Heat kernel asymptotics for magnetic Schrödinger operators

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Abstract. We explicitly construct parametrices for magnetic Schrödinger operators on $\mathbb{R}^d$ and prove that they provide a complete small-$t$ expansion for the corresponding heat kernel, both on and off the diagonal.
1 Introduction

Heat kernel asymptotics have attracted much attention ever since Minakshisundaram and Pleijel [MP49, Min53] proved that the heat kernel for the Laplacian on a compact Riemannian manifold has a complete asymptotic expansion as \( t \to 0^+ \). These asymptotic expansions have since been extended to many elliptic operators of geometric relevance (see, e.g., [BGM71, BGV92, Gil95, Kir01]). Most notably, heat kernel expansions reveal the local nature of heat invariants, i.e., the coefficients in the small-\( t \) asymptotics of the trace of the heat semi-group generated by the operator in question. Among other things, this observation led to novel proofs of index theorems for elliptic complexes [ABP73]. In general, heat kernel expansions turned out to provide powerful tools in spectral geometry.

One would expect similar properties of heat kernels for other (semi-bounded, self-adjoint) operators, too. Schrödinger operators are among the most prominent examples. In particular, magnetic Schrödinger operators are of interest in the context of para- and diamagnetism where heat kernel estimates, including their small-\( t \) behaviour, were used very successfully (see, e.g., [LT97, Erd97]).

In a scattering context, where a Schrödinger operator has a non-empty absolutely continuous spectrum and, therefore, the heat semi-group is not of trace class, a ‘relative heat trace’, as it appears in a Krein trace formula, has been shown to possess a related small-\( t \) expansion (see [CdV81] for the non-magnetic case and [Hit02] for magnetic Schrödinger operators). Moreover, irrespective of whether the heat semi-group of a Schrödinger operator is of trace class, small-\( t \) asymptotics of the diagonal of the heat kernel have been proven (in [HP03] for non-magnetic operators and in [KP03] for the magnetic case). In that context the heat invariants are integrals of the scalar potential and the magnetic field strength as well as their derivatives.

In this paper we consider magnetic Schrödinger operators on \( \mathbb{R}^d \) with smooth and polynomially bounded scalar and vector potentials. Our principal goal is to prove complete asymptotic expansions as \( t \to 0^+ \) of the related full heat kernels (and not only of their diagonals as, e.g., in [KP03]). In order to achieve this we construct parametrices for the heat equations and show that these provide heat kernel asymptotics. We then use the parametrices to determine heat invariants for magnetic Schrödinger operators on some manifolds with and without boundary of the form \( \mathbb{R}^2/\Gamma \), where \( \Gamma \) is a discrete group of reflections and translations. The paper is organised as follows. We first briefly describe the setting of heat kernels and parametrices for magnetic Schrödinger operators in Section 2. The parametrices are then constructed in Section 3 and the main result is summarised in Theorem 3.1. In Section 4 we use the parametrices to construct a Volterra series and prove that this series yields the heat kernel. Moreover, this series turns out to provide an asymptotic expansion for small \( t \). These results are contained in Theorem 4.6. Finally, in Section 5 we discuss some applications to heat trace invariants for magnetic Schrödinger operators on half-planes, infinite cylinders, and tori.
2 Preliminaries

We consider magnetic Schrödinger operators

\[ H = (-i\nabla - A(x))^2 + V(x) , \]

acting on a suitable domain in \( L^2(\mathbb{R}^d) \) with \( d \geq 2 \). For our purposes we require the components \( A_j \) of the vector potential \( A \) and the potential \( V \) to be in

\[ S_m := \{ f \in C^\infty(\mathbb{R}^d); \ \forall \alpha \in \mathbb{N}_0^d \ \exists C_\alpha > 0 \ \text{s.t.} \ |\partial^\alpha_x f(x)| \leq C_\alpha (1 + |x|)^m \} \]

for some fixed \( m \geq 0 \). Moreover, \( V \) shall be bounded from below. Under these conditions \( H \)

is essentially self-adjoint on the domain \( C^\infty_0(\mathbb{R}^d) \), which is indeed true under much weaker conditions (see, e.g., [Sim73, LS81]). The vector potential defines a one-form

\[ A(x) = \sum_{k=1}^d A_k(x) \, dx_k , \]

whose exterior derivative

\[ B(x) := dA(x) = \sum_{k<l} B_{kl}(x) \, dx_l \wedge dx_k , \]

is the two-form of magnetic field strengths, with components

\[ B_{kl}(x) = \frac{\partial A_k(x)}{\partial x_l} - \frac{\partial A_l(x)}{\partial x_k} \]

that are also in \( S_m \).

The heat kernel for \( H \) is a function \( K \in C^\infty((0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d) \) satisfying

\[ \left( \frac{\partial}{\partial t} + H \right) K(t, x, y) = 0 , \quad \lim_{t \to 0^+} K(t, x, y) = \delta(x - y) . \]

The existence of the heat kernel is known and follows, e.g., from a representation in terms of a Feynman-Kac formula (see, e.g., [Sim05]).

Often one is interested in the small-\( t \) behaviour of the heat kernel or of its trace, if the heat semi-group is of trace class. In that case one can infer the distribution of eigenvalues from the asymptotics of the heat semi-group. It is well known that for large classes of operators \( H \) the heat trace allows for an asymptotic expansion of the form

\[ \text{Tr} \ e^{-Ht} = \frac{1}{(4\pi t)^{d/2}} \sum_{j=0}^N \alpha_j t^j + O(t^{-\frac{d}{2}+N+1}) . \]

Operators for which this is known to hold include Laplacians on bounded domains in \( \mathbb{R}^d \), on compact Riemannian manifolds with and without boundary (see, e.g., [MP49, Kac66]).
and certain magnetic and non-magnetic Schrödinger operators (see, e.g., [MS67, Gi95], [HP03, KP03]).

The heat trace coefficients can be obtained from the local heat invariants,

$$\alpha_j = \int a_j(x) \, dx , \quad (2.8)$$

which are determined by the small-\(t\) asymptotics of the diagonal,

$$K(t, x, x) = \frac{1}{(4\pi t)^{d/2}} \sum_{j=0}^{N} a_j(x) \, t^j + O(t^{-2 + N + 1}) . \quad (2.9)$$

It is our intention to determine a complete small-\(t\) asymptotics for the heat kernel of a magnetic Schrödinger operator (2.1), and to compute the first few coefficients explicitly. To achieve this we shall use a parametrix for the heat equation, i.e., an approximate solution of (2.6) for small \(t\). A more precise definition is as follows.

**Definition 2.1.** A parametrix of order \(\lambda \geq 0\) for the heat equation is a function \(k \in C^\infty((0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d)\) such that

1. \((\partial_t - H)k(t, x, y)\) extends to a function in \(C^\infty([0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d)\),
2. there exists a constant \(c_\lambda > 0\) such that \(\left| (\partial_t - H)k(t, x, y) \right| \leq c_\lambda t^\lambda\),
3. \(\lim_{t \to 0^+} k(t, x, y) = \delta(x - y)\).

Parametrices allow to read off the expansion (2.9), including the heat trace invariants \(a_j(x)\). As they approximate the heat kernel itself, and not only its diagonal, parametrices can be used to determine heat trace asymptotics in cases where the heat kernel is determined from a given kernel using a method of images.

## 3 Parametrix construction

In order to obtain a heat parametrix we introduce the ansatz

$$k_N(t, x, y) = \frac{1}{(4\pi t)^{d/2}} e^{-\frac{1}{4t}(x - y)^2} \sum_{k=0}^{N+1} u_k(x, y) \, t^k , \quad \text{where } u_0 \neq 0 , \quad (3.1)$$

and show that one can solve recursively for \(\phi, u_0, u_1, \ldots \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d)\). This procedure will eventually provide us with a complete asymptotic small-\(t\) expansion of the heat kernel.

**Theorem 3.1.** Let \(N \in \mathbb{N}_0\) be such that \(N \geq d/2 - 1\) and define

$$k_N(t, x, y) = \frac{1}{(4\pi t)^{d/2}} e^{-\frac{1}{4t}(x - y)^2} \sum_{k=0}^{N+1} u_k(x, y) \, t^k , \quad (3.2)$$
with leading coefficient

\[ u_0(x, y) = \exp \left( i \int_0^1 A(x(s)) \cdot \dot{x}(s) \, ds \right) \]  

(3.3)

and (recursively defined) higher-order coefficients

\[ u_k(x, y) = -u_0(x, y) \int_0^1 s^{k-1} u_0^{-1}(x(s), y) \left( Hu_{k-1}(x(s), y) \right) \, ds , \quad k \geq 1 , \]  

(3.4)

where \( x(s) = y + s(x - y) \). Then (3.2) is a parametrix of order \( N + 1 - d/2 \) for the heat equation.

**Proof.** Inserting the ansatz (3.1) into (2.6) and ordering terms by powers of \( t \) we obtain

\[
\left( \frac{\partial}{\partial t} + H \right)_{N} = \frac{e^{-\frac{1}{4} \phi}}{(4\pi t)^{d/2}} \sum_{k=0}^{N+1} \left\{ t^{k-2} \left[ \phi - (\nabla \phi)^2 \right] u_k + t^{k-1} \left[ \Delta \phi + \left( k - \frac{d}{2} \right) \right. \right. \\
\left. \left. + 2 (\nabla \phi) \cdot (\nabla - iA) \right] u_k + t^k \left. Hu_k \right\} .
\]  

(3.5)

Requiring the coefficients of \( t^{-j-d/2}, j = -2, \ldots, N \), to vanish independently yields the following hierarchy of conditions,

\[ t^{-2-d/2} : \quad \phi - (\nabla \phi)^2 = 0 , \]  

(3.6)

\[ t^{-1-d/2} : \quad \left[ \phi - (\nabla \phi)^2 \right] u_1 + \left[ \Delta \phi - \frac{d}{2} + 2 (\nabla \phi) \cdot (\nabla - iA) \right] u_0 = 0 , \]  

(3.7)

\[ 0 \leq k \leq N : \quad \left[ \phi - (\nabla \phi)^2 \right] u_{k+2} + \left[ \Delta \phi + k + 1 - \frac{d}{2} + 2 (\nabla \phi) \cdot (\nabla - iA) \right] u_{k+1} + H u_k = 0 . \]  

(3.8)

The solution to the first equation is

\[ \phi(x, y) = \frac{1}{4} (x + b)^2 \]  

(3.9)

with \( b \in \mathbb{R}^d \). The initial condition for \( t \to 0^+ \) for the parametrix implies \( b = -y \), as well as \( u_0(x, x) = 1 \). This means that \( \nabla \phi(x, y) = \frac{1}{2}(x - y) \) and \( \Delta \phi = \frac{d}{2} \).

Substituting the solution for \( \phi \) into eqs. (3.7) and (3.8) we find a homogenous transport equation

\[ (x - y) \cdot (\nabla - iA) u_0(x, y) = 0 \]  

(3.10)

for the lowest order coefficient, and inhomogenous transport equations

\[ [(x - y) \cdot (\nabla - iA) + k] u_k(x, y) = -H u_{k-1}(x, y) \quad \forall k \geq 1 , \]  

(3.11)

for the higher-order coefficients.
In order to solve these equations we introduce the parametrisation

\[ x(s) := y + s(x - y), \quad 0 \leq s \leq 1, \]  

(3.12)

of the line connecting \( y \) and \( x \). Hence, \( x(0) = y \), \( x(1) = x \) and \( \dot{x}(s) = x - y \). Thus,

\[ \left. \left( \frac{d}{ds} - i\dot{x}(s) \cdot A(x(s)) \right) u_k(x(s), y) \right|_{s=1} = (x - y) \cdot (\nabla - iA(x))u_k(x, y). \]  

(3.13)

The homogeneous and inhomogeneous ordinary differential equations for \( u_k(x(s), y) \) can be solved explicitly, providing solutions to the transport equations in the form \( u_k(x, y) = u_k(x(1), y) \). (See [Yos53] for a related approach.)

For the lowest order (homogeneous) transport equation (3.10) we have to solve

\[ \left( \frac{d}{ds} - i\dot{x}(s) \cdot A(x(s)) \right) u_0(x(s), y) = 0, \quad u_0(x(0), y) = 1. \]  

(3.14)

The solution can readily be found to be

\[ u_0(x(s), y) = \exp \left( i \int_0^s A(x(t)) \cdot \dot{x}(t) \, dt \right). \]  

(3.15)

Choosing \( s = 1 \), this gives the lowest-order coefficient \( u_0 \) in the form (3.3).

The inhomogeneous, higher-order transport equations (3.11) can be solved recursively, order by order. We first determine the general solutions

\[ u_k^{\text{hom}}(x, y) = u_0(x, y) v_k(x, y) \]  

(3.16)

of the homogeneous equations corresponding to (3.11). The functions \( v_k \) hence follow from the condition

\[ [(x - y) \cdot \nabla + k] v_k(x, y) = 0, \]  

(3.17)

implying

\[ v_k(x, y) = \frac{f_k(y)}{|x - y|^k}, \]  

(3.18)

with arbitrary \( f_k \). As we require \( u_k \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d) \), we conclude that \( u_k^{\text{hom}} \equiv 0 \).

In order to determine solutions of the inhomogeneous transport equation (3.11) we introduce the ansatz

\[ u_k(x, y) = u_0(x, y) w_k(x, y), \]  

(3.19)

where it is understood that \( w_0 \equiv 1 \). The inhomogeneity requires us to act with \( H \) on \( u_{k-1} \), given in the form (3.19). As a first step, a straightforward calculation yields that

\[ \left( \frac{\partial}{\partial x_j} - iA_j(x) \right) u_0(x, y) = -i \sum_{l=1}^d (x_l - y_l) \int_0^1 t B_{jl}(x(t)) \, dt \, u_0(x, y). \]  

(3.20)
Using this, the inhomogeneity can be brought into the form
\[
-Hu_0(x, y) w_{k-1}(x, y) = - \left( (-i \nabla - A(x))^2 + V(x) \right) u_0(x, y) w_{k-1}(x, y) = u_0(x, y) g_{k-1}(x, y),
\] (3.21)
where, following a straightforward calculation,
\[
g_k(x, y) = - \left[ -\Delta + V(x) + \mathbf{i}(x - y) \cdot \alpha(x, y) + \mathbf{i}(x - y) \cdot \beta(x, y) \nabla \\
+ (x - y) \cdot \gamma(x, y)(x - y) \right] w_k(x, y),
\] (3.22)
and we defined the vector \( \alpha(x, y) \) with components
\[
\alpha_l(x, y) = \sum_{j=1}^d \int_0^1 t^2 \frac{\partial B_{jl}(x(t))}{\partial x_j} dt,
\] (3.23)
and the matrices \( \beta(x, y) \) and \( \gamma(x, y) \) with entries
\[
\beta_{jl}(x, y) := 2 \int_0^1 t B_{jl}(x(t)) dt,
\]
\[
\gamma_{jl}(x, y) := \sum_{m=1}^d \int_0^1 \int_0^1 s B_{ml}(x(t)) B_{mj}(x(s)) dt ds.
\] (3.24)
The functions \( \alpha_l, \beta_{jl}, \gamma_{jl} \) are smooth and polynomially bounded.

Furthermore, using (3.10) on the left-hand side of (3.11) yields
\[
\left( (x - y) \cdot (\nabla - \mathbf{i}A(x)) + k \right) u_0(x, y) w_k(x, y) = u_0(x, y)((x - y) \cdot \nabla + k) w_k(x, y). \tag{3.25}
\]
Hence, the functions \( w_k \) follow from
\[
\left( (x - y) \cdot \nabla + k \right) w_k(x, y) = g_{k-1}(x, y). \tag{3.26}
\]
With the ansatz
\[
w_k(x, y) = \frac{f_k(x, y)}{|x - y|^k},
\] (3.27)
the function \( f_k \), therefore, satisfies the equation
\[
\frac{1}{|x - y|^k} (x - y) \cdot \nabla f_k(x, y) = g_{k-1}(x, y). \tag{3.28}
\]
Along the curve (3.12) this reads
\[
\frac{s^{1-k}}{|x - y|^k} (x - y) \cdot (\nabla f_k)(x(s), y) = g_{k-1}(x(s), y), \tag{3.29}
\]
or
\[
\frac{d}{ds} f_k(x(s), y) = s^{k-1}|x - y|^k g_{k-1}(x(s), y), \tag{3.30}
\]
and is solved by
\[
f_k(x, y) = f_k(y, y) + |x - y|^k \int_0^1 s^{k-1} g_{k-1}(x(s), y) \, ds, \tag{3.31}
\]
i.e.
\[
w_k(x, y) = \frac{f_k(y, y)}{|x - y|^k} + \int_0^1 s^{k-1} g_{k-1}(x(s), y) \, ds. \tag{3.32}
\]
In order to avoid a singularity on the diagonal we have to choose \( f_k(y, y) = 0 \), hence
\[
w_k(x, y) = \int_0^1 s^{k-1} g_{k-1}(x(s), y) \, ds \tag{3.33}
\]
and
\[
u_k(x, y) = u_0(x, y) \int_0^1 s^{k-1} g_{k-1}(x(s), y) \, ds. \tag{3.34}
\]
With (3.21), this implies (3.4).

Finally, if \( N \geq \frac{d}{2} - 1 \),
\[
R_N(t, x, y) := \left( \frac{\partial}{\partial t} + H \right) k_N(t, x, y) = \frac{t^{N+1}}{(4\pi t)^{d/2}} e^{-\frac{1}{4t}(x - y)^2} H u_{N+1}(x, y) \\
- \frac{t^{N+1-d/2}}{(4\pi)^{d/2}} e^{-\frac{1}{4}(x - y)^2} u_0(x, y) g_{N+1}(x, y) \tag{3.35}
\]
extends to \( t = 0 \) such that property (i) in Definition 2.1 is satisfied; property (ii) can be read off too and property (iii) was built in as an initial condition for the lowest-order transport equation.

We remark that the higher-order coefficients \( u_k \) have to be determined recursively; we only do this explicitly for \( u_1 \). As \( w_0 = 1 \), eqs (3.34) and (3.22) with \( k = 1 \) give
\[
u_1(x, y) = \int_0^1 \left[ -V(x(s)) - \sum_{l=1}^d (x_l - y_l) \alpha_l(x(s), y) \right. \\
- s^2 \sum_{j,l=1}^d (x_l - y_l) \gamma_{lj}(x(s), y)(x_j - y_j) \left. \right] ds u_0(x, y). \tag{3.36}
\]
The diagonal terms simplify considerably,
\[
u_k(x, x) = g_{k-1}(x, x) \int_0^1 s^{k-1} \, ds = \frac{1}{k} (\Delta - V(x)) w_{k-1}(x, y) \bigg|_{y=x}. \tag{3.37}
\]
They yield the well-known local heat invariants (compare, e.g., [KP03]); the lowest orders are

\[ \begin{align*}
u_1(x, x) &= -V(x), \\
u_2(x, x) &= \frac{1}{2} V^2(x) - \frac{1}{6} \Delta V(x) + \frac{1}{12} \text{tr} B^2(x). \end{align*} \tag{3.38} \]

The full heat kernel for a magnetic Schrödinger operator is determined by the potentials \( \mathbf{A} \) and \( V \) via (2.6). A parametrix, however, follows from the 'local' transport equations and hence depends only on the potentials along the straight line connecting \( x \) and \( y \).

**Corollary 3.2.** Let \( k_N \) and \( \tilde{k}_N \) be parametrices (of the same order \( N \)) corresponding to potentials \( V, \mathbf{A} \) and \( \tilde{V}, \tilde{\mathbf{A}} \) in the heat equation, respectively. Let \( x, y \) be given and assume that \( V = \tilde{V} \) and \( \mathbf{A} = \tilde{\mathbf{A}} \) along the straight line \( \{x(s); 0 \leq s \leq 1\} \) connecting \( y \) and \( x \). Then \( k_N(t, x, y) = \tilde{k}_N(t, \mathbf{x}, \mathbf{y}) \).

To put our result into perspective we compare it with the well-known case of a constant magnetic field \( B \) in dimension \( d = 2 \). There the heat kernel for the magnetic Schrödinger operator is given by the Mehler kernel (see, e.g., [Sim05, LT97]),

\[ K(t, x, y) = \frac{B}{4\pi \sinh(Bt)} \exp \left\{ -\frac{B}{4} \coth(Bt)(x - y)^2 - \frac{B}{2}(x_1 y_2 - x_2 y_1) \right\}, \tag{3.39} \]

where the gauge

\[ \mathbf{A}(x) = B \left( \begin{array}{c} -x_2 \\ x_2 \end{array} \right) \tag{3.40} \]

has been chosen. Expanding the Mehler kernel for small \( t \) yields

\[ K(t, x, y) = \frac{1}{4\pi t} e^{-\frac{t}{4}(x-y)^2} e^{-\frac{i}{2} B(x_1 y_2 - x_2 y_1)} \left( 1 - \frac{B^2}{12} (x - y)^2 t + O(t^2) \right). \tag{3.41} \]

Inserting the vector potential (3.40) into (3.3) we find

\[ u_0(x, y) = e^{-i \frac{B}{2}(x_1 y_2 - x_2 y_1)}. \tag{3.42} \]

The auxiliary functions (3.23) and (3.24) become \( \gamma_{12} = \gamma_{21} = 0 \) and \( \gamma_{11} = \gamma_{22} = B^2/4 \). Inserting into (3.36) yields

\[ u_1(x, y) = -\frac{B^2}{12} (x - y)^2 u_0(x, y), \tag{3.43} \]

i.e. the parametrix \( k_0 \) agrees with the leading small-\( t \) asymptotics of the Mehler kernel. In the following section we show that it is always true that the parametrix \( k_N \) provides the first \( N + 1 \) terms of the heat kernel asymptotics.
4 Asymptotic expansion of the heat kernel

From the ansatz (3.1) one expects a heat parametrix to be an approximation to the heat kernel for small $t$. It even appears to be a tool to generate an asymptotic expansion for the heat kernel. That this is indeed the case can be proven by generating a Volterra series from a sufficiently regular parametrix, and then to prove that this series converges. This then first implies the existence of the heat kernel, since the Volterra series turns out to represent the heat kernel. As the existence of the heat kernel is known by other means, here the more important consequence of the Volterra series is that it provides an asymptotic expansion of the heat kernel for $t \to 0$.

The approach we follow to construct the Volterra series exists in many variants; it was developed for heat kernels of elliptic operators on manifolds [Min53, Yos53], and was then further extended in many directions. We here take some inspiration from [Gri04].

Recall that $k_N$ as given in Theorem 3.1 is a parametrix of order $\lambda = N + 1 - d/2$ for the heat equation of a magnetic Schrödinger operator, compare (3.35). This requires $N \geq d/2 - 1$, i.e., in two dimensions the simplest choice is $N = 0$, leading to

$$k_0(t, x, y) = \frac{1}{4\pi t} e^{-\frac{1}{4t}(x-y)^2} \left( u_0(x, y) + u_1(x, y) t \right)$$ (4.1)

and, cf. (3.35),

$$R_0(t, x, y) = -\frac{1}{4\pi} e^{-\frac{1}{4t}(x-y)^2} u_0(x, y) g_1(x, y) .$$ (4.2)

In higher dimensions further terms are required.

As a first step towards constructing a Volterra series we need to estimate $R_N$.

Lemma 4.1. Let $V, A_j \in \mathcal{S}_m$ for some $m \geq 0$, cf. (2.2), and let $N \in \mathbb{N}_0$. Then, for every $\varepsilon > 0$ there exists $M_N > 0$ such that

$$|R_N(t, x, y)| \leq M_N t^{N+1-d/2} e^{-\frac{1-\varepsilon}{4t}(x-y)^2} .$$ (4.3)

Proof. According to (3.35), we have to estimate $g_{N+1}(x, y)$. This can be done using (3.22), and taking into account that

$$w_k(x, y) = \frac{u_k(x, y)}{u_0(x, y)} = \int_0^1 s^{k-1} g_{k-1}(x(s), y) \, ds .$$ (4.4)

From (3.22), and the fact that the potentials are assumed to be smooth and polynomially bounded, we see that

$$g_0(x, y) = -V(x) - i(x-y) \cdot \alpha(x, y) - (x-y) \cdot \gamma(x, y)(x-y)$$ (4.5)

is also smooth and polynomially bounded. For $k \geq 1$ the functions $g_k$ are determined recursively through (3.22), (3.33) and (4.4). That way they are also seen to be smooth and polynomially bounded. Hence the estimate (4.3) follows. \qed
To proceed we need the convolution of kernels.

**Definition 4.2.** Let \( f, g \in C((0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d) \). Then their convolution is

\[
(f \ast g)(t, x, y) := \int_0^t \int_{\mathbb{R}^d} f(t - s, x, z) g(s, z, y) \, dz \, ds,
\]

whenever the integrals converge absolutely. The \( n \)-fold convolution of \( f \) with itself is denoted as \( f^n = f \ast \cdots \ast f \).

The following statement on convolutions will be useful.

**Lemma 4.3.** Let \( \alpha > 0 \), \( \kappa_j > 0 \) and \( f_j \in C^\infty((0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d) \), such that

\[
|f_j(t, x, y)| \leq C_j t^{-\frac{d+2}{2} + \kappa_j} e^{-\frac{\alpha}{\tau}(x-y)^2},
\]

where \( C_j > 0 \). Then \( f_1 \ast \cdots \ast f_n \in C^\infty((0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d) \), and

\[
|(f_1 \ast \cdots \ast f_n)(t, x, y)| \leq D_n t^{-\frac{d+2}{2} + \kappa_1 + \cdots + \kappa_n} e^{-\frac{\alpha}{\tau}(x-y)^2},
\]

with some \( D_n > 0 \).

If the constants \( \kappa_j \) are chosen optimally, they can be defined as a degree of \( f_j \). The unusual definition of the power of \( t \) in (4.7) therefore leads to an additivity of the degree under convolution. From Lemma 4.1 one concludes that \( R_N \) has degree \( N + 2 \).

**Proof.** The bounds (4.7) imply that the convolution integrals defining \( f_1 \ast \cdots \ast f_n \) converge absolutely and uniformly, hence \( f_1 \ast \cdots \ast f_n \in C^\infty((0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d) \).

Moreover, the \( n \)-fold convolution of the kernels \( f_j \),

\[
(f_1 \ast \cdots \ast f_n)(t, x, y) = \int_0^t \cdots \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} f_1(t - t_1, x_1, z_1) f_2(t_1 - t_2, z_1, z_2) \cdots f_n(t_{n-1}, z_{n-1}, y) \, dz_{n-1} \cdots dz_1 \, dt_{n-1} \cdots dt_1,
\]

will be estimated based on the bounds (4.7). This includes a convolution of Gaussians,

\[
\int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} e^{-\alpha} \left[ \frac{(x_1 - z_1)^2}{t_1} + \frac{(x_2 - z_2)^2}{t_2} + \cdots + \frac{(x_{n-2} - z_{n-1})^2}{t_{n-2}} + \frac{(x_{n-1} - y)^2}{t_{n-1}} \right] \, dz_{n-1} \cdots dz_1 \nonumber = \left( \frac{\pi}{\alpha} \right)^{(n-1)d/2} \left( \frac{(t - t_1) \cdots (t_{n-2} - t_{n-1}) t_{n-1}}{t} \right)^{d/2} e^{-\frac{\alpha}{\tau}(x-y)^2}.
\]

Hence, with \( \tilde{D}_n = (\pi/\alpha)^{(n-1)d/2} C_1 C_2 \cdots C_n \) we obtain

\[
|(f_1 \ast \cdots \ast f_n)(t, x, y)| \leq \tilde{D}_n e^{-\frac{\alpha}{\tau}(x-y)^2}
\]

\[
\int_0^t \cdots \int_0^{t_{n-2}} \frac{(t - t_1)^{\kappa_1 - 1} \cdots (t_{n-2} - t_{n-1})^{\kappa_{n-1} - 1} t_{n-1}^{\kappa_{n-1}}}{t^{d/2}} \, dt_{n-1} \cdots dt_1
\]

\[
= \tilde{D}_n e^{-\frac{\alpha}{\tau}(x-y)^2} t^{-\frac{d+2}{2} + \kappa_1 + \cdots + \kappa_n}
\]

\[
\int_0^1 \cdots \int_0^{s_{n-2}} (1 - s_1)^{\kappa_1 - 1} \cdots (s_{n-2} - s_{n-1})^{\kappa_{n-1} - 1} s_{n-1}^{\kappa_{n-1}} \, ds_{n-1} \cdots ds_1,
\]

(4.11)
which proves the estimate (4.8).

From this result one obtains the following.

Lemma 4.4. Let \( n \in \mathbb{N} \), then \( R_n^* \in C^\infty((0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d) \). Moreover,

\[
|R_n^*(t, x, y)| \leq \left( \frac{4\pi}{1 - \varepsilon} \right)^{(n-1)d/2} \frac{M_n^n}{(n-1)!} t^{\frac{d+2}{2} + n(N+2)} e^{-\frac{1-\varepsilon}{4\varepsilon}(x-y)^2}.
\] (4.12)

In particular, \( R_n^* \) has degree \( n(N+2) \) and therefore is bounded as \( t \to 0 \) when \( n(N+2) \geq \frac{d+2}{2} \).

Proof. With the bound (4.13) this statement follows almost immediately from Lemma 4.3. We only need to refine the constant \( D_n \) (in terms of \( n \)), which includes the contribution

\[
\int_0^1 \ldots \int_0^{s_{n-2}} (1 - s_1)^{N+1} \ldots (s_{n-2} - s_{n-1})^{N+1} s_{n-1}^{N+1} ds_{n-1} \ldots ds_1 \leq \int_0^1 \ldots \int_0^{s_{n-2}} ds_{n-1} \ldots ds_1 = \frac{1}{(n-1)!}.
\] (4.13)

We also need the following standard result, which is an appropriate version of Duhamel’s principle.

Lemma 4.5. Let \( f \in C^\infty((0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d) \), and \( k_N \) be a heat parametrix. Then

\[
\left( \frac{\partial}{\partial t} + H \right) (k_N * f) = f + R_N * f.
\] (4.14)

One proves this statement by a direct computation. Following a standard procedure, Duhamel’s principle allows us to construct a heat kernel in terms of a Volterra series.

Theorem 4.6. Let \( N \geq d/2 - 1 \) so that \( k_N \) is a heat parametrix. Then the Volterra series

\[
K := k_N + \sum_{n=1}^\infty (-1)^n k_N * R_n^N
\] (4.15)

converges in \( C^\infty((0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d) \). It has degree one and defines a heat kernel for the magnetic Schrödinger operator \( H \).

Moreover, the series (4.15) provides an asymptotic expansion, as \( t \to 0 \), for the heat kernel in such a way that the parametrix \( k_N \) contributes the first \( N + 1 \) terms in that expansion.
Proof. According to Lemma 4.4, $R_N^{*n}$ is bounded as $t \to 0$, if $n \geq \frac{d+2}{2N+4}$. Moreover, in analogy to Lemma 4.1 one finds that

$$|k_N(t, x, y)| \leq C_N t^{-d/2} e^{-\frac{1+\varepsilon}{4\pi t}(x-y)^2},$$

i.e., the degree of $k_N$ is 1 (independent of $N$). The composition Lemma 4.3 then implies the bound

$$|k_N * R_N^{*n}(t, x, y)| \leq \left(\frac{4\pi}{1 - \varepsilon}\right)^{nd/2} C_N M_N^n t^{-\frac{d+2}{2}n(N+2)+1} e^{-\frac{1+\varepsilon}{4\pi t}(x-y)^2}.$$

Choosing $n \geq \frac{d+2}{2N+4}$ as above, this bound ensures uniform convergence (in $x, y$ and $t \in (0, T)$) of the series.

The degree of $K$ is determined by $k_N$ to be one; all other terms in the Volterra series have a higher degree.

Due to the Gaussian factors, any derivative with respect to components of $x, y$ reduces the degree by one, whereas every $t$-derivative reduces the degree by two. Hence, for every derivative of $K$ there exists $l \in \mathbb{N}_0$ such that choosing $n \geq \frac{d+2}{2N+4} + l$ ensures uniform convergence of the series.

As from Lemma 4.5 we have that

$$\left(\frac{\partial}{\partial t} + H\right) k_N * R_N^{*n} = R_N^{*n} + R_N^{*(n+1)},$$

the uniform convergence of the Volterra series and its derivatives implies that after applying $\frac{\partial}{\partial t} + H$ the series telescopes. Therefore, $\left(\frac{\partial}{\partial t} + H\right) K = 0$. The initial condition as $t \to 0$ was built into the construction of $k_N$; all other terms give no contribution to this limit.

The series (4.15) is asymptotic for small $t$ in the sense that $k_N(t, x, y)$ is a sum of terms with a $t$-dependence (on the diagonal $x = y$) of the form $t^{-\frac{d+k}{2}}$, where $k = 0, \ldots, N + 1$. The highest power, i.e., the smallest term as $t \to 0$, therefore is $t^{-\frac{d}{2} + N + 1}$. According to (4.17), however, the smallest power in the remainder, coming from $k_N * R_N$, is $t^{-\frac{d}{2} + N + 2}$.

Informally, Theorem 4.6 can be rephrased as

$$K(t, x, y) = \frac{1}{(4\pi t)^{d/2}} e^{-\frac{1}{4\pi t}(x-y)^2} \sum_{k=0}^{N+1} u_k(x, y) t^k + O(t^{-\frac{d}{2} + N + 2}).$$

A comparison with (2.9) therefore shows that the heat trace invariants are given by

$$a_j(x) = u_j(x, x),$$

cf. (3.38) for the lowest orders.
5 Some applications

One can use the knowledge of a complete asymptotic expansion of the heat kernel for a magnetic Schrödinger operator on \( \mathbb{R}^d \) to, e.g., compute heat invariants as well as the heat trace asymptotics for magnetic Schrödinger operators on manifolds (with or without boundary) of the form \( \mathbb{R}^2 / \Gamma \), where \( \Gamma \) is a discrete subgroup of the isometry group of \( \mathbb{R}^2 \). These include half-planes, cylinders and tori. Below we give some examples in dimension \( d = 2 \). In that case there is only one non-vanishing component

\[
B(x) = B_{21}(x) = -B_{12}(x)
\]

of the field strengths (2.5). This is the magnetic field in \( d = 2 \).

5.1 Half-plane

We consider the heat equation for a magnetic Schrödinger operator (2.1) in the upper half-plane

\[
H_+ := \{ x = (x_1, x_2) \in \mathbb{R}^2; \ x_2 > 0 \}
\]

with Dirichlet- or Neumann boundary conditions along the boundary.

Following a well-known construction, the heat kernels \( K^{-}(t, x, y) \) and \( K^{+}(t, x, y) \) for the upper half-plane with Dirichlet- and Neumann boundary conditions, respectively, can be constructed from the corresponding kernel \( K(t, x, y) \) for the entire plane \( \mathbb{R}^2 \), provided the potentials have been extended suitably to the lower half-plane. Introducing the reflection \( R(x_1, x_2) = (x_1, -x_2) \) on \( \mathbb{R}^2 \) across the boundary, we need potentials on \( \mathbb{R}^2 \) that satisfy

\[
V(Rx) = V(x) \quad \text{and} \quad A(Rx) = RA(x).
\]

The latter condition implies that \( B(Rx) = -B(x) \). Intuitively, this ensures that a particle which is reflected at the boundary with reversed velocity, is subject to a magnetic field with the correct sign. The conditions (5.3) can be achieved by extending the potentials from \( H_+ \) to \( \mathbb{R}^2 \) accordingly. In order for the potentials to be smooth across the boundary, at \( x_2 = 0 \) the odd partial \( x_2 \)-derivatives of \( V \) and \( A_1 \) as well as the even partial \( x_2 \)-derivatives of \( A_2 \) must vanish.

Under these conditions the heat kernel \( K(t, x, y) \) for the extended problem on \( \mathbb{R}^2 \) exists and Theorem 3.1 provides heat parametrices. Then

\[
K^\pm(t, x, y) = K(t, x, y) \mp K(t, x, Ry)
\]

are heat kernels for the Dirichlet- or Neumann problem on \( H_+ \), respectively. The same construction applies to heat parametrices. Their diagonals are

\[
k^\pm_N(t, x, x) = \frac{1}{4\pi t} \sum_{k=0}^{N+1} (u_k(x, x) \mp e^{-\frac{x_2^2}{4t}} u_k(x, Rx)) t^k.
\]

14
Hence, following (4.20) the heat trace invariants are given by
\[ a_k^\pm(x) = u_k(x, x) = a_k(x) . \]  
\[ (5.6) \]

One notices that, due to the second term on the right-hand side of (5.5) the knowledge of heat trace invariants for the extended problem on \( \mathbb{R}^2 \) is not sufficient to construct heat trace invariants on \( H_+ \); one rather requires the coefficients of a parametrix. The resulting heat invariants (5.6) for the half-plane, however, are the same as for the entire plane. The reflection in the boundary produces contributions that are exponentially small and, therefore, are not visible in the heat trace invariants. This is a manifestation of Kac’ principle of not feeling the boundary [Kac66].

It may still be of interest to calculate the first terms of (5.5) from (3.3) and (3.36), e.g.,
\[ u_0(x, x) = e^{-x_1^2} u_0(x, x) = 1 \mp \exp \left\{ -\frac{x_1^2}{t} + 2i x_2 \int_0^1 A_2(x_1, (2s - 1)x_2) \, ds \right\} . \]  
\[ (5.7) \]

5.2 Cylinder

An infinite cylinder can be realised as the plane \( \mathbb{R}^2 \) modulo the discrete subgroup \( \Gamma \cong \mathbb{Z} \) of the euclidean group that is generated by the translation \((x_1, x_2) \mapsto (x_1, x_2 + 1)\). Functions on \( \mathbb{R}^2/\Gamma \) are then functions on \( \mathbb{R}^2 \) with \( f(x_1, x_2) = f(x_1, x_2 + 1) \). A scalar potential on the cylinder can be extended periodically to \( \mathbb{R}^2 \) such that \( V(x_1, x_2) = V(x_1, x_2 + 1) \). The same can be done for the magnetic field (5.1). The vector potential, however, has to be chosen in a particular gauge to allow its components to be periodic, too. In a Fourier representation of the magnetic field,
\[ B(x_1, x_2) = \sum_{n \in \mathbb{Z}} B_n(x_1) e^{2\pi i n x_2} , \]  
\[ (5.8) \]
and of the vector potential
\[ A(x_1, x_2) = \sum_{n \in \mathbb{Z}} A_n(x_1) e^{2\pi i n x_2} , \]  
\[ (5.9) \]
one has to ensure that
\[ B_n(x_1) = \frac{\partial A_{n,2}}{\partial x_1}(x_1) - 2\pi i n A_{n,1}(x_1) , \]  
\[ (5.10) \]
which is always possible. The magnetic Schrödinger operator (2.1) with these potentials can then be defined on the domain \( C_0^\infty(\mathbb{R}^2/\Gamma) \) on which it is essentially self-adjoint.

The heat kernel for such a magnetic Schrödinger operator can be constructed from the respective kernel for the periodically extended problem on \( \mathbb{R}^2 \) via
\[ K^{\text{cyl}}(t, x, y) = \sum_{n \in \mathbb{Z}} K(t, x, (y_1, y_2 + n)) . \]  
\[ (5.11) \]
In the same way a heat parametrix results from the respective parametrix of the periodically extended problem in the plane. Its diagonal then is

\[ k_N^{\text{cyl}}(t, x, x) = \frac{1}{4\pi t} \sum_{k=0}^{N+1} \sum_{n \in \mathbb{Z}} e^{-\frac{n^2}{4t}} u_k(x, (x_1, x_2 + n)) t^k. \]  \( (5.12) \)

Hence the heat trace invariants for the cylinder are

\[ a_k^{\text{cyl}}(x) = u_k(x, x) = a_k(x), \]  \( (5.13) \)

since, again, the corrections coming from summing over the translations in \( \Gamma \) are exponentially small.

The first term in \( (5.12) \) can be calculated to give

\[
\sum_{n \in \mathbb{Z}} e^{-\frac{n^2}{4t}} u_0(x, (x_1, x_2 + n)) = \sum_{n \in \mathbb{Z}} \exp\left\{-\frac{n^2}{4t} - in \int_0^1 A_2(x_1, x_2 + n(1-s)) \, ds\right\} \\
= 1 + \sum_{n \in \mathbb{Z} \setminus \{0\}} \exp\left\{-\frac{n^2}{4t} - in \int_0^1 A_2(x_1, x_2 + n(1-s)) \, ds\right\},
\]

\( (5.14) \)

thus making the exponentially small correction explicit.

5.3 Torus

A torus can be represented as \( \mathbb{R}^2/\Gamma \) in analogy to the cylinder above, however, with a discrete subgroup \( \Gamma \cong \mathbb{Z}^2 \) of the euclidean group that is generated by the two translations \( (x_1, x_2) \mapsto (x_1, x_2 + 1) \) and \( (x_1, x_2) \mapsto (x_1 + 1, x_2) \). Functions on \( \mathbb{R}^2/\Gamma \) can be identified with functions on \( \mathbb{R}^2 \) via \( f(x) = f(x + n) \) for all \( n \in \mathbb{Z}^2 \). The scalar potential and the magnetic field can be chosen periodically on \( \mathbb{R}^2 \), the vector potential, however, does not allow such a choice. A Fourier representation of the magnetic field,

\[ B(x) = \sum_{n \in \mathbb{Z}} B_n e^{2\pi i n \cdot x}, \]  \( (5.15) \)

and of the vector potential

\[ A^{\text{per}}(x) = \sum_{n \in \mathbb{Z}} A_n e^{2\pi i n \cdot x}, \]  \( (5.16) \)

shows that the constant term \( B_0 \) (which equals the flux \( \Phi \) through the torus) cannot be represented in terms of the periodic vector potential. It requires an additional linear contribution \( A^0(x) \) that generates \( B_0 \), hence a constant magnetic field on \( \mathbb{R}^2 \). This is related to the flux quantisation on the torus, i.e., the fact that \( B_0 = \Phi = 2\pi n \), where \( n \in \mathbb{Z} \).
The construction of the heat kernel for the magnetic Schrödinger operator, the heat parametrix and the heat invariants is closely analogous to the case of the cylinder, i.e.,

\[
K_{\text{torus}}(t, x, y) = \sum_{n \in \mathbb{Z}^2} K(t, x, y + n),
\]

leading to the diagonals of parametrices

\[
k_N^{\text{torus}}(t, x, x) = \frac{1}{4\pi t} \sum_{k=0}^{N+1} \sum_{n \in \mathbb{Z}^2} e^{-\frac{n^2}{4t}} u_k(x, x + n) t^k.
\]

The heat trace invariants for the torus, therefore, are

\[
a_k^{\text{torus}}(x) = u_k(x, x) = a_k(x),
\]

since, as for the cylinder the corrections coming from summing over the translations in \( \Gamma \) are exponentially small. Explicitly, the first term in (5.18) is

\[
\sum_{n \in \mathbb{Z}^2} e^{-\frac{n^2}{4t}} u_0(x, x + n) = \sum_{n \in \mathbb{Z}^2} \exp\left\{-\frac{n^2}{4t} - i \int_0^1 n \cdot A(x + (1 - s)n) \, ds\right\}
\]

\[
= 1 + \sum_{n \in \mathbb{Z}^2 \setminus \{0\}} \exp\left\{-\frac{n^2}{4t} - i \int_0^1 n \cdot A(x + (1 - s)n) \, ds\right\}.
\]

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