Simple diamagnetic monotonicities for Schrödinger operators with inhomogeneous magnetic fields of constant direction

Hajo Leschke, Rainer Ruder and Simone Warzel

Institut für Theoretische Physik, Universität Erlangen–Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

E-mail: hajo.leschke@physik.uni-erlangen.de

Abstract. Under certain simplifying conditions we detect monotonicity properties of the ground-state energy and the canonical-equilibrium density matrix of a spinless charged particle in the Euclidean plane subject to a perpendicular, possibly inhomogeneous magnetic field and an additional scalar potential. Firstly, we point out a simple condition warranting that the ground-state energy does not decrease when the magnetic field and/or the potential is increased pointwise. Secondly, we consider the case in which both the magnetic field and the potential are constant along one direction in the plane and give a genuine path-integral argument for corresponding monotonicities of the density-matrix diagonal and the absolute value of certain off-diagonals. Our results complement to some degree results of M. Loss and B. Thaller [*Commun. Math. Phys.* **186** (1997) 95] and L. Erdős [*J. Math. Phys.* **38** (1997) 1289].

PACS numbers: 75.20.-g, 03.65.Ge

Dedicated to John R. Klauder on the occasion of his 70^{th} birthday

1. Introduction

In non-relativistic classical and quantum statistical mechanics of thermal equilibrium the ground-state energy and, more generally, the free energy of the considered particle system does not decrease when its external potential and/or interaction potential is increased. This monotonicity property continues to hold in the presence of a fixed external, possibly inhomogeneous magnetic field, a fact which is trivial in the classical situation, because here the magnetic field can be eliminated in accordance with the Bohr/van Leeuwen theorem [18] on the non-existence of diamagnetism in classical physics. In the non-trivial quantum case a monotonicity with respect to the magnetic field analogous to that in the potentials does not hold in such generality. Only few results are available. The most general one is due to the so-called diamagnetic inequality which implies that the free energy of a system of spinless distinguishable particles or of spinless bosons in an arbitrary magnetic field is not smaller than without [21, 23, 9, 20]. More generally, for such a system the absolute value of its canonical-equilibrium density matrix, that is, of the position representation of the underlying "Boltzmann operator" (in other words: heat kernel) does not decrease when the magnetic field is switched off. As observed by E. Nelson, this is most easily obtained by applying the triangle inequality to the Feynman-Kac(-Itô) path-integral representation of the density matrix [22, 23, 20]. A drawback of the diamagnetic inequality is that it only enables one to compare the two extreme situations with or without magnetic field. It does not supply control when a magnetic field is changed (pointwise) from a given non-zero value to another non-zero one. *Diamagnetic monotonicities* in this more general sense are in fact much harder to obtain and even wrong in general, already for one-particle systems. This has been nicely discussed by L. Erdős [6] in terms of illuminating examples and counterexamples for one-particle Schrödinger and Pauli operators. In deriving some of his results, Erdős was inspired by an interesting diamagnetic-monotonicity result of Loss and Thaller [15] for the density matrix of a spinless electrically charged particle subject exclusively to an inhomogeneous magnetic field of constant direction or, what amounts to the same, of a particle confined to a plane perpendicular to that field. (For a more precise statement, see (14) below.)

The present note is inspired by both works [15, 6]. Given the Schrödinger operator for a spinless charged particle in the Euclidean plane subject to a perpendicular and continuously differentiable but otherwise arbitrary magnetic field and to an additional (scalar) potential, we are going to present two results which to a certain extent complement results in [15, 6] and provide partial positive answers to the open problem [6, II.12]. We first point out a simple sufficient but, in general, somewhat implicit condition for the ground-state energy not to decrease when the magnetic field and/or the potential is increased pointwise. Secondly, a rather direct genuine path-integral argument yields a diamagnetic monotonicity for density matrices under the simplifying condition that both the magnetic field and the potential are constant along (at least) one direction in the plane. As a by-product, the estimate of Loss and Thaller [15] is sharpened for these special fields. The validity of both results and the simplicity of their proofs heavily rely on the fact that under the mentioned conditions the term in the Schrödinger operator which is linear in the canonical momentum can easily be brought under control.

In the remainder of the Introduction we set the stage and fix our basic notation. We consider a spinless charged particle in the Euclidean plane $\mathbb{R}^2$ and choose physical units where the mass and the charge of the particle as well as Planck's constant (divided by 2π) are all equal to one. The corresponding quantum system is characterized by a *Schrödinger operator*, or standard Hamiltonian, informally given by the expression

$$H(b,v) := \tfrac{1}{2}\big(\boldsymbol{P} - \boldsymbol{a}(\boldsymbol{Q})\big)^2 + v(\boldsymbol{Q}) \tag{1}$$

where $\boldsymbol{Q} = (Q_1, Q_2)$ and $\boldsymbol{P} = (P_1, P_2)$ denote the usual two-component vector operators of position and canonical momentum, respectively. Since we are interested in gauge-independent quantities only, we take the liberty to slightly abuse the notation in that the operator (1) actually depends on the vector potential $\boldsymbol{a} = (a_1, a_2)$ (and the scalar potential v) and not just on the magnetic field $b : \mathbb{R}^2 \to \mathbb{R}$ given by $b(\boldsymbol{x}) = \partial a_2(\boldsymbol{x})/\partial x_1 - \partial a_1(\boldsymbol{x})/\partial x_2$, where (x_1, x_2) is the pair of Cartesian co-ordinates of the point $\boldsymbol{x} \in \mathbb{R}^2$. We write $\boldsymbol{x} \cdot \boldsymbol{y} := x_1 y_1 + x_2 y_2$ for the Euclidean scalar product of $\boldsymbol{x}$, $\boldsymbol{y} \in \mathbb{R}^2$ and also $\boldsymbol{x}^2 := \boldsymbol{x} \cdot \boldsymbol{x}$ and $|\boldsymbol{x}| := \sqrt{\boldsymbol{x}^2}$. To avoid technical complications, we will assume throughout that $\boldsymbol{a} : \mathbb{R}^2 \to \mathbb{R}^2$ is continuously differentiable and $v : \mathbb{R}^2 \to \mathbb{R}$ is continuous and bounded from below. This in particular implies that $H(b,v)$ can be defined straightforwardly and uniquely as a self-adjoint bounded below operator acting on a dense domain in the separable Hilbert space $\mathrm{L}^2(\mathbb{R}^2)$ of all (equivalence classes of) Lebesgue square-integrable complex-valued functions on the plane with the usual scalar product $\langle \varphi, \psi \rangle := \int_{\mathbb{R}^2} d^2x\, \varphi(\boldsymbol{x})^* \, \psi(\boldsymbol{x})$, for φ, $\psi \in \mathrm{L}^2(\mathbb{R}^2)$.

The simplest quantity we are going to look at is the *ground-state energy* of $H(b,v)$, that is, the bottom of its spectrum, in symbols

$$e_0(b,v) := \inf \operatorname{spec} H(b,v) = \inf_{\langle\psi,\,\psi\rangle=1} \langle\psi,\, H(b,v)\,\psi\rangle. \tag{2}$$

Here the second infimum is taken over all normalized wave-functions ψ in the domain of $H(b,v)$. The other quantity we will deal with is the canonical-equilibrium *density matrix* of $H(b,v)$, that is, $\langle \boldsymbol{x}|\exp[-\beta H(b,v)]|\boldsymbol{y}\rangle$. It is defined as the in $\boldsymbol{x}$, $\boldsymbol{y} \in \mathbb{R}^2$ jointly continuous Hermitian integral kernel of the self-adjoint, non-negative and bounded "Boltzmann operator" $\exp[-\beta H(b,v)]$ corresponding to inverse temperature $\beta > 0$. In particular, the image $\exp[-\beta H(b,v)]\,\psi \in \mathrm{L}^2(\mathbb{R}^2)$ of an arbitrary $\psi \in \mathrm{L}^2(\mathbb{R}^2)$ has a continuous representative given by the function $\boldsymbol{x} \mapsto \int_{\mathbb{R}^2} d^2y\, \langle \boldsymbol{x}|\exp[-\beta H(b,v)]|\boldsymbol{y}\rangle\, \psi(\boldsymbol{y})$ and the density-matrix diagonal $\langle \boldsymbol{x}|\exp[-\beta H(b,v)]|\boldsymbol{x}\rangle$ is a well-defined, non-negative and continuous function of $\boldsymbol{x} \in \mathbb{R}^2$. For the precise definition of $H(b,v)$ and the existence of a continuous integral kernel of the corresponding "Boltzmann operator" (under much weaker assumptions on b and v), see [5, 23, 3, 4].

2. Monotonicity of ground-state energies

The following two facts, which we recall from [6], show that diamagnetic monotonicity fails in general already for ground-state energies.

Fact 1 ([6, II.10]): There exists a centrally symmetric potential $\hat{v}$ with the function $|\boldsymbol{x}| \mapsto \hat{v}(|\boldsymbol{x}|)$ being decreasing in some neighbourhood of some $|\boldsymbol{x}^{(0)}| > 0$. Moreover, there exist two constant magnetic fields b and $\hat{b}$ such that $0 < b < \hat{b}$ but $e_0(b,\hat{v}) > e_0(\hat{b},\hat{v})$.

Fact 2 ([6, II.11]): There exist two inhomogeneous centrally symmetric magnetic fields b and $\hat{b}$ such that $0 \le b(|\boldsymbol{x}|) \le \hat{b}(|\boldsymbol{x}|)$ for all $\boldsymbol{x} \in \mathbb{R}^2$ but $e_0(b,0) > e_0(\hat{b},0)$.

In both situations the ground-state wave-function $\hat{\psi}_0$ of $H(\hat{b},\hat{v})$, in the *Poincaré gauge*

$$\hat{\boldsymbol{a}}(\boldsymbol{x}) := (-x_2, x_1) \int_0^1 d\xi\, \xi\, \hat{b}\,(\xi\boldsymbol{x})\,, \tag{3}$$

is an eigenfunction of the canonical angular-momentum operator $L_3 := Q_1P_2 - Q_2P_1$ with a non-zero eigenvalue. Hence $\hat{\psi}_0$ is not real-valued. This motivates the additional assumption in

Theorem 1. *Let the Schrödinger operator $H(\hat{b},\hat{v})$ in the Poincaré gauge (3) possess a real-valued ground-state wave-function, that is, $e_0(\hat{b},\hat{v}) = \langle\hat{\psi}_0,\, H(\hat{b},\hat{v})\,\hat{\psi}_0\rangle$ for some real-valued $\hat{\psi}_0$ in the domain of $H(\hat{b},\hat{v})$ with $\langle\hat{\psi}_0,\, \hat{\psi}_0\rangle = 1$. Then the pointwise inequalities $|b(\boldsymbol{x})| \le \hat{b}(\boldsymbol{x})$ and $v(\boldsymbol{x}) \le \hat{v}(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathbb{R}^2$ imply the inequality*

$$e_0(b,v) \le e_0(\hat{b},\hat{v}) \tag{4}$$

for the corresponding ground-state energies.

Before giving a simple proof of the theorem at the end of the section, four remarks are in order:

- An unpleasant feature of Theorem 1 is that the additional assumption uses the special gauge (3) and therefore is not gauge independent. However, this gauge is often convenient, in particular, if $\hat{b}$ and $\hat{v}$ are centrally symmetric, see below. For other gauges the existence of a real-valued ground-state wave-function $\hat{\psi}_0$ is in general not sufficient to imply the monotonicity (4). Conversely, even in the gauge (3) the real-valuedness of $\hat{\psi}_0$ is not necessary for (4) to hold as the diamagnetic inequality $e_0(0, \hat{v}) \leq e_0(\hat{b}, \hat{v})$ illustrates [21]. (See also the Introduction and the first remark following Theorem 2 below.)

- If $e_0(\hat{b}, \hat{v})$ does not belong to the point spectrum of $H(\hat{b}, \hat{v})$, equivalently, if there is no square-integrable ground-state wave-function $\hat{\psi}_0$, assertion (4) remains true, provided there is a generalized real-valued ground-state, that is, a sequence $\{\hat{\psi}_{0,n}\}_{n\in\mathbb{N}}$ of real-valued functions in the domain of $H(\hat{b}, \hat{v})$ such that $\langle \hat{\psi}_{0,n}, \hat{\psi}_{0,n}\rangle = 1$ for all $n \in \mathbb{N}$ and $e_0(\hat{b}, \hat{v}) = \inf_{n\in\mathbb{N}} \langle \hat{\psi}_{0,n}, H(\hat{b}, \hat{v})\, \hat{\psi}_{0,n}\rangle$.
- If $\hat{b}$ is constant, one may use Lieb's inequality [1, App.]
$$e_0(\hat{b}, \hat{v}) \leq \tfrac{1}{2}\,|\hat{b}| + e_0(0, \hat{v}) \tag{5}$$
to further estimates the r.h.s. of (4).
- The subsequent proof shows that analogous statements hold in more than two dimensions and also for spinless (interacting) many-particle systems obeying either Boltzmann or Bose statistics.

If both $\hat{b}$ and $\hat{v}$ are centrally symmetric (or axially symmetric, when taking into account the third dimension along the magnetic-field direction), a ground-state wave-function $\hat{\psi}_0$ of $H(\hat{b}, \hat{v})$, in the gauge (3), is real-valued if and only if it is centrally symmetric or, equivalently, an eigenfunction of L_3 with eigenvalue zero, $L_3\hat{\psi}_0 = 0$. For vanishing magnetic field it is standard textbook wisdom [12, 8] that the ground state in a centrally symmetric potential is always given by a zero angular-momentum eigenfunction. For non-vanishing magnetic fields this is wrong in general, cf. [13, 1, 23]. However, in case the magnetic field $\hat{b} > 0$ is constant, the potential $\hat{v}$ is centrally symmetric and the function $|\boldsymbol{x}| \mapsto \hat{v}(|\boldsymbol{x}|)$ is non-decreasing, then there exists, cf. [2, Thm. 4.6], at least one $\hat{\psi}_0 \neq 0$ with $L_3\hat{\psi}_0 = 0$ in the (in general multi-dimensional) ground-state eigenspace of $H(\hat{b}, \hat{v})$ and the additional assumption of Theorem 1 is fulfilled. This applies for instance to the (centrally symmetric) harmonic-oscillator potential

$$v_{\mathrm{osc}}(\boldsymbol{x}) := \frac{\omega^2}{2}\boldsymbol{x}^2, \qquad \omega \geq 0, \tag{6}$$

and the attractive Coulomb-type potential,

$$v_{\mathrm{cou}}(\boldsymbol{x}) := -\frac{g}{\sqrt{\boldsymbol{x}^2 + \lambda^2}}, \qquad g,\, \lambda > 0. \tag{7}$$

Accordingly, Theorem 1 implies the following upper bounds on the ground-state energy of a spinless charged particle in the plane $\mathbb{R}^2$ subject to one of these potentials and to a perpendicular, possibly inhomogeneous magnetic field b the strength of which not exceeding a certain value, that is, $|b(\boldsymbol{x})| \leq \hat{b}$ for all $\boldsymbol{x} \in \mathbb{R}^2$ with some constant $\hat{b} > 0$,

$$e_0(b, v_{\mathrm{osc}}) \leq e_0(\hat{b}, v_{\mathrm{osc}}) = \sqrt{\left(\hat{b}/2\right)^2 + \omega^2}, \tag{8}$$

$$e_0(b, v_{\mathrm{cou}}) \leq e_0(\hat{b}, v_{\mathrm{cou}}). \tag{9}$$

The equality in (8) follows from the explicitly known [7, 17] spectral properties of $H(\hat{b}, v_{\mathrm{osc}})$ with a constant $\hat{b}$, see also (13) below.

Taking $\omega = 0$ and $\hat{b} = \sup_{\boldsymbol{x}\in\mathbb{R}^2} |b(\boldsymbol{x})|$ in (8) yields the upper bound in the following sandwiching estimate on the ground-state energy of a spinless charged particle in a globally bounded and continuously differentiable but otherwise arbitrary magnetic field $b : \mathbb{R}^2 \to \mathbb{R}$,

$$\tfrac{1}{2} \inf_{\boldsymbol{x}\in\mathbb{R}^2} \big|b(\boldsymbol{x})\big| \leq e_0(b,0) \leq \tfrac{1}{2} \sup_{\boldsymbol{x}\in\mathbb{R}^2} \big|b(\boldsymbol{x})\big|. \tag{10}$$

The lower bound in (10) is a consequence of the continuity of b together with the non-negativity of $H(b,0)$ and that of its associated Pauli operator [5], in symbols, $H(b,0) \geq 0$ and $H(b,0) \pm b(\boldsymbol{Q})/2 \geq 0$.

We close this section with a simple

Proof of Theorem 1. The vector potentials $\boldsymbol{a}$ and $\hat{\boldsymbol{a}}$ defined by (3) satisfy the pointwise inequality

$$|\boldsymbol{a}(\boldsymbol{x})| \leq |\boldsymbol{x}| \int_0^1 d\xi\, \xi\, |b(\xi\boldsymbol{x})| \leq |\boldsymbol{x}| \int_0^1 d\xi\; \xi\; \hat{b}(\xi\boldsymbol{x}) = |\hat{\boldsymbol{a}}(\boldsymbol{x})| \tag{11}$$

by the triangle inequality and the assumption $|b(\boldsymbol{x})| \leq \hat{b}(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathbb{R}^2$. The non-commutative binomial formula gives

$$\begin{aligned}\langle\psi,\, H(\hat{b},\hat{v})\,\psi\rangle &= \langle\psi,\, H(b,v)\,\psi\rangle + \operatorname{Re}\langle\psi, (\boldsymbol{a}(\boldsymbol{Q}) - \hat{\boldsymbol{a}}(\boldsymbol{Q}))\cdot\boldsymbol{P}\,\psi\rangle \\ &\quad + \tfrac{1}{2}\langle\psi, (\hat{\boldsymbol{a}}(\boldsymbol{Q})^2 - \boldsymbol{a}(\boldsymbol{Q})^2)\,\psi\rangle + \langle\psi, (\hat{v}(\boldsymbol{Q}) - v(\boldsymbol{Q}))\,\psi\rangle\end{aligned} \tag{12}$$

for any ψ in the domain of $H(0,0)$, hence in those of $H(b,v)$ and $H(\hat{b},\hat{v})$ by the Kato-Rellich theorem [5]. The real part of $\langle\psi, (\boldsymbol{a}(\boldsymbol{Q}) - \hat{\boldsymbol{a}}(\boldsymbol{Q}))\cdot\boldsymbol{P}\,\psi\rangle$ on the r.h.s. vanishes if ψ is real-valued, because $\boldsymbol{P}$ acts as the gradient divided by the imaginary unit $i = \sqrt{-1}$. Employing (11) and the assumption on the potentials the last two terms on the r.h.s. of (12) are both seen to be non-negative. Altogether this yields $e_0(b,v) \leq \langle\hat{\psi}_0\,, H(b,v)\,\hat{\psi}_0\rangle \leq \langle\hat{\psi}_0\,, H(\hat{b},\hat{v})\,\hat{\psi}_0\rangle = e_0(\hat{b},\hat{v})$ where the first inequality is a consequence of the Rayleigh-Ritz variational principle. $\square$

3. Monotonicity of density matrices

Diamagnetic monotonicity of density matrices (or only of their diagonals) implies monotonicity of the corresponding ground-state energies in the zero-temperature limit. Therefore, Facts 1 and 2 show that the former monotonicity can also neither hold in the presence of general potentials for two homogeneous magnetic fields nor in case of vanishing potential for two general magnetic fields. Accordingly, one can hope to find a diamagnetic monotonicity of density matrices only under additional assumptions on the magnetic fields and/or the potentials.

3.1. Globally constant magnetic fields and harmonic-oscillator potential

In case of a homogeneous, that is, globally constant magnetic field $b \in \mathbb{R}$ and the harmonic-oscillator potential (6), the density matrix is exactly known and, in the gauge

(3), explicitly given [19, 17] in terms of the ground-state energy $\Omega_b := \sqrt{(b/2)^2 + \omega^2}$, cf. (8), and hyperbolic functions by the Mehler-type of formula

$$\langle \boldsymbol{x}|\mathrm{e}^{-\beta H(b,v_{\mathrm{osc}})}|\boldsymbol{y}\rangle = \frac{\Omega_b}{2\pi \sinh{(\beta\Omega_b)}} \exp\left\{ -\frac{\Omega_b}{2\tanh{(\beta\Omega_b)}} \left[\boldsymbol{x}^2 + \boldsymbol{y}^2 - 2\boldsymbol{x}\cdot\boldsymbol{y}\frac{\cosh(\beta b/2)}{\cosh{(\beta\Omega_b)}} \right] \right\}$$
$$\times \exp\left\{ i\,\Omega_b \frac{\sinh(\beta b/2)}{\sinh(\beta\Omega_b)} (x_2 y_1 - x_1 y_2) \right\}. \qquad (13)$$

By discriminating the cases $\boldsymbol{x}\cdot\boldsymbol{y} \geq 0$ and $\boldsymbol{x}\cdot\boldsymbol{y} < 0$, an elementary (but somewhat tedious) calculation shows that the function $|b| \mapsto |\langle \boldsymbol{x}|\exp[-\beta H(b,v_{\mathrm{osc}})]|\boldsymbol{y}\rangle|$ is non-increasing for all $\omega \geq 0$, all $\boldsymbol{x}$, $\boldsymbol{y} \in \mathbb{R}^2$ and all $\beta > 0$. This monotonicity extends (8) in case of a globally constant b and, in view of Fact 1, is a particularity of the harmonic oscillator.

As for the monotonicity in the potential, we remark the following. The function $\omega \mapsto \langle \boldsymbol{x}|\exp[-\beta H(b,v_{\mathrm{osc}})]\,|\boldsymbol{x}\rangle$ is obviously non-increasing for all $b \in \mathbb{R}$, all $\boldsymbol{x} \in \mathbb{R}^2$ and all $\beta > 0$. This property of the harmonic-oscillator density-matrix diagonal is a stronger one than the universally valid (reverse) monotonicity of the free energy $-\beta^{-1}\ln\int_{\mathbb{R}^2} d^2x\,\langle \boldsymbol{x}|\exp[-\beta H(b,v)]\,|\boldsymbol{x}\rangle$ when v is pointwise increased, cf. the Introduction. However, the harmonic oscillator already illustrates that, in contrast to the situation with $b = 0$, monotonicity of the density-matrix off-diagonal in the potential in general ceases to hold for $b \neq 0$. More precisely, by elementary calculations one finds

Fact 3: There exist two constants b, $\beta > 0$ and a non-zero $\boldsymbol{x} \in \mathbb{R}^2$, such that the function $\omega \mapsto |\langle \boldsymbol{x}|\exp[-\beta H(b,v_{\mathrm{osc}})]\,|-\boldsymbol{x}\rangle|$ is increasing in some neighbourhood of some $\omega_0 > 0$.

3.2. Non-constant magnetic fields and vanishing potential

Loss and Thaller [15] studied the density matrix associated with an inhomogeneous magnetic field $\hat{b}$ which is globally bounded from below by a non-negative constant one. In particular, they have shown [15, Thm. 1.3] that the inequality

$$\left|\langle \boldsymbol{x}|\,\mathrm{e}^{-\beta H(\hat{b},0)}\,|\boldsymbol{y}\rangle\right| \leq \frac{b}{4\pi\sinh(\beta b/2)}\,\exp\Big[-\frac{(\boldsymbol{x}-\boldsymbol{y})^2}{2\beta}\Big] \qquad (14)$$

holds for all $\boldsymbol{x}$, $\boldsymbol{y} \in \mathbb{R}^2$ and all $\beta > 0$ as long as $b \leq \hat{b}(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathbb{R}^2$ with some constant $b \geq 0$. The Gaussian in (14) coincides with that of the free density matrix $\langle \boldsymbol{x}|\exp[-\beta H(0,0)]\,|\boldsymbol{y}\rangle$ and the pre-factor with the diagonal $\langle \boldsymbol{x}|\exp[-\beta H(b,0)]\,|\boldsymbol{x}\rangle$, which is actually independent of $\boldsymbol{x} \in \mathbb{R}^2$, see (13) with $\omega = 0$.

Erdős [6] has shown that (14) provides basically the best upper bound on the density-matrix off-diagonal one can hope for, unless $\hat{b} : \mathbb{R}^2 \to \mathbb{R}$ has further properties. More precisely, he proved that (14) cannot be improved universally by replacing its r.h.s. by $|\langle \boldsymbol{x}|\exp[-\beta H(b,0)]|\boldsymbol{y}\rangle|$, which has more rapid Gaussian decay as $|\boldsymbol{x}-\boldsymbol{y}| \to \infty$, cf. (13).

Fact 4 ([6, II.16]): Define $\hat{b}(\boldsymbol{x}) := (1 + x_1^2/\lambda^2)\,b$ with two constants b, $\lambda > 0$. Then $b \leq \hat{b}(\boldsymbol{x})$ for all $\boldsymbol{x} \in \mathbb{R}^2$, but $|\langle \boldsymbol{x}|\exp[-\beta H(\hat{b},0)]|\boldsymbol{y}\rangle| > |\langle \boldsymbol{x}|\exp[-\beta H(b,0)]|\boldsymbol{y}\rangle|$ for some $\lambda > 0$, some $\boldsymbol{x}$, $\boldsymbol{y} \in \mathbb{R}^2$ and some $\beta > 0$.

Nevertheless, in the next subsection it will turn out that (14) can still be improved at the cost of allowing only a restricted class of inhomogeneous magnetic fields (including the one of Fact 4).

3.3. Magnetic fields and potentials which are constant along one direction

In this subsection we will restrict ourselves to the special class of magnetic fields b which do not depend on the second co-ordinate x_2. This class covers the case of globally constant fields, for which the spectrum of the Schrödinger operator $H(b,0)$ is well known [7, 11, 9, 17] to consist only of isolated harmonic-oscillator like eigenvalues $(n-1/2)|b|$, $n \in \mathbb{N}$, of infinite degeneracy, the so-called Landau levels. However, in case such a field is not globally constant, $H(b,0)$ is conjectured [5] to possess only (absolutely) continuous spectrum. The first rigorous proof of this conjecture, was given by Iwatsuka [10] under certain additional assumptions, see also [5, 16]. In acknowledgement of this achievement, for such fields $H(b,0)$ often goes under the name *Iwatsuka model.*

In what follows, it is most convenient to choose the asymmetric gauge defined by

$$a_1(\boldsymbol{x}) := 0, \qquad a_2(x_1) := \int_0^{x_1} dx_1'\, b(x_1'). \tag{15}$$

Then the resulting Schrödinger operator

$$H(b,v) = \tfrac{1}{2}P_1^2 + \tfrac{1}{2}\big(P_2 - a_2(Q_1)\big)^2 + v(Q_1), \tag{16}$$

is translation invariant along the x_2-direction, provided the potential v does not depend on x_2, too. The operator (16) can therefore be decomposed by partial Fourier transformation into the one-parameter family $H_1(k) := P_1^2/2+(k-a_2(Q_1))^2/2+v(Q_1)$, $k \in \mathbb{R}$, of Schrödinger operators for the x_1-direction. As a consequence, one obtains for the density matrix of (16)

$$\begin{aligned}\langle \boldsymbol{x}|\, \mathrm{e}^{-\beta H(b,v)}\, |\boldsymbol{y}\rangle \;&= \int_{\mathbb{R}} \frac{dk}{2\pi}\, \langle x_1|\, \mathrm{e}^{-\beta H_1(k)}\, |y_1\rangle\, \mathrm{e}^{i(x_2-y_2)k} &(17)\\ &= (2\pi\beta)^{-1} \exp\Big[-\frac{(\boldsymbol{x}-\boldsymbol{y})^2}{2\beta}\Big] &(18)\\ &\times \int \mathbb{P}^{0,\beta}_{x_1,y_1}(dw)\, \exp\Big[i\,(x_2-y_2)\,\mu_\beta(a_2\circ w) - \beta\sigma_\beta^2(a_2\circ w) - \beta\mu_\beta(v\circ w)\Big].\end{aligned}$$

For the derivation of the second equality we used the Feynman-Kac formula [23, 20] for the density matrix of $H_1(k)$ in (17), which involves path integration with respect to the probability measure $\mathbb{P}^{0,\beta}_{x_1,y_1}$ of the one-dimensional Brownian bridge going from x_1 at time 0 to y_1 at time β. The latter is the unique normalized Gaussian measure on the set of continuous paths $w : [0,\beta] \to \mathbb{R}$, $\tau \mapsto w(\tau)$ with mean function $\tau \mapsto x_1+(y_1-x_1)\tau/\beta$ and covariance function $(\tau,\tau') \mapsto \min\{\tau,\tau'\} - \tau\tau'/\beta$. In (18) we are making use of the notations

$$\mu_\beta(f\circ w) := \beta^{-1}\int_0^\beta d\tau\, f\big(w(\tau)\big), \tag{19}$$

$$\sigma_\beta^2(f\circ w) := \mu_\beta\big((f\circ w)^2\big) - \big(\mu_\beta(f\circ w)\big)^2 \geq 0 \tag{20}$$

for the mean and variance of the composition $f\circ w$ of a continuous function $f:\mathbb{R}\to\mathbb{R}$ and a path w with respect to the uniform time average $\beta^{-1}\int_0^\beta d\tau\,(\cdot)$. To obtain (18) we also interchanged the (Lebesgue) integration with respect to k and the Browian-bridge integration by referring to the Fubini-Tonelli theorem. Thanks to translation invariance along the x_2-direction the density matrix of (16) depends on x_2 and y_2 only through their difference $x_2 - y_2$. Moreover, a nice feature of the path-integral representation (18) is that its integrand contains the magnetic field but is nevertheless non-negative if $x_2 = y_2$. This enables one to estimate the density matrix of (16) by using standard inequalities of general integration theory (cf. [14]) without loosing the dependence on the magnetic field. For example, the triangle inequality applied to (18) gives the (gauge-independent) estimate

$$\Big|\big\langle \boldsymbol{x}\big|\, \mathrm{e}^{-\beta H(b,v)}\,\big|\boldsymbol{y}\big\rangle\Big| \le \Big|\big\langle (x_1,0)\big|\, \mathrm{e}^{-\beta H(b,v)}\,\big|(y_1,0)\big\rangle\Big| \,\exp\Big[-\frac{(x_2-y_2)^2}{2\beta}\Big], \tag{21}$$

where, in the chosen gauge (15), it would not be necessary to take the absolute value of the r.h.s.. The following theorem provides a generalization of (21). For an interesting application of (18) in case a_2 is a Gaussian random field and $v = 0$, see [24].

Theorem 2. *Let b, $\hat{b}$ and v, $\hat{v}$ be two magnetic fields and two potentials, all four of them not depending on the second co-ordinate x_2. Then the pointwise inequalities $|b(x_1)| \le \hat{b}(x_1)$ and $v(x_1) \le \hat{v}(x_1)$ for all $x_1 \in \mathbb{R}$ imply the inequality*

$$\Big|\big\langle \boldsymbol{x}\big|\, \mathrm{e}^{-\beta H(\hat{b},\hat{v})}\,\big|\boldsymbol{y}\big\rangle\Big| \le \Big|\big\langle (x_1,0)\big|\, \mathrm{e}^{-\beta H(b,v)}\,\big|(y_1,0)\big\rangle\Big| \,\exp\Big[-\frac{(x_2-y_2)^2}{2\beta}\Big] \tag{22}$$

for all $\boldsymbol{x} = (x_1,x_2) \in \mathbb{R}^2$, all $\boldsymbol{y} = (y_1,y_2) \in \mathbb{R}^2$ and all $\beta > 0$.

Three special cases of (22) are worth to be mentioned separately:

- Theorem 2 and translation invariance along the x_2-direction implies monotonicity of the density-matrix diagonal in the magnetic field and the potential in the sense that $\langle \boldsymbol{x}|\exp[-\beta H(\hat{b},\hat{v})]\,|\boldsymbol{x}\rangle \le \langle \boldsymbol{x}|\exp[-\beta H(b,v)]\,|\boldsymbol{x}\rangle$ for all $\boldsymbol{x} \in \mathbb{R}^2$. In particular, in the zero-temperature limit $\beta \to \infty$ the monotonicity $e_0(b,v) \le e_0(\hat{b},\hat{v})$ of the corresponding ground-state energies emerges. In general, this monotonicity is not covered by Theorem 1 as the case $b = 0$ already illustrates.
- If $b > 0$ is globally constant and $v = \hat{v} = 0$, (22) together with (13) yields the following improvement of (14) for the present situation, in which $\hat{b}$ does not depend on x_2,
$$\Big|\big\langle \boldsymbol{x}\big|\, \mathrm{e}^{-\beta H(\hat{b},0)}\,\big|\boldsymbol{y}\big\rangle\Big| \le \frac{b}{4\pi\sinh(\beta b/2)}\,\exp\Big[-\frac{b}{4}\frac{(x_1-y_1)^2}{\tanh(\beta b/2)} - \frac{(x_2-y_2)^2}{2\beta}\Big]. \tag{23}$$
The Gaussian decay on the r.h.s. of (14) as $|x_1 - y_1| \to \infty$ may thus be replaced by that of $|\langle \boldsymbol{x}|\exp[-\beta H(b,0)]\,|\boldsymbol{y}\rangle|$. However, as illustrated by Fact 4, this is not allowed for the Gaussian decay along the perpendicular direction in the plane. In this sense (23) is optimal for the present situation. For given non-negative $\hat{b} : \mathbb{R} \to [0,\infty[$, the r.h.s. of (23) is minimized by taking $b = \inf_{x_1\in\mathbb{R}} \hat{b}(x_1)$.
- If $\hat{b} > 0$ is globally constant and $v = \hat{v} = 0$, (22) together with (13) yields the following lower estimate on certain density-matrix off-diagonals
$$\frac{\hat{b}}{4\pi\sinh\big(\beta\hat{b}/2\big)}\,\exp\left[-\frac{\hat{b}}{4}\frac{(x_1-y_1)^2}{\tanh\big(\beta\hat{b}/2\big)}\right] \le \Big|\big\langle (x_1,0)\,\big|\,\mathrm{e}^{-\beta H(b,0)}\,\big|\,(y_1,0)\big\rangle\Big|. \tag{24}$$
For given $b : \mathbb{R} \to \mathbb{R}$, the l.h.s. of (24) is maximized by taking $\hat{b} = \sup_{x_1\in\mathbb{R}} |b(x_1)|$.

Proof of Theorem 2. Without loosing generality, we may choose for b the gauge (15) and analogously for $\hat{b}$. Then we observe the pathwise non-negativity

$$\begin{aligned}
&\sigma_\beta^2(\hat{a}_2\circ w) - \sigma_\beta^2(a_2\circ w) \\
&= \frac{1}{2\beta^2}\int_0^\beta d\tau \int_0^\beta d\tau' \,\Big\{\big[\hat{a}_2(w(\tau)) - \hat{a}_2(w(\tau'))\big]^2 - \big[a_2(w(\tau)) - a_2(w(\tau'))\big]^2\Big\} \\
&= \frac{1}{2\beta^2}\int_0^\beta d\tau \int_0^\beta d\tau' \,\Big[a_+\big(w(\tau)\big) - a_+\big(w(\tau')\big)\Big]\Big[a_-\big(w(\tau)\big) - a_-\big(w(\tau')\big)\Big] \ge 0.
\end{aligned} \tag{25}$$

Here the non-negativity of the last integrand follows from the fact that the two functions $x_1 \mapsto a_\pm(x_1) := \hat{a}_2(x_1) \pm a_2(x_1) = \int_0^{x_1} dx_1' \left[\hat{b}(x_1') \pm b(x_1')\right]$, cf. (15), are both non-decreasing since $\hat{b}(x_1') \geq |b(x_1')| \geq \mp b(x_1')$ for all $x_1' \in \mathbb{R}$ by assumption. Besides (25) we have $\mu_\beta(v \circ w) \leq \mu_\beta(\hat{v} \circ w)$, also by assumption. Employing both inequalities in (18) with $x_2 = y_2$, the proof is completed with the help of (21) (with b replaced by $\hat{b}$). □

4. Concluding remark

We conclude by specifying part of the open problem [6, II.12] which deals with the complementary situation of (14).

Open problem: Let $b : \mathbb{R}^2 \to \mathbb{R}$ be continuously differentiable and satisfy $|b(\boldsymbol{x})| \leq \hat{b}$ for all $\boldsymbol{x} \in \mathbb{R}^2$ with some constant $\hat{b} > 0$. Prove or disprove the assertion

$$\left|\left\langle \boldsymbol{x} \,\middle|\, \mathrm{e}^{-\beta H(\hat{b},0)} \,\middle|\, \boldsymbol{y} \right\rangle\right| \leq \left|\left\langle \boldsymbol{x} \,\middle|\, \mathrm{e}^{-\beta H(b,0)} \,\middle|\, \boldsymbol{y} \right\rangle\right| \tag{26}$$

for all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^2$ and all $\beta > 0$.

The present note contains partial support for the validity of this assertion. Namely, (26) is true at least in each of the following three limiting cases:

- to logarithmic accuracy in the zero-temperature limit, by the second inequality in (10).
- if b is constant along the x_2-direction and $x_2 = y_2$, by (24).
- if b is globally constant, by (13) with $\omega = 0$.

The third case is well known.

Acknowledgments

This work was partially supported by the Deutsche Forschungsgemeinschaft under grant no. Le 330/12. The latter is a project within the Schwerpunktprogramm "Interagierende stochastische Systeme von hoher Komplexität" (DFG Priority Programme SPP 1033).

References

[1] Avron J, Herbst I and Simon B 1978 Schrödinger operators with magnetic fields. I. General interactions *Duke Math. J.* **45** 847–883
[2] Avron J E, Herbst I W and Simon B 1981 Schrödinger operators with magnetic fields. III. Atoms in homogeneous magnetic field *Commun. Math. Phys.* **79** 529–572
[3] Broderix K, Hundertmark D and Leschke H 2000 Continuity properties of Schrödinger semigroups with magnetic fields *Rev. Math. Phys.* **12** 181–225
[4] Broderix K, Leschke H and Müller P Continuous integral kernels for unbounded Schrödinger semigroups and their spectral projections (in preparation)
[5] Cycon H L, Froese R G, Kirsch W and Simon B 1987 *Schrödinger operators* (Berlin: Springer)
[6] Erdős L 1997 Dia- and paramagnetism for nonhomogenous magnetic fields *J. Math. Phys.* **38** 1289–1317
[7] Fock V 1928 Bemerkung zur Quantelung des harmonischen Oszillators im Magnetfeld (in German) *Z. Physik* **47** 446–448
[8] Galindo A and Pascual P 1990 *Quantum mechanics* I (Berlin: Springer)
[9] Galindo A and Pascual P 1991 *Quantum mechanics* II (Berlin: Springer)
[10] Iwatsuka A 1985 Examples of absolutely continuous Schrödinger operators in magnetic fields *Publ. Res. Inst. Math. Sci.* **21** 385–401

[11] Landau L 1930 Diamagnetismus der Metalle (in German) *Z. Physik* **64** 629–637
[12] Landau L D and Lifshitz E M 1959 *Quantum mechanics: The non-relativistic theory* (London: Pergamon)
[13] Lavine R and O'Carroll M 1977 Ground state properties and lower bounds for energy levels of a particle in a uniform magnetic field and external potential *J. Math. Phys.* **18** 1908–1912
[14] Lieb E H and Loss M 2001 *Analysis* (2^{nd} edition) (Providence: Amer. Math. Soc.)
[15] Loss M and Thaller B 1997 Optimal heat kernel estimates for Schrödinger operators with magnetic fields in two dimensions *Commun. Math. Phys.* **186** 95–107
[16] Măntoiu M and Purice R 1997 Some propagation properties of the Iwatsuka model *Commun. Math. Phys.* **188** 691–708
[17] Matsumoto H 1996 Quadratic Hamiltonians and associated orthogonal polynomials *J. Funct. Anal.* **136** 214–225
[18] Mattis D C 1988 *The theory of magnetism* I (corr. 2^{nd} printing) (Berlin: Springer)
[19] Papadopoulos G J 1971 Magnetization of harmonically bound charges *J. Phys. A: Math. Gen.* **4** 773–781
[20] Roepstorff G 1996 *Path integral approach to quantum physics* (2^{nd} printing) (Berlin: Springer)
[21] Simon B 1976 Universal diamagnetism of spinless Bose systems *Phys. Rev. Lett.* **36** 1083–1084
[22] Simon B 1977 An abstract Kato's inequality for generators of positivity preserving semigroups *Ind. Math. J.* **26** 1067–1073
[23] Simon B 1979 *Functional integration in quantum physics* (New York: Academic)
[24] Ueki N 2000 Simple examples of Lifschitz tails in Gaussian random magnetic fields *Ann. Henri Poincaré* **1** 473–498