens of billions of life-supporting worlds in the universes. These worlds were thought to be scattered throughout space... these speculative scientists were correct.

And it was once believed, by many nonscientists and pseudoscientists and fringe people that there might be – in quite a different way from the first instance – dozens of billions of life-supporting worlds in the universes... These worlds were not to be scattered throughout space. There was not any space in such scatterable sense... And the persons of these wide-eyed groups were quite correct in their assumptions.

There was a third belief that was held by many determined and brilliant, though spotty, folks. This was the belief that there was only one world and that all possible persons were in it... And the persons who held these several similar beliefs were absolutely right to hold them.

And at the same time that these three true theories were current, it was maintained ... that there was no contradiction in these theories and no reason for conflict: that these three beliefs were only three aspects of the same thing, if that is, one should take a tri-mental view of space and of being and of several other things.

R.A. Lafferty, *Not to mention camels*, Wildside Press, September 2000.

Abstract

Starting from the quantum statistical master equation derived in [1] we show how the connection to the semi-classical Boltzmann equation (SCBE) can be established and how irreversibility is is related to the problem of separability of quantum mechanics. Our principle goal is to find a sound theoretical basis for the description of the evolution of an electron gas in the intermediate regime between pure classical behavior and pure quantum behavior.

We investigate the evolution of one-particle properties in a weakly interacting N-electron system confined to a finite spatial region in a near-equilibrium situation that is weakly coupled to a statistical environment. The equations for the reduced n-particle density matrices, with $n < N$ are hierarchically coupled through two-particle interactions. In order to elucidate the role of this type of coupling and of the inter-particle correlations generated by the interaction, we examine first the particular situation where energy transfer between the N-electron system and the statistical environment is negligible, but where the system has a finite memory. We then formulate the general master equation that describes the evolution of the coarse grained one-particle density matrix of an interacting confined electron gas including energy transfer with one or more bath subsystems, which is called the quantum Boltzmann equation (QBE).

The connection with phase space is established by expressing the one-particle states in terms of the overcomplete basis of coherent states, which are localized in phase space. In this way we obtain the QBE in phase space. After performing an additional coarse-graining procedure in phase space, and assuming that the interaction of the electron gas and the bath subsystems is local in real space, we obtain the semi-classical Boltzmann equation. The validity range of the classical description, which introduces local dynamics in phase space is discussed.

Keywords: Non-equilibrium and irreversible thermodynamics, quantum statistical methods, open systems, Boltzmann equation, kinetic theory of electron gases, theories and models of many-electron systems, coherent states, coarse graining, classical and quantum transport

Zusammenfassung

Von der quantenstatistischen Master-Gleichung ([1]) ausgehend, wird gezeigt, dass die Verbindung zur semiklassischen Boltzmann Gleichung hergestellt werden kann und wie Irreversibilität mit dem Problem der Separabilität in der Quantenmechanik in Verbindung steht. Diese Arbeit wurde mit dem Ziel erstellt, eine fundierte theoretische Basis für eine Beschreibung des Bereiches zwischen den Grenzfällen des reinen Quantenverhaltens auf der einen, und des reinen klassichen Verhaltens auf der anderen Seite zu finden.

Es wird die Entwicklung von Einteilcheneigenschaften in einem schwach wechselwirkenden, räumlich beschränkten N-Elektronensystem nahe eines Gleichgewichts untersucht, wobei das Elektronensystem schwach an eine statistiche Umgebung gekoppelt ist. Die Gleichungen für die reduzierten n-Teilchendichtematrizen für $n < N$ sind auf Grund der 2-Teilchen Elektron-Elektron Wechselwirkung hierarchisch miteinander gekoppelt. Um die Rolle dieser Kopplung und der aus der Wechselwirkung folgenden Teilchenkorrelationen aufzuzeigen, untersuchen wir den Fall, in dem der Energieaustausch zwischen dem N-Elektronensystem und der statistischen Umgebung vernachlässigt werden kann, das Elektronensystem aber nur ein endliches Gedächtnis hat. Wir gelangen zur allgemeinen Master-Gleichung, welche die Entwicklung der gemittelten Einteilchendichtematrix eines wechselwirkenden Elektronengases in einem System beschreibt, welches Energieaustausch mit einem oder mehreren Bädern erlaubt.

Die Verbindung mit dem Phasenraum wird durch das Beschreiben der Einteilchenzustände in der übervollständigen Basis der kohärenten Zustände erreicht. Kohärente Zustände sind im Phasenraum lokalisiert, was es ermöglicht die QBE im Phasenraum anzugeben. Nach einer Mittelung im Phasenraum und unter der Annahme, dass die Wechselwirkung zwischen dem Elektronengas und den Bädern räumlich lokal ist, erhalten wir die semiklassische Boltzmanngleichung. Der Gültigkeitsbereich der klassischen Beschreibung, welche eine lokale Dynamik im Phasenraum beschreibt wird diskutiert.

Schlagworte: Nicht-Gleichgewicht und irreversible Thermodynamik, quantenstatistische Methoden, offene Systeme, Boltzmanngleichung, kinetische Theorie des Elektronengases, Theorien und Modelle von Vielelektronensystemen, kohärente Zustände, klassischer Transport und Quanten-Transport.

Contents

Chapter 1

Introduction and outline

Introduction

The question of the link between the quantum mechanical and classical descriptions of physical systems is as old as quantum mechanics. Quantum mechanics has proven its validity to describe small systems, such as single atoms or molecules. It is therefore natural to ask how to describe the behavior of large systems with quantum mechanics. In order to tackle this problem we take a look at the structure of quantum and classical physics. The Geneva-Brussels axiomatic approach of quantum mechanics [2] clearly states the difference between the quantum mechanical and classical descriptions. In this axiomatic formulation of quantum mechanics the classical description is contained as a particular case. The properties of a pure quantum mechanical system can be represented by closed subspaces of a complex separable Hilbert space. At a given time t the state of a system is the set of actual[1] properties of the system. The state is represented by a ray, which itself can again be represented by a vector (*state-vector*) in Hilbert space. All actual properties, of the system in a given state, correspond to subspaces that contain the state-vector. Two different properties are compatible if their associated subspaces are orthogonal. Observables are ensembles of compatible properties[2]. In quantum mechanics, the state-vector can be any non-zero vector in Hilbert space. In relation to an observable, one can introduce the notation "superposition state", often found in the literature. One can chose a certain observable, which corresponds to a set of orthogonal subspaces. If the state of the system is represented by a vector that is not within one of these subspaces, it is called "superposition state"[3]. In the classical description, all properties are imposed to be compatible, i.e., a state-vector must be in a subspace A or in the subspace $A^{\perp}$ orthogonal

[1] For a definition of the word actual, as it is used here, see [2].

[2] In other words: Observables are sets of projectors on orthogonal subspaces.

[3] Note that this superposition is just a mathematical way to describe a vector in Hilbert space relative to a chosen observable and does not contain any additional physical information.

to A. The "superposition states" are excluded. Therefore the Hilbert space associated with a classical system can always be decomposed in orthogonal *one-dimensional* subspaces.

On the basis of the Geneva-Brussels approach it was shown that "two separated quantum entities cannot be described by means of standard quantum mechanics" [3]. This "problem of separability" shows a shortcoming of the quantum mechanical theory[4]. Several attempts have been made to understand the connection between a classical and a quantum description mainly concentrating on the measuring process [6, 7, 8].

In this work we show that in a quantum statistical description one can see how irreversible behavior is related to the problem of separability. A statistical description is adequate to understand experimental results, for example on electronic transport in solids [9, 10, 11, 12]. In the Landauer transport theory one defines a sample connected to separate reservoirs, which inject electrons into the sample. The electronic transport in the sample is calculated using scattering theory. After scattering, the electrons leave the sample into one of the reservoirs again. This one-particle description has proven its validity in particular in mesoscopic transport. It is however not evident why the assumption of statistically independent electronic reservoirs can be made, neither is it clear on what scale this can be justified.

Searching for a classical description, we step into phase space, by introducing the basis of coherent states [13]. Coherent states are centered around different points in phase space and they are related by translation operations. Furthermore, they have a width in position and a width in momentum space. These two widths saturate the Heisenberg inequalities. A coherent state is the natural correspondent of a classical state in the quantum description [14].

Starting from the quantum statistical master equation derived in [1] we will show how the connection to the semi-classical Boltzmann equation (SCBE)[5] can be established. Our principal goal is to find a sound and transparent theoretical basis to describe the intermediate regime in between the two limiting regimes of pure classical behavior and pure quantum mechanical behavior. The intermediate regime is a very interesting and vivid area of both, theory and experiment. This work should be understood as the first step on the path to develop a description of the intermediate regime.

[4] See [4] in relation to the so called "paradox" of Einstein-Podolski-Rosen [5].

[5] The difference between the SCBE and the classical Boltzmann equation is the following. The classical Boltzmann equation describes the evolution of classical particles. The semi-classical Boltzmann equation describes the evolution of classical particles with additional quantum properties. The "Pauli corrected Boltzmann equation" [15] treats classical particles, which have the additional property that states can only being occupied by one of them.

Outline

The theoretical basis of this work is established in chapter 2. Starting from the general approach of [1], we first derive the master equation for the evolution of the coarse grained N-particle density matrix of open many-electron systems. Then we develop a quantum statistical approach, which establishes the theoretical basis to investigate the evolution of one-particle properties in a weakly interacting electronic subsystem in a near-equilibrium situation. We consider an N-electron subsystem confined to a finite spatial region and weakly coupled to a statistical environment. The corresponding equations for the n-particle density operators with $n < N$ are then obtained by trace operations described in in chapter 3. These equations are hierarchically coupled through the two-particle electron-electron interaction.

In order to elucidate the role of this type of coupling and of the interparticle correlations generated by the interaction, we examine in chapter 4 the particular situation where energy transfer between the N-electron subsystem and the statistical environment is negligible, but where the presence of the environment still enables the electronic subsystem to explore different configurations belonging to the same energy. The resulting irreversible evolution is driven by the screened Coulomb interaction. In order to keep the arguments as simple as possible, we consider weakly excited metallic systems, where the screened effective two-particle interaction extends only over a small spatial region. In this case correlations between more than two electrons can be neglected. In our approach we account for this fact by introducing a finite memory time, which hinders the subsystem to build up many-particle correlations involving more than two particles. We derive a master equation for the evolution of the coarse grained one-particle density matrix. Further discussions about the origin of irreversibility for quantum statistical systems can be found in [16, 17]. In the classical approach the problem is hidden in Boltzmann's Stosszahlansatz [18].

In chapter 5, we obtain the general master equation that describes the evolution of the coarse grained one-particle density matrix of an interacting confined electron gas *including* energy transfer with one or more bath subsystems. This equation will be called the quantum Boltzmann equation (QBE).

We show in chapter 6 that the overcomplete basis of coherent states and the concept of quasi-orthogonality finally allow the derivation of the semi-classical Boltzmann equation (SCBE) from the QBE. We start with the representation of the QBE in the basis of coherent states where the one-particle density matrix is expressed in form of the "diagonal representation" [19]. This allows us to study the evolution of the electronic subsystem in phase space. In order to demonstrate the spatial separability on macroscopic scales, we choose sufficiently large cell volumes so that orthogonality between cells can be assumed. We finally discuss the conditions under which the evolution of the averaged densities can be described by the classical Boltzmann equation.

Chapter 2

Dissipative evolution of quantum statistical ensembles

Following the general approach of Reuse, et al. (*Dissipative evolution of quantum statistical ensembles and nonlinear response to a time-periodic perturbation*, [1]), we consider a system composed of two subsystems, a bathed subsystem A and a bath subsystem B, described with the associated Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. The system Hamiltonian is given by

$$H_{\rm tot} = H_0 + H_{\rm int}, \qquad\qquad H_{\rm tot}, H_0, H_{\rm int} \in \mathcal{L}(\mathcal{H}_{\rm A} \otimes \mathcal{H}_{\rm B}).$$

$\mathcal{L}(\mathcal{H}_{\rm A}\otimes\mathcal{H}_{\rm B})$ denotes the space of linear operators in the Hilbert space $\mathcal{H}_A\otimes\mathcal{H}_B$. The operators H_0 and $H_{\rm int}$ can be decomposed as

$$H_0 = H_A \otimes \mathbb{1}_B + \mathbb{1}_A \otimes H_B, \qquad H_A \in \mathcal{L}(\mathcal{H}_{\rm A}), H_B \in \mathcal{L}(\mathcal{H}_{\rm B})$$

and

$$H_{\rm int} = \sum_\alpha Q_\alpha^A \otimes Q_\alpha^B.$$

Without loss of generality the operators $Q_\alpha^A \in \mathcal{L}(\mathcal{H}_{\rm A})$ and $Q_\alpha^B \in \mathcal{L}(\mathcal{H}_{\rm B})$ in the interaction Hamiltonian may be assumed to be self-adjoint[1]. The statistical state of the system is described by the density matrix $D(t) \in \mathcal{L}(\mathcal{H}_{\rm A} \otimes \mathcal{H}_{\rm B})$. The density matrices describing the statistical states of the subsystems are obtained by partial trace operations over the subspaces $\mathcal{H}_{\rm A}$ and $\mathcal{H}_{\rm B}$, i.e.,

$$\begin{aligned} D_A(t) &= {\rm Tr}_{\rm B}\left(D(t)\right), \qquad D_A(t) \in \mathcal{L}(\mathcal{H}_{\rm A}), \\ D_B(t) &= {\rm Tr}_{\rm A}\left(D(t)\right), \qquad D_B(t) \in \mathcal{L}(\mathcal{H}_{\rm B}). \end{aligned}$$

[1] In order to simplify the arguments, we here assume that the Hamiltonian H_A and the operators Q_α^B have already been modified, so that first-order terms in the interaction are absorbed (see equation (7) in [1]).

The density matrices $D(t)$, $D_A(t)$, and $D_B(t)$ satisfy the von Neumann conditions, namely, D is self adjoint

$$D = D^\dagger,$$

positive

$$\langle a|D|a\rangle \geqslant 0, \ \forall \ |a\rangle \in \mathcal{H}$$

with unit trace

$$\mathrm{Tr}\,(D) = 1.$$

One consequence is $D^2 \leqslant D$.

In the following we suppose a discrete spectrum of the Hamiltonian H_A, that the interaction is weak[2] and that the bath is maintained near some statistical equilibrium, which is specified by the density matrix D_B^0. Due to the coupling between the subsystems A and B, the density matrix $D_B(t)$ fluctuates around D_B^0, i.e., we have

$$D_B(t) = \mathrm{Tr_B}\,(D(t)) = D_B^0 + \delta D_B(t), \qquad \text{with } \mathrm{Tr_B}\,(\delta D_B(t)) = 0.$$

The evolution of the *coarse grained* density matrix $\bar{D}_A(t)$ of the bathed system[3] is derived in [1]. One has introduced the time averaged density matrix in the interaction picture

$$\bar{D}_A^I(t) = \frac{1}{\Delta t}\int_{t_0}^{t} D_A^I(t')dt'$$

with the small time interval $\Delta t = t - t_0$.

In the Schrödinger picture we get

$$\frac{d}{dt}\bar{D}_A(t) = \frac{i}{\hbar}\left[\bar{D}_A(t), H_A\right] + \Gamma(\bar{D}_A(t)), \tag{2.1}$$

where Γ is a linear superoperator acting on $\mathcal{L}(\mathcal{H}_\mathrm{A})$.

The generalization to situations where system A interacts with several statistically independent bath subsystems $B_j, j = 1, 2, \ldots$, is straightforward. We simply have to attribute a specific interaction operator

$$H_{\mathrm{int}\,j} = \sum_\alpha Q_{j\alpha}^A \otimes Q_\alpha^{B_j} \tag{2.2}$$

to each bath subsystem B_j. The equilibrium density matrices associated with each bath will be denoted by $D_{B_j}^0$. We then get

$$\Gamma(\bar{D}_A(t)) = \Gamma_1(\bar{D}_A(t)) + \Gamma_2(\bar{D}_A(t)) + \cdots, \tag{2.3}$$

[2]This restriction is stated more precisely in equation (2.15).

[3]We use the term bathed system, for the subsystem A.

where the superoperators Γ_j are associated with the bath subsystems B_j. Equation (2.1) becomes

$$\frac{d}{dt}\bar{D}_A(t) = \frac{i}{\hbar}\left[\bar{D}_A(t), H_A\right] + \Gamma_1(\bar{D}_A(t)) + \Gamma_2(\bar{D}_A(t)) + \cdots . \tag{2.4}$$

The terms $\Gamma_j(\bar{D}_A(t))$ describe the influence of the bath subsystems B_j on subsystem A. They are defined by their matrix elements expressed in the orthonormal eigenbasis of the Hamiltonian H_A. In order to specify the expressions, we denote this eigenbasis by $\{|a\rangle\}$ and the corresponding eigenvalues of H_A by ϵ_a. We further introduce the associated frequencies

$$\omega_a = \frac{\epsilon_a}{\hbar}$$

and the difference frequencies

$$\omega_{ab} = \omega_a - \omega_b.$$

The matrix elements of the superoperator Γ_j can then be written as

$$\left(\Gamma_j(\bar{D}_A(t))\right)_{ab} = \sum_{\{cd|\omega_{ca}=\omega_{db}\}} \left(\Gamma_j\right)_{ab}^{cd} \left(\bar{D}_A(t)\right)_{cd} \tag{2.5}$$

with

$$\left(\Gamma_j\right)_{ab}^{cd} = \begin{cases} \left(\Gamma_{0j}\right)_{ab}^{cd} & -\frac{1}{\hbar}\left(\delta_{ac}\ \left(G_j\right)_{db} + \delta_{bd}\ \left(G_j\right)_{ac}\right) \\ & +\frac{i}{\hbar}\left(\delta_{ac}\left(\Delta H_j\right)_{db} - \delta_{bd}\left(\Delta H_j\right)_{ac}\right) \quad \text{for } \omega_{ca}+\omega_{bd}=0, \\ 0 & \text{else} \end{cases} \tag{2.6}$$

with

$$\left(\Gamma_{0j}\right)_{ab}^{cd} = \left(\left(\Gamma_{0j}\right)_{ba}^{dc}\right)^{\star} = \left(F_j\right)_{ab}^{cd} + \left(\left(F_j\right)_{ba}^{dc}\right)^{\star}, \tag{2.7}$$

$$\left(G_j\right)_{aa'} = \frac{\hbar}{2}\sum_{a''}\left(\Gamma_{0j}\right)_{a''a''}^{a'\,a}, \tag{2.8}$$

$$\left(\Delta H_j\right)_{aa'} = \frac{i\ \hbar}{2}\sum_{a''}\left(\left(F_j\right)_{a''a''}^{a'\ a} - \left(\left(F_j\right)_{a''a''}^{a\ a'}\right)^{\star}\right). \tag{2.9}$$

The terms Γ_{0j} and G_j give rise to the irreversible evolution of subsystem A. The operators ΔH_j describe the self-energy corrections, which account for the dynamical coupling between the states of subsystem A that is induced by the polarization of the bath subsystems B_j. The coefficients $\left(F_j\right)_{ab}^{cd}$ appearing in definitions (2.7), (2.8), and (2.9) are given by

$$\left(F_j\right)_{ab}^{cd} \pm \left(\left(F_j\right)_{ba}^{dc}\right)^{\star} = \frac{1}{\hbar}\sum_{\alpha\beta}\langle a|Q_{j\alpha}^A|c\rangle\ \langle d|Q_{j\beta}^A|b\rangle \times \begin{cases} \chi_{\beta\alpha}^j(\omega_{ca}) \\ i\bar{\chi}_{\beta\alpha}^j(\omega_{ca}), \end{cases} \tag{2.10}$$

where the functions $\chi^j_{\beta\alpha}(\omega)$ and $\bar{\chi}^j_{\beta\alpha}(\omega)$ are themselves directly related to the correlation functions $c^j_{\alpha\beta}(t'-t'')$. The latter are defined as

$$c^j_{\alpha\beta}(t'-t'') = \left(c^j_{\beta\alpha}(t''-t')\right)^\star = \mathrm{Tr_B}\left(D^0_{B_j}\left(Q^{B_j}_\alpha\right)^I(t')\left(Q^{B_j}_\beta\right)^I(t'')\right), \quad (2.11)$$

where the operators

$$\left(Q^{B_j}_\alpha\right)^I(t) = e^{\frac{i}{\hbar}H_B t}\, Q^{B_j}_\alpha\, e^{-\frac{i}{\hbar}H_B t}, \quad H_B = \sum_j H_{B_j}$$

represent the $Q^{B_j}_\alpha$ operators in the interaction picture. We then have

$$\chi^j_{\alpha\beta}(\omega) = \frac{1}{\hbar}\int_{-\infty}^{\infty} c^j_{\alpha\beta}(\tau)e^{i\omega\tau}d\tau, \quad (2.12)$$

$$\bar{\chi}^j_{\alpha\beta}(\omega) = \frac{i}{\hbar}\int_{-\infty}^{\infty} \xi(\tau)c^j_{\alpha\beta}(\tau)e^{i\omega\tau}d\tau, \quad (2.13)$$

where $\xi(\tau)$ is the Heaviside function

$$\xi(\tau) = \begin{cases} -1 & \text{if } \tau < 0 \\ 0 & \text{if } \tau = 0 \\ 1 & \text{if } \tau > 0 \end{cases}. \quad (2.14)$$

We note that equation (2.4) is obtained under the assumption that the correlation functions $c^j_{\alpha\beta}(\tau)$ become negligible for $\tau > \tau^{\mathrm{corr}}_{B_j}$ where the correlation time $\tau^{\mathrm{corr}}_{B_j}$ depends on the interaction Hamiltonian as well as on the density matrix $D^0_{B_j}$. Equation (2.4) is valid for

$$\frac{1}{|\,(\Gamma_j)^{cd}_{ab}\,|} \gg \tau^{\mathrm{corr}}_{max}, \quad \forall\, c,a,b,d, \quad \text{with} \quad \tau^{\mathrm{corr}}_{max} = \sup_j\left\{\tau^{\mathrm{corr}}_{B_j}\right\}. \quad (2.15)$$

The above condition sets an upper limit on the interaction strengths between subsystems A and B_j.

Chapter 3

Reduced density operators

In [1], the evolution of the statistical state of a system in interaction with a bath is investigated. We specify the system we are interested in. Throughout this work we always think of the bathed system as a system of N electrons, with three assumptions: the electron gas has metallic densities, the electron gas is spatially confined, and the electron gas is near an equilibrium state.

It is useful to introduce the Fock space, so that creation and annihilation operators can be defined. The states of the electronic system A of N particles are described by anti-symmetric tensors of the space $\mathcal{H}^{\otimes N}$, where $\mathcal{H}$ denotes the one-particle Hilbert space. The space consisting of the anti-symmetric tensors is $\mathcal{F}^N$

$$\mathcal{F}^N = \mathcal{A}\left(\mathcal{H}^{\otimes N}\right), \tag{3.1}$$

where $\mathcal{A}$ is the antisymmetrizer. The Fock space is given by

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} \mathcal{F}^n \quad \text{with} \quad \mathcal{F}^0 = \mathbb{C}.$$

A set of orthonormal basis vectors $|\nu), \nu = 1, 2, \ldots$, spans the whole one-particle Hilbert space $\mathcal{H}$. Then the vectors

$$|\nu_1, \ldots, \nu_N\rangle = \frac{1}{\sqrt{N!}} \sum_{s \in S_N} \sigma(s) |\nu_{s(1)}) \otimes \cdots \otimes |\nu_{s(N)}), \tag{3.2}$$

which are totally antisymmetric with respect to the action of the permutation group, form an orthonormal basis of $\mathcal{F}^N$. S_N denotes the permutation group of the ensemble $\{1, 2, \ldots, N\}$ and $\sigma(s)$ is the signature of the permutation $s \in S_N$.

The statistical state of the bathed system A is therefore described by an N-particle density matrix $D_{(N)A}$, acting in $\mathcal{F}^N$ and satisfying the normalization condition

$$\mathrm{Tr_A}\left(D_{(N)A}\right) = 1.$$

3.1 One- and two-particle operators

An operator O_A is defined by its action in the one-particle Hilbertspace $\mathcal{H}$. A one-body operator $\tilde{O}_A$ acting in the Fock space is defined by

$$\tilde{O}_A = \sum_{\nu\mu} c_\nu^\dagger (O_A)_{\,\nu\mu}\; c_\mu,$$

where $(O_A)_{\,\nu\mu}$ is the short hand notation for the matrix elements $(\nu|O_A|\mu)$ with $|\nu), |\mu) \in \mathcal{H}$. The creation operator $c_\mu^\dagger$ creates a fermion in the state $|\mu)$, while the annihilation operator c_ν annihilates a fermion in the state $|\nu)$. The creation and annihilation operators of fermions obey the anti-commutation relations

$$\left\{c_\nu, c_\mu^\dagger\right\} = c_\nu c_\mu^\dagger + c_\mu^\dagger c_\nu = \delta_{\nu\mu}\mathbb{1} \tag{3.3}$$

$$\{c_\nu, c_\mu\} = \left\{c_\nu^\dagger, c_\mu^\dagger\right\} = 0. \tag{3.4}$$

The mean value of a one-particle operator is given by

$$\begin{aligned}\left\langle \tilde{O}_A \right\rangle (t) &= \mathrm{Tr_A}\left(\tilde{O}_A D_{(N)A}(t)\right) \\ &= \sum_{\nu\mu} (O_A)_{\nu\mu} \mathrm{Tr_A}\left(c_\mu D_{(N)A}(t) c_\nu^\dagger\right).\end{aligned} \tag{3.5}$$

The trace appearing in equation (3.5) represents the essential information needed to calculate a mean value of a one-body operator. This trace does not contain the full information about all N particles. One can define the general reduced n-particle density operator with $n \in \{1, \ldots, N-1\}$ that appears in the mean value of n-particle observables

$$D^{(n)}_{A\mu_n \ldots \mu_1 \nu_1 \ldots \nu_n}(t) = \frac{1}{n!} \mathrm{Tr}\left(c_{\mu_1} \ldots c_{\mu_n} D_{(N)A}(t) c_{\nu_1}^\dagger \ldots c_{\nu_n}^\dagger\right). \tag{3.6}$$

The mean value (3.5) can now be written with the one-particle density operator $D_A^{(1)}$:

$$D^{(1)}_{A\;\mu\nu} = \mathrm{Tr}\left(c_\mu D_{(N)A} c_\nu^\dagger\right) = (\mu|D_A^{(1)}|\nu) \tag{3.7}$$

as

$$\langle O_A \rangle (t) = \sum_{\nu\mu} (O_A)_{\nu\mu} D^{(1)}_{A\;\mu\nu}(t) \tag{3.8}$$

Note that the trace $\mathrm{Tr_A}(\cdots)$ in equation (3.6) may be extended over the full Fock space $\mathcal{F}$, since non-vanishing contributions are provided only by the $N-n$ particle Fock space.

Let us look at some properties that follow from definition (3.6). The one-particle density operators are normalized as

$$\mathrm{Tr}_1\left(D_A^{(1)}\right) = \sum_\nu \left(D_A^{(1)}\right)_{\nu\nu} = N. \tag{3.9}$$

The density operators $D_A^{(2)}$ and $D_A^{(1)}$ are related by

$$\mathrm{Tr}_1\left(D_A^{(2)}\right)_{\mu\mu'} = \sum_\rho \left(D_A^{(2)}\right)_{\rho\mu\mu'\rho} = \frac{N-1}{2}\left(D_A^{(1)}\right)_{\mu\mu'}. \tag{3.10}$$

According to equations (3.9) and (3.10), we have

$$\mathrm{Tr}_2\left(D_A^{(2)}\right) = \sum_{\rho\mu}(D_A^{(2)})_{\rho\mu\mu\rho} = \frac{N(N-1)}{2}. \tag{3.11}$$

The matrix elements of the reduced two-particle density operator $D^{(2)}$ will be written in this work with the convention:

$$\left(D_A^{(2)}\right)_{\nu\mu\mu'\nu'} = D_{A\ \nu\mu\mu'\nu'}^{(2)} = \langle\nu\mu|D_A^{(2)}|\mu'\nu'\rangle = \frac{1}{2}\mathrm{Tr}\left(c_\nu c_\mu D_{(N)A} c_{\mu'}^\dagger c_{\nu'}^\dagger\right) \tag{3.12}$$

From the anti-commutation relations for the creation and annihilation operators, one finds the symmetry relations for the matrix elements of $D_A^{(2)}$, which must be obeyed by any two-fermion operator O_2, acting in $\mathcal{H}^{\otimes 2}$, namely

$$\begin{aligned} (O_2)_{\rho\mu\mu'\rho'} &= (O_2)_{\mu\rho\rho'\mu'} \\ \left((O_2)_{\rho\mu\mu'\rho'}\right)^\star &= (O_2)_{\rho'\mu'\mu\rho}, \\ (O_2)_{\rho\mu\mu'\rho'} &= -(O_2)_{\mu\rho\mu'\rho'}, \end{aligned} \tag{3.13}$$

where $(O_2)_{\rho\mu\mu'\rho'}$ is the short hand notation for the matrix elements $\langle\rho\mu|O_2|\mu'\rho'\rangle$.

In addition, we use the term *density matrix* for operators that fulfill the von Neumann conditions, while we use the term *density operator* for operators that fulfill the von Neumann conditions except the unit trace condition. As an example, we call $D_{(N)A}$ a density matrix, because $\mathrm{Tr}\left(D_{(N)A}\right) = 1$, while we call $D_A^{(n)}$ with $n < N$ a density operator, because $\mathrm{Tr}\left(D_A^{(n)}\right) = \frac{N!}{(N-n)!n!}$.

3.2 Partial trace operations

When unnecessary, we will suppress the index A for the bathed system from now on.

After having shown how the one-particle operator is related to the reduced one-particle density operator, we return to the evolution of the mean values.

From equation (3.8), we see that it is given by the evolution of the reduced one-particle density operator:

$$\frac{d}{dt}\left\langle \tilde{O}\right\rangle (t)=\sum_{\nu\mu}O_{\nu\mu}\frac{d}{dt}D^{(1)}_{\mu\nu}(t).$$

To determine the evolution of the mean value of a one-body operator, we have to know the evolution of the reduced one-particle density operator $D^{(1)}$. This is the motivation for the next step: derive the equation of motion for the reduced one-particle density operator in the presence of a bath. We start with the equation of motion for the N-particle density matrix, which follows from equation (2.1), by replacing $\bar{D}_A(t)$ with $D_{(N)}$:

$$\frac{d}{dt}D_{(N)}(t)=\frac{i}{\hbar}\left[D_{(N)},H_A\right]+\Gamma\left(D_{(N)}(t)\right), \tag{3.14}$$

where the superoperator Γ describes the action of the statistical environment on the density matrix of the open system.

In equation (3.7), we have seen how the one-particle density operator is obtained from the N-particle density matrix. We multiply equation (3.14) with the creation and annihilation operators $c, c^\dagger$ and calculate the trace:

$$\frac{d}{dt}D^{(1)}_{\nu'\nu}(t)=\frac{i}{\hbar}\mathrm{Tr}\left(\left[D_{(N)}(t),H_A\right]c^\dagger_\nu c_{\nu'}\right)+\mathrm{Tr}\left(\Gamma\left(D_{(N)}(t)\right)c^\dagger_\nu c_{\nu'}\right). \tag{3.15}$$

For the evolution of the n-particle density operator with $n=2$ we get

$$\begin{aligned}\frac{d}{dt}D^{(2)}_{\rho\mu\mu'\rho'}(t) &= \frac{1}{2}\frac{i}{\hbar}\mathrm{Tr}\left(c_\rho c_\mu\left[D_{(N)}(t),H_A\right]c^+_{\mu'}c^+_{\rho'}\right) \\ &\quad +\frac{1}{2}\mathrm{Tr}\left(c_\rho c_\mu\Gamma(D_{(N)}(t))c^+_{\mu'}c^+_{\rho'}\right).\end{aligned} \tag{3.16}$$

In the following section, the terms in equation (3.15) will be treated one after another.

Evaluating the trace over the Hamiltonian contribution

The first term of equation (3.15) describes the non-dissipative evolution

$$\frac{i}{\hbar}\mathrm{Tr}\left(\left[D_{(N)}(t),H_A\right]c^\dagger_\nu c_{\nu'}\right).$$

We suppose that the particle interaction can be described by an effective two-particle interaction.

The Hamiltonian of the bathed system then contains a one-particle part and the two-particle interaction between the particles:

$$\begin{aligned}H_A &= H^{(1)}_A+W^{(2)} \\ &= \sum_{\nu\nu'}c^\dagger_\nu\langle\nu|h|\nu'\rangle c_{\nu'}+\frac{1}{2}\sum_{\mu\nu\mu'\nu'}c^\dagger_\nu c^\dagger_\mu(\nu\mu|w|\nu'\mu')c_{\mu'}c_{\nu'},\end{aligned}$$

where the operator $W^{(2)}$ is self-adjoint and symmetric with respect to the action of the permutation group, i.e., we have

$$\begin{aligned}(\nu\mu|w|\nu'\mu') &= (\mu\nu|w|\mu'\nu'), &(3.17)\\ (\nu\mu|w|\nu'\mu')^\star &= (\nu'\mu'|w|\nu\mu). &(3.18)\end{aligned}$$

The matrix elements $(\nu\mu|w|\nu'\rho')$ describe the screened two-particle interaction potential[1].

For an effective two-particle interaction, we have to treat:

$$\mathrm{Tr}\left(\left[D_{(N)}(t), H_A\right] c_\rho^\dagger c_{\rho'}\right) = \mathrm{Tr}\left(\left[D_{(N)}(t), H_A^{(1)}\right] c_\rho^\dagger c_{\rho'}\right) + \mathrm{Tr}\left(\left[D_{(N)}(t), W^{(2)}\right] c_\rho^\dagger c_{\rho'}\right)$$

with

$$\begin{aligned}\mathrm{Tr}\left(\left[D_{(N)}(t), \sum_{\nu\nu'} h_{\nu\nu'} c_\nu^\dagger c_{\nu'}\right] c_\rho^\dagger c_{\rho'}\right) &= \sum_{\nu\nu'} h_{\nu\nu'} \mathrm{Tr}\left(\left[D_{(N)}(t), c_\nu^\dagger c_{\nu'}\right] c_\rho^\dagger c_{\rho'}\right)\\ &= \sum_{\nu} D^{(1)}_{\rho'\nu} h_{\nu\rho} - \sum_{\nu'} h_{\rho'\nu} D^{(1)}_{\nu\rho}\\ &= \left[D^{(1)}, h\right]_{\rho'\rho}.\end{aligned}$$

The second term will be abbreviated as

$$\begin{aligned}W^{(2\to1)}\left(D^{(2)}\right)_{\rho\rho'} &= \mathrm{Tr}\left(\left[D_{(N)}, W^{(2)}\right] c_\rho^\dagger c_{\rho'}\right)\\ &= \frac{2i}{\hbar}\sum_{\nu\nu'\mu}\left(D^{(2)}_{\rho\nu'\nu\mu}(\nu\mu|w|\nu'\rho') - (\rho\nu'|w|\mu\nu) D^{(2)}_{\mu\nu\nu'\rho'}\right),\end{aligned}$$

where the second line was deduced by using the commutation relations of the creation and annihilation operators (3.3) and (3.4), the definition of the reduced two-particle density matrix (3.12) and the symmetry properties of $W^{(2)}$ (3.17) and (3.18).

Finally we have for the second term of equation (3.15):

$$\frac{i}{\hbar}\mathrm{Tr}\left(\left[D_{(N)}(t), H_A\right] c_\rho^\dagger c_{\rho'}\right) = \frac{i}{\hbar}\left[D^{(1)}, H_A^{(1)}\right]_{\rho'\rho} + W^{(2\to1)}(D^{(2)})_{\rho\rho'}. \quad (3.19)$$

Equation (3.15) is now written as

$$\begin{aligned}\frac{d}{dt} D^{(1)}_{\rho'\rho}(t) &= \frac{i}{\hbar}\left[D^{(1)}, H_A^{(1)}\right]_{\rho'\rho} + W^{(2\to1)}(D^{(2)})_{\rho\rho'}\\ &\quad + \mathrm{Tr}\left(\Gamma\left(D_{(N)}(t)\right) c_\rho^\dagger c_{\rho'}\right). &(3.20)\end{aligned}$$

[1]Note that the vector $|\nu_1, \ldots, \nu_n) = |\nu_1\rangle \otimes \cdots \otimes |\nu_N\rangle$ is the unsymmetrized vector, while $|\nu_1, \ldots, \nu_N\rangle$ is the antisymmetrized (see definition (3.2)) one.

The interaction Hamiltonian

Before we treat the second term of equation (3.15) in appendix B, we take a look at the properties of the bath. So far, we have described the influence of the bath on the evolution of the bathed system by the term containing Γ.

In this section, we will adapt the result of [1] to the case, presented in the last chapter, of a system consisting of N electrons in contact with a bath. We will make two hypotheses. First, we assume that the action of the bath B_j on the bathed system, represented by the interaction Hamiltonian of the form (2.2), can be described by a one-body operator $Q^A_{j\alpha}$:

$$Q^A_{j\alpha} \quad = \sum_{\nu,\nu'} a^{j\,\nu\nu'}_{\alpha}\ c^\dagger_\nu c_{\nu'}, \tag{3.21}$$

with

$$\left(a^{j\nu\nu'}_{\alpha}\right)^* = a^{j\nu'\nu}_{\alpha}. \tag{3.22}$$

Our approach allows interactions with the bath that involve more than two particles[2]. But a two-particle interaction makes the writing as easy as possible, without loosing the essentials. We may describe the action of the bathed system on the bath by a one-body operator $Q^{B_j}_\alpha$:

$$Q^{B_j}_\alpha \quad = \sum_{\mu} b^{j\,\mu}_{\alpha} \left(d^{j\dagger}_\mu + d^j_\mu\right).$$

This restriction is in principle justified in solid state physics. We will assume that $Q^A_{j\alpha}$ and $Q^{B_j}_\alpha$ are described by one-body operators, i.e., the interaction Hamiltonian can be written as the sum of tensor products of the one-body operators $Q^A_{j\alpha}$ and $Q^{B_j}_\alpha$.

3.3 Evolution of the one-particle density operator

The master equation of $D^{(1)}$ is obtained with the results of the appendix B, i.e., inserting equation (3.19) and (B.17) in equation (3.15):

$$\begin{aligned}\frac{d}{dt}D^{(1)}(t) \;=\; & \frac{i}{\hbar}\left[D^{(1)}(t), H^{(1)}\right] + W^{(2\to1)}(D^{(2)}(t)) \\ & +\Gamma_0^{(1\to1)}(D^{(1)}(t)) + \Gamma^{(2\to1)}(D^{(2)}(t)) - \frac{1}{\hbar}\left\{G^{(1)}, D^{(1)}(t)\right\} \\ & +\frac{i}{\hbar}\left[D^{(1)}(t), \Delta H^{(1)}\right] + \Delta H^{(2\to1)}\left(D^{(2)}(t)\right)\end{aligned} \tag{3.23}$$

[2]The consequence would be that the correlations have to be treated up to higher order.

The two terms in the first line on the right-hand side describe the reversible evolution. The second of these terms represents the contribution of the electron-electron interaction. The matrix elements of the operator $W^{(2\to1)}(\bar{D}_A^{(2)}(t))$ are given by equation (3.19)

$$W^{(2\to1)}\left(D^{(2)}\right)_{\rho\rho'} = \frac{2i}{\hbar}\sum_{\nu\nu'\mu}\left(D^{(2)}_{\rho\nu'\nu\mu}(\nu\mu|w|\nu'\rho') - (\rho\nu'|w|\mu\nu)D^{(2)}_{\mu\nu\nu'\rho'}\right).$$

The terms of the second and third line in equation (3.23) result from the interaction with the bath subsystems. In accordance with equation (2.3), each of these contributions is given by a sum over the specific contributions of the different bath subsystems $B_j, j = 1, \ldots$. The second line describes the dissipative evolution induced by the bath subsystems. The action of the superoperators $\Gamma_{0\,j}^{(1\to1)}(\bar{D}_A^{(1)})$ and $\Gamma_{0\,j}^{(2\to1)}(\bar{D}_A^{(2)})$ in the operator space $\mathcal{L}(\mathcal{H}^{\otimes2})$ is expressed in terms of the coefficients C_j, given in equation (B.7)

$$(C_j)^{\nu'\mu}_{\nu\mu'} = \frac{1}{\hbar}\sum_{\alpha\beta}\chi^j_{\alpha\beta}(\omega_{\nu'\nu})a^{j\nu\nu'}_{\alpha}a^{j\mu\mu'}_{\beta},$$

with the functions χ, defined in equation (2.12). According to equation (2.6) we only have to consider coefficients with $\omega_{\mu\mu'} + \omega_{\nu\nu'} = 0$, which satisfy the symmetry relations (B.9)

$$\left((C_j)^{\mu'\nu}_{\mu\nu'}\right)^{\star} = (C_j)^{\nu\mu'}_{\nu'\mu}.$$

We get equation (B.12)

$$\Gamma_{0\,j}^{(1\to1)}\left(D^{(1)}\right)_{\rho\rho'} = \sum_{\nu\mu'}(C_j)^{\mu'\nu}_{\rho\rho'}\,D^{(1)}_{\mu'\nu} \tag{3.24}$$

and equation (B.15)

$$\begin{aligned}\Gamma^{(2\to1)}\left(D^{(2)}\right)_{\rho\rho'} = \sum_{\nu\nu'\mu}\Big(&D^{(2)}_{\rho\nu'\nu\mu}\left((C_j)^{\nu'\mu}_{\nu\rho'} - (C_j)^{\rho'\nu}_{\mu\nu'}\right)\\ &+\left((C_j)^{\nu'\rho}_{\nu\mu} - (C_j)^{\mu\nu}_{\rho\nu'}\right)D^{(2)}_{\mu\nu'\rho'\nu}\Big).\end{aligned}$$

The matrix elements of the operators $G_j^{(1)}$ appearing in the last term on the second line of equation (3.23) are given by (B.11)

$$\left(G_j^{(1)}\right)_{\nu\nu'} = \frac{\hbar}{2}\sum_{\mu}(C_j)^{\mu\mu}_{\nu\nu'}.$$

This term guarantees conservation of $\mathrm{Tr_A}\left(D_A^{(1)}\right)$. The last line in equation (3.23) contains the self-energy terms, which are defined in equation (B.13)

$$\left(\Delta H_j^{(1)}\right)_{\nu\nu'} = \frac{\hbar}{2}\sum_{\mu}\left(\bar{C}_j\right)^{\mu\mu}_{\nu\nu'}$$

and (B.16)

$$\begin{aligned}\Delta H_j^{(2\to1)}\left(D^{(2)}\right)_{\rho\rho'} &= i\sum_{\nu\nu'\mu}\left(D^{(2)}_{\rho\nu'\nu\mu}\left(\left(\bar{C}_j\right)^{\rho'\nu}_{\mu\nu'}+\left(\bar{C}_j\right)^{\nu'\mu}_{\nu\rho'}\right)\right.\\ &\quad\left.-\left(\left(\bar{C}_j\right)^{\mu\nu}_{\rho\nu'}+\left(\bar{C}_j\right)^{\nu'\rho}_{\nu\mu}\right)D^{(2)}_{\mu\nu'\nu\rho'}\right),\end{aligned}$$

with the matrix elements of the superoperators $\bar{C}$ defined in equation (B.8)

$$\left(\bar{C}_j\right)^{\nu'\mu}_{\nu\mu'}=-\frac{1}{\hbar}\sum_{\alpha\beta}\bar{\chi}^j_{\alpha\beta}(\omega_{\nu'\nu})a^{j\nu\nu'}_\alpha a^{j\mu\mu'}_\beta,$$

where the functions $\bar{\chi}$ are defined in equation (2.13). The matrix elements satisfy the symmetry relations (B.10):

$$\left(\left(\bar{C}_j\right)^{\mu'\nu}_{\mu\nu'}\right)^\star=\left(\bar{C}_j\right)^{\nu\mu'}_{\nu'\mu}.$$

The self-energy corrections do not lead to qualitatively new behavior. In most physical situations they may be neglected or they can be treated by a renormalization of the Hamiltonian $H_A^{(1)}$, so that instead of equation (3.23) it is sufficient to consider

$$\begin{aligned}\frac{d}{dt}D^{(1)}(t) &= \frac{i}{\hbar}\left[D^{(1)}(t),H^{(1)}\right]+W^{(2\to1)}(D^{(2)}(t))\\ &\quad+\Gamma_0^{(1\to1)}(D^{(1)}(t))+\Gamma^{(2\to1)}(D^{(2)}(t))-\frac{1}{2}\left\{G^{(1)},D^{(1)}(t)\right\}.\end{aligned}\tag{3.25}$$

The direct two-particle interaction represented by $W^{(2\to1)}$ and the induced two-particle interaction represented by $\Gamma^{(2\to1)}$ lead to a coupling of the one-particle evolution to the two-particle density operator, whose evolution is in turn coupled to the three-particle density operator, and so forth. Continuing this hierarchy of equations, we finally come to a coupling to the evolution of the N-particle density matrix. This set of equations is called the BBGKY[3] hierarchy of equations.

At first sight the reader might have the impression that the reduction to the one-particle density operator, described in this chapter has not lead to any reduction of the complexity – and he would be right. In fact, as long as the hierarchy cannot be truncated, we have only reformulated the problem.

The reduction is valuable, however, because in order to describe a realistic experimental situation, the hierarchy must be truncated. Let us adapt our general description to the example of a metal. In a first approximation we will divide the metal – composed of electrons and nuclei – into two subsystems only. The electrons in the conduction band, treated as a confined electron gas, are assumed to be the bathed subsystem and the phonons are assumed to

[3]BBGKY stands for Born, Bogoliubov, Green, Kirkwood and Yvon.

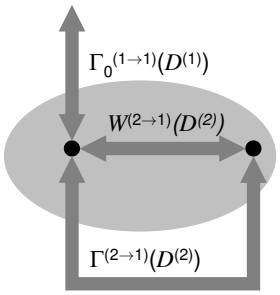

Figure 3.1: Relation between the terms in equation (3.25). The grey ellipsis represents the electronic system, the phonon bath is represented by the white background, the black circles represent electrons and the arrows represent couplings: $W^{(2\to1)}$ represents the screened Coulomb interaction, and $\Gamma_0^{(1\to1)}$ and $\Gamma^{(2\to1)}$ represent the electron-phonon coupling.

form the bath subsystem. The electron-electron interaction (screened Coulomb interaction) is represented by the superoperator $W^{(2\to1)}$, while the interesting part[4] of the electron-phonon interaction is represented by the superoperators $\Gamma_0^{(1\to1)}$ and $\Gamma^{(2\to1)}$ (see figure 3.1).

Let us now address the truncation of the hierarchy in the case of two current models for a metal. In one of the two models, the electron-phonon interaction is assumed to play the important role, while the electron-electron interaction is neglected. In the other model, the electron-electron coupling is assumed to play the important role, while the electron-phonon interaction is neglected.

First, we take the electron-phonon interaction into account and neglect the electron-electron interaction, i.e., $W^{(2\to1)}\left(D^{(2)}\right) = 0$. At first sight, this might describe a non-interacting electron gas. But there is an electron-electron interaction left: the indirect interaction induced by the bath, represented by $\Gamma^{(2\to1)}\left(D^{(2)}\right)$. As shown in the preceding chapter, this influence is of second order in the interaction. In the case of a weak electron-phonon interaction[5] and an initially uncorrelated system, the two particle density operator $D^{(2)}$ is substituted by the antisymmetrized tensor product of one-particle operators depending on the one-particle density matrix

$$D^{(2)} = E[D^{(1)}] \otimes E[D^{(1)}]P_a \tag{3.26}$$

[4]We will not include the terms containing $G_j^1, \Delta H_j^{(1)}$ and $\Delta H_j^{(2\to1)}$ in the following discussion, because they are not important for the truncation of the hierarchy.

[5]Of course, this interaction has to be weak, but still more important, than the electron-electron interaction, we wanted to neglect.

without statistical correlations[6] ($\eta_{(2)} = 0$), and where P_a is the projector[7] on the subspace of antisymmetric tensors in $\mathcal{H}^{\otimes 2}$. Since the generated correlations are at least of third order in the electron-phonon interaction, they can be neglected in the evolution of the one-particle density operator for a small time interval. Equation (3.25) becomes

$$\begin{aligned}&\frac{d}{dt}D^{(1)}(t)\\&= \frac{i}{\hbar}\left[D^{(1)}(t), H^{(1)}\right]\\&\quad +\Gamma_0^{(1\to 1)}(D^{(1)}(t)) + \Gamma^{(2\to 1)}\left(E[D^{(1)}(t)]\otimes E[D^{(1)}(t)]P_a\right) - \frac{1}{2}\left\{G^{(1)}, D^{(1)}(t)\right\}.\end{aligned}$$

The coupling to the two-particle density operator has disappeared, and the hierarchy has thus been truncated. This model is widely used, but a fundamental problem remains. The slowly growing statistical correlations $\eta_{(2)}$ build up with time. Therefore, the two-particle density operator can only be written in the form of equation (3.26) up to a given time. Once correlations have built up the two-particle density operator is no longer described by the antisymmetrized tensor product of the one-particle operators E and the hierarchy of equations comes back into play. The relevance of the hierarchy has just been delayed. By reconsidering the physical situation, we will find a justification of the truncation. This justification will be discussed together with the second model for a metal, where correlations are generated already by first-order terms in the interaction.

We only take the electron-electron interaction into account and neglect the electron-phonon interaction, i.e., the second line of equation (3.25). Now the statistical correlations are created by the electron-electron interaction in first order. Assuming a weak interaction does not change this. Therefore the two-particle density operator $D^{(2)}$ can not be substituted by the antisymmetric tensor product in equation (3.26), but we have to include the correlations $\eta_{(2)}$

$$D^{(2)} = E[D^{(1)}]\otimes E[D^{(1)}]P_a + \eta_{(2)},$$

with $\mathrm{Tr}\left(\eta_{(2)}\right) = 0$.

We thus have to look for some mechanism that hinders the system to build up two-particle correlations $\eta_{(2)}$ in a realistic experimental situation. In fact, up to now we did not take into account the presence in the environment. The distinction between electrons "inside" the sample and electrons "outside" the sample is in conflict with the non-separability problem of a quantum system. We thus have to admit that we have limited knowledge of the electronic system inside the sample. In what follows, we will suppose that the electrons outside the sample form a statistical environment that induces a memory loss in the

[6]See equation (4.18) in the next chapter.

[7]See equation (4.1) in the next chapter.

electronic subsystem inside the sample. We will show that the evolution of the subsystem can be described by a master equation for $D^{(1)}$.

Chapter 4

Evolution of the one-particle density matrix of a system without energy transfer but with memory loss

At the end of the last chapter we have mentioned the origin of the BBGKY hierarchy and the problem of its truncation for the example of a metal. In order to elucidate this problem we will first consider an N-electron system confined to a limited spatial region like a crystal or a quantum dot, which still interacts with its statistical environment, but where energy transfer between the electronic system and the environment is negligible. This type of restricted coupling with the environment, which was not considered in the derivation of equation (3.25), enables the electronic system to explore electronic configurations with the same energy but with different electron-electron correlations. It thus leads to a memory loss in the electronic system. This memory loss changes the situation completely: Starting from an initially uncorrelated N-electron system, it inhibits the generation of high-order correlations. Using the fact that in absence of correlations of order larger than n_{max}, density operators $\bar{D}_A^{(n)}$ with $n > n_{max}$ are fully determined by the density operators $\bar{D}_A^{(k)}, k = 1, \ldots, n_{max}$, we can then truncate the BBGKY hierarchy at the level of $\bar{D}_A^{(n_{max})}$ with $n \leq n_{max} \ll N$. In the following we will assume that the hierarchy can be stopped at the level $n_{max} = 2$, which is adequate for electron densities of usual metallic systems.

4.1 Preparations for the coarse graining

4.1.1 Decomposition of the two-particle density matrix

With the restriction to $n_{max} = 2$, which we have introduced at the end of the last chapter, it becomes convenient to reformulate the problem in the two-particle Hilbert space. We will use the notations

$$\begin{array}{rl}
\mathcal{H} & : \text{one-particle Hilbert space} \\
\mathcal{H}^{\otimes 2} & : \text{two-particle Hilbert space} \\
\mathcal{H}^{\wedge 2} & : \text{subspace of antisymmetric tensors in } \mathcal{H}^{\otimes 2} \\
\mathcal{H}^{\vee 2} & : \text{subspace of symmetric tensors in } \mathcal{H}^{\otimes 2} \\
\frac{1}{\sqrt{2}}\left(|\rho) \otimes |\nu) - |\nu) \otimes |\rho)\right), \rho < \nu & : \text{orthonormal basis in } \mathcal{H}^{\wedge 2} \\
\left.\begin{array}{r} \frac{1}{\sqrt{2}}\left(|\rho) \otimes |\nu) + |\nu) \otimes |\rho)\right), \rho < \nu \\ |\rho) \otimes |\rho), \qquad \rho = \nu \end{array}\right\} & : \text{orthonormal basis in } \mathcal{H}^{\vee 2}.
\end{array}$$

We further introduce the orthogonal projectors

$$\begin{aligned} P_a &: \mathcal{H}^{\otimes 2} \to \mathcal{H}^{\wedge 2}, \\ P_s &: \mathcal{H}^{\otimes 2} \to \mathcal{H}^{\vee 2}, \end{aligned}$$

which can be expressed in the form

$$P_a = \frac{1}{2}\left(\mathbb{1} - S\right), \tag{4.1}$$

$$P_s = \frac{1}{2}\left(\mathbb{1} + S\right), \tag{4.2}$$

where

$$S = \sum_{\rho\nu} |\nu)(\rho| \otimes |\rho)(\nu|. \tag{4.3}$$

From equation (4.3) we obtain

$$S^2 = \mathbb{1}. \tag{4.4}$$

The definitions of P_a (4.1) and P_s (4.2) and equation (4.4) imply

$$P_a^2 = P_a, \qquad P_s^2 = P_s, \qquad P_a P_s = P_s P_a = 0.$$

The orthogonal projectors P_a and P_s can be used to restrict the action of an operator $O \in \mathcal{L}\left(\mathcal{H}^{\otimes 2}\right)$ to one of the subspaces $\mathcal{H}^{\wedge 2}$ or $\mathcal{H}^{\vee 2}$. In the particular case

$$O = A \otimes A, \qquad A \in \mathcal{L}\left(\mathcal{H}\right)$$

we restrict the action of O to $\mathcal{H}^{\wedge 2}$ by the projection

$$\begin{aligned}\mathfrak{P}(A\otimes A) &= P_a(A\otimes A)P_a \\ &= \frac{1}{4}\big(A\otimes A - S(A\otimes A) - (A\otimes A)S + S(A\otimes A)S\big). \quad (4.5)\end{aligned}$$

From the definition(4.3) of S, we get

$$\begin{aligned}S(|\rho)\otimes|\nu)) &= \sum_{\rho'\nu}|\nu')(\rho'|\otimes|\rho')(\nu'|\,(|\rho)\otimes|\nu)) \\ &= |\nu)\otimes|\rho),\end{aligned}$$

which allows us to calculate the matrix elements of the operator defined in equation (4.5)

$$\begin{aligned}\mathfrak{P}(A\otimes A)_{\nu\rho\rho'\nu'} &= (\nu|\otimes(\rho|P_aA\otimes AP_a|\rho')\otimes|\nu') \quad (4.6)\\ &= \frac{1}{2}\left(A_{\rho\rho'}A_{\nu\nu'} - A_{\rho\nu'}A_{\nu\rho'}\right).\end{aligned}$$

In the following, we will use density *matrices* $D_{(n)}$ with

$$\mathrm{Tr}\left(D_{(n)}\right) = 1$$

rather than the density *operators* $D^{(n)}$. Both differ just by a normalization factor. The density matrices $D_{(1)}, D_{(2)}$ are thus given by

$$\begin{aligned}D_{(1)} &= \frac{1}{N}D^{(1)}, \\ D_{(2)} &= \frac{2}{N(N-1)}D^{(2)}. \quad (4.7)\end{aligned}$$

From equations (3.9) and (3.10) we get

$$\begin{aligned}\mathrm{Tr}\left(D_{(1)}\right) &= \sum_{\nu}D_{(1)\nu\nu} = 1, \quad (4.8)\\ \sum_{\nu}D_{(2)\nu\mu\mu'\nu} &= D_{(1)\mu\mu'}. \quad (4.9)\end{aligned}$$

The last equation can be written in operator form

$$\mathrm{Tr}_1\left(D_{(2)}\right) = D_{(1)}. \quad (4.10)$$

Equations (4.8) and (4.10) imply

$$\mathrm{Tr}_2\left(D_{(2)}\right) = \sum_{\nu\mu}D_{(2)\nu\mu\mu'\nu} = \mathrm{Tr}\left(\mathrm{Tr}_1\left(D_{(2)}\right)\right) = 1.$$

In absence of statistical correlations, the two-particle density matrix of the N-electron system is given by a tensor $D^{\mathrm{u}}_{(2)}$ of the form (4.5)

$$D^{\mathrm{u}}_{(2)} = P_a \left(E \otimes E\right) P_a = P_a \left(E \otimes E\right) = \left(E \otimes E\right) P_a, \tag{4.11}$$

where $E \in \mathcal{L}\left(\mathcal{H}\right)$ is a self-adjoint operator, which is completely described by $D_{(1)}$. In order to obtain $E\left(D_{(1)}\right)$, we start from equation (4.6), from which we get

$$D^{\mathrm{u}}_{(2)\nu\rho\rho'\nu'} = \frac{1}{2}\left(E_{\rho\rho'}E_{\nu\nu'} - E_{\rho\nu'}E_{\nu\rho'}\right), \tag{4.12}$$

and thus

$$\left(\mathrm{Tr}_1\left(D^{\mathrm{u}}_{(2)}\right)\right)_{\rho\rho'} = \sum_{\nu} D^{\mathrm{u}}_{(2)\nu\rho\rho'\nu} = \frac{1}{2}\left(\mathrm{Tr}\left(E\right)E - E^2\right)_{\rho\rho'} = D_{(1)\rho\rho'}$$

or

$$\frac{1}{2}\left(\mathrm{Tr}\left(E\right)E - E^2\right) = D_{(1)}. \tag{4.13}$$

The solution of equation (4.13) is given by

$$\begin{aligned} E &= \frac{1}{2}\mathrm{Tr}\left(E\right)\mathbb{1} \pm \sqrt{\frac{1}{4}\left(\mathrm{Tr}\left(E\right)\right)^2\mathbb{1} - 2D_{(1)}} \\ &= \frac{\mathrm{Tr}\left(E\right)}{2}\left(\mathbb{1} \pm \sqrt{\mathbb{1} - \frac{8D_{(1)}}{\left(\mathrm{Tr}\left(E\right)\right)^2}}\right). \end{aligned}$$

The solution with the + sign is not of interest, since it corresponds to $\mathrm{Tr}\left(E\right) = \infty$. We are thus left with

$$E = \frac{\mathrm{Tr}\left(E\right)}{2}\left(\mathbb{1} - \sqrt{\mathbb{1} - \frac{8D_{(1)}}{\left(\mathrm{Tr}\left(E\right)\right)^2}}\right). \tag{4.14}$$

The Taylor expansion around $x = 0$ of the function

$$1 - \sqrt{1-x} = \sum_n a_n \frac{x^n}{n!}$$

has the convergence radius 1. The coefficients are given by

$$a_n = \begin{cases} \frac{1}{2} & n = 1 \\ \frac{1}{2}\frac{(2n-3)!!}{2^{n-1}} & n \geq 2. \end{cases}$$

We thus have

$$\begin{aligned} E &= \frac{\mathrm{Tr}\left(E\right)}{2}\sum_{n=1}^{\infty} a_n \frac{1}{n!}\frac{8{D_{(1)}}^n}{\left(\mathrm{Tr}\left(E\right)\right)^{2n}} \\ &= \frac{\mathrm{Tr}\left(E\right)}{2}\left(\frac{4D_{(1)}}{\left(\mathrm{Tr}\left(E\right)\right)^2} + \sum_{n=2}^{\infty}\frac{(2n-3)!!}{n!}\left(\frac{4D_{(1)}}{\left(\mathrm{Tr}\left(E\right)\right)^2}\right)^n\right). \end{aligned} \tag{4.15}$$

Taking the trace of the above expression, we get

$$\frac{4T_1}{\left(\mathrm{Tr}\,(E)\right)^2} + \sum_{n=2}^{\infty} \frac{(2n-3)!!}{n!} \left(\frac{4^n T_n}{(\mathrm{Tr}\,(E))^{2n}} \right) = 2, \tag{4.16}$$

with

$$T_n = \mathrm{Tr}\left(\left(D_{(1)} \right)^n \right).$$

Equations (4.14) or (4.15) and (4.16) show that the operator E is uniquely determined by $D_{(1)}$. In the following we will consider the case of large N. Then the normalization equation (4.8) and the fact that in the eigenbasis of $D_{(1)}$ we have

$$D_{(1)\nu\nu} \leq \frac{1}{N},$$

imply $T_n \ll 1$ and $T_n \ll T_{n-1}$ for $n = 2, \ldots, \infty$. Accordingly, equations (4.15) and (4.16) yield

$$\begin{aligned} \mathrm{Tr}\,(E) &\approx \sqrt{2}, \\ E &\approx \sqrt{2} D_{(1)}. \end{aligned} \tag{4.17}$$

Obviously, any two-particle density matrix $D_{(2)}$ consistent with a given one-particle density matrix $D_{(1)}$ can be decomposed as

$$D_{(2)} = D^{\mathrm{u}}_{(2)} + \eta_{(2)}, \tag{4.18}$$

where the "uncorrelated two-particle density matrix"

$$D^{\mathrm{u}}_{(2)} = D^{\mathrm{u}}_{(2)} \left[D_{(1)} \right]$$

is a unique functional of $D_{(1)}$, and where $\eta_{(2)}$ describes the inter-particle correlations. The matrix elements of the two-body operators $D^{\mathrm{u}}_{(2)}$ and $\eta_{(2)}$ satisfy the symmetry relations (3.13). Both operators commute with the projector P_a (see also equation (4.11)). Since the condition (4.9) is already satisfied by the uncorrelated two-particle density operator $D^{\mathrm{u}}_{(2)}$, we have

$$\mathrm{Tr}_1\left(\eta_{(2)}\right) = 0, \qquad \mathrm{Tr}_2\left(\eta_{(2)}\right) = 0.$$

From equations (4.11) and (4.18) we get

$$\begin{aligned} D_{(2)} &= \left(E \otimes E + \eta_{(2)} \right) P_a \\ &= \left(E \otimes E \right) P_a + \eta_{(2)}. \end{aligned} \tag{4.19}$$

4.1.2 Evolution of the two-particle density matrix

Let us now consider the evolution of a weakly interacting electronic system of metallic density confined to a finite volume. Excluding here the interaction with supplementary bath subsystems, we can simplify the notation and replace

$$\begin{aligned} D_A^{(1)}(t) &\rightarrow D^{(1)}(t), \\ D_A^{(2)}(t) &\rightarrow D^{(2)}(t), \\ H_A^{(1)} &\rightarrow H^{(1)}, \\ \mathcal{H}_{\mathrm{A}} &\rightarrow \mathcal{H}. \end{aligned}$$

For a closed N-electron system the evolution of the two-particle density operator is given by the von Neumann equation, i.e., it is given by the first term on the right-hand side of equation (3.16),

$$\frac{d}{dt} D^{(2)}_{\rho\mu\mu'\rho'} = \frac{1}{2}\mathrm{Tr}\left(c_\rho c_\mu \frac{i}{\hbar}\left[D_{(N)}(t), H \right] c^+_{\mu'} c^+_{\rho'} \right). \tag{4.20}$$

Following the arguments given at the end of chapter 3, we will introduce a memory loss in the above two-particle evolution. In this way we phenomenologically account for the interaction of the electronic system with an external statistical environment, leading to an irreversible evolution. We suppose that the mean value of the total energy is conserved, but that – on the scale of the finite memory time introduced by the electronic environment – electronic two-particle correlations generated by the electron-electron interaction in the solid are destroyed, so that correlations of higher order become irrelevant for the evolution on short time scales. Density operators $D^{(n)}, n > 2$ are then uniquely determined by $D^{(1)}$ and $D^{(2)}$, so that the BBGKY hierarchy of equations starting from equation (3.23) can be truncated at the level of $n = 2$.

As in the previous section, we will use the density matrices $D_{(n)}$ normalized to 1 rather than the density operators $D^{(n)}$. Since both differ only by a numerical factor, it is clear that under our present assumptions the density matrices $D_{(n)}, n > 2$ are also completely determined by $D_{(1)}$ and $D_{(2)}$. Furthermore, equation (4.10) implies that the evolution of $D_{(1)}$ is determined by the evolution of $D_{(2)}$. The influence of the density matrices $D_n(t) = D_n\left[D_{(1)}(t), D_{(2)}(t)\right]$ with $n > 2$ is contained in the effective interaction Hamiltonian $H_{\mathrm{int}}(t)$, which represents the screened (or "effective") two-particle interaction in the many-particle system. For our weakly excited systems, the time dependence of $H_{\mathrm{int}}(t)$ stemming from the, in principle, time-dependent screening of the evolving two-particle interaction in the many-particle system, is very small and can be neglected for our present considerations. The evolution of the two-particle density matrix in the Schrödinger picture over time intervals much smaller than the memory time is then described by the von Neumann equation (4.20). Expressed in the two-particle

space and with equation (4.7), this equation reads

$$\frac{d}{dt}D_{(2)}(t) = \frac{i}{\hbar}\left[D_{(2)}(t), H_0^{(2)} + H_{\text{int}}\right], \tag{4.21}$$

where

$$H_0^{(2)} = H_0^{(1)} \otimes \mathbf{1} + \mathbf{1} \otimes H_0^{(1)}$$

represents the non-interacting part of the two-particle Hamiltonian. In order to extract the influence of the interaction on the evolution of $D_{(2)}(t)$, we switch to the interaction picture, which corresponds to the unitary transformation

$$(D_{(2)})^I(t) = e^{\frac{i}{\hbar}H_0^{(2)}t} D_{(2)}(t) e^{-\frac{i}{\hbar}H_0^{(2)}t}. \tag{4.22}$$

Equations (4.21) and (4.22) imply

$$\frac{d}{dt}\left(D_{(2)}\right)^I(t) = \frac{i}{\hbar}\left[\left(D_{(2)}\right)^I(t), H_{\text{int}}^I(t)\right]. \tag{4.23}$$

Using equations (4.17) and (4.19) as well as the fact that the operators H_0, $H_{\text{int}}^I(t)$, $\eta_{(2)}$ and $D_{(1)} \otimes D_{(1)}$ commute with the operator P_a (see for example equation (4.11)), we can rewrite equation (4.23) in the form

$$\begin{aligned}
&\frac{d}{dt}\left((D_{(2)}^{\text{u}})^I(t) + \eta_{(2)}^I(t)\right) \\
&\quad = \frac{i}{\hbar}\left[\left(D_{(1)}\right)^I(t) \otimes \left(D_{(1)}\right)^I(t) + \eta_{(2)}^I(t), H_{\text{int}}^I(t)\, P_a\right] \\
&\quad \approx \frac{2i}{\hbar}\left[\left(D_{(1)}\right)^I(t) \otimes \left(D_{(1)}\right)^I(t), \tilde{H}_{\text{int}}^I(t)\right] + \frac{i}{\hbar}\left[\eta_{(2)}^I(t), \tilde{H}_{\text{int}}^I(t)\right]
\end{aligned} \tag{4.24}$$

with

$$\tilde{H}_{\text{int}}^I(t) = H_{\text{int}}^I(t)\, P_a. \tag{4.25}$$

Being symmetric with respect to the particle exchange, $\tilde{H}_{\text{int}}$ can be decomposed as

$$\tilde{H}_{\text{int}} = \sum_\alpha A_\alpha \otimes A_\alpha, \tag{4.26}$$

where the operators A_α are either self-adjoint or anti-self-adjoint

We will give the explicit form of the new operators A_α. The interaction operator acting in $\mathcal{H}^{\otimes 2}$ may be written in the form

$$H_{\text{int}} = \sum_\kappa I_\kappa \otimes I_\kappa, \qquad \kappa = 1, 2, \cdots.$$

In the following we will show that the interaction operator $\tilde{H}_{int}$ including the projector P_a on the anti-symmetric subspace $\mathcal{H}^{\wedge 2}$ may be written in the form (4.26), i.e.,

$$\tilde{H}_{\rm int} = H_{\rm int} P_a = \sum_\alpha A_\alpha \otimes A_\alpha \tag{4.27}$$

For this purpose we first rewrite the operator P_a given in equation (4.1) in the form

$$P_a = \sum_{\rho\nu} \frac{1}{2} \left(|\rho)(\rho| \otimes |\nu)(\nu| - |\nu)(\rho| \otimes |\rho)(\nu| \right)$$

to express it in the symmetric form

$$P_a = \frac{1}{2} \left(\mathbb{1} \otimes \mathbb{1} + \sum_{\nu\rho} S_{1,\nu\rho} \otimes S_{1,\nu\rho} + \sum_{\nu\rho} S_{2,\nu\rho} \otimes S_{2,\nu\rho} \right). \tag{4.28}$$

with

$$\begin{aligned} S_{1,\nu\rho} &= \frac{i}{2} \left(|\nu)(\rho| + |\rho)(\nu| \right), \\ S_{2,\nu\rho} &= \frac{1}{2} \left(|\nu)(\rho| - |\rho)(\nu| \right). \end{aligned}$$

The vectors $|\nu)$, $\nu = 1, 2, \ldots$, form an orthonormal basis in $\mathcal{H}$. From equations (4.27) and (4.28) we obtain

$$\begin{aligned} \tilde{H}_{int} &= \frac{1}{2} \left(\sum_\kappa I_\kappa \otimes I_\kappa \right) \left(\sum_{\rho\nu} S_{1,\nu\rho} \otimes S_{1,\nu\rho} + \sum_{\nu\rho} S_{2,\nu\rho} \otimes S_{2,\nu\rho} \right) \\ &= \frac{1}{2} \left(\sum_\kappa I_\kappa \otimes I_\kappa + \sum_{\kappa\nu\rho} I_\kappa S_{1,\nu\rho} \otimes I_\kappa S_{1,\nu\rho} + \sum_{\kappa\nu\rho} I_\kappa S_{2,\nu\rho} \otimes I_\kappa S_{2,\nu\rho} \right) \\ &= \sum_{\alpha=\{\kappa\nu\rho s\}} A_\alpha \otimes A_\alpha, \quad \kappa, \nu, \rho = 1, 2, \cdots, \quad s = 0, 1, 2 \end{aligned}$$

with

$$A_\alpha = A_{\{\kappa\nu\rho s\}} = \frac{1}{\sqrt{2}} I_\kappa \left(\delta_{\nu 1} \delta_{\rho 1} \delta_{s0} + S_{1,\nu\rho} \delta_{s1} + S_{2,\nu\rho} \delta_{s2} \right).$$

In the following we will only use the compact form of the interaction Hamiltonian, given in equation (4.26).

4.1.3 Evolution of the one-particle density matrix

We determine the evolution of the one-particle density matrix $\left(D_{(1)}\right)^I(t)$, which is driven by the interaction operator $\tilde{H}_{\text{int}}$ given by equation (4.26). By evaluating the trace over the one-particle space in the second position and using the normalization of $D_{(1)}$ (4.8) and the relation between $D_{(2)}$ and $D_{(1)}$ (4.10), we get from the evolution of $D_{(2)}$ (4.24)

$$\begin{aligned} &\frac{d}{dt}\left(D_{(1)}\right)^I(t) \\ &= \frac{2i}{\hbar}\left[\left(D_{(1)}\right)^I(t), \sum_\alpha A^I_\alpha(t)\, a_\alpha\left[D_{(1)}(t)\right]\right] + \frac{i}{\hbar}\sum_\alpha\left[\eta^I_{(1)\alpha}(t), A^I_\alpha(t)\right] \end{aligned} \tag{4.29}$$

with

$$a_\alpha\left[D_{(1)}(t)\right] = \mathrm{Tr}_1\left((D_{(1)})^I(t)A^I_\alpha(t)\right) = \mathrm{Tr}_1\left(D_{(1)}(t)A_\alpha(t)\right)$$

and

$$\begin{aligned} \eta^I_{(1)\alpha}(t) &= \mathrm{Tr}_1\left(\eta^I_{(2)}(t)\left(\mathbf{1}\otimes A^I_\alpha(t)\right)\right) \\ &= \left(\mathrm{Tr}_1\left(\eta_{(2)}\left(\mathbf{1}\otimes A_\alpha\right)\right)\right)^I(t), \end{aligned}$$

where $\mathrm{Tr}_1\left(O^I_{(2)}(t)\left(\mathbf{1}\otimes A^I_\alpha(t)\right)\right)$ denotes the one-body operator that is obtained by evaluating the trace of the two-body operator $O^I_{(2)}(t)\left(\mathbf{1}\otimes A^I_\alpha(t)\right)$ over the one-particle space in the second position.

The first term on the right-hand side of equation (4.29), which represents the linear contribution of the interaction on the evolution of $\left(D_{(1)}\right)^I(t)$, can be eliminated by an adequate redefinition of the operators A_α and H_0. In fact, the total Hamiltonian $H^{(2)}$ can be rewritten as

$$\begin{aligned} H^{(2)} &= H^{(2)}_0 + \tilde{H}_{\text{int}} \\ &= H^{(1)}_0\otimes\mathbf{1} + \mathbf{1}\otimes H^{(1)}_0 + \tilde{H}_{\text{int}} \\ &= \left(H^{(1)}_0 + \sum_\alpha g_\alpha(t)A_\alpha\right)\otimes\mathbf{1} + \mathbf{1}\otimes\left(H^{(1)}_0 + \sum_\alpha g_\alpha(t)A_\alpha\right) \\ &\quad + \sum_\alpha\left(\left(A_\alpha - g_\alpha(t)\,\mathbf{1}\right)\otimes\left(A_\alpha - g_\alpha(t)\,\mathbf{1}\right)\right)P_a \\ &\quad - g_\alpha(t)^2\left(\mathbf{1}\otimes\mathbf{1}\right)P_a, \end{aligned}$$

where $g_\alpha(t)$ is an arbitrary function of time. The last term does not enter the dynamics, since it commutes with any operator in $\mathcal{L}(\mathcal{H}^{\otimes 2})$. It will thus be omitted in what follows. Now, choosing

$$g_\alpha(t) = a_\alpha[D_{(1)}(t)], \tag{4.30}$$

and

$$\hat{H}_0^{(1)}(t) = H_0^{(1)} + \sum_\alpha g_\alpha(t) A_\alpha, \tag{4.31}$$

$$\hat{A}_\alpha(t) = A_\alpha - g_\alpha(t)\mathbf{1}, \tag{4.32}$$

we get

$$\hat{a}_\alpha \left[D_{(1)}(t)\right] = \mathrm{Tr}_1 \left(D_{(1)}(t)\hat{A}_\alpha(t)\right) = \mathrm{Tr}_1 \left(D_{(1)}(t)\left(A_\alpha - g_\alpha(t)\mathbf{1}\right)\right) = 0.$$

From now on we will adopt the Hamiltonian in its new form

$$H^{(2)}(t) = \hat{H}_0^{(1)}(t) \otimes \mathbf{1} + \mathbf{1} \otimes \hat{H}_0^{(1)}(t) + \hat{H}_{\mathrm{int}}(t),$$

where the modified one-particle Hamiltonian $\hat{H}_0^{(1)}(t)$ is given by equations (4.30) and (4.31). The operators $\hat{A}_\alpha(t)$ appearing in the modified interaction Hamiltonian

$$\hat{H}_{\mathrm{int}}(t) = \sum_\alpha \hat{A}_\alpha(t) \otimes \hat{A}_\alpha(t), \tag{4.33}$$

are given by equations (4.30) and (4.32).

Time dependence of the modified Hamiltonian and the interaction picture

In contrast to the old Hamiltonian $H_0^{(1)}$, the modified Hamiltonian $\hat{H}_0^{(1)}(t)$ is time dependent. This time dependency is introduced by the function $g_\alpha(t) = \mathrm{Tr}_1 \left(D_{(1)}(t)A_\alpha\right)$ (see equation (4.31)), which scales with the interaction. As shown in [1], the coarse-graining procedure requires that the interaction between the bathed system and the bath is weak enough, so that the correlation time is much smaller than the evolution time of the bathed system (see equation (2.15)). The evolution time decreases with increasing interaction strength. Let us look at the eigenvalues of the two operators $H_0^{(1)}$ and $\hat{H}_0^{(1)}(t)$. In figure 4.1 a schematic time behavior of an arbitrary eigenvalue of $H_0^{(1)}$ and of $\hat{H}_0^{(1)}(t)$ is shown. The eigenvalue of $H_0^{(1)}$ is constant in time (grey line), while the eigenvalue of $\hat{H}_0^{(1)}(t)$ fluctuates (solid black line). For the supposed weak interaction strength, the eigenvalue of $\hat{H}_0^{(1)}(t)$ fluctuates with a small amplitude. During a time interval Δt we can attribute the amplitude I_{int} to the evolution of the eigenvalue of $\hat{H}_0^{(1)}(t)$. Over the time interval $\Delta t = t - t_0$, the Hamiltonian $\hat{H}_0^{(1)}$ can be assumed to be represented by $\hat{H}_0^{(1)}(t_0)$, i.e.,

$$\hat{H}_0^{(1)}(t') = \hat{H}_0^{(1)}(t_0), \ \forall\ t' \in \Delta t. \tag{4.34}$$

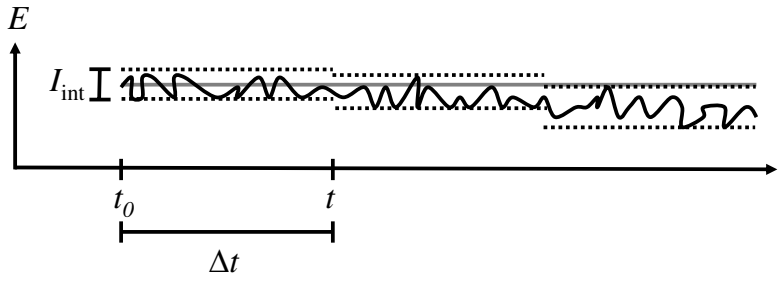

Figure 4.1: Schematic time behaviour of an arbitrary eigenvalue of $H_0^{(1)}$ and the corresponding eigenvalue of $\hat{H}_0^{(1)}(t)$. The eigenvalue of $H_0^{(1)}$ is represented by the grey line. The eigenvalue of $\hat{H}_0^{(1)}(t)$ is represented by the solid black line. The amplitude of the oscillations of the eigenvalue of $\hat{H}_0^{(1)}(t)$ during a time interval Δt is called I_{int}. The time interval $\Delta t = t - t_0$ over which the Hamiltonian can be assumed to be constant, is indicated.

The operators in the *local* interaction picture[1] $\left(O^{(1)}\right)^{\hat{I}}(t)$, are given by

$$\left(O^{(1)}\right)^{\hat{I}}(t) = e^{\frac{i}{\hbar}\hat{H}_0^{(1)}(t_0)t} O^{(1)}(t_0) e^{-\frac{i}{\hbar}\hat{H}_0^{(1)}(t_0)t}, \ \forall\ t \in \Delta t.$$

The time dependence of the operators $\hat{H}_{\text{int}}$, $\hat{A}_\alpha$ and $\hat{H}_0^{(1)}$ in the Schrödinger representation is not explicitly noted in the following expressions. We will see later not only that this dependence is negligible (see also the remark at the beginning of subsection 4.1.2), but also that it has no influence on the evolution of the coarse grained one-particle density matrix. Expressed in terms of $\hat{H}_0^{(1)}$ and $\hat{A}_\alpha$ given by equations (4.31) and (4.32), equation (4.29) becomes

$$\frac{d}{dt}\left(D_{(1)}\right)^{\hat{I}}(t) \;=\; \frac{i}{\hbar}\sum_\alpha \left[\eta_{(1)\alpha}^{\hat{I}}(t), \hat{A}_\alpha^{\hat{I}}(t)\right], \tag{4.35}$$

where the superscript $\hat{I}$ denotes the interaction representation referring to the Hamiltonian $\hat{H}_0^{(2)} = \hat{H}_0^{(1)} \otimes \mathbf{1} + \mathbf{1} \otimes \hat{H}_0^{(1)}$. The term

$$\hat{\eta}_{(1)\alpha}^{\hat{I}}(t) \;=\; \mathrm{Tr}_1\left(\eta_{(2)}^{\hat{I}}(t)\left(\mathbf{1} \otimes \hat{A}_\alpha^{\hat{I}}(t)\right)\right) \tag{4.36}$$

will be calculated from equation (4.24), which can be rewritten in the form

$$\begin{aligned}\frac{d}{dt}\eta_{(2)}^{\hat{I}}(t) \;=\; & \frac{2i}{\hbar}\left[\left(D_{(1)}\right)^{\hat{I}}(t) \otimes \left(D_{(1)}\right)^{\hat{I}}(t), \hat{H}_{\text{int}}^{\hat{I}}(t)\right] \\ & + \frac{i}{\hbar}\left[\eta_{(2)}^{\hat{I}}(t), \hat{H}_{\text{int}}^{\hat{I}}(t)\right] - 2P_a \frac{d}{dt}\left(D_{(1)}^{\hat{I}}(t) \otimes D_{(1)}^{\hat{I}}(t)\right).\end{aligned} \tag{4.37}$$

[1] Local means here local in time.

4.2 Evolution of the coarse grained one-particle density matrix

Starting from equations (4.35) and (4.37), we calculate the evolution of the one-particle density matrix $(D_{(1)})^{\hat{I}}(t)$ in a time interval $t_0 \leq t < t_0 + \Delta t$, assuming that the two-particle density-matrix at some prior time $t_{00} \ll t_0$ is given by

$$(D_{(2)})^{\hat{I}}(t_{00}) = 2P_a \left((D_{(1)})^{\hat{I}}(t_{00}) \otimes (D_{(1)})^{\hat{I}}(t_{00}) \right) P_a + \eta^{\hat{I}}_{(2)}(t_{00}). \qquad (4.38)$$

We further assume that the evolution of the one-particle density matrix is driven only by the electron-electron interaction.

From now on we choose sufficiently small time intervals Δt, so that the evolution of $D_{(1)}{}^{\hat{I}}(t)$ can be described by terms up to the second order in the interaction. For the moment we restrict ourselves to terms that are *formally* of second order. It should be kept in mind, however that - due to the time dependence of the source terms, which is a consequence of the interaction itself - the derived expression implicitly contains terms of higher order. These higher-order contributions will be eliminated in the subsequent coarse-graining procedure where we will keep only true second-order terms.

Integration of equations (4.35) yields

$$\left(D_{(1)}\right)^{\hat{I}}(t) = \left(D_{(1)}\right)^{\hat{I}}(t_0) + \frac{i}{\hbar} \int_{t_0}^{t} dt' \sum_{\alpha} \left[\hat{\eta}^{\hat{I}}_{(1)\alpha}(t'), \hat{A}^{\hat{I}}_{\alpha}(t') \right]. \qquad (4.39)$$

According to the above restriction to terms of second-order we need the first-order contribution to $\eta^{\hat{I}}_{(2)}(t)$. From equation (4.37) we obtain

$$\begin{aligned} \eta^{\hat{I}}_{(2)}(t) \;=\; & \eta^{\hat{I}}_{(2)}(t_0) + \frac{2i}{\hbar} \int_{t_0}^{t} dt' \left[(D_1)^{\hat{I}}(t') \otimes (D_1)^{\hat{I}}(t'), \hat{H}^{\hat{I}}_{\mathrm{int}}(t') \right] \qquad (4.40) \\ & + \frac{i}{\hbar} \int_{t_0}^{t} dt' \left[\eta^{\hat{I}}_{(2)}(t'), \hat{H}^{\hat{I}}_{\mathrm{int}}(t') \right] \\ & - 2P_a \left((D_1)^{\hat{I}}(t) \otimes (D_1)^{\hat{I}}(t) - (D_1)^{\hat{I}}(t_0) \otimes (D_1)^{\hat{I}}(t_0) \right) \\ & + \cdots . \end{aligned}$$

This expression must be inserted into equation (4.36) to obtain $\hat{\eta}^{\hat{I}}_{(1)\alpha}(t')$, which appears in equation (4.39). Presently we admit only for correlations $\eta^{\hat{I}}_{(2)}(t)$ generated by the interaction. It is easily seen that under this condition the third term on the right-hand side of equation (4.40) can be omitted, since in equation (4.39) it leads to a contribution that is at least of third order in the interaction. The first term $\hat{\eta}^{\hat{I}}_{(2)\alpha}(t_0)$ and the second term give rise to a contribution that is at least of second order and must therefore be kept.

Let us now consider the last term in equation (4.40). Clearly, its first non-vanishing contributions would be given by first-order contributions to $\left(D_{(1)}\right)^{\hat{I}}(t)$, which again would give rise to second-order terms in equation (4.39). However, since also none of the other terms in equation (4.40) can generate first-order contributions to $\left(D_{(1)}\right)^{\hat{I}}(t)$, this situation cannot occur, so that the last term in equation (4.40) is never activated. We can therefore omit this term without loss of generality, and restrict to

$$\begin{aligned}\eta^{\hat{I}}_{(2)}(t) &= \eta^{\hat{I}}_{(2)}(t_0) + \frac{2i}{\hbar}\int_{t_0}^{t} dt' \left[(D_1)^{\hat{I}}(t') \otimes (D_1)^{\hat{I}}(t'), \hat{H}^{\hat{I}}_{\rm int}(t') \right] \\ &\quad +\mathcal{O}(2).\end{aligned} \tag{4.41}$$

With the replacements $t \to t_0$ and $t_0 \to t_{00}$ we get in the same approximation

$$\begin{aligned}\eta^{\hat{I}}_{(2)}(t_0) &= \eta^{\hat{I}}_{(2)}(t_{00}) + \frac{2i}{\hbar}\int_{t_{00}}^{t_0} dt' \left[(D_1)^{\hat{I}}(t') \otimes (D_1)^{\hat{I}}(t'), \hat{H}^{\hat{I}}_{\rm int}(t') \right] \\ &\quad +\mathcal{O}(2).\end{aligned} \tag{4.42}$$

From equation (4.41) and using the decomposition equation (4.33) we find

$$\begin{aligned}&\hat{\eta}^{\hat{I}}_{(1)\alpha}(t') = \\ &{\rm Tr}_1\left(\left(\eta^{\hat{I}}_{(2)}(t_0)\left(\mathbf{1}\otimes\hat{A}^{\hat{I}}_{\alpha}(t')\right)\right)\right) \\ &\quad +\frac{2i}{\hbar}\int_{t_0}^{t'} dt''{\rm Tr}_1\left(\left[\left(D_{(1)}\right)^{\hat{I}}(t'')\otimes\left(D_{(1)}\right)^{\hat{I}}(t''), \hat{H}^{\hat{I}}_{\rm int}(t'')\right]\left(\mathbf{1}\otimes\hat{A}^{\hat{I}}_{\alpha}(t')\right)\right) \\ &\quad +\mathcal{O}(2) \\ &= {\rm Tr}_1\left(\eta_{(2)}{}^{\hat{I}}(t_0)\left(\mathbf{1}\otimes\hat{A}^{\hat{I}}_{\alpha}(t')\right)\right) \\ &\quad +\frac{2i}{\hbar}\sum_{\beta}\int_{t_0}^{t'} dt''{\rm Tr}_1\left(\left[\left(D_{(1)}\right)^{\hat{I}}(t'')\otimes\left(D_{(1)}\right)^{\hat{I}}(t''), \hat{A}^{\hat{I}}_{\beta}(t'')\otimes\hat{A}^{\hat{I}}_{\beta}(t'')\right]\left(\mathbf{1}\otimes\hat{A}^{\hat{I}}_{\alpha}(t')\right)\right) \\ &\quad +\mathcal{O}(2),\end{aligned}$$

which can be rewritten as

$$\begin{aligned}&\hat{\eta}^{\hat{I}}_{(1)\alpha}(t') = \\ &\quad {\rm Tr}_1\left(\eta^{\hat{I}}_{(2)}(t_0)\left(\mathbf{1}\otimes\hat{A}^{\hat{I}}_{\alpha}(t')\right)\right) \\ &\quad +\frac{i}{\hbar}\sum_{\beta}\int_{t_0}^{t'} dt''\left(\left(D_{(1)}\right)^{\hat{I}}(t'')\hat{A}^{\hat{I}}_{\beta}(t'')a_{\beta\alpha}(t'',t'',t') - \hat{A}^{\hat{I}}_{\beta}(t'')\left(D_{(1)}\right)^{\hat{I}}(t'')a_{\alpha\beta}(t'',t',t'')\right) \\ &\quad +\mathcal{O}(2)\end{aligned} \tag{4.43}$$

with

$$a_{\alpha\beta}(t,t',t'') = 2{\rm Tr}\left(\left(D_{(1)}\right)^{\hat{I}}(t)\hat{A}^{\hat{I}}_{\alpha}(t')\hat{A}^{\hat{I}}_{\beta}(t'')\right). \tag{4.44}$$

The operators $D_{(1)}$ are self-adjoint, whereas the operators $\hat{A}_\alpha$ are either adjoint or anti-adjoint. We thus obtain the symmetry relations

$$a_{\alpha\beta}(t,t',t'') = a_{\beta\alpha}(t,t'',t')^\star.$$

After insertion of equation (4.43) into equation (4.39) we obtain for the evolution of the one-particle density matrix

$$\begin{aligned}
&\left(D_{(1)}\right)^{\hat{I}}(t) = \qquad (4.45)\\
&\left(D_{(1)}\right)^{\hat{I}}(t_0) + \left(\frac{i}{\hbar}\int_{t_0}^{t} dt' \sum_\alpha \left[\mathrm{Tr}_1\left(\eta_{(2)}^{\hat{I}}(t_0)\left(\mathbf{1}\otimes\hat{A}_\alpha^{\hat{I}}(t')\right)\right), \hat{A}_\alpha^{\hat{I}}(t')\right]\right)\\
&\quad + \left(\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \left[\sum_{\alpha\beta}\left(\left(D_{(1)}\right)^{\hat{I}}(t'')\hat{A}_\beta^{\hat{I}}(t'')a_{\beta\alpha}(t'',t'',t')\right.\right.\\
&\qquad\qquad \left.\left. -\hat{A}_\beta^{\hat{I}}(t'')\left(D_{(1)}\right)^{\hat{I}}(t'')a_{\alpha\beta}(t'',t',t'')\right), \hat{A}_\alpha^{\hat{I}}(t')\right].
\end{aligned}$$

The above expression describes the evolution of the one-particle density matrix $\left(D_{(1)}\right)^{\hat{I}}(t)$ in the time interval $t_0 \le t < t_0+\Delta t$ up to formal second order in the interaction and for the initial condition (4.38). It is expressed in terms of the functions $a_{\alpha\beta}(.,.,.)$ defined in equation (4.44) and of $\eta_{(2)}^{\hat{I}}(t_0)$. Presently, our aim is to describe the evolution of the one-particle density matrix $\left(D_{(1)}\right)^{\hat{I}}(t)$ in a situation where – due to the weak interaction with the environment – the system loses memory over the time interval $[t_{00}, t_0]$, without changing its energy. Thus, looking back from the situation at time t_0 to the situation at time t_{00}, we have to average over all electronic configurations corresponding to

$$\left(D_{(1)}\right)^{\hat{I}}(t_{00}) = \left(D_{(1)}\right)^{\hat{I}}(t_0), \qquad (4.46)$$

but with different two-particle correlations $\eta_{(2)}^{\hat{I}}(t_{00})$, which are compatible with the energy of the electronic system. The condition (4.46) accounts for the fact that the time dependence of $\left(D_{(1)}\right)^{\hat{I}}(t)$ is itself due to the interaction Hamiltonian $\hat{H}_{\mathrm{int}}^{\hat{I}}(t)$. Its inclusion in equation (4.42) would therefore correspond to contributions of higher than first order in the interaction. These contributions are excluded in our present approach, since in equation (4.45) they give rise to terms, which are at least of third order in the interaction.

The contribution of the term $\eta_{(2)}^{\hat{I}}(t_{00})$ in equation (4.45)

$$\frac{i}{\hbar}\int_{t_0}^{t} dt' \sum_\alpha \left[\mathrm{Tr}_1\left(\eta_{(2)}^{\hat{I}}(t_{00})\left(\mathbf{1}\otimes\hat{A}_\alpha^{\hat{I}}(t')\right)\right), \hat{A}_\alpha^{\hat{I}}(t')\right]$$

must be averaged over all correlations $\eta^{\hat{I}}_{(2)}(t_{00})$ with

$$|\mathrm{Tr}_2\left(\eta^{\hat{I}}_{(2)}(t_{00})\hat{H}^{\hat{I}}_{\mathrm{int}}(t_0)\right)| < dE, \tag{4.47}$$

where dE denotes an infinitesimal energy. According to equation (4.45), this contribution is linear in $\eta^{\hat{I}}_{(2)}(t_{00})$. Thus, since all electronic configurations corresponding to different $\eta^{\hat{I}}_{(2)}(t_{00})$ compatible with equation (4.47) possess equal statistical weight, they cancel out under the configurational average. This corresponds to the choice

$$\eta^{\hat{I}}_{(2)}(t_{00}) = 0 \tag{4.48}$$

in equation (4.42).

Let us recall that the above presumed ability of the electronic system to explore the configurations corresponding to all admissible $\left(D_{(2)}\right)^{\hat{I}}(t_{00})$ for fixed $D^{\hat{I}}_{(1)}(t_{00}) = D^{\hat{I}}_{(1)}(t_0)$ or[2], correspondingly, to all admissible $\eta^{\hat{I}}_{(2)}(t_{00})$, results from its unavoidable (*non-dissipative*) coupling with the environment. It is this shuffling of the correlations $\eta_{(2)}$ of the electronic system driven by the external statistical environment, which leads to the loss of the long-time memory in the considered N-electron subsystem.

Inserting equation (4.42) into equation (4.45) and with the choice (4.48) we obtain

$$\begin{aligned}
&\left(D_{(1)}\right)^{\hat{I}}(t) \qquad\qquad (4.49)\\
&= \left(D_{(1)}\right)^{\hat{I}}(t_0) + \left(\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_{00}}^{t'} dt'' \\
&\qquad \left[\sum_{\alpha\beta}\left(\left(D_{(1)}\right)^{\hat{I}}(t'')\hat{A}^{\hat{I}}_{\beta}(t'')a_{\beta\alpha}(t'',t'',t')\right.\right.\\
&\qquad \left.\left.-\hat{A}^{\hat{I}}_{\beta}(t'')\left(D_{(1)}\right)^{\hat{I}}(t'')a_{\alpha\beta}(t'',t',t'')\right), \hat{A}^{\hat{I}}_{\alpha}(t')\right].
\end{aligned}$$

In order to proceed, we have to determine the time behavior of the functions $a_{\alpha\beta}(t,t',t'')$ defined in equation (4.44). Obviously, the time dependence of the operators $\hat{H}^{(1)}_0(t)$, $\hat{A}_\alpha(t)$ and $\left(D_{(1)}\right)^{\hat{I}}(t)$ is itself caused by the interaction. Since we treat the influence of the interaction Hamiltonian from hereon only up to strictly second order, all these operators must be kept independent of time on the right-hand side of equation (4.49), and thus can be evaluated at

[2]Note that the difference $D^{\hat{I}}_{(1)}(t_0) - D^{\hat{I}}_{(1)}(t_{00})$ is at least of first order in the perturbation. Its inclusion would thus give rise to terms of higher than second-order terms in the final expression for the evolution of $D^{\hat{I}}_{(1)}(t)$ in the interval $t_0 \le t \le t_0 + \Delta t$.

$t = t_0$. This justifies our previous omission of the time dependences in the Schrödinger picture (see the remark after equation (4.33)).

In the following we will assume

$$a_{\alpha\beta}(t_0, t, t') \approx 0 \qquad \text{for} \quad |t' - t| > \tau_{\text{corr}}, \tag{4.50}$$

so that the integrands in equation (4.49) depending on these functions vanish for time differences larger than τ_{corr}. This assumption is valid for electronic statistical states close to equilibrium and for interaction operators that couple single-particle states over a wide range of energies, as is the case for the screened Coulomb interaction. Due to equation (4.50), we can extend the integration interval in the second integral in equation (4.49) and replace the lower limit t_{00} by $-\infty$. This allows us to get rid of the unknown parameter t_{00}. We then get

$$\left(D_{(1)}\right)^{\hat{I}}(t) - \left(D_{(1)}\right)^{\hat{I}}(t_0) \;=\; \left(\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{-\infty}^{t'} dt'' J(t_0, t', t'') \tag{4.51}$$

with

$$\begin{aligned} J(t_0, t', t'') = \sum_{\alpha\beta} \Big[& \left(D_{(1)}\right)^{\hat{I}}(t_0) \hat{A}^{\hat{I}}_\beta(t'') a_{\beta\alpha}(t_0, t'', t') \\ & - \hat{A}^{\hat{I}}_\beta(t'') \left(D_{(1)}\right)^{\hat{I}}(t_0) a_{\alpha\beta}(t_0, t', t''), \hat{A}^{\hat{I}}_\alpha(t') \Big]. \end{aligned} \tag{4.52}$$

Inserting the definition (4.44) and expanding the commutator, we obtain

$$\begin{aligned} & J(t_0, t', t'') \\ & = 2 \sum_{\alpha\beta} \Big\{ \left(D_{(1)}\right)^{\hat{I}}(t_0) \hat{A}^{\hat{I}}_\beta(t'') \hat{A}^{\hat{I}}_\alpha(t') \mathrm{Tr} \left(\left(D_{(1)}\right)^{\hat{I}}(t_0) \hat{A}^{\hat{I}}_\beta(t'') \hat{A}^{\hat{I}}_\alpha(t') \right) \\ & \qquad - \hat{A}^{\hat{I}}_\alpha(t') \left(D_{(1)}\right)^{\hat{I}}(t_0) \hat{A}^{\hat{I}}_\beta(t'') \mathrm{Tr} \left(\left(D_{(1)}\right)^{\hat{I}}(t_0) \hat{A}^{\hat{I}}_\beta(t'') \hat{A}^{\hat{I}}_\alpha(t') \right) \\ & \qquad - \hat{A}^{\hat{I}}_\beta(t'') \left(D_{(1)}\right)^{\hat{I}}(t_0) \hat{A}^{\hat{I}}_\alpha(t') \mathrm{Tr} \left(\left(D_{(1)}\right)^{\hat{I}}(t_0) \hat{A}^{\hat{I}}_\alpha(t') \hat{A}^{\hat{I}}_\beta(t'') \right) \\ & \qquad + \hat{A}^{\hat{I}}_\alpha(t') \hat{A}^{\hat{I}}_\beta(t'') \left(D_{(1)}\right)^{\hat{I}}(t_0) \mathrm{Tr} \left(\left(D_{(1)}\right)^{\hat{I}}(t_0) \hat{A}^{\hat{I}}_\alpha(t') \hat{A}^{\hat{I}}_\beta(t'') \right) \Big\}. \end{aligned} \tag{4.53}$$

Using the fact that the trace over a product of operators is invariant with respect to cyclic permutations of the operators, we find

$$\mathrm{Tr}\left(J(t_0, t', t'')\right) = 0, \tag{4.54}$$

which implies that the trace of $D_{(1)}$ is conserved during the evolution described by equation (4.51).

Starting from equation (4.51), we will now calculate the evolution of the time-averaged density matrix

$$\left(\bar{D}_{(1)}\right)^{\hat{I}}(\bar{t}) = \frac{1}{\Delta t}\int_{t_0}^{t_0+\Delta t} dt' \left(D_{(1)}\right)^{\hat{I}}(t'), \qquad \bar{t} = t_0 + \frac{\Delta t}{2},\ \Delta t = t - t_0, \tag{4.55}$$

where the time interval Δt will be chosen later in such a way that the oscillations of $(D_1)^{\hat{I}}(t)$ are suppressed and only the linear contributions with respect to Δt are kept. For our convenience, we define

$$K(\bar{t}) = \frac{\left(\bar{D}_{(1)}\right)^{\hat{I}}(t_0+\Delta t) - \left(\bar{D}_{(1)}\right)^{\hat{I}}(t_0)}{\Delta t}. \tag{4.56}$$

In order to calculate the term $K(\bar{t})$, we first determine the matrix elements of the operator $J(t_0, t', t'')$ given by equation (4.53) in the eigenbasis $|\nu) \in \mathcal{H}$ of the one-particle Hamiltonian $\hat{H}_0^{(1)}$. Like in chapter 2, we introduce the frequencies

$$\omega_\nu = \frac{\epsilon_\nu}{\hbar}$$

corresponding to the eigenvalues ϵ_ν of the one-particle Hamiltonian $\hat{H}_0^{(1)}$, and the short-hand notation

$$\omega_{\nu\mu} = \omega_\nu - \omega_\mu$$

for the difference frequencies. With $t'' = t' - \tau$ we then get from equation (4.53)

$$\begin{aligned}(\nu|J(t_0,t',t'-\tau)|\mu) = 2\left(\frac{i}{\hbar}\right)^2 \sum_{\alpha\beta}\sum_{\gamma,\delta,\epsilon,\kappa,\lambda} \\ \Big\{ D^{\hat{I}}_{(1)\gamma\delta}(t_0)\hat{A}_{\beta,\delta\epsilon}(t_0)\hat{A}_{\alpha,\epsilon\gamma}(t_0)D^{\hat{I}}_{(1)\nu\kappa}(t_0)\hat{A}_{\beta,\kappa\lambda}(t_0)\hat{A}_{\alpha,\lambda\mu}(t_0)e^{i(\omega_{\kappa\mu}+\omega_{\delta\gamma})t'}e^{-i(\omega_{\kappa\lambda}+\omega_{\delta\epsilon})\tau} \\ -D^{\hat{I}}_{(1)\gamma\delta}(t_0)\hat{A}_{\beta,\delta\epsilon}(t_0)\hat{A}_{\alpha,\epsilon\gamma}(t_0)\hat{A}_{\alpha,\nu\kappa}(t_0)D^{\hat{I}}_{(1)\kappa\lambda}(t_0)\hat{A}_{\beta,\lambda\mu}(t_0)e^{i(\omega_{\nu\kappa}+\omega_{\lambda\mu}+\omega_{\delta\gamma})t'}e^{-i(\omega_{\delta\epsilon}+\omega_{\lambda\mu})\tau} \\ -D^{\hat{I}}_{(1)\gamma\delta}(t_0)\hat{A}_{\alpha,\delta\epsilon}(t_0)\hat{A}_{\beta,\epsilon\gamma}(t_0)\hat{A}_{\beta,\nu\kappa}(t_0)D^{\hat{I}}_{(1)\kappa\lambda}(t_0)\hat{A}_{\alpha,\lambda\mu}(t_0)e^{i(\omega_{\nu\kappa}+\omega_{\lambda\mu}+\omega_{\delta\gamma})t'}e^{-i(\omega_{\nu\kappa}+\omega_{\epsilon\gamma})\tau} \\ +D^{\hat{I}}_{(1)\gamma\delta}(t'')\hat{A}_{\alpha,\delta\epsilon}(t_0)\hat{A}_{\beta,\epsilon\gamma}(t_0)\hat{A}_{\alpha,\nu\kappa}(t_0)\hat{A}_{\beta,\kappa\lambda}(t_0)D^{\hat{I}}_{(1)\lambda\mu}(t_0)e^{i(\omega_{\nu\lambda}+\omega_{\delta\gamma})t'}e^{-i(\omega_{\kappa\lambda}+\omega_{\epsilon\gamma})\tau}\Big\}.\end{aligned} \tag{4.57}$$

With the corresponding change of the variable of integration $t'' \to t' - \tau$, the double integral in equation (4.51) becomes

$$\int_{t_0}^{t} dt' \int_{-\infty}^{t'} dt'' \cdots = \int_{t_0}^{t} dt' \int_{0}^{\infty} d\tau \cdots$$

With the relation

$$\int_{t_0}^{t} dt' e^{i\omega t'} = \Delta t \left(g\left(\omega \Delta t\right) e^{i\omega \bar{t}} \right),$$

where

$$g(x) = \frac{\sin\left(x/2\right)}{x/2},$$

we obtain from equations (4.51) and (4.57)[3]

$$\frac{(\nu|\left(D_1\right)^{\hat{I}}\left(t_0+\Delta t\right) - \left(D_1\right)^{\hat{I}}\left(t_0\right)|\mu)}{\Delta t} = 2\left(\frac{i}{\hbar}\right)^2 \sum_{\alpha\beta}\sum_{\gamma,\delta,\epsilon,\kappa,\lambda} \tag{4.58}$$

$$\Bigg\{ D^{\hat{I}}_{(1)\gamma\delta}(t_0)\hat{A}_{\beta,\delta\epsilon}(t_0)\hat{A}_{\alpha,\epsilon\gamma}(t_0)D^{\hat{I}}_{(1)\nu\kappa}(t_0)\hat{A}_{\beta,\kappa\lambda}(t_0)\hat{A}_{\alpha,\lambda\mu}(t_0)e^{i(\omega_{\kappa\mu}+\omega_{\delta\gamma})\bar{t}}$$

$$g\left((\omega_{\kappa\mu}+\omega_{\delta\gamma})\Delta t\right)\right) \int_0^\infty d\tau e^{-i(\omega_{\kappa\lambda}+\omega_{\delta\epsilon})\tau}$$

$$-D^{\hat{I}}_{(1)\gamma\delta}(t_0)\hat{A}_{\beta,\delta\epsilon}(t_0)\hat{A}_{\alpha,\epsilon\gamma}(t_0)\hat{A}_{\alpha,\nu\kappa}(t_0)D^{\hat{I}}_{(1)\kappa\lambda}(t_0)\hat{A}_{\beta,\lambda\mu}(t_0)e^{i(\omega_{\nu\kappa}+\omega_{\lambda\mu}+\omega_{\delta\gamma})\bar{t}}$$

$$g\left((\omega_{\nu\kappa}+\omega_{\lambda\mu}+\omega_{\delta\gamma})\Delta t\right)\right) \int_0^\infty d\tau e^{-i(\omega_{\delta\epsilon}+\omega_{\lambda\mu})\tau}$$

$$-D^{\hat{I}}_{(1)\gamma\delta}(t_0)\hat{A}_{\alpha,\delta\epsilon}(t_0)\hat{A}_{\beta,\epsilon\gamma}(t_0)\hat{A}_{\beta,\nu\kappa}(t_0)D^{\hat{I}}_{(1)\kappa\lambda}(t_0)\hat{A}_{\alpha,\lambda\mu}(t_0)e^{i(\omega_{\nu\kappa}+\omega_{\lambda\mu}+\omega_{\delta\gamma})\bar{t}}$$

$$g\left((\omega_{\nu\kappa}+\omega_{\lambda\mu}+\omega_{\delta\gamma})\Delta t\right)\right) \int_0^\infty d\tau e^{-i(\omega_{\nu\kappa}+\omega_{\epsilon\gamma})\tau}$$

$$+D^{\hat{I}}_{(1)\gamma\delta}(t'')\hat{A}_{\alpha,\delta\epsilon}(t_0)\hat{A}_{\beta,\epsilon\gamma}(t_0)\hat{A}_{\alpha,\nu\kappa}(t_0)\hat{A}_{\beta,\kappa\lambda}(t_0)D^{\hat{I}}_{(1)\lambda\mu}(t_0)e^{i(\omega_{\nu\lambda}+\omega_{\delta\gamma})\bar{t}}$$

$$g\left((\omega_{\nu\lambda}+\omega_{\delta\gamma})\Delta t\right)\right) \int_0^\infty d\tau e^{-i(\omega_{\kappa\lambda}+\omega_{\epsilon\gamma})\tau} \Bigg\}.$$

Choice of Δt

The frequencies appearing in the function g are the sum of difference frequencies $\omega_{\kappa\mu}+\omega_{\delta\gamma}$, $\omega_{\nu\kappa}+\omega_{\lambda\mu}+\omega_{\delta\gamma}$, and $\omega_{\nu\lambda}+\omega_{\delta\gamma}$. Let us abbreviate these sums in the following section by ω, and denote the largest value of these sums $\omega_{\max}$ and the smallest non-zero value of these sums $\Delta\omega$. The latter is of course finite for the here considered spatially confined systems, since we always have a minimum distance between the non-degenerate discrete eigenvalues of the Hamiltonian $\hat{H}_0^{(1)}$.

[3] In the following it is understood that the integrals $\int_{-\infty}^{0} dt\, e^{i\bar{\omega}t}$ and $\int_{-\infty}^{\infty} dt\, e^{i\bar{\omega}t}$ are evaluated as $\lim_{\kappa\to 0}\int_{-\infty}^{0} dt\, e^{i(\bar{\omega}-i\kappa)t}$ and $\lim_{\kappa\to 0}\left(\int_{-\infty}^{0} dt\, e^{i(\bar{\omega}-i\kappa)t} + \int_{0}^{\infty} dt\, e^{i(\bar{\omega}+i\kappa)t}\right)$, respectively. These replacements are justified by Eq. (4.50).

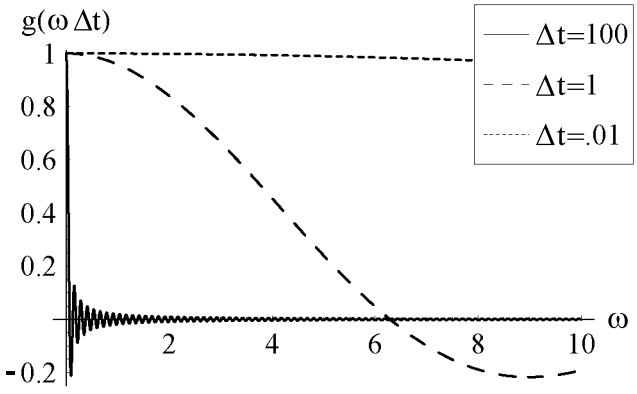

Figure 4.2: The function $g(\omega, \Delta t)$ plotted against ω with three values of $\Delta t = 0.01, 1, 100$. It should illustrate the two cases where g becomes constant ($\Delta t = 0.01$), as it is assumed in the Redfield approach, and when g is zero, except for $\omega = 0$ ($\Delta t = 100$), as it is assumed in the Markov approach.

Looking at the behavior of the function $g(\omega, \Delta t)$ for parameters Δt (see figure 4.2), we distinguish two limiting cases.

The first case is called Redfield approach. It corresponds to a time interval satisfying the inequality $\frac{2\pi}{\omega_{\max}} \gg \Delta t$. Then Δt is so small that the product with the largest ω stays in the vicinity of 0, implying that the function g becomes constant:

$$g(\omega, \Delta t) = 1, \ \forall \ \omega.$$

In figure 4.2, this can be seen for $\Delta t = 0.01$. Note that Δt has still to be much larger than τ_{corr}. This case is called the Redfield approach. In summary, the choice of Δt is limited by

$$\tau_{\text{corr}} \ll \Delta t \ll \frac{2\pi}{\omega_{\max}}.$$

The Redfield approach takes memory effects of the system into account, which are not of interest here.

The second case is called Markov approach. It is valid for time intervals satisfying the inequality $\frac{2\pi}{\Delta\omega} \ll \Delta t$. Then Δt is so large that the product with $\Delta\omega$ is already very large. The function $g(\omega, \Delta t)$ becomes

$$g(\omega, \Delta t) = \begin{cases} 1 & \text{if } \omega = 0 \\ 0 & \text{else} \end{cases}. \tag{4.59}$$

In figure 4.2, this can be seen for $\Delta t = 100$. Here another limiting time comes into play, the timescale on which the irreversible evolution of the bathed

system can be seen. This timescale will be called τ^{evol}. The coarse-graining time interval has to be smaller than that timescale, if not, the evolution, we are interested in will be averaged out[4]. In summary the choice of Δt is limited by

$$\tau_{\text{corr}} \ll \frac{2\pi}{\Delta\omega} \ll \Delta t \ll \tau^{evol}. \tag{4.60}$$

The Markov approach will be the one, we will adopt. We define a finite time interval $\Delta t > \tau_{\text{corr}}$, for which

$$\Delta t\, \Delta\omega \gg 1. \tag{4.61}$$

Note that in the thermodynamic limit (volume $V \to \infty$ and $\frac{N}{V} = const.$) the conditions (4.61) and (4.60) cannot be satisfied, since $\Delta\omega \to 0$.

We assume that Δt remains small enough so that – in accordance with equation (4.51) – the evolution of the one-particle density matrix can still be described by terms up to second order in the electron-electron interaction. This assumption imposes an upper limit on the interaction strength. Taking equation (4.59) and the above property into account, we see that for this choice of Δt the exponentials $e^{i\omega\bar{t}}$ in equation (4.58) can be replaced by 1. Considering here only contributions up to second order in the interaction, and remembering that the time dependence of the operators $D^{\hat{I}}_{(1)}(t)$ and $\hat{A}_\beta(t)$ is solely due the interaction, we may replace the arguments t_0 in equation (4.58) by $\bar{t}$ and replace the density matrix $D^{\hat{I}}_{(1)}$ by the averaged density matrix $\bar{D}^{\hat{I}}_{(1)}$, defined in equation (4.55). Together with equations (4.55), (4.56) and equation

[4]Not all systems have such distinguished time scales, of course.

(4.57) we thus obtain

$$
\begin{aligned}
(\nu|K(\bar{t})|\mu) = K(\bar{t})_{\nu\mu} = 2\left(\frac{i}{\hbar}\right)^2 \sum_{\alpha\beta} \\
\Bigg\{ \sum_{\{\gamma,\delta,\kappa|\omega_{\kappa\mu}+\omega_{\delta\gamma}=0\}} \sum_{\epsilon\lambda} \bar{D}^{\hat{I}}_{(1)\gamma\delta}(\bar{t}) \hat{A}_{\beta,\delta\epsilon}(\bar{t}) \hat{A}_{\alpha,\epsilon\gamma}(\bar{t}) \bar{D}^{\hat{I}}_{(1)\nu\kappa}(\bar{t}) \hat{A}_{\beta,\kappa\lambda}(\bar{t}) \hat{A}_{\alpha,\lambda\mu}(\bar{t}) \\
\int_0^\infty d\tau e^{-i(\omega_{\kappa\lambda}+\omega_{\delta\epsilon})\tau} \\
- \sum_{\{\gamma,\delta,\kappa,\lambda|\omega_{\nu\kappa}+\omega_{\lambda\mu}+\omega_{\delta\gamma}=0\}} \sum_{\epsilon} \bar{D}^{\hat{I}}_{(1)\gamma\delta}(\bar{t}) \hat{A}_{\beta,\delta\epsilon}(\bar{t}) \hat{A}_{\alpha,\epsilon\gamma}(\bar{t}) \hat{A}_{\alpha,\nu\kappa}(\bar{t}) \bar{D}^{\hat{I}}_{(1)\kappa\lambda}(\bar{t}) \hat{A}_{\beta,\lambda\mu}(\bar{t}) \\
\int_0^\infty d\tau e^{-i(\omega_{\delta\epsilon}+\omega_{\lambda\mu})\tau} \\
- \sum_{\{\gamma,\delta,\kappa,\lambda|\omega_{\nu\kappa}+\omega_{\lambda\mu}+\omega_{\delta\gamma}=0\}} \sum_{\epsilon} \bar{D}^{\hat{I}}_{(1)\gamma\delta}(\bar{t}) \hat{A}_{\alpha,\delta\epsilon}(\bar{t}) \hat{A}_{\beta,\epsilon\gamma}(\bar{t}) \hat{A}_{\beta,\nu\kappa}(\bar{t}) \bar{D}^{\hat{I}}_{(1)\kappa\lambda}(\bar{t}) \hat{A}_{\alpha,\lambda\mu}(\bar{t}) \\
\int_0^\infty d\tau e^{-i(\omega_{\nu\kappa}+\omega_{\epsilon\gamma})\tau} \\
+ \sum_{\{\gamma,\delta,\lambda|\omega_{\nu\lambda}+\omega_{\delta\gamma}=0\}} \sum_{\epsilon\kappa} \bar{D}^{\hat{I}}_{(1)\gamma\delta}(\bar{t}) \hat{A}_{\alpha,\delta\epsilon}(\bar{t}) \hat{A}_{\beta,\epsilon\gamma}(\bar{t}) \hat{A}_{\alpha,\nu\kappa}(\bar{t}) \hat{A}_{\beta,\kappa\lambda}(\bar{t}) \bar{D}^{\hat{I}}_{(1)\lambda\mu}(\bar{t}) \\
\int_0^\infty d\tau e^{-i(\omega_{\kappa\lambda}+\omega_{\epsilon\gamma})\tau} \Bigg\}.
\end{aligned}
$$

This expression can be written in the compact form

$$
(K(\bar{t}))_{\nu\mu} = \sum_{\{\gamma\delta\kappa\lambda|\omega_{\nu\mu}+\omega_{\delta\gamma}+\omega_{\lambda\kappa}=0\}} \bar{D}^{\hat{I}}_{(1)\gamma\delta}(\bar{t}) \bar{\Gamma}^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t}) \tag{4.62}
$$

with

$$
\begin{aligned}
\bar{\Gamma}^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t}) &= -\delta_{\nu\gamma} \sum_{\sigma} F^{\mu\delta}_{\sigma\sigma;\kappa\lambda}(\bar{t}) + F^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t}) \\
&\quad + F^{\delta\gamma}_{\mu\nu;\lambda\kappa}(\bar{t})^\star - \delta_{\delta\mu} \sum_{\sigma} F^{\nu\gamma}_{\sigma\sigma;\lambda\kappa}(\bar{t})^\star
\end{aligned} \tag{4.63}
$$

and

$$F^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t}) = \frac{2}{\hbar^2}\bar{D}^{\hat{I}}_{(1)\kappa\lambda}\sum_{\alpha\beta}\hat{A}_{\alpha,\nu\gamma}(\bar{t})\hat{A}_{\beta,\delta\mu}(\bar{t})\sum_{\sigma}\hat{A}_{\beta,\lambda\sigma}(\bar{t})\hat{A}_{\alpha,\sigma\kappa}(\bar{t}) \int_0^\infty d\tau e^{-i\left(\omega_{\delta\mu}+\omega_{\lambda\sigma}\right)\tau} \tag{4.64}$$

$$F^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t})^\star = \frac{2}{\hbar^2}\bar{D}^{\hat{I}}_{(1)\lambda\kappa}\sum_{\alpha\beta}\hat{A}_{\alpha,\gamma\nu}(\bar{t})\hat{A}_{\beta,\mu\delta}(\bar{t})\sum_{\sigma}\hat{A}_{\alpha,\kappa\sigma}(\bar{t})\hat{A}_{\beta,\sigma\lambda}(\bar{t}) \int_0^\infty d\tau e^{i\left(\omega_{\delta\mu}+\omega_{\lambda\sigma}\right)\tau}. \tag{4.65}$$

From equation (4.63) we find

$$\begin{aligned}
\sum_\nu \bar{\Gamma}^{\gamma\delta}_{\nu\nu;\kappa\lambda}(\bar{t}) & \\
&= -\sum_\nu \delta_{\nu\gamma}\sum_\sigma F^{\nu\delta}_{\sigma\sigma;\kappa\lambda}(\bar{t}) + \sum_\nu F^{\gamma\delta}_{\nu\nu;\kappa\lambda}(\bar{t}) \\
&\quad + \sum_\nu F^{\delta\gamma}_{\nu\nu;\lambda\kappa}(\bar{t})^\star - \sum_\nu \delta_{\delta\nu}\sum_\sigma F^{\nu\gamma}_{\sigma\sigma;\lambda\kappa}(\bar{t})^\star \\
&= -\sum_\sigma F^{\gamma\delta}_{\sigma\sigma;\kappa\lambda}(\bar{t}) + \sum_\nu F^{\gamma\delta}_{\nu\nu;\kappa\lambda}(\bar{t}) + \sum_\nu F^{\delta\gamma}_{\nu\nu;\lambda\kappa}(\bar{t})^\star - \sum_\sigma F^{\delta\gamma}_{\sigma\sigma;\lambda\kappa}(\bar{t})^\star \\
&= -\sum_\nu F^{\gamma\delta}_{\nu\nu;\kappa\lambda}(\bar{t}) + \sum_\nu F^{\gamma\delta}_{\nu\nu;\kappa\lambda}(\bar{t}) + \sum_\nu F^{\delta\gamma}_{\nu\nu;\lambda\kappa}(\bar{t})^\star - \sum_\nu F^{\delta\gamma}_{\nu\nu;\lambda\kappa}(\bar{t})^\star \\
&= 0.
\end{aligned} \tag{4.66}$$

Together with equation (4.62) this implies

$$\mathrm{Tr}\left(K(\bar{t})\right) = 0,$$

which corresponds to equation (4.54).

The $\bar{\Gamma}$ coefficients of equation (4.63) can be rewritten in the form

$$\begin{aligned}
\bar{\Gamma}^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t}) = \quad & \bar{\Gamma}_0{}^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t}) \\
& - \left(\frac{1}{\hbar}G_{\nu\gamma\lambda\kappa}(\bar{t}) + \frac{i}{\hbar}\Delta H_{\nu\gamma\lambda\kappa}(\bar{t})\right)\delta_{\delta\mu} \\
& - \left(\frac{1}{\hbar}G_{\delta\mu\lambda\kappa}(\bar{t}) - \frac{i}{\hbar}\Delta H_{\delta\mu\lambda\kappa}(\bar{t})\right)\delta_{\nu\gamma}
\end{aligned} \tag{4.67}$$

with

$$\bar{\Gamma}_0{}^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t}) = F^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t}) + F^{\delta\gamma}_{\mu\nu;\lambda\kappa}(\bar{t})^\star, \tag{4.68}$$

$$\begin{aligned}
G_{\nu\mu\gamma\delta}(\bar{t}) &= \frac{\hbar}{2}\sum_\sigma \bar{\Gamma}_0{}^{\mu\nu}_{\sigma\sigma;\delta\gamma}(\bar{t}) \\
&= \frac{\hbar}{2}\sum_\sigma \left(F^{\mu\nu}_{\sigma\sigma;\delta\gamma}(\bar{t}) + F^{\nu\mu}_{\sigma\sigma;\gamma\delta}(\bar{t})^\star\right),
\end{aligned} \tag{4.69}$$

$$\Delta H_{\nu\mu\gamma\delta}(\bar{t}) = \frac{i\hbar}{2}\sum_\sigma \left(F^{\mu\nu}_{\sigma\sigma;\delta\gamma}(\bar{t}) - F^{\nu\mu}_{\sigma\sigma;\gamma\delta}(\bar{t})^\star\right). \tag{4.70}$$

The matrix elements of the above-defined operators $\bar{\Gamma}_0$, G, and ΔH satisfy the symmetry relations

$$\begin{aligned} \bar{\Gamma}_{0\,\nu\mu;\kappa\lambda}^{\gamma\delta} &= \left(\bar{\Gamma}_{0\,\mu\nu;\lambda\kappa}^{\delta\gamma}\right)^{\star}, \\ G_{\nu\mu\gamma\delta} &= (G_{\mu\nu\delta\gamma})^{\star}, \\ \Delta H_{\nu\mu\gamma\delta} &= (\Delta H_{\mu\nu\delta\gamma})^{\star}, \end{aligned} \tag{4.71}$$

and consequently we have

$$\bar{\Gamma}_{\nu\mu;\kappa\lambda}^{\gamma\delta} = \left(\bar{\Gamma}_{\mu\nu;\lambda\kappa}^{\delta\gamma}\right)^{\star}. \tag{4.72}$$

From equations (4.56) and (4.62) we obtain

$$\frac{d}{dt}\bar{D}_{(1)\nu\mu}^{\hat{I}}(t)|_{t=\bar{t}} = \sum_{\{\gamma\delta\kappa\lambda|\omega_{\nu\mu}+\omega_{\delta\gamma}+\omega_{\lambda\kappa}=0\}} \bar{D}_{(1)\gamma\delta}^{\hat{I}}(\bar{t})\bar{\Gamma}_{\nu\mu;\kappa\lambda}^{\gamma\delta}(\bar{t}). \tag{4.73}$$

Defining

$$\Gamma_{\nu\mu}^{\gamma\delta}(\bar{t}) = \sum_{\{\kappa\lambda|\omega_{\lambda\kappa}+\omega_{\nu\mu}+\omega_{\delta\gamma}=0\}} \bar{\Gamma}_{\nu\mu;\kappa\lambda}^{\gamma\delta}(\bar{t}) \tag{4.74}$$

we can avoid the summation restrictions in equation (4.73), and write

$$\frac{d}{dt}\bar{D}_{(1)\nu\mu}^{\hat{I}}(t)|_{t=\bar{t}} = \sum_{\gamma\delta} \bar{D}_{(1)\gamma\delta}^{\hat{I}}(\bar{t})\,\Gamma_{\nu\mu}^{\gamma\delta}(\bar{t}). \tag{4.75}$$

The one-particle density matrix in the Schrödinger picture is obtained with the transformation

$$\bar{D}_{(1)}(t) = e^{-\frac{i}{\hbar}\hat{H}_0^{(1)}t}\,\bar{D}_{(1)}^{\hat{I}}(t)\,e^{\frac{i}{\hbar}\hat{H}_0^{(1)}t}.$$

From equation (4.75) we obtain

$$\frac{d}{dt}\bar{D}_{(1)}(t)|_{t=\bar{t}} = \frac{i}{\hbar}\left[\bar{D}_{(1)}(\bar{t}), \hat{H}_0^{(1)}(\bar{t})\right] + \Gamma(\bar{t})\big(\bar{D}_{(1)}(\bar{t})\big), \tag{4.76}$$

where

$$\left(\Gamma(\bar{t})(Y)\right)_{\nu\mu} = \sum_{\kappa\lambda}\Gamma_{\nu\mu}^{\kappa\lambda}(\bar{t})Y_{\kappa\lambda}, \quad \forall \quad Y \in \mathcal{L}(\mathcal{H}).$$

Explicitly written, equation (4.76) becomes

$$\frac{d}{dt}\bar{D}_{(1)\nu\mu}(t)|_{t=\bar{t}} = \frac{i}{\hbar}\left[\bar{D}_{(1)}(\bar{t}), \hat{H}_0^{(1)}(\bar{t})\right]_{\nu\mu} + \sum_{\kappa\lambda}\Gamma_{\nu\mu}^{\kappa\lambda}(\bar{t})\bar{D}_{(1)\kappa\lambda}(\bar{t}).$$

This is the master equation that described the coarse grained evolution of an electron gas in a system without energy transfer but with memory loss. We note that the coefficients $\Gamma^{\kappa\lambda}_{\nu\mu}(\bar{t})$, which are obtained from equations (4.63) and (4.74), depend themselves on $\bar{D}_{(1)}$.

It important to note that – in contrast to the situation described in [1] – the superoperator $\Gamma(\bar{t})$ depends itself on the coarse grained density matrix $\bar{D}^{\hat{I}}_{(1)}(\bar{t})$. This dependence results from the fact that the described evolution of $\bar{D}^{\hat{I}}_{(1)}$ is driven by the electron-electron interaction rather than by the interaction of the electronic subsystem with an independent bath subsystem, which is characterized by its proper density matrix.

4.3 Properties of the Γ coefficients and discussion

Let us further inspect the properties of the Γ coefficients, which determine the evolution of the one-particle density matrix (see equation (4.75)). From equations (4.72) and (4.74) we obtain

$$\Gamma^{\gamma\delta}_{\nu\mu} = \left(\Gamma^{\delta\gamma}_{\mu\nu}\right)^{\star}. \tag{4.77}$$

In the spirit of equation (4.74), we define

$$\Gamma_0{}^{\gamma\delta}_{\nu\mu}(\bar{t}) \;=\; \sum_{\{\kappa\lambda|\omega_{\nu\mu}+\omega_{\delta\gamma}+\omega_{\lambda\kappa}=0\}} \bar{\Gamma}_0{}^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t}). \tag{4.78}$$

From equations (4.67), (4.74) and (4.75) it follows that the transition rates from the initial states $|\xi\rangle$ to the final states $|\nu\rangle$ with $\xi \neq \nu$ are given by the diagonal coefficients $\Gamma_0{}^{\xi\xi}_{\nu\nu}(\bar{t})$. For simplicity we assume from now on that all difference frequencies $\omega_{\sigma\tau}$ are non-zero for $\sigma \neq \tau$ and also different[5]. We then get from equation (4.78)

$$\begin{aligned}\Gamma_0{}^{\xi\xi}_{\nu\nu}(\bar{t}) \;&=\; \sum_{\{\kappa\lambda|\omega_{\lambda\kappa}=0\}} \bar{\Gamma}_0{}^{\xi\xi}_{\nu\nu;\kappa\lambda}(\bar{t}) \\ &=\; \sum_{\kappa} \bar{\Gamma}_0{}^{\xi\xi}_{\nu\nu;\kappa\kappa}(\bar{t}),\end{aligned}$$

[5]This assumption can be made without loss of generality. It corresponds to adding some small perturbation to the one-particle Hamiltonian $H_0^{(1)}$ which lifts the $\omega_{\kappa\lambda}$ degeneracies. This allows the identification of the contributions of the single-particle states in the following analysis. After the analysis, the perturbation may be reset to zero again .

and from equations (4.64), (4.65) and (4.68) for $\xi \neq \nu$

$$\begin{aligned}
{\Gamma_0}_{\nu\nu}^{\xi\xi}(\bar{t}) = \Gamma_{\xi\to\nu} &= \sum_{\kappa}\left(F^{\xi\xi}_{\nu\nu;\kappa\kappa}(\bar{t}) + F^{\xi\xi}_{\nu\nu;\kappa\kappa}(\bar{t})^{\star}\right) \qquad (4.79)\\
&= \frac{2\pi}{\hbar^2}\sum_{\kappa\lambda}\sum_{\alpha\beta}\hat{A}_{\alpha,\nu\xi}(\bar{t})\hat{A}_{\beta,\xi\nu}(\bar{t})\hat{A}_{\alpha,\lambda\kappa}(\bar{t})\hat{A}_{\beta,\kappa\lambda}(\bar{t})\bar{D}^{\hat{I}}_{(1)\kappa\kappa}(\bar{t})\delta\left(\omega_{\xi\nu}+\omega_{\kappa\lambda}\right)\\
&= \frac{2\pi}{\hbar^2}\sum_{\kappa\lambda}\sum_{\alpha\beta}\hat{A}_{\alpha,\nu\xi}(\bar{t})\hat{A}_{\beta,\xi\nu}(\bar{t})\hat{A}_{\alpha,\lambda\kappa}(\bar{t})\hat{A}_{\beta,\kappa\lambda}(\bar{t})\bar{D}^{\hat{I}}_{(1)\kappa\kappa}(\bar{t})\delta_{\nu\kappa}\delta_{\xi\lambda}\\
&= \frac{2\pi}{\hbar^2}\bar{D}^{\hat{I}}_{(1)\nu\nu}(\bar{t})\left(\sum_{\alpha}\hat{A}_{\alpha,\nu\xi}(\bar{t})\hat{A}_{\alpha,\xi\nu}(\bar{t})\right)\left(\sum_{\beta}\hat{A}_{\beta,\nu\xi}(\bar{t})\hat{A}_{\beta,\xi\nu}(\bar{t})\right)\\
&= \frac{2\pi}{\hbar^2}\bar{D}^{\hat{I}}_{(1)\nu\nu}(\bar{t})\left(\sum_{\alpha}\left|\hat{A}_{\alpha,\nu\xi}(\bar{t})\right|^2\right)^2\\
&\geq 0,
\end{aligned}$$

which implies

$$\frac{\Gamma_{\xi\to\nu}}{\bar{D}^{\hat{I}}_{(1)\nu\nu}(\bar{t})} = \frac{\Gamma_{\nu\to\xi}}{\bar{D}^{\hat{I}}_{(1)\xi\xi}(\bar{t})}. \qquad (4.80)$$

From equation (4.66) it follows also that

$${\Gamma_0}_{\nu\nu}^{\nu\nu}(\bar{t}) = -\sum_{\{\xi|\xi\neq\nu\}}\Gamma_{\nu\to\xi}.$$

Thus, using equations (4.75), (4.79)) and (4.80), we get

$$\begin{aligned}
\frac{d}{dt}\bar{D}^{\hat{I}}_{(1)\nu\nu}(t)|_{t=\bar{t}} &= \sum_{\xi}\bar{D}^{\hat{I}}_{(1)\xi\xi}(\bar{t})\,\Gamma^{\xi\xi}_{\nu\nu}(\bar{t}), \qquad (4.81)\\
&= \sum_{\{\xi|\xi\neq\nu\}}\Gamma_{\xi\to\nu}\bar{D}^{\hat{I}}_{(1)\xi\xi}(\bar{t}) - \sum_{\{\xi|\xi\neq\nu\}}\Gamma_{\nu\to\xi}\bar{D}^{\hat{I}}_{(1)\nu\nu}(\bar{t})\\
&= \sum_{\{\xi|\xi\neq\nu\}}\Gamma_{\xi\to\nu}\left(\bar{D}^{\hat{I}}_{(1)\xi\xi}(\bar{t}) - \frac{\bar{D}^{\hat{I}}_{(1)\xi\xi}(\bar{t})}{\bar{D}^{\hat{I}}_{(1)\nu\nu}(\bar{t})}\bar{D}^{\hat{I}}_{(1)\nu\nu}(\bar{t})\right)\\
&= 0,
\end{aligned}$$

i.e., the populations remain unchanged throughout the evolution.

The above result is a direct consequence of our assumption that the system energy is conserved during the evolution, which was made to obtain equation (4.49) from equation (4.45). In fact, the energy conservation

$$\left.\frac{d\left\langle\epsilon(t)\right\rangle}{dt}\right|_{t=\bar{t}} = \mathrm{Tr}\left(H_0(\bar{t})\left.\frac{d\bar{D}^{\hat{I}}_{(1)}(t}{dt}\right|_{t=\bar{t}}\right) = 0 \qquad (4.82)$$

follows directly from the conservation of the populations (see equation (4.81)). In order to see this we evaluate the right-hand side of equation (4.82) in the basis of the eigenvectors of $\hat{H}_0^{(1)}$. We then get

$$\begin{aligned}\left.\frac{d\,\langle\epsilon(t)\rangle}{dt}\right|_{t=\bar{t}} &= \sum_{\rho\sigma}\,(\sigma\mid H_0(\bar{t})\mid\rho)\;\;(\rho\mid\;\left.\frac{d\bar{D}^{\hat{I}}_{(1)}(t}{dt}\mid\sigma\right)\Bigg|_{t=\bar{t}}\\ &= \sum_{\sigma}\epsilon_\sigma\;\left.\frac{d\;(\sigma\mid\bar{D}^{\hat{I}}_{(1)}(t\mid\sigma)}{dt}\right|_{t=\bar{t}}\\ &= 0.\end{aligned}$$

Equation (4.81) implies that – in the absence of interactions with external bath subsystems – the evolution of the electronic system is completely determined by the evolution of the coherences. In order to understand this evolution we have to study in more detail the structure of the coefficients $\bar{\Gamma}^{\gamma\delta}_{\nu\mu;\kappa\lambda}$ appearing in equations (4.73) and (4.74). Following the same procedure as for the derivation of equation (4.79), we obtain from the definitions (4.64)

$$\begin{aligned}&F^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t})\pm F^{\delta\gamma}_{\mu\nu;\lambda\kappa}(\bar{t})^\star = \qquad (4.83)\\ &\quad\frac{2}{\hbar^2}\bar{D}^{\hat{I}}_{(1)\kappa\lambda}(\bar{t})\sum_{\alpha\beta}\hat{A}_{\alpha,\nu\gamma}(\bar{t})\hat{A}_{\beta,\delta\mu}(\bar{t})\sum_{\sigma}\hat{A}_{\beta,\lambda\sigma}(\bar{t})\hat{A}_{\alpha,\sigma\kappa}(\bar{t})\int_0^\infty d\tau e^{-i\left(\omega_{\delta\mu}+\omega_{\lambda\sigma}\right)\tau}\\ &\pm\frac{2}{\hbar^2}\bar{D}^{\hat{I}}_{(1)\kappa\lambda}(\bar{t})\sum_{\alpha\beta}\hat{A}_{\alpha,\nu\gamma}(\bar{t})\hat{A}_{\beta,\delta\mu}(\bar{t})\sum_{\sigma}\hat{A}_{\beta,\lambda\sigma}(\bar{t})\hat{A}_{\alpha,\sigma\kappa}(\bar{t})\int_0^\infty d\tau e^{i(\omega_{\kappa\sigma}+\omega_{\gamma\nu})\tau}.\end{aligned}$$

From the above expression and equations (4.68), (4.69), and (4.70) we obtain the coefficients $\bar{\Gamma}_{0\,\cdot;\cdot,\cdot}(\bar{t})$, $G_{\cdot\cdot\cdot\cdot}(\bar{t})$ and $\Delta H_{\cdot\cdot\cdot\cdot}(\bar{t})$, and thus finally the coefficients $\Gamma^{\cdot;\cdot}_{\cdot,\cdot}(\bar{t})$ of equation (4.75), which determine the evolution of $\bar{D}^{\hat{I}}_{(1)}(t)$.

The summation condition $\omega_{\nu\mu}+\omega_{\delta\gamma}+\omega_{\lambda\kappa}=0$ in equation (4.78) can be rewritten as

$$\omega_{\gamma\nu}+\omega_{\kappa\lambda}=\omega_{\delta\mu}. \qquad (4.84)$$

This allows us to rewrite equation (4.83) in the form

$$\begin{aligned}&F^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t})\pm F^{\delta\gamma}_{\mu\nu;\lambda\kappa}(\bar{t})^\star=\frac{2}{\hbar^2}\bar{D}^{\hat{I}}_{(1)\kappa\lambda}(\bar{t})\cdot \qquad (4.85)\\ &\cdot\sum_{\alpha\beta}\hat{A}_{\alpha,\nu\gamma}(\bar{t})\hat{A}_{\beta,\delta\mu}(\bar{t})\sum_{\sigma}\hat{A}_{\beta,\lambda\sigma}(\bar{t})\hat{A}_{\alpha,\sigma\kappa}(\bar{t})\begin{cases}\displaystyle\int_{-\infty}^{\infty}d\tau e^{-i(\omega_{\kappa\sigma}+\omega_{\gamma\nu})\tau}\\ \displaystyle\int_{-\infty}^{\infty}d\tau\xi(\tau)e^{-i(\omega_{\kappa\sigma}+\omega_{\gamma\nu})\tau},\end{cases}\end{aligned}$$

where the Heavyside function $\xi(\tau)$ is defined in (2.14). Alternatively, using the condition (4.84), we can write equation (4.85) in the form

$$F^{\gamma\delta}_{\nu\mu;\kappa\lambda}(\bar{t}) \pm F^{\delta\gamma}_{\mu\nu;\lambda\kappa}(\bar{t})^\star = \begin{cases} \frac{1}{\hbar}\sum_{\alpha\beta} \hat{A}_{\alpha,\nu\gamma}(\bar{t})\hat{A}_{\beta,\delta\mu}(\bar{t})\chi_{\beta\alpha;\lambda\kappa}(\bar{t},-\omega_{\delta\mu}) \\ \frac{1}{\hbar}\sum_{\alpha\beta} \hat{A}_{\alpha,\nu\gamma}(\bar{t})\hat{A}_{\beta,\delta\mu}(\bar{t})\bar{\chi}_{\beta\alpha;\lambda\kappa}(\bar{t},-\omega_{\delta\mu}) \end{cases} \tag{4.86}$$

with

$$\begin{aligned} \chi_{\beta\alpha;\lambda\kappa}(\bar{t},\omega) &= \frac{2\pi}{\hbar}\bar{D}^{\hat{I}}_{(1)\kappa\lambda}(\bar{t})\sum_\sigma \hat{A}_{\beta,\lambda\sigma}(\bar{t})\hat{A}_{\alpha,\sigma\kappa}(\bar{t})\delta\left(\omega-\omega_{\lambda\sigma}\right) \qquad (4.87)\\ \bar{\chi}_{\beta\alpha;\lambda\kappa}(\bar{t},\omega) &= -\frac{2}{\hbar}\bar{D}^{\hat{I}}_{(1)\kappa\lambda}(\bar{t})\sum_\sigma \hat{A}_{\beta,\lambda\sigma}(\bar{t})\hat{A}_{\alpha,\sigma\kappa}(\bar{t})\frac{1}{\omega-\omega_{\lambda\sigma}}. \end{aligned}$$

The Γ_0 coefficients defined in equation (4.78) can then be expressed in terms of the functions $\chi_{\beta\alpha;..}(\bar{t},\omega)$. From equations (4.68), (4.86), and (4.87), we get

$$\begin{aligned} {\Gamma_0}^{\gamma\delta}_{\nu\mu}(\bar{t}) &= \frac{2}{\hbar}\sum_{\alpha\beta}\sum_{\{\kappa\lambda|\omega_{\nu\mu}+\omega_{\lambda\kappa}+\omega_{\delta\gamma}=0\}} \hat{A}_{\alpha,\nu\gamma}(\bar{t})\left(\chi_{\beta\alpha;\lambda\kappa}(\bar{t},\omega_{\mu\delta})\right)\hat{A}_{\beta,\delta\mu}(\bar{t}) \\ &= \frac{2}{\hbar}\sum_{\alpha\beta}\hat{A}_{\alpha,\nu\gamma}(\bar{t})\left(\sum_{\{\kappa\lambda|\omega_{\nu\mu}+\omega_{\lambda\kappa}+\omega_{\delta\gamma}=0\}}\chi_{\beta\alpha;\lambda\kappa}(\bar{t},\omega_{\mu\delta})\right)\hat{A}_{\beta,\delta\mu}(\bar{t}). \end{aligned}$$

The coherences are described by the non-diagonal matrix elements $\bar{D}^{\hat{I}}_{(1)\nu\mu}(\bar{t})$, $\nu\neq\mu$. The evolution of their contribution to the one-particle density matrix $\bar{D}^{\hat{I}}_{(1)}(\bar{t})$ is described by

$$\begin{aligned} &\frac{d}{dt}\left(\sum_{\{\nu\mu|\nu\neq\mu\}}\left|\bar{D}^{\hat{I}}_{(1)\nu\mu}(\bar{t})\right|^2\right)\Bigg|_{t=\bar{t}} \\ &= \frac{d}{dt}\left(\sum_{\{\nu\mu|\nu\neq\mu\}}\bar{D}^{\hat{I}}_{(1)\nu\mu}(\bar{t})\bar{D}^{\hat{I}}_{(1)\mu\nu}(\bar{t})\right)\Bigg|_{t=\bar{t}} \\ &= 2\sum_{\{\nu\mu|\nu\neq\mu\}}\frac{d}{dt}\left(\bar{D}^{\hat{I}}_{(1)\nu\mu}(\bar{t})\right)\Bigg|_{t=\bar{t}}\bar{D}^{\hat{I}}_{(1)\mu\nu}(\bar{t}) \\ &= 2\sum_{\{\nu\mu|\nu\neq\mu\}}\sum_{\gamma\delta}\Gamma^{\gamma\delta}_{\nu\mu}(\bar{t})\bar{D}^{\hat{I}}_{(1)\gamma\delta}(\bar{t})\bar{D}^{\hat{I}}_{(1)\mu\nu}(\bar{t}), \end{aligned} \tag{4.88}$$

where we have used equation (4.75) in the last line. For a nearly diagonal density matrix

$$\bar{D}^{\hat{I}}_{(1)\kappa\lambda}(\bar{t}) \approx \bar{D}^{\hat{I}}_{(1)\kappa\kappa}(\bar{t})\delta_{\kappa\lambda}, \tag{4.89}$$

equations (4.86), (4.87) imply that terms with $\kappa = \lambda$ give the main contributions to the Γ coefficients defined in equation (4.74). According to Eqs. (4.73) and (4.75), the evolution of the coherences $\bar{D}^{\hat{I}}_{1\,\nu\mu}(\bar{t})$ is thus governed by the coefficients $\bar{\Gamma}^{\nu\mu}_{\nu\mu;\kappa\kappa}$ or the corresponding coefficients $\bar{\Gamma}^{\nu\mu}_{\nu\mu}$, so that Eq. (4.88) becomes

$$\begin{aligned} & \frac{d}{dt}\left(\sum_{\{\nu\mu|\nu\neq\mu\}}\left|\bar{D}^{\hat{I}}_{1\,\nu\mu}(\bar{t})\right|^2\right)\Bigg|_{t=\bar{t}} \\ \approx\ & 2\sum_{\{\nu\mu|\nu\neq\mu\}}\sum_{\gamma\delta}\Gamma^{\nu\mu}_{\nu\mu}(\bar{t})\bar{D}^{\hat{I}}_{1\,\gamma\delta}(\bar{t})\bar{D}^{\hat{I}}_{1\,\mu\nu}(\bar{t}). \\ =\ & 2\sum_{\{\nu\mu|\nu\neq\mu\}}\sum_{\gamma\delta}\mathrm{Re}\left(\Gamma^{\nu\mu}_{\nu\mu}(\bar{t})\right)\left|\bar{D}^{\hat{I}}_{1\,\nu\mu}(\bar{t})\right|^2, \end{aligned} \tag{4.90}$$

where we have used the symmetry relation (4.77) to obtain the last line. We then have to investigate the coefficients $\Gamma^{\nu\mu}_{\nu\mu}(\bar{t})$. From equations (4.63) and (4.74) we obtain

$$\begin{aligned} \Gamma^{\nu\mu}_{\nu\mu}(\bar{t}) &= \sum_{\kappa}\bar{\Gamma}^{\nu\mu}_{\nu\mu;\kappa\kappa}(\bar{t}) \\ &= \sum_{\kappa}\left(F^{\nu\mu}_{\nu\mu;\kappa\kappa}(\bar{t}) + F^{\mu\nu}_{\mu\nu;\kappa\kappa}(\bar{t})^\star\right) - \sum_{\kappa\sigma}\left(F^{\mu\mu}_{\sigma\sigma;\kappa\kappa}(\bar{t}) + F^{\nu\nu}_{\sigma\sigma;\kappa\kappa}(\bar{t})^\star\right), \end{aligned}$$

and thus

$$\begin{aligned} & 2\mathrm{Re}\left(\Gamma^{\nu\mu}_{\nu\mu}(\bar{t})\right) \\ &= \sum_{\kappa}\left(F^{\nu\mu}_{\nu\mu;\kappa\kappa}(\bar{t}) + F^{\mu\nu}_{\mu\nu;\kappa\kappa}(\bar{t})^\star\right) + \sum_{\kappa}\left(F^{\nu\mu}_{\nu\mu;\kappa\kappa}(\bar{t})^\star + F^{\mu\nu}_{\mu\nu;\kappa\kappa}(\bar{t})\right) \\ &\quad - \sum_{\kappa\sigma}\left(F^{\nu\nu}_{\sigma\sigma;\kappa\kappa}(\bar{t}) + F^{\nu\nu}_{\sigma\sigma;\kappa\kappa}(\bar{t})^\star\right) - \sum_{\kappa\sigma}\left(F^{\mu\mu}_{\sigma\sigma;\kappa\kappa}(\bar{t}) + F^{\mu\mu}_{\sigma\sigma;\kappa\kappa}(\bar{t})^\star\right). \end{aligned} \tag{4.91}$$

The four terms on the right-hand side can be calculated from equation (4.85). From equations (4.68) and (4.71) we get for the first two terms

$$\begin{aligned} \sum_{\kappa}\left(F^{\nu\mu}_{\nu\mu;\kappa\kappa}(\bar{t}) + F^{\mu\nu}_{\mu\nu;\kappa\kappa}(\bar{t})^\star\right) &= \sum_{\kappa}\left(F^{\nu\mu}_{\nu\mu;\kappa\kappa}(\bar{t})^\star + F^{\mu\nu}_{\mu\nu;\kappa\kappa}(\bar{t})\right) \\ &= \frac{4\pi}{\hbar^2}\sum_{\kappa}\bar{D}^{\hat{I}}_{(1)\kappa\kappa}(\bar{t}) \\ &\quad \sum_{\alpha\beta}\hat{A}_{\alpha,\nu\nu}(\bar{t})\hat{A}_{\beta,\mu\mu}(\bar{t})\hat{A}_{\beta,\kappa\kappa}(\bar{t})\hat{A}_{\alpha,\kappa\kappa}(\bar{t}). \end{aligned} \tag{4.92}$$

The third term is given by

$$\begin{aligned}
&\sum_{\kappa\sigma}\left(F^{\nu\nu}_{\sigma\sigma;\kappa\kappa}(\bar{t})+F^{\nu\nu}_{\sigma\sigma;\kappa\kappa}(\bar{t})^{\star}\right) \qquad (4.93)\\
=\;&\frac{4\pi}{\hbar^2}\sum_{\kappa}\bar{D}^{\hat{I}}_{(1)\kappa\kappa}(\bar{t})\left(\sum_{\alpha\beta}\hat{A}_{\alpha,\nu\nu}(\bar{t})\hat{A}_{\alpha,\kappa\kappa}(\bar{t})\hat{A}_{\beta,\nu\nu}(\bar{t})\hat{A}_{\beta,\kappa\kappa}(\bar{t})\right)\\
&+\frac{4\pi}{\hbar^2}\sum_{\kappa}\bar{D}^{\hat{I}}_{(1)\kappa\kappa}(\bar{t})\sum_{\alpha\beta}\left|\hat{A}_{\alpha,\kappa\nu}(\bar{t})\right|^2\left|\hat{A}_{\beta,\kappa\nu}(\bar{t})\right|^2.
\end{aligned}$$

Replacing the index ν by μ in the above equation we obtain the fourth term

$$\begin{aligned}
&\sum_{\kappa\sigma}\left(F^{\mu\mu}_{\sigma\sigma;\kappa\kappa}(\bar{t})+F^{\mu\mu}_{\sigma\sigma;\kappa\kappa}(\bar{t})^{\star}\right) \qquad (4.94)\\
=\;&\frac{4\pi}{\hbar^2}\sum_{\kappa}\bar{D}^{\hat{I}}_{(1)\kappa\kappa}(\bar{t})\left(\sum_{\alpha\beta}\hat{A}_{\alpha,\mu\mu}(\bar{t})\hat{A}_{\alpha,\kappa\kappa}(\bar{t})\hat{A}_{\beta,\mu\mu}(\bar{t})\hat{A}_{\beta,\kappa\kappa}(\bar{t})\right)\\
&+\frac{4\pi}{\hbar^2}\sum_{\kappa}\bar{D}^{\hat{I}}_{(1)\kappa\kappa}(\bar{t})\sum_{\alpha\beta}\left|\hat{A}_{\alpha,\kappa\mu}(\bar{t})\right|^2\left|\hat{A}_{\beta,\kappa\mu}(\bar{t})\right|^2.
\end{aligned}$$

Inserting equations (4.92), (4.93) and (4.94) into equation (4.91), we define vectors $\mathbf{x}_{\gamma\alpha}$ by their components

$$x_{\gamma\alpha,\kappa}=\frac{2}{\hbar}\sqrt{\pi\bar{D}^{\hat{I}}_{(1)\kappa\kappa}(\bar{t})}\hat{A}_{\alpha,\gamma\gamma}(\bar{t})\hat{A}_{\alpha,\kappa\kappa}(\bar{t})\in\mathbb{R},\qquad\forall\kappa.$$

We introduce the scalar products

$$(\mathbf{x}_{\gamma\alpha},\mathbf{x}_{\delta\beta})=(\mathbf{x}_{\delta\beta},\mathbf{x}_{\gamma\alpha})=\sum_{\kappa}x_{\gamma\alpha,\kappa}\,x_{\delta\beta,\kappa},$$

to obtain

$$\begin{aligned}
&2\mathrm{Re}\left(\Gamma^{\nu\mu}_{\nu\mu}(\bar{t})\right) \qquad (4.95)\\
&=\sum_{\alpha\beta}\left((\mathbf{x}_{\nu\alpha},\mathbf{x}_{\mu\beta})-(\mathbf{x}_{\nu\alpha},\mathbf{x}_{\nu\beta})\right)+\left((\mathbf{x}_{\nu\alpha},\mathbf{x}_{\mu\beta})-(\mathbf{x}_{\mu\alpha},\mathbf{x}_{\mu\beta})\right)-w_{\nu\mu}
\end{aligned}$$

with

$$\begin{aligned}
&w_{\nu\mu} \qquad (4.96)\\
&=\frac{4\pi}{\hbar^2}\sum_{\kappa}\bar{D}^{\hat{I}}_{(1)\kappa\kappa}(\bar{t})\left(\sum_{\alpha\beta}\left|\hat{A}_{\alpha,\kappa\nu}(\bar{t})\right|^2\left|\hat{A}_{\beta,\kappa\nu}(\bar{t})\right|^2+\left|\hat{A}_{\alpha,\kappa\mu}(\bar{t})\right|^2\left|\hat{A}_{\beta,\kappa\mu}(\bar{t})\right|^2\right)\\
&\geq 0.
\end{aligned}$$

The first part of the right hand side of equation (4.95) can be rewritten as

$$\begin{aligned}
&\sum_{\alpha\beta}\left((\mathbf{x}_{\nu\alpha},\mathbf{x}_{\mu\beta})-(\mathbf{x}_{\nu\alpha},\mathbf{x}_{\nu\beta})\right)+\sum_{\alpha\beta}\left((\mathbf{x}_{\nu\alpha},\mathbf{x}_{\mu\beta})-(\mathbf{x}_{\mu\alpha},\mathbf{x}_{\mu\beta})\right) \quad (4.97)\\
&=\sum_{\alpha\beta}\left(\mathbf{x}_{\nu\alpha},\mathbf{x}_{\mu\beta}-\mathbf{x}_{\nu\beta}\right)+\sum_{\alpha\beta}\left(\mathbf{x}_{\mu\beta},\mathbf{x}_{\nu\alpha}-\mathbf{x}_{\mu\alpha}\right)\\
&=\sum_{\alpha\beta}\left(\mathbf{x}_{\nu\alpha},\mathbf{x}_{\mu\beta}-\mathbf{x}_{\nu\beta}\right)+\sum_{\alpha\beta}\left(\mathbf{x}_{\mu\alpha},\mathbf{x}_{\nu\beta}-\mathbf{x}_{\mu\beta}\right)\\
&=-\left(\sum_{\alpha}\left(\mathbf{x}_{\nu\alpha}-\mathbf{x}_{\mu\alpha}\right),\sum_{\beta}\left(\mathbf{x}_{\nu\beta}-\mathbf{x}_{\mu\beta}\right)\right)\leq 0.
\end{aligned}$$

From equations (4.95), (4.96) and (4.97) we obtain

$$\mathrm{Re}\left(\Gamma^{\nu\mu}_{\nu\mu}(\bar{t})\right)\leq 0. \quad (4.98)$$

Equations (4.98) and (4.90) imply that, for an initial one-particle density matrix that is nearly diagonal in the eigenbasis of the one-particle Hamiltonian $\hat{H}_0^{(1)}$ (see equation (4.89)), the weight of the coherences cannot increase with time. Remembering that according to equation (4.81) the populations $\bar{D}_{(1)\nu\nu}, \nu = 1, 2, \ldots$ do not change with time, we find that the density matrix $\bar{D}_{(1)\mathrm{stat}}$ corresponding to the final stationary statistical state is given by $\left(\bar{D}_{(1)\,\mathrm{stat}}\right)_{\nu\mu}=\bar{D}_{(1)\nu\nu}\delta_{\nu\mu}$.

Let us recall that the evolution of the one-particle density matrix $\bar{D}^{\hat{I}}_{(1)}(\bar{t})$ described by equation (4.75) is driven by the electron-electron interaction Hamiltonian $\hat{H}_{\mathrm{int}}$ given by equation (4.33), and that no energy is exchanged with the environment. The remaining weak interaction with the environment, which is unavoidable in a real experimental situation, introduces a memory loss. This memory loss is at the origin of the resulting irreversible evolution of the electronic system. This situation may be regarded as the quantum analog of a weakly interacting classical gas in a box where – independent of the chosen initial conditions and even in absence of energy transfer with the environment – the random noise generated by the environment inhibits the appearance of Poincaré cycles on any time scale, and thus may be used to justify the statistical description based on the "Stosszahlansatz". This Ansatz was introduced by Boltzmann to explain the experimentally observed irreversible evolution towards the statistical state with largest entropy at fixed system energy. The evolution of the one-particle density matrix described by equations (4.81) and (4.98) can be described in a similar way in terms of the von Neumann entropy, which for a given density matrix D is defined by

$$S\left(D\right)=-k_B\mathrm{Tr}\left(D\ln D\right). \quad (4.99)$$

Comparing the entropy $S\left(\bar{D}^{\hat{I}}_{(1)\mathrm{stat}}(\bar{t})\right)$ corresponding to the stationary diagonal density matrix $\bar{D}^{\hat{I}}_{(1)\mathrm{stat}}(\bar{t})$ to the entropy $S\left(\bar{D}^{\hat{I}}_{(1)}(\bar{t})\right)$ associated with

the initial density matrix $\bar{D}^{\hat{I}}_{(1)}(\bar{t})$, which has the same diagonal elements as $\bar{D}^{\hat{I}}_{(1)\mathrm{stat}}(\bar{t})$ but possesses also a small off-diagonal part, we get the quantum analog of the second law of thermodynamics [20]

$$S\left(\bar{D}^{\hat{I}}_{1}(\bar{t})\right) = S\left(\bar{D}_{(1)}(\bar{t})\right) < S\left(\bar{D}^{\hat{I}}_{(1)\mathrm{stat}}(\bar{t})\right) = S\left(\bar{D}_{(1)\,\mathrm{stat}}\right).$$

Chapter 5

Evolution of the one-particle density matrix of a system with energy transfer

Let us now come back to our original problem and consider the evolution of a spatially confined electron gas where the electrons are also dissipatively coupled to bath subsystems such as a phonon bath or a photon bath. In this case, electron-electron coupling is the principal source of statistical correlations $\eta_{(2)}(t)$, since the correlations induced by the interaction with the bath subsystems are at least of second order in the electron-bath interaction. We can thus insert the result given by equation (4.76) into equation (3.23) to describe the evolution of the complete system. With the substitution

$$\Gamma^{\kappa\lambda}_{\nu\mu}(\bar{t}) \to (\Gamma_e)^{\kappa\lambda}_{\nu\mu}(\bar{t}), \qquad \bar{D}_{(1)}(\bar{t}) \to \bar{D}_{(1)A}(\bar{t}),$$

and otherwise using the notations of equation (3.23) we obtain

$$\begin{aligned} \frac{d}{dt}\bar{D}_{(1)A}(t)|_{t=\bar{t}} &= \frac{i}{\hbar}\left[\bar{D}_{(1)A}(\bar{t}), H_A^{(1)}\right] + \Gamma_e(\bar{t})\left(\bar{D}_{(1)A}(\bar{t})\right) \\ &+\Gamma_0^{(1\to1)}(\bar{D}_{(1)A}(\bar{t})) - \frac{1}{\hbar}\left\{\bar{D}_{(1)A}(\bar{t}), G^{(1)}\right\} + \Gamma_0^{(2\to1)}(\bar{D}_{(2)A}(\bar{t})) \\ &+\frac{i}{\hbar}\left[\bar{D}_{(1)A}(t), \Delta H_A^{(1)}\right] + \Delta H_A^{(2\to1)}(\bar{D}_{(2)A}(t)). \end{aligned} \tag{5.1}$$

where the two-particle density matrix is given by equations (4.11), (4.17),

$$\bar{D}_{(2)A}(t) = \bar{D}^{\mathrm{u}}_{(2)A}(t) + \eta_{(2)}(t) \approx 2\bar{D}_{(1)A}(t) \otimes \bar{D}_{(1)A}(t)P_a. \tag{5.2}$$

The latter approximation is justified since the coupling term $\Gamma_0^{(2\to1)}(\bar{D}_{(2)A}(t))$ describes contributions of second order in the interaction with the bath subsystems, while the two-particle correlation $\eta_{(2)}$ is of first order in the electron-electron interaction. Accordingly, under the above condition the $\eta_{(2)}$ contributions to the right-hand side of equation (5.1) are smaller or at most comparable

with the already neglected third-order terms of the electron-electron interaction.

Equation (5.1) can be cast into the form

$$\begin{aligned}\frac{d}{dt}\left(\bar{D}_{(1)A}(t)\right)_{\nu\mu}|_{t=\bar{t}} &= \frac{i}{\hbar}\left[\bar{D}_{(1)A}(\bar{t}),\hat{H}_0^{(1)}(\bar{t})\right]_{\nu\mu} \\ &\quad+\sum_{\kappa\lambda}\left(\Gamma_{\mathrm{tot}}\right)_{\nu\mu}^{\kappa\lambda}(\bar{t})\left(\bar{D}_{(1)A}\right)_{\kappa\lambda}(\bar{t})\end{aligned} \tag{5.3}$$

with

$$\Gamma_{\mathrm{tot}}=\Gamma_e+\sum_j\left(C_j+X_j+\Gamma_{0,j}^{(2\to1)}+\Sigma_j\right), \tag{5.4}$$

where the first superoperator Γ_e is the renamed Γ operator defined in equation (4.74). Equation (5.3) is the QBE in the eigenbasis of $\hat{H}_0^{(1)}$. It describes the evolution driven by the electron-electron interaction. The superoperators C_j, X_j, $\Gamma_{0,j}^{(2\to1)}$ together with the self-energy terms Σ_j give the contributions of the different bath subsystems B_j. The superoperators X_j and $\Gamma_{0,j}^{(2\to1)}$ can be expressed in terms of the superoperators C_j, which were defined in equation (B.7). According to equation (B.12) the latter describe the action of $\Gamma_0^{(1\to1)}$ on $\bar{D}_{(1)A}(\bar{t})$. From equations (B.15), (4.12) and (4.17) we obtain

$$\begin{aligned}(X_j)_{\rho\rho'}^{\nu\nu'} &= -\frac{1}{\hbar}\left(\delta_{\nu\rho}\left(G_j^{(1)}\right)_{\nu'\rho'}+\delta_{\nu'\rho'}\left(G_j^{(1)}\right)_{\rho\nu}\right) \\ &= -\delta_{\nu\rho}\sum_\mu\left(C_j\right)_{\mu\mu}^{\rho'\nu'}-\delta_{\nu'\rho'}\sum_\mu\left(C_j\right)_{\mu\mu}^{\nu\rho}\end{aligned}$$

and

$$\begin{aligned}\left(\Gamma_{0j}^{(2\to1)}\right)_{\rho\rho'}^{\nu\nu'} = &\sum_\mu\left(\left(C_j\right)_{\nu\rho'}^{\nu'\mu}-\left(C_j\right)_{\mu\rho'}^{\nu'\mu}+\left(C_j\right)_{\nu\nu'}^{\rho'\nu}-\left(C_j\right)_{\mu\nu'}^{\rho'\nu}\right)\left(\bar{D}_{(1)A}\right)_{\rho\mu} \\ &+\sum_\mu\left(\left(C_j\right)_{\rho\nu'}^{\mu\nu}-\left(C_j\right)_{\rho\mu}^{\nu'\nu}+\left(C_j\right)_{\nu\nu'}^{\mu\rho}-\left(\Gamma_j\right)_{\nu\mu}^{\nu'\rho}\right)\left(\bar{D}_{(1)A}\right)_{\mu\rho'}.\end{aligned}$$

Similarly, the self-energy terms Σ_j in equation (3.23) can be expressed in terms of the superoperators $\bar{C}_j$ also defined in equation (B.8). With

$$\Sigma_j=\Sigma_j^{(1)}+\Sigma_j^{(2\to1)},$$

where $\Sigma_j^{(1)}$ and $\Sigma_j^{(2\to1)}$ correspond to the two self-energy contributions ($i/\hbar\left[\bar{D}_{(1)A}(t),\Delta H_A^{(1)}\right]$ and $\Delta H_A^{(2\to1)}(\bar{D}_{(2)A}(t))$ in equation (5.1), respectively, we get from equations (B.13), (B.16) and (4.17)

$$\left(\Sigma_j^{(1)}\right)_{\rho\rho'}^{\nu\nu'}=i\left(\delta_{\nu\rho}\sum_\mu(\bar{C}_j)_{\mu\mu}^{\rho'\nu'}-\delta_{\nu'\rho'}\sum_\mu(\bar{C}_j)_{\mu\mu}^{\nu\rho}\right)$$

and

$$\left(\Sigma_j^{(2\to 1)}\right)^{\nu\nu'}_{\rho\rho'} = \quad i\Bigg(\sum_\mu \left((\bar{C}_j)^{\nu'\mu}_{\nu\rho'} + (\bar{C}_j)^{\rho'\nu}_{\mu\nu'} - (\bar{C}_j)^{\nu'\nu}_{\mu\rho'} - (\bar{C}_j)^{\rho'\mu}_{\nu\nu'} \right) \left(\bar{D}_{(1)A}\right)_{\rho\mu} + \sum_\mu \left((\bar{C}_j)^{\mu\rho}_{\nu\nu'} - (\bar{C}_j)^{\nu'\nu}_{\rho\mu} - (\bar{C}_j)^{\nu'\rho}_{\nu\mu} - (\bar{C}_j)^{\mu\nu}_{\rho\nu} \right) \left(\bar{D}_{(1)A}\right)_{\mu\rho'} \Bigg).$$

We will write in what follows the QBE (5.3) in the form

$$\frac{d}{dt}\bar{D}_{(1)}(\bar{t}) = \frac{i}{\hbar}\left[\bar{D}_{(1)}(\bar{t}), \hat{H}_0^{(1)}(\bar{t})\right] + \Gamma(\bar{t})\left(\bar{D}_{(1)}(\bar{t})\right) \tag{5.5}$$

with the replacements

$$\begin{aligned} \bar{D}_{(1)A} &\to \bar{D}_{(1)} \\ \Gamma_{\rm tot} &\to \Gamma. \end{aligned} \tag{5.6}$$

Chapter 6

Towards the semi-classical Boltzmann equation

We have not yet left the quantum statistical description. In this chapter, we investigate how the transition towards a classical description can be made. A "test" of the classical structure will be the derivation of the semi-classical Boltzmann equation (SCBE). First, we discuss some properties of the coherent states and introduce the concept of quasi-orthogonality. Then, we will reformulate the QBE in the basis of coherent states and finally use the quasi-orthogonality for the derivation of the SCBE.

6.1 Coherent states

Equation (5.3) describes the coarse grained evolution of the one-particle density matrix $\bar{D}_{(1)}$ in the basis of the eigenvectors $|\nu\rangle$ of $H_0^{(1)}$. This description is quite different from a classical description, where the statistical state is described in terms of a probability distribution function in the one-particle phase space. In order to relate the evolution of the density matrix $\bar{D}_{(1)}$ with the evolution of the electron gas in phase space, we will from now on abandon the basis of the states $|\nu\rangle$ and switch to a description in terms of coherent states, which are represented by the vectors $|\boldsymbol{\alpha}\rangle, \boldsymbol{\alpha} \in \mathbb{C}^3$. Coherent states are localized in the one-particle phase space. The principal properties of coherent states are summarized in appendix C. There, a one-to-one correspondence between the parameter $\boldsymbol{\alpha}$ and the central position $\mathbf{p}$, $\mathbf{q}$ of the corresponding coherent state $|\boldsymbol{\alpha}\rangle$ in the one-particle phase space is established in equation (C.26),

$$\boldsymbol{\alpha} = \frac{\Delta_q \boldsymbol{p} - i\Delta_p \boldsymbol{q}}{\hbar}. \tag{6.1}$$

The parameter $\Delta \equiv \Delta_q$ specifies the width of the coherent states in position space. The corresponding extension Δ_p of the coherent state in momentum

space is obtained from the fact that the Heisenberg inequality is saturated, i.e.,

$$\Delta_p \Delta_q = \frac{\hbar}{2}. \tag{6.2}$$

The Δ parameters will be kept constant throughout our derivations[1] and can therefore be omitted in our short-hand notation. The correspondence (6.1) allows us to introduce the notation (see equation (C.29))

$$|\boldsymbol{\alpha}\rangle \equiv |\mathbf{p}, \mathbf{q}\rangle. \tag{6.3}$$

For our present purposes it is convenient to replace the complex vector $\boldsymbol{\alpha} \in \mathbb{C}^3$ by the vector $\boldsymbol{z} \in \mathbb{R}^6$, where

$$\begin{aligned} \boldsymbol{z} &\equiv (\mathrm{Re}\,(\boldsymbol{\alpha}), \mathrm{Im}\,(\boldsymbol{\alpha})) \\ &= \left(\frac{\Delta_q}{\pi\hbar}\mathbf{p}, \frac{\Delta_p}{\pi\hbar}\mathbf{q} \right). \end{aligned} \tag{6.4}$$

Adopting this notation, we will identify a coherent state by the real vector $\boldsymbol{z}$ rather than by the complex vector $\boldsymbol{\alpha}$, i.e, instead of equation (6.3) we write

$$\begin{aligned} |\boldsymbol{z}\rangle &\equiv |\mathbf{p}(\boldsymbol{z}), \mathbf{q}(\boldsymbol{z})\rangle \\ &= |\mathbf{p}, \mathbf{q}\rangle. \end{aligned}$$

Including also the spin variable $s = \{\frac{1}{2}, -\frac{1}{2}\}$, we obtain the vectors

$$|\boldsymbol{u}\rangle = |\boldsymbol{z}, s\rangle \equiv |\mathbf{p}, \mathbf{q}, s\rangle, \tag{6.5}$$

which form an overcomplete basis in the one-particle space $\mathcal{H}$. In order to keep the notation as simple as possible, the arguments $\boldsymbol{z}$ in the parameters $\mathbf{p}(\boldsymbol{z})$ and $\mathbf{q}(\boldsymbol{z})$ will be omitted, whenever the reference is unambiguous. From equations (6.2), (6.4), and (6.5) we get

$$\int_{\mathcal{A}} d\boldsymbol{u} \cdots = \sum_s \int_{\mathbb{R}^6} d\boldsymbol{z} \cdots = \frac{1}{(2\pi\hbar)^3} \sum_s \int_{\mathbb{R}^6} d^3\mathbf{p}\, d^3\mathbf{q} \cdots,$$

where

$$\mathcal{A} = \{\mathbb{R}^6, s\}$$

denotes the space of integration over the parameter $\boldsymbol{u}$ including the spin variables s.

[1]For practical applications, the choice of the parameter Δ will be important. As this parameter sets the form of the basis vectors, it influences the form of the overlap between basis vectors and it influences the form of representation of the statistical state of the subsystem. For an application to metals near equilibrium a parameter Δ_q larger than the atomic scale will be adequate in most cases.

Using equation (C.47) and taking the orthogonality of the spin functions into account, we obtain a generalized "completeness relation"

$$\int_{\mathcal{A}} d\boldsymbol{u}\, P(\boldsymbol{u}) = \sum_{s} \int_{\mathbb{R}^6} d\boldsymbol{z}\, |\boldsymbol{z}, s\rangle\langle \boldsymbol{z}, s| = \mathbb{1}, \tag{6.6}$$

where $P(\boldsymbol{u})$ denotes the projector

$$P(\boldsymbol{u}) = |\boldsymbol{u}\rangle\langle \boldsymbol{u}|. \tag{6.7}$$

According to equation (C.52) any one-body operator $O \in \mathcal{L}(\mathcal{H})$ can be expressed in the "diagonal representation"

$$O \;=\; \int_{\mathbb{C}^3} d\boldsymbol{\alpha}\, o\,(\boldsymbol{\alpha})\, |\boldsymbol{\alpha}\rangle\langle \boldsymbol{\alpha}|.$$

This holds in particular for the one-particle density matrix $\bar{D}_{(1)}$, which can be written as

$$\bar{D}_{(1)} = \int_{\mathcal{A}} d\boldsymbol{u}\, \rho(\boldsymbol{u}) P(\boldsymbol{u}). \tag{6.8}$$

Obviously, we have the functional dependence

$$\bar{D}_{(1)} = \bar{D}_{(1)}\,[\rho]\,,$$

which implies that the evolution of $\bar{D}_{(1)}$ is completely determined by the evolution of $\rho(\boldsymbol{u})$.

6.1.1 Quasi-orthogonality

Properties of a system are represented by closed subspaces of a complex Hilbert space (see for example [3] and references therein). In a classical description, all properties are compatible, i.e., they are represented by orthogonal subspaces. Equation (C.38)

$$\langle p, q|p', q'\rangle \;=\; e^{-\frac{(p-p')^2}{8\Delta_p^2}}\, e^{-\frac{(q-q')^2}{8\Delta_q^2}}\, e^{\frac{i(p'q-q'p)}{2\hbar}},$$

shows that the basis of coherent states $Z = \{\boldsymbol{z}\}$ consists of non-orthogonal vectors $\langle \boldsymbol{z}|\boldsymbol{z}'\rangle \neq 0,\ \forall\, \boldsymbol{z}, \boldsymbol{z}' \in Z$.

In order to approach a classical description in phase space, we have to introduce the concept of quasi-orthogonality. We define a volume in phase space

$\Omega(\boldsymbol{z}_0)$, centered at $\boldsymbol{z}_0$, with extension Δ_q^Ω in real space and Δ_p^Ω in momentum space, so the volume $\Omega = \left(\Delta_p^\Omega\right)^3 \left(\Delta_q^\Omega\right)^3$. We define the self adjoint operators

$$P_{\Omega(\boldsymbol{z}_0)} = \sum_s \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z}\, |\boldsymbol{z}, s\rangle\langle \boldsymbol{z}, s| \tag{6.9}$$

$$P_{\Omega_c(\boldsymbol{z}_0)} = \sum_s \int\limits_{\Omega_c(\boldsymbol{z}_0)} d\boldsymbol{z}\, |\boldsymbol{z}, s\rangle\langle \boldsymbol{z}, s|, \tag{6.10}$$

where $\Omega_c(\boldsymbol{z}_0)$ is the complement of $\Omega(\boldsymbol{z}_0)$:

$$\Omega_c(\boldsymbol{z}_0) = \mathbb{R}^6 \setminus \Omega(\boldsymbol{z}_0).$$

Equations (6.9) and (6.10) imply

$$P_{\Omega(\boldsymbol{z}_0)} + P_{\Omega_c(\boldsymbol{z}_0)} = \mathbb{1}.$$

In order to get quasi-orthogonal subspaces associated with the coherent states inside and outside the volume we have to show that

$$\begin{aligned}\left(P_{\Omega(\boldsymbol{z}_0)} + P_{\Omega_c(\boldsymbol{z}_0)}\right)^2 \mathcal{H} &= \left(P^2_{\Omega(\boldsymbol{z}_0)} + P^2_{\Omega_c(\boldsymbol{z}_0)} + 2P_{\Omega(\boldsymbol{z}_0)} P_{\Omega_c(\boldsymbol{z}_0)}\right)\mathcal{H} \\ &\approx \left(P^2_{\Omega(\boldsymbol{z}_0)} + P^2_{\Omega_c(\boldsymbol{z}_0)}\right)\mathcal{H}.\end{aligned}$$

This requires that the Hilbert-Schmidt scalar product $\mathrm{Tr}\left(P_{\Omega(\boldsymbol{z}_0)} P_{\Omega_c(\boldsymbol{z}_0)}\right)$ is negligible with respect to $\mathrm{Tr}\left(P_{\Omega(\boldsymbol{z}_0)} P_{\Omega(\boldsymbol{z}_0)}\right) \ll \mathrm{Tr}\left(P_{\Omega_c(\boldsymbol{z}_0)} P_{\Omega_c(\boldsymbol{z}_0)}\right) = \infty$. We can evaluate the trace, for example in the eigenbasis $\{|\gamma\rangle\}$ of $H_0^{(1)}$:

$$\begin{aligned}Tr(P_{\Omega(\boldsymbol{z}_0)} P_{\Omega_c(\boldsymbol{z}_0)}) &= \sum_\gamma \sum_{s,s'} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z} \int\limits_{\Omega_c(\boldsymbol{z}_0)} d\boldsymbol{z}'\, \langle\gamma|\boldsymbol{z}, s\rangle\langle \boldsymbol{z}, s|\boldsymbol{z}', s'\rangle\langle \boldsymbol{z}', s'|\gamma\rangle \\ &= \sum_{s,s'} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z} \int\limits_{\Omega_c(\boldsymbol{z}_0)} d\boldsymbol{z}'\, \delta_{s,s'} \langle \boldsymbol{z}'|\boldsymbol{z}\rangle\langle \boldsymbol{z}|\boldsymbol{z}'\rangle \sum_\gamma \langle\gamma|\gamma\rangle \\ &= \sum_{s,s'} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z} \int\limits_{\Omega_c(\boldsymbol{z}_0)} d\boldsymbol{z}'\, \delta_{s,s'} g(\boldsymbol{z}, \boldsymbol{z}') \\ &= \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{u} \int\limits_{\Omega_c(\boldsymbol{z}_0)} d\boldsymbol{u}'\, \hat{g}(\boldsymbol{u}, \boldsymbol{u}')\end{aligned} \tag{6.11}$$

where we have defined

$$\hat{g}(\boldsymbol{u}, \boldsymbol{u}') = \delta_{ss'} g(\boldsymbol{z}, \boldsymbol{z}') \tag{6.12}$$

with

$$\begin{aligned} g(\boldsymbol{z},\boldsymbol{z}') &= \left|\langle \boldsymbol{z}|\boldsymbol{z}'\rangle\right|^2 \\ &\overset{(C.38)}{=} e^{-\left(\frac{(\mathbf{p}-\mathbf{p}')\Delta}{\hbar}\right)^2} e^{-\left(\frac{\mathbf{q}-\mathbf{q}'}{2\Delta}\right)^2}. \end{aligned} \tag{6.13}$$

The function $\hat{g}$ is symmetric in $\boldsymbol{u},\boldsymbol{u}'$ and can be expressed as the Hilbert-Schmidt product of the projectors $P(\boldsymbol{u})$ and $P(\boldsymbol{u}')$ defined in equation (6.7),

$$\begin{aligned} \hat{g}(\boldsymbol{u},\boldsymbol{u}') &= \mathrm{Tr}\left(P(\boldsymbol{u})P(\boldsymbol{u}')\right) \\ &= \left|\langle \boldsymbol{u}|\boldsymbol{u}'\rangle\right|^2 \\ &= \hat{g}(\boldsymbol{u}',\boldsymbol{u}). \end{aligned} \tag{6.14}$$

The function $\hat{g}$ satisfies the normalization condition

$$\int\limits_{\mathcal{A}} d\boldsymbol{u}\, \hat{g}(\boldsymbol{u},\boldsymbol{u}') = \langle \boldsymbol{u}'|\boldsymbol{u}'\rangle = 1. \tag{6.15}$$

Equation (6.13) implies

$$\int\limits_{\mathbb{R}^6} d\boldsymbol{z}' g(\boldsymbol{z},\boldsymbol{z}') \approx \int\limits_{\Omega(\boldsymbol{z})} d\boldsymbol{z}' g(\boldsymbol{z},\boldsymbol{z}') \text{ , for } \Delta_q^\Omega \gg \Delta_q \text{ and } \Delta_p^\Omega \gg \Delta_p. \tag{6.16}$$

Equation (6.11) only has contributions from the surface region S_Ω between $\Omega(\boldsymbol{z}_0)$ and $\Omega_c(\boldsymbol{z}_0)$, which is determined by the function g (6.16). The function g is gaussian shaped with respect to the distance of $\boldsymbol{u}$ and $\boldsymbol{u}'$ in phase space (6.13), so the width of the contributing surface volume is about $(2\Delta_p\Delta_q)^3 = \hbar^3$.

The Hilbert-Schmidt scalar product $\mathrm{Tr}\left(P_{\Omega(\boldsymbol{z}_0)}P_{\Omega(\boldsymbol{z}_0)}\right)$ has contributions from the whole volume Ω. Accordingly, we have

$$\left|\frac{\mathrm{Tr}\left(P_{\Omega(\boldsymbol{z}_0)}P_{\Omega_c(\boldsymbol{z}_0)}\right)}{\mathrm{Tr}\left(P_{\Omega(\boldsymbol{z}_0)}P_{\Omega(\boldsymbol{z}_0)}\right)}\right| \approx \frac{S_{\Omega(\boldsymbol{z}_0)}}{\Omega(\boldsymbol{z}_0)} < \epsilon \ll 1. \tag{6.17}$$

For sufficiently large phase space volumes $\Omega(\boldsymbol{z}_0)$ we may assume the projectors $P_{\Omega(\boldsymbol{z}_0)}$ and $P_{\Omega_c(\boldsymbol{z}_0)}$ to be practically orthogonal. The parameter ϵ defines the accuracy to which the subspaces generated by the coherent states centered inside and outside the volume $\Omega(\boldsymbol{z}_0)$ may be considered to be orthogonal. It is always non-zero, but it may be chosen arbitrarily small. A small ϵ corresponds to large volumes Ω.

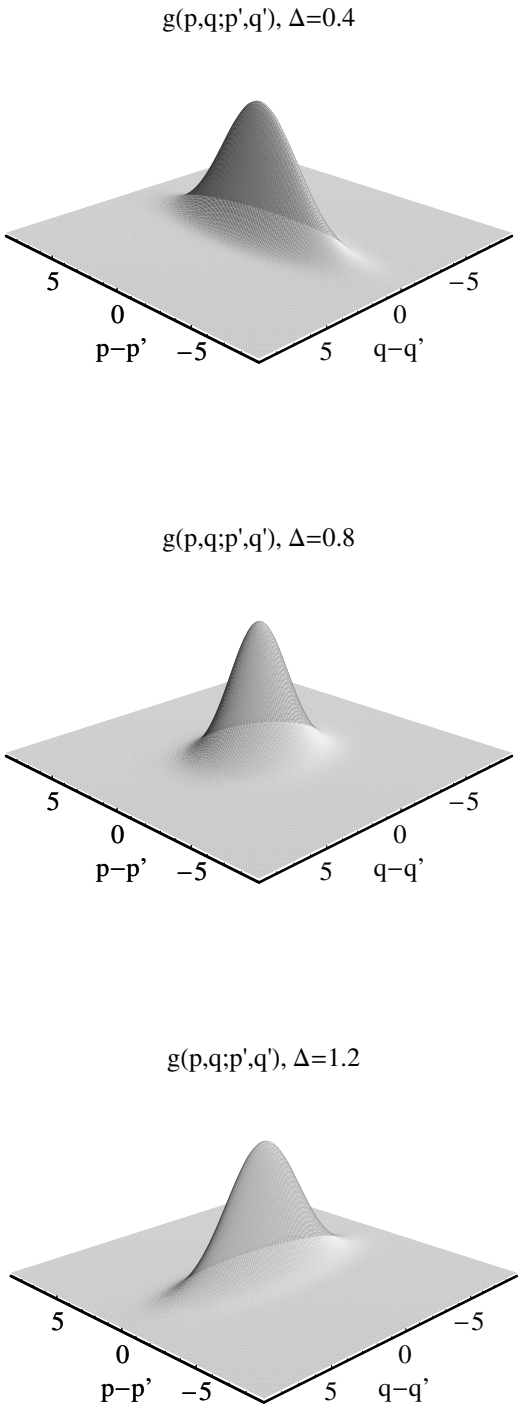

Figure 6.1: Plot of the function $g(\boldsymbol{z}, \boldsymbol{z}') = g(\mathbf{p}, \mathbf{q}; \mathbf{p}', \mathbf{q}')$ (see equation (6.13)) as function of the real space distance $\mathbf{q} - \mathbf{q}'$ and the momentum space distance $\mathbf{p} - \mathbf{p}'$ for three different values of $\Delta = \Delta_q$ and $\hbar = 1$.

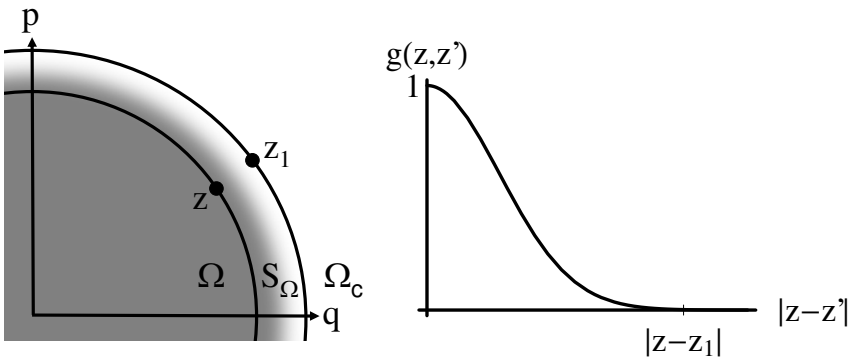

Figure 6.2: The volume Ω, the surface S_Ω, the complement Ω_c and the function $g(\boldsymbol{z}, \boldsymbol{z}')$.

6.1.2 Probability distribution in phase space

We will show that the average $\bar{\rho}_\Omega$ of the function ρ over a volume Ω in phase space can be interpreted as a probability distribution.

From equation (6.8) and the positivity of the one-particle density matrix we get[2]

$$\begin{aligned} p(\boldsymbol{u}) &\equiv \mathrm{Tr}\left(\bar{D}_{(1)} P(\boldsymbol{u})\right) \\ &= \langle \boldsymbol{u}|\bar{D}_{(1)}|\boldsymbol{u}\rangle \\ &= \int\limits_{\mathcal{A}} d\boldsymbol{u}'\, \rho(\boldsymbol{u}')\hat{g}(\boldsymbol{u}, \boldsymbol{u}') \geq 0 \end{aligned} \tag{6.18}$$

with

$$\int\limits_{\mathcal{A}} d\boldsymbol{u}\, p(\boldsymbol{u}) = \int\limits_{\mathcal{A}} d\boldsymbol{u}\, \rho(\boldsymbol{u}) = \mathrm{Tr}\left(\bar{D}_{(1)}\right) = 1. \tag{6.19}$$

The integral equation (6.18) relates the functions $p(\boldsymbol{u})$ and $\rho(\boldsymbol{u})$. We note that, in contrast with $p(\boldsymbol{u})$, the function $\rho(\boldsymbol{u})$ is not necessarily positive everywhere in phase space. Since ρ and p satisfy the normalization condition (6.19) and due to the quasi-orthogonality of subspaces (6.17), it is possible to choose

[2]Strictly speaking, the positivity of the *coarse grained* one-particle density matrix $\bar{D}_{(1)}$ is not always guaranteed, i.e., for some vectors $|\gamma\rangle \in \mathcal{H}$ the expectation value $\langle\gamma|\bar{D}_{(1)}|\gamma\rangle$ may be slightly negative. This deviation from the von Neumann properties of a density matrix is unavoidable if one considers the evolution of the subsystem on the true time scale, but it scales with the strength of the interaction and thus remains negligible. In the following we will assume the positivity of the matrix elements $\langle \boldsymbol{u}|\bar{D}_{(1)}|\boldsymbol{u}\rangle$ where $|\boldsymbol{u}\rangle$ denotes a coherent state.

sufficiently large cell volumes Ω in phase space, so that the mean value taken over a subvolume $\Omega(\boldsymbol{z}_0)$

$$\bar{\rho}_\Omega(\boldsymbol{z}_0, s) \;=\; \frac{1}{\Omega} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z}\; \rho(\boldsymbol{z}, s)$$

becomes positive and can be interpreted as a probability distribution associated with the subvolume $\Omega(\boldsymbol{z}_0)$. Equation (6.18) shows that for a given $\bar{D}_{(1)}$ the function ρ depends on the parameter Δ characterizing the width of the coherent states. We make the assumption that the parameter Δ may be chosen in a way that the one-particle density matrix $\bar{D}_{(1)}(t)$ can be represented by functions

$$|\rho(\boldsymbol{u})| \leq 1. \tag{6.20}$$

See also the comment after equation (C.58). Assumption (6.20) is necessary for the following demonstration and for the derivation of the SCBE only, but it is not necessary for the reformulation of the quantum Boltzmann equation (QBE) in phase space.

From equation (6.16) and (6.20) it follows that in equation (6.18) we can restrict the integration over $|\boldsymbol{z}'\rangle = |\mathbf{p}', \mathbf{q}'\rangle$ to vectors close to $|\boldsymbol{z}\rangle = |\mathbf{p}, \mathbf{q}\rangle$, i.e.,

$$\int\limits_{\mathcal{A}} d\boldsymbol{u}' \rho\left(\boldsymbol{u}'\right) g(\boldsymbol{u}, \boldsymbol{u}') \approx \int\limits_{\Omega(\boldsymbol{z})} d\boldsymbol{z}' \rho\left(\boldsymbol{z}', s\right) g(\boldsymbol{z}, \boldsymbol{z}'). \tag{6.21}$$

Then we get

$$\begin{aligned}
0 \quad &\leq \quad \bar{p}_\Omega(\boldsymbol{z}_0, s) \equiv \frac{1}{\Omega} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z}\, p(\boldsymbol{z}, s) = \frac{1}{\Omega} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z}\;\; \langle \boldsymbol{z}, s | \bar{D}_{(1)} | \boldsymbol{z}, s \rangle \\
&\overset{(6.18)}{=} \quad \frac{1}{\Omega} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z} \int\limits_{\mathbb{R}^6} d\boldsymbol{z}'\, \rho(\boldsymbol{z}', s) g(\boldsymbol{z}, \boldsymbol{z}') \\
&\overset{(6.21)}{\approx} \quad \frac{1}{\Omega} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z}'\, \rho(\boldsymbol{z}', s) g(\boldsymbol{z}, \boldsymbol{z}') \\
&= \quad \frac{1}{\Omega} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z}'\, \rho(\boldsymbol{z}', s) \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z}\, g(\boldsymbol{z}, \boldsymbol{z}') \\
&\overset{(6.17)}{\approx} \quad \frac{1}{\Omega} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z}'\, \rho(\boldsymbol{z}', s) \int\limits_{\mathbb{R}^6} d\boldsymbol{z}\, g(\boldsymbol{z}, \boldsymbol{z}') \\
&\overset{(6.15)}{=} \quad \frac{1}{\Omega} \int\limits_{\Omega(\boldsymbol{z}_0)} d\boldsymbol{z}'\, \rho(\boldsymbol{z}', s) \\
&\equiv \quad \bar{\rho}_\Omega(\boldsymbol{z}_0, s).
\end{aligned} \tag{6.22}$$

From equation (6.19) we get

$$\begin{aligned}\int\limits_{\mathcal{A}} d\boldsymbol{u}\,\rho(\boldsymbol{u}) &= \sum_s \int\limits_{\mathbb{R}^6} d\boldsymbol{z}\,\rho(\boldsymbol{z},s)\\ &= \int\limits_{\mathbb{R}^6} d\boldsymbol{z}\,\frac{1}{\Omega}\int\limits_{\Omega(\boldsymbol{z})} d\boldsymbol{z}'\,\rho(\boldsymbol{z}',s)\\ &= 1\end{aligned}$$

and thus

$$\int\limits_{\mathcal{A}} d\boldsymbol{u}\,\bar{\rho}_\Omega(\boldsymbol{u}) = 1. \tag{6.23}$$

The quasi-orthogonality expressed by equation (6.17), put together with equations (6.22) and (6.23), allows us to interpret $\bar{\rho}_\Omega(\boldsymbol{z},s) \geq 0$ as the probability density in phase space at $\boldsymbol{z}$, which describes the distribution of electrons with spin s on the scale of the volume Ω.

The functions $\rho(\boldsymbol{u})$ and $p(\boldsymbol{u})$ are related by the integral equation Eq. (6.18). A method of is presented in Appendix (C.2).

6.2 Quantum Boltzmann equation in phase space

After it has been shown in the last section, that it is possible to introduce the concept of quasi-orthogonality, the reader should be motivated to continue and to see how the bridge between the QBE derived in chapter 5 and the SCBE can be built, because that is what we will do in this section. We reformulate the QBE in the basis of coherent states and add an assumption about the statistical state of the subsystem.

6.2.1 Transformation into the basis of coherent states

The QBE (5.5)

$$\frac{d}{dt}\bar{D}_{(1)}(t) = \frac{i}{\hbar}\left[\bar{D}_{(1)}(t), \hat{H}_0^{(1)}(t)\right] + \Gamma\big(\bar{D}_{(1)}(t)\big),$$

is transformed into the basis of coherent states. The existence of the "diagonal representation" (6.8) implies that we only need to calculate $\langle\boldsymbol{u}|\ldots|\boldsymbol{u}\rangle$ to completely describe the evolution of $\bar{D}_{(1)}$. Then the QBE reads in the basis of coherent states

$$\begin{aligned}\frac{d}{dt}\left(\langle\boldsymbol{u}|\bar{D}_{(1)}(t)|\boldsymbol{u}\rangle\right) &= \langle\boldsymbol{u}|\frac{i}{\hbar}\left[\bar{D}_{(1)}(t), \hat{H}_0^{(1)}(t)\right]|\boldsymbol{u}\rangle\\ &\quad + \langle\boldsymbol{u}|\Gamma\big(\bar{D}_{(1)}(t)\big)|\boldsymbol{u}\rangle.\end{aligned} \tag{6.24}$$

With (6.18) we obtain the corresponding QBE for $\rho(\boldsymbol{u})$, which defines the complete density matrix $\bar{D}_{(1)}$ (see equations (6.8), (C.47)).

The last term in equation (6.24) expresses the action of the linear superoperator $\Gamma(t) \in \mathcal{L}(\mathcal{L}(\mathcal{H}))$ on $\bar{D}_{(1)}(t) \in \mathcal{L}(\mathcal{H})$. In our derivation of the master equations this superoperator has been defined in terms of its matrix elements $\Gamma^{\kappa\lambda}_{\nu\mu}(t)$ in the basis of the eigenvectors of the one-body operator $H_0^{(1)}$ (see equation (5.4)). According to the replacements (5.6) and remembering that the coherent states satisfy the closure relation (6.6), the action of the superoperator Γ can be expressed in the basis of coherent states as

$$\begin{aligned}&\langle \boldsymbol{u}|\Gamma(Y)|\boldsymbol{u}'\rangle = \\ &\int_{\mathcal{A}} d\boldsymbol{u}'' \int_{\mathcal{A}} d\boldsymbol{u}''' \; \Gamma\left(\boldsymbol{u},\boldsymbol{u}';\boldsymbol{u}'',\boldsymbol{u}'''\right) \; \langle \boldsymbol{u}''|Y|\boldsymbol{u}'''\rangle, \; \forall\, Y \in \mathcal{L}(\mathcal{H})\end{aligned} \tag{6.25}$$

with

$$\Gamma\left(\boldsymbol{u},\boldsymbol{u}';\boldsymbol{u}'',\boldsymbol{u}'''\right) = \sum_{\nu\mu\kappa\lambda} \langle \boldsymbol{u}''|\kappa\rangle\langle \boldsymbol{u}|\nu\rangle \Gamma^{\kappa\lambda}_{\nu\mu} \langle\lambda|\boldsymbol{u}'''\rangle\langle\mu|\boldsymbol{u}'\rangle.$$

Written in the explicit form of equation (6.25), the last term in equation (6.24) reads

$$\langle \boldsymbol{u}|\Gamma\big(\bar{D}_{(1)}(t)\big)|\boldsymbol{u}\rangle = \int_{\mathcal{A}} d\boldsymbol{u}' \int_{\mathcal{A}} d\boldsymbol{u}'' \; \Gamma\left(\boldsymbol{u},\boldsymbol{u};\boldsymbol{u}',\boldsymbol{u}''\right) \; \langle \boldsymbol{u}'|\bar{D}_{(1)}(t)|\boldsymbol{u}''\rangle. \tag{6.26}$$

With the diagonal representation of $\bar{D}_{(1)}$ (equation (C.52)) and the explicit form (6.26), equation (5.5) reads in the basis of coherent states,

$$\begin{aligned}\int_{\mathcal{A}} d\boldsymbol{u}' \hat{g}(\boldsymbol{u},\boldsymbol{u}') \frac{d\rho(\boldsymbol{u}',t)}{dt} \;&=\; \int_{\mathcal{A}} d\boldsymbol{u}' \rho(\boldsymbol{u}',t) \langle \boldsymbol{u}|\frac{i}{\hbar}\left[P(\boldsymbol{u}'), \hat{H}_0^{(1)}(t)\right]|\boldsymbol{u}\rangle \\ &+ \int_{\mathcal{A}} d\boldsymbol{u}' \int_{\mathcal{A}} d\boldsymbol{u}'' \int_{\mathcal{A}} d\boldsymbol{u}''' \rho(\boldsymbol{u}',t) \Gamma\left(\boldsymbol{u},\boldsymbol{u};\boldsymbol{u}'',\boldsymbol{u}'''\right) \\ &\qquad \cdot \langle \boldsymbol{u}''|P(\boldsymbol{u}')|\boldsymbol{u}'''\rangle\end{aligned} \tag{6.27}$$

where we have used equations (6.7) and (6.14).

This equation contains the full quantum statistical information of equation (5.5), no further approximations or assumptions having been made.

6.2.2 Quantum Boltzmann equation

In this section we will make the assumption that the function $\rho(.)$ depends only weakly on its arguments so on the scale of Δ_p, Δ_q it can be described by the first-order terms of a Taylor expansion. Then the second term in equation (6.27) can be treated in more detail.

Expectation values $\langle \boldsymbol{u}| \left[\bar{D}_{(1)}(t), \hat{H}_0^{(1)}(t)\right] |\boldsymbol{u}\rangle$

The one-particle Hamiltonian is composed of the kinetic energy and the potential[3],

$$\hat{H}_0 = T + V.$$

In order to evaluate the commutator $\langle \boldsymbol{u}| \frac{i}{\hbar} \left[\bar{D}_{(1)}, \hat{H}_0^{(1)}(t)\right] |\boldsymbol{u}\rangle$, we treat the contributions T and V separately.

We start with the potential part $\langle \boldsymbol{u}| \frac{i}{\hbar} \left[\bar{D}_{(1)}, V\right] |\boldsymbol{u}\rangle$. For

$$V(\mathbf{x}) = \int\limits_{\mathbb{R}^3} d^3\mathbf{k} e^{i\mathbf{k}\mathbf{x}} \hat{V}(\mathbf{k})$$

and with the real-space representation of the coherent states equation (C.31)

$$\langle \mathbf{x}|\mathbf{p},\mathbf{q}\rangle = \left(\frac{1}{2\pi\Delta^2}\right)^{\frac{3}{4}} e^{-\left(\frac{\mathbf{x}-\mathbf{q}}{2\Delta}\right)^2} e^{\frac{i\mathbf{p}\left(\mathbf{x}-\frac{\mathbf{q}}{2}\right)}{\hbar}},$$

we obtain

$$\begin{aligned} &\langle \mathbf{p},\mathbf{q},s|V|\mathbf{p}',\mathbf{q}',s'\rangle = \\ &\delta_{ss'} \int\limits_{\mathbb{R}^3} d^3\mathbf{k} \hat{V}(\mathbf{k}) e^{-\frac{(\mathbf{q}-\mathbf{q}')^2}{8\Delta^2}} e^{-\frac{\Delta^2(\mathbf{p}-\mathbf{p}'-\hbar\mathbf{k})^2}{2\hbar^2}} e^{\frac{i(\mathbf{p}'\mathbf{q}-\mathbf{p}\mathbf{q}'+\hbar\mathbf{k}(\mathbf{q}+\mathbf{q}'))}{2\hbar}}. \end{aligned} \tag{6.28}$$

For $\mathbf{q}' = \mathbf{q}$, $\mathbf{p}' = \mathbf{p}$ and $s = s'$ this reduces to

$$\begin{aligned} \langle \mathbf{p},\mathbf{q}|V|\mathbf{p},\mathbf{q}\rangle &= \int\limits_{\mathbb{R}^3} d^3\mathbf{k} \hat{V}(\mathbf{k}) e^{-\frac{\Delta^2\mathbf{k}^2}{2}} e^{i\mathbf{k}\mathbf{q}} \\ &= \int\limits_{\mathbb{R}^3} d^3\mathbf{k}\, \hat{\bar{V}}(\mathbf{k})\, e^{i\mathbf{k}\mathbf{q}} \\ &= \bar{V}(\mathbf{q}), \end{aligned}$$

where

$$\hat{\bar{V}}(\mathbf{k}) = e^{-\frac{\Delta^2\mathbf{k}^2}{2}} \hat{V}(\mathbf{k})$$

describes the Fourier components of the one-particle potential, as it is seen on the scale of the coherent states $|\mathbf{p},\mathbf{q}\rangle$. Using the definition (C.45), and introducing the potential operator V^c by

$$V^c = \int\limits_{\mathbb{R}^3} d^3\mathbf{k} \hat{V}(\mathbf{k}) e^{i\mathbf{k}\vec{\mathcal{Q}}_R}, \tag{6.29}$$

[3]In order to simplify the notation, the kinetic energy operator and the potential operator will be denoted V, T instead of $\hat{V}, \hat{T}$ from now on. The hats in the functions $\hat{V}(\mathbf{k})$ are used to denote the Fourier transforms.

we evaluate

$$\begin{aligned}
\langle \mathbf{p},\mathbf{q},s|e^{i\mathbf{k}\vec{\mathcal{Q}}_R}|\mathbf{p}',\mathbf{q}',s'\rangle &= \delta_{s,s'}e^{i\mathbf{k}\mathbf{q}'}\ \langle \mathbf{p},\mathbf{q}|e^{i\mathbf{k}\left(\vec{\mathcal{Q}}_R-\mathbf{q}'\right)}|\mathbf{p}',\mathbf{q}'\rangle \\
&= \delta_{s,s'}e^{i\mathbf{k}\mathbf{q}'}\ \langle \mathbf{p},\mathbf{q}|e^{i\mathbf{k}\left(-i\hbar\frac{\partial}{\partial\mathbf{p}'}|_R-\frac{\mathbf{q}'}{2}\right)}|\mathbf{p}',\mathbf{q}'\rangle \\
&= \delta_{s,s'}e^{\frac{i\mathbf{k}\mathbf{q}'}{2}}\ \langle \mathbf{p},\mathbf{q}|e^{\hbar\mathbf{k}\frac{\partial}{\partial\mathbf{p}'}|_R}|\mathbf{p}',\mathbf{q}'\rangle \\
&= \delta_{s,s'}e^{\frac{i\mathbf{k}\mathbf{q}'}{2}}\langle \mathbf{p},\mathbf{q}|\mathbf{p}'+\hbar\mathbf{k},\mathbf{q}'\rangle \\
&\overset{(C.38)}{=} \delta_{s,s'}e^{\frac{i\mathbf{k}\mathbf{q}'}{2}}e^{-\frac{(\mathbf{p}-\mathbf{p}'-\hbar\mathbf{k})^2\Delta^2}{2\hbar^2}}e^{-\frac{(\mathbf{q}-\mathbf{q}')^2}{8\Delta^2}}e^{\frac{i((\mathbf{p}'+\hbar\mathbf{k})\mathbf{q}-\mathbf{q}'\mathbf{p})}{2\hbar}} \\
&= \delta_{s,s'}e^{\frac{i\mathbf{k}(\mathbf{q}+\mathbf{q}')}{2}}e^{-\frac{(\mathbf{p}-\mathbf{p}'-\hbar\mathbf{k})^2\Delta^2}{2\hbar^2}}e^{-\frac{(\mathbf{q}-\mathbf{q}')^2}{8\Delta^2}}e^{\frac{i(\mathbf{p}'\mathbf{q}-\mathbf{q}'\mathbf{p})}{2\hbar}}.
\end{aligned} \tag{6.30}$$

Comparing equations (6.28) and (6.30) we find that

$$\langle \mathbf{p},\mathbf{q},s|V|\mathbf{p}',\mathbf{q}',s'\rangle = \langle \mathbf{p},\mathbf{q},s|V^c|\mathbf{p}',\mathbf{q}',s'\rangle. \tag{6.31}$$

Equation (6.31) implies that, using the basis of coherent states, we can always replace V by V^c. From the above calculation and the definition of the operator $\vec{\mathcal{Q}}_L$ (C.45)

$$\vec{\mathcal{Q}}_L = \ i\hbar\,\frac{\partial}{\partial\mathbf{p}}\bigg|_L + \frac{\mathbf{q}}{2},$$

it follows immediately that we also have

$$V^c = \int\limits_{\mathbb{R}^3} d^3\mathbf{k}\hat{V}(\mathbf{k})e^{i\mathbf{k}\vec{\mathcal{Q}}_L}.$$

Thus, expressing $\bar{D}_{(1)}$ in the diagonal representation equation (6.8), we can write the expectation value of the commutator $\left[\bar{D}_{(1)},V\right]$ in terms of the expectation value

$$\begin{aligned}
\langle \boldsymbol{u}|\frac{i}{\hbar}\left[\bar{D}_{(1)},e^{i\mathbf{k}\vec{\mathcal{Q}}_{R(L)}}\right]|\boldsymbol{u}\rangle &= \frac{i}{\hbar}\Big(\ \langle \boldsymbol{z}|\bar{D}_{(1)}e^{i\mathbf{k}\vec{\mathcal{Q}}_{R(L)}}|\boldsymbol{z}\rangle - \ \langle \boldsymbol{z}|e^{i\mathbf{k}\vec{\mathcal{Q}}_{R(L)}}\bar{D}_{(1)}|\boldsymbol{z}\rangle\Big) \\
&= \frac{i}{\hbar}\left(e^{i\mathbf{k}\vec{\mathcal{Q}}_R}-e^{i\mathbf{k}\vec{\mathcal{Q}}_L}\right)\ \langle \boldsymbol{z}|\bar{D}_{(1)}|\boldsymbol{z}\rangle.
\end{aligned} \tag{6.32}$$

The operator $\bar{D}_{(1)}$ is given by equation (6.8), so that we have to calculate the terms

$$\frac{1}{(2\pi\hbar)^3}\sum_s\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,\rho(\mathbf{p}',\mathbf{q}',s)\langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle e^{i\mathbf{k}\vec{\mathcal{Q}}_R}\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle \tag{6.33}$$

and

$$\frac{1}{(2\pi\hbar)^3}\sum_s\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,\rho(\mathbf{p}',\mathbf{q}',s)e^{i\mathbf{k}\vec{\mathcal{Q}}_L}\langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle. \tag{6.34}$$

From now on we will make the assumption mentioned at the beginning of this section: we assume that, on the scale of Δ_p and Δ_q the function $\rho(\mathbf{p},\mathbf{q},s)$ depends only weakly on its arguments[4]. Then, due to the presence of the overlap matrix elements $\langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle$ and $\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle$ under the integrals, we can approximate the function $\rho(\mathbf{p}',\mathbf{q}',s)$ by

$$\rho(\mathbf{p}',\mathbf{q}',s) \approx \rho(\mathbf{p},\mathbf{q},s) + \left(\mathbf{p}'-\mathbf{p}\right)\frac{\partial\rho(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}} + \left(\mathbf{q}'-\mathbf{q}\right)\frac{\partial\rho(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{q}}. \quad (6.35)$$

Thus, the first term given by equation (6.33) can be expressed in terms of the integrals

$$\frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,\langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle e^{i\mathbf{k}\vec{\mathcal{Q}}_R}\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle \begin{cases} 1 & \text{(a)} \\ (\mathbf{p}'-\mathbf{p}) & \text{(b)} \\ (\mathbf{q}'-\mathbf{q}) & \text{(c)}\,. \end{cases} \quad (6.36)$$

Similarly, for the second term given by equation (6.34) we have to calculate

$$\frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,e^{i\mathbf{k}\vec{\mathcal{Q}}_L}\langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle \begin{cases} 1 & \text{(a)} \\ (\mathbf{p}'-\mathbf{p}) & \text{(b)} \\ (\mathbf{q}'-\mathbf{q}) & \text{(c)}\,. \end{cases} \quad (6.37)$$

The integrals (6.36) and (6.37) are calculated in appendix C.5. From equations (6.29), (6.32), (6.35), and the results for the integrals (6.36) and (6.37), which are given by equations (C.70), (C.71) for the contributions (a), by equations (C.72), (C.73) for the contributions (b), and by equations (C.74), (C.75) for the contributions (c), we finally obtain

$$\begin{aligned}
\langle \boldsymbol{u}|\frac{i}{\hbar}\left[\bar{D}_{(1)},V\right]|\boldsymbol{u}\rangle &= \frac{i}{\hbar}\sum_s\int\limits_{\mathbb{R}^3} d^3\mathbf{k}\,\hat{V}(\mathbf{k})\,\langle \boldsymbol{u}|\left[\bar{D}_{(1)},e^{i\mathbf{k}\vec{\mathcal{Q}}_L}|s\rangle\langle s|\right]|\boldsymbol{u}\rangle \\
&= \frac{i}{\hbar}\sum_s\int\limits_{\mathbb{R}^3} d^3\mathbf{k}\,\hat{V}(\mathbf{k})\hbar\mathbf{k}e^{-\frac{\Delta^2\mathbf{k}^2}{2}}e^{i\mathbf{k}\mathbf{q}}\frac{\partial\rho(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}} \\
&= \frac{\partial}{\partial\mathbf{q}}\left(\int\limits_{\mathbb{R}^3} d^3\mathbf{k}\,\hat{V}(\mathbf{k})e^{-\frac{\Delta^2\mathbf{k}^2}{2}}e^{i\mathbf{k}\mathbf{q}}\right)\frac{\partial\rho(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}} \\
&= \frac{\partial V^c(\mathbf{q})}{\partial\mathbf{q}}\frac{\partial\rho(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}}. \qquad (6.38)
\end{aligned}$$

[4]The here requested smooth behavior of the function $\rho(\boldsymbol{z},s)$ must be seen as a supplementary condition for the statistical state of the considered subsystem. We remind the reader that we are investigating the conditions for which the evolution of the subsystem can be described by the SCBE. Clearly, we cannot expect or pretend that this covers the whole range of experiments in solid state physics. Nevertheless, the large success of this type of approach indicates that many experimental situations can be described by one-particle density matrices where the functions $\rho(\boldsymbol{z},s)$ satisfy conditions (6.20) and (6.35).

The remaining expectation value

$$\langle \boldsymbol{u}| \frac{i}{\hbar} \left[\bar{D}_{(1)}, T \right] |\boldsymbol{u}\rangle$$

is calculated in appendix C.6. There we obtain equation (C.80)

$$\langle \boldsymbol{u}| \frac{i}{\hbar} \left[\bar{D}_{(1)}, T \right] |\boldsymbol{u}\rangle = -\frac{\mathbf{p}}{m} \frac{\partial \rho(\mathbf{p}, \mathbf{q}, s)}{\partial \mathbf{q}}. \tag{6.39}$$

After insertion of the results (C.76) and (6.39) into equation (6.27), we obtain the QBE for ρ expressed in the basis of coherent states

$$\begin{aligned} \int_{\mathcal{A}} d\boldsymbol{u}' \; \hat{g}\left(\boldsymbol{u}, \boldsymbol{u}'\right) \frac{d\rho(\boldsymbol{u}')}{dt} &= \frac{\partial V^c(\mathbf{q})}{\partial \mathbf{q}} \frac{\partial \rho(\mathbf{p}, \mathbf{q}, s)}{\partial \mathbf{p}} - \frac{\mathbf{p}}{m} \frac{\partial \rho(\mathbf{p}, \mathbf{q}, s)}{\partial \mathbf{q}} \\ &+ \int_{\mathcal{A}} d\boldsymbol{u}' \int_{\mathcal{A}} d\boldsymbol{u}'' \, \Gamma\left(\boldsymbol{u}, \boldsymbol{u}; \boldsymbol{u}', \boldsymbol{u}''\right) \\ &\int_{\mathcal{A}} d\boldsymbol{u}''' \, \rho(\boldsymbol{u}''') \, \langle \boldsymbol{u}'|\boldsymbol{u}'''\rangle \langle \boldsymbol{u}'''|\boldsymbol{u}''\rangle. \end{aligned} \tag{6.40}$$

Note that the function $\hat{g}\left(\boldsymbol{u}, \boldsymbol{u}'\right)$ under the integral on the left-hand side is positive and normalized to 1 (see equations (6.14) and (6.15)). Due to the quasi-orthogonality (6.17) we can restrict the integration over the $\boldsymbol{z}'$-part of $\boldsymbol{u}'$ to a limited region $\Omega(\boldsymbol{z})$, with $\Delta^{\Omega} \gg \Delta$ around $\boldsymbol{z} = (\mathbf{p}, \mathbf{q})$.

Apart from the spin variable s, the first two terms on the right-hand side depend only on $\mathbf{p}$ and $\mathbf{q}$. They have the form of the drift and diffusion terms in the SCBE. It should be kept in mind, however, that the function ρ does not describe a probability distribution.

We note that, apart from equation (6.35), we have not made any restrictive assumptions to derive the QBE in the basis of coherent states (6.40) from the QBE equation in the energy-eigenbasis (5.3). Thus, it is clear that the QBE (6.40) still properly accounts for the "quantum" evolution on small scales. We will show how – based on this equation – also the "classical" evolution on large scales appears. But first we take a closer look at the last term in equation (6.40).

Locality of Γ

The superoperator Γ describes the influence of the electron-electron interaction and of the electron-bath interaction on the evolution of $\langle \boldsymbol{u}|\bar{D}_{(1)}(t)|\boldsymbol{u}\rangle$. It corresponds to the "collision term" in the Boltzmann description of a classical gas. The one-body operators $Q^A_{j\alpha}, A_\alpha \in \mathcal{L}(\mathcal{H})$ entering the interaction Hamiltonian are local operators, i.e.,

$$\begin{aligned} \langle \mathbf{p}, \mathbf{q}, s|A_\alpha|\mathbf{p}', \mathbf{q}', s\rangle &\cong 0 \quad \text{for} \quad \left|\mathbf{q} - \mathbf{q}'\right| > d_q \quad \forall \alpha \\ \langle \mathbf{p}, \mathbf{q}, s|Q^A_{j\alpha}|\mathbf{p}', \mathbf{q}', s\rangle &\cong 0 \quad \text{for} \quad \left|\mathbf{q} - \mathbf{q}'\right| > d_q, \quad \forall j, \, \alpha \end{aligned}$$

with

$$d_q \;>\; \Delta_q.$$

Recognizing that the Γ term represents contributions of second order in the interaction, one sees immediately that the function $\Gamma(\boldsymbol{u},\boldsymbol{u};\boldsymbol{u}',\boldsymbol{u}'')$ only gives significant contributions when the coherent state $|\boldsymbol{u}\rangle = |\boldsymbol{z},s\rangle$ overlaps in real space with $|\boldsymbol{u}'\rangle = |\boldsymbol{z}',s'\rangle$ and also with $|\boldsymbol{u}''\rangle = |\boldsymbol{z}'',s''\rangle$. This implies

$$\begin{aligned} \left|\mathbf{q}'-\mathbf{q}\right| &\leq 2d_q, \\ \left|\mathbf{q}''-\mathbf{q}\right| &\leq 2d_q, \end{aligned} \tag{6.41}$$

i.e., the coherent states $|\boldsymbol{u}'\rangle$ and $|\boldsymbol{u}''\rangle$ leading to non-negligible $\Gamma(\boldsymbol{u},\boldsymbol{u};\boldsymbol{u}',\boldsymbol{u}'')$ contributions are themselves linked by the condition

$$\left|\mathbf{q}'-\mathbf{q}''\right| < 4d_q. \tag{6.42}$$

From equations (6.41) and (6.42) it follows that the "final" states $|\boldsymbol{u}'\rangle$ and $|\boldsymbol{u}''\rangle$ are located in the same spatial region as the "initial" state $|\boldsymbol{u}\rangle$, i.e., the spatial centers $\mathbf{q}'$ and $\mathbf{q}''$ are close to the spatial center $\mathbf{q}$ of the "initial" state.

We make the hypothesis that Δ_q has been chosen to be in the same order of magnitude of d_q

$$\Delta_q \simeq d_q.$$

From the diagonal representation of the one-particle density matrix we obtain

$$\langle \boldsymbol{u}'|\bar{D}_{(1)}(t)|\boldsymbol{u}''\rangle = \int\limits_{\mathbb{C}^3} d\boldsymbol{u}\,\rho(\boldsymbol{u})\,\langle \boldsymbol{u}'|\boldsymbol{u}\rangle\langle \boldsymbol{u}|\boldsymbol{u}''\rangle. \tag{6.43}$$

From condition (6.20) together with equation (6.43) it follows that we can restrict to coherent states $|\boldsymbol{u}\rangle$, $|\boldsymbol{u}'\rangle$, and $|\boldsymbol{u}''\rangle$ that are centered at close positions in phase space, since otherwise

$$\rho(\boldsymbol{u})\,\langle \boldsymbol{u}'|\boldsymbol{u}\rangle\langle \boldsymbol{u}|\boldsymbol{u}''\rangle \approx 0.$$

Non-negligible contributions to the scattering term can then only exist for

$$\begin{aligned} \left|\mathbf{p}'-\mathbf{p}''\right| &< 4\Delta_p, \\ \left|\mathbf{q}'-\mathbf{q}''\right| &< 4\Delta_q. \end{aligned}$$

6.3 Semi-classical Boltzmann equation

In order to arrive at the SCBE, we introduce a sufficiently large volume Ω, on which the quasi-orthogonality (6.17) holds. We average the function ρ over this volume to obtain the probability distribution function $\bar{\rho}_\Omega$ (6.22). We obtain for the left-hand side of equation (6.40) averaged over the volume $\Omega(\boldsymbol{z})$

$$\frac{1}{\Omega}\int\limits_{\Omega(\boldsymbol{z})} d^3\boldsymbol{z}' \int\limits_{\mathcal{A}} d\boldsymbol{u}''\hat{g}(\boldsymbol{u}',\boldsymbol{u}'')\frac{d\rho(\boldsymbol{u}'')}{dt} \overset{(6.22)}{=} \frac{d\bar{\rho}(\mathbf{p},\mathbf{q},s)}{dt}.$$

The following procedure follows closely the standart derivation of the classical Boltzmann equation (see for example [21]). For the first term in equation (6.40) we have to assume that the force $\frac{\partial V^c(\mathbf{q}')}{\partial \mathbf{q}'}$ is constant over the integration domain in the $\mathbf{q}$ subspace and that

$$\frac{1}{\Omega}\int\limits_{\Omega(\boldsymbol{z})} d\boldsymbol{z}' \frac{\partial \rho(\mathbf{p}',\mathbf{q}',s)}{\partial \mathbf{p}'} \approx \frac{\partial \bar{\rho}(\mathbf{p},\mathbf{q},s)}{\partial \mathbf{p}}.$$

Then this term becomes

$$\frac{1}{\Omega}\int\limits_{\Omega(\boldsymbol{z})} d\boldsymbol{z}' \frac{\partial V^c(\mathbf{q}')}{\partial \mathbf{q}'}\frac{\partial \rho(\mathbf{p}',\mathbf{q}',s)}{\partial \mathbf{p}'} \approx \frac{\partial V^c(\mathbf{q})}{\partial \mathbf{q}}\frac{\partial \bar{\rho}(\mathbf{p},\mathbf{q})}{\partial \mathbf{p}}. \tag{6.44}$$

For the second term on the right hand side of equation (6.40) we have to calculate the average

$$\frac{1}{\Omega}\int\limits_{\Omega(\boldsymbol{z})} d\boldsymbol{z}'\ \mathbf{p}'\frac{\partial \rho(\mathbf{p}',\mathbf{q}',s)}{\partial \mathbf{q}'}$$

The factor $\mathbf{p}'$ is one of the integration variables and cannot be assumed to be constant. Nevertheless, recognizing that $\mathbf{p}$ is the average value of $\mathbf{p}'$ in the integration domain, and assuming that $\frac{\partial \rho(\mathbf{p}',\mathbf{q}',s)}{\partial \mathbf{q}'}$ varying weakly over the integration volume Ω, we can approximate the mean value of the product by the product of the mean values, i.e.,

$$\frac{1}{\Omega}\int\limits_{\Omega(\boldsymbol{z})} d\boldsymbol{z}'\ \mathbf{p}'\frac{\partial \rho(\mathbf{p}',\mathbf{q}',s)}{\partial \mathbf{q}'} \approx \mathbf{p}\frac{\partial \bar{\rho}(\mathbf{p},\mathbf{q},s)}{\partial \mathbf{q}}. \tag{6.45}$$

The last term on the right-hand side of the master equation (6.40) depends on the function $\Gamma(\boldsymbol{u},\boldsymbol{u};\boldsymbol{u}'\boldsymbol{u}'')$, which accounts for the effect of the electron-electron, electron-phonon and electron-photon interaction. 'In order to satisfy the conditions

$$\Gamma\left(\boldsymbol{u},\boldsymbol{u};\boldsymbol{u}',\boldsymbol{u}''\right) \cong 0 \qquad \text{if} \quad \mathbf{q}',\mathbf{q}'' \notin \Omega(\boldsymbol{z}) \tag{6.46}$$

$$\Gamma\left(\boldsymbol{u},\boldsymbol{u};\boldsymbol{u}',\boldsymbol{u}''\right) \cong 0 \qquad \text{if} \quad \mathbf{p}',\mathbf{p}'' \in \Omega(\boldsymbol{z}), \tag{6.47}$$

which are required in the classical approach, one has to make an adequate choice of the free parameters Δ_q, $\Delta_q^\Omega > \Delta_q$ and $\Delta_p^\Omega > \Delta_p$ where the latter two parameters characterize the cell volume Ω. Having specified the parameter Δ_q entering the definitions of the coherent states, we can determine the functions $\Gamma(\boldsymbol{u}, \boldsymbol{u}; \boldsymbol{u}', \boldsymbol{u}'')$.

We choose the smallest dimensions Δ_q^Ω and Δ_p^Ω of the sub-volume $\Omega = (\Delta_q^\Omega)^3(\Delta_p^\Omega)^3$ which allow us to satisfy the quasi-orthogonality condition. Clearly, this requires $\Delta_q^\Omega \gg \Delta_q$ and $\Delta_p^\Omega \gg \Delta_p$. The choice $\Delta_q^\Omega \gg \Delta_q$ is also optimal to satisfy condition (6.46). In order to satisfy also condition (6.47), which guarantees that scattering within the cell $\Omega(\mathbf{p}, \mathbf{q})$ can be neglected, we have to choose a sufficiently small Δ_p^Ω.

The general properties of $\Gamma(\boldsymbol{u}, \boldsymbol{u}; \boldsymbol{u}', \boldsymbol{u}'')$ have already been discussed in section 6.2.2. There it was shown that $\Gamma(\boldsymbol{u}, \boldsymbol{u}; \boldsymbol{u}'\boldsymbol{u}'')$ gives non-negligible contributions only if the states $|\boldsymbol{u}'\rangle = |\mathbf{p}', \mathbf{q}', s'\rangle$ and $|\boldsymbol{u}''\rangle = |\mathbf{p}'', \mathbf{q}'', s''\rangle$ are located in the same spatial region as the state $|\boldsymbol{u}\rangle = |\mathbf{p}, \mathbf{q}, s\rangle$. From equation (6.41) it follows that the integrations over $\mathbf{q}'$ and $\mathbf{q}''$ in equation (6.40) can be restricted to a sphere of radius $2\Delta_q^\Omega \gg \Delta_q$ centered at $\mathbf{q}$. Moreover, according to equations (6.8) and (6.12), and assuming that the one-particle density matrix in its diagonal representation is described by a bounded function $\rho(\boldsymbol{u})$ satisfying the condition (6.20), we can further assume that $\mathbf{p}' \approx \mathbf{p}''$, and $|\mathbf{p}' - \mathbf{p}| > \Delta_p^\Omega < |\mathbf{p}'' - \mathbf{p}|$ where $\Delta_p^\Omega \gg \Delta_p$ denotes the dimension of the cell in $\mathbf{p}$ direction, which according to the preliminary arguments given above, is chosen sufficiently small to ensure that scattering into final states lying inside the cell can be neglected. Thus, the integrations over $\mathbf{p}'$ and $\mathbf{p}''$ can be restricted to the same compact $\mathbf{p}$ regions with $\mathbf{p}' \approx \mathbf{p}''$, which lie, however, outside a sphere with radius $\Delta_p^\Omega \gg \Delta_p$ centered at $\mathbf{p}$. From the above considerations it follows that the third term in equation (6.40) couples states with approximately the same position in real space but distant in the $\mathbf{p}$ directions. It thus possesses the basic properties of the collision term in the classical Boltzmann equation (see also the discussion in section 6.2.2).

We can now go back to equation (6.40). For the third term we have to consider

$$\begin{aligned}
&\frac{1}{\Omega} \int\limits_{\Omega(\boldsymbol{z})} d\boldsymbol{z}' \int\limits_{\mathcal{A}} d\boldsymbol{u}_2 \int\limits_{\mathcal{A}} d\boldsymbol{u}_3\, \Gamma((\boldsymbol{z}', s), (\boldsymbol{z}', s); \boldsymbol{u}_2, \boldsymbol{u}_3) \int\limits_{\mathcal{A}} d\boldsymbol{u}_4\, \rho(\boldsymbol{u}_4)\, \langle \boldsymbol{u}_2 | \boldsymbol{u}_4 \rangle \langle \boldsymbol{u}_4 | \boldsymbol{u}_3 \rangle \\
&= \int\limits_{\mathcal{A}} d\boldsymbol{u}_4\, \hat{\Gamma}(\boldsymbol{z}, s; \boldsymbol{u}_4)\, \rho(\boldsymbol{u}_4) \qquad (6.48)
\end{aligned}$$

with the averaged function

$$\begin{aligned}
&\hat{\Gamma}(\boldsymbol{z}, s; \boldsymbol{u}_4) \\
&= \int\limits_{\mathcal{A}} d\boldsymbol{u}_2 \int\limits_{\mathcal{A}} d\boldsymbol{u}_3\, \frac{1}{\Omega} \int\limits_{\Omega(\boldsymbol{z})} d\boldsymbol{z}'\, \Gamma((\boldsymbol{z}', s), (\boldsymbol{z}', s); \boldsymbol{u}_2, \boldsymbol{u}_3) \langle \boldsymbol{u}_2 | \boldsymbol{u}_4 \rangle \langle \boldsymbol{u}_4 | \boldsymbol{u}_3 \rangle.
\end{aligned}$$

The right-hand side of equation (6.48) can be written as

$$\int_{\mathcal{A}} d\boldsymbol{u}'\,\hat{\Gamma}(\boldsymbol{z},s;\boldsymbol{u}')\,\rho(\boldsymbol{u}') = \sum_{s'}\int_{\mathbb{R}^6} d\boldsymbol{z}'\,\hat{\Gamma}(\boldsymbol{z},s;\boldsymbol{z}',s')\,\rho(\boldsymbol{z}',s')$$
$$= \sum_{s'}\int_{\mathbb{R}^6} d\boldsymbol{z}'\,\frac{1}{\Omega}\int_{\Omega(\boldsymbol{z}')} d\boldsymbol{z}''\hat{\Gamma}(\boldsymbol{z},s;\boldsymbol{z}'',s')\,\rho(\boldsymbol{z}'',s'). \tag{6.49}$$

The mean value of the product in the last line of equation (6.49) can be decomposed as the product of mean values

$$\frac{1}{\Omega}\int_{\Omega(\boldsymbol{z}')} d\boldsymbol{z}''\hat{\Gamma}(\boldsymbol{z},s;\boldsymbol{z}'',s')\,\rho(\boldsymbol{z}'',s') = \bar{\Gamma}(\boldsymbol{z},s;\boldsymbol{z}',s')\bar{\rho}(\boldsymbol{z}',s'), \tag{6.50}$$

where we have defined the mean values

$$\begin{aligned}\bar{\rho}(\boldsymbol{z}',s') &= \frac{1}{\Omega}\int_{\Omega(\boldsymbol{z}')} d\boldsymbol{z}''\rho(\boldsymbol{z}'',s')\\ \bar{\Gamma}(\boldsymbol{z},s;\boldsymbol{z}',s') &= \frac{1}{\Omega}\int_{\Omega(\boldsymbol{z}')} d\boldsymbol{z}''\hat{\Gamma}(\boldsymbol{z},s;\boldsymbol{z}'',s').\end{aligned}$$

We assume that conditions (6.46) and (6.47) are satisfied. With equations (6.44), (6.45), and (6.50), we obtain finally for the master equation (6.40) after the averaging procedure (6.22)

$$\begin{aligned}\frac{d\bar{\rho}(\mathbf{p},\mathbf{q},s)}{dt} = \quad & \frac{\partial V^c(\mathbf{q})}{\partial \mathbf{q}}\frac{\partial\bar{\rho}(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{p}} - \frac{\mathbf{p}}{m}\frac{\partial\bar{\rho}(\mathbf{p},\mathbf{q},s)}{\partial\mathbf{q}}\\ & + \sum_{s'}\frac{1}{(2\pi\hbar)^3}\int_{\mathbb{R}^3\setminus\Omega_p(\mathbf{p})} d\mathbf{p}'\int_{\Omega_q(\mathbf{q})} d\mathbf{q}'\,\bar{\Gamma}(\boldsymbol{z},s;\mathbf{p}',\mathbf{q}',s')\bar{\rho}(\mathbf{p}',\mathbf{q}',s')\end{aligned} \tag{6.51}$$

where we have introduced the real space part $\Omega_q(\mathbf{q})$ and the momentum space part $\Omega_p(\mathbf{p})$ of the volume $\Omega(\boldsymbol{z})$.

Equation (6.51) is the SCBE for the evolution of the probability density $\bar{\rho}(\mathbf{p},\mathbf{q},s)$. The three terms on the right-hand side are usually denoted as field term, diffusion term, and collision term.

6.4 Recapitulation

The derivation of the SCBE (6.51) was done in three steps. In the first step we have performed a basis transformation of equation (5.5) from the eigenbasis of the Hamiltonian $H_0^{(1)}$ in the overcomplete basis of coherent states $\{|\boldsymbol{u}\rangle\}$. Within the basis of coherent states, the coarse grained density matrix $\bar{D}_{(1)}$

is fully determined by its diagonal elements, which are a functional of the function ρ. The evolution of the function ρ is given by equation (6.27). This equation contains the full quantum statistical evolution of the density matrix $\bar{D}_{(1)}$.

In the second step, we have assumed a locally homogeneous electronic subsystem, i.e., the function ρ depends weakly on its arguments, so that it can be described on the scale Δ_p, Δ_q by the first-order Taylor expansion (6.35). This assumption allowed us to treat the Hamiltonian contribution in equation (6.27) and to write the QBE in the form of equation (6.40).

In the third step, we have used the concept of quasi-orthogonality (6.17), which can be introduced on the scale of sufficiently large phase space volumes Ω. The dimensions of Ω are imposed by the requested precision. Furthermore we have assumed that the density matrix $\bar{D}_{(1)}$ can be described by a bounded function ρ (see (6.20)). Under the above assumptions one obtains the SCBE (6.51), which describes the evolution of the electronic subsystem on the scale Ω.

Chapter 7

Conclusion

We have shown that starting from a quantum *statistical* description, the transition to the classical statistical description can be achieved. The reason for the irreversibility was related to the separability problem.

In chapter 4 we have in particular studied a spatially confined N-electron subsystem in the situation where the presence of the environment just leads to a memory loss in the electronic subsystem, but where energy transfer between the environment and the electronic subsystem remains negligible. The nature of the subsystem constituting the partner for the coupling is irrelevant in our approach. In the usual experimental situation in solid state physics it can be associated with the ensemble of "external" electrons. The finite memory of the electronic subsystem resulting from the coupling to the environment hinders the subsystem to build up particle-particle correlations involving more than n_{max} electrons. For simplicity, we have assumed $n_{max} = 2$, which is adequate for metallic systems where the radius of the effective screened interaction is of the order of the mean electronic distance. The corresponding results for the evolution of the electronic subsystem have been used to formulate the master equation for the general case where the external bath subsystems can absorb or emit energy. An extension of the present approach to low-density systems, where this approximation does not hold, is straightforward: In this case one would just get a set of $n_{max} - 1$ differential equations for $D_{(n)}, n = 1, \ldots, n_{max}-1$, instead of equation (5.1). This generalized approach is valid for large quantum dots containing a sufficiently large number of mobile electrons, as well as for macroscopic solids as metals or doped semiconductor systems.

The master equation for the reduced one-particle density matrix, describing the evolution of a confined subsystem, with a screened electron-electron interaction and weak electron-bath interactions is still formulated in the basis of eigenvectors of the one-particle Hamilton operator. Let us briefly repeat that coherent states are centered at a point in phase space. A point in phase space corresponds to the expectation value $\mathbf{p}$ of the momentum operator and the expectation value $\mathbf{q}$ of the position operator. The parameter Δ specifies

the width of the wave function of a coherent state in real space, while the width in momentum space is obtained from the Heisenberg relation (6.2). The basis of coherent states is adequate for the following reasons:

- First, it is overcomplete. This overcompleteness becomes obvious in the measure $\frac{1}{(2\pi\hbar)^3}$ in the closure relation (C.47). Due to the overcompleteness a one-body operator O is completely determined by $\langle u|O|u\rangle$ [19]. Thus the evolution of the density matrix $\bar{D}_{(1)}$ is completely determined by the evolution of $\langle \boldsymbol{u}|\bar{D}_{(1)}|\boldsymbol{u}\rangle$.

- Second, it allows to introduce the concept of quasi-orthogonality in phase space. Taking into account that every measurement has a finite precision, a value $\epsilon \ll 1$ can be defined, for which no distinction can be made between 0 and values smaller than ϵ. The rapid decrease of the function g, given in equation (6.13), allows to define quasi-orthogonal subspaces in phase space on a scale Ω (see equation (6.17)).

The quasi-orthogonality properly allows to approach the classical description. Restricting to density matrices satisfying condition (6.20) we have derived in chapter 6 the semi-classical Boltzmann equation (SCBE). This justifies for instance the assumption of statistically independent reservoirs in the Landauer transport theory on the scale[1] Ω.

The key result of this work is the phase space representation of the quantum Boltzmann equation (QBE) in equation (6.40). Based on this equation one can describe both, the classical behavior on scales[2] larger than Ω, and the quantum behavior on scales smaller than Ω. The locality of the electron-electron, electron-phonon and electron-photon interaction and the resulting local dynamics can be discussed in a transparent manner in the frame of equation (6.40). The quasi-orthogonality property reveals the local character of the evolution. Thus equation (6.40) allows us to perform the thermodynamic limit, which was impossible on the basis of equation (5.3).

[1] For instance, as long as the distance between the reservoirs is larger than the real space part of the volume Ω, they can be supposed to be statistically independent.

[2] For example the SCBE.

Appendix A

History of electrical current

One of the motivations for this work was the understanding of experiments with the electrical current. Even though the range of applications of this work is more general, the electrical current provides a typical example. The history of the discovery of electrons going through matter is so exciting, that I couldn't bear not to include this chapter in my thesis. This appendix is mainly based on [**?**].

It started with a shock

He felt a hit in his arms, shoulder and breast that took his breath away and he had to recover from this shock and fear for three days. This is one of the first documented measurements of the electrical current. It is taken from the book of Joseph Priestley (1733 - 1803), published in 1767 *The history and present state of electricity, with original experiments.* Even though Priestley made all the experiments, described in his book on his own, the shocking citation is about the feelings of a man called Pieter van Musschenbroeck, a Dutch professor, who just touched his own invention, he made in Leyden: the *Leyden jar.*

This jar was in fact the first capacitor that lead to man-made electrical discharges that were big enough to cause pain. While Mr. Musschenbroeck was shocked by the feelings the electrical current introduced him to, Mr. Bose, wished to die by an electrical shock to become a part of the French academy annals, while the Benedictine Richmann actually died such a *glorious* death.

An electrical shock is nothing else than feeling the electrical current within your body. As we know today nerves are transmitting information by electrical properties. A current of electrons rushing through our body overloads the nerves and can lead to pain or even death. The latter usually does happen for two reasons. First because the membrane potentials depolarize. Second, because proteins are destroyed (denaturation) by the heat that is produced due to the resistance of the body. The above-mentioned invention of a capacitor

opened the window to the world of electricity beyond the static electrical effects that were the main field of interest before, namely the attracting forces of materials like amber that have been loaded by friction with fur, or with the *electrifying machine*.

As it is the case for really new findings, the first way to explore them is with our body. The first apparatus to measure this new fluid, as electricity was supposed to be at that time, was the human body. And it really did its duty.

To test how many people can feel a shock of a Leyden jar, Abbé Nollet (1700-1770) scientist at the French court, let 180 soldiers feel it in presence of the king. In an abbey in Paris they even managed to have a human chain of 900 Klafter ($\approx 1.5km$), where every man held a metal wire in his hand as a connection to the next man. They all jumped and felt an electric shock at the same time.

Even more astonishing was the precision that was achieved at that time. Henry Cavendish (1731-1810) found that the relation of the conductivity of sea water to the conductivity of iron is $1 : 4 \cdot 10^6$. Today we measure $1 : 2 \cdot 10^6 \frac{S}{m}$[1]. Somewhere in the 1750s Cavendish found that incredible good result by using his algesia. He compared the pain he felt caused by an electric shock once received via iron, and once via sea water (the circuit was build up with a Leyden jar)!

Basic science about electricity started with people like the Swiss academic Johann Georg Sulzer(1720-1779) who found in 1754 that two connected metals lead to a strange flavor on the tongue by closing the metal ring with it. People experienced the electrical current with their own body and by looking at their reactions, they learned about the current's nature.

The invention of current measurements in a more objective way was the logical next step. Using measuring apparatus rather than the own body lead to reproducible experiments. Measurements exploiting the magnetic effects around a wire traversed by a current, were among the first. These experiments were only possible due to another invention, the Galvanic cell, found in 1800 by Allesandro Giuseppe Antonio Anastasio Count of Volta (1745-1827). It is said that frogs' legs and his wife have played an important role in that, but it is for sure that it was the first source of a constant electrical current.

Georg Simon Ohm (1787-1854) published in 1826 and 1827 the nowadays so-called *Ohm's law*, i.e., $U = R \cdot I$ (U is the voltage, R the resistance and I the current). He first used Galvanic cells, but he found out that these measurements were not exact enough. Only after switching to a thermoelectrical current source, he was able to make experiments that proved his law [**?**]. Ohm's law was the first that described the relation between electrical current and voltage.

Today's knowledge about electricity is visible in everyday tools. It helped

[1] S stands for Siemens.

Figure A.1: A comparison of scale: the author (1.90 m) in front of Ohm's galvanic cells (on the left) and the electrifying machine, called *Elektrisiermaschine* (on the right). They are part of the physics exhibition of the Deutsches Museum, Munich, Germany.

us going to the moon. The Apollo space ships of the 1970's had less computer power than a luxury car of 2006. Electricity serves mankind in a way that was not imaginable when the pioneers of electricity, like Ohm, started their work. But it is their testimony.

Microscopic world

Modern use of electricity is based on findings that allowed mankind to produce electricity out of mechanical, thermodynamical and even nuclear energy.

Research on electrical current has never stopped. Well known laws, like Ohm's law, break down for very small systems at low temperatures and new theories are needed. One of formalism is the Landau-Büttiker formalism (see for example [22]). While the resistance in Ohm's law is proportional to the length of a wire it passes through, the resistance becomes independent of the length of a wire, when its temperature is very low and its size becomes very small. The first case is called the (semi-)classical regime, while the latter is the mesoscopic or microscopic regime. Theories for the microscopic, as well as for the macroscopic, "classical regime" were developed between 1782 and 1960.

The transition from the microscopic to the macroscopic regime, is and was a vital field of research since the microscopic theories were developed. It was already studied by the fathers of quantum mechanics Schrödinger, Planck, Pauli, Bohr and Heisenberg in the 1930s. As quantum mechanics is the more general theory, it should contain the classical laws. The astonishing thing about quantum mechanics is that its predictions are in very good agreement with experimental findings. This has to be regarded as a kind of miracle at the moment since the measurement process in quantum mechanics is not yet fully understood.

Appendix B

Calculations for section 3.3

As shown in [1], equation (2.5) and (2.6), can be rewritten[1] as

$$\Gamma_j(D^{(N)}) \;=\; \Gamma_{0,j}(D^{(N)}) - \frac{1}{\hbar}\left\{D^{(N)}, G_j\right\} + \frac{i}{\hbar}\left[D^{(N)}, \Delta H_j\right]. \quad \text{(B.1)}$$

The matrix elements of each term in equation (B.1) can be expressed as

$$\begin{aligned}
\Gamma_{0,j\ \ a_1a_2}^{\ \ a_3a_4} &= \left((\Gamma_{0j})_{a_2a_1}^{a_2'a_1'}\right)^\star = (F_j)_{a_1a_2}^{a_1'a_2'} + \left((F_j)_{a_2a_1}^{a_2'a_1'}\right)^\star, \\
G_{j,a_1a_2} &= \frac{\hbar}{2}\sum_{a_3}(\Gamma_{0j})_{a_3a_3}^{a_2\,a_1}, \\
\Delta H_{j,a_1a_2} &= \frac{i\,\hbar}{2}\sum_{a_3}\left((F_j)_{a_3a_3}^{a_2a_1} - \left((F_j)_{a_3a_3}^{a_1a_2}\right)^\star\right),
\end{aligned}$$

With equation (2.10), we obtain

$$\begin{aligned}
\Gamma_{0,j\ \ a_1a_2}^{\ \ a_3a_4} &= \frac{1}{\hbar}\sum_{\alpha\beta}\langle a_1|Q_{j\alpha}^A|a_3\rangle\langle a_4|Q_{j\beta}^A|a_2\rangle\chi_{\beta\alpha}^j(\omega_{a_3a_1}) \\
G_{j,a_1a_2} &= \frac{1}{2}\sum_{\beta\alpha;\ a_3}\langle a_1|Q_{j\alpha}^A|a_3\rangle\langle a_3|Q_{j\beta}^A|a_2\rangle\chi_{\alpha\beta}^j(\omega_{a_3a_1}) \\
\Delta H_{j,a_1a_2} &= -\frac{1}{2}\sum_{\alpha\beta;\ a_3}\langle a_1|Q_{j\beta}^A|a_3\rangle\langle a_3|Q_{j\alpha}^A|a_2\rangle\bar{\chi}_{\beta\alpha}^j(\omega_{a_2a_3}),
\end{aligned}$$

[1] In the here considered Markov case, i.e. $\omega_{ca} = \omega_{db}$, see equation(2.5).

which leads to the matrix elements:

$$\langle a_1|\Gamma_{0,j}(D_{(N)})|a_2\rangle = \sum_{a_3,a_4} \Gamma_{0,j}{}^{a_3a_4}_{a_1a_2}\langle a_3|D_{(N)}|a_4\rangle \tag{B.2}$$

$$\langle a_1|\left\{D^{(N)},G_j\right\}|a_2\rangle = \sum_{a_3,a_4}\langle a_1|D^{(N)}|a_3\rangle\langle a_3|G_j|a_2\rangle + \langle a_1|G_j|a_4\rangle\langle a_4|D^{(N)}|a_2\rangle \tag{B.3}$$

$$\langle a_1|\left[D^{(N)},\Delta H_j\right]|a_2\rangle = \sum_{a_3,a_4}\langle a_1|D^{(N)}|a_3\rangle\langle a_3|\Delta H_j|a_2\rangle - \langle a_1|\Delta H_j|a_4\rangle\langle a_4|D^{(N)}|a_2\rangle. \tag{B.4}$$

With the assumption of one-body operators (3.21), we can rewrite the matrix elements (B.2):

$$\begin{aligned}
&\langle a_1|\Gamma_{0,j}(D_{(N)})|a_2\rangle \qquad\qquad (B.5)\\
=\;& \frac{1}{\hbar}\sum_{\alpha\beta,a_3,a_4}\langle a_1|Q^A_{j\alpha}|a_3\rangle\langle a_4|Q^A_{j\beta}|a_2\rangle\langle a_3|D_{(N)}|a_4\rangle\chi^j_{\beta\alpha}(\omega_{a_3a_1})\\
=\;& \frac{1}{\hbar}\sum_{\alpha\beta,a_3}\langle a_1|Q^A_{j\alpha}|a_3\rangle\langle a_3|D_{(N)}Q^A_{j\beta}|a_2\rangle\chi^j_{\beta\alpha}(\omega_{a_3a_1})\\
\overset{(3.21)}{=}\;& \frac{1}{\hbar}\sum_{\alpha\beta,a_3,\nu\nu'\mu\mu'}\langle a_1|c^\dagger_\nu c_{\nu'}|a_3\rangle\langle a_3|D_{(N)}c^\dagger_\mu c_{\mu'}|a_2\rangle\chi^j_{\beta\alpha}(\omega_{a_3a_1})a^{j\nu\nu'}_\alpha a^{j\mu\mu'}_\beta.
\end{aligned}$$

To see how this expression is calculated, we write the vectors describing N-particle states as

$$\begin{aligned}
|a_1\rangle &= |\nu_1\cdots\nu_N\rangle\\
|a_3\rangle &= |\mu_1\cdots\mu_N\rangle.
\end{aligned}$$

The matrix element

$$\begin{aligned}
\langle a_1|c^\dagger_\nu c_{\nu'}|a_3\rangle &= \langle\nu_1\cdots\nu_N|c^\dagger_\nu c_{\nu'}|\mu_1\cdots\mu_N\rangle\\
&= \delta_{\nu_1\mu_1}\cdots\delta_{\nu_N\mu_N}\delta_{\nu_i\nu}\delta_{\mu_j\nu'},\ \text{with } i,j\in\{1,\cdots N\},
\end{aligned}$$

is only non-zero, if the two vectors $|a_1\rangle$ and $|a_3\rangle$ differ only in the one-particle vectors $|\nu\rangle$ and $|\nu'\rangle$.

This has immediate consequences on the other factors of equation (B.5). The argument of the χ function is the energy difference $\omega_{a_3a_1}$ of the N-particle vectors $|a_3\rangle$ and $|a_1\rangle$. Since the two vectors differ only by the one-particle states $|\nu\rangle$ and $|\nu'\rangle$, the energy difference between the states $|a_1\rangle$ and $|a_3\rangle$, is just the energy difference of the one-particle energies

$$\omega_{a_3a_1} = \omega_{\nu'\nu}.$$

Finally we get for equation (B.5)

$$\frac{1}{\hbar}\sum_{\alpha\beta,a_3,\nu\nu'\mu\mu'}\langle a_1|c_\nu^\dagger c_{\nu'}|a_3\rangle\langle a_3|D_{(N)}c_\mu^\dagger c_{\mu'}|a_2\rangle\chi^j_{\beta\alpha}(\omega_{a_3a_1})a_\alpha^{j\nu\nu'}a_\beta^{j\mu\mu'}$$
$$=\frac{1}{\hbar}\sum_{\alpha\beta,\nu\nu'\mu\mu'}\langle a_1|c_\nu^\dagger c_{\nu'}D_{(N)}c_\mu^\dagger c_{\mu'}|a_2\rangle\chi^j_{\beta\alpha}(\omega_{\nu'\nu})a_\alpha^{j\nu\nu'}a_\beta^{j\mu\mu'}$$

In the same way we obtain for equations (B.3) and (B.4)

$$\langle a_1|\left\{D_{(N)},G_j\right\}|a_2\rangle =$$
$$\frac{1}{2}\sum_{\alpha\beta,\nu\nu'\mu\mu'}\langle a_1|\left\{c_\nu^\dagger c_{\nu'}c_\mu^\dagger c_{\mu'},D_{(N)}\right\}|a_2\rangle\chi^j_{\alpha\beta}(\omega_{\nu'\nu})a_\alpha^{j\nu\nu'}a_\beta^{j\mu\mu'}$$
$$\langle a_1|\left[D_{(N)},\Delta H_j\right]|a_2\rangle =$$
$$-\frac{1}{2}\sum_{\alpha\beta,\nu\nu'\mu\mu'}\langle a_1|\left[c_\mu^\dagger c_{\mu'}c_\nu^\dagger c_\nu,D_{(N)}\right]|a_2\rangle\bar\chi^j_{\beta\alpha}(\omega_{\mu'\mu})a_\beta^{j\nu\nu'}a_\alpha^{j\mu\mu'}.$$

This leads to the new form of the superoperator Γ:

$$\begin{aligned}\Gamma_j(D_{(N)}) &= \sum_{\nu\nu'\mu\mu'}(C_j)^{\nu'\mu}_{\nu\mu'}\left(c_\mu^\dagger c_{\mu'}D_{(N)}c_\nu^\dagger c_{\nu'}-\frac{1}{2}\left\{c_\nu^\dagger c_{\nu'}c_\mu^\dagger c_{\mu'},D_{(N)}\right\}\right)\\ &\quad+\frac{i}{2}\sum_{\nu\nu'\mu\mu'}\left(\bar C\right)^{\nu'\mu}_{\nu\mu'}\left[c_\nu^\dagger c_{\nu'}c_\mu^\dagger c_{\mu'},D_{(N)}\right],\end{aligned}\tag{B.6}$$

with

$$(C_j)^{\nu'\mu}_{\nu\mu'}=\frac{1}{\hbar}\sum_{\alpha\beta}\chi^j_{\alpha\beta}(\omega_{\nu'\nu})a_\alpha^{j\nu\nu'}a_\beta^{j\mu\mu'}\tag{B.7}$$

$$\left(\bar C_j\right)^{\nu'\mu}_{\nu\mu'}=-\frac{1}{\hbar}\sum_{\alpha\beta}\bar\chi^j_{\alpha\beta}(\omega_{\nu'\nu})a_\alpha^{j\nu\nu'}a_\beta^{j\mu\mu'}.\tag{B.8}$$

We have changed the summation indexes ($\alpha\leftrightarrow\beta$) in the definition of $\bar C_j$ in the last term of equation (B.6).

For $\omega_{\mu\mu'}+\omega_{\nu\nu'}=0$ we have the symmetry relation

$$\left((C_j)^{\mu'\nu}_{\mu\nu'}\right)^\star=(C_j)^{\nu\mu'}_{\nu'\mu}\tag{B.9}$$

$$\left((\bar C_j)^{\mu'\nu}_{\mu\nu'}\right)^\star=(\bar C_j)^{\nu\mu'}_{\nu'\mu}.\tag{B.10}$$

The trace $\mathrm{Tr}\left(D_{(N)}\right)$ is conserved, since

$$\mathrm{Tr}\left(\Gamma(D_{(N)})\right)=0.$$

Furthermore we note that the superoperator C has the property

$$(C_j)^{\nu'\nu'}_{\nu\nu} \geqslant 0,$$

and that it has the symmetry

$$\left((C_j)^{\nu'\mu}_{\nu\mu'}\right)^* = (C_j)^{\mu\nu'}_{\mu'\nu}\,.$$

Now let us calculate the second term of equation (3.15). Using equation (B.6), we get

$$\begin{aligned}
&\mathrm{Tr}\left(\Gamma(D_{(N)})c^\dagger_\rho c_{\rho'}\right) = \\
&\sum_{\mu\mu'\nu\nu'} (C_j)^{\mu'\nu}_{\mu\nu'}\,\mathrm{Tr}\left(D_{(N)}c^\dagger_\mu c_{\mu'}c^\dagger_\rho c_{\rho'}c^\dagger_\nu c_{\nu'} - \frac{1}{2}D_{(N)}c^\dagger_\rho c_{\rho'}c^\dagger_\mu c_{\mu'}c^\dagger_\nu c_{\nu'}\right. \\
&\qquad\qquad \left. -\frac{1}{2}D_{(N)}c^\dagger_\mu c_{\mu'}c^\dagger_\nu c_{\nu'}c^\dagger_\rho c_{\rho'}\right) \\
&+\frac{i}{2}\sum_{\nu\nu'\mu\mu'} (\bar{C}_j)^{\nu'\mu}_{\nu\mu'}\mathrm{Tr}\left(c^\dagger_\nu c_{\nu'}c^\dagger_\mu c_{\mu'}D_{(N)}c^\dagger_\rho c_{\rho'} - D_{(N)}c^\dagger_\nu c_{\nu'}c^\dagger_\mu c_{\mu'}c^\dagger_\rho c_{\rho'}\right).
\end{aligned}$$

With the commutation relations (3.3) and (3.4) we obtain

$$
\begin{aligned}
&\mathrm{Tr}\left(\Gamma(D_{(N)})c^\dagger_\rho c_{\rho'}\right) = \\
&\sum_{\mu\mu'\nu\nu'} (C_j)^{\mu'\nu}_{\mu\nu'}\,\mathrm{Tr}\left(D_{(N)}\frac{1}{2}\left(2\delta_{\mu'\rho}\delta_{\rho'\nu}c^\dagger_\mu c_{\nu'} - \delta_{\rho'\mu}\delta_{\mu'\nu}c^\dagger_\rho c_{\nu'} - \delta_{\mu'\nu}\delta_{\nu'\rho}c^\dagger_\mu c_{\rho'}\right.\right. \\
&\qquad \left.\left. -\delta_{\rho'\nu}c^\dagger_\mu c^\dagger_\rho c_{\mu'}c_{\nu'} - \delta_{\mu'\rho}c^\dagger_\mu c^\dagger_\nu c_{\rho'}c_{\nu'} + \delta_{\rho'\mu}c^\dagger_\rho c^\dagger_\nu c_{\mu'}c_{\nu'} + \delta_{\nu'\rho}c^\dagger_\mu c^\dagger_\nu c_{\mu'}c_{\rho'}\right)\right) \\
&+\frac{i}{2}\sum_{\mu\mu'\nu\nu'} \left(\bar{C}_j\right)^{\nu'\mu}_{\nu\mu'}\,\mathrm{Tr}\left(-\delta_{\nu\rho'}D_{(N)}c^\dagger_\rho c^\dagger_\mu c_{\nu'}c_{\mu'} + \delta_{\mu\nu'}D_{(N)}c^\dagger_\nu c^\dagger_\rho c_{\mu'}c_{\rho'} - \delta_{\nu'\mu}D_{(N)}c^\dagger_\rho c^\dagger_\nu c_{\rho'}c_{\mu'}\right. \\
&\qquad +\delta_{\rho\mu'}D_{(N)}c^\dagger_\nu c^\dagger_\mu c_{\nu'}c_{\rho'} + \delta_{\mu\rho'}D_{(N)}c^\dagger_\rho c^\dagger_\nu c_{\nu'}c_{\mu'} - \delta_{\nu'\rho}D_{(N)}c^\dagger_\nu c^\dagger_\mu c_{\mu'}c_{\rho'} \\
&\qquad \left.+\delta_{\nu\rho'}\delta_{\mu\nu'}D_{(N)}c^\dagger_\rho c_{\mu'} - \delta_{\mu\nu'}\delta_{\mu'\rho}D_{(N)}c^\dagger_\nu c_{\rho'}\right) \\
&= \left(\sum_{\mu\nu'} (C_j)^{\rho\rho'}_{\mu\nu'}\,D^{(1)}_{\nu'\mu} - \frac{1}{2}\sum_{\nu\nu'} (C_j)^{\nu\nu}_{\rho'\nu'}\,D^{(1)}_{\nu'\rho} - \frac{1}{2}\sum_{\mu\nu} (C_j)^{\nu\nu}_{\mu\rho}\,D^{(1)}_{\rho'\mu} - \sum_{\mu\mu'\nu'} (C_j)^{\mu'\rho'}_{\mu\nu'}\,D^{(2)}_{\mu'\nu'\mu\rho}\right. \\
&\qquad \left. - \sum_{\mu\nu\nu'} (C_j)^{\rho\nu}_{\mu\nu'}\,D^{(2)}_{\rho'\nu'\mu\nu} + \sum_{\mu'\nu\nu'} (C_j)^{\mu'\nu}_{\rho'\nu'}\,D^{(2)}_{\mu'\nu'\rho\nu} + \sum_{\mu\mu'\nu} (C_j)^{\mu'\nu}_{\mu\rho}\,D^{(2)}_{\mu'\rho'\mu\nu}\right) \\
&+i\left(\sum_{\mu\mu'\nu} \left(\bar{C}_j\right)^{\mu\mu}_{\nu\mu'}\,D^{(2)}_{\mu'\rho'\nu\rho} - \sum_{\mu\mu'\nu'} \left(\bar{C}_j\right)^{\nu'\mu}_{\rho'\mu'}\,D^{(2)}_{\nu'\mu'\rho\mu} - \sum_{\mu\mu'\nu} \left(\bar{C}_j\right)^{\mu\mu}_{\nu\mu'}\,D^{(2)}_{\rho'\mu'\rho\nu}\right. \\
&\qquad + \sum_{\mu\nu\nu'} \left(\bar{C}_j\right)^{\nu'\mu}_{\nu\rho}\,D^{(2)}_{\nu'\rho'\nu\mu} + \sum_{\mu'\nu\nu'} \left(\bar{C}_j\right)^{\nu'\rho'}_{\nu\mu'}\,D^{(2)}_{\nu'\mu'\rho\nu} - \sum_{\mu\mu'\nu} \left(\bar{C}_j\right)^{\rho\mu}_{\nu\mu'}\,D^{(2)}_{\mu'\rho'\nu\mu} \\
&\qquad \left. +\frac{1}{2}\sum_{\mu\nu} \left(\bar{C}_j\right)^{\mu\mu}_{\rho'\nu}\,D^{(1)}_{\nu\rho} - \frac{1}{2}\sum_{\nu\mu} \left(\bar{C}_j\right)^{\mu\mu}_{\nu\rho}\,D^{(1)}_{\rho'\nu}\right).
\end{aligned}
$$

With the definitions

$$
\left(G^{(1)}_j\right)_{\mu\nu} = \langle\mu|G^{(1)}_j|\rho\rangle = \frac{\hbar}{2}\sum_\nu (C_j)^{\nu\nu}_{\mu\rho} \tag{B.11}
$$

$$
\Gamma^{(1\to 1)}_0(D^{(1)})_{\rho\rho'} = \sum_{\mu\nu'} (C_j)^{\rho\rho'}_{\mu\nu'}\,\langle\nu'|D^{(1)}|\mu\rangle \tag{B.12}
$$

$$
\left(\Delta H^{(1)}_j\right)_{\nu\nu'} = \langle\nu|\Delta H^{(1)}_j|\nu'\rangle = \frac{\hbar}{2}\sum_\mu \left(\bar{C}_j\right)^{\mu\mu}_{\nu\nu'} \tag{B.13}
$$

we get for the terms containing only the one-particle density operator $D^{(1)}$

$$\begin{aligned}
&\frac{1}{\hbar}\left(\sum_{\mu\nu'}(C_j)^{\rho\rho'}_{\mu\nu'}\,D^{(1)}_{\nu'\mu}-\frac{1}{2}\sum_{\nu\nu'}(C_j)^{\nu\nu}_{\rho'\nu'}\,D^{(1)}_{\nu'\rho}-\frac{1}{2}\sum_{\mu\nu}(C_j)^{\nu\nu}_{\mu\rho}\,D^{(1)}_{\rho'\mu}\right)\\
&+\frac{i}{2\hbar}\sum_{\mu\nu}\left((\bar{C}_j)^{\mu\mu}_{\nu\rho}\,D^{(1)}_{\rho'\nu}-(\bar{C}_j)^{\mu\mu}_{\rho'\nu}\,D^{(1)}_{\nu\rho}\right)\\
=\;&\Gamma_0^{(1\to1)}(D^{(1)})_{\rho\rho'}+\frac{1}{\hbar}\left(-\sum_{\nu'}\langle\rho'|G^{(1)}|\nu'\rangle\langle\nu'|D^{(1)}|\rho\rangle-\sum_{\mu}\langle\rho'|D^{(1)}|\mu\rangle\langle\mu|G^{(1)}|\rho\rangle\right)\\
&+\frac{i}{\hbar}\sum_{\nu}\left(\langle\rho'|D^{(1)}|\nu\rangle\langle\nu|\Delta H^{(1)}|\rho\rangle-\langle\rho'|\Delta H^{(1)}|\nu\rangle\langle\nu|D^{(1)}|\rho\rangle\right)\\
=\;&\Gamma_0^{(1\to1)}(D^{(1)})_{\rho\rho'}-\frac{1}{\hbar}\langle\rho'|\left\{G^{(1)},D^{(1)}\right\}|\rho\rangle+\frac{i}{\hbar}\langle\rho'|\left[D^{(1)},\Delta H^{(1)}\right]|\rho\rangle. \qquad \text{(B.14)}
\end{aligned}$$

We can write the terms describing the coupling to the two-particle density operator $D^{(2)}$ in the compact form:

$$\begin{aligned}
\Gamma^{(2\to1)}\left(D^{(2)}\right)_{\rho\rho'} &= \sum_{\nu\nu'\mu}\left(D^{(2)}_{\rho\nu'\nu\mu}\left((C_j)^{\nu'\mu}_{\nu\rho'}-(C_j)^{\rho'\nu}_{\mu\nu'}\right)\right.\\
&\quad\left.+\left((C_j)^{\nu'\rho}_{\nu\mu}-(C_j)^{\mu\nu}_{\rho\nu'}\right)D^{(2)}_{\mu\nu'\rho'\nu}\right) \qquad \text{(B.15)}\\
\Delta H_j^{(2\to1)}\left(D^{(2)}\right)_{\rho\rho'} &= i\sum_{\nu\nu'\mu}\left(D^{(2)}_{\rho\nu'\nu\mu}\left((\bar{C}_j)^{\rho'\nu}_{\mu\nu'}+(\bar{C}_j)^{\nu'\mu}_{\nu\rho'}\right)\right.\\
&\quad\left.-\left((\bar{C}_j)^{\mu\nu}_{\rho\nu'}+(\bar{C}_j)^{\nu'\rho}_{\nu\mu}\right)D^{(2)}_{\mu\nu'\nu\rho'}\right), \qquad \text{(B.16)}
\end{aligned}$$

With (B.14), (B.15) and (B.16), we finally get:

$$\begin{aligned}
\mathrm{Tr}\left(\Gamma(D_{(N)})c^\dagger_\nu c_{\nu'}\right) &= \Gamma_0^{(1\to1)}(D^{(1)})_{\rho\rho'}+\Gamma^{(2\to1)}\left(D^{(2)}\right)_{\rho\rho'}-\frac{1}{\hbar}\left\{G^{(1)},D^{(1)}\right\}_{\rho\rho'}\\
&\quad+\frac{i}{\hbar}\left[D^{(1)},\Delta H^{(1)}\right]_{\rho\rho'}+\Delta H_j^{(2\to1)}\left(D^{(2)}\right)_{\rho\rho'}. \qquad \text{(B.17)}
\end{aligned}$$

Appendix C

Coherent states

C.1 Coherent states, a short summary

Starting from the momentum and position operators $\mathbf{P} = (P_1, P_2, P_3)$ and $\mathbf{Q} = (Q_1, Q_2, Q_3)$, which satisfy the commutation relations

$$[P_k, Q_l] = -i\hbar\delta_{kl}\mathbb{1}, \qquad k, l = 1, 2, 3, \tag{C.1}$$

we define the operator $\mathbf{A} = (A_1, A_2, A_3)$ and its adjoint $\mathbf{A}^\dagger = \left(A_1^\dagger, A_2^\dagger, A_3^\dagger\right)$, where the operators $A_k, k = 1, 2, 3$ are given by

$$A_k = \frac{\Delta_q P_k - i\Delta_p Q_k}{\hbar}, \tag{C.2}$$

$$A_k^\dagger = \frac{\Delta_q P_k + i\Delta_p Q_k}{\hbar}. \tag{C.3}$$

and where

$$\Delta_p\Delta_q = \frac{\hbar}{2}. \tag{C.4}$$

From the commutation relations equation (C.1) we obtain

$$\begin{aligned} \left[A_k, A_l^\dagger\right] &= \delta_{kl}\mathbb{1}, \qquad k, l = 1, 2, 3 \\ [A_k, A_l] &= 0, \\ \left[A_k^\dagger, A_l^\dagger\right] &= 0. \end{aligned} \tag{C.5}$$

By definition, the coherent state $|\mathbf{w}, \mathbf{a}\rangle$ with $\mathbf{w} = \mathbf{0}$ and $\mathbf{a} = \mathbf{0}$ is an eigenvector of the operator $\mathbf{A}$ with zero eigenvalue, i.e., we have

$$A_k|\mathbf{0}, \mathbf{0}\rangle = \mathbf{0}, \quad k = 1, 2, 3. \tag{C.6}$$

The eigenvectors of the self-adjoint operator

$$N = \mathbf{A}^\dagger \cdot \mathbf{A} = \sum_{k=1}^{3} A_k^\dagger A_k \tag{C.7}$$

form a complete orthonormal basis in the one-particle Hilbert space $\mathcal{H}$. N has discrete eigenstates, which can be generated from the coherent state $|\mathbf{0},\mathbf{0}\rangle$. In order to prove this, we start from the commutation relations,

$$\begin{aligned} [N, A_k] &= -A_k, & \text{(C.8)} \\ \left[N, A_k^\dagger\right] &= A_k^\dagger, & \text{(C.9)} \end{aligned}$$

which follow directly from equation (C.5). Let us denote the eigenvectors of N by $|\mathbf{n}\rangle \equiv |n_1, n_2, n_3\rangle$ and the corresponding eigenvalue by $n = n_1 + n_2 + n_3$, so that

$$N|n_1, n_2, n_3\rangle = n|n_1, n_2, n_3\rangle. \tag{C.10}$$

From equations (C.8) and (C.10) we get

$$\begin{aligned} NA_k|n_1, n_2, n_3\rangle &= A_k N|n_1, n_2, n_3\rangle - A_k|n_1, n_2, n_3\rangle \\ &= (n-1)\, A_k|n_1, n_2, n_3\rangle, & \text{(C.11)} \end{aligned}$$

i.e., $A_k|n_1, n_2, n_3\rangle$ is an eigenvector of N with the norm

$$\begin{aligned} \|A_k|n_1, n_2, n_3\rangle\|^2 &= \langle n_1, n_2, n_3|A_k^\dagger A_k|n_1, n_2, n_3\rangle & \text{(C.12)} \\ &= n_k \geq 0. \end{aligned}$$

Similarly, we obtain from equation (C.9)

$$\begin{aligned} NA_k^\dagger|n_1, n_2, n_3\rangle &= A_k^\dagger N|n_1, n_2, n_3\rangle + A_k^\dagger|n_1, n_2, n_3\rangle & \text{(C.13)} \\ &= (n+1)\, A_k^\dagger|n_1, n_2, n_3\rangle. \end{aligned}$$

Thus, if $|\mathbf{n}\rangle = |n_1, n_2, n_3\rangle$ is an eigenvector of N with eigenvalue n, $A_k^\dagger|\mathbf{n}\rangle$ is also an eigenvector $|\mathbf{n} + \mathbf{e}_k\rangle$ with eigenvalue $n+1$, where $\mathbf{e}_k$ is the unit vector in k-direction. equation (C.12) shows that all eigenvalues must be positive or zero. Furthermore, equation (C.6) implies that $|0,0,0\rangle$ is an eigenvector with eigenvalue zero. The state $|0,0,0\rangle$ can thus be identified with the state $|\mathbf{0},\mathbf{0}\rangle$ in equation (C.6). All other mutually orthogonal eigenvectors can then be generated from $|0,0,0\rangle$. We obtain

$$|n_1, n_2, n_3\rangle = d_{n_1,n_2,n_3} \left(A_1^\dagger\right)^{n_1} \left(A_2^\dagger\right)^{n_1} \left(A_3^\dagger\right)^{n_1} |0,0,0\rangle. \tag{C.14}$$

The constant d_{n_1,n_2,n_3} can be used to obtain normalized eigenvectors $|n_1, n_2, n_3\rangle$. From the commutation relations (C.5), the definition (C.7) and equations

(C.13) and (C.14) we obtain

$$\begin{aligned}
&\langle n_1, n_2, n_3 | n_1', n_2', n_3' \rangle \\
&\quad = d^2_{n_1,n_2,n_3} \, \langle 0,0,0| \, (A_1)^{n_1} \, (A_2)^{n_2} \, (A_3)^{n_3} \left(A_1^\dagger\right)^{n_1} \left(A_1^\dagger\right)^{n_1} \left(A_2^\dagger\right)^{n_2} \left(A_3^\dagger\right)^{n_3} |0,0,0\rangle \delta_{\mathbf{n}\mathbf{n}'} \\
&\quad = d^2_{n_1,n_2,n_3} \, \langle 0,0,0| \left(A_1 A_1^\dagger\right)^{n_1} \left(A_2 A_2^\dagger\right)^{n_2} \left(A_3 A_3^\dagger\right)^{n_3} |0,0,0\rangle \delta_{\mathbf{n}\mathbf{n}'} \\
&\quad = d^2_{n_1,n_2,n_3} \, \langle 0,0,0| \, (N_1 + \mathbb{1})^{n_1} \, (N_2 + \mathbb{1})^{n_2} \, (N_3 + \mathbb{1})^{n_3} \, |0,0,0\rangle \delta_{\mathbf{n}\mathbf{n}'} \\
&\quad = d^2_{n_1,n_2,n_3} (n_1! n_2! n_3!) \delta_{\mathbf{n}\mathbf{n}'} \\
&\quad \equiv \delta_{\mathbf{n}\mathbf{n}'}.
\end{aligned}$$

Accordingly, the normalized eigenvectors of N are given by

$$|n_1, n_2, n_3\rangle = \frac{1}{\sqrt{n_1! n_2! n_3!}} \left(A_1^\dagger\right)^{n_1} \left(A_2^\dagger\right)^{n_1} \left(A_3^\dagger\right)^{n_1} |0,0,0\rangle. \tag{C.15}$$

From equations (C.11) and (C.13) we find

$$A_k^\dagger A_k |\mathbf{n}\rangle = n_k |\mathbf{n}\rangle. \tag{C.16}$$

Using the above identity as well as the commutation relations (C.5) we get

$$\begin{aligned}
A_1 |n_1, n_2, n_3\rangle &= \frac{1}{\sqrt{n_1! n_2! n_3!}} \left(A_1 A_1^\dagger\right) \left(A_1^\dagger\right)^{n_1 - 1} \left(A_2^\dagger\right)^{n_1} \left(A_3^\dagger\right)^{n_1} |0,0,0\rangle \\
&= \frac{1}{\sqrt{n_1! n_2! n_3!}} \left(\mathbb{1} + A_1^\dagger A_1\right) \left(A_1^\dagger\right)^{n_1 - 1} \left(A_2^\dagger\right)^{n_1} \left(A_3^\dagger\right)^{n_1} |0,0,0\rangle \\
&= \frac{1 + n_1 - 1}{\sqrt{n_1! n_2! n_3!}} \left(A_1^\dagger\right)^{n_1 - 1} \left(A_2^\dagger\right)^{n_1} \left(A_3^\dagger\right)^{n_1} |0,0,0\rangle \\
&= \frac{\sqrt{n_1}}{\sqrt{(n_1 - 1)! n_2! n_3!}} \left(A_1^\dagger\right)^{n_1 - 1} \left(A_2^\dagger\right)^{n_1} \left(A_3^\dagger\right)^{n_1} |0,0,0\rangle \\
&= \sqrt{n_1} |n_1 - 1, n_2, n_3\rangle.
\end{aligned}$$

The same calculations can be performed for the remaining operators A_2, A_3. We thus obtain

$$A_k |\mathbf{n}\rangle = \sqrt{n_k} |\mathbf{n} - \mathbf{e}_k\rangle.$$

Similarly, we find

$$A_k^\dagger |\mathbf{n}\rangle = \sqrt{n_k + 1} |\mathbf{n} + \mathbf{e}_k\rangle.$$

Let us now define the translation operator

$$T(\mathbf{w}, \mathbf{a}) = e^{G(\mathbf{w}, \mathbf{a})}, \tag{C.17}$$

with

$$G(\mathbf{w}, \mathbf{a}) = \frac{i}{\hbar} \left(\mathbf{w} \cdot \mathbf{Q} - \mathbf{a} \cdot \mathbf{P}\right). \tag{C.18}$$

equations (C.17) and (C.18) imply

$$T(\mathbf{w},\mathbf{a})^\dagger = T(\mathbf{w},\mathbf{a})^{-1} = T(-\mathbf{a},-\mathbf{w}).$$

From the Campbell-Baker-Hausdorff formula

$$e^X Y e^{-X} = \sum_{n=0}^{\infty} \frac{1}{n!}\Omega_n(X,Y)$$

where

$$\begin{aligned}\Omega_n(X,Y) &= [X,\Omega_{n-1}(X,Y)]\,,\\ \Omega_0(X,Y) &= Y,\end{aligned}$$

we obtain also

$$T(\mathbf{w},\mathbf{a})^{-1}\,\mathbf{P}\,T(\mathbf{w},\mathbf{a}) = \mathbf{P} + \mathbf{w}\mathbb{1}, \tag{C.19}$$

$$T(\mathbf{w},\mathbf{a})^{-1}\,\mathbf{Q}\,T(\mathbf{w},\mathbf{a}) = \mathbf{Q} + \mathbf{a}\mathbb{1}. \tag{C.20}$$

The translation operators can be rewritten using the Baker-Hausdorff theorem (see e.g. Ref. [23]),

$$e^{X+Y} = e^X e^Y e^{-\frac{1}{2}[X,Y]} = e^Y e^X e^{+\frac{1}{2}[X,Y]}.$$

For two operators X and Y with

$$[X,Y] = c\mathbb{1}, \quad c \in \mathbb{C},$$

we obtain

$$e^{X+Y} = e^X e^Y e^{-\frac{c}{2}} = e^Y e^X e^{+\frac{c}{2}}. \tag{C.21}$$

Using the commutation relations equation (C.1), we can thus express the translation operators defined in equation (C.17) in the factorized form

$$\begin{aligned}T(\mathbf{w},\mathbf{a}) &= e^{\frac{i}{\hbar}(\mathbf{w}\cdot\mathbf{Q}-\mathbf{a}\cdot\mathbf{P})} \\ &= e^{-\frac{i}{\hbar}\mathbf{a}\cdot\mathbf{P}} e^{\frac{i}{\hbar}\mathbf{w}\cdot\mathbf{Q}} e^{\frac{i}{2\hbar}\mathbf{a}\cdot\mathbf{w}} \\ &= e^{\frac{i}{\hbar}\mathbf{w}\cdot\mathbf{Q}} e^{-\frac{i}{\hbar}\mathbf{a}\cdot\mathbf{P}} e^{-\frac{i}{2\hbar}\mathbf{a}\cdot\mathbf{w}}.\end{aligned} \tag{C.22}$$

Accordingly, we have

$$\left(\mathbf{u}\cdot\frac{\partial}{\partial\mathbf{a}}\right)^n T(\mathbf{w},\mathbf{a}) = \left(\mathbf{u}\cdot\left(-\frac{i}{\hbar}\mathbf{P} + \frac{i}{\hbar}\frac{\mathbf{w}}{2}\right)\right)^n T(\mathbf{w},\mathbf{a}), \tag{C.23}$$

$$\left(\mathbf{u}\frac{\partial}{\partial\mathbf{w}}\right)^n T(\mathbf{w},\mathbf{a}) = \left(\mathbf{u}\cdot\left(\frac{i}{\hbar}\mathbf{Q} - \frac{i}{\hbar}\frac{\mathbf{a}}{2}\right)\right)^n T(\mathbf{w},\mathbf{a}), \tag{C.24}$$

where $\mathbf{u}$ is an arbitrary vector $\mathbf{u} = (u_1, u_2, u_3) \in \mathbb{C}^3$. With equations (C.19) and (C.20) we get

$$T(\mathbf{w}, \mathbf{a})^{-1}\, \mathbf{A}\, T(\mathbf{w}, \mathbf{a}) \;=\; \mathbf{A} + \boldsymbol{\alpha}\mathbb{1}, \tag{C.25}$$

where

$$\boldsymbol{\alpha} = \frac{\Delta_q \mathbf{w} - i\Delta_p \mathbf{a}}{\hbar}. \tag{C.26}$$

We define

$$|\mathbf{w}, \mathbf{a}\rangle = T(\mathbf{w}, \mathbf{a})|\mathbf{0}, \mathbf{0}\rangle. \tag{C.27}$$

equation (C.25) implies

$$\mathbf{A}|\mathbf{w}, \mathbf{a}\rangle = \boldsymbol{\alpha}|\mathbf{w}, \mathbf{a}\rangle. \tag{C.28}$$

This suggests the alternative notation

$$|\boldsymbol{\alpha}\rangle \equiv |\mathbf{w}, \mathbf{a}\rangle. \tag{C.29}$$

so that equation (C.28) becomes

$$\mathbf{A}|\boldsymbol{\alpha}\rangle = \boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle. \tag{C.30}$$

The wavefunctions corresponding to the states $|\boldsymbol{\alpha}\rangle$ in real space representation are given by (see for example figure (C.1))

$$\langle \mathbf{x}|\mathbf{w}, \mathbf{a}\rangle = \left(\frac{1}{2\pi\Delta^2}\right)^{\frac{3}{4}} e^{-\left(\frac{\mathbf{x}-\mathbf{a}}{2\Delta}\right)^2} e^{\frac{i\mathbf{w}\left(\mathbf{x}-\frac{\mathbf{a}}{2}\right)}{\hbar}}, \tag{C.31}$$

where $\mathbf{x}, \mathbf{w}, \mathbf{a}$ denote the three-dimensional vectors

$$\mathbf{x} = (x_1, x_2, x_3), \quad \mathbf{w} = (w_1, w_2, w_3), \quad \mathbf{a} = (a_1, a_2, a_3).$$

In fact, in real space representation the operators Q_k and P_k in equations (C.2) and (C.3) have to be replaced by

$$\begin{aligned} Q_k \quad &\to x_k, \\ P_k \quad &\to \frac{\hbar}{i}\frac{\partial}{\partial x_k}. \end{aligned}$$

It is then easily verified that equation (C.30) is satisfied for the wave functions given by equation (C.31).

From equations (C.2) and (C.3) we get

$$\mathbf{P} \;=\; \frac{\hbar}{2\Delta_q}\left(\mathbf{A}^\dagger + \mathbf{A}\right), \tag{C.32}$$

$$\mathbf{Q} \;=\; \frac{\hbar}{2i\Delta_p}\left(\mathbf{A}^\dagger - \mathbf{A}\right). \tag{C.33}$$

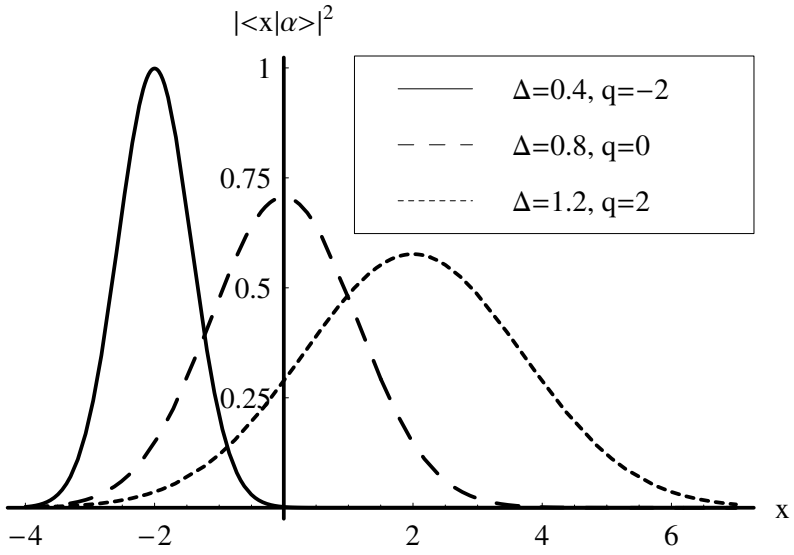

Figure C.1: Absolute value of the wave function of three coherent states $|\alpha\rangle$, with different positions $q = -2, 0, 2$ and with different parameters $\Delta = 0.4, 0.8, 1.2$, respectively.

Accordingly, we obtain from equations (C.26) and (C.28),

$$\langle \mathbf{w}, \mathbf{a}|\mathbf{P}|\mathbf{w}, \mathbf{a}\rangle = \mathbf{w}, \tag{C.34}$$

$$\langle \mathbf{w}, \mathbf{a}|\mathbf{Q}|\mathbf{w}, \mathbf{a}\rangle = \mathbf{a}, \tag{C.35}$$

which shows that the state $|\mathbf{w}, \mathbf{a}\rangle$ is centered at the point $(\mathbf{w}, \mathbf{a})$ in phase space. From equations (C.2), (C.3), (C.26), (C.28), (C.32), (C.33), (C.34) and (C.35) and using equation (C.4) we obtain for the mean square deviations

$$\langle \mathbf{w}, \mathbf{a}| \left(\mathbf{P} - \mathbf{w}\mathbb{1}\right)^2 |\mathbf{w}, \mathbf{a}\rangle = \left(\frac{\hbar}{2\Delta_q}\right)^2 = \Delta_p^2,$$

$$\langle \mathbf{w}, \mathbf{a}| \left(\mathbf{Q} - \mathbf{a}\mathbb{1}\right)^2 |\mathbf{w}, \mathbf{a}\rangle = \left(\frac{\hbar}{2\Delta_p}\right)^2 = \Delta_q^2,$$

i.e., all states $|\mathbf{w}, \mathbf{a}\rangle$ saturate the Heisenberg relation, independent of their position. In fact, by construction (see equation (C.27)) these states are nothing else but the coherent state $|\mathbf{0}, \mathbf{0}\rangle$ translated in phase space.

Using equations (C.22) and (C.27) we can express the scalar product $\langle \mathbf{w}', \mathbf{a}'|\mathbf{w}, \mathbf{a}\rangle$ as

$$\begin{aligned} \langle \mathbf{w}_1, \mathbf{a}_1|\mathbf{w}_2, \mathbf{a}_2\rangle &= \langle \mathbf{0}, \mathbf{0}|T(\mathbf{a}_1, \mathbf{w}_1)^{-1} T(\mathbf{a}_2, \mathbf{w}_2)|\mathbf{0}, \mathbf{0}\rangle \\ &= \langle \mathbf{0}, \mathbf{0}|T(-\mathbf{a}_1, -\mathbf{w}_1) T(\mathbf{a}_2, \mathbf{w}_2)|\mathbf{0}, \mathbf{0}\rangle. \end{aligned} \tag{C.36}$$

In order to evaluate the right-hand side of the above expression, we first calculate the product of translation operators. With

$$\begin{aligned}[G(-\mathbf{a}_1,-\mathbf{w}_1),G(\mathbf{a}_2,\mathbf{w}_2)] &= \left(\frac{i}{\hbar}\right)^2 [-\mathbf{w}_1\cdot\mathbf{Q}+\mathbf{a}_1\cdot\mathbf{P},\mathbf{w}_2\cdot\mathbf{Q}-\mathbf{a}_2\cdot\mathbf{P}] \\ &= \frac{i}{\hbar}\left(\mathbf{w}_2\cdot\mathbf{a}_1-\mathbf{w}_1\cdot\mathbf{a}_2\right)\mathbb{1},\end{aligned}$$

which follows directly from the definition equation (C.18) and the commutation relations equation (C.1), we obtain from equation (C.17) and equation (C.21)

$$\begin{aligned}T(-\mathbf{a}_1,-\mathbf{w}_1)T(\mathbf{a}_2,\mathbf{w}_2) &= e^{G(-\mathbf{a}_1,-\mathbf{w}_1)}e^{G(\mathbf{a}_2,\mathbf{w}_2)} \\ &= e^{G(-\mathbf{a}_1,-\mathbf{w}_1)+G(\mathbf{a}_2,\mathbf{w}_2)}e^{\frac{1}{2}[G(-\mathbf{a}_1,-\mathbf{w}_1),G(\mathbf{a}_2,\mathbf{w}_2)]} \\ &= T(\mathbf{a}_2-\mathbf{a}_1,\mathbf{w}_2-\mathbf{w}_1)e^{\frac{1}{2}[G(-\mathbf{a}_1,-\mathbf{w}_1),G(\mathbf{a}_2,\mathbf{w}_2)]} \\ &= T(\mathbf{a}_2-\mathbf{a}_1,\mathbf{w}_2-\mathbf{w}_1)e^{\frac{i}{2\hbar}(\mathbf{w}_2\cdot\mathbf{a}_1-\mathbf{w}_1\cdot\mathbf{a}_2)}.\end{aligned}$$

We then calculate the matrix element $\langle\mathbf{0},\mathbf{0}|T(\mathbf{w},\mathbf{a})|\mathbf{0},\mathbf{0}\rangle$. From equations (C.18), (C.32), (C.33) and (C.26) we get

$$\begin{aligned}G(-\mathbf{a},-\mathbf{w}) &= \frac{i}{\hbar}\left(\mathbf{w}\cdot\mathbf{Q}-\mathbf{a}\cdot\mathbf{P}\right) \\ &= \boldsymbol{\alpha}\cdot\mathbf{A}^\dagger-\boldsymbol{\alpha}^\star\cdot\mathbf{A}.\end{aligned}$$

With equation (C.21) and the commutation relations equation (C.5) we obtain

$$\begin{aligned}T(\mathbf{w},\mathbf{a}) &= e^{\boldsymbol{\alpha}\cdot\mathbf{A}^\dagger-\boldsymbol{\alpha}^\star\cdot\mathbf{A}} \\ &= e^{\boldsymbol{\alpha}\cdot\mathbf{A}^\dagger}e^{-\boldsymbol{\alpha}^\star\cdot\mathbf{A}}e^{-\frac{\alpha\cdot\alpha^\star}{2}}.\end{aligned}$$

Thus, using equation (C.6) and inserting the definition (C.26) we find

$$\begin{aligned}\langle\mathbf{0},\mathbf{0}|T(\mathbf{w},\mathbf{a})|\mathbf{0},\mathbf{0}\rangle &= e^{-\frac{\alpha\cdot\alpha^\star}{2}}\ \langle\mathbf{0},\mathbf{0}|e^{\boldsymbol{\alpha}\cdot\mathbf{A}^\dagger}e^{-\boldsymbol{\alpha}^\star\cdot\mathbf{A}}|\mathbf{0},\mathbf{0}\rangle \\ &= e^{-\frac{\alpha\alpha^\star}{2}} \\ &= e^{-\frac{1}{2}\left(\frac{\mathbf{w}^2}{(2\Delta p)^2}+\frac{\mathbf{a}^2}{(2\Delta q)^2}\right)}. \qquad \text{(C.37)}\end{aligned}$$

Putting together equations (C.36), C.37) and (C.37), we obtain finally

$$\langle\mathbf{w}_1,\mathbf{a}_1|\mathbf{w}_2,\mathbf{a}_2\rangle = e^{-\frac{1}{2}\left(\frac{(\mathbf{w}_2-\mathbf{w}_1)^2}{(2\Delta p)^2}+\frac{(\mathbf{a}_2-\mathbf{a}_1)^2}{(2\Delta q)^2}\right)}e^{\frac{i}{2\hbar}(\mathbf{w}_2\cdot\mathbf{a}_1-\mathbf{w}_1\cdot\mathbf{a}_2)}. \qquad \text{(C.38)}$$

The states $\mathbf{n}$ defined by equation (C.15) form a complete orthonormal basis in the one-particle Hilbert space $\mathcal{H}$. The closure relation

$$\sum_{n_1,n_2,n_3}|n_1,n_2,n_3\rangle\langle n_1,n_2,n_3| = \mathbb{1}$$

allows us in particular to express $|\mathbf{w}, \mathbf{a}\rangle$ as

$$|\mathbf{w}, \mathbf{a}\rangle = \sum_{n_1,n_2,n_3} |n_1, n_2, n_3\rangle\langle n_1, n_2, n_3|\mathbf{w}, \mathbf{a}\rangle.$$

The coefficients $\langle n_1, n_2, n_3|\mathbf{w}, \mathbf{a}\rangle$, or $\langle n_1, n_2, n_3|\boldsymbol{\alpha}\rangle$ in the notation of equation (C.29), can directly be obtained from equations (C.15) and (C.16). We get immediately

$$\begin{aligned}\langle \mathbf{n}|\boldsymbol{\alpha}\rangle &= \frac{1}{\sqrt{n_1!n_2!n_3!}}\,\langle \mathbf{0}|A_1^{n_1}A_2^{n_2}A_3^{n_3}|\boldsymbol{\alpha}\rangle \\ &= \frac{\alpha_1^{n_1}\alpha_2^{n_2}\alpha_3^{n_3}}{\sqrt{n_1!n_2!n_3!}}\langle \mathbf{0}|\boldsymbol{\alpha}\rangle.\end{aligned}$$

where we have used the property equation (C.28) in the last line. From the closure relation for the states $|\mathbf{n}\rangle$ we get

$$\begin{aligned}1 = \langle \boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle &= \sum_{n_1,n_2,n_3} \langle \boldsymbol{\alpha}|n_1, n_2, n_3\rangle\langle n_1, n_2, n_3|\boldsymbol{\alpha}\rangle \\ &= \sum_{n_1,n_2,n_3} \frac{|\alpha_1|^{2n_1}\,|\alpha_2|^{2n_2}\,|\alpha_3|^{2n_3}}{n_1!n_2!n_3!}\,|\langle \mathbf{0}|\boldsymbol{\alpha}\rangle|^2\,.\end{aligned}$$

From equation (C.38) we obtain

$$\langle \mathbf{0}|\boldsymbol{\alpha}\rangle = e^{-\frac{|\boldsymbol{\alpha}|^2}{2}}$$

so that finally

$$\langle \mathbf{n}|\boldsymbol{\alpha}\rangle = \frac{\alpha_1^{n_1}\alpha_2^{n_2}\alpha_3^{n_3}}{\sqrt{n_1!n_2!n_3!}}e^{-\frac{|\boldsymbol{\alpha}|^2}{2}}. \tag{C.39}$$

Let us now still derive some useful relations involving the coherent states. From equation (C.23) we obtain

$$\begin{aligned}\frac{\partial}{\partial \mathbf{a}}|\mathbf{w}, \mathbf{a}\rangle &= \frac{\partial T(\mathbf{w}, \mathbf{a})}{\partial \mathbf{a}}|\mathbf{0}, \mathbf{0}\rangle \\ &= -\frac{i}{\hbar}\left(\mathbf{P} - \frac{\mathbf{w}}{2}\mathbb{1}\right) T(\mathbf{w}, \mathbf{a})|\mathbf{0}, \mathbf{0}\rangle \\ &= -\frac{i}{\hbar}\left(\mathbf{P} - \frac{\mathbf{w}}{2}\mathbb{1}\right)|\mathbf{w}, \mathbf{a}\rangle,\end{aligned}$$

and thus

$$\mathbf{P}|\mathbf{w}, \mathbf{a}\rangle = \left(i\hbar\frac{\partial}{\partial \mathbf{a}} + \frac{\mathbf{w}}{2}\mathbb{1}\right)|\mathbf{w}, \mathbf{a}\rangle. \tag{C.40}$$

Similarly, we obtain from equation (C.24)

$$\begin{aligned}\frac{\partial}{\partial \mathbf{w}}|\mathbf{w},\mathbf{a}\rangle &= \frac{\partial T(\mathbf{w},\mathbf{a})}{\partial \mathbf{w}}|\mathbf{0},\mathbf{0}\rangle \\ &= \frac{i}{\hbar}\left(\mathbf{Q}-\frac{\mathbf{a}}{2}\mathbb{1}\right)T(\mathbf{w},\mathbf{a})|\mathbf{0},\mathbf{0}\rangle \\ &= \frac{i}{\hbar}\left(\mathbf{Q}-\frac{\mathbf{a}}{2}\mathbb{1}\right)|\mathbf{w},\mathbf{a}\rangle,\end{aligned}$$

and thus

$$\mathbf{Q}|\mathbf{w},\mathbf{a}\rangle = \left(-i\hbar\frac{\partial}{\partial \mathbf{w}}+\frac{\mathbf{a}}{2}\mathbb{1}\right)|\mathbf{w},\mathbf{a}\rangle. \tag{C.41}$$

equations (C.2), (C.40) and (C.41) lead to

$$\begin{aligned}\mathbf{A}|\mathbf{w},\mathbf{a}\rangle &= \frac{1}{\hbar}\left(\Delta_q\left(i\hbar\frac{\partial}{\partial \mathbf{a}}+\frac{\mathbf{w}}{2}\mathbb{1}\right)-i\Delta_p\left(-i\hbar\frac{\partial}{\partial \mathbf{w}}+\frac{\mathbf{a}}{2}\mathbb{1}\right)\right)|\mathbf{w},\mathbf{a}\rangle \\ &= \frac{\Delta_q\mathbf{w}-i\Delta_p\mathbf{a}}{\hbar}|\mathbf{w},\mathbf{a}\rangle, \qquad (C.42)\end{aligned}$$

where the last line is obtained from equations (C.28) and (C.26). Comparing the last two lines of equation (C.42) we find

$$\left(i\hbar\frac{\partial}{\partial \mathbf{a}}-\frac{\mathbf{w}}{2}\right)|\mathbf{w},\mathbf{a}\rangle = -\frac{i\hbar}{2\Delta_q^2}\left(i\hbar\frac{\partial}{\partial \mathbf{w}}+\frac{\mathbf{a}}{2}\right)|\mathbf{w},\mathbf{a}\rangle, \tag{C.43}$$

and by complex conjugation

$$\left(i\hbar\frac{\partial}{\partial \mathbf{a}}+\frac{\mathbf{w}}{2}\right)\langle\mathbf{w},\mathbf{a}| = \frac{i\hbar}{2\Delta_q^2}\left(i\hbar\frac{\partial}{\partial \mathbf{w}}-\frac{\mathbf{a}}{2}\right)\langle\mathbf{w},\mathbf{a}|, \tag{C.44}$$

equations (C.43) and (C.44) suggest to introduce the operators

$$\begin{aligned}\boldsymbol{\mathcal{P}}_R^\star &= -i\hbar\left.\frac{\partial}{\partial \mathbf{a}}\right|_R+\frac{\mathbf{w}}{2}, \qquad \vec{\mathcal{Q}}_R^\star = i\hbar\left.\frac{\partial}{\partial \mathbf{w}}\right|_R+\frac{\mathbf{a}}{2}, \\ \boldsymbol{\mathcal{P}}_L^\star &= i\hbar\left.\frac{\partial}{\partial \mathbf{a}}\right|_L+\frac{\mathbf{w}}{2}, \qquad \vec{\mathcal{Q}}_L^\star = -i\hbar\left.\frac{\partial}{\partial \mathbf{w}}\right|_L+\frac{\mathbf{a}}{2},\end{aligned}$$

where the operators with index R act on the states $|\mathbf{w},\mathbf{a}\rangle$, whereas the operators with index L act on the states $\langle\mathbf{w},\mathbf{a}|$. Written in terms of these operators equations (C.43) and (C.44) become

$$\vec{\mathcal{P}}_R^\star|\mathbf{w},\mathbf{a}\rangle = i\frac{\Delta_p}{\Delta_q}\vec{\mathcal{Q}}_R^\star|\mathbf{w},\mathbf{a}\rangle, \tag{C.45}$$

$$\vec{\mathcal{P}}_L^\star\langle\mathbf{w},\mathbf{a}| = -i\frac{\Delta_p}{\Delta_q}\vec{\mathcal{Q}}_L^\star\langle\mathbf{w},\mathbf{a}|, \tag{C.46}$$

where $\hbar$ has been expressed by equation (C.4).

The coherent states satisfy the generalized closure relation

$$\frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{w}\int d^3\mathbf{a}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}| = \mathbb{1}. \tag{C.47}$$

In order to proof this, we start from equations (C.19) and (C.20), which imply

$$T(\delta\mathbf{a},\delta\mathbf{w})^{-1}\,|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|\,T(\delta\mathbf{a},\delta\mathbf{w}) = |\mathbf{w}+\delta\mathbf{w},\mathbf{a}+\delta\mathbf{a}\rangle\langle\mathbf{w}+\delta\mathbf{w},\mathbf{a}+\delta\mathbf{a}|$$

and thus also

$$\begin{aligned}&\int d^3\mathbf{w}\int d^3\mathbf{a}\,T(\delta\mathbf{a},\delta\mathbf{w})^{-1}\,|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|\,T(\delta\mathbf{a},\delta\mathbf{w}) \\ &= \int d^3\mathbf{w}\int d^3\mathbf{a}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|.\end{aligned} \tag{C.48}$$

For infinitesimal $\delta\mathbf{a}$ and $\delta\mathbf{w}$ we have according to equations (C.17) and (C.18)

$$T(\delta\mathbf{a},\delta\mathbf{w}) \simeq \mathbb{1} + \frac{i}{\hbar}\,(\delta\mathbf{w}\,\mathbf{Q} - \delta\mathbf{a}\,\mathbf{P}).$$

Inserting this expression into equation (C.48), we see that necessarily

$$\begin{aligned}\left[\int d^3\mathbf{w}\int d^3\mathbf{a}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|,\mathbf{P}\right] &= 0,\\ \left[\int d^3\mathbf{w}\int d^3\mathbf{a}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|,\mathbf{Q}\right] &= 0.\end{aligned}$$

Since all operators $X \in \mathcal{L}(\mathcal{H})$ can be written as functions of $\mathbf{P}$ and $\mathbf{Q}$, it follows that

$$\int d^3\mathbf{w}\int d^3\mathbf{a}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}| = c\mathbb{1}, \qquad c\in\mathbb{C}. \tag{C.49}$$

equation (C.47) is obtained for the choice $c = (2\pi\hbar)^3$. This can be seen by calculating the matrix elements $\langle\mathbf{0},\mathbf{0}|\ldots|\mathbf{0},\mathbf{0}\rangle$ of equation (C.49). In fact, adopting the normalization $\langle\mathbf{0},\mathbf{0}|\mathbf{0},\mathbf{0}\rangle = 1$ we get

$$\begin{aligned}&\frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{w}\int d^3\mathbf{a}\,\langle\mathbf{0},\mathbf{0}|\mathbf{w},\mathbf{a}\rangle\langle\mathbf{w},\mathbf{a}|\mathbf{0},\mathbf{0}\rangle \\ &\qquad= \frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{w}\int d^3\mathbf{a}\,e^{-\left(\frac{(\mathbf{w})^2}{(2\Delta p)^2}+\frac{(\mathbf{a})^2}{(2\Delta q)^2}\right)} \\ &\qquad= \langle\mathbf{0},\mathbf{0}|\mathbf{0},\mathbf{0}\rangle \\ &\qquad= 1,\end{aligned}$$

where in the second line we have used the expression (C.38) for the evaluation of the scalar product $\langle\mathbf{0},\mathbf{0}|\mathbf{w},\mathbf{a}\rangle$.

Due to the analytical properties of the coherent states with respect to the parameters $\mathbf{p}, \mathbf{q}$ (or, equivalently, $\boldsymbol{\alpha}$), all matrix elements $\langle\boldsymbol{\alpha}|O|\boldsymbol{\alpha}'\rangle$ of a one-particle operator O can be reconstructed from the "diagonal" matrix elements $\langle\boldsymbol{\alpha}|O|\boldsymbol{\alpha}\rangle$, where the states $|\boldsymbol{\alpha}\rangle$ are written in the short-hand notation (C.29). In order to prove this quite surprising property, which is sometimes referred to as the "diagonal representation", we have to show that

$$\langle\boldsymbol{\alpha}|X|\boldsymbol{\alpha}\rangle = \langle\boldsymbol{\alpha}|Y|\boldsymbol{\alpha}\rangle, \qquad \forall\boldsymbol{\alpha}, \tag{C.50}$$

implies

$$Z \equiv X - Y = 0.$$

We start from the fact that the eigenstates of the self-adjoint operator $\mathbf{A}^\dagger\mathbf{A}$ form a complete orthonormal basis. From equation (C.16) we get

$$\mathbf{A}^\dagger \cdot \mathbf{A}|\mathbf{n}\rangle = n|\mathbf{n}\rangle, \qquad \mathbf{n} = (n_1, n_2, n_3),$$
$$\text{with } n_i = 0, 1, 2, \ldots, \; i = 1, 2, 3.$$

The completeness of the states $|\mathbf{n}\rangle$ implies

$$\sum_{\mathbf{n}} |\mathbf{n}\rangle\langle\mathbf{n}| = \mathbb{1}.$$

Thus, equation (C.50) can be rewritten in the form

$$0 \equiv \langle\boldsymbol{\alpha}|Z|\boldsymbol{\alpha}\rangle = \sum_{\mathbf{n}}\sum_{\mathbf{m}} \langle\boldsymbol{\alpha}|\mathbf{n}\rangle \, \langle\mathbf{n}|Z|\mathbf{m}\rangle\langle\mathbf{m}|\boldsymbol{\alpha}\rangle. \tag{C.51}$$

Inserting equation (C.39), written in the short-hand notation

$$\langle\boldsymbol{\alpha}|\mathbf{n}\rangle = \frac{\boldsymbol{\alpha}^{\star\mathbf{n}}}{\sqrt{\mathbf{n}!}} e^{-\frac{|\boldsymbol{\alpha}|^2}{2}},$$

with $\mathbf{n}! \equiv n_1! n_2! n_3!$ and $\boldsymbol{\alpha}^{\mathbf{n}} \equiv \alpha_1^{n_1}\alpha_2^{n_2}\alpha_3^{n_3}$, into equation (C.51), we obtain the condition

$$\sum_{\mathbf{n}}\sum_{\mathbf{m}} \frac{\boldsymbol{\alpha}^{\star\mathbf{n}}\boldsymbol{\alpha}^{\mathbf{m}}}{\sqrt{\mathbf{n}!\mathbf{m}!}} \, \langle\mathbf{n}|Z|\mathbf{m}\rangle \equiv 0,$$

which implies

$$\langle\mathbf{n}|Z|\mathbf{m}\rangle = 0, \quad \forall\mathbf{n}, \mathbf{m},$$

and thus $Z = 0$. This important property implies in particular, that the operator O can be written in the form

$$\begin{aligned} O &= \int_{\mathbb{R}^6} d^6\boldsymbol{z} \, o(\boldsymbol{z}) \, |\boldsymbol{z}\rangle\langle\boldsymbol{z}| \qquad (C.52) \\ &= \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} d^3\mathbf{w} \int_{\mathbb{R}^3} d^3\mathbf{a} \; o(\mathbf{w}, \mathbf{a}) \, |\mathbf{w}, \mathbf{a}\rangle\langle\mathbf{w}, \mathbf{a}|, \end{aligned}$$

which is the "diagonal representation". From equation (C.52) and the definition of the overlap function $g(\boldsymbol{z}, \boldsymbol{z}')$ given by equation (6.13) we find that the function $o\,(\boldsymbol{z})$ and the diagonal elements $\langle \boldsymbol{z}|O|\boldsymbol{z}\rangle$ are related by the integral equation

$$\langle \boldsymbol{z}|O|\boldsymbol{z}\rangle \;=\; \int_{\mathbb{R}^6} d^6\boldsymbol{z}'\, o(\boldsymbol{z}')g(\boldsymbol{z}, \boldsymbol{z}').$$

C.2 Solution of the integral equation (6.18)

With equation (6.12), the integral equation (6.18) becomes

$$p(\boldsymbol{z}, s) \;=\; \int_{\mathbb{R}^6} d^6\boldsymbol{z}'\, \rho(\boldsymbol{z}', s)g(\boldsymbol{z}, \boldsymbol{z}'). \tag{C.53}$$

This equation can be solved using the matrix inversion method proposed in Ref. [24]. According to equation (6.13) the kernel depends only on the difference $\boldsymbol{z} - \boldsymbol{z}'$, i.e., we may write

$$\begin{aligned} g(\boldsymbol{z}, \boldsymbol{z}') &\equiv h(\boldsymbol{z} - \boldsymbol{z}') \\ &= h_1(\mathbf{q} - \mathbf{q}')h_2(\mathbf{p} - \mathbf{p}') \end{aligned} \tag{C.54}$$

with

$$\begin{aligned} h_1(\mathbf{q} - \mathbf{q}') &= e^{-\left(\frac{\mathbf{q}-\mathbf{q}'}{2\Delta}\right)^2} \\ h_2(\mathbf{p} - \mathbf{p}') &= e^{-\left(\frac{(\mathbf{p}-\mathbf{p}')\Delta}{\hbar}\right)^2}. \end{aligned}$$

We start from the Taylor expansion of $\rho(\boldsymbol{z}', s)$ at $\boldsymbol{z}$,

$$\rho(\boldsymbol{z}', s) = \sum a_n \rho^{(n)}(\boldsymbol{z}) \tag{C.55}$$

with

$$\rho^{(n)}(\boldsymbol{z}, s) \equiv \left(\frac{\partial}{\partial\, \boldsymbol{z}'}\right)^n \rho(\boldsymbol{z}', s)\bigg|_{\boldsymbol{z}'=\boldsymbol{z}}$$

and

$$a_n = \frac{1}{n!}\int_{\mathbb{R}^6} d^6\boldsymbol{z}'\, (\boldsymbol{z}')^n h(\boldsymbol{z}),$$

where $(\boldsymbol{z}')^n$ denotes the 6-dimensional vector

$$(\boldsymbol{z}')^n \equiv \left(\left(\frac{\Delta_q}{\pi\hbar}p_1'\right)^n, \left(\frac{\Delta_q}{\pi\hbar}p_2'\right)^n, \left(\frac{\Delta_q}{\pi\hbar}p_3'\right)^n, \left(\frac{\Delta_p}{\pi\hbar}q_1'\right)^n, \left(\frac{\Delta_p}{\pi\hbar}q_2'\right)^n, \left(\frac{\Delta_p}{\pi\hbar}q_3'\right)^n\right).$$

The symmetry of the function $h(\boldsymbol{z}$ defined in equation (C.54) with respect to the origin implies

$$a_{2n+1} = 0, \quad n = 0, 1, \ldots. \tag{C.56}$$

Inserting equation (C.55) into equation (C.53), we get

$$p(\boldsymbol{z}, s) = \sum_{n=0}^{\infty} a_n \rho^{(n)}(\boldsymbol{z}, s).$$

Taking the derivatives of the above equation

$$\begin{aligned} p^{(1)}(\boldsymbol{z}, s) &= \sum_{n=0}^{\infty} a_n \rho^{(n+1)}(\boldsymbol{z}, s) \\ p^{(2)}(\boldsymbol{z}, s) &= \sum_{n=0}^{\infty} a_n \rho^{(n+2)}(\boldsymbol{z}, s) \\ &\vdots \end{aligned}$$

and assuming that for some given integer m we have

$$p^{(j)}(\boldsymbol{z}, s) \approx 0, \qquad j > m, \tag{C.57}$$

we obtain the linear equation system

$$\begin{pmatrix} p^{(0)}(\boldsymbol{z}, s) \\ p^{(1)}(\boldsymbol{z}, s) \\ \vdots \\ p^{(m)}(\boldsymbol{z}, s) \end{pmatrix} = A \begin{pmatrix} \rho^{(0)}(\boldsymbol{z}, s) \\ \rho^{(1)}(\boldsymbol{z}, s) \\ \vdots \\ \rho^{(m)}(\boldsymbol{z}, s) \end{pmatrix} \tag{C.58}$$

with

$$A = \begin{pmatrix} a_0 & a_1 & a_2 & \cdots & a_m \\ 0 & a_0 & a_1 & \cdots & a_{m-1} \\ & & \ddots & & \\ 0 & 0 & \cdots & & a_0 \end{pmatrix}$$

The tridiagonal matrix A can be easily inverted. We have

$$B \equiv A^{-1} = \begin{pmatrix} b_0 & b_1 & b_2 & \cdots & b_m \\ 0 & b_0 & b_1 & \cdots & b_{m-1} \\ & & \ddots & & \\ 0 & 0 & \cdots & & b_0 \end{pmatrix}$$

where

$$\sum_{i=0}^{n} a_i b_{n-i} = \delta_{0n}, \quad n = 0, 1, \ldots, m. \tag{C.59}$$

From equations (C.56) and (C.59) we get

$$b_{2n+1} = 0, \quad n = 0, 1, \ldots$$

and for the first non-vanishing b coefficients

$$\begin{aligned} b_0 &= \frac{1}{a_0} \\ b_2 &= -\frac{a_2}{a_0^2} \\ b_4 &= \frac{1}{a_0^2}\left(\frac{a_2^2}{a_0} - a_4\right) \\ b_6 &= -\frac{1}{a_0^2}\left(\frac{a_2^3}{a_0^2} - 2\frac{a_2 a_4}{a_0} + a_6\right) \\ &\vdots \end{aligned}$$

Clearly, the solution of equation (C.58)

$$\begin{pmatrix} \rho^{(0)}(\boldsymbol{z}, s) \\ \rho^{(1)}(\boldsymbol{z}, s) \\ \vdots \\ \rho^{(m)}(\boldsymbol{z}, s) \end{pmatrix} = B \begin{pmatrix} p^{(0)}(\boldsymbol{z}, s) \\ p^{(1)}(\boldsymbol{z}, s) \\ \vdots \\ p^{(m)}(\boldsymbol{z}, s) \end{pmatrix} \tag{C.60}$$

satisfies the condition (6.20), if the condition (C.57) is satisfied and if

$$\left| p^{(i)}(\boldsymbol{z}, s) \right| < \infty, \quad i = 1, 2, \ldots, m.$$

The validity of the additional condition (6.35), which finally leads to the conventional form of the drift-term and the field term in the semi-classical Boltzmann equation, requires that we can choose the parameter Δ such that $m = 2$ in equation (C.57). Thus, both conditions (6.20) and (6.35) are satisfied as long as – on the scale of the parameters Δ_q and Δ_p – the expectation values $p^{(0)}(\boldsymbol{z}, s)$ depend only weakly on the position $\mathbf{p}, \mathbf{q}$ in phase space.

C.3 Matrix elements of the position and momentum operators

Any one-body operator $O^{(1)} \in \mathcal{L}(\mathcal{H})$ representing a physical observable can be expressed as

$$O^{(1)} = f\left(\mathbf{p}, \mathbf{q}\right).$$

It is thus worthwhile to calculate the matrix elements of the position operator $\mathbf{q}$ and of the momentum operator $\mathbf{p}$. From equation (C.31) we obtain by direct integration

$$\langle \mathbf{p}, \mathbf{q}|\mathbf{q}|\mathbf{p}', \mathbf{q}'\rangle = \left(\frac{\mathbf{q}+\mathbf{q}'}{2} - i\frac{\Delta_q}{2}\,\frac{\mathbf{p}-\mathbf{p}'}{\Delta_p}\right)\langle \mathbf{p}, \mathbf{q}|\mathbf{p}', \mathbf{q}'\rangle$$

and

$$\langle \mathbf{p}, \mathbf{q}|\mathbf{p}|\mathbf{p}', \mathbf{q}'\rangle = \left(\frac{\mathbf{p}+\mathbf{p}'}{2} + i\frac{\Delta_p}{2}\,\frac{\mathbf{q}-\mathbf{q}'}{\Delta_q}\right)\langle \mathbf{p}, \mathbf{q}|\mathbf{p}', \mathbf{q}'\rangle.$$

In particular we have

$$\langle \mathbf{p}, \mathbf{q}|\mathbf{q}|\mathbf{p}, \mathbf{q}\rangle = \mathbf{q}, \tag{C.61}$$

$$\langle \mathbf{p}, \mathbf{q}|\mathbf{p}|\mathbf{p}, \mathbf{q}\rangle = \mathbf{p}, \tag{C.62}$$

According to equation (C.52), the operators $\mathbf{q}$ and $\mathbf{p}$ can also be written in the form

$$\mathbf{q} = \frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}\, d^3\mathbf{q}\; f_q(\mathbf{p}, \mathbf{q})\;\; |\mathbf{p}, \mathbf{q}\rangle\langle \mathbf{p}, \mathbf{q}|$$

$$\mathbf{p} = \frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}\, d^3\mathbf{q}\; f_p(\mathbf{p}, \mathbf{q})\;\; |\mathbf{p}, \mathbf{q}\rangle\langle \mathbf{p}, \mathbf{q}|,$$

where, according to equation (C.60), the functions $f_q(\mathbf{p}, \mathbf{q})$ and $f_p(\mathbf{p}, \mathbf{q})$ are completely determined by $\langle u|\bar{D}_{(1)}|\boldsymbol{u}\rangle$ (C.61) and (C.62).

C.4 Basis transformation for a one-body operator

The required basis transformation (step (ii) in our general procedure) from the basis $|\nu\rangle$ of one-particle eigenvectors of $H_0^{(1)}$ into the basis of coherent states $|\boldsymbol{z}\rangle = |\mathbf{p}, \mathbf{q}\rangle$ can be performed using the closure relation

$$\sum_\nu |\nu\rangle\langle\nu| = \mathbb{1}, \qquad \nu = 1, 2\ldots. \tag{C.63}$$

Let us first consider the case of a one-body operator $O^{(1)}$, which may e.g. represent the coarse grained one-particle density matrix $\bar{D}_{(1)}$. Its matrix elements in the basis of the eigenvectors of $H_0^{(1)}$ are given as

$$O^{(1)}_{\nu\mu} \equiv \langle\nu|O^{(1)}|\mu\rangle.$$

Similarly, the matrix elements in the basis of the coherent states are

$$O^{(1)}_{\boldsymbol{z}\boldsymbol{z}'} \equiv \langle\boldsymbol{z}|O^{(1)}|\boldsymbol{z}'\rangle.$$

Using the closure relation (C.63) we obtain

$$\langle \boldsymbol{z}|O^{(1)}|\boldsymbol{z}'\rangle = \sum_{\nu\mu}\langle \boldsymbol{z}|\nu\rangle\ \langle\nu|O^{(1)}|\mu\rangle\langle\mu|\boldsymbol{z}'\rangle.$$

Knowing the eigenfunctions $|\nu\rangle$, the coefficients $\langle \boldsymbol{z}|\nu\rangle$,and $\langle\mu|\boldsymbol{z}'\rangle$ can be obtained easily. For a solid with periodic boundary conditions it is convenient to start from the Fourier expansion

$$\langle \mathbf{x}|\nu\rangle = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} c^{\nu}_{\mathbf{k}}\, e^{i\mathbf{k}\mathbf{x}}, \qquad \sum_{\mathbf{k}}|c^{\nu}_{\mathbf{k}}|^2 = 1, \tag{C.64}$$

where the coefficients $c^{\nu}_{\mathbf{k}}$ are determined from equation $H^{(1)}_0|\nu) = \hbar\omega_\nu|\nu)$, and where V is the volume of the solid. Thus, in order to express the matrix elements $O^{(1)}_{\boldsymbol{z}\boldsymbol{z}'}$ in terms of the matrix elements $O^{(1)}_{\nu\mu}$, we need the Fourier transform of the coherent states. For $V = L^3$ and $\Delta \ll L$, the overlap of the coherent states becomes negligible over the crystal dimensions, so that we can approximate

$$\begin{aligned}
\langle \boldsymbol{z}|\nu\rangle &= \int d^3\mathbf{x}\langle \boldsymbol{z}|\mathbf{x}\rangle\langle\mathbf{x}|\nu\rangle \\
&\approx \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2 \int_{-\infty}^{\infty} dx_3 \langle \boldsymbol{z}|\mathbf{x}\rangle\langle\mathbf{x}|\nu\rangle = \int_{\mathbb{R}^3} d^3\mathbf{x}\langle \boldsymbol{z}|\mathbf{x}\rangle\langle\mathbf{x}|\nu\rangle.
\end{aligned} \tag{C.65}$$

From equations (C.31), (C.64) and (C.65) we get

$$\begin{aligned}
\langle \boldsymbol{z}|\nu\rangle &= \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} c^{\nu}_{\mathbf{k}} \left(\frac{1}{2\pi\Delta^2}\right)^{\frac{3}{4}} \int_{\mathbb{R}^3} d^3\mathbf{x} e^{-\left(\frac{|\mathbf{x}-\mathbf{q}|}{2\Delta}\right)^2} e^{-i\frac{\mathbf{p}}{\hbar}\left(\mathbf{x}-\frac{\mathbf{q}}{2}\right)} e^{i\mathbf{k}\mathbf{x}} \\
&= \frac{1}{\sqrt{V}}\left(2\sqrt{2\pi}\Delta\right)^{\frac{3}{2}} \sum_{\mathbf{k}} c^{\nu}_{\mathbf{k}}\, e^{-\frac{\Delta^2(\hbar\mathbf{k}-\mathbf{p})^2}{\hbar^2}} e^{i\frac{(\hbar\mathbf{k}-\frac{\mathbf{p}}{2})\mathbf{q}}{\hbar}} \\
&= \frac{1}{\sqrt{V}}\left(2\sqrt{2\pi}\Delta\right)^{\frac{3}{2}} \sum_{\mathbf{k}} c^{\nu}_{\mathbf{k}}\, e^{-\left(\frac{\hbar\mathbf{k}-\mathbf{p}}{2\Delta_p}\right)^2} e^{\frac{i(\hbar\mathbf{k}-\frac{\mathbf{p}}{2})\mathbf{q}}{\hbar}},
\end{aligned}$$

and finally

$$\begin{aligned}
\langle \mathbf{p},\mathbf{q}|O^{(1)}|\mathbf{p}',\mathbf{q}'\rangle &= \frac{(2\sqrt{2\pi}\Delta)^3}{V}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\nu\mu} c^{\nu}_{\mathbf{k}} c^{\mu\star}_{\mathbf{k}'}\ \langle\nu|O^{(1)}|\mu\rangle \\
&\quad \times e^{-\left(\frac{\hbar\mathbf{k}-\mathbf{p}}{2\Delta_p}\right)^2} e^{-\left(\frac{\hbar\mathbf{k}'-\mathbf{p}'}{2\Delta_p}\right)^2} e^{\frac{i(\hbar\mathbf{k}-\frac{\mathbf{p}}{2})\mathbf{q}}{\hbar}} e^{\frac{-i\left(\hbar\mathbf{k}'-\frac{\mathbf{p}'}{2}\right)\mathbf{q}'}{\hbar}}.
\end{aligned} \tag{C.66}$$

In case of a constant one-particle potential (jellium) the eigenvectors of $H^{(1)}_0$ are given by normalized single plane waves $\frac{1}{\sqrt{V}}e^{i\mathbf{k}\mathbf{x}}$, and the above expression

reduces to

$$\begin{aligned}\langle \mathbf{p},\mathbf{q}|O^{(1)}|\mathbf{p}',\mathbf{q}'\rangle &= \frac{(2\sqrt{2\pi}\Delta)^3}{V}\sum_{\mathbf{k},\mathbf{k}'}\langle \mathbf{k}|O^{(1)}|\mathbf{k}'\rangle \\ &\times e^{-\left(\frac{\hbar\mathbf{k}-\mathbf{p}}{2\Delta_p}\right)^2} e^{-\left(\frac{\hbar\mathbf{k}'-\mathbf{p}'}{2\Delta_p}\right)^2} e^{\frac{i(\hbar\mathbf{k}-\frac{\mathbf{p}}{2})\mathbf{q}}{\hbar}} e^{\frac{-i\left(\hbar\mathbf{k}'-\frac{\mathbf{p}'}{2}\right)\mathbf{q}'}{\hbar}}.\end{aligned} \tag{C.67}$$

The corresponding expressions $\langle \boldsymbol{u}|O^{(1)}|\boldsymbol{u}\rangle$, which determine the one-body operator, are

$$\begin{aligned}\langle \mathbf{p},\mathbf{q}|O^{(1)}|\mathbf{p},\mathbf{q}\rangle &= \frac{(2\sqrt{2\pi}\Delta)^3}{V}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\nu\mu} c_{\mathbf{k}}^{\nu} c_{\mathbf{k}'}^{\mu\star}\ \langle \nu|O^{(1)}|\mu\rangle \\ &\times e^{-\left(\frac{\hbar\mathbf{k}-\mathbf{p}}{2\Delta_p}\right)^2} e^{-\left(\frac{\hbar\mathbf{k}'-\mathbf{p}}{2\Delta_p}\right)^2} e^{i(\mathbf{k}-\mathbf{k}')\mathbf{q}}.\end{aligned}$$

for the general case and

$$\begin{aligned}\langle \mathbf{p},\mathbf{q}|O^{(1)}|\mathbf{p},\mathbf{q}\rangle &= \frac{(2\sqrt{2\pi}\Delta)^3}{V}\sum_{\mathbf{k},\mathbf{k}'}\langle \mathbf{k}|O^{(1)}|\mathbf{k}'\rangle \\ &\times e^{-\left(\frac{\hbar\mathbf{k}-\mathbf{p}}{2\Delta_p}\right)^2} e^{-\left(\frac{\hbar\mathbf{k}'-\mathbf{p}}{2\Delta_p}\right)^2} e^{i(\mathbf{k}-\mathbf{k}')\mathbf{q}}.\end{aligned}$$

for the jellium case. When the operator $O^{(1)}$ represents physical one-particle interaction operators or the operator of the kinetic energy, we have

$$\left|\ \langle \mathbf{k}|O^{(1)}|\mathbf{k}'\rangle\right| \to \infty \qquad \text{for} \quad \text{for}\left|\mathbf{k}-\mathbf{k}'\right| \to 0,$$

which, according to equations (C.66) or (C.67) implies also

$$\left|\ \langle \mathbf{p},\mathbf{q}|O^{(1)}|\mathbf{p}',\mathbf{q}'\rangle\right| \to 0 \qquad \text{for} \quad \text{for}\left|\mathbf{p}-\mathbf{p}'\right| \to \infty.$$

C.5 Matrix elements of the commutator $\left[\bar{D}_{(1)}, V\right]$

According to equation (6.30) we have

$$e^{i\mathbf{k}\vec{\mathcal{Q}}_R}\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle = e^{\frac{i\mathbf{k}\mathbf{q}}{2}}\langle \mathbf{p}',\mathbf{q}'|\mathbf{p}+\hbar\mathbf{k},\mathbf{q}\rangle. \tag{C.68}$$

Similarly, we get for the operators $\vec{\mathcal{Q}}_L$ defined in equation (C.45)

$$e^{i\mathbf{k}\vec{\mathcal{Q}}_L}\langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle = e^{\frac{i\mathbf{k}\mathbf{q}}{2}}\langle \mathbf{p}-\hbar\mathbf{k},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle. \tag{C.69}$$

With equation (C.68) we obtain for the integral (a) in equation (6.36)

$$\begin{aligned}
&\frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,\langle\mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle e^{i\mathbf{k}\vec{\mathcal{Q}}_R}\langle\mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle \\
&\qquad = e^{\frac{i\mathbf{k}\mathbf{q}}{2}}\frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,\langle\mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle\langle\mathbf{p}',\mathbf{q}'|\mathbf{p}+\hbar\mathbf{k},\mathbf{q}\rangle \\
&\qquad = e^{\frac{i\mathbf{k}\mathbf{q}}{2}}\langle\mathbf{p},\mathbf{q}|\mathbf{p}+\hbar\mathbf{k},\mathbf{q}\rangle \\
&\qquad = e^{\frac{i\mathbf{k}\mathbf{q}}{2}}e^{-\frac{\Delta^2\mathbf{k}^2}{2}}e^{\frac{i\mathbf{k}\mathbf{q}}{2}} \\
&\qquad = e^{i\mathbf{k}\mathbf{q}}\,e^{-\frac{\Delta^2\mathbf{k}^2}{2}},
\end{aligned} \tag{C.70}$$

and with equation (C.69) for the integral (a) in equation (6.37)

$$\begin{aligned}
&\frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,e^{i\mathbf{k}\vec{\mathcal{Q}}_L}\langle\mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle\langle\mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle \\
&\qquad = e^{\frac{i\mathbf{k}\mathbf{q}}{2}}\frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,\langle\mathbf{p}-\hbar\mathbf{k},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle\langle\mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle \\
&\qquad = e^{\frac{i\mathbf{k}\mathbf{q}}{2}}\langle\mathbf{p}-\hbar\mathbf{k},\mathbf{q}|\mathbf{p},\mathbf{q}\rangle \\
&\qquad = e^{i\mathbf{k}\mathbf{q}}\,e^{-\frac{\Delta^2\mathbf{k}^2}{2}}.
\end{aligned} \tag{C.71}$$

The integrals (b) and (c) in equations (6.36) and (6.37) are evaluated following the same general procedure. We thus get

$$\begin{aligned}
&\frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,\langle\mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle e^{i\mathbf{k}\vec{\mathcal{Q}}_R}\langle\mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle\,(\mathbf{p}'-\mathbf{p}) \\
&= \frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,\langle\mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle e^{\frac{i\mathbf{k}\mathbf{q}}{2}}\langle\mathbf{p}',\mathbf{q}'|\mathbf{p}+\hbar\mathbf{k},\mathbf{q}\rangle\,(\mathbf{p}'-\mathbf{p}) \\
&= \frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,(\mathbf{p}'-\mathbf{p})\,e^{\frac{i\mathbf{k}\mathbf{q}}{2}}e^{-\frac{(\mathbf{q}-\mathbf{q}')^2}{8\Delta^2}}e^{-\frac{(\mathbf{p}-\mathbf{p}')^2\Delta^2}{2\hbar^2}}e^{\frac{i(\mathbf{p}'\mathbf{q}-\mathbf{q}'\mathbf{p})}{2\hbar}} \\
&\qquad\qquad e^{-\frac{(\mathbf{q}-\mathbf{q}')^2}{8\Delta^2}}e^{-\frac{(\mathbf{p}+\hbar\mathbf{k}-\mathbf{p}')^2\Delta^2}{2\hbar^2}}e^{\frac{i((\mathbf{p}+\hbar\mathbf{k})\mathbf{q}'-\mathbf{q}\mathbf{p}')}{2\hbar}} \\
&= e^{i\mathbf{k}\mathbf{q}}\frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,(\mathbf{p}'-\mathbf{p})\,e^{\frac{i\mathbf{k}(\mathbf{q}'-\mathbf{q})}{2}}e^{-\frac{\Delta^2\mathbf{k}^2}{2}}e^{-\left(\frac{\mathbf{q}-\mathbf{q}'}{2\Delta}\right)^2} \\
&\qquad\qquad e^{-\frac{(\mathbf{p}-\mathbf{p}')^2\Delta^2}{\hbar^2}}e^{-\frac{\Delta^2\mathbf{k}(\mathbf{p}-\mathbf{p}')}{\hbar}} \\
&= e^{i\mathbf{k}\mathbf{q}}\,e^{-\frac{\Delta^2\mathbf{k}^2}{2}}\frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,e^{\frac{i\mathbf{k}\mathbf{q}'}{2}}\,e^{\frac{\Delta^2\mathbf{k}\mathbf{p}'}{\hbar}}e^{-\left(\frac{\mathbf{q}'}{2\Delta}\right)^2}e^{-\left(\frac{\Delta\mathbf{p}'}{\hbar}\right)^2}\mathbf{p}'.
\end{aligned}$$

With

$$\begin{aligned}\int\limits_{\mathbb{R}^3} d^3\mathbf{q}'\, e^{\frac{i\mathbf{k}\mathbf{q}'}{2}} e^{-\left(\frac{\mathbf{q}'}{2\Delta}\right)^2} &= \left(2\Delta\sqrt{\pi}\right)^3 e^{-\frac{\Delta^2\mathbf{k}^2}{4}} \\ \int\limits_{\mathbb{R}^3} d^3\mathbf{p}'\, e^{\frac{\Delta^2\mathbf{k}\mathbf{p}'}{\hbar}} \mathbf{p}' e^{-\left(\frac{\Delta\mathbf{p}'}{\hbar}\right)^2} &= \frac{\hbar\mathbf{k}}{2} e^{\frac{\Delta^2\mathbf{k}^2}{4}} \left(\frac{\hbar\sqrt{\pi}}{\Delta}\right)^3\end{aligned}$$

we get finally for the integral (b) in equation (6.36)

$$\begin{aligned}&\frac{1}{(2\pi\hbar)^3} \int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\, d^3\mathbf{q}'\, \langle \mathbf{p}, \mathbf{q} | \mathbf{p}', \mathbf{q}' \rangle e^{i\mathbf{k}\vec{\mathcal{Q}}_R} \langle \mathbf{p}', \mathbf{q}' | \mathbf{p}, \mathbf{q} \rangle \left(\mathbf{p}' - \mathbf{p}\right) \\ &\qquad = \frac{\hbar\mathbf{k}}{2} e^{i\mathbf{k}\mathbf{q}}\, e^{-\frac{\Delta^2\mathbf{k}^2}{2}}. \end{aligned} \tag{C.72}$$

The integral (b) in equation (6.37) is obtained by complex conjugation of the above result and after the change $\mathbf{k} \to -\mathbf{k}$ (see equation (C.69)), i.e.,

$$\begin{aligned}&\frac{1}{(2\pi\hbar)^3} \int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\, d^3\mathbf{q}'\, e^{i\mathbf{k}\vec{\mathcal{Q}}_L} \langle \mathbf{p}, \mathbf{q} | \mathbf{p}', \mathbf{q}' \rangle \langle \mathbf{p}', \mathbf{q}' | \mathbf{p}, \mathbf{q} \rangle \left(\mathbf{p}' - \mathbf{p}\right) \\ &\qquad = -\frac{\hbar\mathbf{k}}{2}\, e^{i\mathbf{k}\mathbf{q}}\, e^{-\frac{\Delta^2\mathbf{k}^2}{2}}. \end{aligned} \tag{C.73}$$

Correspondingly, we find for the integral (c) in equations (6.36) and (6.37)

$$\begin{aligned}&\frac{1}{(2\pi\hbar)^3} \int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\, d^3\mathbf{q}'\, \langle \mathbf{p}, \mathbf{q} | \mathbf{p}', \mathbf{q}' \rangle e^{i\mathbf{k}\vec{\mathcal{Q}}_R} \langle \mathbf{p}', \mathbf{q}' | \mathbf{p}, \mathbf{q} \rangle \left(\mathbf{q}' - \mathbf{q}\right) \\ &\quad = \frac{1}{(2\pi\hbar)^3} \int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\, d^3\mathbf{q}'\, \langle \mathbf{p}, \mathbf{q} | \mathbf{p}', \mathbf{q}' \rangle e^{\frac{i\mathbf{k}\mathbf{q}}{2}} \langle \mathbf{p}', \mathbf{q}' | \mathbf{p} + \hbar\mathbf{k}, \mathbf{q} \rangle \left(\mathbf{q}' - \mathbf{q}\right) \\ &\quad = e^{i\mathbf{k}\mathbf{q}} e^{-\frac{\Delta^2\mathbf{k}^2}{2}} \frac{1}{(2\pi\hbar)^3} \int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\, d^3\mathbf{q}'\, \mathbf{q}' e^{\frac{i\mathbf{k}\mathbf{q}'}{2}} e^{\frac{\Delta^2\mathbf{k}\mathbf{p}'}{\hbar}} e^{-\left(\frac{\mathbf{q}'}{2\Delta}\right)^2} e^{-\left(\frac{\Delta\mathbf{p}'}{\hbar}\right)^2} \\ &\quad = i\Delta^2\mathbf{k} e^{i\mathbf{k}\mathbf{q}} e^{-\frac{\Delta^2\mathbf{k}^2}{2}}, \end{aligned} \tag{C.74}$$

where the last line3 is obtained from

$$\int\limits_{\mathbb{R}^3} d^3\mathbf{p}' e^{\frac{\Delta^2\mathbf{k}\mathbf{p}'}{\hbar}} e^{-\left(\frac{\Delta\mathbf{p}'}{\hbar}\right)^2} = \left(\frac{\sqrt{\pi}\hbar}{\Delta}\right)^3 e^{\frac{\Delta^2\mathbf{k}^2}{4}}$$

and

$$\int\limits_{\mathbb{R}^3} d^3\mathbf{q}' e^{\frac{i\mathbf{k}\mathbf{q}'}{2}} e^{-\left(\frac{\mathbf{q}'}{2\Delta}\right)^2} \mathbf{q}' = i\Delta^2\mathbf{k} \left(2\sqrt{\pi}\Delta\right)^3 e^{-\frac{\Delta^2\mathbf{k}^2}{4}}.$$

As before, the result for the integral (c) in equation (6.37) is found by complex conjugation of the result of equation (C.74) and after the change $\mathbf{k} \to -\mathbf{k}$,

$$\frac{1}{(2\pi\hbar)^3} \int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\, d^3\mathbf{q}'\, e^{i\mathbf{k}\vec{\mathcal{Q}}_L} \langle \mathbf{p}, \mathbf{q} | \mathbf{p}', \mathbf{q}' \rangle \langle \mathbf{p}', \mathbf{q}' | \mathbf{p}, \mathbf{q} \rangle \left(\mathbf{q}' - \mathbf{q} \right)$$
$$= i\Delta^2 \mathbf{k}\, e^{i\mathbf{k}\mathbf{q}}\, e^{-\frac{\Delta^2 \mathbf{k}^2}{2}}. \tag{C.75}$$

Altogether, from equations (6.29), (6.32), (6.35), and the results for the integrals (6.36) and (6.36), which are given by equations (C.70), (C.71) for the contributions (a), by equations (C.72), (C.73) for the contributions (b), and by equations (C.74), (C.75) for the contributions (c), we obtain finally

$$\begin{aligned}
\langle \boldsymbol{u} | \frac{i}{\hbar} \left[\bar{D}_{(1)}, V \right] | \boldsymbol{u} \rangle &= \frac{i}{\hbar} \sum_s \int\limits_{\mathbb{R}^3} d^3\mathbf{k}\, \hat{V}(\mathbf{k})\, \langle \boldsymbol{u} | \left[\bar{D}_{(1)}, e^{i\mathbf{k}\vec{\mathcal{Q}}_L} | s \rangle \langle s | \right] | \boldsymbol{u} \rangle \\
&= \frac{i}{\hbar} \sum_s \int\limits_{\mathbb{R}^3} d^3\mathbf{k}\, \hat{V}(\mathbf{k}) \hbar \mathbf{k} e^{-\frac{\Delta^2 \mathbf{k}^2}{2}} e^{i\mathbf{k}\mathbf{q}} \frac{\partial \rho(\mathbf{p}, \mathbf{q}, s)}{\partial \mathbf{p}} \\
&= \frac{\partial}{\partial \mathbf{q}} \left(\int\limits_{\mathbb{R}^3} d^3\mathbf{k}\, \hat{V}(\mathbf{k}) e^{-\frac{\Delta^2 \mathbf{k}^2}{2}} e^{i\mathbf{k}\mathbf{q}} \right) \frac{\partial \rho(\mathbf{p}, \mathbf{q}, s)}{\partial \mathbf{p}} \\
&= \frac{\partial V^c(\mathbf{q})}{\partial \mathbf{q}} \frac{\partial \rho(\mathbf{p}, \mathbf{q}, s)}{\partial \mathbf{p}}.
\end{aligned} \tag{C.76}$$

C.6 Matrix elements of the commutator $\left[\bar{D}_{(1)}, T \right]$

We evaluate the expectation values

$$\langle \boldsymbol{u} | \frac{i}{\hbar} \left[\bar{D}_{(1)}, T \right] | \boldsymbol{u} \rangle$$

with the kinetic energy operator

$$T = \frac{\mathbf{p}^2}{2m}.$$

The matrix elements of the one-particle kinetic energy

$$T = \frac{\mathbf{p}^2}{2m}$$

Using the definition of the differential operator $\vec{\mathcal{P}}_R$ (C.45) and the definition of the differential operator $\vec{\mathcal{P}}_L$ (C.45) we obtain

$$
\begin{aligned}
\langle \mathbf{p}, \mathbf{q}, s|T|\mathbf{p}', \mathbf{q}', s'\rangle &= -\frac{\hbar^2}{2m}\delta_{ss'} \int\limits_{\mathbb{R}^3} d^3\mathbf{x}\, \langle \mathbf{p}, \mathbf{q}|\mathbf{x}\rangle \nabla^2 \langle \mathbf{x}|\mathbf{p}', \mathbf{q}'\rangle \qquad \text{(C.77)} \\
&= \delta_{ss'} \int\limits_{\mathbb{R}^3} d^3\mathbf{x}\, \langle \mathbf{p}, \mathbf{q}|\mathbf{x}\rangle \left(i\hbar \frac{\partial}{\partial \mathbf{q}'} + \frac{\mathbf{p}'}{2} \right)^2 \langle \mathbf{x}|\mathbf{p}', \mathbf{q}'\rangle \\
&= \delta_{ss'} \frac{\vec{\mathcal{P}}_R^{\,2}}{2m} \langle \mathbf{p}, \mathbf{q}|\mathbf{p}', \mathbf{q}'\rangle \\
&= \delta_{ss'} \int\limits_{\mathbb{R}^3} d^3\mathbf{x} \left(-i\hbar \frac{\partial}{\partial \mathbf{q}} + \frac{\mathbf{p}}{2} \right)^2 \langle \mathbf{p}, \mathbf{q}|\mathbf{x}\rangle \langle \mathbf{x}|\mathbf{p}', \mathbf{q}'\rangle \\
&= \delta_{ss'} \frac{\vec{\mathcal{P}}_L^{\,2}}{2m} \langle \mathbf{p}, \mathbf{q}|\mathbf{p}', \mathbf{q}'\rangle \\
&= \frac{\hbar^2}{2m}\delta_{ss'} \langle \mathbf{p}, \mathbf{q}|\mathbf{p}', \mathbf{q}'\rangle \\
&\quad \times \left(\left(\frac{\mathbf{p} + \mathbf{p}'}{2\hbar} \right)^2 - \left(\frac{\mathbf{q} - \mathbf{q}'}{4\Delta^2} \right)^2 \right. \\
&\quad \left. + \frac{i\,(\mathbf{p} + \mathbf{p}')\,(\mathbf{q} - \mathbf{q}')}{4\Delta^2\hbar} + \frac{3}{4\Delta^2} \right).
\end{aligned}
$$

The corresponding diagonal elements are

$$
\begin{aligned}
\langle \mathbf{p}, \mathbf{q}, s|T|\mathbf{p}, \mathbf{q}, s\rangle &= -\frac{\hbar^2}{2m} \int\limits_{\mathbb{R}^3} d^3\mathbf{x} \langle \mathbf{p}, \mathbf{q}|\mathbf{x}\rangle \frac{\partial^2}{\partial \mathbf{x}^2} \langle \mathbf{x}|\mathbf{p}, \mathbf{q}\rangle \\
&= \frac{\mathbf{p}^2}{2m} + \frac{3\hbar^2}{8m\Delta^2}.
\end{aligned}
$$

With "diagonal representation" of the density matrix (6.8) and the 3rd and 5th line in equation (C.77) the expectation value of the commutator can be

written in the form

$$\begin{aligned}
&\langle \mathbf{p},\mathbf{q},s|\frac{i}{\hbar}\left[\bar{D}_{(1)},T\right]|\mathbf{p},\mathbf{q},s\rangle \qquad\qquad (C.78)\\
&= \frac{i}{\hbar}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,\rho(\mathbf{p}',\mathbf{q}',s)\,\big(\quad \langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle\ \langle \mathbf{p}',\mathbf{q}'|T|\mathbf{p},\mathbf{q}\rangle\\
&\qquad\qquad - \langle \mathbf{p},\mathbf{q}|T|\mathbf{p}',\mathbf{q}'\rangle\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle \quad\big)\\
&= \frac{i}{\hbar}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,\rho(\mathbf{p}',\mathbf{q}',s)\left(\quad \langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle\frac{1}{2m}\vec{\mathcal{P}}_R^{\,2}\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle\right.\\
&\qquad\qquad \left. -\frac{1}{2m}\vec{\mathcal{P}}_L^{\,2}\langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle \quad\right).
\end{aligned}$$

From equations (C.45) and (C.45) we find

$$\begin{aligned}
\vec{\mathcal{P}}_R^{\,2} &= -\hbar^2\,\frac{\partial^2}{\partial\mathbf{q}^2}\bigg|_R + i\hbar\,\mathbf{p}\,\frac{\partial}{\partial\mathbf{q}}\bigg|_R + \frac{\mathbf{p}^2}{4}\\
\vec{\mathcal{P}}_L^{\,2} &= -\hbar^2\,\frac{\partial^2}{\partial\mathbf{q}^2}\bigg|_L - i\hbar\,\mathbf{p}\,\frac{\partial}{\partial\mathbf{q}}\bigg|_L + \frac{\mathbf{p}^2}{4}.
\end{aligned}$$

Inserting the above expression into equation (C.78) we find that the contribution of the terms $\frac{\mathbf{p}^2}{4}$ cancels, so we are left with

$$\begin{aligned}
&\langle \mathbf{p},\mathbf{q},s|\frac{i}{\hbar}\left[\bar{D}_{(1)},T\right]|\mathbf{p},\mathbf{q},s\rangle \qquad\qquad (C.79)\\
&= \frac{i}{\hbar}\frac{1}{2m}\frac{1}{(2\pi\hbar)^3}\int\limits_{\mathbb{R}^6} d^3\mathbf{p}'\,d^3\mathbf{q}'\,\rho(\mathbf{p}',\mathbf{q}',s)\\
&\qquad\left(\quad \langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle\left(-\hbar^2\frac{\partial^2}{\partial\mathbf{q}^2}\bigg|_R + i\hbar\mathbf{p}\,\frac{\partial}{\partial\mathbf{q}}\bigg|_R\right)\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle\right.\\
&\qquad\left. -\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle\left(-\hbar^2\,\frac{\partial^2}{\partial\mathbf{q}^2}\bigg|_L - i\hbar\mathbf{p}\,\frac{\partial}{\partial\mathbf{q}}\bigg|_L\right)\langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle \quad\right).
\end{aligned}$$

From equations (6.13), (C.45), and (C.45) we get the relations

$$\begin{aligned}
\frac{\partial}{\partial\mathbf{q}}\bigg|_R\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle &= \left(\frac{\mathbf{q}'-\mathbf{q}}{4\Delta^2} - i\frac{\mathbf{p}'}{2\hbar}\right)e^{-\frac{\Delta^2(\mathbf{p}-\mathbf{p}')^2}{2\hbar^2}}e^{-\frac{(\mathbf{q}-\mathbf{q}')^2}{8\Delta^2}}e^{-\frac{i(\mathbf{p}'\mathbf{q}-\mathbf{q}'\mathbf{p})}{2\hbar}}\\
\frac{\partial^2}{\partial\mathbf{q}^2}\bigg|_R\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle &= \left(-\frac{\mathbf{p}'^2}{4\hbar^2} + \frac{(\mathbf{q}-\mathbf{q}')^2}{16\Delta^4} + \frac{i\mathbf{p}'\,(\mathbf{q}-\mathbf{q}')}{4\Delta^2\hbar} - \frac{3}{4\Delta^2}\right)\\
&\qquad e^{-\frac{\Delta^2(\mathbf{p}-\mathbf{p}')^2}{2\hbar^2}}e^{-\frac{(\mathbf{q}-\mathbf{q}')^2}{8\Delta^2}}e^{-\frac{i(\mathbf{p}'\mathbf{q}-\mathbf{q}'\mathbf{p})}{2\hbar}}\\
\frac{\partial}{\partial\mathbf{q}}\bigg|_L\langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle &= \left(\frac{\partial}{\partial\mathbf{q}}\bigg|_R\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle\right)^\star\\
\frac{\partial^2}{\partial\mathbf{q}^2}\bigg|_L\langle \mathbf{p},\mathbf{q}|\mathbf{p}',\mathbf{q}'\rangle &= \left(\frac{\partial^2}{\partial\mathbf{q}^2}\bigg|_R\langle \mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle\right)^\star,
\end{aligned}$$

which are inserted into equation (C.79). With the local expansion (6.35), we can perform the integration and finally obtain

$$\langle \boldsymbol{u}| \frac{i}{\hbar} \left[\bar{D}_{(1)}, T\right] |\boldsymbol{u}\rangle = -\frac{\mathbf{p}}{m} \frac{\partial \rho(\mathbf{p}, \mathbf{q}, s)}{\partial \mathbf{q}}. \tag{C.80}$$

Appendix D

Simulations of spin dependent recombination in silicon

During my thesis I was in the lucky situation, that I got the freedom to do some research besides the subject presented in this work. In collaboration with my old friend Christoph Michel, Philipps Universität, Marburg, Germany, we have implemented a simulation for pulsed electrically detected magnetic resonance experiments (pEDMR). Prof. Christoph Boehme, University of Utah, Salt Lake City, UT, USA, invited us as visiting scientists to work with him on this subject, to better understand recombination processes in silicon.

In solar cells, absorption of light creates pairwise electrons and holes, which carry charges. If these charge carriers arrive at the contacts of the cell, they contribute to the current the cell outputs. Some of the charge carriers annihilate each other before they reach the contacts. During this process, called recombination, the carriers form intermediate pairs. The efficiency of solar cells is therefore reduced by recombination. Dr. Christoph Boehme (University of Utah, Salt Lake City, USA) has developed, amongst other experimental physicists from the Hahn-Meitner-Institut, Berlin, Germany, a new technique to investigate recombination via intermediate pairs: the pulsed electrically-detected magneto resistance (pEDMR) measurements. With a density matrix theory the evolution of the ensemble of intermediate pairs is described, taking the fermionic character (spin 1/2) of the pair partners into account. Our tool numerically solves a set of coupled differential equations and treats intermediate pair parameters such as the exchange coupling and dipole coupling, as well as disorder effects. The insights provided by our simulations serve the understanding and interpretation of the experimental results and enhance the control of the loss mechanism due to recombination. Eventually, these insights will help building more efficient solar cells. First results of our two-month stay are published [25]. We are preparing further results with Christoph Boehme and Klaus Lips, Hahn-Meitner-Institut, Berlin, Germany for publication.

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