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Calculus of Variations

Absence of positive eigenvalues of magnetic Schrödinger operators

Silvana Avramska-Lukarska[1] · Dirk Hundertmark[1,2] · Hynek Kovařík[3]

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Abstract

We study sufficient conditions for the absence of positive eigenvalues of magnetic Schrödinger operators in $\mathbb{R}^d$, $d \geq 2$. In our main result we prove the absence of eigenvalues above certain threshold energy which depends explicitly on the magnetic and electric field. A comparison with the examples of Miller–Simon shows that our result is sharp as far as the decay of the magnetic field is concerned. As applications, we describe several consequences of the main result for two-dimensional Pauli and Dirac operators, and two and three dimensional Aharonov–Bohm operators.

Mathematics Subject Classification 35Q40 · 35P05

1 Introduction and description of main results

The question of the absence of positive eigenvalues of Schrödinger operators has a long history. In 1959 Kato proved that the operator $-\Delta + V$ in $L^2(\mathbb{R}^d)$ has no positive eigenvalues if V is continuous and such that

$$V(x) = o(|x|^{-1}) \qquad |x| \to \infty, \tag{1.1}$$

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✉ Hynek Kovařík
hynek.kovarik@unibs.it

Silvana Avramska-Lukarska
silvana.avramska-lukarska@kit.edu

Dirk Hundertmark
dirk.hundertmark@kit.edu

1 Department of Mathematics, Institute for Analysis, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

2 Department of Mathematics, University of Illinois at Urbana-Champaign, 1409 W. Green Street, Urbana, IL 61801-2975, USA

3 DICATAM, Sezione di Matematica, Università degli studi di Brescia, Brescia, Italy

by deriving suitable lower bounds on solutions of the Schrödinger equation. His lower bound showed that for positive energies these solutions decay so slowly at infinity that they are not normalizable, see [24]. It is known that condition (1.1) is essentially optimal since there exist oscillatory potentials of the Wigner-von Neumann type, decaying as $|x|^{-1}$, which produce positive eigenvalues of the associated Schrödinger operator, see [37, 44] or [36, Ex. VIII.13.1].

Kato's result was generalized by Simon [37], who considered, for $d = 3$, potentials of the class $L^2 + L^\infty$ which are smooth outside a compact set and allow there a decomposition $V = V_1 + V_2$ with $V_1 = o(|x|^{-1})$, $V_2(x) = o(1)$, and

$$\omega_0 = \limsup_{|x|\to\infty} x \cdot \nabla V_2(x) < \infty. \tag{1.2}$$

Under these conditions Simon proved the absence of eigenvalues of $-\Delta + V$ in the interval (ω_0, ∞). Note that $\omega_0 \geq 0$ since $V_2(x) \to 0$ as $|x| \to \infty$. Indeed, since $V_2(x) = V(0) + \int_0^{|x|} s\widehat{x} \cdot \nabla V_2(s\widehat{x}) \, \frac{ds}{s}$ with $\widehat{x} = x/|x|$ one sees that if ω_0 were negative then $\lim_{|x|\to\infty} V_2(x) = -\infty$. Later it was shown by Agmon [1] that under similar assumptions the operator $-\Delta + V$, in any dimension, has no eigenvalues in the interval $(\omega_0/2, \infty)$.

The use of virial identites to exclude positive eigenvalues for specific potentials V, such as the Coulomb potential, has a long tradition in theoretical physics. Rigorous results can be found in [43] and [2], the latter includes also magnetic operators, with strong regularity conditions on the magnetic field B *and the associated vector potential* A, the latter being *not invariant* under gauge transformations. By exploiting a clever exponentially weighted virial identity, Froese, Herbst, and the Hoffmann–Ostenhofs proved the absence of all positive eigenvalues of $-\Delta + V$ under relative compactness conditions on V and $x \cdot \nabla V$, [15, 16] in the non–magnetic case. Their conditions on the regularity and decay on V and $x \cdot \nabla V$ were still global but much more general than the pointwise conditions of Kato, Simon, and Agmon, or the approaches based on virial identities. The use of virial identities before the work [16] is nicely explained in [12].

Yet another approach to the problem is based on Carleman estimates in L^p-spaces. This method allows to further weaken the regularity and decay conditions and to include rough potentials, see the works of Jerison and Kenig [22], Ionescu and Jerison [19], and the article [26] by Koch and Tataru.

Much less is known about the absence of positive eigenvalues for magnetic Schrödinger operators of the form

$$H = (P - A)^2 + V, \qquad P = -i\nabla, \tag{1.3}$$

in particular in dimension two. In the above equation A stands for a magnetic vector potential satisfying curl $A = B$. The results obtained by Koch and Tataru in [26] cover also Schrödinger operators with magnetic fields. But they impose decay conditions on the vector potential A which are *not gauge invariant* and which imply, in the case of dimension two, that the total flux of the magnetic field must vanish. Therefore they cannot be applied to two-dimensional Schrödinger operators with magnetic fields of non-zero flux.

Certain implicit conditions for the absence of eigenvalues of the operator (1.3) in $\mathbb{R}^2$ were recently found by Fanelli, Krejčiřík and Vega in [13], see also [14]. However, their result guarantees absence of *all* eigenvalues of H, not only of the positive ones. Consequently the hypotheses needed in [13] include some smallness conditions on V and B which are not necessary for the absence of positive eigenvalues only. In [18] Ikebe and Saito proved a limiting absorption principle for H under certain pointwise decay conditions on V and B, see Remark 1.5.

A particular case with $V = 0$ was considered by Iwatsuka in [20]. He proved that if B is smooth, non-constant and translationally invariant in one direction, then the spectrum of H in dimension two is purely absolutely continuous. We refer to [9, Sec. 6.5] for further reading on this subject.

In this work we develop quadratic form methods which are an effective tool to rule out positive eigenvalues for a large class of magnetic Schrödinger operators while at the same time allowing the existence of negative eigenvalues, which one does not want to rule out a priori. In addition, intuition from physics and experience from the rigorous study of Schrödinger operators without magnetic fields clearly show that while eigenvalues depend on global properties of the potential and the magnetic field, energies in the essential spectrum depend only on asymptotic properties. Thus, the nonexistence of eigenvalues embedded in the essential spectrum should depend *only on the asymptotic behavior* of the potential and the magnetic field, as long as the local behavior of the potential and magnetic field is not so singular such that it destroys the self–adjointness of the magnetic Schrödinger operator. Our results make this intuition rigorous: the *local behavior* of the magnetic field and the potential is *largely irrelevant* for the non-existence of positive eigenvalues. Our results also cover cases where the magnetic field decays so slowly that no choice of vector potential satisfies the conditions in [26].

In dimension two we identify the magnetic field with a scalar function which, in turn, can be interpreted as a vector field in $\mathbb{R}^3$ perpendicular to the plane $\mathbb{R}^2$. In general dimension the magnetic field is closed two–form, i.e., $dB = 0$, in the sense of distributions, with d the exterior derivative. Hence B can be identified with an antisymmetric matrix–valued function on $\mathbb{R}^d$. The condition $dB = 0$ then is equivalent to the condition

$$\partial_j B_{k,i} + \partial_k B_{i,j} + \partial_i B_{j,k} = 0 \qquad \forall\, i, j, k \in \{1, \ldots, d\}. \tag{1.4}$$

Here $B_{j,k}(x)$ denotes the entries of B at a point $x \in \mathbb{R}^d$. If $d = 3$, then B is an antisymmetric 3×3 matrix

$$\begin{pmatrix} 0 & -B_3 & B_2 \\ B_3 & 0 & -B_1 \\ -B_2 & B_1 & 0 \end{pmatrix}$$

which is in turn identified with a vector field $B = (B_1, B_2, B_3)$. Equation (1.4) thus coincides with the usual divergence free condition

$$\nabla \cdot B = 0 \qquad [\, d = 3\,], \tag{1.5}$$

dictated by Maxwell's equations.
It is well known that as soon as B satisfies (1.4) and certain mild regularity conditions, then there exists a vector potential A, a one–form, such that $B = \mathrm{curl} A$ or $B = dA$, with the exterior derivative.

1.1 The method

Let us briefly describe our method and its most important novel features. As already mentioned above we build upon the technique invented by R. Froese and I. Herbst and M. and Th. Hoffmann–Ostenhof [16] and further developed in [15]. The latter is based on weighted virial identities which require working with dilations and their generator. For non-magnetic Schrödinger operators this is facilitated by the fact that the momentum operator P has very simple commutation relations with dilations. In particular, the domain of P is invariant under dilations. This is not true anymore for the magnetic operators, since the vector potential spoils the dilation invariance of the domain of $P - A$.

One of the crucial new features of our approach shows that to overcome this difficulty one has to work with a vector potential A in the Poincaré gauge and exploit its connection with the dilations and the virial theorem. This connection, which enables us to develop a quadratic form version of the magnetic virial theorem, is explained in Sect. 3. We also show that the rather different conditions of Kato and Agmon–Simon are, in fact, just two sides of the same coin. Kato's condition for the absence of positive eigenvalues can be easily recovered from the quadratic form version of the virial of the potential, see Sect. 3.3 for details.

Moreover, the use of the Poincaré gauge leads to very natural decay conditions on B required for the absence of positive eigenvalues. The well-known example by Miller and Simon, see Sect. 5, shows that these conditions are sharp. In particular, it follows from the Miller-Simon example that no choice of the gauge can provide better decay conditions on B.

1.2 A typical result

In order to describe a typical result with general and easy to verify conditions on the magnetic field B and the potential V, we need some more notation. We denote by $L^p = L^p(\mathbb{R}^d)$, $1 \le p \le \infty$ the usual scale of Lebesgue spaces. Moreover, we need their locally uniform versions

$$L^p_{\mathrm{loc,unif}} = \left\{ V : \sup_{x\in\mathbb{R}^d} \int_{|x-y|\le 1} |V(y)|^p \, dy < \infty \right\} \tag{1.6}$$

with norms

$$\|V\|_{L^p_{\mathrm{loc,unif}}} := \sup_{x\in\mathbb{R}^d} \left(\int_{|x-y|\le 1} |V(y)|^p \, dy \right)^{1/p} \tag{1.7}$$

when $1 \le p < \infty$ and the obvious modification for $p = \infty$. Clearly these spaces are nested, that is, $L^q_{\mathrm{loc,unif}} \subset L^p_{\mathrm{loc,unif}}$ when $1 \le p \le q \le \infty$. Moreover, we need

Definition 1.1 (*Vanishing at infinity locally uniformly (in L^p)*) A function $V \in L^p_{\mathrm{loc,unif}}$ with

$$\lim_{R\to\infty} \|\mathbb{1}_{\ge R} V\|_{L^p_{\mathrm{loc,unif}}} = 0 \tag{1.8}$$

vanishes at infinity locally uniformly in $L^p_{\mathrm{loc,unif}}$.

Here $\mathbb{1}_{\ge R}$ is the characteristic function of the set $\{x \in \mathbb{R}^d : |x| \ge R\}$. In fact, we will only need the $p = 1, 2$ versions of vanishing locally uniformly in L^p at infinity.

This definition is inspired by Section 3 in [23]. It allows us to effectively treat magnetic fields and potentials which can have severe singularities even close to infinity.

Given a magnetic field B and a point $w \in \mathbb{R}^d$ let $\widetilde{B}_w(x) := B(x + w)[x]$. More precisely, $\widetilde{B}_w$ is a vector–field on $\mathbb{R}^d$ with components

$$(\widetilde{B}_w)_j(x) := (B(x + w)[x])_j = \sum_{m=1}^{d} B_{j,m}(x + w)\, x_m\,, \quad j = 1, \dots, d\,. \tag{1.9}$$

Using translations, we will usually assume $w = 0$, in which case we will simply write $\widetilde{B}$. In dimension two, identifying the magnetic field with a scalar, the vector field $\widetilde{B}_w$ is given by $\widetilde{B}_w(x) = B(x + w)(-x_2, x_1)$ and in three dimensions it is given by the cross product $\widetilde{B}_w(x + w) = B(x + w) \wedge x$.

In order to guarantee that there is a locally square integrable vector potential A with $dA = B$, we need

Lemma 1.2 *Given a magnetic field B and $w \in \mathbb{R}^d$ let $\widetilde{B}_w$ be given by (1.9) and assume that*

$$\int_{|x-w|<R} |x-w|^{2-d} \left(\log \frac{R}{|x-w|} \right)^2 |\widetilde{B}_w(x)|^2 \, dx < \infty$$

for all $R > 0$. Then there exists a vector potential $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d)$ with $B = dA$ in the sense of distributions.

In the sequel, given a vector field X on $\mathbb{R}^d$ we write $X \in L^q_{\mathrm{loc,unif}}$ as a shorthand meaning that the Euclidean norm of X belongs to $L^q_{\mathrm{loc,unif}}$.
The simplest version of our results is given by

Theorem 1.3 (Simple version) *Given a magnetic field B assume that $\widetilde{B}_w \in L^p_{loc,unif}$ for some $p > d$ and some $w \in \mathbb{R}^d$. Then there exists a vector potential $A \in L^2_{loc}(\mathbb{R}^d, \mathbb{R}^d)$ with $B = dA$. Moreover, let V be a potential with $V \in L^q_{loc,unif}$ for some $q > d/2$ that allows a splitting $V = V_1 + V_2$ such that $xV_1 \in L^{q_1}_{loc,unif}$ for some $q_1 > d$ and $x \cdot \nabla V_2 \in L^{q_2}_{loc,unif}$ for some $q_2 > d/2$ and assume that $\widetilde{B}$ and xV_1 vanish at infinity locally uniformly in L^2 and V, V_1, and $x \cdot \nabla V_2$ vanish at infinity locally uniformly in L^1.*

Then the magnetic Schrödinger operator $(P - A)^2 + V$, defined via quadratic form methods, has no positive eigenvalues.

Remarks 1.4 (i) The decay condition on xV_1, respectively $x \cdot \nabla V_2$, are generalizations, in terms of local L^p conditions, of the pointwise conditions of Kato [24], respectively Agmon [1] and Simon [37]. For a generalization using only natural quadratic form conditions, see Theorems 1.6 and 4.8 below.

(ii) Even in this simplest version the conditions on B and V allow for strong local singularities and the decay condition at infinity is rather mild: for example, if one splits V in such a way that V_1 is compactly supported. Then xV_1 is zero outside a compact set, so clearly vanishing at infinity. The condition $xV_1 \in L^{q_1}_{\mathrm{loc,unif}}$ for some $q_1 > d$ allows for rather large local singularities. In particular, the virial $x \cdot \nabla V$ has only to exist in a neighborhood of infinity in order to be able to apply Theorem 1.3. One can also include a long range part of V in V_1. Moreover, since $|\widetilde{B}_w(x)| \lesssim |B(x+w)||x|$, the magnetic field can have strong local singularities, in particular at w. The decay of the magnetic field B has to be faster than $\langle x - w \rangle^{-1}$, which is, at leas in dimension two, in line of what one expects from the Miller–Simon examples, see Sect. 5.1.

Let us now briefly describe our main results in full generality.

1.3 Full quadratic form version: absence of all positive eigenvalues

It turns out that the absence of positive eigenvalues depends, in a sense, *only* on the behavior of $\widetilde{B}$, xV and $x \cdot \nabla V$ *at infinity* with respect to the operator $(P - A)^2$. The latter are to be understood in a weak sense according to the following

Definition 1.5 (*Vanishing at infinity*) We say that a potential W vanishes at infinity with respect to $(P - A)^2$ if for some $R_0 > 0$ its quadratic form domain $\mathcal{Q}(W)$ contains all

$\varphi \in \mathcal{D}(P-A)$ with $\mathrm{supp}(\varphi) \in \mathcal{U}^c_{R_0}$ and for $R \geq R_0$ there exist positive α_R, γ_R with $\alpha_R, \gamma_R \to 0$ as $R \to \infty$ such that

$$|\langle\varphi, W\varphi\rangle| \leq \alpha_R \|(P-A)\varphi\|_2^2 + \gamma_R\|\varphi\|_2^2 \quad \text{for all } \varphi \in \mathcal{D}(P-A) \text{ with } \mathrm{supp}(\varphi) \subset \mathcal{U}^c_R \tag{1.10}$$

Here $\mathcal{U}_R = \{x \in \mathbb{R}^d : |x| < R\}$ and $\mathcal{U}^c_R = \mathbb{R}^d \setminus \mathcal{U}_R$ is its complement.

By monotonicity we may assume, without loss of generality, that α_R and γ_R are decreasing in $R \geq R_0$.
We then have

Theorem 1.6 *Given a magnetic field B assume that it fulfills the condition of Lemma 1.2 for some $w \in \mathbb{R}^d$ and that $\widetilde{B}^2_w$ given by (1.9) is relatively form bounded and vanishes at infinity with respect to $(P-A)^2$. Moreover, assume that the potential V is form small and vanishes at infinity with respect to $(P-A)^2$ and allows for a splitting $V = V_1 + V_2$, such that $|xV_1|^2$ and $x \cdot \nabla V_2$ are also form small and vanish at infinity with respect to $(P-A)^2$.*

Then the magnetic Schrödinger operator $(P-A)^2 + V$, defined via quadratic form methods, has essential spectrum $[0, \infty)$ and no positive eigenvalues.

Remarks 1.7 Some comments concerning Theorem 1.6:

(i) We only need relative form boundedness of $\widetilde{B}^2_w$ with respect to $(P-A)^2$. Its relative form bound does not have to be less than one.

(ii) While the conditions on the potential V and the magnetic field B with respect to $(P-A)^2$ might be difficult to check, the diamagnetic inequality

$$\big|P|\varphi|\big| \leq \big|(P-A)\varphi\big| \quad \text{a.e.} \qquad \text{for all } \varphi \in \mathcal{D}(P-A), \tag{1.11}$$

see e.g. [25], shows that it is enough to check them with respect to the non-magnetic kinetic energy P^2, see [4].

(iii) One can again absorb strong local singularities of the potential in a suitable choice of V_1. Thus the local behavior of the potential V and the magnetic field B is *largely irrelevant* for the non-existence of positive eigenvalues. Moreover, the virial $x \cdot \nabla V_2$ has to exist only in a weak quadratic form sense, see Lemma 3.7 and the discussion in Sect. 3.3.

(iv) An inspection of the proof shows that in Theorem 1.6 it is enough to assume that $x \cdot \nabla V$ is bounded from above at infinity by zero, see Definition 1.8 below for the precise meaning. Classically the force is given by $F = -\nabla V$. Thus $x \cdot F = -x \cdot \nabla V$ is negative, i.e., the force is *confining*, if $x \cdot \nabla V$ is positive, otherwise the force is *repulsive*, i.e., it pushes the particle further to infinity. Thus in order to prevent localization of a quantum particle only the positive part of $x \cdot \nabla V$ should have to be small at infinity.

(v) We would like to stress that unlike many other results on the absence of positive eigenvalues for magnetic Schrödinger operators that we are aware of, with the exception of [13] and [18], we impose only conditions on the magnetic field B and not directly on the vector potential A. Decay and regularity conditions on the vector potential A are not invariant under gauge transformations and thus unphysical. The conditions of [13], on the other hand, are quite restrictive. For example, in [13] the authors need that various *global* quantities related to the magnetic field B and to the potential V are absolute form bounded with respect to $(P-A)^2$, i.e. without allowing for lower order terms in the respective bounds and they need an explicit smallness condition for the various constants involved in their bounds. Consequently, the resulting assumptions turn out to be so strong that they rule out existence of any eigenvalue.

However, for a large class of physically relevant potentials and magnetic fields one expects that the corresponding magnetic Schrödinger operator has negative eigenvalues, while it typically should not have positive eigenvalues, at least when the magnetic field and the potential vanish in a suitable sense at infinity. This is exactly what our Theorem 1.6 and its generalizations below provide.

(vi) In order to prove invariance of the essential spectrum, one usually assumes that the potential V is relatively $(P-A)^2$ form compact. We do not assume this! In fact, we show in Theorem 4.8 that if the potential V is form small, i.e., form bounded with relative bound < 1, and vanishes at infinity with respect to $(P-A)^2$, then $\sigma_{\text{ess}}((P-A)^2+V) = \sigma_{\text{ess}}((P-A)^2)$. This shows invariance of the essential spectrum under a large class of perturbations. In particular, it confirms the physical intuition that local singularities, as long as they do not destroy form smallness, cannot influence the essential spectrum, at least as a set. For example, one can have a potential with local Hardy type singularity and even a sequence of suitably decreasing Hardy type singularities moving to infinity. Moreover, using ideas of Combesure and Ginibre [6] and Maz'ya and Verbitzky [31], we can allow perturbations with rather strong oscillations, both locally and at infinity.

(vii) Theorem 1.6 above is the most general formulation of our results, when one considers magnetic fields and potentials vanishing at infinity, in a suitable sense. We can allow for much ore general condition on the potential V and the magnetic field B, see the following section and Sect. 2.3 below for more general assumptions.

1.4 Full quadratic form version: absence of eigenvalues above a positive threshold

If $\widetilde{B}^2$, $|xV_1|^2$ and $x\cdot\nabla V_2$ do not vanish at infinity with respect to $(P-A)^2$, we can still exclude positive eigenvalues above a certain threshold. For this we need

Definition 1.8 (*Bounded at infinity*) A potential W is bounded from above at infinity with respect to $(P-A)^2$ if for some $R_0 > 0$ its quadratic form domain $\mathcal{Q}(W)$ contains all $\varphi \in \mathcal{D}(P-A)$ with $\operatorname{supp}(\varphi) \in \mathcal{U}_{R_0}^c$ and for $R \geq R_0$ there exist positive α_R, γ_R with $\lim_{R\to\infty}\alpha_R = 0$ and $\liminf_{\mathbb{R}\to\infty}\gamma_R < \infty$ such that

$$\langle \varphi, W\varphi\rangle \leq \alpha_R\|(P-A)\varphi\|_2^2 + \gamma_R\|\varphi\|_2 \quad \text{for all } \varphi\in\mathcal{D}(P-A) \text{ with } \operatorname{supp}(\varphi)\subset\mathcal{U}_R^c. \tag{1.12}$$

By monotonicity we may assume, without loss of generality, that α_R and γ_R are decreasing in $R \geq R_0$ in which case we set $\gamma_\infty^+(W) := \lim_{R\to\infty}\gamma_R = \inf_R \gamma_R$, the asymptotic bound upper bound of W (at infinity).

A potential W is bounded from below at infinity with respect to $(P-A)^2$ if $-W$ is bounded from above at infinity. We set $\gamma_\infty^-(W) = \gamma_\infty^+(-W)$.

A potential W is bounded at infinity with respect to $(P-A)^2$ if $\pm W$ are bounded from above at infinity. We set

$$\gamma_\infty(W) := \sup(\gamma_\infty^+(W), \gamma_\infty^-(W)),$$

the asymptotic bound on W (at infinity).

We say that a quadratic form q, not necessarily given by a locally integrable potential W, is bounded from above at infinity w.r.t. $(P-A)^2$ if, for all large enough $R > 0$, its domain $\mathcal{D}(q)$ contains all $\varphi\in\mathcal{D}(P-A)$ with $\operatorname{supp}(\varphi)\subset\mathcal{U}_R^c$ and a bound of the form (1.12) holds with $\langle\varphi, W\varphi\rangle$ replaced by $q(\varphi)$. We define $\gamma_\infty^+(q)$ similarly as for a potential W and set $\gamma_\infty^-(q):=\gamma_\infty^+(-q)$ and $\gamma_\infty(q):=\sup(\gamma_\infty^+(q), \gamma_\infty^-(q))$.

Using the diamagnetic inequality, one can replace $(P-A)^2$ by P^2 in the definition of the asymptotic bounds $\gamma_\infty^+(W)$ and $\gamma_\infty(W)$. We split $V = V_1 + V_2$ and set

$$\beta^2:=\gamma_\infty\big(\widetilde{B}^2\big), \quad \omega_1^2:=\gamma_\infty\big((xV_1)^2\big), \quad \omega_2:=\gamma_\infty^+\big(x\cdot\nabla V_2\big). \tag{1.13}$$

Of course, $\gamma_\infty^+\big(x\cdot\nabla V_2\big)$ is a-priori only defined when the distributional derivative $x\cdot\nabla V_2$ is given by a nice enough function. In the general case, we replace the formal expression $\langle\varphi, x\cdot\nabla V_2\varphi\rangle$ by the quadratic form $q_{x\cdot\nabla V_2}$ associated with this distribution. See (2.21), Lemma 3.7, and the discussion in Sect. 3.3 for the precise meaning of this quadratic form.

Under mild regularity conditions the magnetic Schrödinger operator $(P-A)^2+V$ has $[0,\infty)$ as its essential spectrum and our main result, Theorem 4.8, implies that it has no eigenvalues larger than

$$\Lambda(B,V) = \Lambda := \frac{1}{4}\left(\beta+\omega_1+\sqrt{(\beta+\omega_1)^2+2\omega_2}\right)^2. \tag{1.14}$$

While the β, ω_1, and ω_2 might be difficult to compute directly from the definition it is easy to see

$$\beta \le \limsup_{|x|\to\infty} |\widetilde{B}(x)|, \qquad \omega_1 \le \limsup_{|x|\to\infty} |x|\,|V_1(x)|, \qquad \omega_2 \le \limsup_{|x|\to\infty} x\cdot\nabla V_2(x). \tag{1.15}$$

once the limits are well-defined and finite. We would like to point out that Theorem 4.8 can be applied also in situations in which the limits in (1.15) might not be defined. Morally, $\gamma_\infty(W)$ is the bounded part of W at infinity, modulo terms which are small at infinity uniformly locally in $L^1(\mathbb{R}^d)$: If a potential W is locally uniformly in L^p near infinity, with $p=1$ for $d=1$ and $p>d/2$ for $d\ge 2$, and if $W-W_b$ vanishes at infinity locally uniformly in $L^1(\mathbb{R}^d)$ for some bounded function W_b, then

$$\gamma_\infty(W) \le \|W_b\|_\infty. \tag{1.16}$$

A similar bound holds for $\gamma_\infty^+(W)$. These bounds also hold if W is uniformly locally in L^p, or in the Kato–class, outside of a compact set, see Section A. In particular, Remark A.6 and Propositions A.4 and A.9.

1.5 Relation to previous works

If $B=0$, then by choosing $V_1=V$ and $V_2=0$ we obtain a generalization of the result of Kato [24]. On the other hand, by choosing V_1 such that $V_1(x)=o(|x|^{-1})$, and setting $V_2=V-V_1$ we get $\Lambda=\omega_0/2$, see Eq. (1.2), and recover thus the results of Agmon [1] and Simon [37]. Moreover, Theorem 4.8 extends all the above mentioned results to magnetic Schrödinger operators with magnetic fields which decay fast enough so that $\beta=0$, see Appendix A for more details.

Vice-versa, if $V=0$, then we have $\Lambda=\beta$ which is in agreement with the well–known example by Miller and Simon [32], cf. Sect. 5 if one corrects a calculation error in their examples. The Miller–Simon examples show that our condition on the magnetic field for absence of eigenvalues above a threshold is sharp.

It is tempting to split $V=sV+(1-s)V$ and to optimize the resulting expression for the threshold energy (1.14) with respect to $0\le s\le 1$. This minimization problem can be

explicitly done. It turns out that the minimum is always given by the minimum of the two extreme cases $s = 0$ and $s = 1$, see Corollary C.2 in Appendix C.
Ikebe and Saito proved in [18] a limiting absorption principle, and hence also the absence of eigenvalues of H under the condition that V allows the same decomposition as above with $|V_1(x)| \le C\,|x|^{-1-\delta}$, $|V_2(x)| \le C\,|x|^{-\delta}$, $|x \cdot \nabla V_2(x)| \le C\,|x|^{-\delta}$, and that B is continuous and satisfies $|B(x)| \le C\,|x|^{-1-\delta}$. Here C and δ are positive constants. Note that these pointwise conditions are covered by Theorem 4.8. Indeed, if V and B satisfy these upper bounds, then $\beta = \omega_1 = \omega_2 = 0$, see (1.15).

Remarks 1.9 In [7] it was proved that if the magnetic fields has the form

$$B(x) = \frac{b(\theta)}{r}, \quad x = (r\cos\theta,\, r\sin\theta), \quad b \in L^\infty(\mathbb{S}^1),$$

then the operator $H_{A,}$ has no eigenvalues above $\|b\|^2_{L^\infty(\mathbb{S}^1)}$. Note that in this particular setting $\Lambda = \|b\|^2_{L^\infty(\mathbb{S}^1)}$.

Remarks 1.10 One of the authors of the present paper established in [27] dispersive estimates for the propagator e^{-itH} in weighted L^2-spaces under the condition that H has no positive eigenvalues, see [27, Assumption 2.2]. Theorem 4.8 implies that the latter assumption can be omitted. This was, in fact, one of the main motivations for the present work.

1.6 Essential spectrum

In Sect. 6 we establish new sufficient conditions on B under which

$$\sigma_{\text{ess}}((P - A)^2) = [0, \infty).$$

Roughly speaking we require that $B(x) \to 0$ not uniformly, but only along a certain path connecting to infinity, see Theorem 6.5 and Definition 6.3 for details. For example, in $\mathbb{R}^2$ it suffices that $B(x) \to 0$ in a sector of positive opening angle. As a consequence of this result we show that under the assumptions stated in Sect. 2.3 we have $\sigma_{\text{ess}}((P - A)^2) = [0, \infty)$, cf. Corollary 6.8. We also show that if the potential V is form small and vanishes at infinity w.r.t $(P - A)^2$, then $\sigma_{\text{ess}}((P - A)^2 + V) = \sigma_{\text{ess}}((P - A)^2)$, see Theorem 6.10. For this one usually assumes that V is *relative form compact* w.r.t. $(P - A)^2$ which is a considerably stronger assumption, excluding, for example, Hardy–type singularities. Our result proves invariance of the essential spectrum under a conditions which includes all physically relevant examples, even exotic ones with strong singularities or oscillations.

1.7 Organization of the paper

The article is organized as follows. In Sect. 2 we prove some preliminary results on the properties of the Poincaré gauge and its relation to magnetic Schrödinger operators. In Sect. 3 we establish a magnetic virial theorem together with a weighted version, which is our key technical tool. The main results are stated and proved in Sect. 4. In Sect. 5 we present various examples of applications including Pauli and Dirac operators. Auxiliary material is collected in Appendices.

2 Magnetic Schrödinger operators and the Poincaré gauge

First let us fix some notation. Given a set M and two functions $f_1,\ f_2 : M \to \mathbb{R}$, we write $f_1(x) \lesssim f_2(x)$ if there exists a numerical constant c such that $f_1(x) \le c\, f_2(x)$ for all $x \in M$. The symbol $f_1(x) \gtrsim f_2(x)$ is defined analogously. Moreover, we use the notation

$$f_1(x) \sim f_2(x) \quad \Leftrightarrow \quad f_1(x) \lesssim f_2(x) \ \wedge \ f_2(x) \lesssim f_1(x),$$

and

$$\lim_{|x|\to\infty} f(x) = L \quad \Leftrightarrow \quad \lim_{r\to\infty} \operatorname*{ess\,sup}_{|x|\ge r} |f(x) - L| = 0. \tag{2.1}$$

The quantities $\limsup_{|x|\to\infty} f(x)$ and $\liminf_{|x|\to\infty} f(x)$ are defined in a similar way. We will use $\partial_j = \frac{\partial}{\partial x_j}$ for the usual partial derivatives in the weak sense, i.e., as distributions. For any $u \in L^r(\mathbb{R}^d)$ with $1 \le r \le \infty$ we will use the shorthand

$$\|u\|_r := \|u\|_{L^r(\mathbb{R}^d)}$$

for the L^r-norm of u and

$$\|T\|_{r\to r} := \|T\|_{L^r(\mathbb{R}^d)\to L^r(\mathbb{R}^d)}$$

for a norm of a bounded linear operator $T : L^r(\mathbb{R}^d) \to L^r(\mathbb{R}^d)$. The space $L_{\mathrm{loc}}(\mathbb{R}^d)$ is the space of all complex valued functions f such that $f\mathbb{1}_K \in L^r(\mathbb{R}^d)$ for all compact sets $K \subset \mathbb{R}^d$. Here $\mathbb{1}_K$ stands for the indicator function of K. By $L^r_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d)$ we denote the space of all vector fields v which are locally in L^r, that is, $|v|{:=}(\sum_{j=1}^d v_j^2)^{1/2}\mathbb{1}_K$ is $L^r_{\mathrm{loc}}(\mathbb{R}^d)$.

The space $\mathcal{C}_0^\infty = \mathcal{C}_0^\infty(\mathbb{R}^d)$ is the space of all complex valued test–functions f which are infinitely often differentiable and have compact support. Given measurable complex valued functions $f, g \in L^2(\mathbb{R}^d)$ we denote by

$$\langle f, g\rangle = \int_{\mathbb{R}^d} \overline{f(x)} \cdot g(x)\, dx$$

the usual scalar product on $L^2(\mathbb{R}^d)$. By the symbol

$$\mathcal{U}_R(x) = \{y \in \mathbb{R}^d \ : \ |x - y| < R\}$$

we denote the ball of radius R centered at a point $x \in \mathbb{R}^d$. If $x = 0$, we abbreviate

$$\mathcal{U}_R = \mathcal{U}_R(0).$$

2.1 The magnetic Schrödinger operator

Given a magnetic vector potential $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d)$, the magnetic Sobolev space is defined by

$$\mathcal{H}^1_A{:=}\mathcal{H}^1_A(\mathbb{R}^d){:=}\mathcal{D}(P - A) = \left\{u \in L^2(\mathbb{R}^d) \ : \ (P - A)\,u \in L^2(\mathbb{R}^d)\right\}, \tag{2.2}$$

equipped with the graph norm

$$\|u\|_{\mathcal{H}^1_A} = \left(\|(P - A)u\|_2^2 + \|u\|_2^2\right)^{1/2}. \tag{2.3}$$

Here $P = -i\nabla$ is the momentum operator. It is well-know that

$$q_{A,0}(\varphi, \psi) := \langle (P - A)\varphi, (P - A)\psi \rangle \tag{2.4}$$

is a closed sesqui–linear form on $\mathcal{H}_A^1 \times \mathcal{H}_A^1$, for any magnetic vector potential $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d)$, and that $\mathcal{C}_0^\infty(\mathbb{R}^d)$ is dense in $\mathcal{H}_A^1 = \mathcal{D}(P - A)$, and $\mathcal{C}_0^\infty(\mathbb{R}^d) \times \mathcal{C}_0^\infty(\mathbb{R}^d)$ is dense in $\mathcal{H}_A^1 \times \mathcal{H}_A^1$. see [39, Thm. 2.2]. By a slight abuse of notation, given a sesqui–linear form q with domain $\mathcal{Q} \times \mathcal{Q}$, we will use the notation $q(\varphi) = q(\varphi, \varphi)$, $\varphi \in \mathcal{Q}$, for the associated quadratic form. Hence

$$q_{A,0}(\varphi) = q_{A,0}(\varphi, \varphi) := \langle (P - A)\varphi, (P - A)\varphi \rangle = \|(P - A)\varphi\|_2^2 \tag{2.5}$$

is a closed quadratic form on $\mathcal{H}_A^1$ for any magnetic vector potential $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d)$, and that $\mathcal{C}_0^\infty(\mathbb{R}^d)$ is dense in $\mathcal{D}(P - A)$. We will only consider symmetric sesqui–linear forms $q : \mathcal{Q} \times \mathcal{Q} \to \mathbb{C}$, i.e., $q(\varphi, \psi) = \overline{q(\psi, \varphi)}$ for all $\varphi, \psi \in \mathcal{Q}$. Thus the associated quadratic forms will be real–valued.

Since every closed positive quadratic form on a Hilbert space corresponds to a unique self-adjoint positive operators [35] [42, Theorem 2.14], the quadratic form $q_{A,0}$ defines an operator, which we denote by $H_0 = H_{A,0} = (P - A)^2$. Note that for $u \in \mathcal{D}(P - A)$ one has $Au \in L^1_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d)$. So we only know that $Pu \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ for a typical $u \in \mathcal{D}(P - A)$, which is one of the sources for technical difficulties of Schrödinger operators with magnetic fields. Nevertheless, Kato's inequality shows $|\varphi| \in \mathcal{D}(P)$ for any $\varphi \in \mathcal{D}(P - A)$ and the diamagnetic inequality (1.11), see also [17, 37], yields

$$|((P - A)^2 + \lambda)^{-1}\varphi| \le (P^2 + \lambda)^{-1}|\varphi| \tag{2.6}$$

for all $\lambda > 0$ and $\varphi \in L^2(\mathbb{R}^d)$.

A potential V is a locally integrable, measurable function $V : \mathbb{R}^d \to \mathbb{R}$. Hence its quadratic form domain $\mathcal{Q}(V) = \mathcal{D}(|V|^{1/2})$ contains $\mathcal{C}_0^\infty(\mathbb{R}^d)$. The quadratic form q_V corresponding to V is given by

$$q_V(\varphi) = \left\langle |V|^{1/2}\varphi, \operatorname{sgn}(V)|V|^{1/2}\varphi \right\rangle. \tag{2.7}$$

With a slight abuse of notation, we will often write $q_V(\varphi) = \langle \varphi, V\varphi \rangle$.

A quadratic form q with domain $\mathcal{D}(q)$ is form bounded w.r.t. $(P - A)^2$ if its domain $\mathcal{D}(q)$ contains $\mathcal{D}(P - A)$ and there exists $\alpha, C_\alpha < \infty$ such that

$$|q(\varphi)| \le \alpha \|(P - A)\varphi\|_2^2 + C_\alpha \|\varphi\|_2^2 \quad \text{for all } \varphi \in \mathcal{D}(P - A). \tag{2.8}$$

The infimum

$$\alpha_0 = \inf\{\alpha > 0 : \text{ there exists } C_\alpha < \infty \text{ such that (2.8) holds for all } \varphi \in \mathcal{D}(P - A)\}$$

is called the (relative) form bound of q with respect to $(P - A)^2$.

We say that q is (relative) form small w.r.t $(P - A)^2$ if $\alpha_0 < 1$, i.e., the bound (2.8) holds for some $0 \le \alpha < 1$ and $C_\alpha < \infty$. If $\alpha_0 = 0$ one says that V is infinitesimally form small w.r.t. $(P - A)^2$.

In a similar way this extends to other pairs of operators and their associated quadratic forms. For example, a potential V is form bounded w.r.t $(P-A)^2$ if the associated quadratic form $q_V(\varphi) = \langle \varphi, V\varphi \rangle = \langle \operatorname{sgn} V|V|^{1/2}\varphi, |V|^{1/2}\varphi \rangle$ with domain $\mathcal{D}(q_V) = \mathcal{Q}(V)$ is form bounded w.r.t. $(P-A)^2$. The potential V is form small, respectively, infinitesimally form bounded, w.r.t. $(P-A)^2$ if q_V is form small, repectively, infinitesimally form bounded, w.r.t. $(P-A)^2$.

If a quadratic form q_1 is form small with respect to $(P-A)^2$, the KLMN Theorem, see e.g. [42, Theorem 6.24], [36], shows that the sum

$$q_{A,q_1}(\varphi) := \|(P-A)\varphi\|_2^2 + q_1(\varphi) = \langle (P-A)\varphi, (P-A)\varphi \rangle + q_1(\varphi) \tag{2.9}$$

with domain $\mathcal{D}(q_{A,q_1}) := \mathcal{D}(P-A)$ defines a closed quadratic form which is bounded from below. It corresponds to a unique self-adjoint operator H_{A,q_1}, which is called the form sum of $(P-A)^2$ and q_1.

In case $q_1 = q_V$ is the quadratic form associated to a potential $V \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$, we write

$$q_{A,V}(\varphi) := \|(P-A)\varphi\|_2^2 + q_V(\varphi) = \langle (P-A)\varphi, (P-A)\varphi \rangle + \langle \varphi, V\varphi \rangle \tag{2.10}$$

for the form sum and and $H_{A,V} = (P-A)^2 + V$ for the associated operator. We will sometimes drop the dependence of $H_{A,V}$ and simply write H for the full magnetic Schrödinger operator.

The diamagnetic inequality implies that if a quadratic form q is form bounded, respectively form small w.r.t. P^2, then it is also form bounded, respectively form small w.r.t. $(P-A)^2$ with the same constants, see [4].

Except for Tiktopoulos' formula (2.12), the following is well–known.

Lemma 2.1 *Let q be a (real–valued) quadratic form with domain $\mathcal{D}(q) \supset \mathcal{D}(P-A)$. Then q is form bounded w.r.t. $(P-A)^2$ if and only if for any $\lambda > 0$ the quadratic form given by*

$$q_\lambda(\varphi) := q\left(\left((P-A)^2 + \lambda\right)^{-1/2} \varphi \right) \tag{2.11}$$

corresponds to a bounded linear operator $C_q(\lambda)$ such that $\langle \varphi, C_q(\lambda)\varphi \rangle = q_\lambda(\varphi)$ for all $\varphi \in L^2$. The bound (2.8) holds with

$$\alpha = \|C_\lambda\|_{2\to 2} \qquad \text{and } \beta = \lambda \, \|C_\lambda\|_{2\to 2} \,,$$

and the relative form bound α_0 of q w.r.t. $(P-A)^2$ is given by

$$\alpha_0 = \lim_{\lambda\to\infty} \|C_\lambda\|_{2\to 2} \ .$$

If $q(\varphi) = q_V(\varphi) = \langle \operatorname{sgn}(V)|V|^{1/2}\varphi, |V|^{1/2}\varphi \rangle$ for some potential $V \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$, then

$$C_\lambda := ((P-A)^2 + \lambda)^{-1/2} V ((P-A)^2 + \lambda)^{-1/2} \tag{2.12}$$

Moreover, if $\alpha_0 < 1$ denote by $H_0 = (P-A)^2$ and by H the self-adjoint operator given by the form sum of the quadratic forms $q_{A,0}(\varphi) = \langle (P-A)\varphi, (P-A)\varphi \rangle$ and q. Then Tiktopoulos' formula for the resolvent

$$(H+\lambda)^{-1} = (H_0+\lambda)^{-1/2} \left(1 + C_q(\lambda)\right)^{-1} (H_0+\lambda)^{-1/2} \tag{2.13}$$

holds for all large enough λ.

Proof This is well–known, see [36], [38, Chapter II.3], and, in particular, [42, Theorem 6.30]. Tiktopoulos' formula (2.12) holds once $\lambda > 0$ and $-\lambda \in \rho(H)$, the resolvent set of H (i.e., the resolvents $(H+\lambda)^{-1}$ and $(H_0+\lambda)^{-1}$ are defined) and $\|C_q(\lambda)\|_{2\to 2} < 1$. □

One could extend the above setting by allowing a splitting $V = V_+ - V_-$, where the positive and negative parts of V are given by $V_\pm = \max(\pm V, 0)$. The discussion in [39] shows that for arbitrary $V_+ \in L^1_{\mathrm{loc}}$, the quadratic form

$$q_{A,V_+}(\varphi,\varphi) := \|(P-A)\varphi\|_2^2 + \langle \varphi, V_+\varphi\rangle = \|(P-A)\varphi\|_2^2 + \|\sqrt{V_+}\varphi\|_2^2 \tag{2.14}$$

is well defined and closed on the form domain $\mathcal{D}(Q_{A,V_+}) = \mathcal{D}((P-A)) \cap \mathcal{Q}(V_+)$, where $\mathcal{Q}(V_+) = \mathcal{D}(\sqrt{V_+})$ and that $\mathcal{C}_0^\infty$ is still dense in $\mathcal{D}(Q_{A,V_+})$ in the graph norm $\|\varphi\|_{A,V_+} = (\mathcal{Q}_{A,V_+}(\varphi) + \|\varphi\|_2^2)^{1/2}$. Again this closed quadratic form corresponds to a unique self–adjoint operator H_{A,V_+} and in order to define a self–adjoint operator $H_{A,V}$ via the KLMN theorem. It is enough to assume that V_- is form small w.r.t. H_{A,V_+}.

More important for us is the observation due to Combescure and Ginibre [6] that rather singular potentials V can be form bounded with respect to P^2, and by the diamagnetic inequality then also with respect to $(P-A)^2$.

Lemma 2.2 *Assume that $V = \nabla\cdot\Sigma + W$, where $\Sigma \in L^2_{loc}(\mathbb{R}^d;\mathbb{R}^d)$, and W is locally integrable. Suppose that Σ^2 and W are form bounded w.r.t. $(P-A)^2$, respectively P^2. Then the quadratic form*

$$\langle \varphi, V\varphi\rangle := -2\,\mathrm{Im}\,\langle \Sigma\varphi, (P-A)\varphi\rangle + \langle \varphi, W\varphi\rangle \tag{2.15}$$

is also form bounded w.r.t. $(P-A)^2$, respectively P^2.

Proof For $\varphi \in \mathcal{C}_0^\infty$, an integration by parts shows

$$\langle \varphi, (\nabla\cdot\Sigma)\varphi\rangle = -2\,\mathrm{Im}\,\langle \Sigma\varphi, P\varphi\rangle = -2\,\mathrm{Im}\,\langle \Sigma\varphi, (P-A)\varphi\rangle.$$

Thus, for all $\varepsilon > 0$

$$|\langle \varphi, (\nabla\cdot\Sigma)\varphi\rangle| \le 2\|\Sigma\varphi\|\,\|P\varphi\| \le \varepsilon\|P\varphi\|^2 + \varepsilon^{-1}\|\Sigma\varphi\|^2 \le (\alpha+\varepsilon)\|P\varphi\|^2 + \varepsilon^{-1}C_\alpha\|\Sigma\varphi\|^2$$

when $\|\Sigma\varphi\|^2 = \langle \varphi, \Sigma^2\varphi\rangle \le \alpha\|P\varphi\|^2 + C_\alpha\|\Sigma\varphi\|^2$. The claim follows. □

In the non–magnetic case, the beautiful work of Maz'ya and Verbitsky [32] shows that all potential V which are relatively form bounded w.r.t. P^2 are of the form (2.15).

2.2 The Poincaré gauge

The magnetic field at the point $x \in \mathbb{R}^d$ is given by an antisymmetric two-form $B(x) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, which we identify with a matrix valued function B given by

$$B(x) = (B_{j,m}(x))_{j,m=1}^d,$$

which is antisymmetric, $B_{j,m}(x) = -B_{m,j}(x)$ for all $1 \le j, m \le d$, $x \in \mathbb{R}^d$.

Any vector potential A, or more precisely a one form, generates a magnetic field via the exterior derivative $B = dA$, in the distributional sense. In matrix notation, $B_{j,m} = \partial_j A_m - \partial_m A_j$. In three space dimensions, one can identify the two form B with a vector valued function $B = \mathrm{curl} A$.

For a given magnetic field B and a point $w \in \mathbb{R}^d$ we define the vector field $\widetilde{B}_w$ by equation (1.9), and put

$$A_w(x) := \int_0^1 \widetilde{B}_w(tx)\, dt = \int_0^1 B(tx+w)[tx]\, dt\,, \tag{2.16}$$

which is the vector potential in the Poincaré gauge. Using translations, it is no loss of generality to assume $w = 0$, in which case we will simply write A for the vector potential given by (2.16). By going to spherical coordinates, one easily checks at least for nice, say continuous or even smooth, magnetic fields B, that the above vector potential is well defined and that $dA = B$ in the sense of distributions.

Since B is antisymmetric the vector $\widetilde{B}(x) = B(x)[x]$ is orthogonal to x. Hence, when $w = 0$ the vector potential A given by (2.16) satisfies the transversal, or Poincaré, gauge

$$x \cdot A(x) = 0 \qquad \forall\, x \in \mathbb{R}^d, \tag{2.17}$$

which will be very important in our discussion of dilations and the virial theorem for magnetic Schrödinger operators in Sect. 3. It is easy to see that for A given by (2.16) one has $A \in L^2_{\text{loc}}(\mathbb{R}^d, \mathbb{R}^d)$ for bounded magnetic fields B and this extends to a large class of singular magnetic fields, see Lemma 2.12 below. Except otherwise noted, we will always use the Poincaré gauge in the following. For a nice discussion of the Poincaré gauge from a physics point of view see [21] and from a more mathematical point of view, but still for rather regular magnetic fields, see [41].

2.3 Hypotheses

Recall that we identify the magnetic two form B at a point x with an antisymmetric matrix $B(x)$ and define $\widetilde{B}_w(x) = B(x+w)[x]$ in the sense of the matrix vector product. We will use the following hypotheses on B and V:

Assumption 2.3 The magnetic field B is such that for some $w \in \mathbb{R}^d$ and

$$\mathbb{R}^d \ni x \mapsto |x-w|^{2-d} \log^2\left(\frac{R}{|x-w|}\right) \widetilde{B}_w(x)^2 \in L^1_{\text{loc}}(\mathcal{U}_R(w)) \tag{2.18}$$

for all $R > 0$, where $\mathcal{U}_R(w) = \{x \in \mathbb{R}^d : |x-w| < R\}$ is the open ball of radius R around w.

As already remarked, there is no loss of generality assuming $w = 0$ by using translations. Together with Lemma 2.12 the above mild integrability condition then assures that the corresponding vector potential in the Poincaré gauge is locally square integrable, which is essential in order to define the magnetic Schrödinger operator. The magnetic field B can have severe local singularities, while Assumption 2.3 still holds.

Assumption 2.4 The scalar field $|\widetilde{B}|^2$ is relatively form bounded w.r.t. $(P-A)^2$, where A is the Poincaré gauge vector potential corresponding to B, That is,

$$\langle \varphi, |\widetilde{B}|^2 \varphi \rangle = \|\widetilde{B}\varphi\|_2^2 \lesssim \|(P-A)\varphi\|_2^2 + \|\varphi\|_2^2 \qquad \forall\, \varphi \in \mathcal{D}(P-A). \tag{2.19}$$

Assumption 2.5 The potential V is relatively form small w.r.t. $(P-A)^2$, that is, there exist constants $\alpha_0 < 1$ and $\gamma > 0$ such that

$$|\langle \varphi, V\varphi \rangle| \le \alpha_0 \|(P-A)\varphi\|_2^2 + \gamma \|\varphi\|_2^2 \qquad \forall\, \varphi \in \mathcal{H}^1_A(\mathbb{R}^d). \tag{2.20}$$

We also need similar conditions on the virial $x \cdot \nabla V$ of the potential. Since we don't want to impose strong differentiability conditions on V, one has to be a bit careful: The virial $x \cdot \nabla V$ is, at first, a distribution. When $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, an formal integration by parts argument similar to the one in the proof of Lemma 2.2 shows that

$$\begin{aligned} q_{x\cdot\nabla V}(\varphi) &= \langle \varphi, x \cdot \nabla V \varphi\rangle = -d\langle \varphi, V\varphi\rangle - 2\,\mathrm{Re}\,\langle xV\varphi, \nabla\varphi\rangle \\ &= -d\langle \varphi, V\varphi\rangle - 2\,\mathrm{Im}\,\langle xV\varphi, P\varphi\rangle = -d\langle \varphi, V\varphi\rangle - 2\,\mathrm{Im}\,\langle xV\varphi, (P-A)\varphi\rangle \end{aligned} \tag{2.21}$$

since $\langle xV\varphi, A\varphi\rangle$ is real for all $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d)$. We assume that the form $q_{x\cdot\nabla V}$ extends to a quadratic form whose domain contains all $\mathcal{D}(P-A)$ and, by a slight abuse of notation, will write $q_{x\cdot\nabla V}$ for this extension. A careful discussion when $q_{x\cdot\nabla V}$ is form bounded w.r.t. $(P-A)^2$ is given in Lemma 3.7 and in Sect. 3.3.
For the assumptions which give us control of virial $x \cdot \nabla V$, we decompose the potential $V = V_1 + V_2$. How one splits $V = V_1 + V_2$ is quite arbitrary, as long as the conditions below are met.

Assumption 2.6 If the potential is split as $V = V_1 + V_2$, then $V_1, x^2V_1^2$ and $x \cdot \nabla V_2$ are relatively form bounded w.r.t. $(P-A)^2$.

The above assumptions are all we need to prove a quadratic form version of the virial theorem, see Theorem 5.3. In particular, $\widetilde{B}_w^2$ and the virial $x \cdot \nabla V$ do not have to be form small but only form bounded w.r.t $(P-A)^2$, for the virial theorem to hold.

Behaviour at infinity

We need to quantify the notion that the magnetic field B, the potential V and the virial $x \cdot \nabla V$ are bounded, or even vanish, at infinity.

From physical heuristics, one expect that 'smallness' should not be measured pointwise, but only *relative to* the kinetic energy $(P-A)^2$. The following conditions make this physical intuition precise.

Assumption 2.7 (*Vanishing at infinity*) The potential V vanishes at infinity w.r.t. $(P-A)^2$ in the sense of Definition 1.5. Moreover, if we split $V = V_1 + V_2$ as in Assumption 2.6, then also V_1 vanishes at infinity w.r.t. $(P-A)^2$ in the sense of Definition 1.5.

To state the precise conditions on the magnetic field B and the potential V for being bounded at infinity w.r.t. $(P-A)^2$ we use Definition 1.8.

Assumption 2.8 (*Boundedness of the magnetic field and the virial at infinity*) The scalar field $|\widetilde{B}_w|^2$ is bounded at infinity w.r.t. $(P-A)^2$ in the sense of Definition 1.8. Moreover, splitting the potential $V = V_1 + V_2$ as in Assumption 2.6, we assume that $x^2V_1^2$ and $x \cdot \nabla V_2$, more precisely, the quadratic form corresponding to $x \cdot \nabla V_2$, are bounded from above at infinity w.r.t. $(P-A)^2$.
With the notation from Definition 1.8 we set

$$\beta := \big(\gamma_\infty(|\widetilde{B}_w|^2)\big)^{1/2} \quad \omega_1 := \big(\gamma_\infty(x^2V_1^2)\big)^{1/2} \quad \text{and } \omega_2 := \gamma_\infty^+(x \cdot \nabla V_2)\,. \tag{2.22}$$

The quantities β, ω_1, and ω_2 give a quantitative notion on how large the magnetic field B, respectively, the virial $x \cdot \nabla V$, are at infinity, relative to $(P-A)^2$. Their definition is inspired by Section 3 in [23].

Unique continuation at infinity

For a unique continuation type argument at infinity, we also need a quantitative version of relative form boundedness.

Assumption 2.9 If $V = V_1 + V_2$, then we assume

$$\|\widetilde{B}\varphi\|_2^2 + \|xV_1\varphi\|_2^2 \leq \frac{\alpha_1^2}{4}\,\|(P-A)\varphi\|_2^2 + C_1\|\varphi\|_2^2, \tag{2.23}$$

$$\langle\varphi, x\cdot\nabla V_2\,\varphi\rangle \leq \alpha_2\,\|(P-A)\varphi\|_2^2 + C_2\|\varphi\|_2^2, \tag{2.24}$$

$$|\langle\varphi, V_1\,\varphi\rangle| \leq \alpha_3\,\|(P-A)\varphi\|_2^2 + C_3\|\varphi\|_2^2 \tag{2.25}$$

for some $\alpha_j, C_j > 0$, $j = 1, 2, 3$, all $\varphi \in \mathcal{D}(P-A)$, and

$$\alpha_1 + \alpha_2 + d\alpha_3 < 1. \tag{2.26}$$

The factor d in front of α_3 comes from the Kato form of the virial $x\cdot\nabla V_1$, see Lemma 3.12.

Remarks 2.10 Let us make two comments concerning the above list of conditions. First, all the above hypothesis are either physically motivated or required to be able to define the relevant objects. Secondly, the required conditions are quite weak. In Appendix A we show that Assumptions 2.3–2.9 are satisfied under certain mild and easily verifiable regularity and decay conditions on B and V, see Remark A.6 and Proposition A.2.

Remarks 2.11 In the conditions above, one can use the diamagnetic inequality in order to replace $P-A$ by the nonmagnetic momentum operator P in all relative form boundedness conditions, see [4].

2.4 Regularity of the Poincaré gauge map

Note that the Poincaré gauge map (2.16) is a-priori only well-defined when the magnetic field B is sufficiently regular, say, continuous. Our first result shows that the map (2.16) can be continuously extended to all magnetic field satisfying Assumption 2.3.

Lemma 2.12 *Let $\mathcal{B}$ be the vector space of vector fields $\widetilde{B}$ satisfying*

$$\int_{\mathcal{U}_R} |x|^{2-d}\left(\log\frac{R}{|x|}\right)^2 |\widetilde{B}(x)|^2\,dx < \infty$$

for all $R > 0$. The continuous vector fields are dense in $\mathcal{B}$ and the map $\widetilde{B} \mapsto A{:=}T(\widetilde{B})$ given by

$$A(x) = T(\widetilde{B})(x) := \int_0^1 \widetilde{B}(tx)\,dt \quad \text{for } x \in \mathbb{R}^d\,,$$

extends to a continuous map from $\mathcal{B}$ into $L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d)$. In particular, the Poincaré gauge map given in (2.16) is well defined for all magnetic fields satisfying Assumption 2.3. Moreover,

$$\int_{\mathcal{U}_R} |x|^{2-d}\,|A(x)|^2\,dx \leq 4\int_{\mathcal{U}_R} |x|^{2-d}\left(\log\frac{R}{|x|}\right)^2 |\widetilde{B}(x)|^2\,dx\,, \tag{2.27}$$

for any $R > 0$.

Proof Given $B \in \mathcal{B}$ and $R > 0$ let

$$\|\widetilde{B}\|_{\mathcal{B},R} := \left(\int_{\mathcal{U}_R} |x|^{2-d} \left(\log \frac{R}{|x|} \right)^2 |\widetilde{B}(x)|^2 \, dx \right)^{1/2} .$$

Also let $\mathcal{A}$ be the space of vector potentials A for which

$$\||A\|_{\mathcal{A},R} := \left(\int_{\mathcal{U}_R} |x|^{2-d} \, |A(x)|^2 \, dx \right)^{1/2}$$

is finite for all $R > 0$. This makes $\mathcal{A}$ and $\mathcal{B}$ locally convex metric spaces and by construction, $\mathcal{A} \subset L^2_{\text{loc}}(\mathbb{R}^d, \mathbb{R}^d)$. The metrics consistent with the topologies on $\mathcal{A}$ and $\mathcal{B}$ are, for example,

$$d_{\mathcal{A}}(A_1, A_2) = \sum_{n=0}^{\infty} 2^{-n} \frac{\||A_1 - A_2\|_{\mathcal{A},2^n}}{1 + \|A_1 - A_2\|_{\mathcal{A},2^n}} \quad \text{and}$$

$$d_{\mathcal{B}}(\widetilde{B}_1, \widetilde{B}_2) = \sum_{n=0}^{\infty} 2^{-n} \frac{2\|\widetilde{B}_1 - \widetilde{B}_2\|_{\mathcal{B},2^n}}{1 + 2\|\widetilde{B}_1 - \widetilde{B}_2\|_{\mathcal{B},2^n}} .$$

The standard arguments show that $\mathcal{A}$ and $\mathcal{B}$ are complete metric spaces, see e.g. [35, Sec. V.]. Moreover, the usual cutting and mollifying arguments show that the continuous functions are dense in $\mathcal{B}$. In addition, since the map $0 < s \mapsto \frac{s}{1+s}$ is increasing, $T(\widetilde{B})$ is well defined and locally bounded when $\widetilde{B}$ is continuous, so $T(\widetilde{B}) \in \mathcal{A}$, when $\widetilde{B}$ is continuous. Assuming temporarily (2.27) then gives

$$d_{\mathcal{A}}(T(\widetilde{B}_1), T(\widetilde{B}_2)) = \sum_{n=0}^{\infty} 2^{-n} \frac{\||T(\widetilde{B}_1 - \widetilde{B}_2)\|_{\mathcal{A},2^n}}{1 + \|T(\widetilde{B}_1 - \widetilde{B}_2)\|_{\mathcal{A},2^n}} \le d_{\mathcal{B}}(\widetilde{B}_1, \widetilde{B}_2)$$

so T is uniformly continuous, thus it extends to a map from $\mathcal{B}$ into $\mathcal{A}$ which we continue to denote by T. This shows that the Poincaré gauge map (2.16) is well defined for all magnetic fields B satisfying Assumption 2.3.

Hence it is enough to prove the bound (2.27) and by density, it is enough to prove it for continuous vector fields $\widetilde{B}$. Let g be a radial function, which is positive and finite for almost all $|x| < R$. Since $A(x) = \int_0^1 \widetilde{B}(tx)\, dt$, we have using symmetry

$$\begin{aligned}
\int_{\mathcal{U}_R} g(|x|)|A(x)|^2 \, dx &= \int_0^1 \int_0^1 \int_{\mathcal{U}_R} g(|x|)\widetilde{B}(t_1 x) \cdot \widetilde{B}(t_2 x) \, dx dt_1 dt_2 \\
&= 2 \iint_{0 \le t_1 < t_2 \le 1} \int_{|x| \le R} g(|x|)\widetilde{B}(t_1 x) \cdot \widetilde{B}(t_2 x) \, dx dt_1 dt_2 \\
&= 2 \int_0^1 \int_0^1 \int_{\mathcal{U}_{tR}} g(|y|/t) t^{1-d} \widetilde{B}(uy) \cdot \widetilde{B}(y) \, dy du dt \\
&= 2 \int_{\mathcal{U}_R} \left(\int_{|y|/R}^1 g(|y|/t) t^{1-d} \, dt \right) A(y) \widetilde{B}(y) \, dy \\
&\le 2 \left(\int_{\mathcal{U}_R} g(|y|) |A(y)|^2 \, dy \right)^{1/2} \\
&\quad \left(\int_{\mathcal{U}_R} g(|y|)^{-1} \left(\int_{|y|/R}^1 g(|y|/t) t^{1-d} \, dt \right)^2 |\widetilde{B}(y)|^2 \, dy \right)^{1/2}
\end{aligned}$$

where we also used the substitution $t_1 = ut_2$ and $y = t_2 x$ and then the Cauchy-Schwarz inequality. Thus as soon as $\int_{|x|\le R} g(|x|)|A(x)|^2\, dx$ is finite, we arrive at the a-priori bound

$$\int_{\mathcal{U}_R} g(|x|)|A(x)|^2\, dx \le 4 \int_{\mathcal{U}_R} g(|x|)^{-1} \left(\int_{|x|/R}^1 g(|x|/t) t^{1-d}\, dt \right)^2 |\widetilde{B}(x)|^2\, dx\,. \tag{2.28}$$

It remains to choose g in such a way that the integral weight on the left hand side coincides with the expression in (2.27). Hence we set $g(s) = s^{2-d}$, and calculate

$$g(|x|)^{-1} \left(\int_{|x|/R}^1 g(|x|/t) t^{1-d}\, dt \right)^2 = |x|^{2-d} \left(\log \frac{R}{|x|} \right)^2.$$

Plugging this into (2.28) gives (2.27). We note that $A(x) = \int_0^1 \widetilde{B}(tx)\, dt$ is locally bounded as long as $\widetilde{B}$ is locally bounded. Thus for the above choice of g

$$\int_{\mathcal{U}_R} |x|^{2-d}\, |A(x)|^2\, dx$$

is, as required, finite for all continuous $\widetilde{B}$. Hence the a-priori bound (2.27) holds for all continuous $\widetilde{B}$ and extend by density to all of $\mathcal{B}$. □

For future purposes we will need also a translated and generalized version of inequality (2.27);

Corollary 2.13 *Let assumptions of Lemma 2.12 be satisfied and let $h : \mathbb{R}_+ \to \mathbb{R}_+$ be a non-increasing bounded function. Then*

$$\begin{aligned} &\int_{\mathcal{U}_R(x_0)} |x - x_0|^{2-d}\, h(|x - x_0|)\, |A_{x_0}(x - x_0)|^2\, dx \\ &\quad \le 4 \int_{\mathcal{U}_R} |y|^{2-d} \left(\log \frac{R}{|y|} \right)^2 h(|y|) |\widetilde{B}_{x_0}(y)|^2\, dy\,, \end{aligned} \tag{2.29}$$

holds for any $x_0 \in \mathbb{R}^d$. Recall that $A_{x_0}(x - x_0)$ is given by (2.16).

Proof Since $h(|y|/t) \le h(|y|)$ for all $y \in \mathbb{R}^d$ and $t \le 1$, the result follows from (2.28) upon setting $g(s) = s^{2-d}\, h(s)$ and translating. □

Together with the quadratic form $Q_{A,V}$ we will also need the associated sesqui-linear form

$$q_{A,V}(u, v) = \big\langle (P - A)\, u, (P - A)\, v \big\rangle + \big\langle u, V v \big\rangle = q_{A,0}(u, v) + \big\langle u, V v \big\rangle, \quad u, v \in \mathcal{H}_A^1(\mathbb{R}^d) \tag{2.30}$$

and denote by $H = H_{A,V}$ the self-adjoint operator associated with $Q_{A,V}$.

3 Dilations and the magnetic virial theorem

As already mentioned in the introduction, the aim of this section is to establish a weighted virial theorem for weak eigenfunctions which will be needed later in the proof of absence of positive eigenvalues. This is done in Sects. 3.2 and 3.4 . We will write $H_{A,V} = (P - A)^2 + V$, even though, strictly speaking, the operator is only defined via the sum of the corresponding quadratic forms.

3.1 Dilations and the Poincaré gauge

In this subsection we will study the behavior of the magnetic Schrödinger form $Q_{A,V}$ under the action of the dilation group.
Let D_0 be the operator defined on $C_0^\infty(\mathbb{R}^d)$ by

$$D_0 = \frac{1}{2}\left(P \cdot x + x \cdot P\right), \qquad \mathscr{D}(D_0) = C_0^\infty(\mathbb{R}^d). \tag{3.1}$$

Remarks 3.1 Note that $D_0 = \frac{1}{2}\left((P - A) \cdot x + x \cdot (P - A)\right)$, when A is in the Poincaré gauge (2.17). This is one of the reasons why dilations and the Poincaré gauge work well together.

Lemma 3.2 *D_0 is essentially self-adjoint.*

Proof For $t \in \mathbb{R}$ define the unitary dilation operator U_t by

$$(U_t f)(x) = e^{td/2} f(e^t x) \quad x \in \mathbb{R}^d. \tag{3.2}$$

It is easy to see that U_t is unitary on $L^2(\mathbb{R}^d)$ and forms a group, $U_t U_s = U(t+s)$, for all $t, s \in \mathbb{R}$. In particular, the adjoint is given by $U_t^* = U_{-t}$. Moreover, each U_t leaves $C_0^\infty(\mathbb{R}^d)$ invariant and a direct calculation shows that $t \mapsto U_t$ is strongly differentiable on $C_0^\infty(\mathbb{R}^d)$ with

$$\left(\frac{d}{dt} U_t f\right)\Big|_{t=0} = i D_0 f, \qquad \forall\, f \in C_0^\infty(\mathbb{R}^d). \tag{3.3}$$

The claim now follows from [35, Thm. VIII.10]. □

We denote by D the closure of D_0, which is self-adjoint, and by D_t the operator given by

$$i D_t = \frac{U_t - U_{-t}}{2t}\,. \tag{3.4}$$

D_t is bounded and symmetric. We will use it to approximate D in the limit $t \to 0$.
Let $\varphi \in \mathcal{D}(P)$. It is easy to check the commutation formula

$$U_t^* P U_t = e^t P\,, \tag{3.5}$$

since $(P U_t \varphi)(x) = -i\nabla(e^{td/2}\varphi(e^t x)) = -i e^t e^{td/2}(\nabla\varphi)(e^t x) = e^t (U_t(P\varphi))(x)$. In a similar way, one checks that for a multiplication operator V

$$V_{-t} := U_t^* V(\cdot) U_t = V(e^{-t}\cdot) \tag{3.6}$$

holds on its domain, i.e., for all $\varphi \in \mathcal{D}(V)$ we have $(V(U_t\varphi))(x) = e^{td/2} V(x)\varphi(e^t x) = (U_t(V_t^*\varphi))(x)$ for almost all $x \in \mathbb{R}^d$. A similar result also holds for vector valued multiplication operators, for example,

$$A_{-t} := U_t^* A(\cdot) U_t = A(e^{-t}\cdot). \tag{3.7}$$

For the virial theorem, we want to define the commutator $[H_{A,V}, iD]$, where D is the generator of dilations. Since the two operators involved are unbounded, this usually leads to involved domain considerations. Even worse, in our case we do not know the domain $\mathcal{D}(H_{A,V})$ exactly, nor do we intend to know it, since we prefer to work only with quadratic forms. This seems to make a usable virial theorem impossible to achieve, however, a quadratic form approach turns out to be feasible.

Assume that $u \in \mathcal{D}(H_{A,V})$ and approximate the unbounded generator of dilations D by the bounded approximations D_t. A slightly formal calculation, for $u \in \mathcal{D}(H_{A,V}) \cap \mathcal{C}_0^\infty$ which might be the empty set, however, gives

$$\langle u, [H_{A,V}, iD_t]u\rangle = \langle H_{A,V}u, iD_tu\rangle + \langle iD_tu, H_{A,V}u\rangle = 2\,\mathrm{Re}(\langle H_{A,V}u, iD_tu\rangle) \quad (3.8)$$

since iD_t is antisymmetric. Assume that $\mathcal{D}(P-A)$ is invariant under dilations. Then $iD_tu \in \mathcal{D}(P-A)$ and the right hand side of (3.8) can be identified with $2\,\mathrm{Re}(q_{A,V}(u, iD_tu))$, where $q_{A,V}$ is the quadratic form given by (2.10), which defines the magnetic Schrödinger operator $H_{A,V}$. Since $\mathcal{D}(H_{A,V})$ is dense in $\mathcal{D}(q_{A,V}) = \mathcal{Q}(H_{A,V})$, the latter expression extends to all of $\mathcal{Q}(H_{A,V})$, the quadratic form domain of $H_{A,V}$. So we simply *define the commutator* $[H_{A,V}, iD_t]$ as the quadratic form with domain $\mathcal{Q}(H_{A,V})$ given by

$$\langle u, [H_{A,V}, iD_t]u\rangle := 2\,\mathrm{Re}\left(q_{A,V}(u, iD_tu)\right), \qquad u \in \mathcal{Q}(H_{A,V}). \quad (3.9)$$

Moreover, we can define the commutator $[H, iD]$, again in the sense of quadratic forms, by

$$\left\langle u, i\,[H,D]\,u\right\rangle := \lim_{t\to 0}\langle u, [H_{A,V}, iD_t]u\rangle := \lim_{t\to 0} 2\,\mathrm{Re}\left(q_{A,V}(u, iD_tu)\right), \quad (3.10)$$

provided the limit on the right hand side exists. In the remaining part of this section, we will deal with the proof that the limit in (3.10) exists for all $\varphi \in \mathcal{D}(P-A)$, the calculation of this limit, and, in particular, the claim that $\mathcal{D}(P-A)$ is invariant under dilations under natural conditions on the magnetic field.

By (3.5), the Sobolev space $\mathcal{D}(P)$ is invariant under dilations. To see how one can also get this for the magnetic Sobolev space $\mathcal{D}(P-A)$ let $\varphi \in \mathcal{D}(P-A)$. Then, as distributions,

$$(P-A)U_t\varphi = e^tU_tP\varphi - U_tA_t\varphi = e^tU_t(P-A)\varphi + U_t(e^tA - A_{-t})\varphi\,. \quad (3.11)$$

Since $U_t : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is unitary and $(P-A)\varphi \in L^2(\mathbb{R}^d)$, we have $e^tU_t(P-A)\varphi \in L^2(\mathbb{R}^d)$ for all $t \in \mathbb{R}$. So in order that $U_t\varphi \in \mathcal{D}(P-A)$ we have to check if $(e^tA - A_{-t})\varphi \in L^2(\mathbb{R}^d)$. This is the content of the next proposition.

Proposition 3.3 *Suppose that the magnetic field B satisfies Assumption 2.3, the vector potential A corresponding to B is in the Poincaré gauge, and $\widetilde{B}^2$ is relatively form bounded w.r.t. $(P-A)^2$.*
If $\varphi \in D(P-A) = \mathcal{H}^1_A(\mathbb{R}^d)$, then $(e^tA - A_{-t})\varphi \in L^2(\mathbb{R}^d)$ for all $t \in \mathbb{R}$ and the map $\mathbb{R} \ni t \mapsto (e^tA - A_{-t})\varphi$ is continuous. In particular, $\mathcal{D}(P-A)$ is invariant under dilations.

The main tool for the proof of Proposition 3.3 is the following

Lemma 3.4 *Under the assumptions of Proposition 3.3, if $\varphi \in D(P-A) = \mathcal{H}^1_A(\mathbb{R}^d)$, then*

$$\|(e^tA - A_{-t})\varphi\| \;\le\; e^t\left(e^{C_z|t|} - 1\right)\|(P-A)\varphi\| + \frac{z\,C_z}{C_z \pm 1}\left(e^{(C_z\pm 1)|t|} - 1\right)\|\varphi\| \quad (3.12)$$

for all $t \in \mathbb{R}$ and $z > 0$, where the $+$ sign holds for $t \ge 0$ and the $-$ sign for $t < 0$ and the constant C_z is given by

$$C_z = \sqrt{d}\,\left\|\widetilde{B}\left((P-A)^2 + z^2\right)^{-\frac{1}{2}}\right\|_{2\to 2}.$$

Remarks 3.5 In the above bound we use the convention $\frac{C_z}{C_z-1}\left(e^{(C_z-1)|t|} - 1\right) = |t|$ when $C_z = 1$.

Given Lemma 3.4, the proof of Proposition 3.3 is simple.

Proof of Proposition 3.3 Given $\varphi \in \mathcal{D}(P-A)$, Lemma 3.4 shows that $(e^t A - A_{-t})\varphi \in L^2(\mathbb{R}^d)$ for all $t \in \mathbb{R}$ and then (3.11) shows that $U_t\varphi \in \mathcal{D}(P-A)$ for all $t \in \mathbb{R}$. Thus $\mathcal{D}(P-A)$ is invariant under dilations.

Moreover, the bound (3.12) shows that the map $t \mapsto (e^t A - A_{-t})\varphi$ is continuous at $t=0$. Since, for any $s, t \in \mathbb{R}$,

$$\begin{aligned} e^{t+s}A - A_{-(t+s)} &= e^s\big(e^t A - A_{-t}\big) + e^s A_{-t} - (A_{-s})_{-t} \\ &= e^s\big(e^t A - A_{-t}\big) + U_t^*\big(e^s A - (A_{-s})\big)U_t \end{aligned} \tag{3.13}$$

and $U_t\varphi \in \mathcal{D}(P-A)$ for any $\varphi \in \mathcal{D}(P-A)$, continuity of $t \mapsto \big(e^t A - A_{-t}\big)\varphi$ at $t=0$ implies continuity at all $t \in \mathbb{R}$. □

Proof of Lemma 3.4 First of all, it is enough to prove (3.12) for $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, since this is dense in $\mathcal{D}(P-A)$ in the graph norm: If (3.12) holds for $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, then given $\varphi \in \mathcal{D}(P-A)$, choose a sequence $\varphi_n \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ such that $(P-A)\varphi_n \to (P-A)\varphi$ and $\varphi_n \to \varphi$. By taking a subsequence, if necessary, we can also assume that $\varphi_n \to \varphi$ almost everywhere, hence $(e^t A - A_{-t})\varphi_n \to (e^t A - A_{-t})\varphi$ almost everywhere, in particular, $|(e^t A - A_{-t})\varphi| = \lim_{n\to\infty} |(e^t A - A_{-t})\varphi_n| = \liminf_{n\to\infty} |(e^t A - A_{-t})\varphi_n|$ almost everywhere. Then Fatou's Lemma and (3.12) imply

$$\begin{aligned} \|(e^t A - A_{-t})\varphi\| &= \|\liminf_{n\to\infty} |(e^t A - A_{-t})\varphi_n|\| \le \liminf_{n\to\infty} \|(e^t A - A_{-t})\varphi_n\| \\ &\le e^t\big(e^{C_z|t|}-1\big)\|(P-A)\varphi\| + \frac{z\,C_z}{C_z \pm 1}\big(e^{(C_z\pm 1)|t|}-1\big)\|\varphi\| \end{aligned}$$

for all $\varphi \in \mathcal{D}(P-A)$.

Let $t \in \mathbb{R}$. Since A is in the Poincaré gauge, using the change of variables $t = e^{-s}$, we have

$$A = \int_0^\infty e^{-s}\widetilde{B}(e^{-s}\cdot)\,ds = \int_0^\infty e^{-s}U_s^*\,\widetilde{B}\,U_s\,ds\,. \tag{3.14}$$

From the definition of A_{-t} and (3.14) we get

$$\begin{aligned} e^t\,A - A_{-t} &= e^t\int_0^\infty e^{-s}U_s^*\,\widetilde{B}\,U_s\,ds - \int_0^\infty e^{-s}\,U_t^*U_s^*\,\widetilde{B}\,U_sU_t\,ds \\ &= e^t\int_0^\infty e^{-s}\,U_s^*\,\widetilde{B}\,U_s\,ds - e^t\int_t^\infty e^{t-s}U_s^*\,\widetilde{B}\,U_s\,ds \\ &= e^t\int_0^t e^{-s}\,U_s^*\,\widetilde{B}\,U_s\,ds. \end{aligned} \tag{3.15}$$

Let $\varphi \in C_0^\infty(\mathbb{R}^d)$. The above identity then gives

$$v(t) := (e^t A - A_{-t})\varphi = e^t\int_0^t e^{-s}\,U_s^*\,\widetilde{B}\,U_s\,\varphi\,ds. \tag{3.16}$$

Define the operator $R_z : D(P-A) \to D(H_0)^d$ by

$$R_z := ((P-A)^2 + dz^2)^{-1}\,(P-A-iz). \tag{3.17}$$

Here $(P-A-iz)$ is a vector operator, which maps $\varphi \in \mathcal{D}(P-A)$ to the vector function $(P-A-iz)\varphi = \big((P_j - A_j - iz)\varphi\big)_{j=1,\ldots,d}$. Then $R_z(P-A+iz)\varphi = \varphi$, so

$$\begin{aligned}\widetilde{B}\,U_s\,\varphi &= \widetilde{B}\,R_z(P-A+iz)\,U_s\,\varphi = \widetilde{B}\,R_z\,U_s\big[e^s(P-A)\,\varphi + (e^sA - A_{-s})\,\varphi + iz\varphi\big]\\ &= \widetilde{B}\,R_z\,U_s\big[e^s(P-A)\,\varphi + v(s) + iz\varphi\big],\end{aligned}$$

which in view of (3.16) implies

$$v(t) = \int_0^t e^{t-s}\,U_s^*\widetilde{B}\,R_z\,U_s\big(e^s(P-A)\,\varphi + v(s) + iz\varphi\big)\,ds. \tag{3.18}$$

Note that the map $t \mapsto v(t) \in L^2(\mathbb{R}^d)$ is continuous due to the presence of φ. Hence, if $t \geq 0$,

$$\begin{aligned}w(t) := \|v(t)\| \;&\leq\; K_z \int_0^t e^{t-s}\,\big(e^s\,\|(P-A)\,\varphi\|_2 + w(s) + z\|\varphi\|\big)\,ds\\ &= E(t) + K_z \int_0^t e^{t-s}\,w(s)\,ds,\end{aligned}$$

where

$$K_z := \|\widetilde{B}\,R_z\|_{2\to 2}\,, \tag{3.19}$$

and

$$E(t) = K_z \int_0^t e^{t-s}\,\big(e^s\,\|(P-A)\,\varphi\|_2 + z\|\varphi\|_2\big)\,ds\,.$$

We will derive a suitable bound on K_z at the end of this proof. The Gronwall–type Lemma B.1 in the Appendix yields

$$w(t) \;\leq\; E(t) + K_z \int_0^t e^{(1+K_z)(t-s)}\,E(s)\,ds\,. \tag{3.20}$$

Note

$$\begin{aligned}&\int_0^t e^{(1+K_z)(t-s)}\,E(s)\,ds\\ &\quad= K_z \iint_{0<s<s'<t} e^{(1+K_z)(t-s')}e^{s'}\,ds ds'\,\|(P-A)\,\varphi\|_2\\ &\qquad+ zK_z \iint_{0<s<s'<t} e^{(1+K_z)(t-s')}e^{s'-s}\,ds ds'\,\|\varphi\|_2\\ &\quad= \left(\frac{e^t}{K_z}(e^{K_z t}-1) - te^t\right)\|(P-A)\,\varphi\|_2 + z\left(\frac{1}{K_z+1}\big(e^{(K_z+1)t}-1\big) - \big(e^t-1\big)\right)\|\varphi\|_2\end{aligned}$$

and a straightforward calculation gives

$$E(t) = K_z t e^t\,\|(P-A)\varphi\|_2 + zK_z\big(e^t-1\big)\|\varphi\|_2.$$

Inserting this into (3.20) gives

$$\|(e^tA - A_{-t})\varphi\| = w(t) \leq e^t\big(e^{K_z t}-1\big)\|(P-A)\,\varphi\|_2 + \frac{zK_z}{K_z+1}\big(e^{(K_z+1)t}-1\big)\|\varphi\|_2$$

which gives (3.12), at least for $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$.

If $t < 0$, then setting $\tau = -t > 0$, we get from (3.18)

$$\begin{aligned}\widetilde{w}(\tau) := \|v_{-\tau}\|_2 &\le K_z \int_0^\tau e^{s-\tau} \left(e^{-s}\|(P-A)\,\varphi\|_2 + w(s) + z\|\varphi\|_2\right) ds \\ &= \widetilde{E}(\tau) + K_z \int_0^\tau e^{s-\tau}\,\widetilde{w}(s)\,ds,\end{aligned}$$

with

$$\widetilde{E}(\tau) := K_z \int_0^\tau e^{s-\tau} \left(e^{-s}\|(P-A)\,\varphi\|_2 + z\|\varphi\|_2\right) ds$$

and the second Gronwall–type bound from Lemma B.1 now gives

$$\widetilde{w}(\tau) \le \widetilde{E}(\tau) + K_z \int_0^\tau e^{(K_z-1)(\tau-s)}\,\widetilde{E}(s)\,ds\,. \tag{3.21}$$

Similarly as above one calculates

$$\begin{aligned}&\int_0^\tau e^{(K_z-1)(\tau-s)}\,\widetilde{E}(s)\,ds \\ &\quad= K_z \iint\limits_{0<s<s'<\tau} e^{(K_z-1)\tau-K_z s'}\,ds ds'\,\|(P-A)\,\varphi\|_2 \\ &\qquad+ zK_z \iint\limits_{0<s<s'<t} e^{(K_z-1)\tau-K_z s'+s}\,ds ds'\,\|\varphi\|_2 \\ &\quad= \left(\frac{e^{-\tau}}{K_z}(e^{K_z\tau}-1) - \tau e^{-\tau}\right)\|(P-A)\,\varphi\|_2 \\ &\qquad+ z\left(\frac{1}{K_z-1}\left(e^{(K_z-1)\tau}-1\right) - \left(1-e^{-\tau}\right)\right)\|\varphi\|_2\end{aligned}$$

and

$$\widetilde{E}(\tau) = K_z\tau e^{-\tau}\|(P-A)\,\varphi\|_2 + zK_z(1-e^{-\tau})\|\varphi\|_2\,,$$

and plugging this back into (3.21), using $t = -\tau < 0$ we arrive at

$$\begin{aligned}\|(e^t A - A_{-t})\varphi\|_2 = \widetilde{w}(\tau) &\le e^t\left(e^{K_z|t|}-1\right)\|(P-A)\,\varphi\|_2 \\ &\quad+ \frac{zK_z}{K_z-1}\left(e^{(K_z-1)|t|}-1\right)\|\varphi\|_2\,.\end{aligned}$$

Recalling that we can replace K_z by any upper bound in the above arguments, this proves (3.12), we only have to bound K_z. Let $\psi \in C_0^\infty(\mathbb{R}^d)$. From the definition (3.19) one easily gets

$$\begin{aligned}K_z = \|\widetilde{B}\,R_z\|_{2\to 2} \le \|\widetilde{B}\,((P-A)^2+dz^2)^{-\frac12}\|_{2\to 2}\,\|((P-A)^2+dz^2)^{-\frac12} \\ (P-A-iz)\|_{2\to 2}.\end{aligned}$$

On the other hand, letting $T = ((P-A)^2+dz^2)^{-\frac12}(P-A-iz)$ one sees

$$\begin{aligned}TT^* &= ((P-A)^2+dz^2)^{-\frac12}(P-A-iz)\cdot(P-A+iz)((P-A)^2+dz^2)^{-\frac12} \\ &= ((P-A)^2+dz^2)^{-\frac12}((P-A)^2+dz^2)((P-A)^2+dz^2)^{-\frac12} = \mathbb{1}\,.\end{aligned} \tag{3.22}$$

Hence by duality $\|((P-A)^2+dz^2)^{-\frac{1}{2}}(P-A-iz)\|_{2\to 2} = \|T\|_{2\to 2} = 1$ and thus

$$K_z \;\le\; \|\widetilde{B}(H_0+z^2)^{-\frac{1}{2}}\|_{2\to 2} =: C_z\,. \tag{3.23}$$

□

Since we have defined the commutator $[H, iD]$ as the limit of $[H, iD_t]$, see (3.10) and (3.4), we have to calculate the terms appearing in the latter. The next result concerns the calculation of $\frac{d}{dt}\big(e^t A - A_{-t}\big)\varphi\big|_{t=0}$ for $\varphi \in \mathcal{D}(P-A)$. Recall that given a magnetic field B, the vector field $\widetilde{B}$ is given by $\widetilde{B} = B(x)[x]$, see also Eq. (1.9).

Proposition 3.6 *Suppose that the magnetic field B satisfies Assumption 2.3, the vector potential A corresponding to B is in the Poincaré gauge. Suppose moreover that $\widetilde{B}^2$ is relatively form bounded w.r.t. $(P-A)^2$, i.e. $\widetilde{B}\cdot \in \mathcal{L}_c\big(\mathcal{D}(P-A), L^2(\mathbb{R}^d)\big)$. Then for all $\varphi \in \mathcal{D}(P-A)$ the map $\mathbb{R} \ni t \mapsto (e^t A - A_{-t})\varphi$ is differentiable and*

$$\frac{d}{dt}(e^t A - A_{-t})\varphi\big|_{t=0} = \lim_{t\to 0}\frac{1}{t}(e^t A - A_{-t})\varphi = \widetilde{B}\,\varphi \tag{3.24}$$

where the limit is taken in $L^2(\mathbb{R}^d)$.

Proof Assume that for $\varphi \in \mathcal{D}(P-A)$ the map $t \mapsto \big(e^t A - A_{-t}\big)\varphi$ is differentiable in $t=0$ with derivative given by (3.24). Then (3.13) shows that it is also differentiable in any point $t \in \mathbb{R}$ with derivative

$$\frac{d}{dt}(e^t A - A_{-t})\varphi = \big(e^t A - A_{-t}\big)\varphi + U_t^*\widetilde{B}U_t\varphi \tag{3.25}$$

By assumption, $\widetilde{B} : \mathcal{D}(P-A) \to L^2(\mathbb{R}^d)$ is bounded. Thus the right hand side of (3.25) is in $L^2(\mathbb{R}^d)$ by Proposition 3.3. Hence it is enough to show differentiability at $t=0$. We will prove, for all $\varphi \in \mathcal{D}(P-A)$,

$$\lim_{t\to 0}\frac{1}{|e^t-1|}\big\|(e^t A - A_{-t})\,\varphi - (e^t-1)\,\widetilde{B}\,\varphi\big\| = 0 \quad \text{in } L^2(\mathbb{R}^d), \tag{3.26}$$

which is equivalent to (3.24). First assume that $\varphi \in C_0^\infty(\mathbb{R}^d)$. Using (3.15) we have

$$\begin{aligned}\delta_t &:= (e^t A - A_{-t} - (e^t-1)\,\widetilde{B})\,\varphi = \int_0^t e^{t-s}\,U_s^*\,\widetilde{B}\,U_s\varphi\,ds - (e^t-1)\,\widetilde{B}\,\varphi \\ &= \int_0^t e^{t-s}\,\big(U_s^*\,\widetilde{B}\,U_s - \widetilde{B}\big)\varphi\,ds.\end{aligned} \tag{3.27}$$

Using (3.11) we rewrite the integrand on the right hand side as

$$\begin{aligned}\big(U_s^*\,\widetilde{B}\,U_s - \widetilde{B}\big)\varphi &= U_s^*\widetilde{B}(U_s-1)\varphi + (U_s^*-1)\widetilde{B}\varphi \\ &= U_s^*\widetilde{B}R_z\big((P-A+iz)U_s - (P-A+iz)\big)\varphi + (U_s^*-1)\widetilde{B}\varphi \\ &= U_s^*\widetilde{B}R_z\Big[U_s\big(e^s(P-A)+e^sA-A_{-s}+iz\big)\varphi - (P-A+iz)\varphi\Big] + (U_s^*-1)\widetilde{B}\varphi \\ &= U_s^*\widetilde{B}R_z\Big[U_s\big((e^s-1)(P-A)\varphi + (e^s-1)\widetilde{B}\varphi + \delta_s\big) + (U_s-1)(P-A+iz)\varphi\Big] \\ &\quad + (U_s-1)\widetilde{B}\varphi\,.\end{aligned}$$

Setting $w(s) := \|\delta_s\|_2$, and recalling $\|\widetilde{B}R_z\|_{2\to 2} \le \sqrt{d}\|\widetilde{B}((P-A)^2+z^2)^{-1/2}\| =: C_z$, see (3.23), we get

$$\|\big(U_s^*\,\widetilde{B}\,U_s - \widetilde{B}\big)\varphi\|_2$$

$$\le C_z\Big[|e^s-1|\big(\|(P-A)\varphi\|_2+\|\widetilde{B}\varphi\|_2\big)+w(s)+\|(U_s-1)(P-A+iz)\varphi\|_2\Big]$$
$$+\|(U_s-1)\widetilde{B}\varphi\|_2.$$

This implies the integral inequalities

$$w(t)\le E(t)+C_z\int_0^t e^{t-s}\,w(s)\,ds\quad\text{for } t\ge 0$$

and

$$w(t)\le E(t)+C_z\int_0^{|t|} e^{t+s}\,w(-s)\,ds\quad\text{for } t\le 0,$$

where now

$$E(t)=\int_0^t e^{t-s}\Big[C_z\|(U_s-1)(P-A+iz)\varphi\|_2+\|(U_s-1)\widetilde{B}\varphi\|_2\Big]\,ds$$
$$+\int_0^t e^{t-s}\,(e^s-1)C_z\big(\|(P-A)\varphi\|_2+\|\widetilde{B}\varphi\|_2\big)\,ds\,,$$

for $t\ge 0$, and

$$E(t)=\int_0^{|t|} e^{t+s}\Big[C_z\|(U_s-1)(P-A+iz)\varphi\|_2+\|(U_s-1)\widetilde{B}\varphi\|_2\Big]\,ds$$
$$+\int_0^{|t|} e^{t+s}\,(1-e^{-s})C_z\big(\|(P-A)\varphi\|_2+\|\widetilde{B}\varphi\|_2\big)\,ds\,,$$

for $t\le 0$. Lemma B.1 then yields the upper bounds

$$w(t)\le E(t)+C_z\int_0^t e^{(1+C_z)(t-s)}\,E(s)\,ds\quad\text{for } t\ge 0 \tag{3.28}$$

and

$$w(t)\le E(t)+C_z\int_0^{|t|} e^{(C_z-1)(t-s)}\,E(-s)\,ds\quad\text{for } t\le 0\,. \tag{3.29}$$

To continue it is convenient to use, for $\tau\ge 0$,

$$\kappa(\tau):=\sup_{|s|\le\tau}\|(U_s-1)\widetilde{B}\varphi\|_2+C_z\sup_{|s|\le\tau}\|(U_s-1)(P-A+iz)\varphi\|_2,$$

so that for $t\ge 0$

$$E(t)\le\int_0^t e^{t-s}\,\kappa(s)\,ds+\big(\|(P-A)\varphi\|_2+\|\widetilde{B}\varphi\|_2\big)\int_0^t e^{t-s}\,(e^s-1)\,ds$$
$$\le\kappa(t)(e^t-1)+\big(\|(P-A)\varphi\|_2+\|\widetilde{B}\varphi\|_2\big)(e^t-1)^2,$$

since κ is increasing. Analogously, for $t\le 0$ we have

$$E(t)=\int_0^{|t|} e^{t+s}\kappa(s)\,ds+\big(\|(P-A)\varphi\|_2+\|\widetilde{B}\varphi\|_2\big)\int_0^{|t|} e^{t+s}\,(1-e^{-s})\,ds$$
$$\le\kappa(|t|)(1-e^t)+\big(\|(P-A)\varphi\|_2+\|\widetilde{B}\varphi\|_2\big)(1-e^t)^2\,.$$

So by monotonicity, for $t\ge 0$,

$$\int_0^t e^{(1+C_z)(t-s)}\,E(s)\,ds\le\Big(\kappa(t)(e^t-1)+\big(\|(P-A)\varphi\|_2+\|\widetilde{B}\varphi\|_2\big)(e^t-1)^2\Big)$$

$$\int_0^t e^{(1+C_z)(t-s)}\,ds$$
$$= \frac{(e^{(1+C_z)t}-1)(e^t-1)}{1+C_z}\Big[\kappa(t)+(e^t-1)\big(\|(P-A)\varphi\|_2+\|\widetilde{B}\varphi\|_2\big)\Big]$$

and, similarly, for $t \le 0$ we have

$$\int_0^{|t|} e^{(C_z-1)(t-s)}\,E(-s)\,ds \le \frac{(1-e^{(C_z-1)t})(1-e^t)}{C_z-1}$$
$$\Big[\kappa(|t|)+(1-e^t)\big(\|(P-A)\varphi\|_2+\|\widetilde{B}\varphi\|_2\big)\Big]$$

which in combination with (3.28) and (3.29) implies

$$\frac{w(t)}{|e^t-1|} = \Big\|\frac{e^t\,A - A_{-t}}{e^t-1}\varphi - \widetilde{B}\varphi\Big\|$$
$$\le \left(1+\frac{C_z|e^{(C_z\pm 1)t}-1|}{C_z\pm 1}\right)\Big[\kappa(|t|)+|e^t-1|\big(\|(P-A)\varphi\|_2+\|\widetilde{B}\varphi\|_2\big)\Big], \quad (3.30)$$

where the $+$ sign holds when $t \ge 0$ and the $-$ sign when $t < 0$. Since $P - A : \mathcal{D}(P-A) \to L^2(\mathbb{R}^d)$ and $\widetilde{B} : \mathcal{D}(P-A) \to L^2(\mathbb{R}^d)$ are bounded, (3.30) extends to all $\varphi \in \mathcal{D}(P-A)$, by density. Since $\kappa(t) \to 0$ as $t \to 0$, this proves (3.26). □

We will need a version Proposition 3.6 for the electric potential. Recall that $iD_t = (U_t - U_{-t})/(2t)$, cf. (3.4).

Lemma 3.7 *Let A, B, and $\widetilde{B}$ satisfy the same assumptions as in Proposition 3.6 and let V be any electric potential, with form domain $\mathcal{D}(P-A) \subset \mathcal{Q}(V)$, such that the distribution $x \cdot \nabla V$ extends to a quadratic form $q_{x\cdot\nabla V}$ which is form bounded with respect to $(P-A)^2$. Then with $V_{-t} = U_t^* V U_t = V(e^{-t}\cdot)$ and q_V, respectively, $q_{V_{-t}}$, the quadratic form corresponding to V, respectively, V_{-t}, we have*

$$\lim_{t\to 0}\frac{1}{t}\big(q_V(\varphi,\psi) - q_{V_{-t}}(\varphi,\psi)\big) = q_{x\cdot\nabla V}(\varphi,\psi) \quad (3.31)$$

and

$$\lim_{t\to 0} 2\,\mathrm{Re}\, q_V(\varphi, iD_t\varphi) = -q_{x\cdot\nabla V}(\varphi,\varphi) \quad (3.32)$$

for all $\varphi, \psi \in \mathcal{D}(P-A)$.

Proof We always have $V \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$. Since $V_{-t} = U_t^* V U_t$, we have the identity $q_{V_{-t}}(\varphi,\psi) = \langle\varphi, V_{-t}\psi\rangle = \langle U_t\varphi, VU_t\psi\rangle = q_V(U_t\varphi, U_t\psi)$.

If V is a nice differentiable function, e.g., $V \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, then $\frac{d}{dt}V_{-t} = -e^{-t}x \cdot \nabla V(e^{-t}\cdot) = -e^{-t}U_t^*(x\cdot V)U_t$ so

$$\frac{d}{dt}\langle\varphi, V_{-t}\psi\rangle = -e^{-t}\langle U_t\varphi, x\cdot\nabla V U_t\psi\rangle = -e^{-t}q_{x\cdot\nabla V}(U_t\varphi, U_t\psi)\,. \quad (3.33)$$

Given $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, the map $\mathcal{C}_0^\infty(\mathbb{R}^d) \ni \psi \mapsto q_{V_{-t}}(\varphi,\psi)$ yields a distribution. Approximating V in L^1_{loc} by $\mathcal{C}_0^\infty$ functions and using (3.33) shows that the distributional derivative $W_t{:=}\frac{d}{dt}V_{-t}$ is given by

$$\langle\varphi, W_t\psi\rangle = \frac{d}{dt}\langle\varphi, V_{-t}\psi\rangle = -e^{-t}q_{x\cdot\nabla V}(U_t\varphi, U_t\psi$$

for all $\varphi, \psi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, with $q_{x\cdot\nabla V}$ the sesqui–linear form corresponding to the distribution $x \cdot \nabla V$.

By assumption, the sesqui–linear form $q_{x\cdot\nabla V}$ extends to sesqui–linear form, again denoted by $q_{x\cdot\nabla V}$, which is relatively form bounded with respect to $(P-A)^2$.
We claim that for any $\varphi, \psi \in \mathcal{D}(P-A)$ the map

$$\mathbb{R} \ni s \mapsto q_{x\cdot\nabla V}(U_s\varphi, U_s\psi) \quad \text{is continuous.} \tag{3.34}$$

Assuming this for the moment, the fundamental theorem of calculus shows

$$q_V(\varphi,\psi) - q_{V_{-t}}(\varphi,\psi) = -\int_0^t \frac{d}{ds} q_{V_{-t}}(\varphi,\psi)\, ds = \int_0^t e^{-s} q_{x\cdot\nabla V}(U_s\varphi, U_s\psi)\, ds \tag{3.35}$$

for any $\varphi, \psi \in \mathcal{C}_0^\infty(\mathbb{R}^d) \subset \mathcal{D}(P-A)$. Since $\mathcal{C}_0^\infty(\mathbb{R}^d)$ is dense in $\mathcal{D}(P_A)$ with respect to the graph norm and the involved quadratic forms are form bounded w.r.t $(P-A)^2$, equation (3.35) extend to all $\varphi, \psi \in \mathcal{D}(P-A)$. But then (3.35) implies

$$\frac{d}{dt} q_{V_{-t}}(\varphi,\psi)|_{t=0} = \lim_{t\to 0} \frac{1}{t}\big(q_V(\varphi,\psi) - q_{V_{-t}}(\varphi,\psi)\big) = q_{x\cdot\nabla V}(\varphi,\psi)$$

which proves (3.31). For (3.32) we note

$$\begin{aligned} 2t \operatorname{Re} q_V(\varphi, iD_t\varphi) &= \operatorname{Re}\big(q_V(\varphi, U_t\varphi) - q_V(\varphi, U_{-t}\varphi)\big) = \operatorname{Re}\big(q_V(U_t\varphi, \varphi) - q_V(\varphi, U_{-t}\varphi)\big) \\ &= \operatorname{Re}\big(q_{V_{-t}}(\varphi, U_{-t}\varphi) - q_V(\varphi, U_{-t}\varphi)\big) \end{aligned}$$

and

$$q_{V_{-t}}(\varphi, U_{-t}\varphi) - q_V(\varphi, U_{-t}\varphi = -\int_0^t e^{-s} q_{x\cdot\nabla V}(U_s\varphi, U_sU_{-t}\psi)\, ds$$

again by (3.35). By a simple continuity argument this shows

$$2\operatorname{Re}\langle\varphi, ViD_t\varphi\rangle = -\frac{1}{t}\int_0^t e^{-s} \operatorname{Re} q_{x\cdot\nabla V}(U_s\varphi, U_sU_{-t}\psi)\ ds \to q_{x\cdot\nabla V}(\varphi,\varphi)$$

as $t \to 0$, which yields (3.32).
It remains to prove (3.34): Lemma 2.1 the sesqui–linear form $q_{x\cdot\nabla V}$ being relatively $(P-A)^2$ form bounded is equivalent to the fact that the sesqui–linear form

$$\varphi, \psi \mapsto q_{x\cdot\nabla V}\big(\big((P-A)^2 + dz^2\big)^{-1/2}\varphi, \big((P-A)^2 + dz^2\big)^{-1/2}\psi\big)$$

extends, for $z > 0$, to a bounded sesqui–linear form to all $(\varphi, \psi) \in L^2(\mathbb{R}^d)$. Recalling the definition (3.17) for R_z and (3.22), this is equivalent to

$$\varphi, \psi \mapsto q_{x\cdot\nabla V}\big(\big(R_z\varphi, R_z\psi\big) =: \widetilde{q}(\varphi,\psi)$$

being a bounded quadratic form, more precisely, extending to a bounded quadratic form on all of $L^2(\mathbb{R}^d)$, for all $z > 0$. Using sesqui–linearity, it is easy to see that for all continuous maps $s \mapsto \varphi_s, s \mapsto \psi_s \in L^2(\mathbb{R}^d)$ the map $s \mapsto \widetilde{q}(\varphi_s, \psi_s)$ is continuous for any bounded sesqui–linear form $\widetilde{q}$ on $L^2(\mathbb{R}^d)$.
For $\varphi, \psi \in \mathcal{D}(P-A)$ we have

$$q(U_s\varphi, U_s\psi) = \widetilde{q}((P-A-iz)U_s\varphi, (P-A-iz)U_s\psi)$$

and

$$U_s\varphi = R_z(P-A-iz)U_s\varphi = R_zU_s\big(e^s(P-A) + (e^sA - A_{-s}) - iz\big)\varphi\,.$$

The map $s \mapsto e^s(P-A)\varphi$ is clearly continuous for all $\varphi \in \mathcal{D}(P-A)$ and so is the map $s \to (e^s A - A_s)\varphi$ by Proposition 3.3. Thus $s \mapsto \widetilde{\varphi}_s := \big(e^s(P-A) + (e^s A - A_{-s}) - iz)\varphi$ is continuous for all $\varphi \in \mathcal{D}(P-A)$. Using $s \mapsto U_s$ being strongly continuous and unitary, and

$$U_t\widetilde{\varphi}_t - U_s\widetilde{\varphi}_s = (U_t - U_s)\widetilde{\varphi}_t + U_s(\widetilde{\varphi}_t - \widetilde{\varphi}_s)$$

one sees that the map $s \mapsto \varphi_s := U_s\widetilde{\varphi}_s$ is continuous. Similarly when φ is replaced by $\psi \in \mathcal{D}(P-A)$. Thus

$$\mathbb{R} \ni s \mapsto q(U_s\varphi, U_s\psi) = \widetilde{q}(\varphi_s, \psi_s)$$

is continuous, since $\widetilde{q}$ is a bounded sesqui–linear form. This proves (3.34) and hence the lemma. □

3.2 The commutator as a quadratic form

This section deals with one of our main results, the rigorous identification of the right hand side of (3.10).

Theorem 3.8 (Magnetic virial theorem) *Let B and V satisfy Assumptions 2.3–2.5 and A be the vector potential in the Poincaré gauge corresponding to the magnetic field B. Assume also that the distribution $x \cdot \nabla V$ extends to a quadratic form which is form bounded with respect to $(P-A)^2$. Then for all $\varphi \in \mathcal{D}(P-A)$, the limit $\lim_{t\to 0} 2\,\mathrm{Re}\,\big(q_{A,V}(\varphi, iD_t\varphi)\big)$ exists. Moreover,*

$$\begin{aligned}\big\langle\varphi, [H, iD]\,\varphi\big\rangle &:= \lim_{t\to 0} 2\,\mathrm{Re}\,\big(q_{A,V}(\varphi, iD_t\varphi)\big)\\ &= 2\|(P-A)\varphi\|_2^2 + 2\,\mathrm{Re}\big\langle\widetilde{B}\varphi, (P-A)\,\varphi\big\rangle - \big\langle\varphi, x\cdot\nabla V\varphi\big\rangle.\end{aligned} \tag{3.36}$$

In particular, for any weak eigenfunction ψ of $H_{A,V}$ with eigenvalue E, i.e., $\big\langle\varphi, E\psi,\big\rangle = q_{A,V}(\varphi,\psi)$ for all $\varphi \in \mathcal{D}(P-A)$, we have the virial identity

$$2\|(P-A)\psi\|_2^2 + 2\,\mathrm{Re}\big\langle\widetilde{B}\psi, (P-A)\,\psi\big\rangle - \big\langle\psi, x\cdot\nabla V\psi\big\rangle = 0\,. \tag{3.37}$$

Remarks 3.9 See the proof of Lemma 3.7 for the precise meaning of the quadratic form $\langle\varphi, x\cdot\nabla V\varphi\rangle$.

Proof Recall that, as a quadratic form, we defined $\langle\varphi, [H_{A,V}, iD_t]\varphi\rangle := 2\,\mathrm{Re}\,q_{A,V}(\varphi, iD_t\varphi)$, using the notation from (2.30). See (3.9) and the discussion before it. Once one knows this limit, and its existence, the proof of (3.37) is straightforward. Since ψ is a weak eigenfunction we also have $\big\langle E\psi, \varphi\big\rangle = q_{A,V}(\psi,\varphi)$ for all $\varphi \in \mathcal{D}(P-A)$. Since multiplication with $E \in \mathbb{R}$ and iD_t are bounded operators and multiplication with a constant commutes with any bounded operator, $2\,\mathrm{Re}(q_{A,V}(\psi, iD_t\psi)) = 2\,\mathrm{Re}(\big\langle E\psi, iD_t\psi) = 2\,\mathrm{Re}\,\big\langle\psi, [E, iD_t]\psi\big\rangle = 0$.

Now we will show that the limit in (3.36) exists for all $u \in \mathcal{D}(P-A)$ and is given by the right hand side of (3.36). By (3.11)

$$(P-A)U_t\,u = e^t U_t(P-A)\,u + X_t\,u, \tag{3.38}$$

where

$$X_t\,u = U_t(e^t\,A - A_{-t})\,u\,, \tag{3.39}$$

where we recall $A_{-t} = U_t^*\,A\,U_t = A(e^{-t}\cdot)$. Since

$$2t\,\mathrm{Re}\,\big(q_{A,V}(\varphi, iD_t\varphi)\big) = \mathrm{Re}\,\big(q_{A,V}(\varphi, U_t\varphi) - q_{A,V}(U_{-t}\,\varphi,\varphi)\big)\,,$$

and

$$q_{A,0}(\varphi, U_t\varphi) = \langle (P-A)\varphi, U_t e^t (P-A)\varphi\rangle + \langle (P-A)\varphi, X_t\varphi\rangle\,,$$
$$q_{A,0}(U_{-t}\varphi, \varphi) = \langle (P-A)\varphi, U_t e^{-t} (P-A)\varphi\rangle + \langle X_{-t}\varphi, (P-A)\varphi\rangle\,,$$

we get

$$\begin{aligned}2\,\mathrm{Re}\, q_{A,0}(\varphi, iD_t\varphi) &= \frac{e^t - e^{-t}}{t}\langle (P-A)\varphi, U_t(P-A)\varphi\rangle + \left\langle (P-A)\varphi, \frac{1}{t}X_t\varphi\right\rangle \\ &\quad - \left\langle \frac{1}{t}X_{-t}\varphi, (P-A)\varphi\right\rangle \\ &\to 2\langle (P-A)\varphi, (P-A)\varphi\rangle + 2\,\mathrm{Re}\langle \widetilde{B}\varphi, (P-A)\varphi\rangle\end{aligned}$$

as $t \to 0$, because by Proposition 3.6 we have

$$\lim_{t\to 0}\frac{1}{t}X_{\pm t}\, u = \pm\widetilde{B}u \quad \text{in} \quad L^2(\mathbb{R}^d).$$

Lemma 3.7 gives $\lim_{t\to 0}\mathrm{Re}\, q_V(\varphi, iD_t\varphi)\rangle = -q_{x\cdot\nabla V}(\varphi,\varphi) =: -\langle\varphi, x\cdot\nabla V\varphi\rangle$ and since

$$q_{A,V}(\varphi, iD_t\varphi) = q_{A,0}(\varphi, iD_t\varphi) + q_V(\varphi, iD_t\varphi)\,,$$

this finishes the proof. □

Remarks 3.10 Equation (3.36) is known for smooth magnetic and electric fields, see e.g. [2]. As for its physical interpretation, we note that the virial theorem in classical mechanics states that

$$\big\langle 2T + x\cdot F\big\rangle = 0 \tag{3.40}$$

where T denotes the kinetic energy, F denotes the external force, and $\langle\,\rangle$ stands for an average over (infinitely) large times. The identity (3.40) holds for all initial conditions for which the velocity and position of the system stay bound in time, i.e., the classical version of a bound state.

In our case F is given by the Lorentz force, hence $F = -q\nabla V + qv\wedge B$, and therefore

$$x\cdot F = -qx\cdot\nabla V + q\,x\cdot(v\wedge B) = -q\,x\cdot\nabla V + q\,v\cdot(B\wedge x) = -q\,x\cdot\nabla V + q\,v\cdot\widetilde{B},$$

where we have used the vector identity $a\cdot(b\wedge c) = b\cdot(c\wedge a)$. Since we have $v = \frac{1}{m}(P - qA)$ and $T = \frac{1}{2m}(P-qA)^2$, the quantum analog of (3.40) reads

$$0 = \frac{1}{m}\|(P-qA)\varphi\|_2^2 + \frac{q}{m}\,\mathrm{Re}\big\langle (P-A)\,\varphi, \widetilde{B}\varphi\big\rangle - \big\langle\varphi, x\cdot\nabla V\varphi\big\rangle,$$

which in our system of units, where $q = 1$ and $m = \frac{1}{2}$, coincides with (3.36) when the commutator vanishes.

A proof of (3.40) follows immediately from the observation

$$2T = mv^2 = \dot{x}\cdot p = \frac{d}{dt}(x\cdot p) - x\cdot p = \frac{d}{dt}(x\cdot p) - x\cdot F$$

where v is the velocity, $p = mv$ the momentum and $\dot{p} = F$ by Newton's equation.

An immediate consequence of our magnetic virial theorem is

Corollary 3.11 *Let the assumptions of the magnetic virial Theorem 3.8 above be satisfied. If $\psi \in \mathcal{D}(P-A)$ is a normalised weak eigenfunction of the magnetic Schrödinger operator $H_{A,V}$ corresponding to the energy $E \in \mathbb{R}$, in the sense that $\psi \in \mathcal{D}(P-A)$, $\psi \neq 0$, and*

$$E\langle\varphi, \psi\rangle = q_{A,V}(\varphi, \psi) \tag{3.41}$$

for all $\varphi \in \mathcal{D}(P-A)$, or all $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, then

$$0 = 2E\big\langle\psi, \psi\big\rangle + 2\,\mathrm{Re}\big\langle(P-A)\,\psi, \widetilde{B}\,\psi\big\rangle - \big\langle\psi, (2V + x\cdot\nabla V)\psi\big\rangle \tag{3.42}$$

Proof This follows immediately from (3.37) since $\|(P-A)\psi\|_2^2 = q_{A,V}(\psi,\psi) - \big\langle\psi, V\psi\big\rangle = \big\langle\psi, E\psi\big\rangle - \big\langle\psi, V\psi\big\rangle$. □

Now, of course, the question is for what class of potentials V one can calculate the virial $x\cdot\nabla V$ in a simple way. A typical example is given in the next section.

3.3 The Kato form of the virial

Our standing assumption is that the virial of the potential, given by the distribution $x\cdot\nabla V$, yields a quadratic form $q_{x\cdot\nabla V}$ which is form bounded w.r.t. $(P-A)^2$. If $x\cdot\nabla V$ is given by a function which corresponds to a nice quadratic form, then $q_{x\cdot\nabla V}$ is given by the classical expression $\langle\varphi, x\cdot\nabla V\varphi\rangle$. On the other hand, the virial given by the formal expression $\langle\varphi, x\cdot\nabla V\varphi\big\rangle$ can exist even if V is not at all classically differentiable.

Our next result shows that this can be the case, even without any kind of differentiability of V. Lemma 3.12 result also identifies the quadratic form $q_{x\cdot\nabla V}$ with an expression similar to one already used by Kato in his proof of absence of positive eigenvalues.

Lemma 3.12 *Assume that the magnetic field B satisfies Assumptions 2.3 and 2.4, A is the magnetic vector-potential in the Poincaré gauge, and V and $|x|^2V^2$ are relatively form bounded with respect to $(P-A)^2$. Then the quadratic form $q_{x\cdot\nabla V}$ corresponding to the distribution $x\cdot\nabla V$ extends from $\mathcal{C}_0^\infty(\mathbb{R}^d)$ to a quadratic form which is form bounded w.r.t. $(P-A)^2$. It is given by*

$$\begin{aligned}\big\langle\varphi, x\cdot\nabla V\varphi\big\rangle := q_{x\cdot\nabla V}(\varphi,\varphi) &= 2\,\mathrm{Im}\big\langle xV\varphi, (P-A)\varphi\big\rangle - d\big\langle\varphi, V\varphi\big\rangle \\ &= 2\,\mathrm{Im}\big\langle\varphi, (P-A)\varphi\big\rangle - dq_V(\varphi,\varphi)\end{aligned} \tag{3.43}$$

for all $\varphi \in \mathcal{D}(P-A)$.

Remarks 3.13 Since x^2V^2 is form bounded w.r.t. $(P-A)^2$, $|x|V\varphi \in L^2$ for all $\varphi \in \mathcal{D}(P-A)$. We call (3.43) the Kato form of the virial. Kato did not consider magnetic fields and used the pointwise conditions V bounded and $\lim_{x\to\infty}|x|V(x) = 0$ to conclude absence of positive eigenvalues for non-magnetic Schrödinger operators. Lemma 3.12 allows us not only to extend this to magnetic Schrödinger operators but to replace Kato's pointwise condition by a rather weak and natural smallness condition on the quadratic form $\langle\varphi, |x|^2V^2\varphi\rangle$ at infinity.

Of course, since the vector potential is in the Poincaré gauge $x\cdot A(x) = 0$, so $\big\langle xV\varphi, (P-A)\varphi\big\rangle = \big\langle V\varphi, x\cdot P\varphi\big\rangle$, hence the right hand side of (3.43) does not depend on vector potential A. In fact, since A is a real-valued vector function and V is real-valued $\big\langle xV\varphi, A\varphi\big\rangle$ is real for any function $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$. Keeping $P-A$ in the right hand side of (2.21) is useful, however, see the proof of Lemma 4.4, in particular, the proof of (4.15).

Proof By definition, the virial is given by $\langle\varphi, x \cdot \nabla V\varphi\rangle := -q_{x\cdot\nabla V}(\varphi,\varphi) = \lim_{t\to 0}\operatorname{Re} q_V(\varphi, iD_t\varphi)$ with q_V the quadratic form corresponding to the multiplication operator V. We will calculate this limit slightly differently than in Lemma 3.7. As distributions

$$2itD_t\varphi = \int_{-t}^{t} U_s iD\varphi\,ds = \int_{-t}^{t} U_s ix\cdot P\varphi\,ds + \frac{d}{2}\int_{-t}^{t} U_s\varphi\,ds$$

and

$$\frac{1}{|x|}\int_{-t}^{t} U_s ix\cdot P\varphi\,ds = i\int_{-t}^{t} e^s U_s\big(\tfrac{x}{|x|}\cdot P\varphi\big)\,ds = i\int_{-t}^{t} e^s U_s\big(\tfrac{x}{|x|}\cdot (P-A)\varphi\big)\,ds$$

since any vector potential in the Poincaré gauge is transversal, that is, $x\cdot A(x) = 0$ for all $x\in\mathbb{R}^d$. Altogether, we have

$$iD_t\varphi = \frac{i}{2t}|x|\int_{-t}^{t} e^s U_s\big(\tfrac{x}{|x|}\cdot(P-A)\varphi\big)\,ds\ + \frac{d}{4t}\int_{-t}^{t} U_s\varphi\,ds$$

at least when $\varphi\in\mathcal{C}_0^\infty(\mathbb{R}^d)$. Thus, in this case,

$$\begin{aligned} q_V(\varphi, iD_t\varphi) &= i\left\langle |x|V\varphi, \frac{1}{2t}\int_{-t}^{t} e^s U_s\big(\tfrac{x}{|x|}\cdot(P-A)\varphi\big)\,ds\right\rangle + \frac{d}{2}\left\langle V\varphi, \frac{1}{2t}\int_{-t}^{t} U_s\varphi\,ds\right\rangle \\ &= i\left\langle |x|V\varphi, \frac{1}{2t}\int_{-t}^{t} e^s U_s\big(\tfrac{x}{|x|}\cdot(P-A)\varphi\big)\,ds\right\rangle + \frac{d}{2}q_V\left(\varphi, \frac{1}{2t}\int_{-t}^{t} U_s\varphi\,ds\right) \end{aligned} \tag{3.44}$$

Since $\frac{x}{|x|}\cdot(P-A)\varphi\in L^2(\mathbb{R}^d)$ for all $\varphi\in\mathcal{D}(P-A)$, the maps $s\mapsto U_s(\frac{x}{|x|}(P-A)\varphi)$ and $s\mapsto U_s\varphi$ are continuous. Moreover, the map $s\mapsto U_s\varphi$ is continuous in the graph norm corresponding to $P-A$ for any $\varphi\in\mathcal{D}(P-A)$ by a similar argument as in the proof of Lemma 3.7. Also $|x|V\varphi\in L^2(\mathbb{R}^d)$ for any $\varphi\in\mathcal{D}(P-A)$, since xV is relatively $P-A$ bounded, that is, $|x|^2V^2$ is relatively $(P-A)^2$ form bounded, by assumption. But then (3.44) also extends to all $\varphi\in\mathcal{D}(P-A)$ by continuity.

Since for $\varphi\in\mathcal{D}(P-A)$ the map $s\mapsto U_s$ is continuous in the graph norm of $P-A$, we also have $\frac{1}{2t}\int_{-t}^{t} U_s\varphi\,ds\to\varphi$ in the graph norm. In addition, $\frac{1}{2t}\int_{-t}^{t} e^s U_s\big(\frac{x}{|x|}\cdot(P-A)\varphi\big)\,ds\to\frac{x}{|x|}\cdot(P-A)\varphi$ in $L^2(\mathbb{R}^d)$ as $t\to 0$. Then (3.44) and continuity of the quadratic form q_V in the graph norm of $P-A$ yields

$$\lim_{t\to 0}\langle\varphi, ViD_t\varphi\rangle = i\langle |x|V\varphi, \tfrac{x}{|x|}\cdot(P-A)\varphi\rangle + \frac{d}{2}q_V(\varphi,\varphi)$$

which, taking real parts, finishes the proof of Lemma 3.12. □

Remarks 3.14 Slightly informally, an alternatively way to derive (3.43) is as follows: For $u, w\in\mathcal{C}_0^\infty(\mathbb{R}^d)$, which is dense in the domain of $P-A$, the quadratic form $\langle u, x\cdot\nabla Vw\rangle$ is given as a distribution by

$$\begin{aligned} \langle u, x\cdot\nabla Vw\rangle &= \langle u, x\cdot\nabla(Vw) - Vx\cdot\nabla w\rangle = -\langle\nabla\cdot(xu), Vw\rangle - \langle Vu, x\cdot\nabla w\rangle \\ &= -d\langle u, Vw\rangle - \langle Vu, x\cdot\nabla w\rangle - \langle x\cdot\nabla u, Vw\rangle \\ &= -d\langle u, Vw\rangle - i\big(\langle xVu, (P-A)w\rangle - \langle (P-A)u, xVw\rangle\big) \end{aligned} \tag{3.45}$$

since the vector potential A is in the Poincaré gauge and $P=-i\nabla$. Under the conditions on V this extends to all $\varphi\in\mathcal{D}(P-A)$.

Corollary 3.15 *Assume that the magnetic field B satisfies Assumptions 2.3 and 2.4, A is the magnetic vector-potential in the Poincaré gauge, and the potential V splits as $V = V_1 + V_2$ where V_1 and $|x|^2 V_1^2$ are relatively form bounded with respect to $(P-A)^2$ and the distribution $x \cdot \nabla V_2$ extend to a quadratic form which is form bounded with respect to $(P-A)^2$. Then, with a slight abuse of notation,*

$$- \langle \varphi, x \cdot \nabla V \varphi \rangle = -2 \operatorname{Im} \langle x V_1 \varphi, (P-A)\varphi \rangle + d \langle \varphi, V_1 \varphi \rangle - \langle \varphi, x \cdot \nabla V_2 \varphi \rangle \tag{3.46}$$

for all $\varphi \in \mathcal{D}(P-A)$.

Proof Simply combine Lemmas 3.7 and 3.12. □

3.4 The exponentially weighted magnetic virial

The proof of our main result, see Theorem 4.8 below, is based on finding two different expressions for the commutator $\langle e^F \psi, [H, iD] e^F \psi \rangle$, when F is a suitable weight function and ψ is a weak eigenfunction, see (3.41). This is done in

Lemma 3.16 *Assume that the magnetic field B and the electric potential V satisfy Assumptions 2.3, 2.4, and 2.5, and A is the vector potential corresponding to B in the Poincaré gauge. Moreover assume that the distribution $x \cdot \nabla V$ extend to a quadratic form, which is form bounded with respect to $(P-A)^2$. Let $F : \mathbb{R}^d \to \mathbb{R}$ be a smooth and bounded radial function, such that $\nabla F(x) = g(x)x$, and assume that $g \geq 0$ and that the functions $\nabla(|\nabla F|^2)$, $(1+|\cdot|^2)g$, $x \cdot \nabla g$ and $(x \cdot \nabla)^2 g$ are bounded. Let $\psi \in \mathcal{D}(P-A)$ be a weak eigenfunction of the magnetic Schrödinger operator $H_{A,V}$, i.e., $E\langle \varphi, \psi \rangle = q_{A,V}(\varphi, \psi)$ for some $E \in \mathbb{R}$ and all $\varphi \in \mathcal{D}(P-A)$, where $q_{A,V}$ is the sesqui–linear form corresponding to the magnetic Schrödiner operator $H_{A,V}$ and set $\psi_F = e^F \psi$. Then*

$$\begin{aligned} \langle \psi_F, [H, iD] \psi_F \rangle &= \langle \psi_F, (E + |\nabla F|^2) \psi_F \rangle + 2 \operatorname{Re} \langle (P-A) \psi_F, \widetilde{B} \psi_F \rangle \\ &\quad + \|(P-A)\psi_F\|_2^2 - \langle \psi_F, (V + x \cdot \nabla V) \psi_F \rangle, \end{aligned} \tag{3.47}$$

and

$$\langle \psi_F, [H, iD] \psi_F \rangle = -4 \|\sqrt{g}\, D \psi_F\|_2^2 + \langle \psi_F, ((x \cdot \nabla)^2 g - x \cdot \nabla |\nabla F|^2) \psi_F \rangle. \tag{3.48}$$

Remarks 3.17 Of course, $\langle \varphi, (V + x \cdot \nabla V) \varphi \rangle$ is given by the sum $q_V + q_{x \cdot \nabla V}$ of the quadratic forms. Rearranging the terms in the derivation of (3.47) a little bit also shows that

$$\begin{aligned} \langle \psi_F, [H, iD] \psi_F \rangle &= \langle \psi_F, 2(E + |\nabla F|^2) \psi_F \rangle + 2 \operatorname{Re} \langle (P-A) \psi_F, \widetilde{B} \psi_F \rangle \\ &\quad - \langle \psi_F, (2V + x \cdot \nabla V) \psi_F \rangle . \end{aligned}$$

Thus (3.47) and (3.48) are a quadratic form version of the bounds of [16], in which the authors considered only the nonmagnetic case. Also note that the conditions in [16] are stronger, since they work with operators and not with forms.
To get an idea why the bounds from Lemma 3.16 are useful for excluding eigenfunctions for positive energies $E > 0$, think of $\langle \psi_F, (E + |\nabla F|^2) \psi_F \rangle$, respectively $-4 \|\sqrt{g}\, D \psi_F\|^2$, as the main terms in (3.47) and (3.48), and the other terms as lower order. Then (3.47) and (3.48) contradict each other when $E > 0$ unless $\psi = 0$.

Before we prove Lemma 3.16 we first collect some auxiliary results, to simplify the calculations. First note that as distributions,

$$(P-A)\psi_F = e^F (P-A)\psi - i e^F \nabla F \psi . \tag{3.49}$$

Hence since F and ∇F are bounded we have $\psi_F \in \mathcal{D}(P-A)$ for any $\psi \in \mathcal{D}(P-A)$, so $\langle \psi_F, i\,[H, D]\,\psi_F \rangle$ is well-defined.

Secondly, note that the operators $\nabla F \cdot P$ and $P \cdot \nabla F$ are well defined on $\mathcal{D}(P-A)$. Indeed, since F is radial we have $\nabla F = gx$ for some function g depending only on $|x|$. This implies $\nabla F \cdot A = 0$, see also (2.17). Hence, as distributions,

$$\nabla F \cdot Pu = gx \cdot Pu = gx \cdot (P-A)u \in L^2(\mathbb{R}^d) \tag{3.50}$$

for all $u \in \mathcal{D}(P-A)$. Similarly,

$$\begin{aligned}
P \cdot \nabla F\, u &= P \cdot (gx)u = gP \cdot xu - i(x \cdot \nabla g)u \\
&= gx \cdot (P-A)u - igdu - i(x \cdot \nabla g)u \in L^2(\mathbb{R}^d)\,, \\
\langle x \rangle^{-1} D\, u &= \frac{1}{2\langle x \rangle}\big(x \cdot P + P \cdot x\big)u = \frac{x}{\langle x \rangle} \cdot P\, u - \frac{i}{2\langle x \rangle} u \\
&= \langle x \rangle^{-1} x \cdot (P-A)\, u - \frac{i}{2\langle x \rangle} u \in L^2(\mathbb{R}^d), \\
gD\, u &= \frac{g}{2}\big(x \cdot P + P \cdot x\big)u \\
&= gx \cdot P\, u - \frac{ig}{2} u = gx \cdot (P-A)\, u - \frac{ig}{2} u \in L^2(\mathbb{R}^d), \\
\sqrt{g} D\, u &= \sqrt{g} x \cdot (P-A)\, u - \frac{i\sqrt{g}}{2} u \in L^2(\mathbb{R}^d), \\
\langle x \rangle g D\, u &= \langle x \rangle g x \cdot (P-A)\, u - \frac{i\langle x \rangle g}{2} u \in L^2(\mathbb{R}^d),
\end{aligned} \tag{3.51}$$

and

$$D_{\nabla F}\, u := \frac{1}{2}\big(\nabla F \cdot P + P \cdot \nabla F\big)u = gDu - \frac{i}{2}(x \cdot \nabla g)u \in L^2(\mathbb{R}^d) \tag{3.52}$$

for all $u \in \mathcal{D}(P-A)$, by the assumptions on g. Note also that $D_{\nabla F}$ is symmetric.

The next result is needed also later, so we single it out.

Lemma 3.18 *Under the conditions of Lemma 3.16 we have*

$$q_{A,V}(u,v) = q_{A,V}(e^{-F}u, e^{F}v) + 2i\,\langle D_{\nabla F}\, u, v \rangle + \langle \nabla F\, u, \nabla F\, v \rangle \tag{3.53}$$

for all $u, v \in \mathcal{D}(P-A)$. In particular, if ψ is a weak eigenfunction corresponding to the energy E of the magnetic Schrödinger operator $H_{A,V}$, then

$$q_{A,V}(\psi_F, \psi_F) = \langle \psi_F, (E + |\nabla F|^2)\psi_F \rangle. \tag{3.54}$$

Proof A straightforward calculation using the above equations and (3.49) yields

$$\begin{aligned}
q_{A,0}(e^{-F}u, e^{F}v) &= \langle (P - A + i\nabla F)u, (P - A - i\nabla F)v \rangle \\
&= q_{A,0}(u,v) - i\big(\langle \nabla F u, (P-A)v \rangle + \langle (P-A)u, \nabla F v \rangle\big) \\
&\quad - \langle \nabla F u, \nabla F v \rangle \\
&= q_{A,0}(u,v) - 2i\langle D_{\nabla F}\, u, v \rangle - \langle \nabla F u, \nabla F v \rangle.
\end{aligned} \tag{3.55}$$

In particular, since $\langle e^{-F}\, u, Ve^{F}\, v \rangle = \langle u, Vv \rangle$ and $q_{A,0}(u,v) = q_{A,0}(u,v) + \langle u, Vv \rangle$ this gives (3.53).

If ψ is a weak eigenfunction of $H_{A,V}$ then $q_{A,V}(\psi, v) = E\langle\psi, v\rangle$ for all $v \in \mathcal{D}(P - A)$. Since $D_{\nabla F}$ is symmetric, $\langle D_{\nabla F}\psi_F, \psi_F\rangle$ s real and (3.53) implies

$$\begin{aligned} q_{A,V}(\psi_F, \psi_F) &= \operatorname{Re} q_{A,V}(\psi_F, \psi_F) = \operatorname{Re} q_{A,V}(\psi_F, e^F\psi_F) + \operatorname{Re}\langle\nabla F\psi_F, \nabla F\psi_F\rangle \\ &= \operatorname{Re} E\langle\psi_F, e^F\psi_F\rangle + \operatorname{Re}\langle\nabla F\psi_F, \nabla F\psi_F\rangle = \operatorname{Re}\langle\psi_F, (E + |\nabla F|^2)\psi_F\rangle \end{aligned}$$

□

Proof of Lemma 3.16 From (3.49) we know that $\psi_F \in \mathcal{D}(P - A) = \mathcal{Q}(H_{A,V})$. Thus for any $\psi \in \mathcal{Q}(H_{A,V})$ our magnetic virial Theorem 3.8 shows

$$\langle\psi_F, [H, iD]\psi_F\rangle = 2q_{A,0}(\psi_F, \psi_F) + 2\operatorname{Re}\langle\widetilde{B}\psi_F, (P - A)u\rangle - \langle\psi_F, x\cdot\nabla V\psi_F\rangle.$$

with $q_{A,0}(\psi_F, \psi_F) = \langle(P - A)\psi_F, (P - A)\psi_F\rangle$. If ψ is a weak eigenfunction of $H_{A,V}$ with energy E, then

$$\begin{aligned} \langle\psi_F, i[H, D]\psi_F\rangle &= q_{A,V}(\psi_F, \psi_F) - \langle\psi_F, V\psi_F\rangle + q_{A,0}(\psi_F, \psi_F) \\ &\quad + 2\operatorname{Re}\langle\widetilde{B}\psi_F, (P - A)\psi_F\rangle - \langle\psi_F, x\cdot\nabla V\psi_F\rangle \\ &= \langle\psi_F, (E + |\nabla F|^2)\psi_F) + q_{A,0}(\psi_F, \psi_F) \\ &\quad + 2\operatorname{Re}\langle\widetilde{B}\psi_F, (P - A)\psi_F\rangle - \langle\psi_F, (V + x\cdot\nabla V)\psi_F\rangle \end{aligned}$$

by (3.54). This proves the first claim of Lemma 3.16.

Applying (3.53) with $u = \psi_F$ and $v = iD_t\psi_F$ one sees

$$\begin{aligned} q(\psi_F, iD_t\psi_F) &= q(\psi, e^F iD_t\psi_F) + 2i\langle D_{\nabla F}\psi_F, iD_t\psi_F\rangle + \langle\nabla F\,\psi_F, \nabla F\, iD_t\psi_F\rangle \\ &= E\,\langle\psi_F, iD_t\psi\rangle - 2\langle D_{\nabla F}\psi_F, D_t\psi_F\rangle + \langle\psi_F, |\nabla F|^2 iD_t\psi_F\rangle, \end{aligned}$$

where we again used $q_{A,V}(\psi, v) = E\langle\psi, v\rangle$ for all $v \in \mathcal{D}(P-A)$ and any weak eigenfunction ψ with energy E. Notice that $\langle\psi_F, iD_t\psi_F\rangle = i\langle\psi_F, D_t\psi_F\rangle$ is purely imaginary since D_t is symmetric, so taking the real part above shows

$$2\operatorname{Re} q(\psi_F, iD_t\psi_F) = -4\operatorname{Re}\langle D_{\nabla F}\,\psi_F, D_t\psi_F\rangle + 2\operatorname{Re}\langle\psi_F, |\nabla F|^2 iD_t\psi_F\rangle. \quad (3.56)$$

Lemma 3.7 gives $2\operatorname{Re}\langle\psi_F, |\nabla F|^2 iD_t\psi_F\rangle \to -\langle\psi_F, x\cdot\nabla(|\nabla F|^2)\psi_F\rangle$ as $t \to 0$. Hence (3.56) implies (3.48) as long as

$$\lim_{t\to 0}\operatorname{Re}\langle D_{\nabla F}\,\psi_F, D_t\psi_F\rangle = \|\sqrt{g}D\psi_F\|_2^2 - \frac{1}{4}\langle\psi_F, ((x\cdot\nabla)^2 g)\psi_F\rangle. \quad (3.57)$$

Using $D_{\nabla F}u = gDu - \frac{i}{2}(x\cdot\nabla g)u$ for all $u \in \mathcal{D}(P - A)$, we get

$$\langle D_{\nabla F}\,u, D_t u\rangle = \langle gD\,u, D_t u\rangle + \frac{1}{2}\langle(x\cdot\nabla g)u, iD_t u\rangle$$

and we already know from Lemma 3.7 that $\frac{1}{2}\operatorname{Re}\langle(x\cdot\nabla g)u, iD_t u\rangle \to -\frac{1}{4}\langle u, ((x\cdot\nabla)^2 g)u\rangle$ as $t \to 0$. Moreover,

$$\langle x\rangle^{-1}D_t u = \frac{1}{2t}\int_{-t}^{t}\langle x\rangle^{-1}U_s(Du)\,ds = \frac{1}{2t}\int_{-t}^{t}\frac{\langle e^s x\rangle}{\langle x\rangle}U_s(\langle x\rangle^{-1}Du)\,ds$$

initially for $u \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, but by density and since $\langle x\rangle^{-1}D : \mathcal{D}(P - A) \to L^2(\mathbb{R}^d)$ is bounded, this extends to all $u \in \mathcal{D}(P - A)$. Thus, by continuity, $\langle x\rangle^{-1}D_t u \to \langle x\rangle^{-1}Du$ in $L^2(\mathbb{R}^d)$ as $t \to 0$ and

$$\langle gD\,u,\,D_t u\rangle = \langle\langle x\rangle gD\,u,\,\langle x\rangle^{-1}D_t u\rangle \to \langle\langle x\rangle gD\,u,\,\langle x\rangle^{-1}Du\rangle = \|\sqrt{g}Du\|_2^2$$

as $t \to 0$ for all $u \in \mathcal{D}(P-A)$. This completes the proof of (3.57) and of the Lemma. □

For a type of unique continuation at infinity argument, we will also need the following

Lemma 3.19 *Let B and V satisfy Assumptions 2.3, 2.5, and 2.9. Assume that ψ and F satisfy conditions of Lemma 3.16. Then there exists $\kappa > 0$ and $c_\kappa > 0$ such that*

$$\left\langle \psi_F,\,[H,iD]\,\psi_F\right\rangle \geq \kappa\left\langle \psi_F,|\nabla F|^2\,\psi_F\right\rangle - c_\kappa\|\psi_F\|_2^2\,. \tag{3.58}$$

Proof In what follows the value of a constant c might change from line to line. Since $\psi_F \in \mathcal{H}_A^1(\mathbb{R}^d)$, Lemma 3.16, the Cauchy-Schwarz inequality and Assumption 2.6 give

$$\begin{aligned}\left\langle \psi_F,\,[H,iD]\,\psi_F\right\rangle &\geq \|(P-A)\psi_F\|_2^2 - 2\|(P-A)\psi_F\|_2\big(\|\widetilde{B}\psi_F\|_2 + \|xV_1\psi_F\|_2\big)\\ &\quad - (\alpha_2 + d\,\alpha_3)\|(P-A)\psi_F\|_2^2 - c\|\psi_F\|_2^2\,.\end{aligned}$$

Therefore using (3.54) and Assumption 2.5 we find that for any $\kappa > 0$

$$\begin{aligned}\left\langle \psi_F,\,[H,iD]\,\psi_F\right\rangle &\geq (1-\kappa)\|(P-A)\psi_F\|_2^2 + \kappa\left\langle \psi_F,|\nabla F|^2\,\psi_F\right\rangle\\ &\quad - (\alpha_2 + d\alpha_3 + \kappa\alpha_0)\,\|(P-A)\psi_F\|_2^2\\ &\quad - 2\|(P-A)\psi_F\|_2\big(\|\widetilde{B}\psi_F\|_2 + \|xV_1\psi_F\|_2\big) - c\|\psi_F\|_2^2.\end{aligned}$$

On the other hand Assumption 2.6 implies that

$$\begin{aligned}2\|(P-A)\psi_F\|_2\big(\|\widetilde{B}\psi_F\|_2 + \|xV_1\psi_F\|_2\big) &\leq \alpha_1\|(P-A)\psi_F\|_2^2\\ &\quad + 2\,c_1\|(P-A)\psi_F\|_2\,\|\psi_F\|_2\\ &\leq (\alpha_1+\kappa)\,\|(P-A)\psi_F\|_2^2 + \frac{c_1}{\kappa}\,\|\psi_F\|_2^2.\end{aligned}$$

Hence

$$\begin{aligned}\left\langle \psi_F,\,[H,iD]\,\psi_F\right\rangle &\geq (1-2\kappa-\kappa\alpha_0-\alpha_1-\alpha_2-d\,\alpha_3)\,\|(P-A)\psi_F\|_2^2\\ &\quad + \kappa\left\langle \psi_F,|\nabla F|^2\,\psi_F\right\rangle - (c+\kappa^{-1}c_1)\,\|\psi_F\|_2^2,\end{aligned}$$

and the result follows upon setting

$$\kappa = \frac{1-\alpha_1-\alpha_2-d\,\alpha_3}{2+\alpha_0} > 0,$$

see (2.26). □

4 Absence of positive eigenvalues

We will give the proof of absence of positive eigenvalues in two steps. The first is that putative eigenfunctions corresponding to positive energies have to decay faster than exponentially. In a second step, we prove that any such eigenfunction has to be zero.

4.1 Ridiculously fast decay

We set $\langle x\rangle_\lambda := \sqrt{\lambda + |x|^2}$ for $x \in \mathbb{R}^d$, $\lambda > 0$. For $\lambda = 1$, we write simply $\langle x\rangle_1 = \langle x\rangle$. We have

Proposition 4.1 (Fast decay) *Assume that B and V satisfy Assumptions 2.3–2.8 and that the magnetic field A corresponding to B is in the Poincaré gauge. Furthermore, assume that ψ is a weak eigenfunction of the magnetic Schrödinger operator $H_{A,V}$ corresponding to the energy $E \in \mathbb{R}$, and that there exist $\overline{\mu} \geq 0$ and $\lambda > 0$ such that $x \mapsto e^{\overline{\mu}\langle x\rangle_\lambda}\,\psi(x) \in L^2(\mathbb{R}^d)$. If $E + \overline{\mu}^2 > \Lambda$ with Λ given by (1.14), then*

$$x \mapsto e^{\mu\langle x\rangle_\lambda}\,\psi(x) \in L^2(\mathbb{R}^d) \qquad \forall\,\mu > 0, \quad \forall\,\lambda > 0. \tag{4.1}$$

Before we start with the proof, we make some preparations. Obviously it suffices to prove the statement for $\lambda = 1$. We will first consider the case $\overline{\mu} = 0$, i.e., we only know that $\psi \in \mathcal{D}(P - A) \subset L^2(\mathbb{R}^d)$. The choice

$$F_{\mu,\varepsilon}(x) = \frac{\mu}{\varepsilon}\left(1 - e^{-\varepsilon\,\langle x\rangle}\right), \tag{4.2}$$

for the weight function, for some $\mu \geq 0$ and $\varepsilon > 0$, will be convenient. We have $F_{\mu,\varepsilon}(x) \to \mu\langle x\rangle$ as $\varepsilon \to 0$. Also, since

$$\nabla F_{\mu,\varepsilon} = \mu\langle x\rangle^{-1} e^{-\varepsilon\langle x\rangle} x \tag{4.3}$$

we have

$$g_{\mu,\varepsilon}(x) = \mu\langle x\rangle^{-1} e^{-\varepsilon\langle x\rangle}\,. \tag{4.4}$$

Moreover, let

$$\mu_* = \sup\left\{\mu \geq 0 \,:\, e^{\mu\langle x\rangle}\psi \in L^2(\mathbb{R}^d)\right\},$$

the maximal exponential decay rate of the weak eigenfunction ψ. The bound (4.1) is equivalent to $\mu_* = \infty$, so we have to exclude $0 \leq \mu_* < \infty$. If $0 \leq \mu_* < \infty$, then there exist sequences $\mu_n \searrow \mu_*$, $\varepsilon_n \searrow 0$ as $n \to \infty$, i.e., both sequences are decreasing and $\mu_n \to \mu_*$, $\varepsilon_n \to 0$, as $n \to \infty$, with

$$a_n := \|e^{F_n}\,\psi\|_2 \;\to\; \infty \quad \text{as} \quad n \to \infty, \tag{4.5}$$

where we put $F_n := F_{\mu_n,\varepsilon_n}$. Moreover, we let $g_n(x) := g_{\mu_n,\varepsilon_n}$ and define φ_n by

$$\varphi_n = \frac{e^{F_n}\,\psi}{\|e^{F_n}\,\psi\|}\,. \tag{4.6}$$

Since

$$F_n(x) \;\leq\; \mu_n\langle x\rangle\,, \tag{4.7}$$

the function e^{F_n} is bounded uniformly in $n \in \mathbb{N}$ on compact subsets of $\mathbb{R}^d$. This implies that for any compact subset $K \subset \mathbb{R}^d$ one has

$$\left\langle\varphi_n, \mathbb{1}_K\varphi_n\right\rangle \to 0 \quad \text{as } n \to \infty$$

where $\mathbb{1}_K$ is the characteristic function of K. In turn, this implies that for any bounded function W with $W(x) \to 0$ as $x \to \infty$ one has

$$\left\langle\varphi_n, W\varphi_n\right\rangle \to 0 \quad \text{as } n \to \infty. \tag{4.8}$$

The last equation is the central point of the argument used in the proof of Proposition 4.1. It will allow us to show that in the virial identity applied to φ_n certain terms vanish as $n \to \infty$. This turns crucial when applying 3.16 to prove Proposition 4.1 by contradiction.

Lemma 4.2 *Let F_n, g_n, ψ, and φ_n be given as above. If $0 < \mu_* < \infty$, then*

$$\lim_{n\to\infty} \langle e^{F_n}\psi, \varepsilon_n \langle x\rangle e^{F_n}\psi\rangle = 0 \,. \tag{4.9}$$

Moreover, if $0 \le \mu_* < \infty$, then

$$\lim_{n\to\infty} \big\langle \nabla F_n\varphi_n, \nabla F_n\varphi_n\big\rangle = \mu_*^2 \tag{4.10}$$

and

$$\lim_{n\to\infty} \big\langle \varphi_n, \big((x\cdot\nabla)^2 g_n - x\cdot\nabla|\nabla F_n|^2\big)\varphi_n\big\rangle = 0 \tag{4.11}$$

Remarks 4.3 If $\mu_* > 0$, then ψ decays exponentially and since F_n is bounded for fixed $n \in \mathbb{N}$ we have $\langle e^{F_n}\psi, \langle x\rangle e^{F_n}\psi\rangle < \infty$ for all n.

Lemma 4.4 *Let $0 \le \mu_* < \infty$ and F_n, g_n, and φ_n be given as above. If the potential V is relative form small and vanishes at infinity w.r.t $(P-A)^2$, i.e satisfies Assumptions 2.5 and 2.7, then*

$$\lim_{n\to\infty} \langle\varphi_n, V\varphi_n\rangle = 0 \tag{4.12}$$

$$\lim_{n\to\infty} \langle (P-A)\varphi_n, (P-A)\varphi_n\rangle = E + \mu_*^2 \,. \tag{4.13}$$

Moreover, if the magnetic field B satisfy Assumptions 2.4, and 2.8, then

$$\limsup_{n\to\infty} |\big\langle \widetilde{B}\,\varphi_n, (P-A)\,\varphi_n\big\rangle| \le \beta(E+\mu_*^2)^{1/2} \,. \tag{4.14}$$

and if one splits $V = V_1 + V_2$, with V_1 and V_2 satisfying Assumptions 2.6 and 2.8 then

$$\limsup_{n\to\infty} \big\langle\varphi_n, x\cdot\nabla V\varphi_n\big\rangle \le 2\omega_1(E+\mu_*^2)^{1/2} + \omega_2. \tag{4.15}$$

Here β, ω_1, and ω_2 from (1.13) measure the strength of the magnetic field and the virial of the potential near infinity.

Remarks 4.5 For the proof of similar results in [16], the assumption that V and $x\cdot\nabla V$ are relatively form compact with respect to P^2 is made. Thus they only deal with potentials which are relatively form bounded with relative bound zero. They also do not consider conditions on the Kato form of the virial $x\cdot\nabla V$.

We will prove these two Lemmas later in this section.

Proof of Proposition 4.1 Assume that $0 \le \mu_*^2 < \infty$. It is easy to check that F_n and g_n satisfy the assumptions of the exponentially weighted magnetic virial Lemma 3.16. Thus Lemmas 3.16 and 4.2 show

$$\limsup_{n\to\infty} \big\langle\varphi_n, \ [H, iD]\,\varphi_n\big\rangle \le 0 \,. \tag{4.16}$$

On the other hand the first equality from Lemma 3.16 together with Lemma 4.4 shows

$$\begin{aligned}\liminf_{n\to\infty} \big\langle\varphi_n, \ [H, iD]\,\varphi_n\big\rangle &\ge 2(E+\mu_*^2) - 2(\beta+\omega_1)(E+\mu_*^2)^{1/2} - \omega_2 \\ &= 2\left[\left(\sqrt{E+\mu_*^2} - \frac{\beta+\omega_1}{2}\right)^2 - \left(\frac{\beta+\omega_1}{2}\right)^2 - \frac{\omega_2}{2}\right] > 0\end{aligned} \tag{4.17}$$

if $\sqrt{E+\mu_*^2} > \frac{1}{2}\big(\beta+\omega_1+\sqrt{(\beta+\omega_1)^2+2\omega_2}\big) = \sqrt{\Lambda}$. Clearly, (4.16) and (4.17) contradict each other. Thus $\mu_* = \infty$, which is equivalent to (4.1). □

It remains to prove Lemmas 4.2 and 4.4.

Proof of Lemma 4.2 Clearly, for any $\delta > 0$

$$\begin{aligned}\langle\varphi_n, \varepsilon_n\langle x\rangle\varphi_n\rangle &= \langle\varphi_n, \mathbb{1}_{\{\varepsilon_n\langle x\rangle<\delta\}}\varphi_n\rangle + \langle\varphi_n, \mathbb{1}_{\{\varepsilon_n\langle x\rangle\geq\delta\}}\varepsilon_n\langle x\rangle\varphi_n\rangle \\ &\leq \delta + \langle\varphi_n, \mathbb{1}_{\{\varepsilon_n\langle x\rangle>\delta\}}\varepsilon_n\langle x\rangle\varphi_n\rangle\end{aligned}$$

One easily checks that the mapping $t \mapsto \frac{1-e^{-t}}{t}$ is decreasing on $(0, \infty)$. Thus

$$\overline{\gamma}_\delta := \sup_{t\geq\delta}\frac{1-e^{-t}}{t} = \frac{1-e^{-\delta}}{\delta} < 1 \tag{4.18}$$

which shows

$$F_n = \frac{\mu_n\langle x\rangle}{\varepsilon_n\langle x\rangle}(1-e^{-\varepsilon_n\langle x\rangle}) \leq \mu_n\overline{\gamma}_\delta\langle x\rangle \quad \text{for all } x \text{ with } \varepsilon_n\langle x\rangle \geq \delta\,.$$

Given $\delta > 0$ choose any κ with $\overline{\gamma}_\delta < \kappa < 1$. If $0 < \mu_* < \infty$ then ψ decays exponentially with any rate μ with $\kappa\mu_* < \mu < \mu_*$, by the definition of μ_*. Thus

$$\begin{aligned}\limsup_{n\to\infty}\langle e^{F_n}\psi, \mathbb{1}_{\{\varepsilon_n\langle x\rangle>\delta\}}\langle x\rangle e^{F_n}\psi\rangle &\leq \limsup_{n\to\infty}\langle e^{\mu_n\overline{\gamma}_\delta\langle x\rangle}\psi, \langle x\rangle e^{\mu_n\overline{\gamma}_\delta\langle x\rangle}\psi\rangle \\ &\leq \langle e^{\kappa\mu_*\langle x\rangle}\psi, \langle x\rangle e^{\kappa\mu_*\langle x\rangle}\psi\rangle < \infty\end{aligned}$$

since, $\mu_n\gamma_\delta \to \gamma_\delta\mu_* < \kappa\mu_*$ as $n \to \infty$. In view of (4.5) this implies (4.9).
For the proof of the remaining part of Lemma 4.2, we note that from (4.3) one gets

$$|\nabla F_n|^2 = \mu_n^2\big(1-\langle x\rangle^{-2}\big)e^{-2\varepsilon_n\langle x\rangle}\,. \tag{4.19}$$

Since φ_n is normalized this gives

$$\begin{aligned}\mu_n^2 - \langle\nabla F_n\varphi_n, \nabla F_n\varphi_n\rangle &= \langle\varphi_n, (\mu_n^2 - |\nabla F_n|^2)\varphi_n\rangle \\ &= \mu_n^2\left(\langle\varphi_n, (1-e^{-2\varepsilon_n\langle x\rangle})\varphi_n\rangle + \langle\varphi_n, \langle x\rangle^{-2}e^{-2\varepsilon_n\langle x\rangle}\varphi_n\rangle\right).\end{aligned} \tag{4.20}$$

Recall that $\mu_n \searrow \mu_*$. If $\mu_* = 0$, then (4.20) shows

$$\left|\mu_n^2 - \langle\nabla F_n\varphi_n, \nabla F_n\varphi_n\rangle\right| \leq 2\mu_n^2 \to 0 \quad \text{as } n \to \infty\,.$$

If $0 < \mu_* < \infty$, then using $0 \leq 1 - e^{-2\varepsilon_n\langle x\rangle} \leq 2\varepsilon_n\langle x\rangle$ in (4.20) gives

$$\left|\mu_n^2 - \langle\nabla F_n\varphi_n, \nabla F_n\varphi_n\rangle\right| \leq \mu_n^2\left(2\langle\varphi_n, \varepsilon_n\langle x\rangle\varphi_n\rangle + \langle\varphi_n, \langle x\rangle^{-2}\varphi_n\rangle\right) \to 0 \quad \text{as } n \to \infty$$

due to (4.9) and (4.8). This proves (4.10).

Using the definitions of F_n and g_n a relatively short calculation shows

$$\left|(x\cdot\nabla)^2 g_n - x\cdot\nabla|\nabla F|^2\right| \lesssim \mu_n(\mu_n+1)\left[\langle x\rangle^{-2} + \langle x\rangle^{-1} + \varepsilon_n\langle x\rangle + \varepsilon_n^2\langle x\rangle\right]e^{-\varepsilon_n\langle x\rangle} \tag{4.21}$$

Since $0 \leq t \mapsto te^{-t}$ is bounded, (4.21) implies, if $\mu_* = 0$,

$$\left|\langle\varphi_n, \big((x\cdot\nabla)^2 g_n - x\cdot\nabla|\nabla F|^2\big)\varphi_n\rangle\right| \lesssim \mu_n(\mu_n+1) \to 0 \quad \text{as } n \to \infty.$$

If $0 < \mu_* < \infty$, then (4.21) shows

$$\left|\left\langle \varphi_n, \left((x\cdot\nabla)^2 g_n - x\cdot\nabla|\nabla F|^2\right)\varphi_n\right\rangle\right| \lesssim \left\langle \varphi_n, \left(\langle x\rangle^{-2} + \langle x\rangle^{-1}\right)\varphi_n\right\rangle + \left\langle \varphi_n, \varepsilon_n\langle x\rangle\varphi_n\right\rangle \to 0 \quad \text{as } n\to\infty$$

using again (4.9) and (4.8). This proves (4.11). □

In the proof of Lemma 4.4 we need the following auxiliary tool.

Lemma 4.6 *Assume that the potential V is relatively form bounded w.r.t $(P-A)^2$. Then for any family of real-valued bounded function $\xi_j \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, $j\in I$, for which $\sup_{j\in I}\|\xi_j\|_\infty$ and $\sup_{j\in I}\|\nabla\xi_j\|_\infty$ are finite, we have*

$$\sup_{j\in I}\sup_{n\in\mathbb{N}} \|(P-A)\xi_j\varphi_n\| < \infty\,. \tag{4.22}$$

where φ_n is the sequence defined in (4.6). Moreover, if $\xi\in\mathcal{C}_0^\infty(\mathbb{R}^d)$ is a real-valued function with compact support, then

$$\limsup_{n\to\infty} \|(P-A)\xi\varphi_n\| = 0\,. \tag{4.23}$$

We give the proof of this Lemma after the

Proof of Lemma 4.4 One easily checks that if ξ is an infinitely often differentiable cut–off function with bounded derivative, then $\xi\varphi\in\mathcal{D}(P-A)$ for any $\varphi\in\mathcal{D}(P-A)$.

Let $\chi_l : [0,\infty)\to\mathbb{R}_+$, $l=1,2$, be infinitely often differentiable on $(0,\infty)$ with $\chi_1(r)=1$ for $0\le r\le 1$, $\chi_1(r)>0$ for $r\le 3/2$, $\chi_1(r)=0$ for $r\ge 7/4$, and $\chi_2(r)=0$ for $r\le 5/4$, $\chi_2(r)>0$ for $r\ge 3/2$, $\chi_2(r)=1$ for $r\ge 2$. Then $\inf_{r\ge 0}(\chi_1^2(r)+\chi_2^2(r))>0$ and thus

$$\xi_1 := \frac{\chi_1}{\sqrt{\chi_1^2+\chi_2^2}}\,,\quad \xi_2 := \frac{\chi_2}{\sqrt{\chi_1^2+\chi_2^2}}$$

are infinitely often differentiable with bounded derivatives and $\xi_1^2+\xi_2^2=1$. Given $R\ge 1$ we set

$$\xi_{<R}(x) := \xi_1(|x|/R),\quad \xi_{\ge R}(x) := \xi_2(|x|/R)$$

which yields a family of infinitely often differentiable real-valued localization functions on $\mathbb{R}^d$ with bounded derivatives. Note that $\xi_{<R}$ has compact support and $\operatorname{supp}(\xi_{\ge R})\subset\mathcal{U}_R^c = \{x\in\mathbb{R}^d : |x|\ge R\}$. By construction, we have

$$\left\langle \varphi_n, V\varphi_n\right\rangle = \left\langle \xi_{<R}^2\varphi_n, V\varphi_n\right\rangle + \left\langle \xi_{\ge R}^2\varphi_n, V\varphi_n\right\rangle$$

and, recalling that V is form bounded with respect to $(P-A)^2$, we have for fixed $R\ge 1$

$$|\langle \xi_{<R}^2\varphi_n, V\varphi\rangle| = |\langle \xi_{<R}\varphi_n, V\xi_{<R}\varphi_n\rangle| \lesssim \|(P-A)\xi_{<R}\varphi_n\|_2^2 + \|\xi_{<R}\varphi_n\|_2^2 \to 0\,,\ \text{as } n\to\infty$$

by Lemma 4.6 and (4.8), since $\xi_{<R}$ has compact support. Since V vanishes at infinity w.r.t. $(P-A)^2$, there exist α_R, γ_R with $\alpha_R,\gamma_R\to 0$ as $R\to\infty$ such that

$$|\langle \xi_{\ge R}^2\varphi_n, V\varphi_n\rangle| = |\langle \xi_{\ge R}\varphi_n, V\xi_{\ge R}\varphi_n\rangle| \le \alpha_R\|(P-A)\xi_{\ge R}\varphi_n\|_2^2 + \gamma_R\|\xi_{\ge R}\varphi_n\|_2^2\,.$$

Lemma 4.6 then shows

$$\limsup_{n\to\infty} |\langle \xi_{\geq R}^2 \varphi_n, V\varphi_n\rangle| \lesssim \alpha_R + \gamma_R \to 0\,, \text{ as } R \to \infty\,,$$

which proves (4.12).
Moreover, from Lemma 3.18, we get

$$\begin{aligned}\langle (P-A)\varphi_n, (P-A)\varphi_n\rangle &= E + \langle \nabla F_n\varphi_n, \nabla F_n\varphi_n\rangle - \langle \varphi_n, V\varphi_n\rangle \\ &\to E + \mu_*^2 \quad \text{as } n \to \infty\end{aligned}$$

using also (4.12) and (4.9). This proves (4.13).
For $\widetilde{B}^2$ one can argue exactly the same way as above for V to see that for fixed R

$$\limsup_{n\to\infty} \langle \varphi_n, |\widetilde{B}|^2\varphi_n\rangle \leq \limsup_{n\to\infty} \langle \xi_{\geq R}^2\, \varphi_n,\ |\widetilde{B}|^2\varphi_n\rangle \leq C\varepsilon_R + \beta_R^2$$

where we also used Assumption 2.8 and put $C = \sup_{j\in\mathbb{N}} \limsup_{n\to\infty} \|(P-A)\xi_j\varphi_n\|_2^2$, which due to Lemma 4.6 is finite. Since $\varepsilon_R \to 0$ and $\beta_R \to \beta$, as $R \to \infty$, we get

$$\limsup_{n\to\infty} \|\widetilde{B}\varphi_n\| \leq \beta\,,$$

Because of $|\langle \widetilde{B}\,\varphi_n, (P-A)\,\varphi_n\rangle| \leq \|\widetilde{B}\,\varphi_n\|\|(P-A)\,\varphi_n\|$ and (4.13) this proves (4.14).
If the potential splits as $V = V_1 + V_2$ with V_1, V_2 satisfying Assumptions 2.6 and 2.8, then one can argue exactly as above to see that

$$\limsup_{n\to\infty} |\langle x V_1\varphi_n, (P-A)\varphi_n\rangle| \leq\ \omega_1$$

and

$$\limsup_{n\to\infty} |\langle \varphi_n, x\cdot \nabla V_2\varphi_n\rangle| \leq\ \omega_2\,.$$

Moreover, if V_1 and $(xV_1)^2$ are form bounded w.r.t. $(P-A)^2$ and $\varphi \in \mathcal{D}(P-A)$ with $\mathrm{supp}(\varphi) \subset \{|x| \geq R\}$, then

$$\begin{aligned}|\langle \varphi, V_1\,\varphi\rangle| &= |\langle |x|^{-1}\varphi, |x|V_1\varphi\rangle| \leq \||x|^{-1}\varphi\|\||x|V_1\varphi\| \\ &\lesssim R^{-1}\|\varphi\|\left(\|(P-A)\varphi\|_2^2 + \|\varphi\|_2^2\right)^{1/2}\,,\end{aligned}$$

so V_1 vanishes at infinity w.r.t. $(P-A)^2$. Thus $\lim_{n\to\infty}\langle \varphi_n, V_1\,\varphi_n\rangle = 0$ and using the mixed form of the virial from Corollary 3.15 yields

$$\limsup_{n\to\infty} \langle \varphi, x\cdot\nabla V\varphi\rangle \leq 2\omega_1(E+\mu_*^2)^{1/2} + \omega_2\,.$$

□

Remarks 4.7 Note that $\Lambda < \beta + \omega$ as soon as $\omega > 0$.

Now we give the

Proof of Lemma 4.6 Let $\psi \in \mathcal{D}(P-A)$ be a weak eigenfunction of the magnetic Schrödinger operator $H_{A,V}$ with eigenvalue E and F_n, $\psi_n = e^{F_n}\psi$ and $\varphi_n = \psi_n/\|\psi_n\|$ as in (4.6). In particular, we have $\sup_n \|\nabla F_n\| \leq \sup_n \mu_n < \infty$. Since V is relatively form bounded with respect to $(P-A)^2$

$$\|(P-A)\varphi\|_2^2 = q_{A,V}(\varphi,\varphi) - \langle \varphi, V\varphi\rangle \leq q_{A,V}(\varphi,\varphi) + \alpha_0\|(P-A)\varphi\|_2^2 + C\|\varphi\|_2^2$$

for some $0 \le \alpha_0 < 1$, $C > 0$, and all $\varphi \in \mathcal{D}(P - A)$. Thus

$$\|(P-A)\varphi\|_2^2 \le (1-\alpha_0)^{-1}\left(q_{A,V}(\varphi,\varphi) + C\|\varphi\|_2^2\right)$$

From the IMS localization formula (D.1) we get

$$\begin{aligned} q_{A,V}(\xi\psi_n, \xi\psi_n) &= \mathrm{Re}\, q_{A,V}(\xi^2 e^{2F_n}\psi, \psi) + \left\langle \psi, |\nabla(\xi e^{F_n})|^2\psi\right\rangle \\ &\le E\|\xi\psi_n\|_2^2 + 2\|(\nabla\xi)\psi_n\|_2^2 + 2\|(\nabla F_n)\xi\psi_n\|_2^2 \end{aligned}$$

since ψ is a weak eigenfunction with energy E. Thus

$$\|(P-A)\xi_j\varphi_n\|_2^2 \lesssim \|\xi_j\varphi_n\|_2^2 + \|(\nabla\xi_j)\varphi_n\|_2^2$$

where the implicit constant is independent of $j \in I$ and $n \in \mathbb{N}$. Since φ_n is normalized, this proves the first claim.

On the other hand, if ξ has compact support then so does $\nabla\xi$. Thus, from (4.8) we get $\|\xi\varphi_n\| \to 0$ and $\|(\nabla\xi)\varphi_n\| \to 0$, as $n \to \infty$. Hence,

$$\|(P-A)\xi\varphi_n\|_2^2 \lesssim \|\xi\varphi_n\|_2^2 + \|(\nabla\xi)\varphi_n\|_2^2 \to 0\,,$$

as $n \to \infty$. □

4.2 Absence of positive eigenvalues

Now we are in position to prove our main result.

Theorem 4.8 *Let B and V satisfy Assumptions 2.3–2.8. Then the magnetic Schrödinger operator $H_{A,V}$ has no eigenvalues in the interval (Λ, ∞), where Λ is given by (1.14).*

Moreover, if $E \le \Lambda$ is an eigenvalue of $H_{A,V}$ then any weak eigenfunction ψ with energy E cannot decay faster than $e^{\sqrt{\Lambda - E}|x|}$, in the sense that if $x \mapsto e^{\overline{\mu}|x|}\psi(x) \in L^2(\mathbb{R}^d)$ for some $\overline{\mu} > \sqrt{\Lambda - E}$, then ψ is the zero function.

Proof Let $q_{A,V}$ be the quadratic from corresponding to $H_{A,V}$ and assume that $E\langle\varphi,\psi\rangle = q_{A,V}(\varphi,\psi)$ for all $\varphi \in \mathcal{D}(q_{A,V}) = \mathcal{D}(P - A)$. Furthermore, assume that either $E > \Lambda$ or $E + \overline{\mu}^2 > \Lambda$ for some $\overline{\mu} > 0$ and $x \mapsto e^{\overline{\mu}|x|}\psi(x) \in L^2(\mathbb{R}^d)$. Then from Proposition 4.1 we know that

$$x \mapsto e^{\mu\langle x\rangle_\lambda}\,\psi(x) \in L^2(\mathbb{R}^d) \qquad \forall\,\mu > 0, \quad \forall\,\lambda > 0.$$

where $\langle x\rangle_\lambda = (\lambda + x^2)^{1/2}$.

Let $\mu > 0$, $\varepsilon > 0$, $\lambda > 0$, and define

$$F(x) = F_{\mu,\varepsilon,\lambda}(x) = \frac{\mu}{\varepsilon}\left(1 - e^{-\varepsilon\,\langle x\rangle_\lambda}\right)\,,$$

so that

$$\nabla F_{\mu,\varepsilon,\lambda}(x) = x g_{\mu,\varepsilon,\lambda}(x), \quad g_{\mu,\varepsilon,\lambda}(x) = \frac{\mu\, e^{-\varepsilon\,\langle x\rangle_\lambda}}{\sqrt{\lambda + |x|^2}}\,.$$

Denote $\psi_{\mu,\varepsilon,\lambda} = e^{F_{\mu,\varepsilon,\lambda}}\,\psi$. Lemma 3.19 and Eq. (3.48) then give

$$\begin{aligned} \kappa\left\langle\psi_{\mu,\varepsilon,\lambda}, |\nabla F_{\mu,\varepsilon,\lambda}|^2\,\psi_{\mu,\varepsilon,\lambda}\right\rangle &\le \left\langle\psi_{\mu,\varepsilon,\lambda}, \left((x\cdot\nabla)^2 g_{\mu,\varepsilon,\lambda} - x\cdot\nabla|\nabla F_{\mu,\varepsilon,\lambda}|^2\right)\psi_{\mu,\varepsilon,\lambda}\right\rangle \\ &\quad + C\,\|\psi_{\mu,\varepsilon,\lambda}\|_2^2 \end{aligned} \tag{4.24}$$

for all $\mu, \varepsilon, \lambda > 0$ and some constant C independent of μ, λ and ε. Moreover, a direct calculation shows

$$\lim_{\varepsilon\to 0} x \cdot \nabla |\nabla F_{\mu,\varepsilon,\lambda}(x)|^2 = 2\lambda\mu^2 \langle x\rangle_\lambda^{-1}(1 - \langle x\rangle_\lambda^{-2}) > 0 \tag{4.25}$$

and

$$\lim_{\varepsilon\to 0} (x \cdot \nabla)^2 g_{\mu,\varepsilon,\lambda}(x) = -2\lambda\mu \langle x\rangle_\lambda^{-3} |x|^2 < 0\,. \tag{4.26}$$

Since

$$\lim_{\varepsilon\to 0} F_{\mu,\varepsilon,\lambda}(x) := F_{\mu,\lambda}(x) = \mu\langle x\rangle_\lambda\,,$$

in view of Proposition 4.1 we can pass to limit $\varepsilon \to 0$ in (4.24) to obtain

$$\kappa\,\mu^2 \left\langle \psi_{\mu,\lambda}, \frac{|x|^2}{\lambda + |x|^2}\,\psi_{\mu,\lambda}\right\rangle \leq C\,\|\psi_{\mu,\lambda}\|_2^2 \qquad \forall\,\mu,\lambda > 0, \tag{4.27}$$

where

$$\psi_{\mu,\lambda}(x) := e^{\mu\langle x\rangle_\lambda}\,\psi(x)\,.$$

Using Proposition 4.1 again and the monotone convergence theorem we finally obtain, by letting $\lambda \to 0$,

$$\kappa\,\mu^2\,\|\psi_\mu\|_2^2 \leq C\,\|\psi_\mu\|_2^2 \qquad \forall\,\mu > 0, \tag{4.28}$$

where $\psi_\mu(x) = e^{\mu|x|}\,\psi(x)$. This is of course impossible for μ large enough. Hence $\psi_\mu = 0$. The the first part of the claim, i.e. the absence of eigenvalues above Λ, thus follows from the case $E > \Lambda$. The second part of the claim is covered by the case $E + \overline{\mu}^2 > \Lambda$ for some $\overline{\mu} > 0$. □

Remarks 4.9 Notice that in view of Corollary 6.8 we have $(\Lambda, \infty) \subseteq \sigma_{\text{ess}}(H)$. Hence Theorem 4.8 excludes the presence of all embedded eigenvalues of H above Λ.

On the other hand, the possibility of Λ being an eigenvalue of H cannot be in general excluded. Indeed, if B is continuous and compactly supported with $|\int_{\mathbb{R}^2} B| > 2\pi$, and if $V = -B$, then by the Aharonov-Casher theorem, see e.g. [9, Sec. 6.4], $\Lambda = 0$ is an eigenvalue of $H = (P - A)^2 - B$. Sufficient conditions for the absence of positive eigenvalues of the Pauli operator are proved in Sect. 5.4 , see 5.5.

5 Examples

We recall a couple of examples which show that the decay assumptions on B and V stated in Theorems 1.3, 1.6, and 4.8, and Proposition A.2 cannot be improved.

5.1 Miller–Simon revisited

In [32] Miller and Simon considered, in dimension two, the case $V = 0$ and radial magnetic field $B(x) = b(r)$, $r = |x|$. They proved that

(1) If $b(r) = r^{-\alpha} + O(r^{-1-\varepsilon})$ with $0 < \alpha < 1$ and $\varepsilon > 0$ then the spectrum of H is dense pure point,

(2) If $b(r) = b_0 r^{-1} + O(r^{-1-\varepsilon})$ for some $\varepsilon > 0$ then the spectrum of H is dense pure point in $[0, b_0^2)$ and absolutely continuous in $[b_0^2, \infty)$,
(3) If $b(r) = \mathcal{O}(r^{-\alpha})$ with $\alpha > 1$ then the spectrum of H is purely absolutely continuous in $(0, \infty)$.

Remarks 5.1 Note that $\beta = \limsup_{|x|\to\infty} |\widetilde{B}(x)| = +\infty$ in the case (1). On the other hand, Theorem 4.8 guarantees the absence of eigenvalues in the interval (b_0^2, ∞) for the case (2), in which case $\beta = b_0$, and in the interval $(0, \infty)$ for the case (3), even for non–radial magnetic fields. In particular, the Miller–Simon examples show that our result on absence of eigenvalues is *sharp*. These examples even have dense point spectrum in $[0, b_0^2]$.

Since there is a calculation error in the original Miller-Simon paper and also in the book [9], we sketch their argument: Assume that the radial magnetic field b is reasonable, e.g., bounded and use x, y as coordinates in $\mathbb{R}^2$ and $r = (x^2 + y^2)^{1/2}$.

The first observation of Miller and Simon is that if the magnetic field, radial or not, B goes pointwise to zero at infinity, then $\sigma_{\text{ess}}((P - A)^2) = [0, \infty)$ (this is sharpened in Theorem 6.5).

For radial magnetic fields we have $\widetilde{B}(x) = (-y, x)b(r)$, so the Poincaré gauge the magnetic vector potential is

$$A(x, y) = (-y, x) \int_0^1 b(tr)t\, dt = \frac{(-y, x)}{r} h(r)$$

with $h(r) = r^{-1} \int_0^r b(s)s\, ds$. Expanding $(P - A)^2$ one sees

$$(P - A)^2 = (P_x - A_x)^2 + (P_y - A_y)^2 = P^2 + h(r)^2 - 2\frac{h(r)}{r} L$$

where $L = xP_y - yP_x$ is the angular momentum in the plane. It is well-known that L has eigenvalues $(0, \pm 1, \pm 2, \ldots)$ and it commutes with P^2 and with the radial potential $h(r)^2$. So restricted to the angular momentum channel $\{L = m\}$, the operator $(P - A)^2$ is given by

$$H_m := (P - A)^2\big|_{\{L=m\}} = \left(P^2 + V_m\right)|_{\{L=m\}} \quad \text{with } V_m(r) = h(r)^2 - \frac{2mh(r)}{r}$$

Due to the angular momentum barrier the divergence of V_m for small r when $m \neq 0$ is irrelevant.

If $b_0 = \lim_{r\to\infty} r\, b(r) = \infty$, then $h(r) \to \infty$, so V_m is trapping and all operators H_m have discrete spectrum. But if also $b(r) \to 0$ as $r \to \infty$, then $\sigma_{\text{ess}}(H_A) = [0, \infty)$, so $(P - A)^2$ has necessarily dense point spectrum in $[0, \infty)$, proving the first claim (1) above.

If $b_0 = \lim_{r\to\infty} r\, b(r) < \infty$, then $h(r) \to b_0$ and $V_m(r) \to b_0^2$ as $r \to \infty$, so H_m has only discrete spectrum below b_0^2 for any $m \in \mathbb{Z}$. Since $b(r) \to 0$ for $r \to \infty$, the operator has essential spectrum $[0, \infty]$, which must be dense point spectrum in $[0, b_0^2]$.

For any reasonable choice of radial magnetic field b, the effective potential V_m is smooth with decaying derivatives for large r, so the spectrum of H_m above b_0^2 is absolutely continuous for all $m \in \mathbb{Z}$. Thus $(P - A)^2$ has absolutely continuous spectrum in (b_0^2, ∞), which proves the last two claims.

Remarks 5.2 In [32] the choice of the vector potential contains a wrong factor of $1/2$ and in the example in [9] there is a mistake in the calculation of the magnetic field. Thus in their examples they concluded incorrectly that the effective potential has the asymptotic $V_m(r) \to b_0^2/4$ for large r.

5.2 Wigner–von Neumann potential

Suppose that $B = 0$. Wigner and von Neumann showed that the operator $-\Delta + V$ in $L^2(\mathbb{R}^3)$ with the radial potential

$$V(r) = -\frac{32\sin r\big[g(r)^3\cos r - 3g^2(r)\sin^3 r + g(r)\cos r + \sin^3(r)\big]}{(1+g(r)^2)^2},$$
$$g(r) = 2r - \sin(2r), \tag{5.1}$$

has eigenvalue $+1$, see [37, 44] and [36, Ex. VIII.13.1]. As pointed out in [37] for large r

$$V(r) = -\frac{8\sin(2r)}{r} + \mathcal{O}(r^{-2}). \tag{5.2}$$

Theorem 4.8 implies that $-\Delta + V = -\Delta + V_1 + V_2$ has no eigenvalues larger than

$$\Lambda = \frac{1}{2}\left(\omega_1 + \omega_2 + \sqrt{\omega_1^2 + 2\omega_1\omega_2}\,\right),$$

with ω_1 and ω_2 defined by Eq. (1.15). We can thus optimize the splitting $V = V_1 + V_2$ in order to minimize Λ. A quick calculation using (5.2) shows that the optimal choice is $V_1 = 0,\ V_2 = V$, see also Lemma C.1. With this choice we get $\Lambda = 8$ which coincides with [1, Thm. 4]. Note that [37, Thm. 2] implies absence of eigenvalues in the interval $(16, \infty)$. The Wigner-von Neumann example was further generalized in [3] where Arai and Uchiyama constructed, for each $|k| > 2$, bounded radial potentials which are asymptotically of the form

$$V(x) = \frac{k\sin(2|x|)}{|x|} + O(|x|^{-1-\varepsilon}) \quad \text{as } |x| \to \infty \tag{5.3}$$

for some $\varepsilon > 0$ such that $P^2 + V$ has eigenvalue 1. In these examples also $x \cdot \nabla V$ is bounded and $\omega_1 = \limsup_{|x|\to\infty}(x \cdot \nabla V(x))_+ = 2|k|$. Thus we can conclude that $P^2 + V$ has no eigenvalues $E > |k|^2/2$.

5.3 Aharonov Bohm vector potentials

In two dimensions the prototypical Aharonov Bohm magnetic vector potential is given by

$$A^{ab}(x, y) = \frac{(-y, x)}{x^2 + y^2}\, B_0\,, \tag{5.4}$$

for some $B_0 \in \mathbb{R}$. This yields a locally square integrable vector potential on $\mathbb{R}^2 \setminus \{0\}$, it corresponds to a singular magnetic field, which is concentrated in zero, i.e., $B = \partial_x A^{ab}_y - \partial_y A^{ab}_x = 0$ in $\mathbb{R}^2 \setminus \{0\}$, but for any smooth curve S circling once around zero, the line integral along S is given by

$$\int_S (A_x dx + A_y dy) = 2\pi B_0$$

that is, the 'magnetic field' corresponding to A has total flux $2\pi B_0$. The corresponding magnetic Schrödinger operator H^{ab}_0 is now defined as the closure of the quadratic form $q_{ab,0}$ defined first on $\mathcal{C}_0^\infty(\mathbb{R}^2 \setminus \{0\})$ as

$$q_{ab,0}(\varphi, \varphi) = \big\langle (P - A^{ab})\varphi, (P - A^{ab})\varphi)\big\rangle$$

and for any potential V which is form small w.r.t. H_0^{ab}, the operator H_V^{ab} is defined as the form sum

$$q_{ab,V}(\varphi,\varphi):=q_{ab,0}(\varphi,\varphi)+\langle\varphi, V\varphi\rangle.$$

For such type of singular magnetic Schrödinger operators we still have a virial theorem and a result on absence of positive eigenvalues for the following simple reasons:

For dilation, it makes no difference if one works on $\mathbb{R}^2$ or on $\mathbb{R}^2\setminus\{0\}$. Thus we can still use dilations to derive a virial theorem. In fact, this is easy.

The first thing one has to check if $\mathcal{D}(P-A^{ab})$ is invariant under dilations. Recall Eq. (3.11), which for the Aharonov Bohm vector potential reads

$$\begin{aligned}(P-A^{ab})U_t\varphi &= e^t U_t P\varphi - U_t A_t^{ab}\varphi = e^t U_t(P-A^{ab})\varphi + U_t(e^t A^{ab}-A_{-t}^{ab})\varphi\\ &= e^t U_t(P-A^{ab})\varphi \end{aligned}\tag{5.5}$$

since, the Aharonov Bohm vector potential is homogeneous of degree -1, we have $e^t A^{ab} - A_{-t}^{ab} = 0$ for all $t>0$. That is, the Aharonov Bohm magnetic momentum operator $P-A^{ab}$ has the same commutation properties with dilations as the free momentum P, which drastically simplifies the analysis!

Theorem 5.3 (Aharonov Bohm magnetic virial theorem) *Let A^{ab} be the Aharonov Bohm vector potential and V satisfy Assumptions 2.5. Assume also that the distribution $x\cdot\nabla V$ extends to a quadratic form which is form bounded with respect to $(P-A^{ab})^2$. Then for all $\varphi\in\mathcal{D}(P-A^{ab})$, the limit $\lim_{t\to 0} 2\,\mathrm{Re}\,\big(q_{ab}(\varphi, iD_t\varphi)\big)$ exists. Moreover,*

$$\langle\varphi,[H_V^{ab}, iD]\,\varphi\rangle:=\lim_{t\to 0} 2\,\mathrm{Re}\,\big(q_{ab,V}(\varphi, iD_t\varphi)\big) = 2\|(P-A^{ab})\varphi\|_2^2 - \langle\varphi, x\cdot\nabla V\varphi\rangle. \tag{5.6}$$

This is proven exactly as Theorem 3.8, the extra term from the magnetic field disappears because of the scaling of the Aharonov Bohm vector potential.

Of course, this theorem then also implies absence of positive eigenvalues under the same conditions on the potential V as in Theorem 4.8, now with $\beta=0$. For the Aharonov–Bohm Hamiltonian H_V^{ab} no eigenvalues E with

$$E>\frac{1}{4}\left(\omega_1+\sqrt{\omega_1^2+2\omega_2}\right)^2 \tag{5.7}$$

exist.

Remarks 5.4 (i) One can also allow for an angular dependence in the Aharonov–Bohm type potential as in [29].

(ii) In addition to the Aharonov–Bohm potential, one can also allow for an additional regular magnetic field B satisfying Assumptions 2.3 and 2.4. One has to modify the right hand sides of (5.6) and of (5.7) accordingly.

(iii) On can also consider the Aharonov–Bohm effect in $\mathbb{R}^3$ where the magnetic field is singular along a line l through the origin.

We leave the straightforward modifications of the technical details to the interested reader.

5.4 Pauli and magnetic Dirac operators

In this section we state two consequences of Theorem 4.8 and Proposition A.2. Let $B : \mathbb{R}^2 \to \mathbb{R}$ be given and consider the Pauli operator

$$P(A) = \begin{pmatrix} (i\nabla + A)^2 + B & 0 \\ 0 & (i\nabla + A)^2 - B \end{pmatrix}$$

in $L^2(\mathbb{R}^2, \mathbb{C}^2)$. It is well-known that the operator $P(B)$ is non-negative, and that if $|\int_{\mathbb{R}^2} B| > 2\pi$, then zero is an eigenvalue of $P(B)$, see also Remark 4.9.

Corollary 5.5 *Assume that* $B \in L^p_{\text{loc}}(\mathbb{R}^2)$ *for some* $p > 2$ *and that* $B(x) = \mathcal{O}(|x|^{-1})$ *as* $|x| \to \infty$. *Let* $A \in L^2_{\text{loc}}(\mathbb{R}^2)$ *be such that* $\operatorname{curl} A = B$. *Then the operator* $P(A)$ *has no eigenvalues in the interval* $(4\beta^2, \infty)$*, with* β *given by* (1.15).
If moreover there exists a compact set $K \subset \mathbb{R}^2$ *such that* $B \in C^1(\mathbb{R}^2 \setminus K)$*, then the operator* $P(A)$ *has no eigenvalues in the interval* $\big(\Lambda_P, \infty\big)$*, with*

$$\Lambda_P := \min\left\{4\beta^2, \frac{1}{4}(\beta + \omega + \sqrt{(\beta+\omega)^2 + 2\omega})^2\right\} \tag{5.8}$$

and

$$\omega = \max\left\{\limsup_{|x|\to\infty} x \cdot \nabla B(x), \ -\liminf_{|x|\to\infty} x \cdot \nabla B(x)\right\}.$$

Proof The first part of the statement follows from Theorem 4.8, the definition 1.13 of the asymptotic bounds and Proposition A.2, applied to the components of the Pauli operator with the splitting $V_1 = \pm B$, $V_2 = 0$. The second part follows from the first part and from the application of Theorem 4.8 and Proposition A.2 with the splitting $V_1 = 0$, $V_2 = \pm B$. □

Remarks 5.6 A couple of comments are in order:

(i) The example of Miller and Simon [32], see Sect. 5.1, applies to two-dimensional Pauli operators as well. In particular, a quick inspection shows that if $B(r) = b_0\, r^{-1} + \mathcal{O}(r^{-2})$, then the spectrum of $P(A)$ is dense pure point in $[0, b_0^2)$ and absolutely continuous in $[b_0^2, \infty)$. Note that in this case Corollary 5.5 guarantees the absence of eigenvalues for $P(A)$ in the interval (b_0^2, ∞), so this result is *sharp*.
(ii) Under the hypotheses of Corollary 5.5 the essential spectrum of $P(A)$ coincides with $[0, \infty)$, see Corollary 6.8 below.
(iii) Using the main results of our paper, one can significantly relax the regularity assumption on the magnetic field B. We leave this to the interested reader.
(iv) Absence of positive eigenvalues of the Pauli operator in $\mathbb{R}^3$ will be treated elsewhere.

The second application of Theorem 4.8 concerns magnetic Dirac operators in $L^2(\mathbb{R}^2, \mathbb{C}^2)$ which in the standard representation have the form

$$\mathbb{D} = \begin{pmatrix} m & \mathrm{Q} \\ \mathrm{Q}^* & -m \end{pmatrix}, \qquad \mathrm{Q} = (P_1 - A_1) + i(P_2 - A_2), \tag{5.9}$$

where m is the mass of the particle. We have

Corollary 5.7 *Let* B *satisfy the assumptions of Corollary* 5.5 *and let* $A \in L^2_{\text{loc}}(\mathbb{R}^2)$ *be such that* $\operatorname{curl} A = B$. *Then the Dirac operator* $\mathbb{D}$ *defined on* $\mathcal{D}(P - A)$ *has no eigenvalues in*

$$\big(-\infty, -\sqrt{\Lambda_P + m^2}\,\big) \cup \big(\sqrt{\Lambda_P + m^2}, \infty\big).$$

Proof Note that

$$\mathbb{D}^2 = P(A) + m^2 \mathbb{1} \tag{5.10}$$

in the sense of sesqui-linear forms on $\mathcal{D}(P-A)\otimes\mathcal{D}(P-A)$. Hence if $\mathbb{D}\psi = E\psi$ for some $\psi \in \mathcal{D}(P-A)\otimes\mathcal{D}(P-A)$, then ψ is a weak eigenfunction of $P(A)$ relative to eigenvalue $E^2 - m^2$. In view of Corollary 5.5 we thus have $E^2 - m^2 \le \Lambda_P$. □

Remarks 5.8 Sufficient conditions for the absence of the entire point spectrum of Pauli and Dirac operators with electromagnetic fields where recently found in [8], see also Remark 1.7.(v).

6 The essential spectrum

We have the following dichotomy.

Lemma 6.1 (Dichotomy) *Let* $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d)$. *Then either* $\inf \sigma((P-A)^2) > 0$ *or* $\sigma((P-A)^2) = [0,\infty)$.

Remarks 6.2 The Landau Hamiltonian, where the vector potential A corresponds to a constant magnetic field, provides an example where $\inf \sigma((P-A)^2) > 0$, see [28].

Proof Write $H_0 = (P-A)^2$. It suffices to prove the implication

$$0 \in \sigma(H_0) \quad \Rightarrow \quad \sigma(H_0) = [0,\infty). \tag{6.1}$$

Let $D(H_0)$ denote the domain of H_0. To prove (6.1) suppose that $0 \in \sigma(H_0)$. Hence there exits a sequence $\{\widetilde{\varphi}_n\}_{n\in\mathbb{N}} \subset D(H_0)$ such that $\|\widetilde{\varphi}_n\|_2 = 1$ for all $n \in \mathbb{N}$ and

$$\|H_0\, \widetilde{\varphi}_n\|_2 \;\to\; 0 \qquad n \to \infty. \tag{6.2}$$

Now we define

$$\phi_n(x) = e^{ik\cdot x}\, \widetilde{\varphi}_n(x), \tag{6.3}$$

where $k \in \mathbb{R}^d$ is arbitrary. Then $\phi_n \in D(H_0)$ for every $n \in \mathbb{N}$, and we have

$$(P-A)\,\phi_n(x) = e^{ik\cdot x}\,(P - A + k)\,\widetilde{\varphi}_n(x),$$

and

$$H_0\,\phi_n(x) = (P-A)^2\,\phi_n(x) = e^{ik\cdot x}\, H_0\,\widetilde{\varphi}_n(x) + 2e^{ik\cdot x} k\cdot(P-A)\widetilde{\varphi}_n(x) + |k|^2\phi_n(x).$$

with the derivatives meant in the sense of distributions. Since $\|\widetilde{\varphi}_n\|_2 = 1$, it follows that $H_0\,\phi_n \in L^2(\mathbb{R}^d)$. Hence $\phi_n \in D(H_0)$. Moreover the above calculations and the Cauchy-Schwarz inequality show that

$$\begin{aligned}\|(H_0 - |k|^2)\,\phi_n\|_2 &\le \|H_0\,\widetilde{\varphi}_n\|_2 + 2|k|\,\|(P-A)\widetilde{\varphi}_n\|_2 \;=\; \|H_0\,\widetilde{\varphi}_n\|_2 + 2|k|\sqrt{\langle\widetilde{\varphi}_n, H_0\,\widetilde{\varphi}_n\rangle}\\ &\le\; \|H_0\,\widetilde{\varphi}_n\|_2 + 2|k|\,\|H_0\,\widetilde{\varphi}_n\|_2^{1/2}.\end{aligned}$$

By (6.2) we thus have $\|(H_0 - |k|^2)\,\phi_n\|_2 \to 0$ for any $k \in \mathbb{R}^d$. Hence $[0,\infty) \subseteq \sigma_{\mathrm{ess}}(H_0)$ and since $H_0 \ge 0$, we conclude that $\sigma(H_0) = \sigma_{\mathrm{ess}}(H_0) = [0,\infty)$. □

Next we formulate a condition on B under which $\sigma((P-A)^2) = [0,\infty)$ for any locally square integrable vector potential A with $B = dA$.

Definition 6.3 (*Vanishing somewhere at infinity*) We say that the magnetic field B *vanishes somewhere at infinity* if there exist sequences $\{R_n\}_{n\in\mathbb{N}} \subset \mathbb{R}$ and $\{x_n\}_{n\in\mathbb{N}} \subset \mathbb{R}^d$ such that $R_n \to \infty$, $|x_n| \to \infty$ as $n \to \infty$, and

$$\lim_{n\to\infty} R_n^{-d} \int_{\mathcal{U}_{R_n}} \left(\frac{|y|}{R_n}\right)^{2-d} \left(1 - \frac{|y|}{R_n}\right)^2 \left(\log \frac{R_n}{|y|}\right)^2 \left|\widetilde{B}_{x_n}(y)\right|^2 dy = 0. \tag{6.4}$$

Remarks 6.4 This vanishing condition is quite weak. For example, if $d = 2$ and if B decays uniformly in a cone S_ω with an opening angle $\omega \in (0, \pi)$, meaning that $\sup_{|\theta|<\omega} |B(r,\theta)| \to 0$ as $r \to \infty$, then B vanishes somewhere at infinity. Indeed, given a sequence $R_n \to \infty$ one can choose $x_n = (x_1^n, 0)$ with x_1^n growing fast enough, depending on B and R_n, such that $\mathcal{U}_{R_n}(x_n) \subset S_\omega$ for all n, and such that

$$R_n^{-d} \int_{\mathcal{U}_{R_n}(0)} \left(\log \frac{R_n}{|y|}\right)^2 \left|\widetilde{B}_{x_n}(y)\right|^2 dy \lesssim R_n^2 \left(\sup_{\mathcal{U}_{R_n}(x_n)} |B|^2\right) \to 0, \qquad n \to \infty.$$

Also, we do not require that the magnetic field $B = dA$ exists as a classical vector field outside the sequence of balls $\mathcal{U}_{R_n}(x_n)$.

Theorem 6.5 *Suppose that A is a locally square integrable magnetic vector potential such that the magnetic field $B = dA$ vanishes somewhere at infinity in the sense of Definition 6.3. Then*

$$\sigma((P - A)^2) = \sigma_{\mathrm{ess}}((P - A)^2) = [0, \infty).$$

Remarks 6.6 In case that the magnetic field goes to zero pointwise at infinity, the above result was already shown by Miller and Simon, [9, 32]. As pointed out in [32] the invariance of the essential spectrum is quite remarkable, since the the vector potential A corresponding to the magnetic field B might not have any decay at infinity, i.e., the magnetic kinetic energy $(P - A)^2$ is not a small perturbation of the non–magnetic kinetic energy P^2, in general.

Proof Let R_n and x_n be the sequences defined in Definition 6.3 and let

$$A_n(x) = \int_0^1 B(x_n + t(x - x_n))\,[t(x - x_n)]\,dt \tag{6.5}$$

be the vector potential related to B via the Poincaré gauge centred at x_n. Then curl $A_n =$ curl $A = B$ for all $n \in \mathbb{N}$, and therefore there exits a scalar gauge field $\chi_n \in H^1_{\mathrm{loc}}(\mathbb{R}^2; \mathbb{R})$ with $\nabla\chi_n \in L^2(\mathbb{R}^2)$ such that

$$A_n = A - \nabla\chi_n, \tag{6.6}$$

and for all $\varphi \in L^2(\mathbb{R}^2)$ with $(P - A_n)\varphi \in L^2(\mathbb{R}^2)$ we have $e^{i\chi}\varphi \in \mathcal{D}(P - A)$ and $(P - A)e^{i\chi_n}\varphi = e^{i\chi_n}(P - A_n)\varphi$, see [30]. To simplify the notation we denote

$$\mathcal{U}_n = \mathcal{U}_{R_n}(x_n).$$

Due to the Dichotomy Lemma 6.1 we only have to show that $0 \in \sigma((P - A)^2)$. To this end we will construct a sequence $\{\phi_n\}_n \subset \mathcal{D}(P - A)$ with $\mathrm{supp}(\phi_n \in \mathcal{U}_n)$ and $\|\phi_n\|_2 = 1$ such that

$$\|(P - A)\,\phi_n\|_2^2 \to 0 \qquad n \to \infty. \tag{6.7}$$

We choose $\phi_n = e^{i\chi_n}\,\varphi_n$, where

$$\varphi_n(x) = C_d\, R_n^{-\frac{d}{2}} \left(\frac{|x-x_n|}{R_n}\right)^{\frac{2-d}{2}} \left(1-\frac{|x-x_n|}{R_n}\right)_+ ,$$

where the constant C_d depends only on d and is chosen such that $\|\phi_n\| = \|\varphi_n\| = 1$. Then by the above gauge invariance

$$\|(P-A)\,\phi_n\|_2^2 = \|(P-A_n)\,\varphi_n\|_2^2 \le \big(\|P\varphi_n\| + \|A_n\varphi_n\|\big)^2. \tag{6.8}$$

We have

$$\|P\varphi_n\|_2^2 \lesssim R_n^{-2} \to 0 \qquad n\to\infty.$$

Hence by setting $h(s) = (1-s/R)_+^2$ in (2.29) we obtain, in view of (6.5),

$$\begin{aligned}\|A_n\varphi_n\|_2^2 &\lesssim R_n^{-2}\int_{\mathcal{U}_n}\left(1-\frac{|x-x_n|}{R_n}\right)^2 |x-x_n|^{2-d}\,|A_n(x)|^2\,dx\\ &\le 4R_n^{-d}\int_{\mathcal{U}_{R_n}(0)}\left(\frac{|y|}{R_n}\right)^{2-d}\left(1-\frac{|y|}{R_n}\right)^2 \log^2(R_n/|y|)\,\big|\widetilde{B}_{x_n}(y)\big|^2\,dy. \end{aligned}\tag{6.9}$$

Thus the assumption that B vanishes somewhere at infinity implies $\|A_n\varphi_n\|_2 \to 0$ as $n\to\infty$. By (6.8) this shows

$$\|(P-A)\,\phi_n\|_2^2 \to 0$$

as $n\to\infty$, which proves (6.7). Since $\|\phi_n\|_2 = \|\varphi_n\|_2 = 1$ for all $n\in\mathbb{N}$, it follows that $0\in\sigma(H_0)$ and applying Lemma 6.1 then gives $\sigma_{\rm ess}((P-A)^2) = [0,\infty)$. □

To prove that the magnetic B vanishes somewhere at infinity it is convenient to impose following additional condition.

Assumption 6.7 Suppose that there exist $\kappa > 0$ and sequences $\{x_n\}\subset\mathbb{R}^d, \{R_n\}\subset\mathbb{R}_+, \{\alpha_n\}\subset\mathbb{R}_+$ and $\{\gamma_n\}\subset\mathbb{R}_+$ such that $|x_n|\to\infty$, $R_n\to\infty, \alpha_n\to 0$, $\gamma_n\to 0$, and such that

$$\big\langle\varphi,\, |\cdot - x_n|^\kappa\, \big|\widetilde{B}_{x_n}(\cdot - x_n)\big|^2\,\varphi\big\rangle \le \alpha_n\|(P-A)\varphi\|_2^2 + \gamma_n\|\varphi\|_2^2 \tag{6.10}$$

for all $\varphi\in D(P-A)$ with $\operatorname{supp}\varphi\subset\mathcal{U}_{R_n}(x_n)$.

Corollary 6.8 *Suppose that the magnetic field satisfies Assumptions 2.3 and 6.7. Then for any locally square integrable magnetic vector potential A with $dA = B$ we have*

$$\sigma_{ess}((P-A)^2) = [0,\infty)\,. \tag{6.11}$$

Proof Let $\widetilde{R}_n, x_n, \alpha_n$ and γ_n be the sequences given by Assumption 6.7. We define

$$u_n = \widetilde{R}_n^{-\frac{d}{2}}\left(\frac{|x-x_n|}{\widetilde{R}_n}\right)^{\frac{2-d+\kappa}{2}}\left(1-\frac{|x-x_n|}{\widetilde{R}_n}\right)_+ \log_+(\widetilde{R}_n/|x-x_n|)\,.$$

and

$$\widetilde{C}_n = \widetilde{R}_n^\kappa\,\big\langle u_n,\, |\cdot - x_n|^{-\kappa}\,\big|\widetilde{B}_{x_n}(\cdot - x_n)\big|^2\, u_n\big\rangle.$$

Note that $u_n\in L^2(\mathbb{R}^d)$, $|\nabla u_n|\in L^2(\mathbb{R}^d)$ and

$$\|u_n\|_2 = \mathcal{O}(1), \qquad \|P\,u_n\|_2 = \mathcal{O}(\widetilde{R}_n^{-1}) \qquad n\to\infty.$$

Hence by (6.10) and (6.5)

$$\begin{aligned} \widetilde{C}_n &\le 2\widetilde{R}_n^{\kappa}\,\alpha_n \|P\,u_n\|_2^2 + 2\widetilde{R}_n^{\kappa}\,\alpha_n \|A_n u_n\|_2^2 + \widetilde{R}_n^{\kappa}\,\gamma_n \|u_n\|_2^2 \\ &\lesssim \widetilde{R}_n^{\kappa-2}\,\alpha_n + \widetilde{R}_n^{\kappa}\,\gamma_n + \widetilde{R}_n^{\kappa}\,\alpha_n \|A_n u_n\|_2^2. \end{aligned} \tag{6.12}$$

Now, the bound $\sup_{0<s<1} s^{\kappa}|\log s|^2 < \infty$ in combination with inequality (2.29) implies

$$\begin{aligned} \|A_n u_n\|_2^2 &= \widetilde{R}_n^{-d} \int_{\mathcal{U}_{\widetilde{R}_n}} \left(\frac{|x-x_n|}{\widetilde{R}_n}\right)^{2-d+\kappa} \\ &\quad \left(1-\frac{|x-x_n|}{\widetilde{R}_n}\right)^2 \left(\log_+(\widetilde{R}_n/|x-x_n|)\right)^2 |A(x_n+y)|^2\,dy \\ &\lesssim \widetilde{R}_n^{-d} \int_{\mathcal{U}_{\widetilde{R}_n}} \left(\frac{|x-x_n|}{\widetilde{R}_n}\right)^{2-d} \left(1-\frac{|x-x_n|}{\widetilde{R}_n}\right)^2 |A(x_n+y)|^2\,dy \\ &\lesssim \widetilde{R}_n^{-d} \int_{\mathcal{U}_{\widetilde{R}_n}} \left(\frac{|y|}{\widetilde{R}_n}\right)^{2-d} \left(1-\frac{|y|}{\widetilde{R}_n}\right)^2 \left(\log_+(\widetilde{R}_n/|y|)\right)^2 |B_{x_n}(y)|^2\,dy = \widetilde{C}_n\,. \end{aligned}$$

Inserting this into (6.12) gives

$$\widetilde{C}_n \lesssim \widetilde{R}_n^{\kappa-2}\,\alpha_n + \widetilde{R}_n^{\kappa}\,\gamma_n + \widetilde{R}_n^{\kappa}\,\alpha_n\,\widetilde{C}_n\,.$$

At this point we redefine

$$R_n := \min\left\{\widetilde{R}_n,\, \alpha_n^{-\frac{1}{2\kappa}},\, \gamma_n^{-\frac{1}{2\kappa}}\right\}, \tag{6.13}$$

and

$$\varphi_n(x) = R_n^{-\frac{d}{2}} \left(\frac{|x-x_n|}{R_n}\right)^{\frac{2-d}{2}} \left(1-\frac{|x-x_n|}{R_n}\right)_+ \log_+(R_n/|x-x_n|)\,.$$

Note that $R_n \to \infty$ as $n \to \infty$. Repeating the above bounds with $\widetilde{R}_n$ replaced by R_n and u_n replaced by φ_n then leads to

$$\begin{aligned} C_n := \langle \varphi_n,\, \widetilde{B}_{x_n}(\cdot - x_n)\,\varphi_n\rangle &\lesssim R_n^{\kappa-2}\,\alpha_n + R_n^{\kappa}\,\gamma_n + R_n^{\kappa}\,\alpha_n\,C_n \\ &\lesssim R_n^{-2}\sqrt{\alpha_n} + \sqrt{\gamma_n} + \sqrt{\alpha_n}\,C_n, \end{aligned}$$

where, in the second step, we have used $R_n^{\kappa}\,\alpha_n \le \sqrt{\alpha_n}$ and $R_n^{\kappa}\,\gamma_n \le \sqrt{\gamma_n}$, which follows from (6.13). Hence $C_n \to 0$ as $n \to \infty$, and since

$$C_n = R_n^{-d} \int_{\mathcal{U}_{R_n}} \left(\frac{|y|}{R_n}\right)^{2-d} \left(1-\frac{|y|}{R_n}\right)^2 \left(\log\frac{R_n}{|y|}\right)^2 \left|\widetilde{B}_{x_n}(y)\right|^2 dy,$$

the claim follows from Theorem 6.5. □

Remarks 6.9 The condition imposed by Assumption 6.7 rather weak. Indeed, if we set

$$W_n(x) = \mathbb{1}_{\mathcal{U}_n}(x)\,|x-x_n|^{-\kappa} \left|\widetilde{B}_{x_n}(x-x_n)\right|^2,$$

then by the discussion in Section A.4 it follows that (6.10) holds if W_n is, uniformly for large n, in $L^p_{\mathrm{loc,unif}}(\mathbb{R}^d)$ and vanishes at infinity locally uniformly in L^1. The discussion in Section A.4 also shows that (6.10) holds with

$$\alpha_n = \|(P^2+\lambda)^{-1}\,W_n\|_\infty, \qquad \gamma_n = \lambda\|(P^2+\lambda)^{-1}\,W_n\|_\infty,$$

and any $\lambda > 0$. Hence Assumption 6.7 is satisfied whenever

$$\lim_{n\to\infty} \|(P^2+\lambda)^{-1} W_n\|_\infty = 0.$$

This allows for strong local singularities of the magnetic field near infinity.

Theorem 6.10 *Suppose that A is a locally square integrable magnetic vector potential and the potential V is form small and vanishes at infinity w.r.t $(P-A)^2$. Then*

$$\sigma_{\mathrm{ess}}(H_{A,V}) = \sigma_{\mathrm{ess}}((P-A)^2). \tag{6.14}$$

Proof Since V is form small with respect to $(P-A)^2$, the quadratic form $q_{A,V}$ is closed and bounded from below on the form domain $\mathcal{D}(P-A)$. Hence there exists $\lambda \geq 1$ such that the operators $H_{A,0}+\lambda$ and $H_{A,V}+\lambda$ are invertible in $L^2(\mathbb{R}^d)$. We are going to prove that the resolvent difference

$$(H_{A,0}+\lambda)^{-1} - (H_{A,V}+\lambda)^{-1} \quad \text{is compact in } \ L^2(\mathbb{R}^d). \tag{6.15}$$

for some large enough $s \geq 1$, which by Weyl's theorem implies that the essential spectra of $H_{A,V}$ and $(P-A)^2$ coincide.

In the following, we will abbreviate $H_0 = H_{A,0}$. Let $C(\lambda){:=}(H_0+\lambda)^{-1/2}V(H_0+\lambda)$, more precisely, $C(\lambda))$ is the bounded operator associated with the bounded form

$$q_\lambda(\varphi,\varphi){:=}q_V((H_0+\lambda)^{-1/2}\varphi, (H_0+\lambda)^{-1/2}\varphi)\,,$$

and the relative form bound of V w.r.t $(P-A)^2$ is given by $\lim_{\lambda\to\infty}\|C(\lambda)\|_{2\to 2} < 1$, see Lemma 2.1. Choose λ large enough, such that $\|C(\lambda)\| < 1$. Then Tiktopoulos' formula (2.12) shows

$$(H_{A,V}+\lambda)^{-1} = (H_0+\lambda)^{-1/2}(1-C(\lambda))^{-1}(H_0+\lambda)^{-1/2}\,.$$

Hence

$$(H_0+\lambda)^{-1} - (H_0+\lambda)^{-1} = (H_0+\lambda)^{-1/2}(1-C_s)^{-1}C_s(H_0+\lambda)^{-1/2}$$

so we only have to show that

$$C(\lambda)(H_0+\lambda)^{-1/2} = (H_0+\lambda)^{-1/2}V(H_0+\lambda)^{-1}$$

is a compact operator. For this let $\xi_{<R}, \xi_{\geq R}$ the smooth partition from the proof of Lemma 4.4 with $\xi_{<R}^2+\xi_{\geq R}^2 = 1$, $\mathrm{supp}(\xi_{<R}) \subset \mathcal{U}_{2R}$, $\mathrm{supp}(\xi_{\geq R}) \subset \mathcal{U}_R^c$, and $\|\nabla\xi_{<R}\|_\infty, \|\nabla\xi_{\geq R}\|_\infty \lesssim R^{-1}$. With

$$J_{<R}{:=}(H_0+\lambda)^{-1/2}\xi_{<R}^2 V(H_0+\lambda)^{-1} \tag{6.16}$$

$$J_{\geq R}{:=}(H_0+\lambda)^{-1/2}\xi_{\geq R}^2 V(H_0+\lambda)^{-1} \tag{6.17}$$

we obviously have $(H_0+\lambda)^{-1/2}V(H_0+\lambda)^{-1} = J_{<R}+J_{\geq R}$.

We will show that $\lim_{R\to\infty}\|J_{\geq R}\|_{2\to 2} = 0$. So $(H_0+\lambda)^{-1/2}V(H_0+\lambda)^{-1}$ is the norm limit of $J_{<R}$ as $R\to\infty$, in particular, it is a compact operators if $J_{<R}$ is compact for all large R. Since

$$\|J_{\geq R}\|_{2\to 2} = \sup_{\|f\|=1} |\langle f, J_{\geq R} f\rangle| \tag{6.18}$$

and with $\varphi = (H_0+\lambda)^{-1/2}f$

$$|\langle f, J_{\geq R} f\rangle| = |\langle \xi_{\geq R}\varphi, V\xi_{\geq R}\varphi\rangle| \leq \alpha_R\|(P-A)\xi_{\geq R}\varphi\|_2^2 + \gamma_R\|\xi_{\geq R}\varphi\|_2^2$$

$$\le \alpha_R\Big(\|(P-A)\varphi\| + \|\nabla\xi_{\ge R}\|\|\varphi\|\Big)^2 + \gamma_R\|\varphi\|_2^2$$
$$\lesssim \big(\alpha_R(1+R^{-1})^2 + \gamma_R\big)\|f\|_2^2$$

since $(P-A)\xi_{\ge R}\varphi = \xi_{\ge R}(P-A)\varphi - i(\nabla\xi_{\ge R})\varphi$, $\|(P-A)\varphi\| \le \|f\|$ and $\|\varphi\| \le \lambda^{-1}\|f\|$. From this and (6.18) one immediately gets $\|J_{\ge R}\|_{2\to 2} \lesssim \alpha_R(1+R^{-1})^2 + \gamma_R \to 0$ for $R\to\infty$.

To prove that $J_{<R}$ is compact, we first note that the domain of $H_0 = (P-A)^2$ is given by all $\varphi \in \mathcal{D}(P-A)$ for which with $\psi = (P-A)\varphi$ the distribution $(P-A)\psi$ is also in $L^2(\mathbb{R}^d)$. Thus for all $\varphi \in \mathcal{D}((P-A)^2)$ we have

$$(H_0+\lambda)^{-1}(P-A+is)\cdot(P-A-is)\varphi = (H_0+\lambda)^{-1}(H_0+ds^2)\varphi = \varphi$$

when $\lambda = ds^2$. Moreover, when $\varphi \in \mathcal{D}((P-A)^2)$ and χ is a bounded $\mathcal{C}^2$ function such that $\nabla\chi$ and $\Delta\chi$ are bounded, then

$$\begin{aligned}(P-A-is)\chi\varphi &= \chi(P-A-is)\varphi - i(\nabla\chi)\varphi \in L^2(\mathbb{R}^d)\,,\\ (P-A+is)\cdot(P-A-is)\chi\varphi &= \chi(P-A+is)\cdot(P-A-is)\varphi - 2i(\nabla\chi)\cdot\\ &\qquad (P-A)\varphi - (\Delta\chi)\varphi\\ &= \chi(H_0+ds^2)\varphi - 2i(\nabla\chi)\cdot(P-A)\varphi - (\Delta\chi)\varphi \in L^2(\mathbb{R}^d)\end{aligned}$$

so also $\chi\varphi \in \mathcal{D}((P-A)^2)$.

Use $\varphi = (H_0+\lambda)^{-1}f$ with $f \in L^2(\mathbb{R}^d)$ and choose $ds^2 = \lambda$. Then the last equality yields

$$\begin{aligned}\chi(H_0+\lambda)^{-1}f = \chi\varphi &= (H_0+\lambda)^{-1}(P-A+is)\cdot(P-A-is)\chi\varphi\\ &= (H_0+\lambda)^{-1}\chi f - 2i(H_0+\lambda)^{-1}(\nabla\chi)\cdot(P-A)(H_0+\lambda)^{-1}f\\ &\quad - (H_0+\lambda)^{-1}(\Delta\chi)(H_0+\lambda)^{-1}f\,.\end{aligned}$$

Setting $\chi = \xi_{<R}^2$ one sees that $J_{<R}$ can be written as

$$J_{<R} = C(\lambda)\Big(J_1 - 2iJ_2\cdot(P-A)(H_0+\lambda)^{-1} - J_3(H_0+\lambda)^{-1}\Big). \tag{6.19}$$

where we abbreviated $J_1 = (H_0+\lambda)^{-1/2}\chi$, $J_2 = (H_0+\lambda)^{-1/2}(\nabla\chi)$, and $J_3 = (H_0+\lambda)^{-1/2}(\Delta\chi)$.

Note that $C(\lambda)$ is bounded and so are $(P-A)(H_0+\lambda)^{-1}$ and $(H_0+\lambda)^{-1}$. Moreover, since $\chi = \xi_{<R}^2$ has compact support, it is well–know that the operators $\chi(P^2+\lambda)^{-1/2}$, $(\nabla\chi)(P^2+\lambda)^{-1/2}$, and $(\Delta\chi)(P^2+\lambda)^{-1/2}$ are compact operators on $L^2(\mathbb{R}^d)$, see [10, Thm. 5.7.3], for example. The diamagnetic inequality and the Dodds–Fremlin–Pitt theorem [11, 33] then imply that the operators $\chi(H_0+\lambda)^{-1/2}$, $(\nabla\chi)(H_0+\lambda)^{-1/2}$, and $(\Delta\chi)(H_0+\lambda)^{-1/2}$ are also compact, and by duality so are J_1, J_2, and J_3. Thus by (6.19) the operator $J_{<R}$ is a compact operator for all $R > 0$. □

Corollary 6.11 *Suppose that B satisfies Assumptions 2.3, 6.7, and that V satisfies Assumptions 2.5 and 2.8. Then*

$$\sigma_{\mathrm{ess}}(H_{A,V}) = [0,\infty). \tag{6.20}$$

Proof Combine Theorem 6.5 and Corollary 6.8. □

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Appendix A. Pointwise conditions and the Kato–class

Below we show that Assumptions 2.3–2.9 are satisfied under mild explicit regularity and decay conditions on the magnetic field B and the potential V. In particular, we give local L^p conditions, which in a natural way extend the pointwise bounds on the potential from in [1, 37].

A.1. Uniformly local L^p conditions

Recall that the space $L^p_{loc,unif}(\mathbb{R}^d)$ of uniformly local real-valued L^p functions is given by (measurable) functions $f : \mathbb{R}^d \to \mathbb{R} \cup \{-\infty, \infty\}$ such that for $1 \le p < \infty$

$$\|f\|_{L^p_{loc,unif}} := \sup_{x\in\mathbb{R}^d} \left(\int_{|x-y|\le 1} |f(y)|^p \, \mathrm{d}y \right)^{1/p} < \infty \,, \tag{A.1}$$

with the obvious replacement for $p = \infty$, $L^\infty_{\mathrm{loc,unif}}(\mathbb{R}^d) = L^\infty(\mathbb{R}^d)$.

We note that unlike the L^p spaces, the spaces $L^p_{\mathrm{loc,unif}}(\mathbb{R}^d)$ are nested in the sense that for $1 \le q \le p \le \infty$ one has $L^p_{\mathrm{loc,unif}}(\mathbb{R}^d) \subset L^q_{\mathrm{loc,unif}}(\mathbb{R}^d) \subset L^1_{\mathrm{loc,unif}}(\mathbb{R}^d)$.

Proposition A.1 *Let $p = 1$ if $d = 1$ and $p > d/2$ when $d \ge 2$. If $|\widetilde{B}|^2 \in L^p_{\mathrm{loc,unif}}(\mathbb{R}^d)$ then Assumptions 2.3 and 2.4 are satisfied. If $V \in L^p_{\mathrm{loc,unif}}(\mathbb{R}^d)$ then Assumption 2.5 is satisfied. Moreover, assume that one can split $V = V_1 + V_2$, where the distributional derivative $x \cdot \nabla V_2$ is given by a function and $V_1, x^2 V_1^2, x \cdot \nabla V_2 \in L^p_{\mathrm{loc,unif}}(\mathbb{R}^d)$ then Assumptions 2.6 and 2.9 are satisfied.*

Before we prove this, we give a simple additional pointwise condition on $|\widetilde{B}|, V_1, V_2$ which guarantees that the remaining assumptions on being bounded at infinity are satisfied.

We say that V is bounded at infinity, if there exists a compact set $K \subset \mathbb{R}^d$ such that $V \in L^\infty(\mathbb{R}^d \setminus K)$. We also say that V goes to zero pointwise at infinity, if it is bounded at infinity and $\limsup_{x\to\infty} |V(x)| = 0$.

Proposition A.2 *Assume that V goes to zero pointwise at infinity and that V splits as $V = V_1 + V_2$ where V_1 goes to zero pointwise at infinity. Then Assumption 2.7 is satisfied.*

Moreover, if the distribution $x \cdot \nabla V_2$ is given by a function and $|\widetilde{B}|, x^2 V_1^2, x \cdot \nabla V_2$ are bounded from above at infinity, then Assumption 2.8 is satisfied and we have the bounds

$$\beta \le \limsup_{|x|\to\infty} |\widetilde{B}(x)|, \quad \omega_1 \le \limsup_{|x|\to\infty} |x\, V_1(x)|^2, \quad \omega_2 \le \limsup_{|x|\to\infty} x \cdot \nabla V_2(x) \,. \tag{A.2}$$

Remark A.3 So, under the assumptions of Propositions A.1 and A.2 all our Assumptions 2.3–2.9 are satisfied and the upper bounds from (A.2) hold for β, ω_1, and ω_2.

Of course, the above pointwise conditions are in general way too strong. Below we show how some of the assumptions of Proposition A.2 can be relaxed for potentials $V \in L^p_{\mathrm{loc,unif}}(\mathbb{R}^d)$, or even potentials in the Kato-class, see Remark A.6 and Propositions A.4 and A.9.

Proof of Proposition A.2 Let W be bounded at infinity and set $M := \limsup_{x\to\infty} W(x)$. Given $\delta > 0$ there exists $R = R_\delta < \infty$ such that

$$\langle \varphi, W\varphi\rangle \leq (M+\delta)\|\varphi\|^2 \tag{A.3}$$

for any $\varphi \in L^2(\mathbb{R}^d)$ with $\text{supp}(\varphi) \subset \mathcal{U}^c_{R_\delta}$. From this observation, the claims of Propostion A.2 follow straightforwardly. □

Proof of Proposition A.1 Of course, magnetic fields exist only in dimensions $d \geq 2$. Nevertheless, for any $d \geq 1$ and $w \in \mathbb{R}^d$, Assumption 2.3 follows from $|\widetilde{B}|^2 \in L^p_{\text{loc}}(\mathbb{R}^d)$, with $p = 1$ if $d = 1$ and $p > d/2$ when $d \geq 2$, by a simple application of Hölder's inequality.

In the following, let $p \geq 1$ for $d = 1$ and $p > d/2$ when $d \geq 2$. It is well-know, at least for specialists, that a potential $V \in L^p(\mathbb{R}^d)$ is infinitesimally form bounded with respect to P^2. That is, for any choice $\alpha_0 > 0$ there exists $C_\varepsilon < \infty$ such that

$$|\langle \varphi, V\varphi\rangle| \leq \langle \varphi, |V|\varphi\rangle \leq \varepsilon\|P\varphi\|^2 + C_\varepsilon\|\varphi\|^2 \qquad \text{for all } \varphi \in \mathcal{D}(P)\,. \tag{A.4}$$

Using the diamagnetic inequality this also implies

$$|\langle \varphi, V\varphi\rangle| \leq \langle |\varphi|, |V||\varphi|\rangle \leq \varepsilon\|(P-A)\varphi\|^2 + C_\varepsilon\|\varphi\|^2 \qquad \text{for all } \varphi \in \mathcal{D}(P-A)\,, \tag{A.5}$$

for any magnetic vector potential $A \in L^2_{\text{loc}}(\mathbb{R}^d, \mathbb{R}^d)$.

Less known is the fact that (A.4), hence also (A.5), continue to hold for $V \in L^p_{\text{loc,unif}}(\mathbb{R}^d)$. This follows, for example, from the fact that under the above conditions on p in terms of the dimension d one knows that $L^p_{\text{loc,unif}}(\mathbb{R}^d) \subset K_d$, where K_d is the Kato–class of potentials, and all potentials $V \in K_d$ are infinitesimally form bounded w.r.t. P^2, see [9, 40] .

Given this observation, one sees that Assumption 2.5 is satisfied when $V \in L^p_{\text{loc,unif}}(\mathbb{R}^d)$ and Assumptions 2.6 and 2.9 are satisfied when we split $V = V_1 + V_2$ with $V_1, x^2V_1^2, x\cdot\nabla V_2 \in L^p_{\text{loc,unif}}(\mathbb{R}^d)$. This proves all claims of Proposition A.1.

However, in order to derive a simple local L^p condition for a potential to vanish at infinity w.r.t. P^2 we need a quantitative bound for dependence of the constant C_ε in the bounds (A.4) and (A.5) depends on ε and on the norm $\|V\|_{L^p_{\text{loc,unif}}}$. For this reason, and the convenience of the reader, we sketch the derivation of a quantitative version of (A.4):

If $p \geq 1$ for $d = 1$ and $p > d/2$ when $d \geq 2$, an argument similar to the proof of Theorem X.20 in [36] shows that there exists a function $G : \mathbb{R}_+ \times \mathbb{R}_+ \to [0, \infty)$, with $G(s_1, s_2)$ separately increasing in $(s_1, s_2) \in R^2_+$ and $\lim_{s_2\to 0} G(s_1, s_2) = 0$ for all $s_1 > 0$, such that

$$|\langle \varphi, V\varphi\rangle| \leq \langle \varphi, |V|\varphi\rangle \leq \varepsilon\|P\varphi\|^2 + G\big(\varepsilon^{-1}, \|V\|_p\big)\|\varphi\|^2 \qquad \text{for all } \varphi \in \mathcal{D}(P)\,. \tag{A.6}$$

Indeed, Hölder's inequality gives $\langle \varphi, |V|\varphi\rangle \leq \|V\|_p\|\varphi\|^2_{\frac{2p}{p-1}}$. Since $\frac{2p}{p-1} \geq 2$ the Hausdorff–Young inequality shows $\langle \varphi, |V|\varphi\rangle \leq \|V\|_p\|\widehat{\varphi}\|^2_q$ with $\widehat{\varphi}$ the Fourier transform of φ and $\frac{1}{q} = 1 - \frac{p-1}{2p} = \frac{1}{2} + \frac{1}{2p} \leq 1$. Let $t > 0$ and write $\widehat{\varphi} = (1+t\eta^2)^{-1/2}(1+t\eta^2)^{1/2}\widehat{\varphi}$. Since $\frac{1}{q} = \frac{1}{2p} + \frac{1}{2}$ we can use again Hölder's inequality to get

$$\|\widehat{\varphi}\|^2_q \leq \|(1+t\eta^2)^{-1/2}\|^2_{2p}\|(1+t\eta^2)^{1/2}\widehat{\varphi}\|^2_2 \leq C_{p,q}t^{-d/2p}(t\|P\varphi\|^2_2 + \|\varphi\|^2_2)$$

with $C_{p,d} = \|(1+\eta^2)^{-1/2}\|^2_{2p}$. Note that $\mathbb{R}^d \ni \eta \mapsto (1+\eta^2)^{-1/2} \in L^{2p}(\mathbb{R}^d)$ for any $p \geq 1$ if $d = 1$ and $p > d/2$ if $d \geq 2$. Altogether we have

$$\langle \varphi, |V|\varphi\rangle \leq 2C_{p,d}\|V\|_p t^{-d/(2p)}(t\|P\varphi\|^2 + \|\varphi\|^2)$$

for any $t > 0$ and all $\varphi \in \mathcal{D}(P)$. Rescaling in $t > 0$ one sees that a bound of the form (A.6) holds with $G(s_1, s_2) = C s_1^{-\frac{d}{2p-d}} s_2^{\frac{2p-d}{2p}}$ for some constant C depending only on d and p.

Now we extend this to potentials $V \in L^p_{\mathrm{loc,unif}}(\mathbb{R}^d)$. Let $\chi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ with $0 \le \chi \le 1$ and $\chi(x) = 1$ for $\|x\|_\infty \le 3/2$ and $\chi(x) = 0$ when $\|x\|_\infty \ge 2$. For $j \in \mathbb{Z}^d$ define $\chi_j(x) = \chi(x - j)$ for $x \in \mathbb{R}^d$. Then $\chi_j \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ for all $j \in \mathbb{Z}^d$. Since the supports of the χ_j have the finite intersection property, there exist a constant $c > 1$ such that $1 \le \sum_{j\in\mathbb{Z}^d} \chi_j^2 \le c$. Moreover, $\sum_{j\in\mathbb{Z}^d} \chi_j^2 \in \mathcal{C}^\infty(\mathbb{R}^d)$ and all partial derivatives of $\sum_{j\in\mathbb{Z}^d} \chi_j^2$ are bounded functions. We define

$$\xi_j := \frac{\chi_j}{(\sum_{k\in\mathbb{Z}^d} \chi_k^2)^{1/2}} . \tag{A.7}$$

Since $1 \le \sum_{k\in\mathbb{Z}^d} \chi_k^2 \le c_1$ the cutoff functions ξ_j are well–defined and $\xi_j \in \mathcal{C}_0^\infty(\mathbb{R}^d)$. By construction

$$\sum_{j\in\mathbb{Z}^d} \xi_j^2 = 1 . \tag{A.8}$$

Hence the family of cutoff functions $(\xi_j)_{j\in\mathbb{Z}^d}$ is a smooth quadratic partition of unity. Using again that the supports of the χ_j have the finite intersection property, it is also easy to see that there exists a constant $0 < L < \infty$ such that

$$\sum_{j\in\mathbb{Z}^d} |\nabla \xi_j|^2 \le L. \tag{A.9}$$

Lastly, let $K_j = \mathrm{supp}(\xi_j) = \mathrm{supp}(\chi_j)$ and notice that there exist $0 < \kappa < \infty$ such that

$$\sup_{j\in\mathbb{Z}^d} \|\mathbb{1}_{K_j} V\|_p \le \kappa \|V\|_{L^p_{\mathrm{loc,unif}}} \tag{A.10}$$

for all $V \in L^p_{\mathrm{loc,unif}}(\mathbb{R}^d)$. In fact, it is straightforward to show that the two norms in (A.10) are equivalent.

Given $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, we have $\varphi = \sum_{j\in\mathbb{Z}^d} \xi_j^2 \varphi$ because of (A.8). Note also that we can arbitrarily rearrange this sum, and similar sums below, since $\mathrm{supp}(\xi_j) \cap \mathrm{supp}(\varphi) \ne \emptyset$ for only finitely many $j \in \mathbb{Z}^d$. In particular, we have $\langle \varphi, |V|\varphi\rangle = \sum_j \langle \xi_j\varphi, |V_j|\xi_j\varphi\rangle$ with $V_j = \mathbb{1}_{K_j} V$. Using (A.6) one gets

$$|\langle \varphi, V\varphi\rangle| \le \langle \varphi, |V|\varphi\rangle \le \sum_{j\in\mathbb{Z}^d} \Big(\varepsilon \|P(\xi_j\varphi)\|_2^2 + G\big(\varepsilon^{-1}, \|V_j\|_p\big)\|\xi_j\varphi\|_2^2\Big) . \tag{A.11}$$

Because of (A.10) and since G is increasing in its second variable, we have $\sup_{j\in\mathbb{Z}^d} G\big(\varepsilon^{-1}, \|V_j\|_p\big) \le G\big(\varepsilon^{-1}, \kappa\|V\|_{L^p_{\mathrm{loc,unif}}}\big)$ for some constant $0 < \kappa < \infty$ and all $V \in L^p_{\mathrm{loc,unif}}(\mathbb{R}^d)$. Moreover, because of (A.8) we have

$$\sum_{j\in\mathbb{Z}^d} \|\xi_j\varphi\|^2 = \langle \varphi, \xi_j^2\varphi\rangle = \langle \varphi, \sum_{j\in\mathbb{Z}^d} \xi_j^2\varphi\rangle = \|\varphi\|^2 .$$

The IMS localization formula D.1 together with (A.8) and (A.9) yields

$$\sum_{j\in\mathbb{Z}^d} \|P(\xi_j\varphi)\|^2 = \sum_{j\in\mathbb{Z}^d} \langle P(\xi_j\varphi), P(\xi_j\varphi)\rangle = \sum_{j\in\mathbb{Z}^d} \Big(\mathrm{Re}\langle P(\xi_j^2\varphi), P\varphi\rangle + \langle \varphi, |\nabla\xi_j|^2\varphi\rangle\Big)$$

$$= \mathrm{Re}\Big\langle P(\sum_{j\in\mathbb{Z}^d} \xi_j^2\varphi), P\varphi\Big\rangle + \Big\langle \varphi, \sum_{j\in\mathbb{Z}^d} |\nabla\xi_j|^2\varphi\Big\rangle \le \|P\varphi\|_2^2 + L\|\varphi\|_2^2 .$$

Using (A.11) we arrive at

$$|\langle\varphi, V\varphi\rangle| \leq \langle\varphi, |V|\varphi\rangle \leq \varepsilon\|P\varphi\|_2^2 + \Big(\varepsilon L + G\big(\varepsilon^{-1}, \kappa\|V\|_{L^p_{\mathrm{loc,unif}}}\big)\Big)\|\varphi\|_2^2 \tag{A.12}$$

for all $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$ and all $\varepsilon > 0$, as soon as a local bound of the form (A.6) holds. Since $\mathcal{C}_0^\infty(\mathbb{R}^d)$ is dense in $\mathcal{D}(P)$ with respect to the graph norm, the bound (A.12) extends to all $\varphi \in \mathcal{D}(P)$. This shows that any potential $V \in L^p_{\mathrm{loc,unif}}(\mathbb{R}^d)$ is infinitesimally form bounded w.r.t. P^2. The bound (A.12) also holds with P replaced by $P - A$ and $\varphi \in \mathcal{D}(P - A)$ for any vector potential $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d)$ thanks to the diamagnetic inequality (1.11). □

A.2. Potentials vanishing at infinity

Recall the Definitions 1.5, respectively 1.8, for a potential V to vanish, respectively being bounded, at infinity w.r.t. $(P - A)^2$. Assume that V can be split as $V = W_1 + W_2$ with the quadratic form domains $\mathcal{Q}(W_1)$ and $\mathcal{Q}(W_2)$ containing, for all large enough $R > 0$, all $\varphi \in \mathcal{D}(P - A)$ with $\mathrm{supp}(\varphi) \subset \mathcal{U}_R^c$. Then it is straightforward to see that

$$\gamma_R(V) \leq \gamma_R(W_1) + \gamma_R(W_2) \text{ and } \gamma_R^+(V) \leq \gamma_R^+(W_1) + \gamma_R^+(W_2)$$

for all large enough $R > 0$. Hence

$$0 \leq \gamma_\infty(V) = \lim_{R\to\infty} \gamma_R(V) \leq \gamma_\infty(W_1) + \gamma_\infty(W_2) \tag{A.13}$$

and

$$\gamma_\infty^+(V) = \lim_{R\to\infty} \gamma_R^+(V) \leq \gamma_\infty^+(W_1) + \gamma_\infty^+(W_2)\,. \tag{A.14}$$

If W_1 and W_2 vanish at infinty w.r.t. $(P_A)^2$, then $\gamma_\infty(W_1) = \gamma_\infty(W_2) = 0$. Thus $\gamma_\infty(V) = 0$, that is, V vanishes at infinity w.r.t $(P - A)^2$. Moreover, the bound (A.14) shows that V is bounded from above at infinity w.r.t. $(P - A)^2$ with upper bound $\gamma_\infty^+(W_1) + \gamma_\infty^+(W_2)$. This simple observation proves the first part of

Proposition A.4 a) *If $V = W_1 + W_2$ and W_1 and W_2 vanish at infinity, respectively, are bounded from above at infinity, w.r.t. $(P - A)^2$, then V vanishes at infinity, respectively, is bounded from above at infinity, w.r.t. $(P - A)^2$. Moreover, in the latter case (A.14) holds.*

b) *If $V = \nabla \cdot \Sigma$ for some real-valued vector field Σ and if Σ^2 is form bounded respectively vanish at infinity w.r.t. $(P - A)^2$, then V is form bounded respectively vanishes at infinity w.r.t. $(P - A)^2$.*

Remark A.5 (i) Again, the diamagnetic inequality implies that one only has to check form boundedness and vanishing w.r.t. P^2.

(ii) It is not true, in general, that Σ^2 bounded at infinity implies that $\nabla \cdot \Sigma$ is bounded at infinity w.r.t $(P - A)^2$.

(iii) The choice $\Sigma(x) = x\langle x\rangle^{-\varepsilon}\sin(e^{1/|x|}) = O(\langle x\rangle)^{-\varepsilon}$, for some $\varepsilon > 0$, yields a potential $V = \nabla \cdot \Sigma$ with

$$V(x) = -|x|^{-1}e^{1/|x|}\langle x\rangle^{-\varepsilon}\cos(e^{1/|x|}) + O(\langle x\rangle^{-\varepsilon}) \tag{A.15}$$

which has a severe singularity at zero. Since Σ^2 is infinitesimally for bound and vanishing at infinity w.r.t P^2, the above result shows that so does V. That V vanishes at infinity w.r.t. P^2, which might not be too surprising, since the singularity is local.

(iv) The choice $\Sigma(x) = x\langle x\rangle^{-\varepsilon}\sin(e^{|x|}) = O(\langle x\rangle)^{-\varepsilon}$, for some $\varepsilon > 0$, yields a potential $V = \nabla\cdot\Sigma$ with

$$V(x) = |x|e^{|x|}\langle x\rangle^{-\varepsilon}\cos(e^{|x|}) + O(\langle x\rangle^{-\varepsilon}) \tag{A.16}$$

which has again severe oscillations, now at infinity. Nevertheless, it is infinitesimally form bounded and vanishes at infinity w.r.t. P^2 since Σ^2 does. In particular, despite the severe oscillations of V at infinity, our Theorem 6.10 below shows that the perturbation V does not change the essential spectrum.

Proof The first claim was already proven in the discussion just before the proposition. For the second claim let $\varphi \in \mathcal{C}_0^\infty$, and note that Lemma 2.2 shows that the distribution $\nabla\cdot\Sigma$ yields the quadratic form

$$\langle\varphi, \nabla\cdot\Sigma\varphi\rangle = -2\,\mathrm{Im}\,\langle\Sigma\varphi, P\varphi\rangle = -2\,\mathrm{Im}\,\langle\Sigma\varphi, (P-A)\varphi\rangle$$

since $\langle\Sigma\varphi, A\varphi\rangle$ is real. Thus the right hans side above extend to all $\varphi \in \mathcal{D}(P-A)$ if Σ^2 is form bounded w.r.t. $(P-A)^2$ and $|\langle\varphi, \nabla\cdot\Sigma\varphi\rangle| \le \|\Sigma\varphi\|\|(P-A)\varphi\|$. So if $\|\Sigma\varphi\|_2^2 \le \alpha\|(P-A)\varphi\|_2^2 + \gamma\|\varphi\|_2^2$, then

$$\begin{aligned}|\langle\varphi, \nabla\cdot\Sigma\varphi\rangle| &\le 2(\alpha\|(P-A)\varphi\|_2^2 + \gamma\|\varphi\|_2^2)^{1/2}\|(P-A)\varphi\| \\ &\le (\varepsilon^{-1}\alpha + \varepsilon)\|(P-A)\varphi\|_2^2 + \varepsilon^{-1}\gamma\|\varphi\|_2^2\end{aligned} \tag{A.17}$$

for all $\varepsilon > 0$, which proves that $\nabla\cdot\Sigma$ is form bounded w.r.t. $(P-A)^2$. If W is also form bounded w.r.t $(P-A)^2$, then so is their sum $V = \nabla\cdot\Sigma + W$.

Lastly, because of the first part, we only have to show that $\nabla\cdot\Sigma$ vanishes at infinity as soon as Σ^2 vanishes at infinity w.r.t $(P-A)^2$. So assume that there exist α_R and γ_R decreasing with $\alpha_R, \gamma_R \to 0$ as $R \to \infty$ and

$$\|\Sigma\varphi\|_2^2 \le \alpha_R\|(P-A)\varphi\|_2^2 + \gamma_R\|\varphi\|_2^2$$

for all $\varphi \in \mathcal{D}(P-A)$ with $\mathrm{supp}(\varphi) \in \mathcal{U}_R^c$. Setting $\varepsilon = \max(\alpha_R, \gamma_R)^{1/2}$ in (A.17) yields

$$|\langle\varphi, \nabla\cdot\Sigma\varphi\rangle| \le \max(\alpha_R, \gamma_R)^{1/2}\Big(2\|(P-A)\varphi\|_2^2 + \|\varphi\|_2^2\Big)$$

for all $\varphi \in \mathcal{D}(P-A)$ with $\mathrm{supp}(\varphi) \subset \mathcal{U}_R^c$ and large enough R. This shows that $\nabla\cdot\Sigma$ vanishes at infinity w.r.t. $(P-A)^2$. □

Remark A.6 The two bounds (A.13) and (A.14) also show that

$$\gamma_\infty(V) = \inf\{\gamma_\infty(V-W) : \gamma_\infty(W) = 0\} \tag{A.18}$$

and

$$\gamma_\infty^+(V) = \inf\{\gamma_\infty^+(V-W) : \gamma_\infty^+(W) = 0\}\,. \tag{A.19}$$

As upper bounds these statements follow immediately from (A.13) and (A.14). The reverse inequality follows by choosing $W = 0$. Thus when trying to calculate the asymptotic bounds $\beta, \omega_1, \omega_2$ from (1.13), see also Assumption 2.8 one can modify the involved potentials by arbitrary vanishing potentials. Efficient criteria for this are derived in the next two sections.

A.3. A local L^p condition for vanishing at infinity

We say that V is locally uniformly L^p *near infinity*, or $V \in L^p_{\text{loc,unif}}$ *near infinity* if there exists a compact set $K \subset \mathbb{R}^d$ such that $\mathbb{1}_{K^c} V \in L^p_{\text{loc,unif}}(\mathbb{R}^d)$.

In the following we will always assume that $p = 1$ for $d = 1$ and $p > d/2$ for $d \geq 2$. If $V \in L^p_{\text{loc,unif}}$ near infinity, then (A.12) and the diamagnetic inequality shows that the quadratic form domain $\mathcal{Q}(V)$ contains all $\varphi \in \mathcal{D}(P - A)$ with $\text{supp}(\varphi) \subset \mathcal{U}_R^c = \{x \in \mathbb{R}^d : |x| \geq R\}$ as soon as $R > 0$ is large enough.

Recalling the notation of Definition 1.5, the bound (A.12) also shows that for any R large enough and all $\varepsilon > 0$ we have

$$\alpha_R \leq \varepsilon \text{ and } \gamma_R \leq \varepsilon L + G\big(\varepsilon^{-1}, \kappa \|V_R\|_{L^p_{\text{loc,unif}}}\big) \tag{A.20}$$

with $V_R = \mathbb{1}_{\mathcal{U}_R^c} V$.

Now assume that V vanishes at infinity locally uniformly in L^p, that is,

$$\lim_{R \to \infty} \|V_R\|_{L^p_{\text{loc,unif}}} = 0\,. \tag{A.21}$$

Since $\lim_{s_2 \to 0} G(s_1, s_2) = 0$ for any $s_1 > 0$ we can, for any $n \in \mathbb{N}$, inductively choose $R_n \to \infty$ such that $G\big(n, \kappa \|V_R\|_{L^p_{\text{loc,unif}}}\big) \to 0$ as $n \to \infty$. Clearly, (A.20) shows that $\alpha_{R_n} \to 0$ and $\gamma_{R_n} \to 0$ as $n \to \infty$. Since we can also assume, without loss of generality, that α_R and γ_R are decreasing in $R \geq R_0$, once they exist for some $R_0 > 0$, this shows that V vanishes at infinity w.r.t. $(P - A)^2$ as soon as it vanishes at infinity locally uniformly in L^p.

With an additional trick it turns out that it is enough to only assume that V is locally uniformly L^p at infinity and vanished at infinity locally uniformly in L^1.

Proposition A.7 *Let $p = 1$ for $d = 1$ and $p > d/2$ for $d \geq 2$. Assume that the potential $W \in L^p_{\text{loc,unif}}$ near infinity and that it vanishes at infinity locally uniformly in L^1, that is, with $\mathbb{1}_{\mathcal{U}_R^c}$ the characteristic function of $\mathcal{U}_R^c = \{x \in \mathbb{R}^d : |x| \geq R\}$ and $W_R := \mathbb{1}_{\mathcal{U}_R^c} W$ we have*

$$\lim_{R \to \infty} \|W_R\|_{L^1_{loc,unif}} = 0\,. \tag{A.22}$$

Then W vanishes at infinity w.r.t. P^2 in the sense of Definition 1.5.

Moreover, if $V = \nabla \cdot \Sigma + W$ for some vector field $\Sigma \in L^2_{loc}$ and a potential $W \in L^1_{loc}$ and Σ^2 and W satisfy the above assumptions, then V also vanishes at infinity w.r.t. P^2 in the sense of Definition 1.5.

Proof The discussion just before Proposition A.7 shows that W vanishes at infinity w.r.t. P^2 in the sense of Definition 1.5 if we use the norm $\|\cdot\|_{L^p_{\text{loc,unif}}}$ instead of the norm $\|\cdot\|_{L^1_{\text{loc,unif}}}$ in (A.22). If $p = 1$, i.e., $d = 1$, then there is nothing to prove.

So assume $d \geq 2$ and $p > d/2 \geq 1$. Pick $R_0 > 0$ so large that $W_{R_0} \in L^p_{\text{loc,unif}}(\mathbb{R}^d)$. Since $p > d/2 \geq 1$, there exist $1 \leq d/2 < q < p$. Replacing p by q in the discussion just before Proposition A.7 shows that W vanishes at infinity w.r.t $(P - A)^2$ as soon as one knows $\lim_{R \to \infty} \|W_R\|_{L^q_{\text{loc,unif}}} = 0$. This is easy. Since $1 \leq d/2 < q < p$ there exists $0 < \theta < 1$ with $q = \theta 1 + (1 - \theta)p$. Thus for all $R \geq R_0$ Hölder's inequality implies

$$\|W_R\|_{L^q_{\text{loc,unif}}} \leq \|W_R\|^{1-\theta}_{L^p_{\text{loc,unif}}} \|W_R\|^{\theta}_{L^1_{\text{loc,unif}}} \leq \|W\|^{1-\theta}_{L^p_{\text{loc,unif}}} \|W_R\|^{\theta}_{L^1_{\text{loc,unif}}} \to 0 \text{ as } R \to \infty$$

The second claim of Proposition A.7 follows from the first and the second part of Proposition A.4. □

A.4. Vanishing at infinity for potentials in the Kato–class

To get a replacement for the borderline case $p = d/2$ one can use the Kato–class, which we recall.

Definition A.8 (*Kato–class*) A real-valued and measurable function V on $\mathbb{R}^d$ is in the Kato–class K_d if

$$\lim_{\alpha\to 0} \sup_{x\in\mathbb{R}^d} \int_{|x-y|\le\alpha} g_d(x-y)|V(y)|\,dy = 0 \tag{A.23}$$

where

$$g_d(x) := \begin{cases} |x|^{2-d} & \text{if } d \ge 3 \\ |\ln|x|| & \text{if } d = 2 \end{cases}. \tag{A.24}$$

One also defines the Kato–norm

$$\|V\|_{K_d} := \begin{cases} \sup_{x\in\mathbb{R}^d} \int_{|x-y|\le 1} |x-y|^{d-2}|V(y)|\,dy\,, & \text{if } d \ge 3 \\ \sup_{x\in\mathbb{R}^2} \int_{|x-y|\le 1/2} |\ln(|x-y|)||V(y)|\,dy\,, & \text{if } d = 2 \end{cases}. \tag{A.25}$$

It is well-known that any Kato–class potential is infinitesimally form bounded with respect to P^2, see e.g. [5, Thm. 1.4], thus also with respect to $(P-A)^2$ for any vector potential $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathbb{R}^d)$. It is also clear that $K_d \subset L^1_{\mathrm{loc,unif}}(\mathbb{R}^d)$ and using Hölder's inequality one easily sees $L^p_{\mathrm{loc,unif}}(\mathbb{R}^d) \subset K_d$ for all $p > d/2$.

Lastly, we say that a potential V is in the Kato–class outside a compact set, if there exists a compact set $K \subset \mathbb{R}^d$ such that $\mathbb{1}_{K^c} V \in K_d$. Here $\mathbb{1}_{K^c}$ is the characteristic function of the complement of K.

For potentials which are in the Kato–class outside of a compact set we also desire a simple criterium for vanishing.

Proposition A.9 *Given a potential W assume that it is in the Kato–class outside a compact set and that it vanishes at infinity locally uniformly in L^1, that is,*

$$\lim_{R\to\infty} \|\mathbb{1}_{\ge R} W\|_{L^1_{loc,unif}} = 0\,. \tag{A.26}$$

with $\mathbb{1}_{\ge R}$ the characteristic function of $\{x \in \mathbb{R}^d : |x| \ge R\}$. Then W vanishes at infinity w.r.t. P^2 in the sense of Definition 1.5.

Moreover, if $V = \nabla\cdot\Sigma + W$ for some vector field $\Sigma \in L^2_{loc}$ and a potential $W \in L^1_{loc}$ and Σ^2 and W satisfy the above assumptions, then V also vanishes at infinity w.r.t. P^2 in the sense of Definition 1.5.

In the proof of Proposition A.9 we need

Lemma A.10 *Given a potential W in the Kato-class assume that there exist $R_0 > 0$ and $\alpha_{R,\lambda}, \gamma_{R,\lambda} \ge 0$ for $R_0 > 0$ and $R \ge R_0$, $\lambda > 0$ such that*

$$\langle \varphi, W\varphi\rangle \le \alpha_{R,\lambda}\|(P-A)\varphi\|_2^2 + \gamma_{R,\lambda}\|\varphi\|_2^2 \tag{A.27}$$

for all $\varphi \in \mathcal{D}(P-A)$ with $\mathrm{supp}(\varphi) \in \mathcal{U}_R^c$. Moreover, assume that $R_0 \le R \mapsto \alpha_{R,\lambda}, \gamma_{R,\lambda}$ are decreasing for fixed $\lambda > 0$ and $\lim_{\lambda\to\infty} \alpha_{R,\lambda} = 0$ for fixed $R \ge R_0$.

Then W is bounded from above at infinity w.r.t $(P-A)^2$ with asymptotic bound

$$\gamma_\infty^+(W) \le \liminf_{\lambda\to\infty} \lim_{R\to\infty} \gamma_{R,\lambda}\,. \tag{A.28}$$

Remark A.11 The order of the limits in (A.28) is important, since typically one has $\liminf_{\lambda\to\infty}\gamma_{R,\lambda}=\infty$ for any fixed R.

Given any $\alpha_{R,\lambda},\gamma_{R,\lambda}$ for which (A.27) holds, one can, by a simple monotonicity argument, replace them with $\alpha'_{R,\lambda}:=\inf_{R_0\le L\le R}\alpha_{L,\lambda}$ and $\gamma'_{R,\lambda}:=\inf_{R_0\le L\le R},\gamma_{L,\lambda}$, i.e., the required monotonicity in R in Lemma A.10 is not a restriction.

Proof Let $\widetilde{\gamma}_\lambda=\lim_{R\to\infty}\gamma_{R,\lambda}$. Pick any $\lambda_0>0$ and given R_n,λ_n for $n\in\mathbb{N}_0$ choose inductively $\lambda_{n+1}\ge\lambda_n+1$ with $\alpha_{R_n,\lambda_{n+1}}\le\frac{1}{n+1}$ and then $R_{n+1}\ge R_n+1$ with $\gamma_{R_{n+1},\lambda_{n+1}}\le\frac{1}{n+1}+\widetilde{\gamma}_{\lambda_{n+1}}$.

Take a subsequence n_j with $\widetilde{\gamma}_j:=\widetilde{\gamma}_{n_j}\to\liminf_{n\to\infty}\tilde{\gamma}_n$ as $j\to\infty$ and set $\alpha_R:=\frac{1}{n_j+1}$ and $\gamma_R:=\frac{1}{n_j+1}+\widetilde{\gamma}_j$ for $R\in[R_{n_j},R_{n_{j+1}})$. With this choice Definition 1.8 is satisfied, so W is asymptotically bounded at infinity w.r.t. $(P-A)^2$ and $\gamma_\infty(W)=\lim_{R\to\infty}\gamma_R=\lim_{j\to\infty}\widetilde{\gamma}_j=\liminf_{\lambda\to\infty}\lim_{R\to\infty}\gamma_{R,\lambda}$. □

Proof of Proposition A.9 Given a locally square integrable magnetic vector potential A we abbreviate $H_0=(P-A)^2$ for the free magnetic Schrödinger operator defined by quadratic form methods. Given a potential W in the Kato–class, $\varphi\in\mathcal{D}(P-A)=\mathcal{Q}(H_0)$, and $\lambda>0$ let $f=(H_0+\lambda)^{1/2}\varphi\in L^2$. Then

$$\begin{aligned}|\langle\varphi,W\varphi\rangle|&\le\langle\varphi,|W|\varphi\rangle=\langle f,(H_0+\lambda)^{-1/2}|W|(H_0+\lambda)^{-1/2}f\rangle\\&\le\|(H_0+\lambda)^{-1/2}|W|(H_0+\lambda)^{-1/2}\|_{2\to2}\|f\|_2^2\\&=\|(H_0+\lambda)^{-1/2}|W|(H_0+\lambda)^{-1/2}\|_{2\to2}\left(\|((P-A)^2\varphi\|_2^2+\lambda\|\varphi\|_2^2\right)\end{aligned}$$

By duality, $\|(H_0+\lambda)^{-1/2}|W|(H_0+\lambda)^{-1/2}\|_{2\to2}=\||W|^{1/2}(H_0+\lambda)^{-1}|W|^{1/2}\|_{2\to2}$. Assume that $|W|$ is bounded, then for $0\le\mathrm{Re}(z)\le1$ the operator family $T_z=|W|^z(H_0+\lambda)^{-1}|W|^{1-z}$ is analytic and bounded.

Using the diamagnetic inequality and duality we have

$$\begin{aligned}\||W|(H_0+\lambda)^{-1}\|_{1\to1}=\|(H_0+\lambda)^{-1}|W|\|_{\infty\to\infty}&=\|(H_0+\lambda)^{-1}|W|\|_\infty\\&\le\|(P^2+\lambda)^{-1}|W|\|_\infty\,,\end{aligned}$$

which is finite for any $\lambda>0$ and bounded W. Thus T_z is bounded from $L^1\to L^1$ for $\mathrm{Re}(z)=0$ and from $L^\infty\to L^\infty$ for $\mathrm{Re}(z)=1$ and as in [9] one can use the Stein interpolation theorem [35] to see

$$\|(H_0+\lambda)^{-1/2}|W|(H_0+\lambda)^{-1/2}\|_{2\to2}\le\|(P^2+\lambda)^{-1}|W|\|_\infty\,.$$

at least for bounded W. If $\mathrm{supp}(\varphi)\subset\mathcal{U}_R^c$, one can replace W by $W_R=\mathbb{1}_{\ge R}W$. Thus

$$|\langle\varphi,W\varphi\rangle|=|\langle\varphi,W_R\varphi\rangle|\le\alpha_{R,\lambda}\|(P-A)\varphi\|_2^2+\gamma_{R,\lambda}\|\varphi\|_2^2$$

for all $\varphi\in\mathcal{D}(P-A)$ with $\mathrm{supp}(\varphi)\subset\mathcal{U}_R^c$, choosing

$$\begin{aligned}\alpha_{R,\lambda}&=\|(P^2+\lambda)^{-1}|W_R|\|_\infty\,,\\\gamma_{R,\lambda}&=\lambda\|(P^2+\lambda)^{-1}|W_R|\|_\infty\,.\end{aligned}\tag{A.29}$$

If W_R is unbounded, replace W_R by $\min(|W_R|,n)$ and take the limit $n\to\infty$ to see that the above bounds work also for unbounded W, as long as the right hand side of (A.29) is finite.

Clearly, $\alpha_{R,\lambda}$ and $\gamma_{R,\lambda}$ are decreasing in R for fixed $\lambda>0$. One even has $\lim_{\lambda\to\infty}\|(P^2+\lambda)^{-1}|W|\|_\infty=0$ if and only if W is in the Kato–class, which is well–known, see [9, 40]. However, we also clearly have $\lim_{\lambda\to\infty}\gamma_{R,\lambda}=\|W_R\|_\infty$, which is finite, if and only if W_R

is bounded. Nevertheless, if W_R is in the Kato class for some, hence all, large enough R and $\lim_{R\to\infty} \|W_R\|_{L^1_{\mathrm{loc,unif}}} = 0$ then

$$\lim_{R\to\infty} \|(P^2+\lambda)^{-1}|W_R|\|_\infty = 0\,, \tag{A.30}$$

which together with Lemma A.10 shows $\gamma_\infty(W) = 0$. This proves the first part of Proposition A.9. The other claim of Proposition A.9 follows from the above since by Proposition A.4 $W = \nabla\cdot\Sigma$ vanishes w.r.t $(P-A)^2$ as soon as Σ^2 does.

For the proof of (A.30), we claim that for any potential W and any $0<\alpha\le 1$

$$\|(P^2+\lambda)^{-1}|W|\|_\infty \lesssim \sup_{x\in\mathbb{R}^d} \int_{|x-y|\le\alpha} g_d(x-y)|W(y)|\,dy + \frac{e^{-\sqrt{\lambda}\alpha/4}}{\sqrt{\lambda}\alpha}\|W\|_{L^1_{\mathrm{loc,unif}}} \tag{A.31}$$

where the implicit constant depend only on d. This clearly proves (A.30), since replacing W by $W_R = \mathbb{1}_{\ge R} W$ it yields

$$\limsup_{R\to\infty} \|(P^2+\lambda)^{-1}|W_R|\|_\infty \le C_{\lambda,d} \sup_{x\in\mathbb{R}^d} \int_{|x-y|\le\alpha} g_d(x-y)|W_{R_0}(y)|$$

for any fixed R_0, $\lambda>0$ and all $0\le\alpha\le 1$ as soon as $\lim_{R\to\infty}\|W_R\|_{L^1_{\mathrm{loc,unif}}} = 0$. Since W_{R_0} is in the Kato–class, we can then take the limit $\alpha\to 0$ to get (A.30).

It remains to prove (A.31). Note

$$\|(P^2+\lambda)^{-1}|W|\|_\infty = \sup_{x\in\mathbb{R}^d}\int_{\mathbb{R}^d} G(x,y,\lambda)|W(y)|\,dy$$

where $G(x,y),\lambda = (P^2+\lambda)^{-1}(x,y)$ is the Green's function, i.e., the kernel of $(P^2+\lambda)^{-1}$. We split the integral above in the two regions $|x-y|\le\alpha$ and $|x-y|>\alpha$. The bounds

$$G(x,y,\lambda) \lesssim \lambda^{-1}|x-y|^{-d}e^{-\sqrt{\lambda}|x-y|/2} \tag{A.32}$$

and for $|x-y|\le 1/2$ and $\lambda\ge 1$

$$G(x,y,\lambda) \lesssim \begin{cases} |x-y|^{2-d} & \text{if } d\ge 3\\ |\ln|x-y|| & \text{if } d=2\end{cases} \tag{A.33}$$

are well-know. The second bound immediately gives

$$\sup_{x\in\mathbb{R}^d}\int_{|x-y|\le\alpha} G(x,y,\lambda)|W(y)|\,dy \lesssim \sup_{x\in\mathbb{R}^d}\int_{|x-y|\le\alpha} g_d(x-y)|W(y)|\,dy$$

at least for all $0<\alpha\le 1/2$ and the first one shows

$$\int_{|x-y|>\alpha} G(x,y,\lambda)|W(y)|\,dy \lesssim \lambda^{-1}\int_{|x-y|\ge\alpha} |x-y|^{-d}e^{-\sqrt{\lambda}|x-y|/2}|W(y)|\,dy\,.$$

Integrating over shells $\alpha n\le|x-y|<\alpha(n+1)$ leads to

$$\sup_{x\in\mathbb{R}^d}\int_{|x-y|>\alpha} G(x,y,\lambda)|W(y)|\,dy \lesssim \lambda^{-1}\sum_{n=1}^\infty e^{-\sqrt{\lambda}\alpha n/2}\frac{(\alpha(n+1))^d-(\alpha n)^d}{(\alpha n)^d}\|W\|_{L^1_{\mathrm{loc,unif}}}$$

$$\lesssim \lambda^{-1}\sum_{n=1}^\infty e^{-\sqrt{\lambda}\alpha n/2}\|W\|_{L^1_{\mathrm{loc,unif}}} = \frac{e^{-\sqrt{\lambda}\alpha/2}}{\lambda(1-e^{-\sqrt{\lambda}\alpha/2})}\|W\|_{L^1_{\mathrm{loc,unif}}} \lesssim \frac{e^{-\sqrt{\lambda}\alpha/4}}{\sqrt{\lambda}\alpha}\|W\|_{L^1_{\mathrm{loc,unif}}}$$

since $0<t\mapsto \frac{te^{-t/2}}{1-e^{-t}}$ is bounded. This proves (A.31).

We sketch the proof of the bounds (A.32) and (A.33), for the convenience of the reader: The kernel of the heat semigroup is $e^{-P^2 t}(x,y) = (4\pi t)^{-d/2} e^{-\frac{|x-y|^2}{4t}}$. Since $(P^2+\lambda)^{-1} = \int_0^\infty e^{-P^2 s - \lambda s}\, ds$ we have

$$\begin{aligned} G(x,y,\lambda) &= \int_0^\infty (4\pi s)^{-d/2} e^{-\frac{|x-y|^2}{4s}} e^{-\lambda s}\, ds \\ &= |x-y|^{2-d} \int_0^\infty (4\pi u)^{-d/2} e^{-\frac{1}{4u}} e^{-\lambda |x-y|^2 u}\, du \end{aligned}$$

Moreover, $\frac{1}{4u} + \lambda|x-y|^2 u \geq \sqrt{\lambda}|x-y|$ for all $u > 0$, so

$$\begin{aligned} G(x,y,\lambda) &\leq |x-y|^{2-d} e^{-\sqrt{\lambda}|x-y|/2} \int_0^\infty (4\pi u)^{-d/2} e^{-\frac{1}{8u}} e^{-\lambda|x-y|^2 u/2}\, du \\ &= \frac{|x-y|^{-d} e^{-\sqrt{\lambda}|x-y|/2}}{\lambda} \int_0^\infty (4\pi u)^{-d/2} e^{-\frac{1}{8u}} \lambda |x-y|^2 u e^{-\lambda|x-y|^2 u/2} \frac{du}{u} \\ &\lesssim \frac{|x-y|^{-d} e^{-\sqrt{\lambda}|x-y|/2}}{\lambda} \end{aligned}$$

since $0 < t \mapsto t e^{-t}$ is bounded and $c_d = \int_0^\infty (4\pi u)^{-d/2} e^{-\frac{1}{4u}} \frac{du}{u} < \infty$ for all $d \geq 1$. This proves (A.32).

On the other hand,

$$G(x,y,\lambda) = |x-y|^{2-d} \int_0^\infty (4\pi u)^{-d/2} e^{-\frac{1}{4u}} e^{-\lambda|x-y|^2 u}\, du \leq \widetilde{c}_d |x-y|^{2-d}$$

where $\widetilde{c}_d = \int_0^\infty (4\pi u)^{-d/2} e^{-\frac{1}{4u}}\, du < \infty$ if $d \geq 3$, which proves (A.33) when $d \geq 3$.

If $d = 2$, then for $0 < |x-y| \leq 1/2$, one has

$$\begin{aligned} G(x,y,\lambda) = (4\pi)^{-1} \int_0^\infty e^{\frac{1}{4u}} e^{-\lambda|x-y|^2 u} \frac{du}{u} &\lesssim \int_0^1 e^{\frac{1}{4u}} \frac{du}{u} \\ &+ \int_1^{|x-y|^{-2}} \frac{du}{u} + \int_{|x-y|^{-2}}^\infty e^{-\lambda|x-y|^2 u} \frac{du}{u} \end{aligned}$$

Since $\int_0^1 e^{\frac{1}{4u}} \frac{du}{u} \lesssim 1$ and $\int_{|x-y|^{-2}}^\infty e^{-\lambda|x-y|^2 u} \frac{du}{u} = \int_1^\infty e^{-\lambda u} \frac{du}{u} \leq 1$ for $\lambda \geq 1$, this proves (A.33) when $d = 2$. □

Appendix B. Gronwall type bounds

Lemma B.1 *Let $T > 0$ and let $w, E : [0,T] \to [0,\infty)$. If for some $c > 0$*

$$w(t) \leq E(t) + c \int_0^t e^{t-s} w(s)\, ds, \tag{B.1}$$

for all $t \in [0,T]$, then

$$w(t) \leq E(t) + c \int_0^t e^{(1+c)(t-s)} E(s)\, ds \qquad \forall t \in [0,T]. \tag{B.2}$$

Moreover, if

$$w(t) \leq E(t) + c \int_0^t e^{s-t}\, w(s)\, ds, \tag{B.3}$$

for all $t \in [0, T]$, *then*

$$w(t) \leq E(t) + c \int_0^t e^{(c-1)(t-s)}\, E(s)\, ds \qquad \forall\, t \in [0, T]. \tag{B.4}$$

Proof Put $v(t) := \int_0^t e^{t-s}\, w(s)\, ds$. Then $v(0) = 0$ and, assuming (B.1),

$$v'(t) = v(t) + w(t) \leq E(t) + (1 + c)v(t)$$

Hence

$$\frac{d}{dt}\Big(e^{-(1+c)t}\, v(t)\Big) = e^{-(1+c)t}(v'(t) - (1 + c)v(t)) \leq e^{-(1+c)t}\, E(t).$$

It follows that

$$e^{-(1+c)t}\, v(t) = \int_0^t \frac{d}{ds}\Big(e^{-(1+c)s}\, v(s)\Big)\, ds \leq \int_0^t e^{-(1+c)s}\, E(s)\, ds\, .$$

This implies

$$v(t) \leq \int_0^t e^{(1+c)(t-s)}\, E(s)\, ds,$$

and (B.2) follows, cf. (B.1). □

Appendix C. Optimizing the threshold

It is tempting to split the potential $V = V_1 + V_2$ at infinity in order to optimize the threshold above which one can exclude existence of eigenvalues. Using $V_1 = sV$ and $V_2 = (1 - s)V$, Theorem 4.8 shows the non–existence of eigenvalues with

$$E > \frac{1}{4}\Big(\beta + \omega_1 s + \sqrt{(\beta + \omega_1 s)^2 + 2\omega_2(1 - s)}\Big)^2 = \frac{\omega_1^2}{4}(g(s))^2$$

where for $0 \leq s \leq 1$ we set

$$g(s){:=}b + s + \sqrt{(b + s)^2 + 2c(1 - s)} \tag{C.1}$$

with $b = \beta/\omega_1$ and $c = \omega_2/\omega_1^2$. The goal is to minimize g over $s \in [0, 1]$.

Lemma C.1 (Bang–Bang type Lemma) *For* g *given in* (C.1) *we have* $\min_{0\leq s\leq 1} g(s) = \min(g(0), g(1))$. *More precisely,*

$$\min_{0\leq s\leq 1} g(s) = \begin{cases} g(0) \text{ if } c < 2b + 2 \\ g(1) \text{ if } c > 2b + 2 \end{cases} \tag{C.2}$$

and g *is constant if* $c = 2b + 2$.

Proof Write $c = 2b + 2 + r$. Then $(b+s)^2 + 2c(1-s) = (b+2-s)^2 + 2r(1-s)$, hence

$$g(s) = b + s + \sqrt{(b+2-s)^2 + 2r(1-s)}$$

for all $0 \le s \le 1$. Note that g is clerly constant on $[0, 1]$ if $r = 0$. On $[0, 1]$ the derivative of g is given by

$$g'(s) = 1 + ((b+2-s)^2 + 2r(1-s))^{-1/2}\big(s - (b+2+r)\big).$$

Fix $0 \le s \le 1$. A calculation shows

$$\Big(((b+2-s)^2 + 2r(1-s))^{-1/2}\big(s - (b+2+r)\big)\Big)^2 > 1$$

if and only if $0 < r(r+2b+2) = rc$. Since $c \ge 0$, this implies that if $r < 0$, i.e., $c < 2b+2$, we have $g' > 0$ on $[0, 1]$, i.e., g is strictly increasing on $[0, 1]$.

On the other hand, if $c > 2b + 2$, then also $c - b > b + 2 \ge 2$ and $r < 0$, so $g' < 0$ on $[0, 1]$, i.e., g is strictly decreasing on $[0, 1]$. This proves the lemma. □

Corollary C.2 *Setting*

$$\beta^2 := \gamma_\infty\big(\widetilde{B}^2\big), \quad \omega_1^2 := \gamma_\infty\big((xV)^2\big), \quad \omega_2 := \gamma_\infty^+\big(x \cdot \nabla V\big) \tag{C.3}$$

the threshold $\Lambda(B, V)$ *defined in* (1.14) *optimized for splitting the potential as* $V = V_1 + V_2$ *with* $V_1 = sV$, $V_2 = (1-s)V$ *and* $0 \le s \le 1$ *is given by*

$$\widetilde{\Lambda}(B, V) = \begin{cases} \frac{1}{2}\left(\beta^2 + \omega_2 + \beta\sqrt{\beta + 2\omega_2}\right) & \text{if } \omega_2 \le 2\omega_1(\beta + \omega_1) \\ (\beta + \omega_1)^2 & \text{if } \omega_2 > 2\omega_1(\beta + \omega_1) \end{cases} \tag{C.4}$$

Proof Given Lemma C.1 this is just a simple calculation. □

Appendix D. IMS localization formula

In one step in the proof of Lemma 4.6 we need a quadratic form version of the well-known IMS localization formula under minimal assumptions on the quadratic form of the magnetic Schrödinger operator. This result is not new, see e.g. [34, pp. 98, Prop. 4.2]. For the sake of completeness we include a short proof.

Theorem D.1 (IMS localization formula) *Let* A *be a locally square integrable magnetic vector potential and* V *form small w.r.t.* $(P - A)^2$. *Then for all bounded real–valued* $\xi \in \mathcal{C}^\infty(\mathbb{R}^d)$ *such that* $\nabla\xi$ *is also bounded and all* $\varphi \in \mathcal{D}(P - A)$, *also* $\xi\varphi$ *and* $\xi^2\varphi \in \mathcal{D}(P - A)$ *and*

$$\operatorname{Re} q_{A,V}(\xi^2\varphi, \varphi) = q_{A,V}(\xi\varphi, \xi\varphi) - \big\langle \varphi, |\nabla\xi|^2\varphi \big\rangle \tag{D.1}$$

Proof As before, one easily checks that $\xi\varphi$ and $\xi^2\varphi$ are in the domain of $P - A$ when φ is. Moreover, the potential V commutes with the multiplication operator ξ, so as quadratic forms $\langle \xi^2\varphi, V\varphi\rangle = \langle \xi\varphi, V\xi\varphi\rangle$ and we only have to check the kinetic energy term. Since $(P - A)(\xi^2\varphi) = \xi(P - A)(\xi\varphi) + (P\xi)\xi\varphi$ a short calculation reveals

$$\begin{aligned}\big\langle (P-A)(\xi^2\varphi), (P-A)\varphi \big\rangle &= \big\langle (P-A)(\xi\varphi), (P-A)(\xi\varphi) \big\rangle + \big\langle (P\xi)\varphi, (P-A)(\xi\varphi) \big\rangle \\ &\quad - \big\langle (P-A)(\xi\varphi), (P\xi)\varphi) \big\rangle - \big\langle \varphi, |\nabla\xi|^2\varphi \big\rangle,\end{aligned}$$

so

$$\begin{aligned}\operatorname{Re} q_{A,0}(\xi^2 \varphi, \varphi) &= \operatorname{Re}\big\langle (P-A)(\xi^2\varphi), (P-A)\varphi\big\rangle \\ &= \big\langle (P-A)(\xi\varphi), (P-A)(\xi\varphi)\big\rangle + \big\langle \varphi, |\nabla\xi|^2\varphi\big\rangle\end{aligned}$$

which proves (D.1). □

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