# Dia- and paramagnetism for nonhomogeneous magnetic fields

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**Abstract**

Diamagnetism of the magnetic Schrödinger operator and paramagnetism of the Pauli operator are rigorously proven for nonhomogeneous magnetic fields in the large field, in the large temperature and in the semiclassical asymptotic regimes. New counterexamples are presented which show that neither dia- nor paramagnetism are true in a robust sense (without asymptotics). In particular, we demonstrate that the recent diamagnetic comparison result by Loss and Thaller [1] is essentially the best one can hope.

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# Contents



# 1 Introduction

We consider a single electron subject to a nonhomogeneous magnetic field $B(x)$ and an external potential $V(x)$, $x \in \mathbf{R}^d$. The magnetic field is generated by a vectorpotential $\mathbf{A}$, which is a 1-form (canonically identified with a vectorfield), and the magnetic field $B := \mathrm{d}\mathbf{A}$ is a 2-form. Its *pointwise strength* is defined as $\|B(x)\| := \mathrm{Tr}|\mathcal{B}(x)| = \sum_{j=1}^{[d/2]} |B_j(x)|$, where $\mathcal{B}(x)$ is the skew-symmetric matrix with entries $(\frac{1}{2}B(x)(e_\alpha, e_\beta))_{\alpha,\beta=1}^d$ (for any orthonormal basis $\{e_\alpha\}_{\alpha=1}^d$) with eigenvalues $\pm\frac{1}{2}iB_j(x)$ (in odd dimensions there is an extra zero eigenvalue). Here [ ] denotes the integer part. We will also need the *local energy norm* of the magnetic field, defined as $\|B(x)\|_2 = \Big(\mathrm{Tr}|\mathcal{B}(x)|^2\Big)^{1/2} = \Big(\sum_j |B_j(x)|^2\Big)^{1/2}$.

The Hamiltonian of this system is either the Pauli operator

$$H_{Pauli}(B,V) := [\boldsymbol{\sigma}\cdot(-i\nabla - \mathbf{A})]^2 + V \tag{1.1}$$

or the Schrödinger operator

$$H_{Sch}(B,V) := (-i\nabla - \mathbf{A})^2 + V,$$

depending on whether the electron is considered with or without spin. In the first case the underlying Hilbert space is the space of spinors $L^2(\mathbf{R}^d, \mathbf{C}^2) = L^2(\mathbf{R}^d) \oplus L^2(\mathbf{R}^d)$, while in the second case it is the usual $L^2(\mathbf{R}^d)$. We fix the representation of Pauli matrices, i.e.

$$\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3) = \left( \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right).$$

We shall consider the Pauli operator only in $d = 2, 3$, while the Schrödinger operator shall be treated in any dimension $d \geq 2$ for most of our results.

In $d = 2$ the Pauli operator uses only the first two Pauli matrices and it decouples in the spin space as follows

$$H_{Pauli}(B, V) = \Big(H_{Sch}(B, V) - B\Big) \bigoplus \Big(H_{Sch}(B, V) + B)\Big) = \Big(H_{Sch}(B, V - B)\Big) \bigoplus \Big(H_{Sch}(B, V + B)\Big). \tag{1.2}$$

In $d = 3$ the magnetic field $B = \mathrm{d}\mathbf{A}$ can be identified with a vectorfield $\mathbf{B}$ and

$$H_{Pauli}(\mathbf{B}, V) = (-i\nabla - \mathbf{A})^2 - \boldsymbol{\sigma} \cdot \mathbf{B} + V. \tag{1.3}$$

Note that we slightly abused the notation, as these operators depend on the vectorpotential and not just on the magnetic field, but all our statements will be gauge invariant, therefore depend only on the field.

The goal of our work is to investigate the monotonicity of these operators in terms of the physical data; the magnetic field and the external potential. The potential is just a function on $\mathbf{R}^d$, so we can easily introduce a (partial) ordering; we say that $V_1$ is smaller than $V_2$ if $V_1(x) \leq V_2(x)$ for all $x \in \mathbf{R}^d$,

Magnetic fields can be ordered in three ways. $B_1$ is smaller than $B_2$ in the sense of pointwise strength or local energy norm if $\|B_1(x)\| \leq \|B_2(x)\|$ or $\|B_1(x)\|_2 \leq \|B_2(x)\|_2$ (for all $x \in \mathbf{R}^d$), respectively. Finally we say that $B_1$ is smaller than $B_2$ as a 2-form if $|\mathcal{B}_1(x)| \leq |\mathcal{B}_2(x)|$ as nonnegative matrices for all $x$. Note that all these comparisons coincide in $d = 2$ and in $d = 3$ if the magnetic fields have the same constant direction. The first two notions coincide in $d = 3$ for any field.

Now we define various (partial) orderings of selfadjoint operators. Here are some possibilities to say that an operator $H_2$ majorizes $H_1$ (assuming that both are semibounded, defined on $L^2(\mathbf{R}^d)$ and the kernels below exist)

- (I.) (Operator sense): $H_1 \leq H_2$;
- (II.) (Heat kernel pointwise): $|\exp(-tH_2)(x, y)| \leq |\exp(-tH_1)(x, y)|$ for all $x, y \in \mathbf{R}^d$, $t > 0$;

- (III.) (Heat kernel diagonal pointwise): $\exp(-tH_2)(x,x) \le \exp(-tH_1)(x,x)$ for all $x \in \mathbf{R}^d$, $t > 0$;
- (IV.) (Trace of the heat kernel): $\mathrm{Tr}\exp(-tH_2) \le \mathrm{Tr}\exp(-tH_1)$ for all $t > 0$;
- (V.) (Infimum of the spectrum): $\inf \mathrm{Spec} H_1 \le \inf \mathrm{Spec} H_2$;
- (VI.) (Heat kernel $L^p \to L^q$-norm): $\|\exp(-tH_2)\|_{p,q} \le \|\exp(-tH_1)\|_{p,q}$ $(1 \le p \le q \le \infty)$.

In the case of the Pauli operator we shall always consider the partial trace, $\mathrm{Tr}_{\mathbf{C}^2}$, with respect to the spin variables to reduce it to an operator on $L^2(\mathbf{R}^d)$.

Obviously these definitions are related; some of them imply some others (for example $(II.) \Longrightarrow (III.) \Longrightarrow (IV.) \Longrightarrow (V.)$). From physical point of view $(I.), (IV.)$ and $(V.)$ are the most important ones.

If the magnetic field is zero, then the following statement is well known:

**Proposition 1.1** *Assume that $V_1 \le V_2$ pointwise. Then $H_2 = -\Delta + V_2$ majorizes $H_1 = -\Delta + V_1$ in any of the senses above in any dimension.*

Perhaps the easiest proof uses the Feynman-Kac formula for $H = -\Delta + V$:

$$e^{-tH}(x,y) = p_d(t,x,y)\mathbf{E}_{0,x}^{2t,y} e^{-\frac{1}{2}\int_0^{2t} V(W_s)ds}$$

where $p_d(t,x,y) = (4\pi t)^{-d/2}\exp(-(x-y)^2/4t)$ is the heat kernel of the $d$-dimensional Laplacian and $\mathbf{E}_{0,x}^{2t,y}$ denotes the expectation with respect to the measure of the Brownian bridge $\{W_{0\le s\le 2t} : W(0) = x, W(2t) = y\}$. To show $(VI.)$, one also uses the positivity preserving property of the heat kernel. $\square$

A naive way to summarize this proposition is to say that the energy increases as the external potential increases.

Our goal is to find analogous statements if the magnetic field increases. Due to the coupling between the spin and the magnetic field, the Schrödinger and Pauli operators can and will behave differently. Though Feynman-Kac formula (under various conditions, see [2, 3]) is still available,

$$e^{-tH_{Sch}(B,V)}(x,y) = p_d(t,x,y)\mathbf{E}_{0,x}^{2t,y} e^{-i\int_0^{2t}\mathbf{A}(W_s)\circ \mathrm{d}W_s - \frac{1}{2}\int_0^{2t} V(W_s)ds} \tag{1.4}$$

(and similarly for $H_{Pauli}$, see [4], [5], [6]); the heat kernel is neither positive nor positivity preserving any more, which makes pathwise estimates impossible ($\circ$ denotes the Stratanovich stochastic integral).

Nevertheless, one can formulate naive conjectures:

*Diamagnetic conjecture:* The Schrödinger operator "increases" as the magnetic field increases pointwise.

*Paramagnetic conjecture:* The Pauli operator "decreases" as the magnetic field increases pointwise.

Several arguments support these conjectures. The simplest one is based upon explicit formulas for the diagonal element of the corresponding heat kernel for constant magnetic field and zero potential. This quantity is of physical interest as it expresses the local energy density at positive temperature. We have, in $d = 2$,

$$e^{-tH_{Sch}(B=const,V=0)}(x,x) = \frac{B}{4\pi \sinh Bt} \tag{1.5}$$

and

$$\mathrm{Tr}_{\mathbf{C}^2} e^{-tH_{Pauli}(B=const,V=0)}(x,x) = \frac{B\cosh Bt}{2\pi \sinh Bt}, \tag{1.6}$$

which are easily seen to be decreasing and, respectively, increasing functions of $|B|$.

There also have been various asymptotic calculations, in particular both conjectures have been checked in the semiclassical and in the weak field limits (perhaps the best modern reference is [7]; for classical references, see [8]).

It turns out that the picture is much more complicated and none of these conjectures are correct in such a robust way as in the nonmagnetic case. In this paper we prove some related results, we present new counterexamples which show that certain natural conjectures are false and we formulate open questions. The highlights of the paper are the following.

We prove both conjectures in the short time (large temperature) limit (which will include the semiclassical asymptotics as well) and we show that the local energy norm, $\|B(x)\|_2$ determines the ordering (Sections 2.3, 3.1).

We also verify these conjectures in the large field limit, but the paramagnetic conjecture is proven only in a weaker sense (ground state result). In contrast to the short time, in the case of the large field limit the field strength $\|B(x)\|$ determines the ordering (Sections 2.4, 3.2).

Finally we investigate whether these conjectures hold in a robust sense, i.e. without any limiting procedure. The answer is essentially no, and we demonstrate it via various counterexamples. In particular, we show that the recent result by Loss and Thaller [1] (which is the only nontrivial robust comparison result for nonhomogeneous fields) is essentially the best one could hope; its several possible extensions are incorrect (Sections 2.5, 2.6, 3.3).

Physically, our results concern either a single charged particle or a noninteracting system with Bose statistics (recall that the trace of the heat kernel is the positive temperature partition function). As to noninteracting fermions, we remark that monotonicity (even for constant field) is not expected by the well-known de Haas–van Alphen effect. More interestingly, the flux phase phenomenon shows that, at a high density of fermions, the Schrödinger operator can be paramagnetic. This has been proven rigorously on a finite lattice (in the Hubbard model) by Lieb [9] (see also the earlier paper by Lieb and Loss [10] for some special planar graphs).

# 2 Diamagnetism for the Schrödinger operator

The standard diamagnetic inequality compares $H_{Sch}(B, V)$ with $H_{Sch}(B = 0, V)$ (see [11, 12, 2]) in sense $(II.)$ i.e. one obtains, in any dimension, that

$$\left|e^{-tH_{Sch}(B,V)}(x, y)\right| \le \left|e^{-tH_{Sch}(B=0,V)}(x, y)\right|. \tag{2.1}$$

The proof is obvious from the Feynman-Kac formula. From this, the corresponding relations $(III.), (IV.), (V.)$ immediately follow, and noting again that the heat kernel of $H_{Sch}(B = 0, V)$ is positive and positivity preserving, we obtain $(VI.)$ as well.

A natural generalization would be to consider two magnetic fields, $B_1, B_2$, the corresponding operators $H_i = H_{Sch}(B_i, V)$, and ask whether $H_2$ majorizes $H_1$ in some sense if $B_2$ majorizes $B_1$ in some sense.

## 2.1 Constant field

If both $B_1$ and $B_2$ are *constant* and $V = 0$, then the heat kernels can be compared explicitly, as they are given by the Mehler kernel (in $d = 2$ see [2, p. 168], in higher dimensions the generalization is straightforward). Any constant 2-form $B$ can be written as

$$B = \sum_{j=1}^{[d/2]} B_j \mathrm{d}x_{2j-1} \wedge \mathrm{d}x_{2j} \tag{2.2}$$

with some constants $B_j = B_{2j-1,2j} \ge 0$ in an appropriate coordinate system $\{x_1, x_2, \ldots x_d\}$, with orthonormal basis vectors $\{e_1, e_2, \ldots e_d\}$, where $B_{\alpha,\beta} = B(e_\alpha, e_\beta)$. Note that in this basis $B_{\alpha,\beta} = 0$ unless $\{\alpha, \beta\} = \{2j - 1, 2j\}$ for some $1 \le j \le [d/2]$ and $B_{2j-1,2j} = -B_{2j,2j-1}$. Then the Mehler kernel is

$$e^{-tH_{Sch}(B=const,V=0)}(x, y) = p_1(t, x_{2[d/2]+1}, y_{2[d/2]+1}) \tag{2.3}$$

$$\times \prod_{j=1}^{[d/2]} \frac{B_j}{4\pi \sinh B_j t} \exp\Big(-\frac{B_j[(x_{2j-1}-y_{2j-1})^2+(x_{2j}-y_{2j})^2]}{4}\coth(B_j t)+i\frac{B_j}{2}(x_{2j}y_{2j-1}-x_{2j-1}y_{2j})\Big)$$

in the standard gauge

$$\mathbf{A}(x) = \sum_{j=1}^{[d/2]} \frac{B_j}{2}(x_{2j-1}\mathrm{d}x_{2j} - x_{2j}\mathrm{d}x_{2j-1}). \tag{2.4}$$

The first factor (one dimensional free heat kernel) is present only in odd dimension. Since the functions $x \to x/\sinh x$ and $x \to -x\coth x$ both are monotonically decreasing, so the comparison $(II.)$ (therefore $(III.), (IV.)$ and $(V.)$ as well) follows if the magnetic fields are ordered in the sense of 2-forms.

Because of the lack of positivity, the comparison $(VI.)$ is not trivial any more. In two dimensions, due to a theorem of E. Lieb about Gaussian kernels ([13]), when computing the norm $\|e^{-tH_{Sch}(B,V=0)}\|_{p,q}$, it is enough to maximize $\sup_u \|e^{-tH_{Sch}(B,V=0)}u\|_p/\|u\|_q$ over Gaussian functions $u$ (here we assume that $1 < p \le q < \infty$). This idea enabled Loss and Thaller [1, Theorem 1.1] to compute all these heat kernel norms explicitly. Moreover, they proved a more general statement (Theorem 1.2) from which comparison $(VI.)$ follows under certain conditions on $p, q, B_1$ (if $p < q < 2$ or $2 < p < q$ then $B_1 t$ should be small enough, for $p \le 2 \le q$ there is no restriction on $B_1 t$). For the constant field case, one could try to verify $(VI.)$ directly just by showing that $\frac{\partial}{\partial B_1}\|e^{-tH(B_1)}\|_{p,q} \le 0$ where $\|e^{-tH(B_1)}\|_{p,q}$ is given in Theorem 1.1 of [1]. This is a horrendous, though elementary computation, which we could carry out only for the case $p = q$. The general case is still open, though various special cases and numerical examples leave no doubt on its validity. We remark that the theorem by Loss and Thaller settles this question in the cases when it applies.

## 2.2 Nonhomogeneous field

Now we turn to the case of nonhomogeneous fields $B_1$ and $B_2$, such that $B_1$ is "smaller" than $B_2$ in some of the senses discussed above. The main reason, apart from (1.5) mentioned above, why one expects that $H_1 = H_{Sch}(B_1, V)$ is majorized by $H_2 = H_{Sch}(B_2, V)$ in senses $(II.) - (VI.)$ is the stochatic phase factor $\int_0^{2t} \mathbf{A}(W_s) \circ \mathrm{d}W_s$ in the Feynman-Kac formula (1.4). By Stokes theorem (recall that the Stratanovich integral allows one to use standard calculus), intuitively this integral is equal to a constant (depending on the gauge) plus the random magnetic flux (area integral of the magnetic field, counted with sign and mulitplicity) within the stochastic domain bounded by the straight segment joining $x, y$ and by the Brownian bridge $W_s$ (strictly speaking this area integral is not defined directly, rather by the line integral above). This suggests that if the magnetic field pointwise increases, then the oscillatory effect due to this phase factor should increase, which in turn should decrease the value of the expectation.

A natural simplification is to introduce large or small scaling parameters in the magnetic field and/or in the time. The semiclassical and the weak field limits were studied in [7]. One can also study the strong field limit for the operator $\exp(-tH_{Sch}(LB, V = 0)) = \exp(-t(-i\nabla - L\mathbf{A})^2)$, where $B$ is a fixed magnetic field and $L$ is a large parameter (note that large $L$ *along with* small time of order $L^{-2}$ is equivalent to the semiclassical limit).

First we investigate the short time case, where $\|B(x)\|_2$ determines the ordering. In particular, this includes the semiclassical limit with the result obtained in [7] but our approach is more general and mathematically rigorous (a rigorous proof of the main term in the semiclassical limit is found in [14], but this is not enough to deduce comparison). Then we study the strong field limit. In Section 2.5 we present a counterexample showing that the naturally expected general form of the diamagnetic conjecture is wrong. Finally we show that the expected robust offdiagonal bound (see the remark after Theorem 1.3 [1]) is wrong as well.

## 2.3 Short time and semiclassics

We shall consider short time and (possibly) strong field simultaneously under the constraint that $tL \to 0$ ($L \geq 1$ is the scaling parameter of the field). In particular, this includes the semiclassical limit with $t =: \beta h^2$, $L := h^{-1}$ where $\beta$ is the inverse temperature and $h$ is the semiclassical parameter (Planck constant). Therefore all our results include the corresponding semiclassical statements by a simple change of parameters, $(t, L) \leftrightarrow (\beta, h)$, but we keep using $t$ and $L$ and we do not formulate each statement twice.

In the case of the short time asymptotics ($t \to 0$), the oscillatory effect goes to zero as the Brownian loop converges to a point. This is even valid if only $Lt \to 0$ is assumed. Spectrally this corresponds to a Weyl type large energy asymptotics, which is proven even with including nonzero external potential. The earliest theorem, which includes the effect of the magnetic field in a nontrivial way, is perhaps due to [15] (see also [16]), and later Matsumoto got more precise results [17, 18, 19, 20]. For example, Proposition 2.1 in [19] states, under some general conditions, that

$$\operatorname{Tr} e^{-tH_{Sch}(B,V)} = (4\pi t)^{-d/2}(1 + o(1)) \int e^{-tV(x)} \prod_{j=1}^{[d/2]} \frac{tB_j(x)}{\sinh tB_j(x)} \mathrm{d}x$$

as $t \to 0$, where, as before, $\pm\frac{1}{2}iB_j(x)$ are the eigenvalues of the skew-symmetric matrix $\mathcal{B}(x) = \frac{1}{2}B(x)(e_\alpha, e_\beta)$ (and there is an extra zero eigenvalue in odd dimensions). This statement does not yet imply majorization in sense (*III.*) or (*IV.*) for short times, unless the error term can be effectively controlled.

Since the work of Matsumoto aimed at eigenvalue asymptotics, neither pointwise heat kernel results nor precise controll of the error terms were emphasized. Nevertheless, the proof of the following statement is close to the spirit of [17], though it requires slightly finer estimates. To keep the proof short, we are not looking for the most general conditions (especially we do not investigate increasing magnetic fields which were Matsumoto's main concern), but due to the localization given by the short time, the extensions are obvious.

**Proposition 2.1** *Let $V$ be semibounded, continuously differentiable, let $\|B\|_\infty + \|\nabla B\|_\infty < \infty$, and let $L \geq 1$ be a scaling parameter, then for any $x \in \mathbf{R}^d$*

$$e^{-tH_{Sch}(LB,V)}(x,x) = (4\pi t)^{-d/2}(1 + O(t^{5/2}L^2 + t^4L^4))e^{-tV(x)} \prod_{j=1}^{[d/2]} \frac{tLB_j(x)}{\sinh tLB_j(x)} \tag{2.5}$$

$$+\Big(e^{-tH_{Sch}(B=0,V)}(x,x) - e^{-tV(x)}e^{-tH_{Sch}(B=0,V=0)}(x,x)\Big)$$

*as $t \to 0$ and $tL \to 0$. The error depends on the $C^1$-norm of $B$, on $V_0 := \min_{y\in\mathbf{R}^d} V(y)$ and on $\max_{y:\,|y-x|\leq 1} |\nabla V(y)|$.*

*Remark.* If $V \in C^2$, then for the last term we have

$$\Big(e^{-tH_{Sch}(B=0,V)}(x,x) - e^{-tV(x)}e^{-tH_{Sch}(B=0,V=0)}(x,x)\Big) = (4\pi t)^{-d/2}O(t^2) \tag{2.6}$$

with an error depending on $V_0$ and $\max_{y:\,|y-x|\leq 1} |\nabla^2 V(y)|$. Therefore

$$e^{-tH_{Sch}(B,V)}(x,x) = (4\pi t)^{-d/2}(1 + O(t^2 + t^{5/2}L^2 + t^4L^4))e^{-tV(x)} \prod_{j=1}^{[d/2]} \frac{tLB_j(x)}{\sinh tLB_j(x)},$$

but this result is not precise enough for the corollary below.

We have the following comparison in sense $(III.)$ and $(IV.)$:

**Corollary 2.2** *If the magnetic fields $B_1$ and $B_2$ with finite $C^1$-norm satisfy $\|B_1(x)\|_2 < \|B_2(x)\|_2$ and $V$ is semibounded, continuously differentiable, then for any $x$*

$$e^{-tH_{Sch}(LB_1,V)}(x,x) - e^{-tH_{Sch}(LB_2,V)}(x,x) \geq C^*(4\pi t)^{-d/2}e^{-tV(x)}t^2L^2(\|B_2(x)\|_2^2 - \|B_1(x)\|_2^2) > 0, \tag{2.7}$$

*for some constant $C^*$ and for small enough $tL \leq \varepsilon_0$, $t \leq \varepsilon_0$, where $\varepsilon_0, C^*$ depend on the $C^1$-norm of $B_1, B_2$, on $V_0 = \min_{y\in\mathbf{R}^d} V(y)$ and on $\max_{y:|y-x|\leq 1} |\nabla V(y)|$. If, in addition, $\int \exp(-tV(x))\mathrm{d}x$ is finite for all $t > 0$ and the $C^1$ norm of $V$ is finite, then comparison in sense $(IV.)$ is valid as well for small enough $t$.*

The proof of (2.7) is obvious from $X/\sinh X = 1 - X^2/6 + O(X^4)$. In particular, $C^* \to 1/6$ as $tL \to 0$ and $t \to 0$. The trace inequality follows from the fact that, under the stronger condition $\|V\|_\infty + \|\nabla V\|_\infty < \infty$, $\varepsilon_0$ can be chosen uniformly for all $x$.

*Remark.* From Propositions 1.1 and 2.1 it is obvious that the diamagnetic comparison in sense (*III.*) and (*IV.*) is true more generally if we allow different potentials $V_1 \le V_2$ in the operators $H_{Sch}(LB_i, V_i)$ to be compared $(i = 1, 2)$.

*Proof of Proposition 2.1.* Since $B$ and $V$ are continuously differentiable, the existence of the diagonal element of the heat kernel follows from general continuity results for the heat kernels (for the best available result see [21], but the present case is essentially covered in [5]). For notational symplicity we can assume that $x = 0$, and by adding a constant it is enough to consider $V(x) = V(0) = 0$. We choose a coordinate system in which the constant magnetic field $B(0)$ has the form given in (2.2). Let $\mathbf{A}_0$ be the standard gauge generating $B(0)$ (see (2.4)), i.e.

$$\mathbf{A}_0(x) := \sum_{j=1}^{[d/2]} \frac{B_{2j-1,2j}(0)}{2} \Big[x_{2j-1}\mathrm{d}x_{2j} - x_{2j}\mathrm{d}x_{2j-1}\Big]. \tag{2.8}$$

Obviously

$$|\mathbf{A}_0(x)| \le C_0|x| \tag{2.9}$$

with some $C_0$ depending on the $C^0$-norm of $B$. By the well known Poincaré formula we can choose a gauge $\mathbf{A}$ for the original magnetic field $B$ as follows

$$\mathbf{A}(x) := \mathbf{A}_0(x) + \sum_{1 \le \alpha < \beta \le d} \Big(\int_0^1 \tau(B_{\alpha\beta}(\tau x) - B_{\alpha\beta}(0))\mathrm{d}\tau\Big)(x_\alpha \mathrm{d}x_\beta - x_\beta \mathrm{d}x_\alpha) \tag{2.10}$$

(see [22]). This gauge satisfies

$$|\mathbf{A}(x) - \mathbf{A}_0(x)| \le C_1|x|^2, \quad |\mathbf{A}(x)| \le C_1|x|, \quad |\mathrm{div}\mathbf{A}(x)| \le C_1|x|, \tag{2.11}$$

where $C_1$ is a constant depending on the $C^1$-norm of $B$. From now on we work in this gauge.

The proof of (2.5) immediately follows from these two lemmas below:

**Lemma 2.3** *With the notations above*

$$\Big|e^{-tH_{Sch}(LB,V)}(0,0) - e^{-tH_{Sch}(LB(0),V)}(0,0)\Big| \le C_2(4\pi t)^{-d/2}(t^{5/2}L^2 + t^4L^4) \tag{2.12}$$

*for $t < 1$ with some $C_2$ depending on $V_0$ and on the $C^1$-norm of $B$.*

**Lemma 2.4** *With the notations above*

$$\Big|e^{-tH_{Sch}(LB(0),V)}(0,0)-e^{-tH_{Sch}(LB(0),V=0)}(0,0)-\Big(e^{-tH_{Sch}(B=0,V)}(0,0)-e^{-tH_{Sch}(B=0,V=0)}(0,0)\Big)\Big|$$

$$\le C_3(4\pi t)^{-d/2}t^3L^2 \tag{2.13}$$

*for* $t<1$ *and with some* $C_3$ *depending on* $B$, $V_0=\min V$ *and* $\max_{|x|\le 1}|\nabla V(x)|$.

We need the following simple technical lemma:

**Lemma 2.5** *For any vectorfield* $\mathbf{F}$, *satisfying* $|\mathbf{F}(x)|\le C|x|^k$ *(with* $k=1,2$*) and* $|div\,\mathbf{F}(x)|\le C|x|$ *we have for* $n\ge 1$

$$\mathbf{E}^{2t,0}_{0,0}\Big|\int_0^{2t}\mathbf{F}(W_s)\circ \mathrm{d}W_s\Big|^n\le C'(t^{n(k+1)/2}+t^{3n/2}) \tag{2.14}$$

*with some* $C'$ *depending on* $C$ *and* $n$.

*Proof of Lemma 2.5.* By Lemma 4.3 from [22],

$$\mathbf{E}^{2t,0}_{0,0}\Big|\int_0^{2t}\mathbf{F}(W_s)\circ \mathrm{d}W_s\Big|^n$$

$$\le 2^{n-1}\Big[\mathbf{E}^{2t,0}_{0,0}\Big(\int_0^{2t}\mathbf{F}(W_s)\mathrm{d}W_s\Big)^{2n}\Big]^{1/2}+2^{n-1}\Big[\mathbf{E}^{2t,0}_{0,0}\Big(\frac12\int_0^{2t}\mathrm{div}\mathbf{F}(W_s)\mathrm{d}s\Big)^{2n}\Big]^{1/2}$$

$$\le c_nt^{n/2}\Big[\mathbf{E}^{2t,0}_{0,0}\frac{1}{2t}\int_0^{2t}|\mathbf{F}(W_s)|^{8n}\mathrm{d}s\Big]^{1/8}+2^{n-1}\Big[\mathbf{E}^{2t,0}_{0,0}\Big(\frac12\int_0^{2t}\mathrm{div}\mathbf{F}(W_s)\mathrm{d}s\Big)^{2n}\Big]^{1/2}$$

with some $n$-dependent constant $c_n$. Using the estimates for $\mathbf{F}$ and div$\mathbf{F}$ and the scaling of the Brownian loop, i.e. $\mathbf{E}^{2t,0}_{0,0}\int_0^{2t}|W_s|^n\mathrm{d}s\sim t^{1+n/2}$, we easily get (2.14). □

*Proof of Lemma 2.3.* By the Feynman-Kac formula, the fact that the diagonal element of the heat kernel is real and that $\mathrm{Re}\,e^{iX}=\cos X=1-X^2/2+O(X^4)$ for any real $X$, we obtain

$$\Big|e^{-tH_{Sch}(LB,V)}(0,0)-e^{-tH_{Sch}(LB(0),V)}(0,0)\Big| \tag{2.15}$$

$$=(4\pi t)^{-d/2}\Big|\mathbf{E}^{2t,0}_{0,0}e^{-\frac12\int_0^{2t}V(W_s)\mathrm{d}s}\mathrm{Re}\Big(e^{-iL\int_0^{2t}\mathbf{A}(W_s)\circ\mathrm{d}W_s}-e^{-iL\int_0^{2t}\mathbf{A}_0(W_s)\circ\mathrm{d}W_s}\Big)\Big|$$

$$=\frac12(4\pi t)^{-d/2}\Big|\mathbf{E}^{2t,0}_{0,0}e^{-\frac12\int_0^{2t}V(W_s)\mathrm{d}s}\Big\{\Big[L\int_0^{2t}\mathbf{A}_0(W_s)\circ\mathrm{d}W_s\Big]^2-\Big[L\int_0^{2t}\mathbf{A}(W_s)\circ\mathrm{d}W_s\Big]^2$$

$$+O\Big(\Big[L\int_0^{2t}\mathbf{A}_0(W_s)\circ\mathrm{d}W_s\Big]^4+\Big[L\int_0^{2t}\mathbf{A}(W_s)\circ\mathrm{d}W_s\Big]^4\Big)\Big\}\Big|.$$

Now we can use Lemma 2.5 to estimate various terms on the right hand side of (2.15). The potential term is estimated by a universal constant $e^{-V_0}$, since $V$ is bounded from below by $V_0$, and $t < 1$ can be assumed. Then, by Lemma 2.5,

$$\mathbf{E}_{0,0}^{2t,0}\Big|\Big(\Big[L\int_0^{2t}\mathbf{A}_0(W_s)\circ \mathrm{d}W_s\Big]^2 - \Big[L\int_0^{2t}\mathbf{A}(W_s)\circ \mathrm{d}W_s\Big]^2\Big)\Big|$$

$$\leq L^2\Big(\mathbf{E}_{0,0}^{2t,0}\Big|\int_0^{2t}(\mathbf{A}-\mathbf{A}_0)(W_s)\circ \mathrm{d}W_s\Big|^2\cdot \mathbf{E}_{0,0}^{2t,0}\Big|\int_0^{2t}(\mathbf{A}+\mathbf{A}_0)(W_s)\circ \mathrm{d}W_s\Big|^2\Big)^{1/2} \leq C_4 t^{5/2}L^2$$

using (2.9) and (2.11), and, furthermore,

$$\mathbf{E}_{0,0}^{2t,0}\Big[L\int_0^{2t}\mathbf{A}(W_s)\circ \mathrm{d}W_s\Big]^4 \leq C_5 t^4 L^4 \tag{2.16}$$

with some $C_4, C_5$ depending on the $C^1$ norm of $B$; and the same estimate is valid for the quartic term containing $\mathbf{A}_0$. Therefore (2.15) yields (2.12) and Lemma 2.3 is proven. □

*Proof of Lemma 2.4.*

$$\Big|e^{-tH_{Sch}(LB(0),V)}(0,0) - e^{-tH_{Sch}(LB(0),V=0)}(0,0) - \Big(e^{-tH_{Sch}(B=0,V)}(0,0) - e^{-tH_{Sch}(B=0,V=0)}(0,0)\Big)\Big| \tag{2.17}$$

$$= (4\pi t)^{-d/2}\Big|\mathrm{Re}\,\mathbf{E}_{0,0}^{2t,0}\Big(e^{-iL\int_0^{2t}\mathbf{A}_0(W_s)\circ\mathrm{d}W_s}-1\Big)\Big(e^{-\frac{1}{2}\int_0^{2t}V(W_s)\mathrm{d}s}-1\Big)\Big|$$

$$= (4\pi t)^{-d/2}\Big|\mathbf{E}_{0,0}^{2t,0}\Big(1-\cos\Big[L\int\mathbf{A}_0\Big]\Big)\Big(e^{-\int V}-1\Big)\Big|,$$

where, for brevity, we used $\int \mathbf{A}_0 := \int_0^{2t}\mathbf{A}_0(W_s)\circ \mathrm{d}W_s$ and $\int V := \frac{1}{2}\int_0^{2t}V(W_s)\mathrm{d}s$.

On the complement of the set $\mathcal{E} := \{\sup_{0\leq s\leq 2t}|W_s| \leq 1\}$ each term can be estimated trivially and we obtain for $t \leq 1$

$$\Big|\mathbf{E}_{0,0}^{2t,0}\chi(\mathcal{E}^c)\Big(e^{-\int V}-1\Big)\Big(1-\cos\Big[L\int\mathbf{A}_0\Big]\Big)\Big| \leq 4e^{-V_0}\mathbf{E}_{0,0}^{2t,0}\chi(\mathcal{E}^c) \leq ce^{-V_0}e^{-c/t} \leq ce^{-V_0}t^3 \tag{2.18}$$

for some universal constant $c$ (using $\int V \geq V_0$ and a standard large deviation estimate for the Brownian loop).

On the set $\mathcal{E}$ we have

$$\Big|\mathbf{E}_{0,0}^{2t,0}\chi(\mathcal{E})\Big(e^{-\int V}-1\Big)\Big(1-\cos\Big[L\int\mathbf{A}_0\Big]\Big)\Big| \tag{2.19}$$

$$\leq L^2\mathbf{E}_{0,0}^{2t,0}\Big[\chi(\mathcal{E})\Big|\int V\Big|e^{-V_0}\Big(\int\mathbf{A}_0\Big)^2\Big] \leq L^2 e^{-V_0}\Big[\mathbf{E}_{0,0}^{2t,0}\chi(\mathcal{E})\Big(\int V\Big)^2\cdot\mathbf{E}_{0,0}^{2t,0}\Big(\int\mathbf{A}_0\Big)^4\Big]^{1/2}$$

using that $V_0 \leq 0$ and that $|1-\cos X| \leq \frac{1}{2}X^2$ and $|e^{-X}-1| \leq 2|X|\exp(-\min\{X,0\})$ for any real $X$. For the second factor we use (2.14) to get $O(t^4)$ (see (2.16)). In the first factor we estimate $|V(W_s)| \leq |W_s| \sup_{|x|\leq 1} |\nabla V(x)|$ on the set $\mathcal{E}$ (recall that $V(0)=0$). The result is

$$\Big|\mathbf{E}^{2t,0}_{0,0}\chi(\mathcal{E})\Big(e^{-\int V}-1\Big)\Big(1-\cos\Big[L\int \mathbf{A}_0\Big]\Big)\Big| \leq C_6 t^{7/2} L^2$$

where $C_6$ depends on $V_0$ and on the $C^1$-norm of $B$ and on $\sup_{|x|\leq 1}|\nabla V(x)|$, and Lemma 2.4 is proven, which also completes the proof of Proposition 2.1. $\square$

*Proof of (2.6).* (See the remark after Proposition 2.1.) Here one has to estimate $\mathbf{E}(e^{-\int V} - 1)$. On the set $\mathcal{E}^c$ the most trivial estimate (2.18) works. Then one can easily verify that on the set $\mathcal{E}$,

$$\Big|e^{-\int V} - 1 + \int V\Big| \leq C_7\Big(\int V\Big)^2 \leq C_8\Big(\int |W_s|\mathrm{d}s\Big)^2,$$

and therefore

$$\mathbf{E}^{2t,0}_{0,0}\chi(\mathcal{E})\Big|e^{-\int V} - 1 + \int V\Big| \leq C_9 t^3$$

with some $C_7, C_8, C_9$ depending on $V_0$ and $\max_{|x|\leq 1}|\nabla V(x)|$.

Finally, for the term $\int V$ we use $V(W_s) = \nabla V(0)\cdot W_s + C_{10}|W_s|^2$ on the set $\mathcal{E}$ and the fact that by the $W_s \to -W_s$ symmetry

$$\mathbf{E}^{2t,0}_{0,0}\chi(\mathcal{E})\int_0^{2t} W_s \mathrm{d}s = 0, \tag{2.20}$$

to get

$$\Big|\mathbf{E}^{2t,0}_{0,0}\chi(\mathcal{E})\int V\Big| \leq C_{11}t^2.$$

Here $C_{10}, C_{11}$ depends on $\max_{y:\,|y-x|\leq 1}|\nabla^2 V(y)|$. $\square$

## 2.4 Large time and/or large field asymptotics

The large time and/or large field asymptotics of the heat kernel is typically harder since the oscillation (the flux encircled by the Brownian bridge) is big. In $d=2$ it is easy to see that

$$\inf \mathrm{Spec} H_{Sch}(B, V=0) \geq \mathrm{Ess}\inf_{x\in\mathbf{R}^2} B(x)$$

since $H_{Sch}(B, V=0) - B$ is a nonnegative operator (being one component of the Pauli operator). By variational principle, using a very localized Gaussian trial function (see later), one can easily get for a $C^1$ field $\lim_{L\to\infty} L^{-1}\inf \mathrm{Spec} H_{Sch}(LB, V=0) = \inf_{x\in\mathbf{R}^2} B(x)$, which shows that comparison $(V.)$ is true in the large field limit.

From now on we discuss any dimension $d \geq 2$ and the final result of this section will be summarized in Theorem 2.8.

Based upon the Gaussian type localization due to a strong magnetic field, one expects that the ground state is again given by the infimum of the magnetic field, at least in the strong field limit. The first theorem in this direction is due to Malliavin [23], proving that in $d = 3$

$$\liminf_{L\to\infty} \frac{1}{L} \inf Spec H_{Sch}(LB, V=0) \geq e^{-1} \inf_{x\in\mathbf{R}^3} \|B(x)\|.$$

Note that this result is off by a factor of $e^{-1}$ from our expectation. With similar technique Malliavin also proved an $L^\infty$ result (see [24]):

$$\limsup_{t\to\infty} \frac{1}{t} \log \|e^{-tH_{Sch}(LB,V=0)}\|_{\infty\to\infty} \leq -\Phi(C) L \inf_{x\in\mathbf{R}^3} \|B(x)\|$$

for curl-free magnetic fields $B(x)$, $0 < \inf \|B(x)\| \leq \|B(x)\| \leq C \inf_x \|B(x)\|$, with some function $0 < \Phi(C) < 1$.

Later the optimal constant was obtained in any dimension for any $L^p \to L^q$ norm ($1 \leq p \leq q \leq \infty$) in the large field limit for a $C^1$ magnetic field with a $C^1$ strength and with uniform positive lower bound, i.e. $\|B\| \geq C > 0$ (see [22]):

$$\frac{1}{t} \log \|e^{-tH_{Sch}(LB,V=0)}\|_{p\to q} \leq -C_L L \inf_{x\in\mathbf{R}^d} \|B(x)\| + O\Big(t^{-1}(1 + |\log t|)\Big) \tag{2.21}$$

with some constant $C_L = 1 - O(L^{-\alpha} \log L)$ as $L \to \infty$, for some explicit $0 < \alpha < 1/4$, $t \geq L^{-\alpha}$; and the constants in the error terms depend only on the dimension, on $p, q$ and on the $C^1$ norm of the field. In this section by $C^1$ field we mean that $B(x)(e_\alpha, e_\beta)$ (for all $\alpha, \beta$) and $\|B(x)\|$ must be $C^1$ functions. [The condition $t \geq L^{-\alpha}$ can be easily removed but then the error term is replaced by $O(t^{-1}(1 + |\log t|) \log L)$. For, one can notice that $tL^\alpha$ should be replaced by $\max\{1, tL^\alpha\}$ on the right hand side of (9) of [22], and the proof goes through without any changes.]

For the infimum of the spectrum (from which the $L^2 \to L^2$ heat kernel estimate follows), the following better estimate was proven in [25, Theorem 3.1]

$$\frac{1}{L} \inf \mathrm{Spec}\, H_{Sch}(LB, V=0) \geq \inf_x \|B(x)\| - CL^{-1/4} \tag{2.22}$$

with some constant $C$ for large enough $L$.

Note that (2.21) is only a one sided estimate, but we claim a similar lower bound:

**Proposition 2.6** *For a $C^1$ magnetic field $B$ with uniform positive lower bound we have*

$$\frac{1}{t}\log\|e^{-tH_{Sch}(LB,V=0)}\|_{p\to q} \geq -D_L L \inf_{x\in\mathbf{R}^d}\|B(x)\| - O\Big(t^{-1}(1+|\log t|)\Big) \tag{2.23}$$

*with some $D_L = 1 + O(L^{-1/4}\log L)$ as $L\to\infty$,*

*Proof.* For $p=q=2$ (2.23) follows from

$$\inf \mathrm{Spec} H_{Sch}(LB, V=0) \leq L(1+CL^{-1/4}) \inf_{x\in\mathbf{R}^d}\|B(x)\| \tag{2.24}$$

with some $C$ depending only on $B$. Combining it with (2.22) we get

$$\lim_{L\to\infty}\frac{1}{L}\inf\mathrm{Spec}\, H_{Sch}(LB, V=0) = \inf_x \|B(x)\|, \tag{2.25}$$

in particular, the comparison in sense ($V$.) is true in the strong field limit.

The bound (2.24) was proven in [25] even with a better error term ($CL^{-1/3}$ instead of $CL^{-1/4}$). In its simpler form it was also essentially proven in [26] by constructing a suitable trial function (there the error term was slightly worse and the computation longer because the authors focused on low lying eigenvalues as well, not just on the lowest one, see Theorem 11.1). Here, for completeness, we just give the simple trial function ([25] used an approximation which is one order better).

Let $x^{(0)}$ be a point such that $\|B(x^{(0)})\| = \min_{x\in\mathbf{R}^d}\|B(x)\|$, we can assume that $x^{(0)}=0$. Let $L^{-1/2} < \varepsilon_L < 1$ and define

$$f_L(x) = \exp\Big(-\frac{1}{2\varepsilon_L^2}\sum_{j=2r+1}^{d} x_j^2\Big)\prod_{j=1}^{r}\exp\left(-\frac{LB_j(0)}{4}[x_{2j-1}^2 + x_{2j}^2]\right) \tag{2.26}$$

using a coordinate system in which the constant 2-form, which is equal to $B(0)$ everywhere, has the form $B(0) = \sum_{j=1}^r B_{2j-1,2j}(0)\mathrm{d}x_{2j-1}\wedge \mathrm{d}x_{2j}$ and $B_j(0) := B_{2j-1,2j} > 0$ (here $r$ is the rank of the 2-form $B(0)$).

We can choose a gauge $\mathbf{A}$ for the original magnetic field $B$ such that it satisfies $|\mathbf{A}(x) - \mathbf{A}_0(x)| \leq C'|x|^2$, exactly as in (2.10), where $C'$ is a constant depending on the $C^1$ norm of $B$.

Then by computation (for any $0<\delta_L<1$)

$$(f_L, H_{Sch}(LB, V=0)f_L) \leq (1+\delta_L)L\|B(0)\|\|f_L\|_2^2 + C''(\varepsilon_L^{-2} + \delta_L^{-1}L^2\varepsilon_L^4)\|f_L\|_2^2$$

with some constant $C''$ depending only on $B$. Choose $\varepsilon_L = \delta_L^{1/6}L^{-1/3}$, and $\delta_L = L^{-1/4}$ we obtain (2.24).

This implies that (2.23) is true for $p = q = 2$ with $D_L = 1 + O(L^{-1/4})$, moreover

$$\|e^{-tH} f_L\|_2 \geq \exp\Big(-tL(1 + CL^{-1/4})\|B(0)\|\Big)\|f_L\|_2. \tag{2.27}$$

Hence

$$\|e^{-tH} f_L\|_q = \sup_{g\in L^{q'}} \frac{|(g, e^{-tH} f_L)|}{\|g\|_{q'}} \geq \frac{|(e^{-t\eta_L H} f_L, e^{-tH} f_L)|}{\|e^{-t\eta_L H} f_L\|_{q'}} \geq \frac{\|\exp\Big(-t\frac{1+\eta_L}{2}H\Big) f_L\|_2^2}{\|e^{-t\eta_L H}\|_{q'\to q'}\|f_L\|_{q'}}$$

with the choice $g = e^{-t\eta_L H} f_L$ and with $q'$ being the dual exponent $q/(q-1)$, From this (2.23) easily follows by choosing $\eta_L = L^{-1/4}$, using (2.27), (2.21) and that $|\log\|f_L\|_p| = c\log L$ with some nonzero $c$ depending only on $B$ and $p$. $\square$

Therefore one gets comparison $(VI.)$ in the large field limit for all $t > 0$:

**Corollary 2.7** *For any $1 \leq p \leq q \leq \infty$,*

$$\lim_{L\to\infty} \frac{1}{L}\|e^{-tH_{Sch}(LB_2,V=0)}\|_{p\to q} \leq \lim_{L\to\infty} \frac{1}{L}\|e^{-tH_{Sch}(LB_1,V=0)}\|_{p\to q} \tag{2.28}$$

*for any $B_1, B_2 \in C^1$ fields if $0 < \|B_1(x)\| \leq \|B_2(x)\|$ (in fact only $\inf_{x\in\mathbf{R}^d}\|B_1(x)\| \leq \inf_{x\in\mathbf{R}^d}\|B_2(x)\|$ was needed).*

It is not stated explicitly in [22], but that proof obviously shows that an unscaled smooth semibounded potential can be included without effecting the final result in (2.21) and similarly in (2.28) since its effect vanishes in the $L \to \infty$ limit. The same is valid for the ground state results. For more details about potential and magnetic wells, see [25, 26] and references therein.

Finally, one can easily check from the proof of (2.21) that the comparison in sense $(IV.)$ is also valid in the large field limit if one adds a confining potential $V$. Assume that $V(x) \to \infty$ such that $\exp(-t(-\Delta + V))$ is of trace class for any $t > 0$, then

$$\frac{1}{t}\lim_{L\to\infty} \frac{1}{L}\log \mathrm{Tr}\, e^{-tH_{Sch}(LB(x),V)} = -\inf_{\mathbf{R}^d}\|B(x)\| \tag{2.29}$$

for any $t$. The proof is simple, let $0 < \varepsilon < 1/2$,

$$\begin{aligned} e^{-tH_{Sch}(LB(x),V)} &= e^{-t\varepsilon H_{Sch}(LB(x),V)} e^{-t(1-2\varepsilon)H_{Sch}(LB(x),V)} e^{-t\varepsilon H_{Sch}(LB(x),V)} \\ &\leq \exp\Big(-t(1-2\varepsilon)C_L L \inf_{x\in\mathbf{R}^d}\|B(x)\|\Big) e^{-2t\varepsilon H_{Sch}(LB(x),V)}, \end{aligned} \tag{2.30}$$

where we used (2.22). Then, by the diamagnetic inequality (2.1),

$$\operatorname{Tr} e^{-2t\varepsilon H_{Sch}(LB(x),V)} \leq \operatorname{Tr} e^{-2t\varepsilon(-\Delta+V)}, \tag{2.31}$$

and putting (2.30) and (2.31) together, letting first $L \to \infty$ then $\varepsilon \to 0$ one obtains (2.29).

To summarize our results, we have the following theorem:

**Theorem 2.8** *Assume that $B_1$ and $B_2$ are two $C^1$ magnetic fields such that $0 < \|B_1(x)\| \leq \|B_2(x)\|$ and let $V$ be a smooth semibounded potential. Then the comparisons (IV.), (V.) and (VI.) are true for the operators $H_i = H(LB_i, V)$ in the $L \to \infty$ limit (for (VI.) we need the additional hypothesis that* $\exp(-t(-\Delta + V))$ *is of trace class for all $t > 0$).* □

We remark that for $p = q = 2$ (which is equivalent to the infimum of the spectrum) Ueki in [27] gave a result similar to (2.25) even for manifolds, but without effective error terms (later this was improved in [25]). This establishes comparison in sense ($V.$) even for manifolds. The reason again is that on the effective scale of the magnetic field (which is the size of the cyclotronic radius, and is of order $L^{-1/2}$), the geometry is flat.

It is not clear how to get pointwise comparison (in sense ($II.$) or ($III.$)) from these results. A convenient upper bound on $|\exp(-tH_{Sch}(LB,V))(x,y)|$ is of course the $L^1 \to L^\infty$ norm given in (2.21), but apparently there is no lower bound for offdiagonal elements. Nevertheless we conjecture that the comparison in sense ($III.$) is true (i.e. for diagonal elements):

**Open Problem 2.9** *Prove that*

$$\lim_{L\to\infty} \frac{1}{L} \log e^{-tH_{Sch}(LB_2,V)}(x,x) \leq \lim_{L\to\infty} \frac{1}{L} \log e^{-tH_{Sch}(LB_1,V)}(x,x)$$

*for all $x$ and $t$, for smooth, bounded magnetic fields with* $0 < \|B_1\| \leq \|B_2\|$.

Note that while the previous three comparisons ($IV., V., VI.$) used only the fact that $\inf_x \|B_1(x)\| \leq \inf_x \|B_2(x)\|$, here we expect that the full strength of the condition $\|B_1(x)\| \leq \|B_2(x)\|$ has to be used. This statement is presumably harder than the similar semiclassical limits, as here the effective time is not small. Therefore large loops effectively participate in the Feynman-Kac formula.

## 2.5 Comparison without asymptotics

The most complicated case is when no limiting procedure is involved; we study this case only in $d = 2$ dimensions and we assume that $B(x) \geq 0$. As we pointed out in Section 2.1, comparison of two *homogeneous* magnetic fields, without external potential, is straightforward (except certain $L^p \to L^q$ norms). Therefore, the next natural step is either to relax the homogeneity assumption or to include a potential. The paper [1] by Loss and Thaller followed the first path, and they allowed an inhomogeneous magnetic field for the bigger field $B_2$, but kept the smaller field $B_1$ constant ($0 \leq B_1 = B_1(x) \leq B_2(x)$) and there was no external potential. In this case they managed to prove comparison in sense $(VI.)$ (see Theorem 1.2 of [1]). Their method is very elegant, but apparently there is no way to extend it to cover more general cases (neither to compare two inhomogeneous fields nor include potential). Here we present two counterexamples which show that the theorem by Loss and Thaller is essentially the best one could hope in general. (There was one more, slightly annoying and probably only technical condition in [1], namely in the case when $p < q < 2$ or $2 < p < q$ one has to assume that $B_1 t$ is small. Though it is certainly an interesting question to settle this issue, here we do not focus on it.)

**Counterexample 2.10** *There exist a potential $V$ and two constant magnetic fields $0 < B_1 < B_2$ such that*

$$\inf\ \mathit{Spec} H_{Sch}(B_2, V) < \inf\ \mathit{Spec} H_{Sch}(B_1, V). \tag{2.32}$$

**Counterexample 2.11** *There exists two inhomogeneous magnetic fields $0 \leq B_1(x) \leq B_2(x)$ such that*

$$\inf\ \mathit{Spec} H_{Sch}(B_2, V = 0) < \inf\ \mathit{Spec} H_{Sch}(B_1, V = 0). \tag{2.33}$$

*Remark 1.* Though in the second counterexample we are going to present $B_1(x)$ is not positive everywhere, but from the strict inequality and continuity it follows that $B_1$ could be chosen strictly positive. Also, essentially the same counterexample can show that the monotonicity is not true even in the following weaker sense: there exists a magnetic field $B(x)$ such that $L \mapsto \inf \mathrm{Spec} H_{Sch}(LB, V = 0)$ is not monotone increasing. For brevity we just present the proof of the simplest case formulated above.

*Remark 2.* Obviously these counterexamples show that comparison in sense $(V.)$ cannot be true. This, of course, excludes the comparison in senses $(II.) - (IV.)$ as well, at least for all times (the short time case has been discussed in Section 2.3). Also it shows that the $L^2 \to L^2$ norms of the heat kernels cannot be compared in sense $(VI.)$, which probably would have been expected to be easiest case in a possible extension of [1]. The following interesting case remains open, which is the opposite setup of [1], and where we expect positive answer:

**Open Problem 2.12** *Assume that the bigger field $B_2$ is constant and the smaller one $0 \leq B_1(x) \leq B_2$ is nonhomogeneous. Prove a diamagnetic comparison in some sense.*

The idea behind both counterexamples is the same: we confine the electron (either by a strong electric or magnetic barrier) in a narrow ringshaped domain. It turns out that the ground state energy of the electron depends on whether the total magnetic flux inside the ring is close to $(2\pi)$-times an integer or not. In the second case there is a frustration; on one hand the phase factor of the ground state wave function must change by $(2\pi)$-times an integer as we go around the ring once (since it is a continuous function into $S^1$), on the other hand the magnetic field would favor a phase factor shift close to the total enclosed flux. The continuity requirement could be removed by forcing Dirichlet boundary conditions on a line somewhere across the ring, but this would mean an increase of the energy, too.

In both counterexamples we shall consider a radially symmetric situation, so we fix the notations for both proofs simulteneously. The magnetic field is $B(x) = B(|x|) = B(r)$ using $x = (r, \theta)$ radial coordinates. We choose the radial gauge $\mathbf{A}(r, \theta) := (-a(r)\sin\theta, a(r)\cos\theta)$, with $a(r) := (1/r)\int_0^r B(s)s\mathrm{d}s$ (in the constant field case $a(r) = Br/2$). The potential (in Counterexample 2.10) is also chosen to be radial, $V(x) = V(r)$. We decompose the Hilbert space $L^2(\mathbf{R}^2)$ into angular momentum sectors

$$L^2(\mathbf{R}^2) \cong \mathcal{H} := \bigoplus_{n=-\infty}^{\infty} L^2(\mathbf{R}, 2\pi r\mathrm{d}r), \tag{2.34}$$

$$f \in L^2(\mathbf{R}^2) \mapsto (\dots, f_{-1}, f_0, f_1, \dots) \in \mathcal{H},$$

where $f(r, \theta) = \sum_n e^{in\theta} f_n(r)$. For simplicity, we continue to denote the elements of $\mathcal{H}$ by $f$. In general, $\int f$ will stand for the integral on $\mathbf{R}^2$ with the Lebesgue measure or on $\mathbf{R}_+$ with the measure $2\pi r\mathrm{d}r$, depending on whether the function has one or two variables. We shall integrate radial functions only and then these two notions coincide anyway.

The operator $H_{Sch} = \bigoplus_n H_n$, under the isomophism (2.34), acts on $\mathcal{H}$ as follows

$$(H_{Sch} f)_n(r) := (H_n f_n)(r) := -\Delta f_n(r) + U_n(r) f_n(r) + V(r) f_n(r) \tag{2.35}$$

with $U_n(r) := (n/r - a(r))^2$. Here $-\Delta = -\partial_r^2 - (1/r)\partial_r$ denotes the usual Laplacian on the half line with the domain of the usual two-dimensional Laplacian restricted to the radial functions (in our problem it is convenient to think of $\Delta f_n$ as the radial part of the radially symmetric two-dimensional function $\Delta \tilde{f}_n$ with $\tilde{f}_n(x) := f_n(|x|)$).

We need a well known statement from the general theory of Schrödinger operators whose proof is postponed to the Appendix.

**Lemma 2.13** *(i.) Suppose that $0 \le V_n(x) \nearrow V(x)$ almost everywhere pointwise and all potentials are assumed to be in $L^1_{loc}(\mathbf{R}^d \setminus G)$, where $G$ is a zero measure set. Let us assume* *that the bottom of the spectrum of $-\Delta+V_n$ and $-\Delta+V$ is an eigenvalue, $\lambda_n$ and $\lambda$, respectively. Then*

$$\lambda_n \to \lambda \quad as \quad n \to \infty. \tag{2.36}$$

*(ii.) If $V = \infty$ on an open set $\Omega$ with regular (e.g. smooth) boundary then the statement is still true, provided that $-\Delta + V$ is defined on $L^2(\mathbf{R}^d \setminus \Omega)$ with Dirichlet boundary conditions.*

*Proof of Counterexample 2.10.*

Let $B \geq 1$ be a constant magnetic field. Let $a_n := (2nB^{-1})^{1/2}$ be the unique zero of $U_n$ for $n \geq 0$, then note that $U_n(r) \geq \frac{1}{4}B(r-a_n)^2$ for $n \geq 0$, and $U_n(r) \geq \frac{1}{4}B^2r^2$ for $n < 0$. Let $\mathcal{R} := \{1-\varepsilon \leq |x| \leq 1+\varepsilon\} \subset \mathbf{R}^2$ be a ring ($\varepsilon < 1$ to be chosen later), and let the potential be $V(x) = 2K \cdot \chi(x \notin \mathcal{R})$ with some huge constant $K$ (one can safely think of Dirichlet boundary conditions on $\mathcal{R}$). Here $\chi(\cdot)$ is the characteristic function of a set.

Fix $m \geq 2$ integer and assume that $B$ is such that $a_{m-1} < 1 \leq a_m$ (i.e. $2(m-1) < B \leq 2m$). Assume that $\varepsilon \leq (12m)^{-1}$.

Let $\lambda_{\varepsilon,K}$ denote the lowest eigenvalue of $H_0 = -\Delta+V$, and $\lambda_\varepsilon$ denote the lowest eigenvalue of the Dirichlet Laplacian on $\mathcal{R}$; then

$$\lim_{K\to\infty} \lambda_{\varepsilon,K} = \lambda_\varepsilon \tag{2.37}$$

for any fixed $\varepsilon$ by Lemma 2.13.

*Lower bound*

For the lower bound we choose $B = B_1 = 2m-1$. Then $1 - a_{m-1} \geq (6m)^{-1}$ and $a_m - 1 \geq (6m)^{-1}$, therefore $\mathcal{R}$ is at least at a distance $(12m)^{-1}$ from the set $\{a_n\}_{n=0}^\infty$.

It is obvious that $H_{Sch}(B_1, V)$ has a ground state, say $f = \sum_n e^{in\theta} f_n(r)$. From the estimates on $U_n$ and $2m-1 \geq 3m/2$ it easily follows that

$$\int (U_n+V)|f_n|^2 \geq \frac{1}{384m}\int_{\mathcal{R}} |f_n|^2 + K\int_{\mathcal{R}^c} |f_n|^2 \geq \frac{1}{384m}\int |f_n|^2$$

for any $n$. Therefore

$$H_{Sch}(B_1, V) \geq \lambda_{\varepsilon,K} + \frac{1}{384m}, \tag{2.38}$$

since the same estimate is valid for each $H_n$ on each sector.

*Upper bound*

For the upper bound, choose $B = B_2 = 2m$ and let $\psi$ be the lowest energy eigenfunction of the Laplacian with Dirichlet boundary condition on $\mathcal{R}$. Since $a_m = 1$, we have $U_m(r) \le 3m^2\varepsilon^2$ for $|r-1| \le \varepsilon$, i.e. on $\mathcal{R}$. Let $f = e^{im\theta}\psi$ be a trial function, which gives

$$\inf \operatorname{Spec} H_{Sch}(B_2, V) \le \lambda_\varepsilon + 3m^2\varepsilon^2. \tag{2.39}$$

Choosing $K$ sufficiently large and $\varepsilon$ sufficiently small, (2.37), (2.39) and (2.38) completes the proof of Counterexample 2.10. $\square$

*Proof of Counterexample 2.11.*

Strong magnetic field can act as a confining potential. We shall create a magnetic field which is zero on a ring, huge outside and has a $(2\pi)$-flux inside, such that the ground state is in the $n = 1$ angular momentum sector. Then by slightly decreasing this magnetic field, we show that the energy increases.

Let $B, K > 1$, $\varepsilon \ge 0$ be numbers to be chosen later, and consider the magnetic field $B(x) = 2(1-\varepsilon)B \cdot \chi(|x| \le B^{-1/2}) + 2K \cdot \chi(|x| \ge 1)$, which is generated by a radial gauge $a(r) = a_{B,K,\varepsilon}(r)$

$$a(r) := \begin{cases} (1-\varepsilon)Br & \text{for} \quad r < B^{-1/2} \\ (1-\varepsilon)r^{-1} & \text{for} \quad B^{-1/2} \le r < 1 \\ \Big[1-\varepsilon + K(r^2-1)\Big]r^{-1} & \text{for} \quad 1 \le r. \end{cases} \tag{2.40}$$

Let $\lambda_n(B, K, \varepsilon)$ denote the lowest eigenvalue of $H_n := -\Delta + U_n(r)$, where $U_n(r) = U_n^{B,k,\varepsilon}(r) = (n/r - a_{B,K,\varepsilon}(r))^2$ as before (usually we omit the dependence on $B, K, \varepsilon$ in $U_n(r)$ and $a(r)$). The following two lemmas will prove Counterexample 2.11.

**Lemma 2.14** *For large enough $B$ and $K$ and small enough $\varepsilon \ge 0$ we have*

$$\lambda_1(B, K, \varepsilon) < \lambda_n(B, K, \varepsilon) \tag{2.41}$$

*for all $n \ne 1$.*

**Lemma 2.15** *For large enough $K$ and $B \ge 1$ we have*

$$\liminf_{\varepsilon \to 0+0} \frac{\lambda_1(B, K, \varepsilon) - \lambda_1(B, K, \varepsilon = 0)}{\varepsilon^2} \ge \frac{1}{2}.$$

*Proof of Lemma 2.14.*

First we define $\tilde{U}_n(r)$ which coincides with $U_n(r)$ except for $r \in (1, \sqrt{1+K^{-1}(n-1+\varepsilon)})$ *and* $n \geq 1$, when we let $\tilde{U}_n(r) = 0$. Let $\tilde{\lambda}_n(B, K, \varepsilon)$ be the corresponding eigenvalue, which is smaller than $\lambda_n(B, K, \varepsilon)$ for any $n$. Note that $|U_1(r) - \tilde{U}_1(r)| \leq \varepsilon^2$, therefore

$$\tilde{\lambda}_1(B, K, \varepsilon) \leq \lambda_1(B, K, \varepsilon) \leq \tilde{\lambda}_1(B, K, \varepsilon) + \varepsilon^2. \tag{2.42}$$

Elementary computation shows that $\tilde{U}_n(r)$ is increasing as $K \to \infty$, and the limit function is $U_n(r)$ for $r \leq 1$ and infinity otherwise. By Lemma 2.13 $\lim_{K\to\infty} \tilde{\lambda}_n(B, K, \varepsilon) = \lambda_n(B, \varepsilon)_{|x|\leq 1}$, where this latter is the lowest eigenvalue of $-\Delta + U_n(r)$ on $|x| \leq 1$ with Dirichlet boundary condition. Therefore

$$\lambda_n(B, \varepsilon)_{|x|\leq 1} = \lim_{K\to\infty} \tilde{\lambda}_n(B, K, \varepsilon) \leq \liminf_{K} \lambda_n(B, K, \varepsilon) \tag{2.43}$$

for any $n$.

Now we compare $U_n(r)$ and $U_1(r)$ for $r \leq 1$ $(n \neq 1)$. For $\varepsilon < 1/2$ obviously $U_n(r) > U_1(r) + (1-\varepsilon)^2$ if $B^{-1/2} \leq r \leq 1$, and $U_n(r) > U_1(r) + B$ for $r \leq B^{-1/2}$ if $n \neq 0, 1$. This shows that $\lambda_n(B, \varepsilon)_{|x|\leq 1} \geq \lambda_1(B, \varepsilon)_{|x|\leq 1} + 1/4$ (if $\varepsilon < 1/2$, $B \geq 1/4$), which, along with (2.42), (2.43) shows (2.41) for $n \neq 0$.

Finally, to settle $n = 0$, we define $\overline{U}_0(r)$ to be equal to $U_0(r)$ for $r \geq B^{-1/2}$ and zero otherwise and let $\overline{\lambda}_0(B, \varepsilon)$ be the corresponding eigenvalue (on $\{|x| \leq 1\}$ with Dirichlet boundary condition). As $B \to \infty$, $\overline{U}_0(r)$ monotonically increases to $(1-\varepsilon)^2 r^{-2}$, so

$$\liminf_{B\to\infty} \lambda_0(B, \varepsilon) \geq \lim_{B\to\infty} \overline{\lambda}_0(B, \varepsilon) \geq \lambda^* \tag{2.44}$$

where $\lambda^*$ is the lowest eigenvalue of $-\Delta + (2r)^{-2}$ on $\{|x| \leq 1\}$. Consider the normalized eigenfunction $f^*$ corresponding to $\lambda^*$, this is a radial function, and use it as a trial function for $\lambda_1(B, \varepsilon)$ if $\varepsilon < 1/4$:

$$\lambda_1(B, \varepsilon) \leq \int_{|x|\leq 1} |\nabla f^*|^2 + U_1(|x|)|f^*(x)|\mathrm{d}x \leq \lambda^* + \int_{|x|\leq 1} (U_1(|x|) - (2|x|)^{-2})|f^*(x)|^2 \mathrm{d}x$$

$$\leq \lambda^* - 2\pi \int_{B^{-1/2}}^1 \frac{1}{8r^2}|f^*(r)|^2 r\mathrm{d}r + 2\pi \int_0^{B^{-1/2}} \frac{1}{r^2}|f^*(r)|^2 r\mathrm{d}r.$$

But $\int |x|^{-2}|f^*(x)|^2$ is finite, therefore

$$\limsup_{B\to\infty} \lambda_1(B, \varepsilon) \leq \lambda^* - 2\pi \int_0^1 \frac{1}{8r^2}|f^*(r)|^2 r\mathrm{d}r \leq \lambda^* - \frac{1}{8}.$$

Combining this with (2.44), we have

$$\liminf_{B\to\infty} \lambda_0(B,\varepsilon) \geq \limsup_{B\to\infty} \lambda_1(B,\varepsilon) + \frac{1}{8}$$

which, along with (2.42), (2.43) gives (2.41) for $n=0$ if $\varepsilon < 1/4$ and $B$ is large enough. $\square$

*Proof of Lemma 2.15.*
For any $\varepsilon > 0$ we have

$$\liminf_{K\to\infty} \frac{\lambda_1(B,K,\varepsilon) - \lambda_1(B,K,\varepsilon=0)}{\varepsilon^2}$$

$$\geq \liminf_{K\to\infty} \frac{\tilde\lambda_1(B,K,\varepsilon) - \tilde\lambda_1(B,K,\varepsilon=0)}{\varepsilon^2} = \frac{\lambda_1(B,\varepsilon)_{|x|\leq 1} - \lambda_1(B,\varepsilon=0)_{|x|\leq 1}}{\varepsilon^2}$$

using (2.42). Simple computation shows that $U_1^{B,K,\varepsilon}(r) \geq U_1^{B,K,\varepsilon=0}(r) + \varepsilon^2$ for $r \leq 1$ if $B \geq 1$, which, by recalling the definition of $\lambda_1(B,\varepsilon)_{|x|\leq 1}$, completes the proof. $\square$

## 2.6 Off-diagonal elements

Mehler formula (2.3) for constant magnetic field $B$ shows two essential features in two dimensions (similar statements are valid for higher dimensions, but for simplicity we restrict ourselves to $d=2$ in this Section). One is that the size of the diagonal element of the heat kernel decays as $e^{-Bt}$ for large $Bt$ (due to the $\sinh Bt$ factor). The other feature is the Gaussian type offdiagonal decay which is at least $\exp(-B(x-y)^2/4)$ for large $Bt$ (for small $Bt$ one obtains the usual decay of the free heat kernel, $\exp(-(x-y)^2/4t)$). The results in Section 2.5 show that the first feature is not robust (though it is true in the strong field limit, see Section 2.4). In this section we show that the second feature is not robust either, by answering a question of Loss and Thaller (see remark after Theorem 1.3. [1]):

**Counterexample 2.16** *There exists a continuous magnetic field $B(x) \geq B > 0$ in two dimensions, and there exist $t \in \mathbf{R}$, $x, y \in \mathbf{R}^2$ such that*

$$\left| e^{-tH_{Sch}(B(x),V=0)}(x,y) \right| > \left| e^{-tH_{Sch}(B,V=0)}(x,y) \right|.$$

*Remark.* Loss and Thaller proved that

$$\left| e^{-tH_{Sch}(B(x),V=0)}(x,y) \right| \leq \frac{B}{4\pi \sinh Bt} e^{-\frac{(x-y)^2}{4t}}$$

which means that the offdiagonal decay is at least as fast as in the nonmagnetic case. Our example shows that the expected stronger magnetic Gaussian decay is not always true.

*Proof.* Let $B(x) = B + 3bx_2^2$ where $B, b > 0$ and $x = (x_1, x_2) \in \mathbf{R}^2$. What we show is that

$$\frac{\partial}{\partial b}\Big|_{b=0} \Big| e^{-tH_{Sch}(B(x), V=0)}(x, y) \Big|^2 > 0 \tag{2.45}$$

for some $x, y, t$.

Before the proof, which is a long computation, let us indicate the intuition. It is well known that the homogeneous magnetic field has a strong confining effect, which classically corresponds to closed circular orbits; quantum mechanically it corresponds to the strongly (Gaussian) localized eigenfunctions. It is less known that this situation is very unstable; typically a magnetic field which has some gradient induces delocalization in the transversal direction. Iwatsuka [28], [29] considered a magnetic field, which takes one value $B_1$ on the $\{x_1 \leq 0\}$ half plane, and another value $B_2 \neq B_1$ on the other half plane. It is easy to see that any classical orbit intersecting the line $x_1 = 0$ is an unbounded spiral, i.e. the classical electron escapes to infinity. Iwatsuka showed the quantum analogue of this phenomenon, namely that the spectrum of the corresponding Schrödinger operator is absolutely continuous.

The idea behind our counterexample is to detect delocalization in the direction transversal to the gradient of the field, i.e. in our case we expect that turning on $b > 0$, the offdiagonal decay in the first coordinate direction becomes weaker.

The basic technical problem is that Mehler formula is the result of the explicit computation related to the exact solvability of the harmonic oscillator. There is no other known magnetic field whose heat kernel could be computed explicitly, or precisely enough for our purpose. The magnetic field $B(x)$ given in our counterexample is not exactly solvable either (since it leads to a usual Schrödinger operator with a polynomial potential of sixth degree), but the derivative of the heat kernel, with respect to $b$ at the point $b = 0$, is expressible by Gaussian integrals.

Choose a special gauge $\mathbf{A}(x) = (Bx_2 + bx_2^3, 0)$. First we compute the derivative of the heat kernel by the Duhamel formula:

$$\frac{\partial}{\partial b}\Big|_{b=0} e^{-t[(-i\partial_1 - Bx_2 - bx_2^3)^2 - \partial_2^2]}(x, y) = \frac{1}{2\pi} \int \mathrm{d}p_1 e^{ip_1(x_1 - y_1)} \tag{2.46}$$

$$\times \int_0^t \mathrm{d}s \int_{-\infty}^{\infty} \mathrm{d}z_2 e^{-s[-\partial_2^2 + (p_1 - Bx_2)^2]}(x_2, z_2) \Big[2z_2^3(p_1 - Bz_2)\Big] e^{-(t-s)[-\partial_2^2 + (p_1 - Bx_2)^2]}(z_2, y_2).$$

Now we use the Mehler formula for the one dimensional shifted harmonic oscillator:

$$e^{-s[-\partial_2^2+(p_1-Bx_2)^2]}(u,v) \tag{2.47}$$
$$= \frac{\sqrt{B}}{\sqrt{2\pi\sinh(2sB)}}\exp\Big[-\frac{(Bu-p_1)^2+(Bv-p_1)^2}{2B}\coth(2Bs)+\frac{(Bu-p_1)(Bv-p_1)}{B\sinh(2Bs)}\Big].$$

After inserting this formula into (2.46) we can explicitly perform the d$z_2$-integration. The formula is very lengthy, so we immediately apply it to $x_2=y_2=0$, the result is

$$\frac{\partial}{\partial b}\Big|_{b=0} e^{-t[(-i\partial_1-Bx_2-bx_2^3)^2-\partial_2^2]}\Big((x_1,0),(y_1,0)\Big) \tag{2.48}$$
$$= -\frac{2\exp\Big(-\frac{(x_1-y_1)^2}{4K}\Big)}{(2\pi)^{3/2}B^3}\int_0^t \mathrm{d}s\frac{1}{\sqrt{\sinh(2Bs)\sinh(2B(t-s))}}\int_{-\infty}^{\infty}\mathrm{d}q\, e^{-Kq^2}$$
$$\times\frac{1}{\sqrt{2E}}\Big\{\frac{3}{(2E)^2}+\frac{3}{2E}\Big(q+\frac{i(x_1-y_1)}{2K}\Big)^2\Big(1-\frac{H}{2BE}\Big)\Big(1-\frac{H}{BE}\Big)-\Big(q+\frac{i(x_1-y_1)}{2K}\Big)^4\Big(1-\frac{H}{2BE}\Big)^3\frac{H}{2BE}\Big\},$$

where, for brevity, we introduced

$$E:=\frac{\sinh(2Bt)}{2B\sinh(2Bs)\sinh(2B(t-s))};\quad H:=\frac{1}{\sinh(2Bs)}+\frac{1}{\sinh(2B(t-s))};\quad K:=\frac{\cosh(2Bt)-1}{B\sinh(2Bt)}.$$

In order to compute the derivative of the square of the heat kernel one needs its value at the given point as well which can also be given using (2.47):

$$e^{-t[(-i\partial_1-Bx_2)^2-\partial_2^2]}\Big((x_1,0),(y_1,0)\Big)=\frac{B}{4\pi\sinh(Bt)}\exp\Big[-\frac{B(x_1-y_1)^2}{4}\coth(Bt)\Big]. \tag{2.49}$$

Combining (2.48) and (2.49) and considering that the derivative of the absolute value is real we obtain, with $z:=x_1-y_1$,

$$\frac{\partial}{\partial b}\Big|_{b=0}\Big|e^{-tH_{Sch}(B(x),V=0)}\Big((x_1,0),(y_1,0)\Big)\Big|^2 \tag{2.50}$$
$$= -\frac{2\exp\Big(-\frac{Bz^2}{4}\coth(Bt)-\frac{z^2}{4K}\Big)}{(2\pi)^{5/2}B^2\sinh(Bt)}\int_0^t\mathrm{d}s\frac{1}{\sqrt{\sinh(2Bs)\sinh(2B(t-s))}}\int_{-\infty}^{\infty}\mathrm{d}q\,e^{-Kq^2}$$
$$\times\frac{1}{\sqrt{2E}}\Big\{\frac{3}{(2E)^2}+\frac{3}{2E}\Big[q^2-\Big(\frac{z}{2K}\Big)^2\Big]\Big(1-\frac{H}{2BE}\Big)\Big(1-\frac{H}{BE}\Big)$$

$$-\Big[q^4 - 6q^2\Big(\frac{z}{2K}\Big)^2 + \Big(\frac{z}{2K}\Big)^4\Big]\Big(1 - \frac{H}{2BE}\Big)^3 \frac{H}{2BE}\Big\}.$$

The d$q$-integration can be done explicitly and we arrive at

$$\frac{\partial}{\partial b}\Big|_{b=0}\Big|e^{-tH_{Sch}(B(x),V=0)}\Big((x_1,0),(y_1,0)\Big)\Big|^2 = -\frac{2\sqrt{Y}\exp\Big(-\frac{Bz^2}{4}\coth(Bt) - \frac{Yz^2}{2}\Big)}{(2\pi)^2 B^{3/2}\sinh(Bt)\sqrt{\sinh(2Bt)}}$$

$$\times \int_0^t \mathrm{d}s\,\Big\{3U^2 + 3UXY(2X-1)(1-z^2Y) - \Big[z^4Y^2 - 6z^2Y + 3\Big]Y^2X^3(1-X)\Big\}$$

with

$$X := 1 - \frac{\sinh(2Bs) + \sinh(2B(t-s))}{\sinh(2Bt)}; \quad Y := \frac{1}{2K}; \quad U := \frac{1}{2E}.$$

In order to show (2.45), it is enough to prove that the integral is negative. Notice that $0 \le X \le 1$ and $U, X, Y$ are independent of $z$. Viewing this integral as a polynomial in $z$, we notice that the coefficient of the highest degree term, $z^4$ is negative: $-z^4Y^4\int_0^t \mathrm{d}s\,X^3(1-X)$. Choosing $z$ large enough, we complete the proof. $\square$.

# 3 Paramagnetism for the Pauli operator

In $d = 2$ (and also in $d = 3$ if the magnetic field has a constant direction), the paramagnetism due to the spin coupling obviously decreases the energy (see (1.2), (1.3)). The ground state $\psi$ is entirely in the more favorable spin subspace (where the spin points in the direction of the field), which means a net energy decrease by $\int \|B(x)\||\psi(x)|^2\mathrm{d}x$ compared to the Schrödinger case, while at a positive temperature, a bigger part of the state is in the lower energy spin sector. But of course in the case of dynamical electrons, diamagnetic effects are always present and they compete with the spin-coupling paramagnetism.

This competition can be seen in the formula for the constant field (1.6). Here diamagnetism is responsible for the factor $B/\sinh(Bt)$ (compare with (1.5)), while $\cosh(Bt)$ is due to paramagnetism.

In Section 3.1 we prove paramagnetism in the short time (and semiclassical) regime in $d = 2, 3$. Then we restrict ourselves to $d = 2$ and prove paramagnetism in the strong field and large time limit, and finally we show that paramagnetism does not necessarily hold in a robust sense, without asymptotics.

A very interesting open problem is to investigate paramagnetism in $d = 3$ for a general magnetic field away from the short time regime. While for *constant direction* field many ideas can be used from the $d = 2$ case, for general fields the energy likely depends on the geometric structure of the field lines and not just on the field strength (or local field energy). The example of Loss and Yau [30] shows a remarkable conspiracy between the field strength and the field line geometry which yields an unexpected zero energy ground state. We are far from understanding this phenomenon. How generic or rigid these states are would obviously influence any paramagnetic monotonicity. Naively it seems that the zero eigenvalue of the Loss-Yau state disappears by essentially *any* perturbation of the magnetic field, but no rigorous argument is known. This would mean that the ground state density function also disappears immediately, excluding any large time heat kernel comparison.

## 3.1 Short time and semiclassics

For large temperature (short time in the heat kernel) the diamagnetic and paramagnetic effects can be compared and we have the following general result in $d = 2, 3$. Again, this statement includes the semiclassical result by using $t := \beta h^2$, $L := h^{-1}$.

**Proposition 3.1** *Let $V$ be semibounded, continuously differentiable, let $B \in C^3$ with $\|B\|_\infty + \|\nabla B\|_\infty < \infty$ and let $L \geq 1$ be a scaling parameter. In $d = 2, 3$, for any $x \in \mathbf{R}^d$,*

$$Tr_{\mathbf{C}^2} e^{-tH_{Pauli}(LB,V)}(x,x) = 2(4\pi t)^{-d/2}(1 + O(t^{5/2}L^2 + t^4L^4))e^{-tV(x)}\frac{tLB(x)\cosh tLB(x)}{\sinh tLB(x)} \tag{3.1}$$

$$+2\Big(e^{-tH_{Sch}(B=0,V)}(x,x) - e^{-tV(x)}e^{-tH_{Sch}(B=0,V=0)}(x,x)\Big)$$

*as $t \to 0$ and $tL \to 0$. The error depends on the $C^1$-norm of $B$, on $\max_{y:\,|y-x|\leq 1}[|\nabla^2 B(y)| + |\nabla^3 B(y)|]$, on $V_0 := \min_{y\in\mathbf{R}^d} V(y)$ and on $\max_{y:\,|y-x|\leq 1}|\nabla V(y)|$. In $d = 3$ we use the notation $B(x) := \|\mathbf{B}(x)\|_2 = \|\mathbf{B}(x)\|$ in (3.1) but $\mathbf{B}$ replaces $B$ everywhere in the first and in the previous sentence.*

This implies the paramagnetic comparison in the senses $(III.)$ and $(IV.)$

**Corollary 3.2** *Let the magnetic fields $B_1$, $B_2$ be three times continuously differentiable and have finite $C^1$-norm, and let the semibounded pontential $V$ be continuously differentiable. In $d = 2, 3$, for any $x$ satisfying $B_1(x) < B_2(x)$, we have*

$$Tr_{\mathbf{C}^2} e^{-tH_{Pauli}(LB_2,V)}(x,x) - Tr_{\mathbf{C}^2} e^{-tH_{Pauli}(LB_1,V)}(x,x) \tag{3.2}$$

$$\geq C^*(4\pi t)^{-d/2}e^{-tV(x)}t^2L^2\Big(B_2^2(x) - B_1^2(x)\Big) > 0$$

*for small enough $tL \leq \varepsilon_0$, $t < \varepsilon_0$ and some constant $C^*$. The constants $\varepsilon_0, C^*$ depend on global lower bound $V$, on the global $C^1$-norm of $B_1$ and $B_2$, and on $\max_{y:\,|y-x|\leq 1}[|\nabla V(y)| +$*

$|\nabla^2 B(y)|+|\nabla^3 B(y)|]$. *If, in addition,* $\int \exp(-tV(x))\mathrm{d}x$ *is finite for all* $t$*, and the* $C^1$*-norm of* $V$ *and the* $C^3$*-norms of* $B_1, B_2$ *are bounded, then comparison in sense (IV.) is valid for small enough* $t$*. In* $d=3$ *we use the notation* $B_i(x) = \|\mathbf{B}_i(x)\|_2 = \|\mathbf{B}_i(x)\|$ *in (3.2) but* $\mathbf{B}_i$ *replaces* $B_i$ *everywhere in the first and in the previous two sentences.*

The proof of this Corollary is obvious from $X \coth X = 1 + X^2/3 + O(X^4)$. In particular $C^* \to 1/3$ as $tL \to 0, t \to 0$.

*Proof of Proposition 3.1.* We can assume that $x=0$, $V(0)=0$, $t \le 1$ and $Lt \le 1$.

*Two dimensions.*

From (2.5) and (1.2) we immediately get

$$\mathrm{Tr}_{\mathbf{C}^2} e^{-tH_{Pauli}(LB,V)}(0,0) = 2(4\pi t)^{-1}(1+O(t^{5/2}L^2+t^4L^4))\frac{tLB(0)\cosh tLB(0)}{\sinh tLB(0)} + \Lambda_1 + \Lambda_2$$

with

$$\Lambda_1 = \sum_{\pm}\Big[e^{-tH_{Sch}(B=0,V\pm B)}(0,0) - e^{\mp tLB(0)}e^{-tH_{Sch}(B=0,V)}(0,0)\Big]$$

and

$$\Lambda_2 = 2\cosh(tLB(0))\Big[e^{-tH_{Sch}(B=0,V)}(0,0) - e^{-tH_{Sch}(B=0,V=0)}(0,0)\Big].$$

Using $\cosh X = 1 + O(X^2)$ and a simplified version of (2.6) (we expand $V$ only up to first order as in (2.19)):

$$\Lambda_2 = 2\Big[e^{-tH_{Sch}(B=0,V)}(0,0) - e^{-tH_{Sch}(B=0,V=0)}(0,0)\Big] + (4\pi t)^{-1}O(t^{7/2}L^2)$$

with the error depending on $V_0$ and on $\max_{|y|\le 1}|\nabla V(y)|$ and the $C^0$ norm of $B$.

By the Feynman-Kac formula

$$\Lambda_1 = (4\pi t)^{-1}\sum_{\pm} e^{\mp tLB(0)}\mathbf{E}_{0,0}^{2t,0} e^{-\frac{1}{2}\int_0^{2t} V(W_s)\mathrm{d}s}\Big(e^{\mp\frac{L}{2}\int_0^{2t}(B(W_s)-B(0))\mathrm{d}s} - 1\Big).$$

Similarly to the proof of (2.6) in Section 2.3, on the set $\mathcal{E}^c$ the estimate is trivial. Next we write

$$\Lambda_1 = (4\pi t)^{-1}\Big[\sum_{\pm} e^{\mp tLB(0)}\mathbf{E}_{0,0}^{2t,0}\Big(e^{\mp L\int(B-B(0))}-1\Big)+\sum_{\pm} e^{\mp tLB(0)}\mathbf{E}_{0,0}^{2t,0}\Big(e^{-\int V}-1\Big)\Big(e^{\mp L\int(B-B(0))}-1\Big)\Big]$$

using the shorthand notations introduced in Section 2.3 and $\int(B-B(0)) = \frac{1}{2}\int_0^{2t}(B(W_s)-B(0))\mathrm{d}s$. The second term in the square bracket is smaller than $C_{12}t^3L$ by Schwarz, similarly to (2.19), the constant depending on $V_0$, $\max_{|y|\le 1}|\nabla V(y)|$ and the $C^1$-norm of $B$.

For the first term we use

$$\mathbf{E}_{0,0}^{2t,0}\chi(\mathcal{E})\Big|e^{\mp L\int(B-B(0))}-1\pm L\int(B-B(0))\Big|\le C_{13}t^3L^2$$

with some $C_{13}$ depending on $\max_{|y|\le 1}|\nabla B(y)|$.

Finally for the remaining linear term we use

$$B(W_s)=B(0)+\nabla B(0)\cdot W_s+\frac{1}{2}(W_s,\nabla^2B(0)\cdot W_s)+C_{14}|W_s|^3,$$

and the symmetry as in (2.20), which gives

$$\Big|\sum_{\pm}e^{\mp tLB(0)}\mathbf{E}_{0,0}^{2t,0}\chi(\mathcal{E})\Big\{\mp L\int(B-B(0))\Big\}\Big|$$

$$\le\mathbf{E}_{0,0}^{2t,0}\chi(\mathcal{E})\Big\{\sinh(tLB(0))\int_0^{2t}L(W_s,\nabla^2B(0)\cdot W_s)\mathrm{d}s+2C_{14}e^{tLB(0)}L\int_0^{2t}|W_s|^3\mathrm{d}s\Big\}\le C_{15}t^{5/2}L^2$$

with $C_{14},C_{15}$ depending on $B(0)$ and on $\max_{|y|\le1}[|\nabla^2B(y)|+|\nabla^3B(y)|]$.

*Three dimensions.*

We can assume that $\mathbf{B}(0)$ points in the positive direction of the third coordinate axis, and in this proof we use the notation $\mathbf{B}=(B_1,B_2,B_3)$. The generalized Feynman-Kac formula (involving a joint Wiener-Poisson process) gives a representation of the heat kernel (for details see [4], [6]):

$$\mathrm{Tr}_{\mathbf{C}^2}\,e^{-tH_{Pauli}(LB,V)}(0,0)=\sum_{\sigma=\pm}\frac{\cosh(2t)}{(4\pi t)^{3/2}}\mathbf{E}_W^0\mathbf{E}_\nu^\sigma e^{-iL\int\mathbf{A}}e^{-\int V}e^{\frac{L}{2}\int_0^{2t}B_3(W_s)(-1)^{\nu_s}\mathrm{d}s}$$

$$\times\exp\Big(\int_0^{2t}\log\Big[\frac{L}{2}(B_1(W_s)-i(-1)^{\nu_s}B_2(W_s))\Big]\mathrm{d}\nu_s\Big),$$

where $\nu_s$ is a Poisson jump process on $\mathbf{Z}$ with unit intensity $\mathbf{E}\mathrm{d}\nu_s=\mathrm{d}s$. We used the notation $\mathbf{E}_W^0:=\mathbf{E}_{0,0}^{2t,0}$ for the expectation with respect to the Brownian bridge, and $\mathbf{E}_\nu^\sigma:=\mathbf{E}_{0,\sigma}^{2t,\sigma}$ for the "Poisson bridge", where $\sigma\in\{+,-\}$ and the "bridge" means $\nu_0\equiv\nu_{2t}\equiv\frac{1-\sigma}{2}\ (\mathrm{mod}2)$, or, equivalently, $(-1)^{\nu_0}=(-1)^{\nu_{2t}}=\sigma$. Therefore

$$\mathrm{Tr}_{\mathbf{C}^2}\,e^{-tH_{Pauli}(LB,V)}(0,0)=\sum_{\sigma=\pm}(4\pi t)^{-3/2}\mathbf{E}_W^0e^{-iL\int\mathbf{A}}e^{-\int V}e^{\frac{L}{2}\sigma\int_0^{2t}B_3(W_s)\mathrm{d}s}-\Omega_1-\Omega_2+\Omega_3 \quad (3.3)$$

with

$$\Omega_1:=\sum_{\sigma=\pm}(4\pi t)^{-3/2}\mathbf{E}_W^0\mathbf{E}_\nu^\sigma e^{-iL\int\mathbf{A}}e^{-\int V+\sigma L\int B_3}$$

$$\times\Big\{1-\cosh(2t)\exp\Big(\int_0^{2t}\log\Big[\frac{L}{2}(B_1(W_s)-i(-1)^{\nu_s}B_2(W_s))\Big]\mathrm{d}\nu_s\Big)\Big\}$$

$$\Omega_2 := \sum_{\sigma=\pm}\frac{\cosh(2t)}{(4\pi t)^{3/2}}\mathbf{E}^0_W\mathbf{E}^\sigma_\nu\Big\{1-\exp\Big(\sigma L\int_0^{2t}B_3(W_s)(\sigma(-1)^{\nu_s}-1)\mathrm{d}s\Big)\Big\}$$

and

$$\Omega_3 := \sum_{\sigma=\pm}\frac{\cosh(2t)}{(4\pi t)^{3/2}}\mathbf{E}^0_W\mathbf{E}^\sigma_\nu\Big(1-e^{-iL\int\mathbf{A}-\int V+\sigma L\int B_3+\int\log L(B_1-iB_2)}\Big)$$

$$\times\Big\{1-\exp\Big(\sigma L\int_0^{2t}B_3(W_s)(\sigma(-1)^{\nu_s}-1)\mathrm{d}s\Big)\Big\}$$

where we used the shorthand $\int B_3$ for $\frac{1}{2}\int_0^{2t}B_3(W_s)\mathrm{d}s$ and $\int\log L(B_1-iB_2)$ for $\int\log\Big[\frac{L}{2}(B_1(W_s)-i(-1)^{\nu_s}B_2(W_s))\Big]\mathrm{d}\nu_s$.

The main term in (3.3) is treated exactly as in $d=2$ (note that the dimension was used only in the power of the prefactor $(4\pi t)^{-d/2}$ in the two dimensional proof). This gives the two main terms in (3.1), noting that $B_3(0)=\|\mathbf{B}(0)\|$.

In $\Omega_1$ the expectation with respect to the Poisson process can be estimated as follows (see Eq. (72) in [6], which is true for random anticipatory functions as well)

$$\Big|\mathbf{E}^\sigma_\nu\Big\{1-\cosh(2t)\exp\Big(\int_0^{2t}\log\Big[\frac{L}{2}(B_1(W_s)-i(-1)^{\nu_s}B_2(W_s))\Big]\mathrm{d}\nu_s\Big)\Big\}\Big|$$

$$\leq\Big|1-\mathbf{E}^\sigma_\nu\cosh\Big(\int_0^{2t}\Big[\frac{L}{2}(B_1(W_s)-i(-1)^{\nu_s}B_2(W_s))\Big]\mathrm{d}s\Big)\Big|\leq C_{16}L^2\Big(\int_0^{2t}\Big(B_1^2(W_s)+B_2^2(W_s)\Big)^{1/2}\mathrm{d}s\Big)^2.$$

Since $B_1(0)=B_2(0)=0$, therefore

$$\Omega_1\leq C_{17}(4\pi t)^{-3/2}L^2\mathbf{E}^0_W\Big(\int_0^{2t}\Big(B_1^2(W_s)+B_2^2(W_s)\Big)^{1/2}\mathrm{d}s\Big)^2\leq C_{18}(4\pi t)^{-3/2}t^3L^2$$

where $C_{16}, C_{17}, C_{18}$ depend on $V_0$, and the $C^1$-norm of $\mathbf{B}$.

$\Omega_2$ is zero on the set $\mathcal{F}:=\{(-1)^{\nu_s}\equiv\sigma\ :\ 0\leq s\leq 2t\}$. On the complement set, it is estimated as follows

$$\Omega_2\leq\sum_{\sigma=\pm}\frac{\cosh(2t)}{(4\pi t)^{3/2}}\mathbf{E}^0_W\mathbf{E}^\sigma_\nu\chi(\mathcal{F}^c)\Big[\Big(-\sigma L\int_0^{2t}B_3(W_s)(\sigma(-1)^{\nu_s}-1)\mathrm{d}s\Big) \tag{3.4}$$

$$+\Big(1+\sigma L\int_0^{2t}B_3(W_s)(\sigma(-1)^{\nu_s}-1)\mathrm{d}s-\exp\Big\{\sigma L\int_0^{2t}B_3(W_s)(\sigma(-1)^{\nu_s}-1)\mathrm{d}s\Big\}\Big)\Big].$$

The first term vanishes, after summation over $\sigma = \pm$, by the symmetry $\sigma \to -\sigma$, $\nu_s \to \nu_s + 1$ for each realization of $W_s$. The other term in (3.4) gives $O(t^2 L^2)$ after taking the Wiener expectation uniformly for each realization of $\nu_s$. Finally one uses that $\mathbf{E}_\nu^\sigma \chi(\mathcal{F}^c) \le 2t$ for small enough $t$. Therefore we obtain

$$\Omega_2 \le C_{19}(4\pi t)^{-3/2} t^3 L^2$$

with $C_{19}$ depending on the $C^0$-norm of $\mathbf{B}$.

Finally we use a weighted Schwarz for $\Omega_3$:

$$\Omega_3 \le \sum_{\sigma=\pm} \frac{\cosh(2t)}{(4\pi t)^{3/2}} \Big[ t^{1/2} \mathbf{E}_W^0 \mathbf{E}_\nu^\sigma \Big| 1 - e^{-iL\int \mathbf{A} - \int V + \sigma L \int B_3 + \int \log L(B_1 - iB_2)} \Big|^2 \tag{3.5}$$

$$+ t^{-1/2} \mathbf{E}_W^0 \mathbf{E}_\nu^\sigma \Big| 1 - \exp\Big( \sigma L \int_0^{2t} B_3(W_s)(\sigma(-1)^{\nu_s} - 1) \mathrm{d}s \Big) \Big|^2 \Big].$$

The second term in the square bracket is zero on $\mathcal{F}$ and is of order $t^{-1/2} O(t^2 L^2)$ on $\mathcal{F}^c$, after taking the Wiener expectation uniformly for each $\nu_s$ (use $|e^X - 1| \le |X| e^{|X|}$). Since the probability of $\mathcal{F}^c$ is of order $t$, we obtain a bound of order $t^{5/2} L^2$.

The first term in (3.5) is estimated by $2(\Omega_4 + \Omega_5)$ with

$$\Omega_4 = t^{1/2} \sum_{\sigma=\pm} \frac{\cosh(2t)}{(4\pi t)^{3/2}} \mathbf{E}_W^0 \mathbf{E}_\nu^\sigma \Big| 1 - e^{-iL\int \mathbf{A} - \int V + \sigma L \int B_3} \Big|^2,$$

and

$$\Omega_5 = t^{1/2} \sum_{\sigma=\pm} \frac{\cosh(2t)}{(4\pi t)^{3/2}} \mathbf{E}_W^0 \mathbf{E}_\nu^\sigma e^{-2\int V + 2\sigma L \int B_3} \Big| 1 - e^{\int \log L(B_1 - iB_2)} \Big|^2.$$

We can assume that $\mathbf{A}$ is chosen such that $|\mathbf{A}(x)| \le C_1 |x|$, $|\mathrm{div}\, \mathbf{A}(x)| \le C_1 |x|$ (see (2.11)). By simple estimates $\Omega_4 \le C_{20}(4\pi t)^{-3/2} t^{5/2} L^2$ where $C_{20}$ depends on $V_0$, $\max_{|y|\le 1} |\nabla V|$ and on the $C^1$-norm of $\mathbf{B}$.

Finally for $\Omega_5$ we perform the squaring and apply again Eq. (72) [6]:

$$\Omega_5 \le C_{21} t^{1/2} \sum_{\sigma=\pm} (4\pi t)^{-3/2} \mathbf{E}_W^0 \mathbf{E}_\nu^\sigma$$

$$\Big\{ \cosh(2t) - 2\mathrm{Re}\cosh\Big( \int_0^{2t} \Big[ \frac{L}{2}(B_1(W_s) - i(-1)^{\nu_s} B_2(W_s)) \Big] \mathrm{d}s \Big) + \cosh\Big( \int_0^{2t} \frac{L^2}{4}(B_1^2(W_s) + B_2^2(W_s)) \mathrm{d}s \Big) \Big\}$$

$$\le C_{22} t^{1/2} \sum_{\sigma=\pm} (4\pi t)^{-3/2} \mathbf{E}_W^0 \mathbf{E}_\nu^\sigma \Big\{ t^2 + \Big( \int_0^{2t} \frac{L}{2} \sqrt{B_1^2(W_s) + B_2^2(W_s)} \mathrm{d}s \Big)^2 + \Big( \int_0^{2t} \frac{L^2}{4}(B_1^2(W_s) + B_2^2(W_s)) \mathrm{d}s \Big)^2 \Big\}$$

$$\le C_{23}(4\pi t)^{-3/2} t^{1/2} (t^2 + t^3 L^2 + t^4 L^4),$$

where $C_{21}, C_{22}, C_{23}$ depend on $V_0$ and on the $C^0$-norm of $\mathbf{B}$. This completes the proof of the three dimensional case in Proposition 3.1. □

## 3.2 Large field and time

For low temperature (large time) and strong field both the diamagnetic and the paramagnetic effects are huge (the corresponding factors, $B/\sinh(Bt)$ and $\cosh(Bt)$, respectively, behave exponentially for large $|B|t$). These two exponential factors essentially cancel each other, and we are left with a linear factor $B$, representing the fact that eventually paramagnetism prevails. This heavy cancellation makes the problem especially difficult and for nonhomogeneous fields we have only a ground state result in $d = 2$.

For a magnetic field $B(x) \geq 0$ let $P_B(x)$ be the ground state density of the Pauli operator. It can be defined as $\sum_j |f_j(x)|^2$ for any orthonormal family of functions in the kernel of $(-i\nabla - \mathbf{A})^2 - B$, since $H_{Pauli}(B, V = 0)$ has no ground state in the other spin subspace – see (1.2). If the operator $P_B$ has a continuous kernel $P_B(x, y)$, then $P_B(x) = P_B(x, x)$. We recall the main result from [5]:

**Proposition 3.3** *In $d = 2$ suppose that $0 \leq B \in C^1$ and it does not grow faster than a quadratic function at infinity.*

*(i) If, in addition, $B(x) \geq B_0 > 0$ then for any sequence $L_n \to \infty$ (as $n \to \infty$)*

$$\lim_{n\to\infty} \frac{1}{L_n} P_{L_n B}(x) = \frac{B(x)}{2\pi}$$

*for almost all $x$.*

*(ii) If $B(x)$ is compactly supported then*

$$\frac{1}{L} P_{LB}(x) \to \frac{B(x)}{2\pi}$$

*in $L^p$-sense ($1 \leq p < \infty$).*

**Corollary 3.4** *Assume that $B_1, B_2 \in C^1(\mathbf{R}^2)$, do not grow faster than a quadratic function at infinity, and $0 < B_0 \leq B_1(x) \leq B_2(x)$. Let $H_i(L) = H_{Pauli}(LB_i, V = 0)$ for brevity. Then the comparison in the sense (III.) is true in the large time and large field limit, i.e. for any sequence $L_n \to \infty$ (as $n \to \infty$)*

$$\lim_{n\to\infty} \frac{1}{L_n} \liminf_{t\to\infty} e^{-tH_1(L_n)}(x,x) = \lim_{n\to\infty} \frac{1}{L_n} \limsup_{t\to\infty} e^{-tH_1(L_n)}(x,x) \quad (= B_1(x))$$

$$\leq \lim_{n\to\infty} \frac{1}{L_n} \liminf_{t\to\infty} e^{-tH_2(L_n)}(x,x) = \lim_{n\to\infty} \frac{1}{L_n} \limsup_{t\to\infty} e^{-tH_2(L_n)}(x,x) \quad (= B_2(x))$$

*for almost all $x$.*

*Remark.* Notice that we are not comparing the heat kernels on a logarithmic scale as in Section 2.4.

*Proof of the Corollary.* By the continuity of the heat kernel (see Appendix B in [5])

$$\liminf_{t\to\infty} e^{-tH_{Pauli}(LB,V=0)}(x,x) \geq P_{LB}(x)$$

for any $L$ and almost all $x$. By Eq. (25) in [5] and the monotonicity of the diagonal elements of the heat kernel in time,

$$\limsup_{t\to\infty} e^{-tH_{Pauli}(LB,V=0)}(x,x)$$

$$\leq e^{-t_L H_{Pauli}(LB,V=0)}(x,x) \leq P_{LB}(x) + e^{-t_L LB_0} e^{-\frac{1}{2}t_L H_{Pauli}(LB,V=0)}(x,x)$$

for all $x$ and for $t_L = \log L/(LS)$ where $S$ can be chosen large enough, depending on a compact neighbourhood of $x$. Dividing by $L$ and using Main Lemma 2.2. from [5], the statement follows from Proposition 3.3. $\square$

## 3.3 Comparison without asymptotics

Finally, as in the case of diamagnetism, one can ask again whether paramagnetism is true in a robust sense. Apparently this question was asked first by Hogreve, Schrader and Seiler [7] in the sense ($IV.$) for the special case when $B_1(x) = 0 < B_2(x)$. It was positively answered by E. Lieb in the sense ($V.$) if $B_2$ is constant [31, Appendix]. Later this was extended by Avron and Seiler [32] for certain polynomial magnetic fields $B_2(x)$. Finally Avron and Simon gave a counterexample [33], again in the sense ($V.$), where essentially the Aharonov-Bohm effect [34] was used; a strong potential shielded the electron away from the magnetic field, which excluded the paramagnetic effect of the coupling between the field and the spin, but the diamagnetism was still effective due to the nonlocality of the vectorpotential.

Here we are presenting a counterexample in the sense ($III.$) without potential. The point is that without potential the bottom of the spectrum of the Pauli operator is zero (under some general conditions, see [35, 29, 5]), therefore a more refined comparison is needed. We shall compare ground state densities which implies comparison in the sense ($III.$) for large $t$. By adding a strongly concentrated potential well one can obviously obtain comparison in the sense ($IV.$) as well.

The mechanism in our counterexample will be different from the Aharonov-Bohm effect used in [33]. Similarly to Section 2.5, we use the phenomenon that the magnetic operator is sensitive to the fractional part of the flux/$(2\pi)$ in a nonmonotonic way.

**Counterexample 3.5** *In $d = 2$ there exist two magnetic fields $0 \le B_1(x) \le B_2(x)$ and a number $R$ such that*

$$P_{B_1}(x) > P_{B_2}(x)$$

*for all $|x| \ge R$.*

**Corollary 3.6** *In $d = 2$ there exist two magnetic fields $0 \le B_1(x) \le B_2(x)$ such that the comparison in the sense $(III.)$ is not true, i.e.*

$$Tr_{\mathbf{C}^2}\, e^{-tH_{Pauli}(B_1,V=0)}(x,x) > Tr_{\mathbf{C}^2}\, e^{-tH_{Pauli}(B_2,V=0)}(x,x)$$

*for some $t$ and $x$.*

*Proof of Counterexample 3.5.* For compactly supported magnetic fields, the ground states can explicitly be given by following the proof of the Aharonov-Casher theorem [35, 29]. Let $B(x) = B \cdot \chi\{|x| \le 1\}$ and let $Q = B/2$ be the total flux divided by $2\pi$. The unnormalized orthogonal ground states are

$$g_n(z) := z^n \cdot \begin{cases} e^{-Q/2}|z|^{-Q} & \text{for} \quad |z| > 1 \\ e^{-Q|z|^2/2} & \text{for} \quad |z| \le 1 \end{cases} \tag{3.6}$$

for $n = 0, 1, 2, \ldots \lfloor Q \rfloor - 1$, where $\lfloor\ \rfloor$ denotes the lower integer part (i.e. $\lfloor x \rfloor = x - 1$ for integer $x$, otherwise $\lfloor x \rfloor = [x]$). Here we used the identification $\mathbf{C} \cong \mathbf{R}^2$, $z = x_1 + ix_2 = (x_1, x_2)$.

The ground state density function is radially symmetric and

$$P_B(|z|) = P_B(r) = \frac{1}{\pi} \sum_{n=0}^{\lfloor Q \rfloor - 1} \frac{r^{2(n-Q)}}{\frac{1}{Q-n-1} + \frac{e^Q}{Q^{n+1}} \int_0^Q t^n e^{-t} \mathrm{d}t}.$$

Let $B = 2 + 2\varepsilon$, $Q = 1 + \varepsilon$, where $0 < \varepsilon \le 1/2$, then

$$P_B(r) = P_{2+2\varepsilon}(r) = \frac{1}{\pi} \frac{r^{-2(1+\varepsilon)}}{\varepsilon^{-1} + (1+\varepsilon)^{-1}(e^{1+\varepsilon} - 1)}$$

Differentiation with respect to $\varepsilon$ shows that for large enough $r$ the ground state density decreases as $\varepsilon$ increases. For more detailed asymptotic behaviour see [36, Appendix B]. □

*Proof of the Corollary 3.6.* Let $\Pi_B$ be the ground state projection operator of $H_{Pauli}(B, V = 0)$ ($B$ is either $B_1$ or $B_2$). This is equal to $P_B \oplus 0$ according to the decomposition (1.2). By direct inspection, the ground state eigenfunctions, obtained in the proof of the Proposition 3.5, are uniformly continuous, therefore the operator kernel $\mathrm{Tr}_{\mathbf{C}^2}\Pi_B(x,y) = P_B(x,y)$ is uniformly continuous.

Now we show that the heat kernel $e^{-tH}(x,y)$ is continuous in $x,y$, uniformly for $t \geq 2$. Let $f_x(y) = \exp(-H_{Pauli}(B, V=0))(x,y)$, then

$$\Big|e^{-tH_{Pauli}(B,V=0)}(x,y) - e^{-tH_{Pauli}(B,V=0)}(x,y')\Big| = \Big|\Big(f_x, e^{-(t-2)H_{Pauli}(B,V=0)}(f_y - f_{y'})\Big)\Big| \leq \|f_x\| \|f_y - f_{y'}\|,$$

since the Pauli operator is nonnegative. By the estimates in the Appendix B of [5] (also in [21]), $f_{y'}(x) \to f_y(x)$ as $y' \to y$, uniformly in $x$ and $y$ (note that in our case all the important data, $B$ and $\mathbf{A}$, are bounded). Therefore $f_{y'} \to f_y$ in $L^2$ as $y' \to y$, uniformly in $y$, since $f_y$ and $f_{y'}$ are both dominated by a uniformly rapidly decaying function (free heat kernel). This proves the continuity of the heat kernel uniformly in time. Note that in [5] the continuous differentiability of $B$ was needed only to assure that there is a continuous gauge $\mathbf{A}$ with continuous divergence, which, in our case, is true anyway. The continuity of $B$ was used only in the first term of Eq. (76), and it can be relaxed to $B$ being in the Kato class (see [37]).

Fix a point $|x_0| > R$, then $P_{B_1}(x_0) > P_{B_2}(x_0)$ by Proposition 3.5. Let $\tilde{h}_\delta(x) = (\pi\delta^2)^{-1}\chi\{|x - x_0| \leq \delta\}$, be a function, and $h_\delta = (\tilde{h}_\delta, 0)$ be a spinor, according the the decomposition (1.2). By the continuity of the kernels $\lim_{\delta\to 0}(h_\delta, \Pi_B h_\delta) = \mathrm{Tr}_{\mathbf{C}^2}\, \Pi_B(x_0,x_0) = P_B(x_0)$ and

$$\lim_{\delta\to 0}(h_\delta, e^{-tH_{Pauli}(B,V=0)}h_\delta) = \mathrm{Tr}_{\mathbf{C}^2}\, e^{-tH_{Pauli}(B,V=0)}(x_0,x_0) - e^{-tH_{Sch}(B,V=B)}(x_0,x_0)$$

uniformly in $t$. Finally by the spectral theorem $(h_\delta, e^{-tH_{Pauli}(B,V=0)}h_\delta) \to (h_\delta, \Pi_B h_\delta)$ as $t \to \infty$ and by the diamagnetic inequality $|e^{-tH_{Sch}(B,V=B)}(x_0,x_0)| \leq (4\pi t)^{-1}$. Therefore

$$\limsup_{\delta\to 0}\limsup_{t\to\infty}\Big|\mathrm{Tr}_{\mathbf{C}^2}\, e^{-tH_{Pauli}(B,V=0)}(x_0,x_0) - P_B(x_0)\Big| = 0,$$

which completes the proof of Corollary 3.6. □

# A Appendix: Proof of Lemma 2.13

*Proof.* (*i.*) Obviously $\lambda_n \leq \lambda$ and is increasing. First consider the case $V \in L^1_{loc}(\mathbf{R}^d \setminus G)$. By Kato's theorem [11, Thm. VIII. 3.11] $H_n := -\Delta + V_n \to H := -\Delta + V$ in strong resolvent sense (since they converge on a common core), therefore

$$\lim_{n\to\infty} t^{-1}\log\Big(f, e^{-tH_n}f\Big) = t^{-1}\log\Big(f, e^{-tH}f\Big) \leq -\lambda$$

for all $t$, $\|f\| = 1$, and, by monotonicity of $H_n \nearrow H$ we know that the limit can be changed to infimum. On the other hand,

$$\lambda_n = -\lim_{t\to\infty} t^{-1}\log(f, e^{-tH_n}f) = -\inf_t t^{-1}\log(f, e^{-tH_n}f)$$

for any nonnegative, not identically zero function $f$ (since such a function is not orthogonal to the ground state). Therefore

$$\inf_n(-\lambda_n) = \inf_n \inf_t t^{-1}\log(f, e^{-tH_n}f) \leq -\lambda,$$

and (2.36) follows.

(*ii.*) If $V = \infty$ on $\Omega$, then one can define $V_{n,K} := \min\{K, V_n\}$, $V_K := \min\{K, V\}$, with the corresponding principal eigenvalues $\lambda_{n,K}$ and $\lambda_K$, which are monotonic increasing in $K$. For these potentials $\lim_{n\to\infty}(-\lambda_{n,K}) = \inf_n(-\lambda_{n,K}) = -\lambda_K$ for any $K$ using (*i.*). Now let $\lambda_\Omega$ be the lowest eigenvalue of $H_\Omega := -\Delta + V$ with Dirichlet boundary condition on $\mathbf{R}^d \setminus \Omega$. By variational principle $\lambda_K \geq \lambda_\Omega$. On the other hand

$$\lim_{K\to\infty}\Big(f, e^{-t(-\Delta+V_K)}f\Big) = \Big(f, e^{-tH_\Omega}f\Big) \tag{A.1}$$

for any $f$ which is positive on $\mathbf{R}^d \setminus \Omega$ and zero otherwise. This statement follows from the Feynman-Kac representation of both sides, since

$$\Big(f, e^{-t(-\Delta+V_K)}f\Big) - \Big(f, e^{-tH_\Omega}f\Big) = \int \mathrm{d}\mu(W) e^{-\frac{1}{2}\int_0^{2t} V_K(W_s)\mathrm{d}s}\chi(\tau(W) < 2t) f(W_0) f(W_{2t})$$

where $\tau$ is the first hitting time of the boundary $\partial\Omega$ and $\mathrm{d}\mu(W)$ is the $d$-dimensional Wiener measure. By the dominated convergence theorem $\int_0^{2t} V_K(W_s)\mathrm{d}s \to \infty$ as $K \to \infty$ for all path for which $\tau(W) < 2t$, since for these path $\{s : W_s \in \Omega\}$ has positive measure, and $V_K(W_s) = K$ if $W_s \in \Omega$ (similar proof, without potential, was given in [38, Lemma 1.2]).

Since the left hand side of (A.1) is decresing in $K$, we can replace the limit by infimum. We obtain

$$\inf_K(-\lambda_K) = \inf_t \inf_K t^{-1}\log\Big(f, e^{-t(-\Delta+V_K)}f\Big) = \inf_t t^{-1}\log\Big(f, e^{-tH_\Omega}f\Big) = -\lambda_\Omega$$

which completes the proof (see also [39] for a more general setup). □

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