LARGE TIME BEHAVIOR OF THE HEAT KERNEL OF TWO-DIMENSIONAL MAGNETIC SCHRÖDINGER OPERATORS

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Abstract. We study the heat semigroup generated by two-dimensional Schrödinger operators with compactly supported magnetic field. We show that if the field is radial, then the large time behavior of the associated heat kernel is determined by its total flux. We also establish some on-diagonal heat kernel estimates and discuss their applications for solutions to the heat equation. An exact formula for the heat kernel, and for its large time asymptotic, is derived in the case of the Aharonov-Bohm magnetic field.

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1. Introduction

The Hamiltonian of a charged quantum particle in $\mathbb{R}^d$ interacting with a magnetic field B is given formally by the differential operator

$$H_B = (i\nabla + A)^2 \tag{1.1}$$

in $L^2(\mathbb{R}^d)$, where A is the vector potential of the magnetic field; $B = \text{rot}A$ (for $d = 2, 3$). The object of our interest in the present paper is the integral kernel $e^{-tH_B}(x, y)$ of the heat semigroup generated by H_B. In particular, we are interested in the dependence of $e^{-tH_B}(x, y)$ on t. A well known semiclassical result, [Er97, Ma] says that under certain conditions on B we have

$$\lim_{t\to 0} t^{\frac{d}{2}}\, e^{-tH_B}(x, x) = (4\pi)^{-d/2}. \tag{1.2}$$

In other words, the leading term of $e^{-tH_B}(x, x)$ in the short time limit is not affected by the magnetic field. However, the situation changes in the large time limit, where the diagonal element of the heat kernel decays exponentially fast provided the size of the magnetic field is bounded from below by a positive constant, [Er94, Mal]. More precisely, the estimate

$$\lim_{t\to\infty} \frac{1}{t} \log \|e^{-tH_{LB}}\|_{L^1\to L^\infty} \,\leq\, -C_L\, L \min_{x\in\mathbb{R}^d} \|B(x)\| \tag{1.3}$$

holds true with $C_L = 1 + o(1)$ as $L \to \infty$, see [Er94]. From the Mehler formula for the heat kernel of the two-dimensional Schrödinger operator with a constant magnetic field, see [Si1, Sect.II.4-6], it follows that the factor $\min_{x\in\mathbb{R}^d} \|B(x)\|$ in (1.3) cannot be improved. Later, a uniform pointwise bound on the two-dimensional magnetic heat kernel in the form

$$\|e^{-tH_B}\|_{L^1\to L^\infty} \,\leq\, \frac{B_0}{4\pi \sinh(\frac{B_0 t}{2})}\,, \quad B_0 = \min_{x\in\mathbb{R}^2} |B(x)|, \quad t > 0, \quad d = 2 \tag{1.4}$$

was obtained in [LT] under the assumption that $B_0 > 0$. This bound is the best possible since there is equality for $B = B_0$. The latter follows again by the Mehler formula.

In this paper we focus on the the case $d = 2$ and address the following question: what is the large time behavior of $e^{-tH_B}(x, y)$ when $B(x)$ is of compact support? Note that for a compactly supported

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magnetic field we have $B_0 = \min_{x\in\mathbb{R}^2} |B(x)| = 0$ in (1.3) and (1.4). This of course reflects the fact that $\inf \operatorname{spect}(H_B) = 0$ and therefore no exponential decay of the heat kernel is possible.

On the other hand, Laptev and Weidl showed in [LW] that under certain conditions on B the operator H_B satisfies a Hardy type inequality

$$H_B \,\geq\, \frac{C_B}{1+|x|^2} \tag{1.5}$$

in the sense of quadratic forms on $H^1(\mathbb{R}^2)$, see also [W]. Inequality (1.5) implies that H_B is a subcritical operator. The criticality theory then suggests that the integral

$$\int_0^\infty e^{-tH_B}(x,y)\, dt \tag{1.6}$$

should be finite for all $x \neq y$. Hence in the limit of large times the magnetic heat kernel $e^{-tH_B}(x,y)$ should behave differently than the heat kernel of the usual Laplace operator in $\mathbb{R}^2$. Our motivation is to find out how exactly the large time behavior of $e^{-tH_B}(x,y)$ depends on the magnetic field.

One of our main results, Theorem 4.1, shows that for radially symmetric and weak magnetic fields the time decay of $e^{-tH_B}(x,y)$ is completely determined by the total flux of the magnetic field. The key point of the proof is to show that $e^{-tH_B}(x,y)$ is asymptotically (as $t\to\infty$) equivalent to the heat kernel of certain two-dimensional Schrödinger operator with positive potential, see (3.1). In section 5 we establish some pointwise and L^p-estimates on the magnetic semigroup e^{-tH_B} in terms of the distance between the total flux and the set of integers, see Theorem 5.1 and Proposition 5.2. One of the main technical tools used in the proofs is Lemma 3.3, in which we derive a formula for the heat semigroup of certain family of one-dimensional Schrödinger operators. This also enables us to write an explicit expression for the heat kernel of the Aharonov-Bohm operator, Proposition 6.1, and consequently to calculate its exact large time asymptotic, see Theorem 6.3.

Remark 1.1. Let us make a brief remark on the properties of the heat kernel under gauge transformations. It is a matter of fact that the vector potential A is not uniquely determined by the magnetic field B. However, if $\operatorname{rot}A = \operatorname{rot}\tilde{A} = B \in C(\mathbb{R}^2,\mathbb{R})$, then there exists a scalar field ϕ such that $\tilde{A} = A + \nabla\phi$. So the respective Hamiltonians H_B and $\tilde{H}_B$ are unitarily equivalent; $\tilde{H}_B = e^{i\phi}\, H_B\, e^{-i\phi}$, and their heat kernels are linked through the equation

$$e^{-t\tilde{H}_B}(x,y) = e^{i(\phi(x)-\phi(y))}\, e^{-tH_B}(x,y).$$

Hence changing the gauge does not change the time dependence of the heat kernel. In other words, the decay rate in time is gauge invariant.

2. Preliminaries

Given two functions f_1, f_2 on a set Ω we will use the notation $f_1 \simeq f_2$ to indicate that there exist positive constants c, C such that the inequalities $c\, f_1 \leq f_2 \leq C\, f_1$ hold on Ω. Accordingly, the notation $f_1(t,x) \simeq f_2(t,x)$ as $t\to\infty$ means that $f_1 \simeq f_2$ holds for all t large enough. Moreover, given two points $x, y \in \mathbb{R}^2$, we will often use the polar coordinate representation $e^{-tH_B}(x,y) = e^{-tH_B}(r,r',\theta,\theta')$ of the heat kernel which corresponds to the identification $x = r(\cos\theta, \sin\theta)$ and $y = r'(\cos\theta', \sin\theta')$. Finally, we denote $\mathbb{R}_+ = (0,\infty)$ and $\dot{\mathbb{R}}_+ = [0,\infty)$. We will need the following hypotheses.

Assumption 2.1. Let the magnetic field be given as $B(|x|)$, $x\in\mathbb{R}^2$, where $B : \dot{\mathbb{R}}_+ \to \mathbb{R}$ is a continuous function with the support contained in some interval $[0,R]$, $R<\infty$.

We introduce a vector potential $A : \dot{\mathbb{R}}_+ \times [0,2\pi) \to \mathbb{R}^2$ which in polar coordinates (r,θ) reads as follows

$$A(r,\theta) = a(r)\,(-\sin\theta,\, \cos\theta), \quad a(r) = \frac{1}{r}\int_0^r B(t)\, t\, dt.$$

Then A generates the magnetic field B. Hamiltonian H_B is associated with the closed quadratic form

$$Q_B[u] = \int_0^\infty \int_0^{2\pi} \left(|\partial_r u|^2 + r^{-2} |i\,\partial_\theta u + b(r) u|^2\right) r\,dr d\theta, \quad u \in H^1(\mathbb{R}_+ \times (0,2\pi)), \tag{2.1}$$

where

$$b(r) = r a(r) = \int_0^r B(t)\,t\,dt = \frac{1}{2\pi} \int_{\{|x|\leq r\}} B(|x|)\,dx$$

is the flux of the magnetic field through the disc of radius r centered in the origin. Moreover, we denote by α the total flux of the magnetic field through the plane. By assumption 2.1 we have

$$b(r) = \alpha \qquad \forall\, r > R. \tag{2.2}$$

By expanding a given function $u \in L^2(\mathbb{R}_+ \times (0,2\pi))$ into a Fourier series with respect to the basis $\{e^{im\theta}\}_{m\in\mathbb{Z}}$ of $L^2((0,2\pi))$, we obtain a direct sum decomposition

$$L^2(\mathbb{R}^2) = \sum_{m\in\mathbb{Z}} \oplus\, \mathcal{L}_m, \tag{2.3}$$

where $\mathcal{L}_m = \left\{ g \in L^2(\mathbb{R}^2) \,:\, g(x) = f(r)\, e^{im\theta}\ a.e.,\ \int_0^\infty |f(r)|^2\, r\,dr < \infty \right\}$. Since the magnetic field B is radial, the operator H_B can be decomposed accordingly to the direct sum

$$H_B = \sum_{m\in\mathbb{Z}} \oplus\, (h_m \otimes \mathrm{id})\, \Pi_m, \tag{2.4}$$

where h_m are operators generated by the closures, in $L^2(\mathbb{R}_+, r dr)$, of the quadratic forms

$$Q_m[f] = \int_0^\infty \left(f'^2 + \frac{(b(r)+m)^2}{r^2}\, f^2 \right) r\,dr \tag{2.5}$$

defined initially on $C_0^\infty(0,\infty)$, and $\Pi_m : L^2(\mathbb{R}^2) \to \mathcal{L}_m$ is the projector acting as

$$(\Pi_m u)(r,\theta) = \frac{1}{2\pi} \int_0^{2\pi} e^{im(\theta-\theta')}\, u(r,\theta')\, d\theta'.$$

Note that Π_m commutes with $h_m \otimes \mathrm{id}$. Hence the integral kernel of e^{-tH_B} splits as follows:

$$e^{-tH_B}(x,y) = \frac{1}{2\pi} \sum_{m\in\mathbb{Z}} p_m(r,r',t)\, e^{im(\theta-\theta')}\,. \tag{2.6}$$

Here $p_m(r,r',t)$ denotes $e^{-th_m}(r,r')$ which is real and positive for all $m \in \mathbb{Z}$. The idea behind the proof of Theorem 4.1 is to show that if the magnetic flux is small enough, then the large time behavior of $e^{-tH_B}(x,y)$ is determined by the contribution from $m=0$ in (2.6).

3. Heat kernel of the reduced operators

In this section we will study the heat kernels $p_m(r,r',t)$. First we prove a result which allows us to quantify the large time behavior of $p_0(r,r',t)$. To this end we consider an auxiliary Schrödinger operator

$$\mathcal{A} = -\Delta + \frac{b^2(|x|)}{|x|^2} \quad \text{in} \quad L^2(\mathbb{R}^2). \tag{3.1}$$

The operator $\mathcal{A}$ can be defined in the usual way through the corresponding closed quadratic form

$$Q_{\mathcal{A}}[f] = \int_{\mathbb{R}^2} \left(|\nabla f|^2 + f^2\, \frac{b^2(|x|)}{|x|^2} \right) dx, \qquad f \in D(Q_{\mathcal{A}}) = H^1(\mathbb{R}^2).$$

Lemma 3.1. *Assume that $b(\cdot)$ is not identically zero. Then there exists a positive radial function $h \in C^2(\mathbb{R}^2)$ such that $\mathcal{A}\, h = 0$. Moreover, any such function satisfies*

$$h(x) = h(|x|) \simeq \begin{cases} |x|^{|\alpha|} & if \quad \alpha \neq 0\,, \\ 1 + |\log |x|| & if \quad \alpha = 0. \end{cases} \qquad |x| > R. \tag{3.2}$$

Finally, there exist positive constants C and c such that the heat kernel of $\mathcal{A}$ admits for all $x, y \in \mathbb{R}^2$ and all $t > 0$ the following estimate,

$$e^{-t\mathcal{A}}(x,y) \simeq C\, \frac{h(x)\, h(y)}{t\, h(|x| + \sqrt{t})\, h(|y| + \sqrt{t})}\; e^{-c\, \frac{|x-y|^2}{t}}. \tag{3.3}$$

Here we use, with a slight abuse of notation, the same symbol for the function h on $\mathbb{R}^2$ and for its natural identification on $\dot{\mathbb{R}}_+$.

Proof. Since $b(|x|) = \alpha$ for $|x| > R$, the spectrum of $\mathcal{A}$ coincides with the positive half-line $[0, \infty)$. Hence by the Allegretto-Piepenbrink theorem, see e.g. [MP], there exists a positive solution u to the equation $\mathcal{A}\, u = 0$. Since the potential term $b^2(|x|)/|x|^2$ in $\mathcal{A}$ is Hölder continuous, see assumption 2.1, the elliptic regularity ensures that $u \in C^2(\mathbb{R}^2)$. The radial function h given by

$$h(|x|) = \int_0^{2\pi} u(|x|, \theta)\, d\theta,$$

then also satisfies $\mathcal{A}\, h = 0$ and for $|x| > R$ we have

$$h(x) = h(|x|) = a\, |x|^{|\alpha|} + b\, |x|^{-|\alpha|}, \quad \alpha \neq 0 \tag{3.4}$$

$$h(x) = h(|x|) = c + d\, |\log |x||, \qquad \alpha = 0. \tag{3.5}$$

The positivity of h implies that $a \geq 0$, $d \geq 0$. On the other hand, h satisfies $r(r\, h'(r))' = h(r)\, b^2(r)$ with $r = |x|$ and therefore it is easy to see that h is an increasing function of r. This means that $a > 0$, $d > 0$. A straightforward verification now shows that the manifold $\mathbb{R}^2$ equipped with the Lebesgue measure and the function h satisfy hypothesis of [Gr05, Thm.10.10.(i)]. The latter yields the heat kernel estimate (3.3). □

Corollary 3.2. *There exists a positive radial function $h \in C^2(\mathbb{R}^2)$ such that $H_B\, h = 0$. Moreover, if $b(\cdot)$ is not identically zero, then any such function satisfies* (3.2).

Proof. This follows from Lemma 3.1 and the fact that the operators H_B and $\mathcal{A}$ coincide on the set of radial functions. □

In order to control the terms in (2.6) with $m \neq 0$ we will make use of Lemma 3.3 below which gives an explicit formula for the heat semigroup generated by the operators which are associated with the quadratic form

$$\mathcal{Q}_\beta[u] = \int_0^\infty \left(u'^2 + \frac{\beta^2}{r^2}\, u^2 \right) r\, dr, \qquad \beta \in \mathbb{R} \tag{3.6}$$

defined on $C_0^\infty(\mathbb{R}_+)$. This form is closable, see e.g. [Da, Sec.1.8], and its closure generates a self-adjoint operator $\mathcal{H}_\beta$ in $L^2(\mathbb{R}_+, rdr)$. By the Beurling-Deny criteria $\mathcal{H}_\beta$ generates on $L^2(\mathbb{R}_+, rdr)$ a symmetric submarkovian semigroup $e^{-t\mathcal{H}_\beta}$. Let $e^{-t\mathcal{H}_\beta}(r, r')$ be its integral kernel.

Lemma 3.3. *Let $\mathcal{H}_\beta$ be the operator in $L^2(\mathbb{R}_+, rdr)$ associated with closure of the form $\mathcal{Q}_\beta$. Then for all $r, r' \in \mathbb{R}_+$ and all $t > 0$ it holds*

$$e^{-t\,\mathcal{H}_\beta}(r, r') = \frac{1}{2t}\; I_{|\beta|} \left(\frac{r\, r'}{2t} \right) e^{-\frac{r^2 + r'^2}{4t}}, \tag{3.7}$$

where $I_{|\beta|}$ is the modified Bessel function of the first kind, see e.g. [AS, Chap.9].

Proof. Consider the operators

$$L_\beta = U\,\mathcal{H}_\beta\,U^{-1} \qquad \text{in} \qquad L^2(\mathbb{R}_+, dr), \tag{3.8}$$

where $U : L^2(\mathbb{R}_+, r\,dr) \to L^2(\mathbb{R}_+, dr)$ is a unitary mapping acting as $(Uf)(r) = r^{1/2} f(r)$. Note that L_β is subject to Dirichlet boundary condition at 0 and that it coincides with the Friedrichs extension of the differential operator

$$-\frac{d^2}{dr^2} + \frac{\beta^2 - \frac{1}{4}}{r^2}$$

defined on $C_0^\infty(\mathbb{R}_+)$. Denote by $D(L_\beta)$ the domain of L_β. Now let λ be a complex number from some fixed neighborhood of $\mathbb{R}_+$. A straightforward calculation using the standard technique of the Sturm-Liouville theory shows that the integral kernel of the resolvent operator $(L_\beta - \lambda)^{-1}$ for $r < r'$ is given as follows

$$(L_\beta - \lambda)^{-1}(r, r') = \frac{\pi i}{2}\sqrt{rr'}\; J_{|\beta|}(r\sqrt{\lambda}\,)\left(J_{|\beta|}(r'\sqrt{\lambda}\,) + i\,Y_{|\beta|}(r'\sqrt{\lambda}\,)\right), \qquad \operatorname{Im}\lambda > 0$$

$$(L_\beta - \lambda)^{-1}(r, r') = -\frac{\pi i}{2}\sqrt{rr'}\; J_{|\beta|}(r\sqrt{\lambda}\,)\left(J_{|\beta|}(r'\sqrt{\lambda}\,) - i\,Y_{|\beta|}(r'\sqrt{\lambda}\,)\right), \quad \operatorname{Im}\lambda < 0,$$

where $J_{|\beta|}$ and $Y_{|\beta|}$ are the Bessel functions of the first and second kind respectively. Next we introduce the function $g(r,\lambda) = \sqrt{r}\, J_{|\beta|}(r\sqrt{\lambda})$, and note that $L_\beta\, g = \lambda\, g$ and $g(0,\lambda) = 0$. Hence the Weyl-Titchmarsh-Kodaira Theorem, see [DSch, Chap.13], says that

$$W_\beta\, L_\beta\, W_\beta^{-1}\,\varphi(\lambda) = \lambda\,\varphi(\lambda), \quad \varphi \in W_\beta(D(L_\beta)), \tag{3.9}$$

where the mapping W_β and its inverse W_β^{-1} given by

$$(W_\beta\, u)(\lambda) = \int_0^\infty u(r)\sqrt{r}\, J_{|\beta|}(r\sqrt{\lambda})\, dr, \quad (W_\beta^{-1}\varphi)(r) = \int_0^\infty \varphi(\lambda)\sqrt{r}\, J_{|\beta|}(r\sqrt{\lambda})\,\frac{d\lambda}{2} \tag{3.10}$$

defined initially on $C_0^\infty(\mathbb{R}_+)$ extend to unitary operators from $L^2(\mathbb{R}_+)$ onto itself. Given $f \in C_0^\infty(\mathbb{R}_+)$, in view of (3.9) we then get

$$\begin{aligned}\left(e^{-tL_\beta}\, f\right)(r) &= \left(W_\beta^{-1}\, e^{-t\lambda}\, W_\beta\, f\right)(r) = \int_0^\infty \sqrt{rr'} \int_0^\infty e^{-t\lambda} J_{|\beta|}(r\sqrt{\lambda})\, J_{|\beta|}(r'\sqrt{\lambda})\,\frac{d\lambda}{2}\, f(r')\, dr' \\ &= \frac{1}{2t}\int_0^\infty \sqrt{rr'}\; I_{|\beta|}\left(\frac{r\,r'}{2t}\right) e^{-\frac{r^2+r'^2}{4t}}\, f(r')\, dr',\end{aligned} \tag{3.11}$$

where we have used Fubini's theorem to switch the order of integration and [Erd, Eq.8.11(23)] to evaluate the $\lambda-$integral. Moreover, since $\sqrt{r'}\; I_{|\beta|}(rr'/2t)\, e^{-\frac{r^2+r'^2}{4t}} \in L^2(\mathbb{R}_+)$ for all $r, t > 0$, see [AS, Chap.9.7], identity (3.11) extends by density to all $f \in L^2(\mathbb{R}_+)$. Hence

$$e^{-tL_\beta}(r, r') := \frac{1}{2t}\sqrt{rr'}\; I_{|\beta|}\left(\frac{r\,r'}{2t}\right) e^{-\frac{r^2+r'^2}{4t}} \tag{3.12}$$

is the integral kernel of e^{-tL_β}, and by (3.8) we conclude that

$$e^{-t\mathcal{H}_\beta}(r, r') = \frac{1}{\sqrt{r\,r'}}\; e^{-tL_\beta}(r, r') = \frac{1}{2t}\; I_{|\beta|}\left(\frac{r\,r'}{2t}\right) e^{-\frac{r^2+r'^2}{4t}}. \tag{3.13}$$

$\square$

Lemma 3.4. *Let $|\alpha| < 1$. Then for all $x, y \in \mathbb{R}^2$ it holds*

$$\lim_{t\to\infty} e^{-t\mathcal{A}}(x, y)\,(p_0(|x|, |y|, t))^{-1} = 1. \tag{3.14}$$

Proof. Operator $\mathcal{A}$ admits the decomposition

$$\mathcal{A} = \sum_{m\in\mathbb{Z}} \oplus \left(\mathcal{A}_m \otimes \mathrm{id}\right) \Pi_m, \tag{3.15}$$

where $\mathcal{A}_m$ are operators in $L^2(\mathbb{R}_+, r\, dr)$ generated by the closures of the quadratic forms

$$a_m[f] = \int_0^\infty \left(f'^2 + \frac{b(r)^2+m^2}{r^2}\, f^2 \right) r\, dr$$

defined on $C_0^\infty(0,\infty)$. Note that $\mathcal{A}_0 = h_0$ and hence

$$e^{-t\mathcal{A}}(x,y) = p_0(|x|,|y|,t) + \sum_{m\neq 0} e^{-t\mathcal{A}_m}(|x|,|y|)\, e^{im(\theta-\theta')}. \tag{3.16}$$

In order to estimate the sum on the right hand side of the last equation, we note that by the Trotter product formula

$$e^{-t\mathcal{A}_m}(r,r') \,\leq\, e^{-t\mathcal{H}_m}(r,r') \qquad \forall\, r,r' \in \mathbb{R}_+, \quad \forall\, m\neq 0, \tag{3.17}$$

where $\mathcal{H}_m$ is the operator defined in Lemma 3.3. By the same Lemma we get

$$\Big| \sum_{m\neq 0} e^{-t\mathcal{A}_m}(|x|,|y|)\, e^{im(\theta-\theta')} \Big| \,\leq\, C\, z \sum_{m\neq 0} I_{|m|}(z)\,, \quad z := \frac{|xy|}{2t}, \tag{3.18}$$

where the constant C depends on x and y. Assume first that $\alpha\neq 0$. From the integral representation

$$I_\nu(z) = \frac{z^\nu}{2^\nu\, \Gamma(\nu+\frac12)\Gamma(\frac12)} \int_{-1}^1 (1-s^2)^{\nu-\frac12}\, e^{zs}\, ds \tag{3.19}$$

for I_ν, see e.g. [AS, Chap.9], it is then easy to see that

$$\begin{aligned}
\limsup_{t\to\infty}\, t^{1+|\alpha|}\, \Big| \sum_{m\neq 0} e^{-t\mathcal{A}_m}(|x|,|y|)\, e^{im(\theta-\theta')}\Big| &\leq\, c\, \limsup_{z\to 0} \sum_{n\geq 1} \frac{z^{n-|\alpha|}}{2^n\, \Gamma(n+\frac12)} \\
&\leq\, c\, \limsup_{z\to 0}\, z^{1-|\alpha|} \sum_{n\geq 1} \frac{1}{2^n\, \Gamma(n+\frac12)} = 0,
\end{aligned}$$

where c' depends on x and y. Since

$$e^{-t\mathcal{A}}(x,y) \,\simeq\, t^{-1-|\alpha|} \qquad t\to\infty, \quad \alpha\neq 0,$$

by Lemma 3.1, we conclude from (3.16) that equation (3.14) holds true in the case $\alpha\neq 0$. On the other hand, if $\alpha = 0$, then Lemma 3.1 gives

$$e^{-t\mathcal{A}}(x,y) \,\simeq\, t^{-1}\, (\log t)^{-2} \qquad t\to\infty, \quad \alpha = 0.$$

From (3.18) and (3.19) we find

$$\limsup_{t\to\infty}\, t\, (\log t)^2\, \Big| \sum_{m\neq 0} e^{-t\mathcal{A}_m}(|x|,|y|)\, e^{im(\theta-\theta')}\Big| \,\leq\, c\, \limsup_{z\to 0} \sum_{n\geq 1} \frac{(\log z)^2\, z^n}{2^n\, \Gamma(n+\frac12)} = 0.$$

This proves (3.14) for $\alpha = 0$. □

4. Large time asymptotic of $e^{-tH_B}(x,y)$

Below we formulate our main result regarding the large time behavior of the magnetic heat kernel $e^{-tH_B}(x,y)$. It shows that if the magnetic field is sufficiently small, then the decay rate of $e^{-tH_B}(x,y)$ is completely determined by the total flux α.

Theorem 4.1. *Let $B(x)$ satisfy assumption 2.1 and suppose that $|b(r)| < 1/2$ for all $r \in \mathbb{R}_+$. Let $h \in C^2(\mathbb{R}^2)$ be a positive radial function such that $H_B\, h = 0$. Then there exist constants C and c such that the inequalities*

$$c \,\leq\, \liminf_{t\to\infty}\, t^{1+|\alpha|}\, \frac{e^{-tH_B}(x,y)}{h(x)h(y)} \,\leq\, \limsup_{t\to\infty}\, t^{1+|\alpha|}\, \frac{e^{-tH_B}(x,y)}{h(x)h(y)} \,\leq\, C, \qquad \alpha\neq 0 \tag{4.1}$$

and

$$c \leq \liminf_{t\to\infty}\, t\,(\log t)^2\, \frac{e^{-tH_B}(x,y)}{h(x)h(y)} \,\leq\, \limsup_{t\to\infty}\, t\,(\log t)^2\, \frac{e^{-tH_B}(x,y)}{h(x)h(y)} \,\leq\, C, \quad \alpha = 0 \tag{4.2}$$

hold true for all $x, y \in \mathbb{R}^2$.

Remark 4.2. Similar connection between the large time asymptotic of the heat kernel $e^{-tP}(x,y)$ and the ground state of the corresponding generator is known when P has an eigenvalue at the bottom of its spectrum, see e.g. [CK, P, Si3].

Remark 4.3. Equation (4.2) shows that $e^{-tH_B}(x,y)$ is integrable with respect to t at infinity even if the total flux is zero. The latter reflects the fact that H_B satisfies a Hardy type inequality also in this case, see [W].

Proof of Theorem 4.1. The existence of the ground state h is guaranteed by Corollary 3.2. By Lemma 3.1 it suffices to show that

$$\lim_{t\to\infty} \frac{e^{-t\mathcal{A}}(x,y)}{e^{-tH_B}(x,y)} = 1 \qquad \forall\, x, y \in \mathbb{R}^2. \tag{4.3}$$

Let $\alpha \neq 0$. By assumption we have $(b(r)+m)^2 \geq m^2/4$ for all $m \neq 0$ and all $r \in \mathbb{R}_+$. Hence the Trotter product formula gives

$$p_m(r,r',t) \,\leq\, e^{-t\,\mathcal{H}_{m/2}}(r,r') \qquad \forall\; r, r' \in \mathbb{R}_+,\; t>0,\, m\neq 0.$$

With the notation of equation (3.18) we get from (3.19) and Lemma 3.3

$$\limsup_{t\to\infty}\, t^{1+|\alpha|} \sum_{m\neq 0} p_m(r,r',t) \leq\, c\, \limsup_{z\to 0}\, z \sum_{m\neq 0} I_{|m/2|}(z) \,\leq c\, \lim_{z\to 0} \sum_{n\geq 1} \frac{z^{\frac{n}{2}-|\alpha|}}{2^{n/2}\,\Gamma((n+1)/2)} = 0,$$

where we have used the fact that $|\alpha| < 1/2$. In view of equations (2.6), (3.3) and Lemma 3.4, this proves (4.3). If $\alpha = 0$, we obtain in the same way as above

$$\limsup_{t\to\infty}\, t\,(\log t)^2 \sum_{m\neq 0} p_m(r,r',t) = 0.$$

Equation (4.3) thus holds also in this case. $\square$

In the case $|\alpha| \geq 1/2$ we give an asymptotic upper bound on the heat kernel.

Proposition 4.4. *Let $B(x)$ satisfy assumption 2.1. Let $\varrho = \min_{k\in\mathbb{Z}} |k+\alpha|$ be the distance between the flux α and the set of integers. Then there exists a constant C such that*

$$\limsup_{t\to\infty}\, t^{1+\varrho}\, |e^{-tH_B}(x,y)| \,\leq\, C\,(1+|x|)^{\varrho}\,(1+|y|)^{\varrho} \tag{4.4}$$

holds for all $x, y \in \mathbb{R}^2$.

Proof. We introduce the operators T_m generated by the quadratic forms

$$t_m[f] = \int_0^\infty \left(f'^2 + \Theta(r-R)\, \frac{(b(r)+m)^2}{r^2}\, f^2 \right) r\, dr,$$

defined initially on $C_0(\mathbb{R}_+)$ and then closed in $L^2(\mathbb{R}, r\, dr)$. Here $\Theta(\cdot)$ denotes the Heaviside function. By the Trotter product formula we have

$$e^{-th_m}(r,r') \,\leq\, e^{-t\,T_m}(r,r') \qquad \forall\, r, r' \in \mathbb{R}_+, \quad m \in \mathbb{Z}. \tag{4.5}$$

In view of (2.2) it follows that the functions $\psi_m \in C^1(\mathbb{R}_+, \mathbb{R}_+)$, defined by

$$\psi_m(r) = 1, \quad r < R, \quad \psi_m(r) = \frac{1}{2}\left(\frac{r}{R}\right)^{\sigma_m} + \frac{1}{2}\left(\frac{R}{r}\right)^{\sigma_m} \qquad r \geq R, \quad \sigma_m = |\alpha + m| \tag{4.6}$$

solve the Cauchy problems

$$\Theta(r-R)\, \frac{(b(r)+m)^2}{r}\, \psi_m = (r\, \psi_m')', \quad \psi_m(R) = 1,\ \psi_m'(R) = 0.$$

The operators

$$S_m = \psi_m^{-1}\, T_m\, \psi_m \qquad \text{in} \quad L^2(\mathbb{R}_+,\, \psi_m^2(r)\, r dr),$$

are thus unitarily equivalent to T_m and their heat kernels satisfy

$$e^{-t\, T_m}(r, r') = \psi_m(r)\, \psi_m(r')\, e^{-tS_m}(r, r'). \tag{4.7}$$

A direct calculation shows that S_m is associated with the quadratic form

$$s_m[u] = t_m[u\, \psi_m] = \int_0^\infty (u')^2\, \psi_m^2\, r\, dr, \qquad u \in D(s_m) = H^1(\mathbb{R}_+, \psi_m^2\, r\, dr).$$

We now apply Theorem A.1 with $\mu(x) = \nu(x) = x\, \psi_m^2(x)$, $p = 2$ and $q = (2 + 2\sigma_m)/\sigma_m$. Hence for each m there exists a constant c_m, such that

$$s_m[u] \,\geq\, c_m \left(\int_0^\infty u^{\frac{2+2\sigma_m}{\sigma_m}}\, \psi_m^2\, r\, dr \right)^{\frac{\sigma_m}{1+\sigma_m}} \qquad \forall\, u \in D(s_m). \tag{4.8}$$

By the Beurling-Deny criteria, S_m generates on $L^2(\mathbb{R}_+, \psi_m(r) dr)$ a symmetric submarkovian semigroup e^{-tS_m}. This allows us to apply [Da, Thm.2.4.2], see also [Var], to obtain

$$\| e^{-tS_m} \|_{\infty,2} \,\leq\, C_m\, t^{-\frac{1+\sigma_m}{2}}$$

for some constant C_m. By duality this implies that

$$\sup_{r,r'} e^{-tS_m}(r, r') = \| e^{-tS_m} \|_{\infty,1} \,\leq\, \| e^{-tS_m} \|_{\infty,2}^2 \,\leq\, C_m^2\, t^{-1-\sigma_m} \qquad \forall\, t > 0.$$

In view of equations (4.5) , (4.6) and (4.7) this yields

$$e^{-t\, T_m}(r, r') \leq C_m^2\; t^{-1-\sigma_m}\, (1+r)^{\sigma_m}\, (1+r')^{\sigma_m} \qquad t > 0,\ r, r' \in \mathbb{R}_+. \tag{4.9}$$

Now define $n_0 := \inf\{n \in \mathbb{N} \,:\, n > 2 \sup_{r>0} |b(r)|\}$. From (4.5) and (4.9) we obtain

$$\limsup_{t \to \infty}\, t^{1+\varrho} \sum_{m=-n_0}^{n_0} p_m(r, r', t) \leq\, C\, (1+r)^{\varrho} (1+r')^{\varrho}. \tag{4.10}$$

To estimate the rest of the sum in (2.6) we note that

$$(b(r)+m)^2 \geq \frac{m^2}{4} \qquad \forall\ r > 0, \quad m\, :\, |m| > n_0.$$

Hence mimicking the arguments used in the proof of Theorem 4.1 it is easy to see that

$$\limsup_{t \to \infty}\, t^{1+\varrho} \sum_{|m| > n_0} p_m(r, r', t) = 0.$$

By (2.6) this completes the proof. $\square$

5. Heat kernel estimates

In this section we use Theorem 4.1 and Proposition 4.4 in order to prove certain point-wise heat kernel estimates. We use the notation introduced in Proposition 4.4, i.e. $\varrho = \min_{k\in\mathbb{Z}} |k+\alpha|$.

Theorem 5.1. *Under assumption 2.1 there exists a constant C such that the inequality*

$$e^{-tH_B}(x,x) \,\leq\, C \, \min\left\{t^{-1}, \, (1+|x|)^{2\varrho} \, t^{-1-\varrho}\right\} \tag{5.1}$$

holds for all $x \in \mathbb{R}^2$ and all $t>0$.

Proof. Adopting the notation of the proof of Theorem 4.4, it follows from (4.9) that

$$p_m(r,r,t) \leq C\, t^{-1-\sigma_m} \,(1+r)^{2\,\sigma_m} \qquad \forall\, m \in \{-n_0,\dots,n_0\}.$$

On the other hand, the diamagnetic inequality

$$\left|e^{-tH_B}(x,y)\right| \,\leq e^{t\Delta}(x,y) = \frac{1}{4\pi t}\, e^{-\frac{|x-y|^2}{4t}}, \qquad x,y\in\mathbb{R}^2, \quad t>0, \tag{5.2}$$

see e.g. [AHS, HS, Si2], clearly implies that $p_m(r,r,t) \leq 1/(2t)$ for all m. Hence

$$p_m(r,r,t) \leq C\,(t^{-1-\sigma_m}\,(1+r)^{2\,\sigma_m})^{\frac{\varrho}{\sigma_m}}\, t^{-(1-\frac{\varrho}{\sigma_m})} = C\, t^{-1-\varrho}\,(1+r)^{2\,\varrho} \quad |m|\leq n_0. \tag{5.3}$$

Next we introduce the variable $z=\frac{|x|^2}{t}$. From the proof of Theorem 4.1 and from Lemma 3.3 we get

$$z^{-\varrho} \sum_{|m|>n_0} t\, p_m(|x|,|x|,t) \leq \, z^{-\varrho} \sum_{|m|>n_0} t\, e^{-t\,\mathcal{H}_{m/2}}(|x|,|x|) = c\, z^{-\varrho}\, e^{-z} \sum_{|m|>n_0} I_{|m/2|}(z). \tag{5.4}$$

On the other hand, inequality (5.2) shows that

$$\sum_{|m|>n_0} t\, p_m(|x|,|x|,t) \leq \sum_{m\in\mathbb{Z}} t\, p_m(|x|,|x|,t) = 2\pi\, t\, e^{-tH_B}(x,x) \leq \frac{1}{2}.$$

This in combination with (5.4) gives

$$\sup_{t,r>0} \frac{|x|^{2\varrho}}{t^\varrho} \sum_{|m|>n_0} p_m(|x|,|x|,t) \,\leq\, c\, \max\left\{ \sup_{z\leq 1} z^{-\varrho} \sum_{|m|>n_0} I_{|m/2|}(z)\,,\, \sup_{z>1} z^{-\varrho}\right\} \leq C.$$

Indeed, in view of (3.19) the series $\sum_{|m|>n_0} I_{|m/2|}(z)$ converges uniformly with respect to z on $[0,1]$. Hence $z^{-|\alpha|}\sum_{|m|>n_0} I_{|m/2|}(z)$ is continuous on $(0,1]$ and since it tends to zero as $z\to 0$, see the proof of Theorem 4.1, it is bounded. From equation (5.3) we thus get

$$\sum_{m\in\mathbb{Z}} p_m(|x|,|x|,t) \,\leq\, C\,(1+|x|)^{2\varrho}\, t^{-1-\varrho}, \qquad \forall\, x\in\mathbb{R}^2, \quad t>0.$$

The statement now follows by (2.6) and (5.2). □

As a consequence of inequality (5.1) we get an estimate on the norm of e^{-tH_B} acting on certain weighted L^p spaces. To formulate our result we introduce the following family of subspaces:

$$L^p_\beta := \left\{ f \,:\, \|f\|_{L^p_\beta} < \infty \right\}, \quad \|f\|_{L^p_\beta} := \left(\int_{\mathbb{R}^2} |f|^p\,(1+|x|)^\beta\, dx\right)^{\frac{1}{p}}, \qquad \beta\in\mathbb{R}.$$

We then have

Proposition 5.2. *Let assumptions 2.1 be satisfied. Assume that $p\in[1,2]$ and let $q\in[2,\infty]$ be such that $\frac{1}{p}+\frac{1}{q}=1$. Then for any $\beta > 2+2\,\varrho$ there exists a constant $C=C(\varrho,\beta)$ such that*

$$\|e^{-tH_B}\|_{L^p_\beta\to L^q} \,\leq\, C\; t^{\frac{1-q}{q}-\frac{\varrho}{2}} \qquad \forall\, t\geq 1. \tag{5.5}$$

Proof. We use the shorthand $k(t,x,y) = e^{-tH_B}(x,y)$. Since e^{-tH_B} is self-adjoint, we have $k(t,y,x) = \overline{k(t,x,y)}$. The semigroup property of e^{-tH_B} and the Cauchy-Schwarz inequality then yield

$$\begin{aligned} |k(2t,x,y)| &= \Big| \int_{\mathbb{R}^2} k(t,x,z)\, k(t,z,y)\, dz \Big| \le \Big(\int_{\mathbb{R}^2} |k(t,x,z)|^2\, dz \Big)^{\frac{1}{2}} \Big(\int_{\mathbb{R}^2} |k(t,z,y)|^2\, dz \Big)^{\frac{1}{2}} \\ &= \sqrt{k(2t,x,x)}\ \sqrt{k(2t,y,y)}. \end{aligned} \tag{5.6}$$

This in combination with estimate (5.1) and diamagnetic inequality (5.2) gives

$$|k(t,x,y)| \le C\, t^{-1-\varrho\frac{\mu_1+\mu_2}{2}}\, (1+|x|)^{\mu_1\,\varrho} (1+|y|)^{\mu_2\,\varrho}, \quad \forall\, \mu_1,\, \mu_2 \in [0,1]. \tag{5.7}$$

Now fix $f \in L^2(\mathbb{R}^2)$ and let $t \ge 1$. Chose $\mu_1 = \mu_2 = 1$ in (5.7). In view of (5.6), Cauchy-Schwarz inequality and Fubuni's theorem we have

$$\begin{aligned} \|e^{-tH_B}\, f\|_{L^2}^2 &= \int_{\mathbb{R}^2} \Big| \int_{\mathbb{R}^2} k(t,x,y) f(y)\, dy \Big|^2 dx \le \|f\|^2_{L^2_\beta} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |k(t,x,y)|^2 (1+|y|)^{-\beta}\, dy\, dx \\ &= \|f\|^2_{L^2_\beta} \int_{\mathbb{R}^2} k(2t,y,y)\, (1+|y|)^{-\beta}\, dy \le C'\ t^{-1-\varrho}\ \|f\|^2_{L^2_\beta}. \end{aligned} \tag{5.8}$$

This shows that

$$\|e^{-tH_B}\|_{L^2_\beta \to L^2} \le C'\, t^{-(1+\varrho)/2}. \tag{5.9}$$

On the other hand, choosing $\mu_1 = 0$ and $\mu_2 = 1$ in (5.7) it is easily seen that

$$\|e^{-tH_B}\|_{L^1_\beta \to L^\infty} \le C\, t^{-1-\varrho/2}. \tag{5.10}$$

Inequality (5.5) now follows from (5.9), (5.10) and the Riesz-Thorin interpolation theorem. □

Remark 5.3. In the absence of magnetic field we have

$$\|e^{-tH_0}\|_{L^p_\beta \to L^q} = \|e^{t\Delta}\|_{L^p_\beta \to L^q} \simeq C\ t^{\frac{1-q}{q}} \qquad \forall\, \beta > 2. \tag{5.11}$$

Indeed, the upper bound in (5.11) follows by mimicking the proof of Proposition 5.2 with $k(t,x,y)$ replaced by $e^{t\Delta}(x,y) = e^{-\frac{|x-y|^2}{4t}}/(4\pi t)$. This leads to equations (5.9) and (5.10) with $\varrho = 0$. In order to prove the lower bound in (5.11) let us consider the solution of the heat equation with the initial data $f(x) = e^{-|x|^2}$. An easy calculation gives

$$u(t,x) = \big(e^{t\Delta} f\big)(x) = \frac{1}{1+4t}\ e^{-\frac{|x|^2}{1+4t}}, \qquad \|u(t,\cdot)\|_{L^q} = c\,(1+4t)^{\frac{1-q}{q}}.$$

Proposition 5.2 thus says that the L^q norm of the solution to the heat equation

$$\partial_t u + H_B\, u = 0, \qquad u(0,x) = f(x),$$

decays faster (with respect to the case $B = 0$), if we restrict the initial data f to a smaller subspace of $L^p(\mathbb{R}^2)$. Note also that similar estimates were recently obtained, in the case $p = q = 2$, for the heat semigroup of Dirichlet-Laplace operator in twisted waveguides; see [KZ].

6. Example: The Aharonov-Bohm operator

A natural question which arises from theorem 4.1 is whether the limit

$$\lim_{t\to\infty} t^{1+|\alpha|}\, e^{-tH_B}(x,y) \tag{6.1}$$

always exists and how it depends on x and y. In this section we calculate the limit (6.1) in the case of the so-called Aharonov-Bohm magnetic field. This field is characterized by the property that the flux $b(r)$ through a disc of radius r is constant. It is generated by the vector potential A whose radial and azimuthal components (in the polar coordinates) are given by

$$A(r,\theta) = (a_1(r,\theta),\, a_2(r)), \qquad a_1 = 0, \quad a_2(r) = \Big(0, \frac{\alpha}{r}\Big). \tag{6.2}$$

The associated operator $(i\nabla+A)^2$ defined on $C_0^\infty(\mathbb{R}^2\setminus\{0\})$ has deficiency indices $(2,2)$, see [AT, PR]. We will consider the Hamiltonian H_α as its Friedrichs extension. In other words, we define H_α as a non negative self-adjoint operator in $L^2(\mathbb{R}^2)$ generated by the closure of the quadratic form

$$Q_\alpha[u]=\int_0^{2\pi}\int_0^\infty \left(|\partial_r u|^2+r^{-2}\,|(-i\partial_\theta+\alpha)\,u|^2\right) r\,drd\theta,\quad u\in C_0^\infty((0,\infty)\times[0,2\pi)).$$

Proposition 6.1. *Let $t>0$ and $r,r'\in\mathbb{R}_+$. Then the heat kernel of the Aharonov-Bohm Hamiltonian H_α is given by the absolutely convergent series*

$$e^{-tH_\alpha}(x,y)=\frac{1}{4\pi t}\,e^{-\frac{r^2+r'^2}{4t}}\sum_{m\in\mathbb{Z}} I_{|m+\alpha|}\left(\frac{r\,r'}{2t}\right)e^{im(\theta-\theta')}. \tag{6.3}$$

Proof. We note that

$$H_\alpha=\sum_{m\in\mathbb{Z}}\oplus\left(\mathcal{H}_{m+\alpha}\otimes\mathrm{id}\right)\Pi_m, \tag{6.4}$$

where $\mathcal{H}_{m+\alpha}$ are the operators in $L^2(\mathbb{R}_+,rdr)$ defined in Lemma 3.3. Hence

$$e^{-tH_\alpha}(x,y)=\frac{1}{2\pi}\sum_{m\in\mathbb{Z}} e^{-t\,\mathcal{H}_{m+\alpha}}(r,r')\,e^{im(\theta-\theta')}\,, \tag{6.5}$$

Equation (6.3) now follows from Lemma 3.3. The absolute convergence of the series is easily seen from the integral representation of the Bessel function I_ν, see equation (3.19). □

Remark 6.2. For $\alpha\in\mathbb{Z}$ we get by [AS, Eq.9.6.33]

$$e^{-tH_\alpha}(x,y)=\frac{1}{4\pi t}\,e^{-\frac{r^2+r'^2}{4t}}\,e^{\frac{rr'}{2t}\,\cos(\theta-\theta')}\,e^{i\alpha(\theta'-\theta)}=\frac{1}{4\pi t}\,e^{-\frac{|x-y|^2}{4t}}\,e^{i\alpha(\theta'-\theta)}. \tag{6.6}$$

This reflects the well known fact that for integer values of the flux the Aharonov-Bohm operator is unitarily equivalent to the Laplacian in $L^2(\mathbb{R}^2)$ under the unitary mapping $f\mapsto e^{-i\alpha\,\theta}f$, see also Remark 1.1. Equation (6.3) also implies that it is no loss of generality if we suppose that $\alpha\in[-1/2,\,1/2]$.

Theorem 6.3. *We have*

$$\lim_{t\to\infty} t^{1+|\alpha|}\,e^{-tH_\alpha}(x,y)=\frac{1}{4\pi\Gamma(1+|\alpha|)}\left(\frac{r\,r'}{4}\right)^{|\alpha|}\qquad \textit{if}\quad |\alpha|<1/2, \tag{6.7}$$

$$\lim_{t\to\infty} t^{\frac32}\,e^{-tH_\alpha}(x,y)=\frac{1}{4\pi\Gamma(3/2)}\left(\frac{r\,r'}{4}\right)^{\frac12}\left(1+e^{\mp i(\theta-\theta')}\right)\qquad \textit{if}\quad \alpha=\pm1/2. \tag{6.8}$$

Proof. From equation (3.7) and the asymptotic behavior of $I_\nu(z)$ for small z, see [AS, Chap.9], we get

$$\lim_{t\to\infty} t^{1+|m+\alpha|}\,e^{-t\mathcal{H}_{m+\alpha}}(r,r')=\frac{r^{|m+\alpha|}\,r'^{|m+\alpha|}}{2^{2|m+\alpha|+1}\,\Gamma(1+|m+\alpha|)}\,. \tag{6.9}$$

Assume first that $|\alpha|<1/2$. In view of (3.19) we obtain

$$e^{-\frac{r^2+r'^2}{4t}}\,I_{|m+\alpha|}\left(\frac{r\,r'}{2t}\right)\le t^{-|m+\alpha|}\,\frac{(rr')^{|m+\alpha|}}{2^{|m+\alpha|}\,\Gamma(|m+\alpha|+\frac12)\Gamma(\frac12)}\,e^{\frac{-(r-r')^2}{4t}}\,.$$

Since $\inf_{m\neq0}|m+\alpha|>|\alpha|$, it follows that

$$\lim_{t\to\infty} t^{|\alpha|}e^{-\frac{r^2+r'^2}{4t}}\sum_{m\neq0} I_{|m+\alpha|}\left(\frac{r\,r'}{2t}\right)e^{im(\theta-\theta')}=0,$$

which, in combination with (6.9), proves equation (6.7). The proof in the case $|\alpha|=1/2$ follows the same line. □

Appendix A

For the reader's convenience, and also because equation (13) of [M, Sec.1.3.1] contains a missprint, we recall below a simplified version of [M, Thm.1.3.1.3].

Theorem A.1 (Maz'ya). *Let $1 \leq p \leq q \leq \infty$ and let $\mu, \nu \in L^1(\mathbb{R}_+)$ be nonnegative. Then the inequality*

$$\left(\int_0^\infty |u|^q \, \mu(x) \, dx \right)^{\frac{1}{q}} \leq C \, \left(\int_0^\infty |u'|^p \, \nu(x) \, dx \right)^{\frac{1}{p}} \tag{A.1}$$

holds for all $u \in W^{1,p}(\mathbb{R}_+, \, \nu(x)dx)$ and some constant C, independent of u, if and only if

$$\sup_{r>0} \left(\int_0^r \mu(x) \, dx \right)^{\frac{1}{q}} \left(\int_r^\infty \nu(x)^{-\frac{1}{p-1}} \, dx \right)^{\frac{p-1}{p}} < \infty. \tag{A.2}$$

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