Semiclassical eigenvalue estimates for the Pauli operator with strong non-homogeneous magnetic fields

II. Leading order asymptotic estimates

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Abstract

We give the leading order semiclassical asymptotics for the sum of the negative eigenvalues of the Pauli operator (in dimension two and three) with a strong non-homogeneous magnetic field. As in [LSY-II] for homogeneous field, this result can be used to prove that the magnetic Thomas-Fermi theory gives the leading order ground state energy of large atoms. We develop a new localization scheme well suited to the anisotropic character of the strong magnetic field. We also use the basic Lieb-Thirring estimate obtained in our companion paper [ES-I].

Contents

1 Introduction

This work is the continuation of our previous paper [ES-I] on studying semiclassical limits of the Pauli operator with both electric and magnetic fields. Our main concern, compared to most other works in the subject, is to allow for non-homogeneous magnetic fields. This transition from homogeneous to non-homogeneous field is highly non-trivial, partly because of challenging technical difficulties and partly because the non-homogeneous field can exhibit qualitatively different behaviour.

We shall be concerned with dimensions two and three. Though, it may seem that dimension three is the physically most important case, certain new experimental techniques (see an extensive review in [LSY-III]) allows one to study effectively two dimensional systems, like quantum dots. For these two dimensional systems laboratory magnetic fields actually have a stronger influence on the structure than for most three dimensional systems.

The other reason why we treat the two dimensional case as well is pedagogical; some of our basic ideas can be presented without less technicalities in dimension two.

The three dimensional Pauli operator is the following operator acting on the space $L^2(\mathbf{R}^3; \mathbf{C}^2)$ of spinor valued functions.

$$H(h, \mathbf{A}, V) := [\boldsymbol{\sigma} \cdot (-ih\nabla + \mathbf{A}(x))]^2 + V(x) = (-ih\nabla + \mathbf{A}(x))^2 + V(x) + h\boldsymbol{\sigma} \cdot \mathbf{B}(x), \quad (1.1)$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the vector of Pauli spin matrices, i.e.,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The magnetic field $\mathbf{B} : \mathbf{R}^3 \to \mathbf{R}^3$ is a divergence free field related to the vector potential $\mathbf{A} : \mathbf{R}^3 \to \mathbf{R}^3$ by $\mathbf{B} = \nabla \times \mathbf{A}$. The potential $V(x)$ describes the electric field. As usual h is the semiclassical parameter. Throughout the paper we shall use the convention of writing $-i\nabla = \mathbf{p}$. Let $B(x) := |\mathbf{B}(x)|$ and $\mathbf{n}(x) := \mathbf{B}(x)/B(x)$ be the field strength and direction, respectively.

The two dimensional Pauli operator has essentially the same form as the three dimensional operator above. The modifications are rather obvious. The magnetic field is a function $B : \mathbf{R}^2 \to \mathbf{R}$, the vector potential is a vector field $\mathbf{A} : \mathbf{R}^2 \to \mathbf{R}^2$ and we shall write as before $B = \nabla \times \mathbf{A}$ with the obvious interpretation. We apply the convention that $\boldsymbol{\sigma} \cdot v := \boldsymbol{\sigma} \cdot (v, 0)$ for any $v \in \mathbf{R}^2$, $\boldsymbol{\sigma} \cdot \mathbf{p} = \boldsymbol{\sigma} \cdot (\mathbf{p}, 0)$ for the two dimensional momentum operator $\mathbf{p}$, and similarly for the vectorproduct of a 3D and a 2D vector (in particular, we define $\mathbf{n} := (0, 0, 1)$ and let $\mathbf{n} \times v \in \mathbf{R}^2$ be $\mathbf{n} \times v := (-v_2, v_1)$ for $v \in \mathbf{R}^2$). We may then write

$$H^{(2)}(h, \mathbf{A}, V) := [\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A}(x))]^2 + V(x) = (h\mathbf{p} + \mathbf{A}(x))^2 + V(x) + h\sigma_3 B(x). \quad (1.2)$$

Since we shall consider $\mathbf{B} \in L^\infty(\mathbf{R}^3)$ and $B \in L^\infty(\mathbf{R}^2)$, we consider the last terms in (1.1) and (1.2) as a multiplication operator on the corresponding L^2 space.

The Pauli operator describes the motion of a non-relativistic electron, where the electron spin is important because of its interaction with the magnetic field. For simplicity we have not included any physical parameters (i.e., the electron mass, the electron charge, the speed of light, or Planck's constant $\hbar$) in the expressions for the operators. In place of Planck's constant we have the semiclassical parameter h, which we let tend to zero.

The last identities in (1.1) and (1.2) can easily be checked. If we note that $\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A}(x))$ is in fact the three dimensional Dirac operator, we recognize the last identity in (1.1) as the Lichnerowicz formula. As a consequence of these identities one sees a significant difference between the Pauli operator and the 'magnetic' Schrödinger operator $(h\mathbf{p} + \mathbf{A}(x))^2 + V(x)$. In particular, for reasonable potentials and reasonable magnetic fields the essential spectrum of the Pauli operator starts at zero. (See [ES-I] for more details.)

The physically as well as mathematically interesting quantities connected with the eigenvalues are the number and the sum of the eigenvalues below the essential spectrum (in this case, the negative eigenvalues). Recall that the sum of the negative eigenvalues represents the energy of the non-interacting fermi gas in the external potential V and magnetic field $\mathbf{B}$.

In the case of a constant magnetic field it is known [Sol, Sob-1986] that even for a smooth compactly supported potential V, which is negative, there will be *infinitely* many negative eigenvalues. This holds in both two and three dimensions. It was, however, proved in [LSY-II] (three dimensions) and [LSY-III] (two dimensions) that the *sum* of the negative eigenvalues is finite.

The goal in [LSY-II] was to analyze the eigenvalue sum in the semiclassical limit, i.e., as the semiclassical parameter h tends to zero. In the case where one fixes the magnetic field $\mathbf{B}$ and let $h \to 0$ one finds that the leading order contribution to the sum of the eigenvalues becomes independent of the magnetic field[1]. It is therefore equal to the non-magnetic Weyl term, which in three dimensions is $-2(15\pi^2)^{-1}h^{-3}\int_{\mathbf{R}^3}[V]_-^{5/2}$ and in two dimensions is $-h^{-2}(8\pi)^{-1}\int_{\mathbf{R}^2}[V]_-^2$ ($[V]_-$ denotes the negative part of the function V). This type of semiclassical limit is therefore not very well suited to the study of the effect of magnetic fields. One could maybe hope that higher order terms in the expansion would reveal information about the magnetic field. In this context we should point out, however, that without some assumptions on the classical Hamiltonian flow one cannot establish non-vanishing higher order corrections to the above Weyl term.

The observation made in [LSY-II] for homogeneous magnetic fields is that one can establish a semiclassical expression for the sum of the negative eigenvalues which is asymptotically exact uniformly in the magnetic field strength. In contrast to the above standard semiclassical Weyl term, the generalized semiclassical expression, indeed, depends on the magnetic field. In case of three dimensions this formula is given by

$$E_{scl}(h, \mathbf{B}, V) := -h^{-3} \int_{\mathbf{R}^3} P(h|\mathbf{B}(x)|, [V(x)]_-) \mathrm{d}x \tag{1.3}$$

[1] We believe that this result in its greatest generality was also first proved in [LSY-II], or rather follows from the result in [LSY-II]. In fact, to prove the semiclassics of the sum of all the negative eigenvalues for fixed $\mathbf{B}$ one needs to know that the sum is finite, which was first established by the Lieb-Thirring (LT) estimate in [LSY-II].

with

$$P(B,W) := \frac{B}{3\pi^2}\left(W^{3/2} + 2\sum_{\nu=1}^{\infty}[2\nu B - W]_-^{3/2}\right) = \frac{2}{3\pi}\sum_{\nu=0}^{\infty} d_\nu B[2\nu B - W]_-^{3/2} \tag{1.4}$$

being the pressure of the three dimensional Landau gas ($B, W \geq 0$). Here $d_0 = (2\pi)^{-1}$ and $d_\nu = \pi^{-1}$ if $\nu \geq 1$. Observe that if $\|\mathbf{B}\| = o(h^{-1})$ then E_{scl} reduces to leading order to the standard Weyl term as $h \to 0$. If $B(x)h \to \infty$ for all x, then only the lowest Landau band gives the main contribution, i.e. E_{scl} reduces to leading order to a similar expression where only the first term ($\nu = 0$) is kept in (1.4). Here and throughout the paper $\|\cdot\|$ refers to the supremum norm.

In [LSY-III] the two dimensional problem was studied, but since this paper was aimed mainly at applications the semiclassical formula did not appear explicitly. It is

$$E_{scl}^{(2)}(h, B, V) := -h^{-2}\int_{\mathbf{R}^2} P^{(2)}(hB(x), [V(x)]_-)\mathrm{d}x \tag{1.5}$$

with

$$P^{(2)}(B,W) := \frac{B}{2\pi}\left(W + 2\sum_{\nu=1}^{\infty}[2\nu B - W]_-\right) = \sum_{\nu=0}^{\infty} d_\nu B[2\nu B - W]_- \tag{1.6}$$

being the pressure of the two dimensional Landau gas (d_ν is as above). Again if $\|\mathbf{B}\| = o(h^{-1})$ then $E_{scl}^{(2)}$ reduces to the standard Weyl term.

Our goal in this paper is to show that these semiclassical formulas are exact also for non-homogeneous fields. Of course, for non-homogeneous fields it is more subtle exactly what one means by uniformity in the field, since the field is now no longer determined by just one parameter. We shall return to this question later.

The physical motivations for studying these issues are explained in [ES-I]. Here we just recall, as one of the most important applications, that the problem of the ground state energy of large atoms in strong magnetic fields can be reduced to the semiclassical limit of the eigenvalue sum, using Thomas-Fermi theories. We shall investigate this question in our context of non-homogeneous magnetic fields.

In typical applications, it is usually a good approximation to consider the magnetic field as homogeneous. There are several reasons, however, why one would still like to extend the analysis to non-homogeneous fields. First of all it is of course natural to ask whether the features found for homogeneous fields are really stable. Furthermore, a detailed mathematical study often requires one to be able to locally vary the field, even if one is mainly interested in the constant field case. Even though we will find that the semiclassical results known for constant fields really carry over to non-constant fields, we will also see that, in fact, not all features of the constant case are stable.

Of course the problem is also of independent interest and raises, as we shall see, many extremely interesting mathematical issues. The homogeneous field case is comparatively simple because the kinetic energy part is an exactly solvable quantum mechanical model.

The semiclassical analysis of eigenvalues is really twofold. One must first of all establish non-asympotic, Lieb-Thirring type estimates on the sum of the negative eigencvalues, allowing one to control errors and contributions coming from non-semiclassical regions. In our context this is the subject of [ES-I].

The second part of the semiclassical study is to show that when all the errors have been controlled one can indeed get the asymptotic formula. This is the main subject of the present paper. There are a multitude of highly developed methods for this part of the analysis, e.g., pseudo-differential operator and Fourier integral operator methods (see e.g., [Sob-1994, Sob-1995] which generalizes results in [LSY-II] using these methods, or the book [R], or the preprints [I]). Depending on certain properties of the classical Hamiltonian flow, these results even give higher order corrections to the leading term. However, these methods require, in general, strong regularity assumptions on the data. Also, without some non-asymptotic Lieb-Thirring type apriori estimates, these results usually either refer to only a part of the spectrum which is strictly away form the essential spectrum or compute only quantities which are localized in space, what is called local traces or local eigenvalue moments. Within this context non-Weyl type formulas similar to (1.3) and (1.5) are studied in the preprints [I].

Our approach to the problem is the more elementary coherent state method also used in [LSY-II, LSY-III]. In addition to the conceptual simplicity, it reveals some important geometric features related to the magnetic field.

As always, semiclassical methods require controlling localization errors. For a homogeneous field one simply has to localize in regions where the potential does not vary too much. In the case of non-homogeneous fields one is, however, forced to also localize on the often much shorter scale where the vector potential is nearly constant. This scale turns out to be so small that the standard IMS localization procedure would be too expensive.

We have elaborated a new localization scheme, particularly suitable for magnetic problems. Similarly to the proof of the Lieb-Thirring estimate in [ES-I], we shall use a two step localization. First we have a larger scale isotropic localization. On this length scale, the field direction is almost constant and also the field strength does not vary too much. As usual in IMS type arguments, the actual localization function is not essential, only its length scale is determined. In dimension two the field direction is of course stable, therefore this step is only necessary to control the variation of the field strength (this strategy allows us to treat fields whose strength has no uniform positive lower bound).

The second localization is reminiscent of the cylindrical localization in the LT proof since the localization function is supported in a typically elongated cylindrical domain, corresponding to the effective anisotropic character of the magnetic field. The key point is that, in contrast to the standard localization approach, the function itself is very specially chosen. It essentially must be a zero mode of the associated two dimensional Pauli operator with a locally constant field. In a strong magnetic field, the zero mode can be chosen as a well localized Gaussian function. It allows one to localize very strongly (much beyond the IMS localization), essentially for free (the price we pay appears as a slight modification in the magnetic field).

To understand this phenomenon, recall that in the typical IMS scheme one pays the price of the lowest eigenvalue of the Dirichlet Laplacian for localization. This is of course an expression of the uncertainity principle. It should be, however, noted that while the uncertainity principle between position and momentum is a universal fact about quantum systems, large momentum does not necessarily imply large energy. This is exactly the case for the two dimensional Pauli operator, where the magnetic field and spin coupling can, and in the right sector does, compensate the "spinless" kinetic energy. This is the reason behind the existence of the Aharonov-Casher zero modes (see [AC], [CFKS]), which carry large (angular) momentum, but have no energy.

We should mention that probably the first asymptotic formula for eigenvalues of an operator with non-homogeneous magnetic field appeared in [CdV, T], and later was extended in [H], [Mat-1994]. All these works consider the large eigenvalue asymptotics for the 'magnetic' Schrödinger operator with a magnetic field increasing at infinity (magnetic bottles). This operator has pure point spectrum (and compact resolvent), therefore the problem is considerably simpler than ours. The analogy to our result is that in both problems the asymptotic formula for the non-homogeneous magnetic field is obtained by simply inserting the strength of the non-homogeneous field into the formula for homogeneous field.

The organization of the paper is the following. In the next two subsections we explain the main results in the simplest setup. In Section 2 we present our new localization method, which is one of the key point of our analysis. The other key point is the analysis of the geometry of the three dimensional magnetic field (in particular a careful choice of a suitable gauge), which was already used in [ES-I]. For the reader's convenience we recall the necessary results in the Appendix.

In Section 3 we work out the two dimensional case. We start with a short presentation of the necessary Lieb-Thirring inequality. Then we apply the localization scheme to estimate the quadratic form of the kinetic energy with a non-homogeneous field, by a similar expression with a locally homogeneous field. Finally we work out separately the lower bound, using Lieb-Thirring inequality, and the upper bound, using coherent states and variational principle. In both cases we heavily rely on the structure of the Pauli operator with a constant magnetic field (e.g. Landau levels).

Section 4 contains the three dimensional semiclassics. Approximating the true kinetic energy by a (locally) constant field kinetic energy requires choosing an 'economical' gauge for the approximating field, we use the results from the Appendix. Once this approximation is done, the lower and upper bounds for the eigenvalue sum are obtained essentially in the same way as in the two dimensional case. For the lower bound, one has to use the more complicated three dimensional Lieb-Thirring inequality. The formulas are somewhat lengthy, as one has complicated error terms, but their basic structure resembles the simpler two dimensional setup. Therefore the reader is advised to start with the two dimensional proof.

The last Section is devoted to the proof of the validity of the Magnetic Thomas Fermi (MTF) theory introduced and studied, even for non-homogeneous fields, in [LSY-II]. The validity of this theory, as an approximation to the ground state energy of large atoms in strong magnetic fields, was proved for homogeneous fields in [LSY-II]. Here we have to cope with two new difficulties, compared to the constant field case in [LSY-II]. First is that our Lieb-Thirring inequality does not provide a kinetic energy inequality via Legendre transform (because of an extra gradient term, see (1.12) later). The other complication is that one needs more information on the magnetic Thomas Fermi potential, again because of the extra terms in our LT inequality, i.e., one has to prove that these terms are negligible for the potential of MTF theory.

1.1 Main results in semiclassics

We shall throughout the paper assume the following conditions on the magnetic field, $\mathbf{B} : \mathbf{R}^3 \to \mathbf{R}^3$, in dimension three

$$\|B\| < \infty, \tag{1.7}$$

$$l(\mathbf{B})^{-1} := \|\nabla \mathbf{n}\| = \|\nabla \frac{\mathbf{B}}{B}\| < \infty, \tag{1.8}$$

$$L(\mathbf{B})^{-1} := \|\frac{|\nabla B|}{B}\| < \infty. \tag{1.9}$$

Here $l = l(\mathbf{B})$ describes the length scale on which the field line geometry changes, while $L = L(\mathbf{B})$ is the length scale on which the field strength varies. Note that the conditions imply that $B(x) := |\mathbf{B}(x)|$ never vanishes. We are especially interested in the case when $l \gg L$. In particular, for $l = \infty$, $L < \infty$, we obtain the constant direction (but non-homogeneous) case.

In dimension two we assume conditions analoguous to (1.7), (1.9)

$$\|B\| < \infty \tag{1.10}$$

$$
\|\frac{|\nabla B|}{B}\| < \infty \tag{1.11}
$$

for the two dimensional magnetic field $B : \mathbf{R}^2 \to \mathbf{R}$.

Notice, that we do not assume more than a bound[2] on the first derivative of the magnetic field in contrast to the more traditional SC approach which uses pseudodifferential operators and therefore assumes strong regularity conditions on the data.

The potential V is naturally assumed to be in the corresponding L^p spaces which make the semiclassical formulas (1.3), (1.5) finite, that is we assume $V \in L^{5/2}(\mathbf{R}^3) \cap L^{3/2}(\mathbf{R}^3)$ in the three dimensional case, and $V \in L^1(\mathbf{R}^2) \cap L^2(\mathbf{R}^2)$ in dimension two. As it is explained in [ES-I], in dimension two these natural assumptions are sufficient since we have a Lieb-Thirring inequality which scales exactly as the semiclassical expression. In fact, in the simple case of a bounded field, which is our concern here, the combination of the methods in [E-1995] and [LSY-III] gives a very simple proof which we present in Section 3.1 (for references on unbounded fields, see [ES-I]).

However, in dimension three, our Lieb-Thirring inequality (the main theorem in [ES-I]) bounds the sum of the negative eigenvalues of H in (1.1) by

$$
C_1\Bigg(h^{-3}\int_{\mathbf{R}^3}[V]_-^{5/2} + \int_{\mathbf{R}^3}(h^{-1}B + d^{-2})h^{-1}\,[V]_-^{3/2} \tag{1.12}
$$

$$
+ \int_{\mathbf{R}^3}(h^{-1}B + d^{-2})d^{-1}\,[V]_- + \int_{\mathbf{R}^3}(h^{-1}B + d^{-2})\,|\nabla[V]_-|\Bigg),
$$

where

$$
d = d(h, \mathbf{B}) := \min\{h^{1/4}\|B\|^{-1/4}l(\mathbf{B})^{1/2}, L(\mathbf{B}), l(\mathbf{B})\}.
$$

This estimate contains two extra terms which, to be finite, require $[V]_- \in W^{1,1}(\mathbf{R}^3)$. These terms are of lower order as far as the large field semiclassics is concerned, but at least the term involving $\int[V]_-$ cannot be eliminated (see [ES-I]). The other term, with $\int|\nabla[V]_-|$, is a conceptual error coming from our method, also has to be considered.

Our theorem in dimension two is the following.

Theorem 1.1 (2D Semiclassics) *Assume that the potential V satisfies $V \in L^1(\mathbf{R}^2)\cap L^2(\mathbf{R}^2)$ and the magnetic field B satisfies (1.10)-(1.11). For $h, b > 0$ let $e_1(h,b), e_2(h,b), \ldots$ denote the negative eigenvalues of the operator $H = H^{(2)}(h, b\mathbf{A}, V)$ in (1.2). Then*

$$
\lim_{h\to 0}\left|\frac{\sum_k e_k(h,b)}{E^{(2)}_{scl}(h, bB, V)} - 1\right| = 0
$$

[2] We strictly speaking only need the magnetic field to be Lipschitz

uniformly in b.

Later we shall in fact prove a slighty stronger result. Instead of considering magnetic fields depending only on the parameter b, we shall prove a statement that is uniform on more general families of magnetic fields. We shall make it more precise in Section 3.

The formulation of the three dimensional result is more complicated than the two dimensional result, since we do not prove a fully uniform statement.

Theorem 1.2 (3D Semiclassics) *Assume that the potential V satisfies $V \in L^{5/2}(\mathbf{R}^3) \cap L^{3/2}(\mathbf{R}^3)$, $[V]_- \in W^{1,1}(\mathbf{R}^3)$ and the magnetic field $\mathbf{B}$ satisfies (1.7)–(1.9). For $h, b > 0$ let $e_1(h,b), e_2(h,b), \ldots$ denote the negative eigenvalues of the operator $H = H(h, b\mathbf{A}, V)$ in (1.1). Then*

$$\lim_{\substack{h\to 0\\ bh^3\to 0}} \left| \frac{\sum_k e_k(h,b)}{E_{scl}(h, b\mathbf{B}, V)} - 1 \right| = 0. \tag{1.13}$$

We shall again prove a slightly stronger result. The reason for this generalization is that in our main application the magnetic Thomas-Fermi theory, the potential will depend slightly on the magnetic field and on the effective Planck constant. The details are explained in Section 5.

There is a fundamental technical reason for the condition $bh^3 \to 0$. We already explained it in [ES-I], since a similar condition plays a role in the proof of our Lieb-Thirring inequality.

Part of the motivation for believing that the semiclassical formula for homogeneous or even constant direction fields should generalize to fully non-homogeneous fields is that these fields on the relevant quantum scales should behave approximately like constant direction fields. This is, however, not true if the field is too strong. A charged particle moving in a magnetic field essentially occupies a region in space of the shape of a cylinder with axis parallel to the magnetic field. For particles of fixed energy e the radius of the cylinder is the Landau radius $r \sim b^{-1/2}h^{1/2}$ and the height is of order $s = he^{-1/2}$ (particles localized in regions of length $he^{-1/2}$ in one dimension have energies of order e). The condition that one can approximate the magnetic field within this region by a constant direction field is that the field lines remain within this cylinder, i.e., that $l(\mathbf{B})^{-1}s^2 \ll r$. This condition is simply that $bl(\mathbf{B})^{-2} \ll h^{-3}e^2$.

Although the above restriction on the magnetic field might seem natural, we believe that it can be removed by an additional geometrical analysis which is beyond the scope of the present work. We intend to return to this issue in the future.

1.2 Application to the magnetic Thomas-Fermi theory

As an application of our semiclassical analysis we shall here generalize Theorem 5.1 in [LSY-II] on the energy of large atoms in strong *exterior* magnetic fields. We shall work in dimension three, but we are convinced that a very similar analysis can be carried over in dimension two, similarly to [LSY-III]. We consider again a magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$ which satisfies (1.7–1.9). Our generalization will be to allow a much more general class of three dimensional exterior fields than in [LSY-II], where only homogeneous fields were treated.

The quantum mechanical Hamiltonian for an atom with nuclear charge Z and with N electrons in such an exterior magnetic field is given by

$$H_{N,\mathbf{A},Z} := \sum_{i=1}^{N} \left\{ [\boldsymbol{\sigma}_i \cdot (\mathbf{p}_i + \mathbf{A}(x_i))]^2 - Z|x_i|^{-1} \right\} + \sum_{i<j}^{N} |x_i - x_j|^{-1}. \tag{1.14}$$

It operates on spinor-valued wave functions $\psi \in \bigwedge^N L^2(\mathbf{R}^3; \mathbf{C}^2)$. We have here used units in which twice the electron mass $2m_e$, the electron charge e, and Plancks constant $\hbar$ are all equal to unity. We have also used the infinite mass approximation for the nucleus, which is situated at the origin.

We define the ground state energy of this atom

$$E(N, \mathbf{B}, Z) := \inf_{\|\psi\|=1} \langle \psi \mid H_{N,\mathbf{A},Z} \mid \psi \rangle, \tag{1.15}$$

which, of course, depends only on the magnetic field.

In order to state our main result we must introduce the magnetic Thomas-Fermi (MTF) theory of [LSY-II]. It is defined in terms of the energy functional

$$\begin{aligned} \mathcal{E}[\rho; B, Z] \;\; := \;\; & \int_{\mathbf{R}^3} \tau(B(x), \rho(x)) \mathrm{d}x - \int_{\mathbf{R}^3} Z|x|^{-1} \rho(x) \mathrm{d}x \\ & + \tfrac{1}{2} \iint_{\mathbf{R}^3 \times \mathbf{R}^3} \rho(x) |x-y|^{-1} \rho(y) \mathrm{d}x \mathrm{d}y, \end{aligned} \tag{1.16}$$

where $\rho \mapsto \tau(B, \rho)$ is the Legendre transform of the Landau pressure function $W \mapsto P(B, W)$ defined in (1.4), i.e.,

$$\tau(B, \rho) := \sup_{W \geq 0} [\rho W - P(B, W)], \tag{1.17}$$

and conversely, since $W \mapsto P(B, W)$ is convex,

$$P(B, W) = \sup_{\rho \geq 0} [\rho W - \tau(B, \rho)].$$

The energy in MTF theory is defined by

$$E^{\mathrm{MTF}}(N,B,Z) := \inf_{0\leq\rho,\ \int\rho\leq N} \mathcal{E}[\rho;B,Z]. \tag{1.18}$$

We here use the convention that $\mathcal{E}[\rho;B,Z] = +\infty$ unless all integrals are finite. Note that $E^{\mathrm{MTF}}(N,B,Z)$ depends only on the magnitude of $B(x) = |\mathbf{B}(x)|$ of the magnetic field. The minimization problem (1.18) was studied in great detail in Section IV of [LSY-II], and the necessary results will be recalled later.

Our main result on the energy of large atoms is given in the following theorem.

Theorem 1.3 *Let $\mathbf{B} = \nabla\times\mathbf{A} : \mathbf{R}^3 \to \mathbf{R}^3$ be a fixed magnetic field satisfying (1.7–1.9). If $Z, N\to\infty$ with N/Z fixed and $b/Z^3 \to 0$, then*

$$E(N,b\mathbf{B},Z)/E^{\mathrm{MTF}}(N,bB,Z)\to 1.$$

In this theorem we introduced a field strength parameter b. The point is that we allow the field strength to be large in comparison to powers of Z. The condition $b/Z^3\to 0$ is identical to the condition in [LSY-II].

In Section 5 we shall slightly generalize this result by allowing more complicated relations between the magnetic field and the atomic parameters. In particular, we shall give conditions for when the field is allowed to vary on the scale of the size of the atom.

2 Localization for operators with magnetic fields

As usual one of the important ingredients in the proof of leading order semiclassics is to control localization errors. The most commonly used estimate in this context is often referred to as the IMS formula. It is given in the following lemma.

Lemma 2.1 (IMS) *Let $n=2$ or $n=3$. For $k\in C^\infty(\mathbf{R}^n,\mathbf{C}^2)$ and $g\in C^\infty(\mathbf{R}^n)$ we have for all $0<\delta<1$ the pointwise inequalities*

$$\begin{aligned} |g(x)\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}(x))k(x)|^2 &\geq (1-\delta)\,|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}(x))\,(gk)(x)|^2 - c\delta^{-1}h^2|\nabla g(x)|^2|k(x)|^2 \\ |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}(x))(gk)(x)|^2 &\leq (1+\delta)\,|g(x)\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}(x))\,k(x)|^2 + c\delta^{-1}h^2|\nabla g(x)|^2|k(x)|^2. \end{aligned}$$

Moreover, on average, even an identity is valid (IMS formula), if, in addition, g is real and compactly supported

$$\langle k|g^2(\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}))^2|k\rangle + \langle k|(\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}))^2g^2|k\rangle = 2\langle kg|(\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}))^2|gk\rangle - 2h^2\langle k|(\nabla g)^2k\rangle. \tag{2.1}$$

Proof. The first two inequalities are straightforward to prove using Leibniz formula. These inequalities are of course essentially identical. The IMS formula can be seen as follows

$$
\begin{aligned}
&\langle \boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gk|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gk\rangle \\
&= \langle g\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})k|g\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})k\rangle + h^2\langle k|(\nabla g)^2|k\rangle + 2\mathrm{Re}\langle g\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})k|(h\boldsymbol{\sigma}\cdot\mathbf{p}g)k\rangle \\
&= \tfrac{1}{2}\langle k|g^2(\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}))^2|k\rangle + \tfrac{1}{2}\langle k|(\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}))^2g^2|k\rangle + h^2\langle k|(\nabla g)^2|k\rangle \\
&\quad +2\mathrm{Re}\langle g\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})k|(h\boldsymbol{\sigma}\cdot\mathbf{p}g)k\rangle + \mathrm{Re}\langle(h\boldsymbol{\sigma}\cdot\mathbf{p}g^2)(\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}))k|k\rangle.
\end{aligned}
$$

We used integration by parts, and, by reality of g, one finally sees that the last two terms above cancel. □

In turns out, as we shall explain below, that the above localization estimates are not adequate for the Pauli operator with strong magnetic fields. In this case it is better to use a very specific localization function. Namely, the function $\eta^{(0)}\in C^\infty(\mathbf{R}^2,\mathbf{C}^2)$ given by

$$\eta^{(0)}(x) = w^{-1}e^{-w^{-2}x^2},$$

where $w>0$ represents the localization scale. That this function does not have compact support turns out to be just a minor difficulty.

Lemma 2.2 (Magnetic localization) *Let B_0 be any constant and $k\in C^\infty(\mathbf{R}^2,\mathbf{C}^2)$. Then with the explicit choice of $\eta^{(0)}$ we have for all $0<\delta<1$*

$$
\begin{aligned}
&|\eta^{(0)}(x)\boldsymbol{\sigma}\cdot(h\mathbf{p}+(1/2)B_0\mathbf{n}\times x)k(x)|^2 \\
&\geq (1-\delta)\left|\boldsymbol{\sigma}\cdot\Big(h\mathbf{p}+(1/2)(B_0+4hw^{-2})\mathbf{n}\times x\Big)(\eta^{(0)}k)(x)\right|^2 \\
&\quad - c\delta^{-1}h^2w^{-2}|xw^{-1}|^2|P_+(\eta^{(0)}k)(x)|^2
\end{aligned}
\tag{2.2}
$$

and

$$
\begin{aligned}
&|\boldsymbol{\sigma}\cdot(h\mathbf{p}+(1/2)B_0\mathbf{n}\times x)(\eta^{(0)}k)(x)|^2 \\
&\leq (1+\delta)\left|\eta^{(0)}(x)\boldsymbol{\sigma}\cdot\Big(h\mathbf{p}+(1/2)(B_0-4hw^{-2})\mathbf{n}\times x\Big)k(x)\right|^2 \\
&\quad + c\delta^{-1}h^2w^{-2}|xw^{-1}|^2|P_+(\eta^{(0)}k)(x)|^2.
\end{aligned}
\tag{2.3}
$$

Proof. Using Leibniz formula a simple computation gives

$$
\begin{aligned}
&\boldsymbol{\sigma}\cdot(h\mathbf{p}+(1/2)B_0\mathbf{n}\times x)\,(\eta^{(0)}k)(x) \\
&= \eta^{(0)}(x)\boldsymbol{\sigma}\cdot\Big(h\mathbf{p}+(1/2)(B_0-4hw^{-2})\mathbf{n}\times x\Big)k(x) + 4ihw^{-2}\eta^{(0)}(x)(\boldsymbol{\sigma}\cdot x)P_+k(x).
\end{aligned}
$$

A simple application of a Cauchy-Schwarz inequality then gives (2.3). Replacing B_0 by $B_0 + 4hw^{-2}$ we similarly get (2.2). □

We shall use both the magnetic localization and the IMS Lemma. The magnetic localization shall be used to approximate the variable magnetic field by a constant field. We shall now explain why the magnetic localization is superior to the IMS formula for this purpose.

Imagine that we attempt to approximate the variable field by a constant field over a region of length w. The approximation error for the vector potential is then $\|B\|L^{-1}w^2$ using that $|\nabla B| \leq \|B\|L^{-1}$ and (A.9). [This error will appear squared in the estimate on the Hamiltonian (see e.g. (3.20) and (3.21)) below, but this is unimportant for the present discussion.] Since we want to prove estimates uniform in $\|B\|$ we must choose w proportional to $\|B\|^{-1/2}$. The IMS formula would then give an error $w^{-2} \sim \|B\|$, which is not independent of $\|B\|$.

The magnetic localization seems at first sight to give the same error. In fact, this is the order of the last terms in (2.2) and (2.3). [Since $\int \eta^{(0)}(x)^2 x \mathrm{d}x = cw$ we should think of $|xw^{-1}|$ being of order one.] The important observation is that the error terms in the magnetic localization contain the spin up projection P_+. If the magnetic field B is bounded below then the free Pauli operator restricted to the spin up subspace is not just positive but, indeed, bounded below by a positive amount proportional to the lower bound on B [see (3.28)]. If the ratio of the supremum of B is bounded relative the infimum of B then the *relative* localization error (compared to the main term) in the magnetic localization is independent of $\|B\|$ and this is the important fact.

We shall not actually assume that the magnetic field is bounded below. This is just a minor technical problem. In fact, as should be clear from the above discussion, it is only the ratio of the maximum of the field to the minimum that counts. We therefore simply use the standard IMS Lemma to localize in regions where this ratio is bounded.

3 Semiclassics in two dimensions

In the introduction we stated our semiclassical result in Theorem 1.1 for fixed potential. First we formulate our more general result for potentials which are allowed to depend mildly on B and h. To describe the precise result, we introduce the **2D magnetic Lieb-Thirring error functional**

$$\mathcal{E}^{(2)}_{h,B}(V) := h^{-2}\int |V|^2 + \|B\|h^{-1}\int |V| \tag{3.1}$$

(in Section 3 all integrals are on $\mathbf{R}^2$, unless otherwise specified). With this notation, the Lieb-Thirring inequality Theorem 3.2 in Section 3.1 states that the sum of the negative eigenvalues

$e_1(H), e_2(H), \ldots$ of $H = H^{(2)}(h, \mathbf{A}, V)$ satisfies the bound

$$\sum_k |e_k(H)| \le c\mathcal{E}^{(2)}_{h,B}([V]_-) \le c\mathcal{E}^{(2)}_{h,B}(V)$$

if the magnetic field satisfies (1.10).

Define the following set for $L > 0$

$$\mathcal{C}_L := \Big\{ 0 < B(x) \in L^\infty(\mathbf{R}^2) \; : \; \sup_x \frac{|\nabla B(x)|}{B(x)} \le L^{-1} \Big\}.$$

We may now introduce the conditions on the potential.

$$C_+(V) := \sup_{B \in \mathcal{C}_L,\, 0<h<1} \frac{\mathcal{E}^{(2)}_{h,B}(V)}{\|B\|h^{-1} + h^{-2}} < \infty \tag{3.2}$$

$$\varepsilon_1(V, y) := \sup_{B \in \mathcal{C}_L,\, 0<h<1} \frac{\mathcal{E}^{(2)}_{h,B}([V]_\pm - [V(\cdot - y)]_\pm)}{\|B\|h^{-1} + h^{-2}} \to 0 \quad \text{as } y \to 0 \tag{3.3}$$

$$\varepsilon_2(V, \varrho) := \sup_{B \in \mathcal{C}_L,\, 0<h<1} \frac{\mathcal{E}^{(2)}_{h,B}([V\chi_\varrho]_- - [V]_-)}{\|B\|h^{-1} + h^{-2}} \to 0 \quad \text{as } \varrho \to \infty, \tag{3.4}$$

where χ_ϱ denotes the characteristic function of the ball of radius ϱ centered at the origin. Furthermore, we require a joint condition on B and V

$$C_-(B, V) := \inf_{0<h<1} \frac{|E^{(2)}_{scl}(h, B, V)|}{\|B\|h^{-1} + h^{-2}} > 0. \tag{3.5}$$

Note that (3.2), (3.5), and $P^{(2)}(B, W) \le c(BW + W^2)$ imply that

$$c \le \frac{\mathcal{E}^{(2)}_{h,B}(V)}{|E^{(2)}_{scl}(h, B, V)|} \le \frac{C_+(V)}{C_-(B, V)} \tag{3.6}$$

for all $0 < h < 1$ and all $B \in \mathcal{C}_L$.

For $C, L > 0$ introduce the set

$$\mathcal{C}_{C,L}(V) := \left\{ 0 < B(x) \in L^\infty(\mathbf{R}^2) \; : \; \sup_x \frac{|\nabla B(x)|}{B(x)} \le L^{-1}, \; C_-(B, V) \ge C \right\}.$$

Theorem 3.1 (2D Semiclassics) *Let $V \in L^1(\mathbf{R}^2) \cap L^2(\mathbf{R}^2)$ and let $e_1(H), e_2(H), \ldots$ denote the negative eigenvalues of the operator $H = H^{(2)}(h, \mathbf{A}, V)$ in (1.2). For any $C, L > 0$ we have*

$$\lim_{h\to 0}\left(\sup_{B\in\mathcal{C}_{C,L}(V)}\left|\frac{\sum_k e_k(H)}{E^{(2)}_{scl}(h,B,V)} - 1\right|\right) = 0.$$

Remark. What we really need about V and B for the semiclassical limit is the conditions (3.2)–(3.5). For a fixed potential, these conditions follow simply from $V \in L^1 \cap L^2$ and $B \in \mathcal{C}_{C,L}(V)$.

Following [LSY-III], there are two ingredients in the proof: Lieb-Thirring inequality and localization.

3.1 Two dimensional Lieb-Thirring inequality

For completeness, we formulate here the necessary Lieb-Thirring inequality.

Theorem 3.2 *For any $\gamma \geq 1$ there exists a universal constant C_γ such that the following estimate is valid for the γ^{th} moment of the negative eigenvalues $\{e^{(2)}_m\}_{m=1,2\ldots}$ of the two dimensional operator $H^{(2)}(1, \mathbf{A}, V) = [\boldsymbol{\sigma}\cdot(\mathbf{p}+\mathbf{A})]^2 + V$*

$$\sum_m |e^{(2)}_m|^\gamma \leq C_\gamma\left(\|B\|\int [V]_-^\gamma + \int [V]_-^{\gamma+1}\right). \tag{3.7}$$

In particular we get an estimate for the sum of the eigenvalues (the case $\gamma = 1$).

Remark. Magnetic Lieb-Thirring inequalities for nonhomogeneous magnetic field were first proven in [E-1995]. There only the three dimensional case was discussed, though the corresponding two dimensional results follow analogously. In fact, [E-1995] mainly focuses on the constant direction case, which essentially requires a two dimensional analysis. The only difficulty stems from the fact that the exponent $\gamma = 1$ is critical in two dimensions, which has to be treated, using Fan's theorem, analogously to [LSY-III].

Later Sobolev [Sob-1996(1)], with a different approach, proved Theorem 3.2 in a more general setting which allows fairly general unbounded magnetic fields. We would like to point out, however, that Theorem 3.2, in the present form, i.e. for bounded field, has a simple proof which follows immediately from [E-1995] and [LSY-III]. Without going into the details, here we just outline the steps.

Steps of the proof. Since $B(x) > 0$, it is enough to consider the operator on the spin-down subspace and we can replace V by $-[V]_-$. Therefore we are left with the operator

$H_- := (\mathbf{p}+\mathbf{A})^2 - B - [V]_-$ acting on $L^2(\mathbf{R}^2)$. We introduce the Birman-Schwinger kernel $K_E := [V]_-^{1/2}((\mathbf{p}+\mathbf{A})^2 - B + E)^{-1}[V]_-^{1/2}$ (there is no need to add part of E to the potential, see the proof of Theorem 5.1. in [LSY-III]), and decompose it into a lower and an upper part, $K_E = K_{E,L}^< + K_{E,L}^>$ with

$$K_{E,L}^< := [V]_-^{1/2}\Pi_L((\mathbf{p}+\mathbf{A})^2 - B + E)^{-1}\Pi_L[V]_-^{1/2}$$

$$K_{E,L}^> := [V]_-^{1/2}(I-\Pi_L)((\mathbf{p}+\mathbf{A})^2 - B + E)^{-1}(I-\Pi_L)[V]_-^{1/2},$$

where Π_L is the spectral projection, onto $[0, L]$, of the operator $(\mathbf{p}+\mathbf{A})^2 - B$. Here we cannot separate the lowest Landau level from the rest of the spectrum, as the field is not constant. Nevertheless we artifically cut the spectrum at level L (to be chosen $2\|B\|$ later) by inserting the spectral projections Π_L, $I - \Pi_L$ (similarly to (26), (27) in [E-1995], but we now omit the kinetic energy in the third direction). Using the method of [LSY-III] one easily gets, as in (49) of [E-1995], the following bound on N_E, the number of eigenvalues of H_- below $-E$,

$$N_E \le \#\{\text{ev.'s of } \Pi_L[V]_-\Pi_L \text{ bigger than } E/4\} + 4\mathrm{Tr}[K_{E,L}^>]$$

Therefore, analogously to (50) in [E-1995], we have the following bound on the γ^{th} moment of the negative eigenvalues of H_-

$$\sum_i |e_i(H_-)|^\gamma \le 4^\gamma\gamma\mathrm{Tr}\left([V]_-^{\gamma/2}\Pi_L[V]_-^{\gamma/2}\right) + 4\gamma\int_0^\infty \mathrm{Tr}[K_{E,L}^>]E^{\gamma-1}\mathrm{d}E. \tag{3.8}$$

By the diamagnetic inequality

$$\Pi_L(x,x) \le e^{tL}e^{-tH_-}(x,x) \le e^{tL}e^{t\|B\|}e^{t\Delta}(x,x)$$

Making the particular choice of $L = 2\|B\|$ and $t = (3\|B\|)^{-1}$ we therefore see (as in Proposition 3.1. of [E-1995]) from the explicit formula for the heat kernel $e^{t\Delta}(x,x)$ that $\Pi_L(x,x) \le c\|B\|$. This yields the first term in the present Lieb-Thirring inequality (3.7).

The second term in (3.8) is estimated by using the obvious operator inequality

$$(I-\Pi_L)\left((\mathbf{p}+\mathbf{A})^2 - B + E\right)^{-1}(I-\Pi_L) \le \left(\frac{1}{2}[(\mathbf{p}+\mathbf{A})^2 - B] + \frac{L}{2} + E\right)^{-1},$$

and the pointwise inequality

$$\left(\frac{1}{2}[(\mathbf{p}+\mathbf{A})^2 - B] + \frac{L}{2} + E\right)^{-1}(x,x) \le \left(\frac{1}{2}\mathbf{p}^2 + E\right)^{-1}(x,x), \tag{3.9}$$

which is obtained by rewriting the resolvent kernel as the Laplace transform of the heat kernel then using the diamagnetic inequality and the monotonicity of the nonmagnetic heat kernel, i.e.

$$\begin{aligned}\exp\left[-t\left(\frac{1}{2}[(\mathbf{p}+\mathbf{A})^2-B]+\frac{L}{2}+E\right)\right](x,x) &\le \exp\left[-t\left(\frac{1}{2}[\mathbf{p}^2-B]+\frac{L}{2}+E\right)\right](x,x)\\ &\le \exp\left[-t\left(\frac{1}{2}\mathbf{p}^2+E\right)\right](x,x),\end{aligned}$$

since $B \le L/2$. From (3.9) one finishes the proof along the lines of [LSY-III] (the $\gamma > 1$ case requires obvious modification). □

3.2 Constant field approximation

In this section we rewrite the kinetic energy part of the Pauli operator in terms of a spatial average of operators with constant magnetic field plus error terms.

Define spin-up and spin-down projections $P_\pm := \frac{1}{2}(1 \pm \sigma_3)$. For each $u \in \mathbf{R}^2$ we define the function $\eta^u := \eta^{(0),u}\zeta$, where $\eta^{(0),u}(x) := c_{norm,u} w_u^{-1} e^{-w_u^{-2}x^2}$ (modulo the constant) is the magnetic localization function introduced in Lemma 2.2 and $\zeta \in C_0^\infty(\mathbf{R}^2)$, $\zeta \equiv 1$ on $B(0,\lambda(h)/2)$, $\operatorname{supp}\zeta \subset B(0,\lambda(h))$ and $|\nabla\zeta| \le c\lambda(h)^{-1}$. The scale w_u of $\eta^{(0),u}$ we choose to be

$$w_u := w_u(h,B) = \Lambda(h) B^\#(u)^{-1/2} h^{1/2},$$

where $\Lambda(h)$ is any function satisfying $\Lambda(h) \to \infty$ and $\Lambda(h)h^{1/2} \to 0$ as $h \to 0$. We have introduced the notation

$$B^\#(u) := \sup_{|x-u|<2L} \{B(x)\}.$$

We also require $\Lambda(h) \ge 4e$. The constant $c_{norm,u}$ is chosen such that $\int(\eta^u)^2 = 1$. In particular we have an estimate of the moments

$$\int \eta^u(v)^2 v^{2k} \mathrm{d}v \le c \min\{w_u, \lambda(h)\}^{2k} \tag{3.10}$$

for $k = 0, 1, 2$. It is easy to see that there exists a constant c such that we then also have

$$c^{-1} < \int_{\operatorname{supp}\zeta} (\eta^{(0),u})^2 < c.$$

Let $\eta^u_v(x) := \eta^u(x-v)$ and $\zeta_v(x) := \zeta(x-v)$. We shall choose $\lambda(h)$ to be any function such that $\lambda(h) < (8e^2)^{-1}L$, $\lambda(h) \to 0$ and $h\lambda(h)^{-1} \to 0$ as $h \to 0$.

As explained in the discussion after the magnetic localization Lemma (Lemma 2.2) we shall localize into regions where the maximum of the magnetic field strengths is bounded relative to the minimum. To do this we use that for all $\mathbf{B} \in \mathcal{C}_L$ we have $e^{-2} \leq B(x)/B(y) \leq e^2$ for all $|x-y| < 2L$. Thus from the definition of $B^\#(u)$ we conclude that

$$e^{-2}B^\#(u) \leq B(u) \leq B^\#(u). \tag{3.11}$$

With the above definition of w_u and the assumptions on $\lambda(h)$ and $\Lambda(h)$ we can now prove the main result of this subsection.

Proposition 3.3 *Given $\mathbf{B} \in \mathcal{C}_L$. There exists $\varepsilon(h) > 0$, depending only on h and L such that $\varepsilon(h) \to 0$ as $h \to 0$; and for each $u, v \in \mathbf{R}^2$ there exist a (phase) function $\phi_{u,v}$ in $C^1(\mathbf{R}^2)$ and constant magnetic fields $\hat{B}^\pm_{u,v}$ satisfying*

$$|B(u) - \hat{B}^\pm_{u,v}| \leq \varepsilon(h)B(u), \quad \textit{for all } v \textit{ with } |u-v| \leq 2\lambda(h) \tag{3.12}$$

such that the following is valid. For any $f \in C^\infty(\mathbf{R}^2, \mathbf{C}^2)$ and $g \in C_0^\infty(B(u, \lambda(h)), \mathbf{R})$ we have

$$\begin{aligned} &\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gf|^2 \\ &\geq \int\!\!\int \Big[(1-\varepsilon(h))|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}^+_{u,v})(e^{i\phi_{u,v}}\eta^u_v gf)(x)|^2 - \varepsilon(h)|(e^{i\phi_{u,v}}\eta^u_v gf)(x)|^2\Big]\,\mathrm{d}x\mathrm{d}v \end{aligned} \tag{3.13}$$

and for any fixed $v \in \mathbf{R}^2$

$$\begin{aligned} &\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})(e^{-i\phi_{u,v}}\eta^u_v gf)(x)|^2\mathrm{d}x \\ &\leq \int (\eta^u_v g)^2(x)\Big[(1+\varepsilon(h))|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}^-_{u,v})f(x)|^2 + \varepsilon(h)W_{u,v}(x)|f(x)|^2 \\ &\quad +\varepsilon(h)W^+_{u,v}(x)|P_+f(x)|^2\Big]\,\mathrm{d}x + ch^2\int|\nabla(\zeta_v g)(x)|^2|(\eta^{(0),u}_v f)(x)|^2\mathrm{d}x, \end{aligned} \tag{3.14}$$

where

$$W_{u,v}(x) = w_u^{-4}(x-v)^4 \quad \textit{and} \quad W^+_{u,v}(x) = cB^\#(u)hw_u^{-2}(x-v)^2.$$

and the vector potentials

$$\hat{\mathbf{A}}^\pm_{u,v}(x) := \frac{1}{2}\hat{B}^\pm_{u,v}\mathbf{n}\times x, \tag{3.15}$$

generate the constant magnetic fields $\hat{B}^\pm_{u,v}$

Proof.
Since u is fixed we shall omit the u subscript in the proof.

Step 1. Separation

The separation of the spin up and spin down subspaces is trivial since $P_\pm$ commutes with $\sigma_3 B$:

$$\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gf|^2 = \int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gP_- f|^2 + \int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gP_+ f|^2 \tag{3.16}$$

Step 2. Localization

We separately consider the kinetic energies of $P_\pm f =: f_\pm$. For the lower bound we write

$$\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gf_\pm|^2 = \int\int \eta_v(x)^2 |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})(gf_\pm)(x)|^2 \mathrm{d}x\,\mathrm{d}v. \tag{3.17}$$

Note that the above integrals can be restricted to $x, v \in B(u, 2\lambda(h))$. For all $x, v \in B(u, 2\lambda(h))$, we can, since $\lambda(h) < L$, approximate the magnetic field by the constant field $B_v := B(v)$, such that

$$|B(x) - B_v| \le |x-v| B^\#(u) L^{-1}. \tag{3.18}$$

We can then approximate $\mathbf{A}$ by $\mathbf{A}_v$, $\operatorname{rot}\mathbf{A}_v = B_v$, such that

$$|\mathbf{A}(x) - \mathbf{A}_v(x)| \le cB^\#(u)|x-v|^2 L^{-1} \tag{3.19}$$

(using the Poincaré formula, see (A.9) in the Appendix).

Using a Cauchy-Schwarz inequality, we have, for any $0 < \delta < 1$,

$$\begin{aligned}\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gf_\pm|^2 \;\; &\ge \;\; (1-\delta)\int\int \eta(x-v)^2 |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(gf_\pm)(x)|^2 \mathrm{d}x\,\mathrm{d}v \\ &\quad - c\delta^{-1}\int\int \eta(x-v)^2 |\mathbf{A}(x)-\mathbf{A}_v(x)|^2 |gf_\pm(x)|^2 \mathrm{d}x\,\mathrm{d}v.\end{aligned} \tag{3.20}$$

For the upper bound, we fix $v \in \mathbf{R}^2$, and we consider

$$\begin{aligned}\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})(e^{-i\phi_v}\eta_v g f_\pm)(x)|^2 \mathrm{d}x \;\; &\le \;\; (1+\delta)\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(e^{-i\phi_v}\eta_v g f_\pm)(x)|^2 \mathrm{d}x \\ &\quad + c\delta^{-1}\int \eta(x-v)^2 |\mathbf{A}(x)-\mathbf{A}_v(x)|^2 |gf_\pm(x)|^2 \mathrm{d}x\end{aligned} \tag{3.21}$$

where the phase function $\phi_v : \mathbf{R}^2 \to \mathbf{R}$ will be chosen below.

To control the error in (3.20), we shall apply the following estimate

$$\begin{aligned}\delta^{-1}\int \eta_v(x)^2|\mathbf{A}(x)-\mathbf{A}_v(x)|^2\mathrm{d}v &\leq c\delta^{-1}B^{\#}(u)^2L^{-2}\int \eta(v)^2v^4\,\mathrm{d}v\\ &\leq c\delta^{-1}B^{\#}(u)^2L^{-2}w^4,\end{aligned} \tag{3.22}$$

which is a consequence of (3.10) and (3.19).

We are left with considering the quadratic forms

$$\int\int \eta_v(x)^2|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(gf_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v = \int\int \eta_v(x)^2|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v-\nabla\phi_v)(e^{i\phi_v}gf_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v, \tag{3.23}$$

and

$$\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(e^{-i\phi_v}\eta_v gf_\pm)(x)|^2\mathrm{d}x = \int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v-\nabla\phi_v)(\eta_v gf_\pm)(x)|^2\mathrm{d}x \tag{3.24}$$

in (3.20) and (3.21), where we again introduced the gauge transformation ϕ_v. We choose ϕ_v such that

$$(\mathbf{A}_v-\nabla\phi_v)(x) = (1/2)B_v\mathbf{n}\times(x-v),$$

this determines ϕ_v (up to an irrelevant constant).

Step 3. Magnetic localization

Using the estimates in Lemma 2.2 and $k(x)=\zeta(x)(gf)(x+v)$ (and including a phase factor in the case of (2.3)), then shifting $x\to x-v$, we obtain from (3.23), (3.24), (3.10), and the estimates in the IMS Lemma (once for ζ_v and once for $g\zeta_v$) that

$$\begin{aligned}&\iint \eta_v(x)^2|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(gf_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v \qquad (3.25)\\ &\geq (1-\delta)\iint |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_v^+)(e^{i\phi_v}\eta_v gf_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v\\ &\quad -(1-\delta)h^2\iint |\nabla\zeta_v(x)|^2|(\eta_v^{(0)}gf_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v\\ &\quad -c\delta^{-1}h^2w^{-2}\iint |P_+(\eta_v gf_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v\end{aligned}$$

and for each v

$$\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(e^{-i\phi_v}\eta_v gf_\pm)(x)|^2\mathrm{d}x \tag{3.26}$$

$$
\begin{aligned}
&\leq\ (1+\delta)\int \eta(x-v)^2 g(x)^2 |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_v^-)f_\pm(x)|^2 \mathrm{d}x \\
&\quad + (1+\delta)h^2 \int |\nabla(g\zeta_v(x))|^2 |(\eta_v^{(0)} f_\pm)(x)|^2 \mathrm{d}x \\
&\quad + c\delta^{-1}h^2 w^{-4} \int (x-v)^2 |P_+(\eta_v g f_\pm)(x)|^2 \mathrm{d}x
\end{aligned}
$$

where the vector potentials $\hat{\mathbf{A}}_v^\pm$ defined in (3.15) generate the constant fields $\hat{B}_v^\pm := B_v \pm 4hw^{-2}$.

It follows from (3.11) that for $|u-v| \leq 2\lambda(h)(< 2L)$ we have

$$
\begin{aligned}
|\hat{B}_v^\pm - B(u)| &\leq |B(u)-B(v)| + 4hw^{-2} \\
&\leq 2B^\#(u)L^{-1}\lambda(h) + 4e^2 hw^{-2} B^\#(u)^{-1} B(u) \\
&\leq 2e^2(\lambda(h)L^{-1} + 2\Lambda(h)^{-2})B(u).
\end{aligned}
$$

In order to prove the (3.12) we must therefore show that we can choose $\varepsilon(h)$ such that

$$
2e^2(\lambda(h)L^{-1} + 2\Lambda(h)^{-2}) \leq \varepsilon(h). \tag{3.27}
$$

We also get the lower bound (recall that we assumed $\lambda(h) \leq (8e^2)^{-1}L$ and $\Lambda(h) \geq 4e$)

$$
\hat{B}_v^\pm \geq (1 - 2e^2(\lambda(h)L^{-1} + 2\Lambda(h)^{-2}))B(u) \geq (1/2)e^{-2}B^\#(u)
$$

for all v such that $|v-u| \leq 2\lambda(h)$.

Since for all $k \in C_0^\infty(\mathbf{R}^2, \mathbf{C}^2)$ we have

$$
\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_v^\pm)P_+k|^2 \geq h\hat{B}_v^\pm \int |P_+k|^2 \geq (1/2)e^{-2}hB^\#(u)\int |P_+k|^2, \tag{3.28}
$$

we see that the last error term in (3.25), which is nonzero only for f_+, can be absorbed into the kinetic energy if

$$
\begin{aligned}
R &:= c\delta^{-1}h^2 w^{-2}(B^\#(u)h)^{-1} \\
&= c\delta^{-1}\Lambda(h)^{-2} < 1.
\end{aligned} \tag{3.29}
$$

We put together (3.16), (3.20), (3.22), (3.23) and (3.25), the final lower bound of this section is

$$
\begin{aligned}
&\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gf|^2 \\
&\geq \int\!\!\int \Big[(1-\delta)^2 |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_v^+)(e^{i\phi_v}\eta_v g P_- f)(x)|^2 - (Q + c\lambda(h)^{-2}h^2)|(e^{i\phi_v}\eta_v g P_- f)(x)|^2 \\
&\quad + (1-\delta)^2(1-R)|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_v^+)(e^{i\phi_v}\eta_v g P_+ f)(x)|^2 \\
&\quad - (Q + c\lambda(h)^{-2}h^2)|(e^{i\phi_v}\eta_v g P_+ f)(x)|^2\Big] \mathrm{d}x\, \mathrm{d}v
\end{aligned} \tag{3.30}
$$

with

$$Q := c\delta^{-1}B^{\#}(u)^2L^{-2}w^4 = c\delta^{-1}L^{-2}\Lambda(h)^4h^2.$$

We also used $|\nabla\zeta| \le c\lambda(h)^{-1}$ and $\int_{\mathrm{supp}\,\zeta}(\eta^{(0)})^2 < c$.

For the upper bound we use (3.16) for $f = e^{-i\phi_v}\eta_v f$, then combine it with (3.21), (3.22), (3.24) and (3.26) to obtain

$$\begin{aligned}
&\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})(e^{-i\phi_v}\eta_v gf)(x)|^2\mathrm{d}x \\
\le\ &\int \eta_v(x)^2g(x)^2\Big[(1+\delta)^2|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_v^-)(P_-f)(x)|^2 + Qw^{-4}(x-v)^4|P_-f(x)|^2 \\
&\quad + (1+\delta)^2|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_v^-)(P_+f)(x)|^2 \\
&\quad + [Qw^{-4}(x-v)^4 + RB^{\#}(u)hw^{-2}(x-v)^2]|P_+f(x)|^2\Big]\mathrm{d}x \\
&\quad + ch^2\int |(\nabla(g\zeta_v))(x)|^2|\eta_v^{(0)}f(x)|^2\mathrm{d}x.
\end{aligned} \tag{3.31}$$

In order to prove the proposition we must show that we can choose $\varepsilon(h)$ such that $\varepsilon(h)\to 0$ as $h\to 0$ and such that (3.27) and the following requirements are met

$$R \le \varepsilon(h),\ Q + c\lambda(h)^{-2}h^2 \le \varepsilon(h),\ (1+\delta)^2 \le (1+\varepsilon(h)),\ (1-\delta)^2(1-R) \ge (1-\varepsilon(h)).$$

In particular this will imply (3.29). Since $\Lambda(h)\to\infty$, $\Lambda(h)h^{1/2}\to 0$, and $h\lambda(h)^{-1}\to 0$ as $h\to 0$ it is clear that we can find δ as a function of h such that all these requirements are simultaneously satisfied. This finishes the proof of Proposition 3.3. □

3.3 Lower bound

We shall here prove the one-sided bound

$$\limsup_{h\to 0}\frac{\sum_k e_k(H)}{E_{scl}^{(2)}(h,B,V)} \le 1, \tag{3.32}$$

uniformly for B in $\mathcal{C}_{C,L}$. Since $E_{scl}^{(2)}(h,B,V)\le 0$ this is a *lower* bound on the eigenvalue sum $\sum_k e_k(H)$.

For this bound, we can replace V by its negative part, $-[V]_-$.

We introduce a spherically symmetric function $0\le\theta_\lambda\in C_0^\infty(\mathbf{R}^2)$, which localizes at scale $\lambda(h)$, i.e. $\int_{\mathbf{R}^2}\theta_\lambda^2 = 1$, $\mathrm{supp}\,\theta_\lambda\subset B(0,\lambda(h))$ and $\int(\nabla\theta_\lambda)^2 = c\lambda(h)^{-2}$. Let $\theta_{u,\lambda}(x) = \theta_\lambda(x-u)$.

Instead of the original Pauli operator H, we are going to study

$$\tilde{H} := (1 - 2\delta_1)\Theta_\varrho[\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})]^2 \Theta_\varrho - [V\chi_\varrho]_- * (\theta_\lambda)^2, \tag{3.33}$$

where χ_ϱ is the characteristic function of the ball of radius ϱ centered at the origin in $\mathbf{R}^2$ and $\Theta_\varrho \in C_0^\infty(\mathbf{R}^2)$ satisfies $\Theta_\varrho(x) = 1$ on $B(0, \varrho + \lambda(h))$, vanishes outside $B(0, \varrho + 2\lambda(h))$ and $|\nabla\Theta_\varrho| \le c\lambda(h)^{-1}$. Here $0 < \delta_1 < 1/4$.

We then use the localization formula (2.1) to write

$$\langle f|\tilde{H}|f\rangle = \int \langle f\theta_{u,\lambda}|\tilde{H}_u|\theta_{u,\lambda} f\rangle \mathrm{d}u - c(1 - 2\delta_1)h^2\lambda(h)^{-2}\langle f|\Theta_\varrho^2|f\rangle,$$

for any $f \in C_0^\infty(\mathbf{R}^2, \mathbf{C}^2)$, where

$$\tilde{H}_u = (1 - 2\delta_1)\Theta_\varrho[\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})]^2\Theta_\varrho - [V\chi_\varrho(u)]_-.$$

The relation between the kinetic energy parts of H and $\tilde{H}$ is given by the pointwise inequality in Lemma 2.1

$$\langle f|[\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})]^2|f\rangle \ge (1 - \delta_1)\langle f|\Theta_\varrho[\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})]^2\Theta_\varrho|f\rangle - c\delta_1^{-1}h^2\langle f|(\nabla\Theta_\varrho)^2|f\rangle. \tag{3.34}$$

In order to merge the two error terms from these two localizations, we note that

$$c(1 - 2\delta_1)h^2\lambda^{-2}\Theta_\varrho^2 + c\delta^{-1}h^2(\nabla\Theta_\varrho)^2 \le c\delta_1^{-1}h^2\lambda^{-2}(\chi_{\rho+2\lambda})^2. \tag{3.35}$$

Therefore we may write, using (3.34), (3.35)

$$\langle f|H|f\rangle \ge \int \langle f\theta_{u,\lambda}|\tilde{H}_u|\theta_{u,\lambda} f\rangle \mathrm{d}u + \langle f|H_{err}|f\rangle, \tag{3.36}$$

where

$$H_{err} := \delta_1[\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})]^2 + W_{err} \tag{3.37}$$

with

$$W_{err} = [V\chi_\varrho]_- * (\theta_\lambda)^2 - [V]_- - c\delta_1^{-1}h^2\lambda^{-2}(\chi_{\rho+2\lambda})^2.$$

To estimate the effect of H_{err}, we use the 2D-magnetic Lieb-Thirring error functional. We have

$$\begin{aligned}
\mathcal{E}_{h,B}^{(2)}\left(\delta_1^{-1}W_{err}\right) &\le c\delta_1^{-2}\Big\{\mathcal{E}_{h,B}^{(2)}\left([V\chi_\varrho]_- * (\theta_\lambda)^2 - [V]_- * (\theta_\lambda)^2\right) \\
&\quad + \mathcal{E}_{h,B}^{(2)}\left([V]_- * (\theta_\lambda)^2 - [V]_-\right) + \mathcal{E}_{h,B}^{(2)}\left(c\delta_1^{-1}h^2\lambda^{-2}(\chi_{\rho+2\lambda})^2\right)\Big\} \\
&\le c\delta_1^{-2}\Big\{\mathcal{E}_{h,B}^{(2)}\left([V\chi_\varrho]_- - [V]_-\right) \\
&\quad + \mathcal{E}_{h.B}^{(2)}\left([V]_- * (\theta_\lambda)^2 - [V]_-\right) + \mathcal{E}_{h,B}^{(2)}\left(c\delta_1^{-1}h^2\lambda^{-2}(\chi_{\rho+2\lambda})^2\right)\Big\},
\end{aligned}$$

where we used Jensen's inequality. Note that Jensen also implies that

$$\mathcal{E}^{(2)}_{h,B}\left([V]_- * (\theta_\lambda)^2 - [V]_-\right) \;\leq\; \int \mathcal{E}^{(2)}_{h,B}([V]_- - [V(\cdot - y)]_-)\theta_\lambda(y)^2 dy.$$

The integrand vanishes unless $|y| \leq \lambda(h)$. Since $\lambda(h) \to 0$ as $h \to 0$ it follows, from (3.2–3.2) and (3.6), that this term tends to zero relative to $|E^{(2)}_{scl}(h, B, V)|$ as $h \to 0$. If we also use condition (3.4) we see that

$$\begin{aligned}\frac{\mathcal{E}^{(2)}_{h,B}\left(\delta_1^{-1} W_{err}\right)}{|E^{(2)}_{scl}(h, B, V)|} \;&\leq\; c\delta_1^{-2} C_-(B, V)^{-1}\Big(\varepsilon_2(V, \varrho) + \sup_{|y|\leq\lambda(h)} \varepsilon_1(V, y) \\ &\quad + \left(\lambda(h)^{-2}h^2 + (\lambda(h)^{-2}h^2)^2\right)(\varrho + 2\lambda(h))^2\Big).\end{aligned}$$

Let $f_1, f_2, \dots f_N$ be a family of compactly supported smooth orthonormal spinors and we want to estimate

$$\sum_{j=1}^N \langle f_j|H|f_j\rangle \geq \sum_{j=1}^N \int \langle f_j\theta_{u,\lambda}|\tilde{H}_u|\theta_{u,\lambda} f_j\rangle \mathrm{d}u + \sum_{j=1}^N \langle f_j|H_{err}|f_j\rangle \tag{3.38}$$

uniformly in N.

By the Lieb-Thirring inequality we have

$$\sum_{j=1}^N \langle f_j|H_{err}|f_j\rangle \geq -c\delta_1 \mathcal{E}^{(2)}_{h,B}\left(\delta_1^{-1} W_{err}\right) \tag{3.39}$$

which shall be controlled using (3.38).

For the main term, we use

$$\sum_{j=1}^N \langle f_j\theta_{u,\lambda}|\tilde{H}_u|\theta_{u,\lambda} f_j\rangle \tag{3.40}$$

$$\geq \sum_{j=1}^N \int \left[(1-\delta_1)|\boldsymbol{\sigma}\cdot(h\mathbf{p} + \mathbf{A})(\Theta_\varrho\theta_{u,\lambda} f_j)(x)|^2 - \int \left\{[V\chi_\varrho(u)]_- |(\theta_{u,\lambda}\eta^u_v\Theta_\varrho f_j)(x)|^2\right\} \mathrm{d}v\right] \mathrm{d}x.$$

For each $\nu \in \mathbf{N}$ and $u, v \in \mathbf{R}^2$ we define the following positive operators via their kernel

$$\Pi^\pm(\nu, u, v)(x, y) \tag{3.41}$$

$$:= \theta_\lambda(x-u)\eta^u(x-v)e^{-i\phi_{u,v}(x)}\Pi^{\nu,\pm}_{u,v}(x, y)e^{i\phi_{u,v}(y)}\eta^u(y-v)\theta_\lambda(y-u)$$

where $\Pi^{\nu,\pm}_{u,v}$ is the ν^{th} Landau level projection corresponding to the constant field $\hat{\mathbf{B}}^{\pm}_{u,v}$ and to the gauge $\hat{\mathbf{A}}^{\pm}_{u,v}$, obtained in Proposition 3.3. Note that $\Pi^{\pm}(\nu,u,v)=0$ unless $|v-u|\le 2\lambda$. In this section we shall use $\Pi^{+}(\nu,u,v)$ only, the other operator will be useful in Section 3.4.

Since $\theta_{u,\lambda}$ has support in $B(u,\lambda(h))$ we see from (3.13) that

$$
\begin{aligned}
&\sum_j \langle f_j\theta_{u,\lambda}|\tilde{H}_u|\theta_{u,\lambda}f_j\rangle \qquad (3.42)\\
\geq\ & \sum_j \iint \Big[(1-\delta_1)(1-\varepsilon(h))|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}^{+}_{u,v})(e^{i\phi_{u,v}}\eta^u_v\Theta_\varrho\theta_{u,\lambda}f_j)(x)|^2\\
&\quad -([V(u)]_- +\varepsilon(h))|(e^{i\phi_{u,v}}\eta^u_v\Theta_\varrho\theta_{u,\lambda}f_j)(x)|^2\Big]\mathrm{d}x\,\mathrm{d}v\\
=\ & (1-\delta_2)\sum_j\sum_{\nu=0}^{\infty}\int\Big\{2\nu h\hat{B}^{+}_{u,v}-(1-\delta_2)^{-1}([V(u)]_- +\varepsilon(h))\Big\}\\
&\quad\times\langle f_j|\Theta_\varrho\Pi^{+}(\nu,u,v)\Theta_\varrho|f_j\rangle\mathrm{d}v.
\end{aligned}
$$

Here

$$(1-\delta_2):=(1-\delta_1)(1-\varepsilon(h)). \qquad (3.43)$$

Observe now that for each $\nu\in\mathbf{N}$ we have from (3.12) that

$$\Pi^{\nu,\pm}_{u,v}(x,x)=d_\nu h^{-1}\hat{B}^{\pm}_{u,v}\le d_\nu h^{-1}(1+\varepsilon(h))B(u). \qquad (3.44)$$

if $|u-v|\le 2\lambda(h)$.

Therefore

$$
\begin{aligned}
&\int\sum_j\langle f_j|\Theta_\varrho\Pi^{+}(\nu,u,v)\Theta_\varrho|f_j\rangle\mathrm{d}v\\
&\le\int\mathrm{Tr}[\Pi^{+}(\nu,u,v)]\mathrm{d}v\le d_\nu h^{-1}(1+\varepsilon(h))B(u), \qquad (3.45)
\end{aligned}
$$

where d_ν was defined in (1.6). In the last estimate above we used (3.12).

Thus, combining (3.45) with (3.40), (3.42), both the upper and lower bounds of (3.12), and the definition (1.6) of $P^{(2)}$, we have

$$
\begin{aligned}
\sum_{j=1}^{N}\int\langle f_j\theta_{u,\lambda}|\tilde{H}_u|\theta_{u,\lambda}f_j\rangle\mathrm{d}u\ &\geq\ -h^{-2}(1-\varepsilon(h)^2)(1-\delta_2)\int_{|u|<\varrho+3\lambda}P^{(2)}\left(hB(u),\frac{[V(u)]_- +\varepsilon(h)}{1-\delta_3}\right)\mathrm{d}u\\
&\geq\ -h^{-2}\int_{|u|<\varrho+3\lambda}P^{(2)}\left(hB(u),\frac{[V(u)]_- +\varepsilon(h)}{1-\delta_3}\right)\mathrm{d}u \qquad (3.46)
\end{aligned}
$$

independently of N, with

$$(1-\delta_3) := (1-\delta_2)(1-\varepsilon(h)) = (1-\delta_1)(1-\varepsilon(h))^2. \tag{3.47}$$

We used that the integral on the left side of (3.46) vanishes unless $|u| \leq \varrho + 3\lambda(h)$.

Putting together (3.38), (3.39) and (3.46), we see that

$$\sum_j \langle f_j|H|f_j\rangle \geq -h^{-2}\int_{|u|<\varrho+3\lambda} P^{(2)}\left(hB(u), \frac{[V(u)]_- + \varepsilon(h)}{1-\delta_3}\right) \mathrm{d}u - c\delta_1 \mathcal{E}^{(2)}_{h,B}\left(\delta_1^{-1}W_{err}\right). \tag{3.48}$$

Clearly

$$0 \leq \partial_2 P(B,W) := \frac{\partial}{\partial W} P(B,W) \leq cB + cW. \tag{3.49}$$

Therefore, using $0 \leq P(B, W+V) - P(B,W) \leq V\partial_2 P(B, W+V)$ for any $V \geq 0$, and (1.10), we obtain if $\varepsilon(h) \leq 1$ and $\delta_3 \leq 1/2$

$$\begin{aligned}
0 &\leq h^{-2}\int_{|u|<\varrho+3\lambda}\left[P^{(2)}\left(hB(u), \frac{[V(u)]_- + \varepsilon(h)}{1-\delta_3}\right) - P^{(2)}(hB(u),[V(u)]_-)\right]\mathrm{d}u \\
&\leq ch^{-2}\int_{|u|<\varrho+3\lambda}(\varepsilon(h) + \delta_3[V(u)]_-)\left[\|B\|h + ([V(u)]_- + \varepsilon(h))\right]\mathrm{d}u \\
&\leq c\left[\varepsilon(h)(\varrho+3\lambda(h))^2[\|B\|h^{-1} + h^{-2}] + (\varepsilon(h)+\delta_3)\mathcal{E}^{(2)}_{h,B}([V]_-)\right].
\end{aligned} \tag{3.50}$$

Here we also used the simple estimate

$$h^{-2}\varepsilon(h)\int_{|u|<\varrho+3\lambda}[V(u)]_- \mathrm{d}u \leq ch^{-2}\varepsilon(h)(\varrho+3\lambda)^2 + c\varepsilon(h)h^{-2}\int_{|u|<\varrho+3\lambda}[V(u)]_-^2\mathrm{d}u. \tag{3.51}$$

Using (1.5), (3.48), (3.50), (3.2–3.5), (3.38)

$$\begin{aligned}
\frac{\sum_j\langle f_j|H|f_j\rangle}{E^{(2)}_{scl}(h,B,V)} &\leq 1 + cC_-(B,V)^{-1}\Big[\varepsilon(h)(\varrho+3\lambda(h))^2 + (\varepsilon(h)+\delta_3)C_+(V) \\
&\quad + \delta_1^{-2}\Big(\varepsilon_2(V,\varrho) + \sup_{|y|\leq\lambda(h)}\varepsilon_1(V,y) + \left(\lambda(h)^{-2}h^2 + (\lambda(h)^{-2}h^2)^2\right)(\varrho + 2\lambda(h))^2\Big)\Big].
\end{aligned} \tag{3.52}$$

This estimate is valid independently of N, the ratio of the sum of the negative eigenvalues $\sum_k e_k(H)$ of $H = H^{(2)}(h,\mathbf{A},V)$, to $E^{(2)}_{scl}(h,B,V)$ is therefore estimated above by the right side of (3.52).

It is clear, using (3.4–3.5) and the fact that $B \in \mathcal{C}_{C,L}(V)$ implies $C_-(B,V) \geq C$, that we can choose δ_1 and ϱ as functions of h such that the error in (3.52) tends 0 as $h \to 0$. This yields (3.32).

3.4 Upper bound

In this section we shall show the opposite asymptotic bound

$$\liminf_{h\to 0} \frac{\sum_k e_k(H)}{E^{(2)}_{scl}(h,B,V)} \geq 1, \tag{3.53}$$

uniformly for B in $\mathcal{C}_{C,L}$. For each $\nu \in \mathbf{N}$, $v \in \mathbf{R}^2$ we define the following coherent state operators via their kernel

$$\Pi(\nu,u,v)(x,y) := \theta_\lambda(x-u)\eta^u(x-v)e^{-i\phi_{u,v}(x)}\Pi^{\nu,-}_{u,v}(x,y)e^{i\phi_{u,v}(y)}\eta^u(y-v)\theta_\lambda(y-u)$$

(we used the notations from Section 4.1) and the Landau level projection $\Pi^{\nu,-}_{u,v}$ corresponding to the constant field $\hat{B}^-_{u,v}$ and to the gauge $\hat{\mathbf{A}}^-_{u,v}$. Note that $\Pi(\nu,u,v)=0$ unless $|v-u|<2\lambda(h)$.

The following relations are immediate to check

$$\sum_{\nu=0}^{\infty}\iint \Pi(\nu,u,v)\mathrm{d}v\mathrm{d}u = 1_{L^2(\mathbf{R}^2,\mathbf{C}^2)}, \tag{3.54}$$

$$\mathrm{Tr}\Pi(\nu,u,v) = d_\nu h^{-1}\hat{B}^-_{u,v}\Phi(u,v) \tag{3.55}$$

with

$$\Phi(u,v) = \int \theta_\lambda(x-u)^2\eta^u(x-v)^2\mathrm{d}x$$

and from (3.12)

$$\int \mathrm{Tr}[V\Pi(\nu,u,v)]\mathrm{d}v \leq d_\nu h^{-1}B(u)\left(\{(1+\varepsilon(h))[V]_+ - (1-\varepsilon(h))[V]_-\} * (\theta_\lambda)^2\right)(u). \tag{3.56}$$

In order to calculate the kinetic energy we first note that since $\Pi^{\nu,-}_{u,v}$ is a projection we can write $\Pi(\nu,u,v)=\Xi(\nu,u,v)\Xi(\nu,u,v)^*$, where $\Xi(\nu,u,v)$ has the integral kernel

$$\Xi(\nu,u,v)(x,y) = \theta_\lambda(x-u)\eta^u(x-v)e^{-i\phi_{u,v}(x)}\Pi^{\nu,-}_{u,v}(x,y).$$

We therefore have

$$\begin{aligned}\int \mathrm{Tr}\left([\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})]^2\Pi(\nu,u,v)\right)\mathrm{d}v &= \int \mathrm{Tr}\left[(\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})\Xi(\nu,u,v))^*(\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})\Xi(\nu,u,v))\right]\mathrm{d}v \\ &= \iiint \left|[\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})\Xi(\nu,u,v)](x,y)\right|^2\mathrm{d}x\mathrm{d}y\mathrm{d}v \end{aligned} \tag{3.57}$$

To estimate this we use (3.14) for each fixed y with $f(x) = \Pi_{u,v}^{\nu,-}(x,y)$ and $g = \theta_{\lambda,u}$. We begin by examining the error terms. From the spectral denisty expression (3.44), the moment estimate (3.10), the field comparison (3.12) and the normalization of $\theta_{\lambda,u}$ we find

$$\begin{aligned}\int (\eta_v^u\theta_{\lambda,u})^2(x)W_{u,v}(x)|\Pi_{u,v}^{\nu,-}(x,y)|^2\mathrm{d}y\mathrm{d}x\mathrm{d}v &= \int w_u^{-4}(x-v)^4(\eta_v^u(x))^2\theta_{\lambda,u}^2(x)|\Pi_{u,v}^{\nu,-}(x,x)|\mathrm{d}x\mathrm{d}v \\ &\leq cd_\nu h^{-1}(1+\varepsilon(h))B(u), \qquad (3.58)\end{aligned}$$

where the first identity follows since $\Pi_{u,v}^{\nu,-}$ is a projection.

Since P_+ commutes with $\Pi_{u,v}^{\nu,-}$ we have $[P_+\Pi_{u,v}^{\nu,-}P_+](x,x) \leq \Pi_{u,v}^{\nu,-}(x,x)$. For the second error term we therefore get in the same manner as above that

$$\begin{aligned}\int (\eta_v^u\theta_{\lambda,u})^2(x)W_{u,v}^+(x)|P_+\Pi_{u,v}^{\nu,-}(x,y)|^2\mathrm{d}y\mathrm{d}x\mathrm{d}v &\leq c\nu(hB^\#(u))d_\nu h^{-1}(1+\varepsilon(h))B(u) \\ &\leq c\nu(hB(u))d_\nu h^{-1}(1+\varepsilon(h))B(u). \ (3.59)\end{aligned}$$

In the last line we used (3.11) to estimate $B^\#(u)$ in terms of $B(u)$. Note that we inserted a ν in the estimate. This is clearly allowed for $\nu \geq 1$. For $\nu = 0$ it follows simply because $P_+\Pi_{u,v}^{0,-} = 0$ (i.e., the lowest Landau level contains only spinors with spin down).

For the last error term in (3.14) we just have to recall that $\int_{\mathrm{supp}\,\zeta}(\eta^{(0),u})^2 < c$ to conclude that

$$\int |\nabla(\zeta_v\theta_{\lambda,u})(x)|^2|(\eta_v^{(0),u})(x)\Pi_{u,v}^{\nu,-}(x,y)|^2\mathrm{d}x\mathrm{d}y\mathrm{d}v \leq c\lambda(h)^{-2}d_\nu h^{-1}(1+\varepsilon(h))B(u). \qquad (3.60)$$

If we insert (3.57–3.60) into (3.14) we arrive at

$$\begin{aligned}&\int \mathrm{Tr}\left([\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})]^2\Pi(\nu,u,v)\right)\mathrm{d}v \\ &\leq\ (1+\varepsilon(h))\int\!\!\int\!\!\int \eta_v^u(x)^2\theta_{\lambda,u}(x)^2\left|\left[\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_{u,v}^-)\Pi_{u,v}^{\nu,-}\right](x,y)\right|^2\mathrm{d}x\mathrm{d}y\mathrm{d}v \\ &\qquad + cd_\nu h^{-1}(1+\varepsilon(h))B(u)\Big[\varepsilon(h)+\nu(hB(u))\varepsilon(h)+h^2\lambda(h)^{-2}\Big].\end{aligned}$$

To compute the first term we observe that since $\Pi_{u,v}^{\nu,-}$ is an eigenprojection for $\left[\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_{u,v}^-)\right]^2$ it commutes with $\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_{u,v}^-)$. Hence, using again the spectral density expression (3.44), we get

$$\begin{aligned}&\int \left|\left[\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_{u,v}^-)\Pi_{u,v}^{\nu,-}\right](x,y)\right|^2\mathrm{d}y = \left[\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_{u,v}^-)\Pi_{u,v}^{\nu,-}\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_{u,v}^-)\right](x,x) \\ &= \left[\left[\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_{u,v}^-)\right]^2\Pi_{u,v}^{\nu,-}\right](x,x) = 2\nu h\hat{B}_{u,v}^-\Pi_{u,v}^{\nu,-}(x,x) = 2\nu h\hat{B}_{u,v}^-(d_\nu h^{-1}\hat{B}_{u,v}^-).\end{aligned}$$

If we insert this identity into the estimate above we conclude, again using the field comparison (3.12) that

$$\begin{aligned}
&\int \mathrm{Tr}\left([\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})]^2 \Pi(\nu,u,v)\right) \mathrm{d}v \\
&\quad \le\; d_\nu h^{-1}(1+\varepsilon(h))B(u)\Big[(1+c\varepsilon(h))2\nu h B(u) + c\varepsilon(h) + ch^2\lambda(h)^{-2}\Big]. \qquad (3.61)
\end{aligned}$$

Fix $\varrho > 0$ for the moment, and let $M(\nu,u)$ be the characteristic function of the set

$$\{(\nu,u) \,:\, 2\nu h B(u) < [V(u)]_-, |u| \le \varrho\}.$$

Note that $M(\nu,u) = 0$ if $V(u) \ge 0$. Define the operator γ on $L^2(\mathbf{R}^2,\mathbf{C}^2)$ by

$$\gamma = \sum_{\nu=0}^{\infty} \int M(\nu,u)\Pi(\nu,u,v)\mathrm{d}v\mathrm{d}u,$$

which satisfies the density matrix condition $0 \le \gamma \le 1_{L^2(\mathbf{R}^2,\mathbf{C}^2)}$ by (3.54).

From the variational principle, (3.56) and (3.61) we have (recall that $\lambda(h)^{-2}h^2 \le \varepsilon(h)$)

$$\begin{aligned}
\sum_k e_k(H) \;&\le\; \mathrm{Tr}[H\gamma] \qquad (3.62)\\
&\le\; \sum_\nu \int M(\nu,u) d_\nu h^{-1}(1+\varepsilon(h))B(u)\Bigg\{ \Big[(1+c\varepsilon(h))2\nu h B(u) + c\varepsilon(h)\Big] \\
&\quad + \left(\left\{ [V]_+ - \frac{1-\varepsilon(h)}{1+\varepsilon(h)}[V]_- \right\} * (\theta_\lambda)^2 \right)(u) \Bigg\} \mathrm{d}u.
\end{aligned}$$

Moreover, for u such that $V(u) < 0$ and $|u| \le \varrho$ we have

$$\sum_\nu d_\nu h^{-1} B(u) M(\nu,u) = h^{-2}\partial_2 P^{(2)}(hB(u),[V(u)]_-)$$

therefore we can continue the estimate (3.62)

$$\begin{aligned}
\sum_k e_k(H) \;&\le\; -(1+c\varepsilon(h))^2 h^{-2} \int_{|u|\le\varrho} P^{(2)}(hB(u),[V(u)]_-)\mathrm{d}u + \mathrm{Error}(h) \\
&\le\; -h^{-2}\int_{|u|\le\varrho} P^{(2)}(hB(u),[V(u)]_-)\mathrm{d}u + \mathrm{Error}(h)
\end{aligned}$$

with

$$\begin{aligned}
\mathrm{Error}(h) \;&:=\; h^{-2} \int_{\substack{|u|\le\varrho \\ V(u)<0}} (1+\varepsilon(h))\partial_2 P^{(2)}\left(hB(u),[V(u)]_-\right) \qquad (3.63)\\
&\quad \times \left((1+c\varepsilon(h))[V(u)]_- + \left(\left\{ [V]_+ - \frac{1-\varepsilon(h)}{1+\varepsilon(h)}[V]_- \right\} * (\theta_\lambda)^2 \right)(u) + c\varepsilon(h) \right) \mathrm{d}u.
\end{aligned}$$

Therefore, using (3.49), we have if ($\varepsilon(h) < 1$)

$$\begin{aligned}
\mathrm{Error}(h) &\leq h^{-2}\int_{|u|\leq\varrho} c(h\|B\| + [V(u)]_-)\Big[\Big|[V]_- - [V]_- * (\theta_\lambda)^2\Big|(u) \\
&\quad + \Big|[V]_+ * (\theta_\lambda)^2 - [V]_+\Big|(u) + \varepsilon(h)[V(u)]_- + \varepsilon(h)\Big]\mathrm{d}u \\
&\leq c\Big\{\varepsilon(h)[h^{-1}\|B\| + h^{-2}]\varrho^2 + \varepsilon(h)\mathcal{E}^{(2)}_{h,B}([V]_-) \\
&\quad + \sum_{\pm}\Big(\mathcal{E}^{(2)}_{h,B}\Big([V]_\pm - [V]_\pm * (\theta_\lambda)^2\Big) + \mathcal{E}^{(2)}_{h,B}\Big([V]_\pm - [V]_\pm * (\theta_\lambda)^2\Big)^{1/2}\mathcal{E}^{(2)}_{h,B}([V]_-)^{1/2}\Big)\Big\}
\end{aligned} \tag{3.64}$$

where we used also used (3.51) as in the lower bound.

Considering (3.2–3.5), and (3.3) we get, using Jensen's inequality as in the lower bound, that for fixed ϱ

$$\frac{\mathrm{Error}(h)}{|E^{(2)}_{scl}(h,B,V)|} \to 0$$

uniformly for B in $\mathcal{C}_{C,L}(V)$ as $h \to 0$. Hence for all $\varrho > 0$ we have

$$\liminf_{h\to 0}\frac{\sum_k e_k(H)}{E^{(2)}_{scl}(h,B,V)} \geq \left(1 - \limsup_{h\to 0}\frac{h^{-2}\int_{|u|\geq\varrho}P^{(2)}(hB(u),[V(u)]_-)\mathrm{d}u}{|E^{(2)}_{scl}(h,B,V)|}\right). \tag{3.65}$$

By (3.4) and $C_-(B,V) \geq C$,

$$h^{-2}\int_{|u|\geq\varrho}P^{(2)}(hB(u),[V(u)]_-)\mathrm{d}u = h^{-2}\int P^{(2)}(hB(u),[V(1-\chi_\varrho)(u)]_-)\mathrm{d}u$$

$$\leq \mathcal{E}^{(2)}_{h,B}([V - V\chi_\varrho]_-) = \mathcal{E}^{(2)}_{h,B}([V\chi_\varrho]_- - [V]_-) \leq \varepsilon_2(V,\varrho)|E^{(2)}_{scl}(h,B,V)|/C_-(B,V)$$

we obtain the final result (3.53). $\square$

4 Semiclassics in three dimensions

In the introduction we stated our semiclassical result in Theorem 1.2 for fixed potential and a simple one parameter family of magnetic fields but we shall in fact prove a slightly stronger result, which includes more general family of magnetic fields and which allows the potential to depend mildly on $\mathbf{B}$ and h.

We always take $h \to 0$, and we also would like to allow $\|\mathbf{B}\| \to \infty$ simultaneously (otherwise the leading term in the semiclassical limit becomes independent of the magnetic field), but always with the restrictions that $hL(\mathbf{B})^{-1} \to 0$, $hl(\mathbf{B})^{-1} \to 0$ and $h^3\|\mathbf{B}\|l(\mathbf{B})^{-2} \to 0$. The first two conditions are natural, as they require that the magnetic field should not change considerably on the usual semiclassical distance scale h. The role of the third condition was explained in the Introduction after Theorem 1.2. This means that instead of a single magnetic field, we consider a one-parameter family of magnetic fields, $\mathbf{B}_\tau$, parametrized by a real parameter $\tau \in (0,1)$. We also allow the potential $V = V_\tau$ and the semiclassical parameter $h = h_\tau$ depend on τ in such a way that $h_\tau < 1$, $\lim_{\tau\to 0} h_\tau = 0$, i.e. we consider a triple of one-parameter family of data $(h_\tau, \mathbf{B}_\tau, V_\tau)$. Let $\mu(h, \mathbf{B}) := h \max\{L(\mathbf{B})^{-1}, l(\mathbf{B})^{-1}\}$, $\kappa(h,\mathbf{B}) := h^3\|\mathbf{B}\|l(\mathbf{B})^{-2}$ and let $\mu(\tau) := \mu(h_\tau, \mathbf{B}_\tau)$, $\kappa(\tau) := \kappa(h_\tau, \mathbf{B}_\tau)$ for shortness, then we require that these functions go to zero as $\tau \to 0$.

To describe how the potential is allowed to depend on $\mathbf{B}$ and h (via τ), we introduce the **full 3D magnetic Lieb-Thirring error functional**

$$\mathcal{F}_{h,\mathbf{B}}(V) := h^{-3}\int |V|^{5/2} + (h^{-1}\|\mathbf{B}\| + d(h,\mathbf{B})^{-2})h^{-1}\int |V|^{3/2} \tag{4.1}$$

$$+(h^{-1}\|\mathbf{B}\| + d(h,\mathbf{B})^{-2})d(h,\mathbf{B})^{-1}\int |V| + (h^{-1}\|\mathbf{B}\| + d(h,\mathbf{B})^{-2})\int |\nabla V|,$$

where

$$d(h,\mathbf{B}) := \min\left\{h^{1/4}\|\mathbf{B}\|^{-1/4}l(\mathbf{B})^{1/2}, L(\mathbf{B}), l(\mathbf{B})\right\},$$

and we also introduce the **reduced 3D magnetic Lieb-Thirring error functional**

$$\mathcal{E}_{h,\mathbf{B}}(V) := h^{-3}\int |V|^{5/2} + \|\mathbf{B}\|h^{-2}\int |V|^{3/2} \tag{4.2}$$

(in Section 4 all the integrals are on $\mathbf{R}^3$ unless otherwise specified). Recall that in the case of a large magnetic field (which is our main concern), namely if $\|\mathbf{B}\| \geq \max\{L(\mathbf{B})^{-2}, l(\mathbf{B})^{-2}\}$, $\mathcal{F}_{h,\mathbf{B}}$ is of order

$$h^{-3}\int |V|^{5/2} + \|B\|h^{-2}\int |V|^{3/2} + \|B\|^{5/4}h^{-5/4}l^{-1/2}\int |V| + \|B\|h^{-1}\int (|\nabla V| + |V|)\,. \tag{4.3}$$

With this notation, the Lieb-Thirring inequality in [ES-I] states that the sum of the negative eigenvalues $e_1(H), e_2(H), \ldots$ of the operator $H = H(h, \mathbf{A}, V)$ satisfies the bound

$$\sum_k |e_k(H)| \leq c\mathcal{F}_{h,\mathbf{B}}([V]_-) \leq c\mathcal{F}_{h,\mathbf{B}}(V)$$

for any magnetic field $\mathbf{B}$ satisfying (1.7), (1.8), (1.9).

We may now introduce that set of conditions on the triple $(h_\tau, \mathbf{B}_\tau, V_\tau)$ which involve the potential. We require the following

$$C_- := \liminf_{\tau\to 0} C_-(\tau) := \liminf_{\tau\to 0} \frac{|E_{scl}(h_\tau, \mathbf{B}_\tau, V_\tau)|}{\|\mathbf{B}_\tau\| h_\tau^{-2} + h_\tau^{-3}} > 0, \tag{4.4}$$

$$C_+ := \limsup_{\tau\to 0} C_+(\tau) := \limsup_{\tau\to 0} \frac{\mathcal{E}_{h_\tau, \mathbf{B}_\tau,}([V_\tau]_-)}{\|\mathbf{B}_\tau\| h_\tau^{-2} + h_\tau^{-3}} < \infty, \tag{4.5}$$

and

$$\lim_{\tau, r\to 0} \sup_{\sigma\le\tau} \varepsilon_\pm(\sigma, r) = 0, \qquad \lim_{\varrho\to\infty} \sup_{\tau\in(0,1)} \varepsilon_2(\tau, \varrho) = 0 \tag{4.6}$$

where

$$\varepsilon_+(\tau, r) := \sup_{|y|\le r} \frac{\mathcal{E}_{h_\tau, \mathbf{B}_\tau}([V_\tau]_+ - [V_\tau(\cdot - y)]_+)}{\|\mathbf{B}_\tau\| h_\tau^{-2} + h_\tau^{-3}}, \tag{4.7}$$

$$\varepsilon_-(\tau, r) := \sup_{|y|\le r} \frac{\mathcal{F}_{h_\tau, \mathbf{B}_\tau}([V_\tau]_- - [V_\tau(\cdot - y)]_-)}{\|\mathbf{B}_\tau\| h_\tau^{-2} + h_\tau^{-3}}, \tag{4.8}$$

$$\varepsilon_2(\tau, \varrho) := \frac{\mathcal{F}_{h_\tau, \mathbf{B}_\tau}([V_\tau \chi_\varrho]_- - [V_\tau]_-)}{\|\mathbf{B}_\tau\| h_\tau^{-2} + h_\tau^{-3}} \tag{4.9}$$

and here χ_ϱ denotes the characteristic function of the ball of radius ϱ centered at the origin. Note that (4.4), (4.5) and $P(B, W) \le c(BW^{3/2} + W^{5/2})$ imply that

$$c \le \frac{\mathcal{E}_{h_\tau, \mathbf{B}_\tau}(V)}{|E_{scl}(h_\tau, \mathbf{B}_\tau, V_\tau)|} \le \frac{C_+(\tau)}{C_-(\tau)}. \tag{4.10}$$

Remark. If V is independent of τ (i.e. of $\mathbf{B}_\tau$ and h_τ), then the conditions follow simply from $V \in L^{5/2} \cap L^{3/2}$, $[V]_- \in W^{1,1}$, $|E_{scl}(h\tau, \mathbf{B}_\tau, V)| \ge C(\|\mathbf{B}_\tau\| h_\tau^{-2} + h_\tau^{-3})$ and $\mu(\tau), \kappa(\tau) \to 0$ (use that $d(h, \mathbf{B})^{-2} \le h^{-2}(\mu^2(h, \mathbf{B}) + \kappa(h, \mathbf{B})^{1/2})$).

Theorem 4.1 (3D Semiclassics) *Let $e_1(H_\tau), e_2(H_\tau), \dots$ denote the negative eigenvalues of the operator $H_\tau = H(h_\tau, \mathbf{A}_\tau, V_\tau)$ in (1.1). Assume that the triple of the physical data $(h_\tau, \mathbf{B}_\tau, V_\tau)$ is such that $\mu(\tau) = h_\tau \max\{L(\mathbf{B}_\tau)^{-1}, l(\mathbf{B}_\tau)^{-1}\} \to 0$, $\kappa(\tau) = h_\tau^3 \|\mathbf{B}_\tau\| l(\mathbf{B}_\tau)^{-2} \to 0$ (as $\tau \to 0$), and it satisfies (4.4–4.6) then*

$$\lim_{\tau\to 0} \left| \frac{\sum_k e_k(H_\tau)}{E_{scl}(h_\tau, \mathbf{B}_\tau, V_\tau)} - 1 \right| = 0. \tag{4.11}$$

Remark 1. From our proof it will be clear that in order to get the corresponding upper bound on the eigenvalue sum in (4.11), we can relax the condition (4.6) involving ε_- and ε_2 by replacing $\mathcal{F}_{h_\tau,\mathbf{B}_\tau}$ to $\mathcal{E}_{h_\tau,\mathbf{B}_\tau}$ in their definitions (4.8)-(4.9).

Remark 2. The reader might wonder to what extent our result is uniform, i.e. if we can say something without restricting ourselves to a one-parameter family of data. Our proof, in fact, immediately provides a uniform statement but its precise formulation is fairly complicated due to the interrelations between various control parameters (like $\kappa, \mu, \varepsilon_\pm, \varepsilon_2$), therefore we omit it.

4.1 Constant field approximation

Fix $\mu, \kappa > 0$, $h \in (0,1)$ and consider a magnetic field $\mathbf{B}$ such that $hL(\mathbf{B})^{-1}, hl(\mathbf{B})^{-1} \leq \mu$ and $h^3\|\mathbf{B}\|l(\mathbf{B})^{-2} \leq \kappa$. The goal of this section is to rewrite the kinetic energy part of the Pauli operator in terms of a spatial average of operators with constant magnetic field plus error terms. The error terms will go to zero as $\mu, \kappa, h \to 0$, (notice that, in addition to h, κ and μ also play the role of the small parameters). Later, this representation will be used to obtain precise lower and upper bounds on the eigenvalue sum. The final result of this section is Proposition 4.2 below, but we have to introduce some notations before stating it.

First we introduce a spherically symmetric functions $\theta_\lambda = \lambda^{-3/2}\theta(x/\lambda)$ with $\theta \in C_0^\infty(\mathbf{R}^3)$, which localizes at scale $\lambda = \lambda(\kappa, \mu, h)$, i.e. $\int_{\mathbf{R}^3} \theta_\lambda^2 = 1$, $\operatorname{supp}\theta_\lambda \subset B(0,\lambda)$ and $\int(\nabla\theta_\lambda)^2 \leq c\lambda^{-2}$. Here the function $\lambda = \lambda(\kappa, \mu, h)$ will be chosen later, but it is required to go to zero as $\kappa, \mu, h \to 0$.

Let $f \in C_0^\infty(\mathbf{R}^3, \mathbf{C}^2)$, then by the IMS localization formula (Lemma 2.1)

$$\langle f|[\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})]^2|f\rangle = \iint |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}(x))\theta_\lambda(x-u)f(x)|^2 \mathrm{d}x\,\mathrm{d}u - h^2\langle f|f\rangle\int(\nabla\theta_\lambda)^2, \quad (4.12)$$

(the gradient operator $\mathbf{p}$ always acts on the x variable).

We fix a point u and now study

$$\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}(x))\theta_\lambda(x-u)f(x)|^2\mathrm{d}x = \int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gf|^2, \quad (4.13)$$

where $g(x) := \theta_\lambda(x-u)$ (for the rest of this section u and λ remain fixed, so we omit them from the notation).

Note that (4.13) is invariant under orthogonal coordinate transformation, so we can choose a coordinate system such that $\mathbf{B}(u) = (0,0,B(u))$, i.e. $\mathbf{n}(u) = (0,0,1)$. Throughout this section we shall work in this coordinate system. We also define the spin projections as

$$P_\pm^u = P_\pm := \frac{1}{2}(1 \pm \boldsymbol{\sigma}\cdot\mathbf{n}(u)). \quad (4.14)$$

Moreover, we define the transversal coordinates, denoted by $x_\perp \in \mathbf{R}^2$, by

$$x = (x_\perp, x_3) := (\pi_{1,2}(x - x \cdot \mathbf{n}(u)), x \cdot \mathbf{n}(u))$$

($\pi_{1,2}$ is the standard projection on the first two components from $\mathbf{R}^3 \to \mathbf{R}^2$), and $p_\perp$, $\sigma_\perp$ are defined analogously. Strictly speaking the notions of "perpendicular" and "third direction" depend on u, i.e. formally the notation $(x_\perp, x_3) = (x_{\perp(u)}, x_{3(u)})$ would be meticulous, but in this Section we omit the u dependence.

We shall need a second localization, which is essentially identical to the localization given in Section 3.2. For the reader's convenience we recall that for any u it is given by a function $\eta^u \in C_0^\infty(\mathbf{R}^2)$ with $\operatorname{supp} \eta^u \subset B(0, \lambda(\kappa, \mu, h)) \subset \mathbf{R}^2$ which has the form $\eta^u := \eta^{(0),u}\zeta$. Here $\zeta \in C_0^\infty(\mathbf{R}^2)$, $\operatorname{supp} \zeta \subset B(0, \lambda(\kappa, \mu, h))$, $|\nabla \zeta| \leq c\lambda(\kappa, \mu, h)^{-1}$, $\zeta \equiv 1$ on $B(0, \lambda(\kappa, \mu, h)/2)$, $0 \leq \zeta \leq 1$; and the function $\eta^{(0)} = \eta^{(0),u}$ is defined as

$$\eta^{(0)}(v) = \eta^{(0),u}(v) := c_{norm,u} w_u^{-1} e^{-w_u^{-2} v^2}$$

with a normalization constant chosen such that $\int_{\mathbf{R}^2} (\eta^u)^2 = 1$. It is easy to see that

$$c^{-1} < \int_{\operatorname{supp} \zeta} (\eta^{(0),u})^2 < c$$

with a universal constant. The scale $w_u = w_u(\kappa, \mu, h)$ of $\eta^{(0),u}$ is chosen as

$$w_u := \Lambda(\kappa, \mu, h)(B^\#(u))^{-1/2} h^{1/2},$$

where $\Lambda(\kappa, \mu, h)$ is a function to be chosen later, which satisfies $\Lambda(\kappa, \mu, h) \to \infty$ as $\kappa, \mu, h \to 0$. Here we introduced the notation

$$B^\#(u) := \sup_{x\,:\,|x-u|<2L(\mathbf{B})} \{|\mathbf{B}(x)|\},$$

and since $e^{-2} \leq B(x)/B(y) \leq e^2$ for all $|x - y| \leq 2L(\mathbf{B})$, we note that

$$e^{-2} B^\#(u) \leq B(u) \leq B^\#(u). \tag{4.15}$$

Notice that w_u, the scale of $\eta^{(0),u}$, depends on u, but in general we omit it from the notation in this section. In particular we have

$$\int_{\mathbf{R}^2} \eta^u(v)^2 v^{2k} \mathrm{d}v \leq c \min\{w_u, \lambda(\kappa, \mu, h)\}^{2k} \tag{4.16}$$

for $k = 0, 1, 2$.

We define

$$\eta_v^u(x) = \eta_v(x) := \eta(x_\perp - v),$$

and similarly

$$\zeta_v^u(x) = \zeta_v(x) := \zeta(x_\perp - v),$$
$$\eta_v^{(0),u}(x) = \eta_v^{(0)}(x) := \eta^{(0)}(x_\perp - v)$$

(note that η_v, $\eta_v^{(0)}$ and ζ_v are functions on $\mathbf{R}^3$ and the u-dependence is hidden in $\perp = \perp(u)$).

Armed with these notations and definitions, we can state the main result of this section.

Proposition 4.2 *There exist two universal constants $c_0 \le 1$ and $c_1 \ge 1$, and there exists a function $\varepsilon(\kappa, \mu, h) : (0, c_0) \times (0, c_0) \times (0, c_0) \to (0, 1/4)$, $\varepsilon(\kappa, \mu, h) \to 0$ as $\kappa, \mu, h \to 0$ (in fact the function $\varepsilon(\kappa, \mu, h) = c_1 \max\{\kappa^{1/6}, \mu^{1/3}, h^{2/3}\}$ would do) with following property: for any $0 < h, \kappa, \mu < c_0$, for any magnetic field $\mathbf{B}$ satisfying $hL(\mathbf{B})^{-1}, hl(\mathbf{B})^{-1} \le \mu$, $h^3\|\mathbf{B}\| l(\mathbf{B})^{-2} \le \kappa$ and for any $u \in \mathbf{R}^3$, $v \in \mathbf{R}^2$ there exist a phase function $\phi_{u,v}$, constant magnetic fields $\hat{\mathbf{B}}_{u,v}^{\pm}$ (with strengths $\hat{B}_{u,v}^{\pm}$), parallel with $\mathbf{B}(u)$, satisfying*

$$|B(u) - \hat{B}_{u,v}^{\pm}| \le \varepsilon(\kappa, \mu, h) B(u), \quad \text{for all } v \text{ with } |v - u_{\perp(u)}| \le 2\lambda(\kappa, \mu, h) \tag{4.17}$$

with

$$\lambda(\kappa, \mu, h) := \min\{c_1 h \varepsilon(\kappa, \mu, h)^{-1}, 10^{-4} h \mu^{-1}, \varepsilon(\kappa, \mu, h)\}, \tag{4.18}$$

such that for any $f \in C^\infty(\mathbf{R}^3, \mathbf{C}^2)$ and $g \in C_0^\infty(B(u, \lambda(\kappa, \mu, h)), \mathbf{R})$ we have

$$\int |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A}) g f|^2 \tag{4.19}$$

$$\ge \int_{\mathbf{R}^2} \int \Big[(1 - \varepsilon(\kappa, \mu, h)) |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \hat{\mathbf{A}}_{u,v}^{+})(e^{i\phi_{u,v}} \eta_v^u g f)(x)|^2 - \varepsilon(\kappa, \mu, h) |(e^{i\phi_{u,v}} \eta_v^u g f)(x)|^2 \Big] \mathrm{d}x\, \mathrm{d}v,$$

and for any v-dependent spinor $f^v \in C^\infty(\mathbf{R}^3, \mathbf{C}^2)$

$$\int_{\mathbf{R}^2} \int |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})(e^{-i\phi_{u,v}} \eta_v^u g f^v)(x)|^2 \mathrm{d}x\, \mathrm{d}v \tag{4.20}$$

$$\le \int_{\mathbf{R}^2} \int (\eta_v^u g)(x)^2 \Big[(1 + \varepsilon(\kappa, \mu, h)) |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \hat{\mathbf{A}}_{u,v}^{-}) f^v(x)|^2 + \varepsilon(\kappa, \mu, h) W_{u,v}(x_\perp)) |f^v(x)|^2$$
$$+ \varepsilon(\kappa, \mu, h) W_{u,v}^{+}(x_\perp) |P_+ f^v(x)|^2 \Big] \mathrm{d}x \mathrm{d}v + ch^2 \int_{\mathbf{R}^2} \int |\nabla(\zeta_v g)(x)|^2 |(\eta_v^{(0),u} f^v)(x)|^2 \mathrm{d}x\, \mathrm{d}v$$

where

$$W_{u,v}(x_\perp) = w_u^{-4}(x_\perp - v)^4 + w_u^{-2}(x_\perp - v)^2 + 1,$$
$$W_{u,v}^{+}(x_\perp) = hB^{\#}(u) w_u^{-2}(x_\perp - v)^2,$$
$$w_u = w_u(\kappa, \mu, h) := \Lambda(\kappa, \mu, h)(B^{\#}(u))^{-1/2} h^{1/2}$$

with

$$\Lambda(\kappa, \mu, h) := c_1 \varepsilon(\kappa, \mu, h)^{-1},$$

and the vector potentials

$$\hat{\mathbf{A}}_{u,v}^{\pm} := \frac{1}{2} \hat{B}_{u,v}^{\pm} \mathbf{n}(u) \times x \tag{4.21}$$

generating the constant fields $\hat{\mathbf{B}}_{u,v}^{\pm}$.

Proof. Since u is fixed, we shall omit it from the notation, but we recall that f^v, w, $\mathbf{A}_v^{\pm}$, ϕ_v, $P^{\pm}$ and $\perp$ can and will depend on u in the application. To simplify the formulas, we also drop the arguments from $\varepsilon = \varepsilon(\kappa, \mu, h)$, $\lambda = \lambda(\kappa, \mu, h)$ and $\Lambda = \Lambda(\kappa, \mu, h)$ in this proof.

Step 1. Separation of the spin up and spin down subspaces

Let $\alpha = \alpha(\kappa, \mu, h) \le (32e^2)^{-1}$ be chosen later. For any function ψ (to be applied for $\psi = gf$) we have

$$\begin{aligned}
\int |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})\psi|^2 &= \int |(h\mathbf{p} + \mathbf{A})\psi|^2 - \int (\psi, h\boldsymbol{\sigma} \cdot \mathbf{B}\psi) \\
= \int |(h\mathbf{p} + \mathbf{A})P_-\psi|^2 &- \int (P_-\psi, h\boldsymbol{\sigma} \cdot \mathbf{B}P_-\psi) + \int |(h\mathbf{p} + \mathbf{A})P_+\psi|^2 - \int (P_+\psi, h\boldsymbol{\sigma} \cdot \mathbf{B}P_+\psi) \\
&- \int (P_-\psi, h\boldsymbol{\sigma} \cdot \mathbf{B}P_+\psi) - \int (P_+\psi, h\boldsymbol{\sigma} \cdot \mathbf{B}P_-\psi) \\
= \int |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})P_-\psi|^2 &+ \int |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})P_+\psi|^2 - \int (P_-\psi, h\boldsymbol{\sigma} \cdot \mathbf{B}P_+\psi) - \int (P_+\psi, h\boldsymbol{\sigma} \cdot \mathbf{B}P_-\psi),
\end{aligned} \tag{4.22}$$

where we here used that $P_\pm$ commute with $h\mathbf{p} + \mathbf{A}$. Therefore we obtain

$$\begin{aligned}
&\left| \int |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})gf|^2 - \int |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})gP_-f|^2 - \int |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})gP_+f|^2 \right| \\
&\le \ 2hB^{\#}(u) \left(\alpha^{-1} l(\mathbf{B})^{-2} \lambda^2 \int |gP_-f|^2 + \alpha \int |gP_+f|^2 \right),
\end{aligned} \tag{4.23}$$

using

$$
\begin{aligned}
h|(P_+\psi(x), \boldsymbol{\sigma}\cdot\mathbf{B}(x)P_-\psi(x))| &= hB(x)|(P_+\psi(x), \boldsymbol{\sigma}\cdot(\mathbf{n}(x)-\mathbf{n}(u))P_-\psi(x))| \\
&\le 2hB^{\#}(u)l(\mathbf{B})^{-1}\lambda|P_+\psi(x)||P_-\psi(x)| \\
&\le hB^{\#}(u)(\alpha|P_+\psi(x)|^2+\alpha^{-1}l(\mathbf{B})^{-2}\lambda^2|P_-\psi(x)|^2), \qquad (4.24)
\end{aligned}
$$

which is valid by Cauchy-Schwarz and $P_+\boldsymbol{\sigma}\cdot\mathbf{n}(u)P_-=0$ for any function $\psi(=gf)$ supported in the ball $B(u,\lambda)$.

Therefore, we have a lower bound

$$
\begin{aligned}
\int|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gf|^2 &\ge \int\left[|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gP_-f|^2-2hB^{\#}(u)\alpha^{-1}l(\mathbf{B})^{-2}\lambda^2|gP_-f|^2\right] \\
&\quad+\int\left[|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gP_+f|^2-2hB^{\#}(u)\alpha|gP_+f|^2\right], \qquad (4.25)
\end{aligned}
$$

and, similarly, an upper bound,

$$
\begin{aligned}
\int|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gf|^2 &\le \int\left[|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gP_-f|^2+2hB^{\#}(u)\alpha^{-1}l(\mathbf{B})^{-2}\lambda^2|gP_-f|^2\right] \\
&\quad+\int\left[|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gP_+f|^2+2hB^{\#}(u)\alpha|gP_+f|^2\right]. \qquad (4.26)
\end{aligned}
$$

Step 2. Second localization

We separately consider the kinetic energies of $P_\pm f =: f_\pm$ appearing in (4.25) and (4.26). For the lower bound we write

$$
\int|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gf_\pm|^2=\int_{\mathbf{R}^2}\int\eta(x_\perp-v)^2|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})(gf_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v. \qquad (4.27)
$$

Since $\operatorname{supp} g\subset B(u,\lambda)\,(\subset\mathbf{R}^3)$ and $\operatorname{supp}\eta\subset B(0,\lambda)\,(\subset\mathbf{R}^2)$, therefore the above integral can be restricted to $x\in B(u,\lambda)\subset\mathbf{R}^3$ and $v\in B(u_\perp,2\lambda)\subset\mathbf{R}^2$. For any $v\in B(u_\perp,2\lambda)$, we can approximate the magnetic field by a constant field $\mathbf{B}_v=(0,0,B_v)$ such that for all $x\in B(u,2\lambda)$

$$
|\mathbf{B}(x)-\mathbf{B}_v|\le cB^{\#}(u)\lambda l(\mathbf{B})^{-1}+cB^{\#}(u)L(\mathbf{B})^{-1}|x_\perp-v|, \qquad (4.28)
$$

by applying Corollary A.2 from the LT proof with the particular choice of a cylinder with center in (v,u_3), length 4λ and radius $|x_\perp-v|\le 4\lambda$, and using $\lambda L(\mathbf{B})^{-1}\le\lambda h^{-1}\mu\le 10^{-4}$ and a similar estimate for $\lambda l(\mathbf{B})^{-1}$. Notice that the proof of Corollary A.2 requires $\lambda l(\mathbf{B})^{-1}\le[(6+3\sqrt{3})(8+\sqrt{3})]^{-1}$ (see (A.1)), but this is satisfied given $\lambda\le 10^{-4}h\mu^{-1}$ and $l(\mathbf{B})^{-1}\le h^{-1}\mu$.

We can then approximate $\mathbf{A}$ by $\mathbf{A}_v$, rot $\mathbf{A}_v = \mathbf{B}_v$, applying the formula (A.7) from Proposition A.3 and using (A.3) to estimate $\nabla(\mathbf{B}(x) - \mathbf{B}_v) = \nabla\mathbf{B}(x)$, such that

$$|\mathbf{A}(x) - \mathbf{A}_v(x)| \leq cB^{\#}(u)\lambda l(\mathbf{B})^{-1}|x_\perp - v| + cB^{\#}(u)L(\mathbf{B})^{-1}|x_\perp - v|^2 \tag{4.29}$$

for all $x \in B(u,\lambda)$, $v \in B(u_\perp, 2\lambda)$. Using a Cauchy-Schwarz, we have, for any $0 < \delta < 1/2$,

$$\begin{aligned}\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})gf_\pm|^2 \;\geq\; & (1-\delta)\int_{\mathbf{R}^2}\int \eta(x_\perp - v)^2|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(gf_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v \\ & -c\delta^{-1}\int_{\mathbf{R}^2}\int \eta(x_\perp - v)^2|\mathbf{A}(x)-\mathbf{A}_v(x)|^2|(gf_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v\end{aligned} \tag{4.30}$$

For the upper bound, we have to consider functions f^v depending on v, and we shall need the bound

$$\begin{aligned}& \int_{\mathbf{R}^2}\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})(e^{-i\phi_v}\eta_v g f^v_\pm)(x)|^2\mathrm{d}x\mathrm{d}v \\ \leq\; & (1+\delta)\int_{\mathbf{R}^2}\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(e^{-i\phi_v}\eta_v g f^v_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v \\ & +c\delta^{-1}\int_{\mathbf{R}^2}\int \eta(x_\perp - v)^2|\mathbf{A}(x)-\mathbf{A}_v(x)|^2|(gf^v_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v,\end{aligned} \tag{4.31}$$

where the phase function $\phi_v : \mathbf{R}^3 \to \mathbf{R}$ will be chosen below.

To control the error in (4.30), we shall apply the following estimate, which is valid uniformly for all $x \in B(u,\lambda)$

$$\begin{aligned}& \delta^{-1}\int_{|v-u_\perp|\leq 2\lambda}\eta(x_\perp - v)^2|\mathbf{A}(x)-\mathbf{A}_v(x)|^2\mathrm{d}v \\ \leq\; & c\delta^{-1}(B^{\#}(u))^2\int_{\mathbf{R}^2}\eta(v)^2\left[\lambda^2 l(\mathbf{B})^{-2}v^2 + L(\mathbf{B})^{-2}v^4\right]\mathrm{d}v \\ \leq\; & c\delta^{-1}(B^{\#}(u))^2(w^2\lambda^2 l(\mathbf{B})^{-2} + h^{-2}\mu^2 w^4)\end{aligned} \tag{4.32}$$

using (4.29), (4.16) and, in the applications, for the error term in (4.31), we will need a uniform upper bound for $f^v(x)$.

We choose a gauge transformation $\phi_{u,v} = \phi_v$ such that

$$(\mathbf{A}_v - \nabla\phi_v)(x) = (1/2)B_v\mathbf{n}(u)\times(x-(v,x_3)),$$

that determines ϕ_v (up to an irrelevant constant). Notice that $\mathbf{A}_v - \nabla\phi_v$ does not depend on x_3 and has zero third component. Therefore the main terms in (4.30) and (4.31) can be written as

$$\int_{\mathbf{R}^2}\int \eta(x_\perp - v)^2|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(gf_\pm)(x)|^2\mathrm{d}x\,\mathrm{d}v \tag{4.33}$$

$$= \int_{\mathbf{R}^2}\int \eta(x_\perp - v)^2 \Big[|\sigma_\perp \cdot (h\mathbf{p} + \mathbf{A}_v - \nabla\phi_v)_\perp (e^{i\phi_v} g f_\pm)(x)|^2 + |hp_3(e^{i\phi_v} g f_\pm)(x)|^2 \Big] \mathrm{d}x\,\mathrm{d}v,$$

and

$$\begin{aligned}
&\int_{\mathbf{R}^2}\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(e^{-i\phi_v}\eta_v g f^v_\pm)(x)|^2 \mathrm{d}x\,\mathrm{d}v \\
&\quad = \int_{\mathbf{R}^2}\int \Big[|\sigma_\perp \cdot (h\mathbf{p} + \mathbf{A}_v - \nabla\phi_v)_\perp (\eta_v g f^v_\pm)(x)|^2 + |hp_3(\eta_v g f^v_\pm)(x)|^2 \Big] \mathrm{d}x\,\mathrm{d}v. \qquad (4.34)
\end{aligned}$$

Step 3. Magnetic localization

Using the estimates in Lemma 2.2 with the same δ as above and $k(x_\perp) = \zeta(x_\perp)(gf_\pm)(x_\perp + v, x_3)$ for each x_3 (and including the phase factor in the case of (2.3)), then shifting $x_\perp \to x_\perp - v$, we obtain from (4.33), (4.34), (4.16) and the estimates in the IMS Lemma 2.1 (once for ζ_v, once for $g\zeta_v$) that

$$\begin{aligned}
&\int_{\mathbf{R}^2}\int \eta(x_\perp - v)^2 |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(gf_\pm)(x)|^2 \mathrm{d}x\,\mathrm{d}v \qquad (4.35)\\
&\geq \int_{\mathbf{R}^2}\int \eta^{(0)}(x_\perp - v)^2 |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(\zeta_v g f_\pm)(x)|^2 \mathrm{d}x\,\mathrm{d}v - ch^2 \sup(\nabla\zeta)^2 \cdot \int |gf_\pm|^2 \\
&\geq (1-\delta)\int_{\mathbf{R}^2}\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}^+_v)(e^{i\phi_v}\eta_v g f_\pm)(x)|^2 \mathrm{d}x\,\mathrm{d}v \\
&\quad -ch^2\lambda^{-2}\int |gf_\pm|^2 - c\delta^{-1}h^2 w^{-2}\int |P_+ g f_\pm|^2 \qquad (4.36)
\end{aligned}$$

and

$$\begin{aligned}
&\int_{\mathbf{R}^2}\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_v)(e^{-i\phi_v}\eta_v g f^v_\pm)(x)|^2 \mathrm{d}x\,\mathrm{d}v \qquad (4.37)\\
&\leq (1+\delta)\int_{\mathbf{R}^2}\int \eta^{(0)}(x_\perp - v)^2 |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}^-_v)(\zeta_v g f^v_\pm)(x)|^2 \mathrm{d}x\,\mathrm{d}v \\
&\quad +c\delta^{-1}h^2 w^{-2}\int_{\mathbf{R}^2}\int |P_+(\eta_v g f^v_\pm)(x)|^2 \mathrm{d}x\mathrm{d}v \\
&\leq (1+\delta)\int_{\mathbf{R}^2}\int \eta_v(x)^2 g(x)^2 |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}^-_v) f^v_\pm(x)|^2 \mathrm{d}x\,\mathrm{d}v \\
&\quad +(1+\delta)h^2\int_{\mathbf{R}^2}\int |\nabla(\zeta_v g)(x)|^2 |\eta^{(0)}_v f^v(x)|^2 \mathrm{d}x\,\mathrm{d}v \\
&\quad +c\delta^{-1}h^2 w^{-4}\int_{\mathbf{R}^2}\int (x_\perp - v)^2 |P_+(\eta_v g f^v_\pm)(x)|^2 \mathrm{d}x\mathrm{d}v, \qquad (4.38)
\end{aligned}$$

where the vector potentials $\hat{\mathbf{A}}^\pm_{u,v} = \hat{\mathbf{A}}^\pm_v(x)$ defined in (4.21) generate the constant fields $\hat{\mathbf{B}}^\pm_{u,v} = \hat{\mathbf{B}}^\pm_v := (0, 0, B_v \pm 4hw^{-2})$.

To estimate how well this constant field approximates to original one, for $|v - u_\perp| \le 2\lambda$ we obtain (using (4.28) for $x = (v, u_3)$, $L(\mathbf{B})^{-1}, l(\mathbf{B})^{-1} \le h^{-1}\mu$) that

$$\begin{aligned} |B(u) - \hat{B}_v^\pm| &\le |\mathbf{B}(u) - \hat{\mathbf{B}}_v^\pm| \\ &\le |\mathbf{B}(u) - \mathbf{B}(v, u_3)| + |\mathbf{B}(v, u_3) - \mathbf{B}_v| + 4hw^{-2} \qquad (4.39) \\ &\le 2B^\#(u)h^{-1}\mu\lambda + cB^\#(u)\lambda l(\mathbf{B})^{-1} + 4hw^{-2} \\ &\le cB^\#(u)(h^{-1}\mu\lambda + \Lambda^{-2}) \le cB(u)(h^{-1}\mu\lambda + \Lambda^{-2}). \qquad (4.40) \end{aligned}$$

In the last step we used (4.15). In order to prove (4.17) we must therefore choose $\varepsilon = \varepsilon(\kappa, \mu, h)$ such that

$$c(h^{-1}\mu\lambda + \Lambda^{-2}) \le \varepsilon, \tag{4.41}$$

We also get a lower bound ($\varepsilon \le 1/2$)

$$\hat{B}_v^\pm \ge (1 - \varepsilon)B(u) \ge (1/2)e^{-2}B^\#(u)$$

for all v such that $|v - u_\perp| \le 2\lambda$ (in particular (4.39) and (4.41) imply that $\mathbf{B}(u)$, $\hat{\mathbf{B}}_v^-$ and $\hat{\mathbf{B}}_v^+$ point in the same direction).

Since for all $k \in C_0^\infty(\mathbf{R}^3, \mathbf{C}^2)$ we have

$$\int |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \hat{\mathbf{A}}_v^\pm)P_+k|^2 \ge h\hat{B}_v^\pm \int |P_+k|^2 \ge (1/2)e^{-2}hB^\#(u) \int |P_+k|^2, \tag{4.42}$$

we see that the last error terms in (4.25), (4.26) and (4.35), which are nonzero only for f_+, can be absorbed into the kinetic energy (with the constant direction magnetic field $\hat{\mathbf{B}}_v^\pm$) if $\alpha \le (32e^2)^{-1}$ and

$$R := c\delta^{-1}h^2w^{-2}(hB^\#(u))^{-1} = c\delta^{-1}\Lambda^{-2} = cc_1^{-2}\delta^{-1}\varepsilon^2 < (8e^2)^{-1} \tag{4.43}$$

(using the definition of w and Λ).

We put together (4.25), (4.30), (4.32), (4.33) and (4.35), the final lower bound of this section is

$$\begin{aligned} &\int |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A})gf|^2 \qquad (4.44) \\ \ge\ &\int_{\mathbf{R}^2} \int \Big[(1-\delta)^2 |\boldsymbol{\sigma} \cdot (h\mathbf{p} + \hat{\mathbf{A}}_v^+)(e^{i\phi_v}\eta_v g P_- f)(x)|^2 \\ &-(S + Q + ch^2\lambda^{-2})|(e^{i\phi_v}\eta_v g P_- f)(x)|^2 \\ &+[(1-\delta)^2(1-R) - 4e^2\alpha]|\boldsymbol{\sigma} \cdot (h\mathbf{p} + \hat{\mathbf{A}}_v^+)(e^{i\phi_v}\eta_v g P_+ f)(x)|^2 \\ &-(Q + ch^2\lambda^{-2})|(e^{i\phi_v}\eta_v g P_+ f)(x)|^2 \Big] \mathrm{d}x\, \mathrm{d}v \qquad (4.45) \end{aligned}$$

with

$$S := 2hB^{\#}(u)\alpha^{-1}l(\mathbf{B})^{-2}\lambda^2$$
$$Q := Q_1 + Q_2$$

where

$$Q_1 := c\delta^{-1}(B^{\#}(u))^2 w^2\lambda^2 l(\mathbf{B})^{-2} \quad \text{and} \quad Q_2 := c\delta^{-1}(B^{\#}(u))^2 h^{-2}\mu^2 w^4.$$

Using $h^3\|\mathbf{B}\|l(\mathbf{B})^{-2} \leq \kappa$, $B^{\#}(u) \leq \|\mathbf{B}\|$ and the definitions of w and Λ we see that

$$S \leq 2h^{-2}\alpha^{-1}\lambda^2\kappa$$
$$Q \leq cc_1^2\delta^{-1}h^{-2}\varepsilon^2\lambda^2\kappa + cc_1^4\delta^{-1}\varepsilon^{-4}\mu^2. \tag{4.46}$$

For the upper bound we use (4.26) for $f = e^{-i\phi_v}\eta_v f^v$, then combine it with (4.31), (4.32), (4.34) and (4.37) to obtain

$$\begin{aligned}
&\int_{\mathbf{R}^2}\int |\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A})(e^{-i\phi_v}\eta_v g f^v)(x)|^2 \mathrm{d}x\,\mathrm{d}v & (4.47)\\
\leq\ & \int_{\mathbf{R}^2}\int \eta(x_\perp - v)^2 g(x)^2\Big[(1+\delta)^2|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_v^-)(P_- f^v)(x)|^2 \\
&+\left\{S + Q_1 w^{-2}(x_\perp - v)^2 + Q_2 w^{-4}(x_\perp - v)^4\right\}|P_- f^v(x)|^2 \\
&+[(1+\delta)^2 + 4e^2\alpha]|\boldsymbol{\sigma}\cdot(h\mathbf{p}+\hat{\mathbf{A}}_v^-)(P_+ f^v)(x)|^2 \\
&+\left\{(RB^{\#}(u)h + Q_1)w^{-2}(x_\perp - v)^2 + Q_2 w^{-4}(x_\perp - v)^4\right\}|P_+ f^v(x)|^2\Big]\mathrm{d}x\,\mathrm{d}v \\
&+ch^2\int_{\mathbf{R}^2}\int |(\nabla(g\zeta_v))(x)|^2|\eta_v^{(0)} f^v(x)|^2 \mathrm{d}x\,\mathrm{d}v. & (4.48)
\end{aligned}$$

In order to prove the proposition we must show that we can choose numbers c_0, c_1 and positive functions $\varepsilon = \varepsilon(\kappa,\mu,h) \leq 1/4$, $\delta = \delta(\kappa,\mu,h)$ and $\alpha = \alpha(\kappa,\mu,h) \leq (32e^2)^{-1}$ defined on $(0,c_0)\times(0,c_0)\times(0,c_0)$ such that $\varepsilon(\kappa,\mu,h)\to 0$ (as $\kappa,\mu,h\to 0$) and such that (4.41) and the following requirements are met with $\Lambda(\kappa,\mu,h) := c_1\varepsilon(\kappa,\mu,h)^{-1}$

$$R \leq \varepsilon,\ Q + ch^2\lambda^{-2} + S \leq \varepsilon,\ (1+\delta)^2 + 4e^2\alpha \leq (1+\varepsilon),\ (1-\delta)^2(1-R) - 4e^2\alpha \geq (1-\varepsilon). \tag{4.49}$$

In particular, $R \leq \varepsilon$, and therefore a small enough choice of c_0 will imply (4.43).

One possible choice is $\varepsilon := c_1\max\{\kappa^{1/6}, \mu^{1/3}, h^{2/3}\}$, $\delta := \varepsilon/10$, $\alpha := \varepsilon/(8e^2)$. Then a short calculation, with the help of (4.46) shows that all the requirements are met for small enough (universal) c_0 and large enough (universal) c_1 (appearing in (4.18)). This finishes the proof of Proposition 4.2. □

4.2 Lower bound

We shall here prove the one-sided bound

$$\limsup_{\tau\to 0} \frac{\sum_k e_k(H_\tau)}{E_{scl}(h_\tau, \mathbf{B}_\tau, V_\tau)} \leq 1, \tag{4.50}$$

in Theorem 4.1. Since $E_{scl}(h_\tau, \mathbf{B}_\tau, V_\tau) \leq 0$, this is a *lower* bound on the eigenvalue sum $\sum_k e_k(H_\tau)$.

For this bound, we can replace V_τ by its negative part, $-[V_\tau]_-$. Obviously for small enough h_τ we have $h_\tau L(\mathbf{B}_\tau)^{-1} \leq c_0$, $h_\tau l(\mathbf{B}_\tau)^{-1} \leq c_0$ and $h_\tau^3 \|\mathbf{B}_\tau\| l(\mathbf{B}_\tau)^{-2} \leq c_0$, therefore we can apply Proposition 4.2 with $\mathbf{B} = \mathbf{B}_\tau$ and $\kappa = \kappa(\tau)$, $\mu = \mu(\tau)$ where $\kappa(\tau) = h_\tau^3 \|\mathbf{B}_\tau\| l(\mathbf{B}_\tau)^{-2}$ and $\mu(\tau) = h_\tau \max\{L(\mathbf{B}_\tau)^{-1}, l(\mathbf{B}_\tau)^{-1}\}$. We also introduce $d_\tau := h_\tau \min\{\kappa(\tau)^{1/4}, \mu(\tau)\}$. Define $\tilde\lambda(\tau) := \lambda(\kappa(\tau), \mu(\tau), h_\tau)$ and $\tilde\varepsilon(\tau) := \varepsilon(\kappa(\tau), \mu(\tau), h_\tau)$, where the functions $\lambda(\kappa, \mu, h)$ and $\varepsilon(\kappa, \mu, h)$ were obtained in Proposition 4.2. Remark that $\tilde\lambda(\tau) \leq \tilde\varepsilon(\tau) \to 0$ as $\tau \to 0$.

Instead of the original Pauli operator H_τ, we are going to study

$$\tilde H_\tau := (1 - 2\delta_1)\Theta_\varrho [\boldsymbol{\sigma}\cdot(h_\tau \mathbf{p} + \mathbf{A}_\tau)]^2 \Theta_\varrho - [V_\tau \chi_\varrho]_- * \theta_\lambda^2, \tag{4.51}$$

where θ_λ is the function defined in Section 4.1 with lengthscale $\lambda = \tilde\lambda(\tau)$ (for brevity we use λ for $\tilde\lambda(\tau)$) and χ_ϱ denotes the characteristic function of the ball of radius $\varrho \geq 1$ centered at the origin in $\mathbf{R}^3$, and $\Theta_\varrho \in C_0^\infty(\mathbf{R}^3)$ satisfies $\Theta_\varrho(x) = 1$ on $B(0, \varrho + \lambda)$, $\operatorname{supp}\Theta_\varrho \subset B(0, \varrho + 2\lambda)$, and $|\nabla \Theta_\varrho| \leq c\lambda^{-1}$. Here $0 < \delta_1 < 1/4$.

Let $\theta_{u,\lambda}(x) := \theta_\lambda(x - u)$. We then use the localization formula (2.1) to write

$$\langle f|\tilde H_\tau|f\rangle = \int \langle f\theta_{u,\lambda}|\tilde H_{u,\tau}|\theta_{u,\lambda} f\rangle \, du - c(1-2\delta_1)h_\tau^2 \lambda^{-2} \langle f|\Theta_\varrho^2|f\rangle,$$

for any $f \in C_0^\infty(\mathbf{R}^3, \mathbf{C}^2)$, where

$$\tilde H_{u,\tau} = (1 - 2\delta_1)\Theta_\varrho [\boldsymbol{\sigma}\cdot(h_\tau \mathbf{p} + \mathbf{A}_\tau)]^2 \Theta_\varrho - [V_\tau \chi_\varrho(u)]_-.$$

The relation between the kinetic energy parts of H_τ and $\tilde H_\tau$ is given by the pointwise inequality in Lemma 2.1

$$\langle f|[\boldsymbol{\sigma}\cdot(h_\tau \mathbf{p} + \mathbf{A}_\tau)]^2|f\rangle \geq (1-\delta_1)\langle f|\Theta_\varrho[\boldsymbol{\sigma}\cdot(h_\tau \mathbf{p} + \mathbf{A}_\tau)]^2\Theta_\varrho|f\rangle - c\delta_1^{-1} h_\tau^2 \langle f|(\nabla\Theta_\varrho)^2|f\rangle. \tag{4.52}$$

In order to merge the two error terms from these two localizations, we introduce the function $\Theta_\varrho^* \in C_0^\infty(\mathbf{R}^3)$, satisfying $\Theta_\varrho^*(x) = 1$ on $B(0, \varrho + 2\lambda)$, $\operatorname{supp}\Theta_\varrho^* \subset B(0, \varrho + 3\lambda)$, and $|\nabla\Theta_\varrho^*| \leq c\lambda^{-1}$. Then obviously

$$c(1-2\delta_1)h_\tau^2\lambda^{-2}\Theta_\varrho^2 + c\delta^{-1} h_\tau^2 (\nabla\Theta_\varrho)^2 \leq c\delta_1^{-1} h_\tau^2 \lambda^{-2} (\Theta_\varrho^*)^2. \tag{4.53}$$

Therefore we may write, using (4.52), (4.53)

$$\langle f|H_\tau|f\rangle \geq \int \langle f\theta_{u,\lambda}|\tilde{H}_{u,\tau}|\theta_{u,\lambda}f\rangle \mathrm{d}u + \langle f|H_{err,\tau}|f\rangle, \tag{4.54}$$

where

$$H_{err,\tau} := \delta_1[\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\mathbf{A}_\tau)]^2 + W_{err,\tau} \tag{4.55}$$

with

$$W_{err,\tau} = [V_\tau\chi_\varrho]_- * (\theta_\lambda)^2 - [V_\tau]_- - c\delta_1^{-1}h_\tau^2\lambda^{-2}(\Theta_\varrho^*)^2.$$

$H_{err,\tau}$ shall be treated by the LT inequality.

To estimate the effect of $H_{err,\tau}$, we use the full 3D magnetic Lieb-Thirring error functional. We have

$$\begin{aligned}
\mathcal{F}_{h_\tau,\mathbf{B}_\tau}\left(\delta_1^{-1}W_{err,\tau}\right) &\leq C\delta_1^{-5/2}\Big\{\mathcal{F}_{h_\tau,\mathbf{B}_\tau}\left([V_\tau\chi_\varrho]_- * \theta_\lambda^2 - [V_\tau]_- * \theta_\lambda^2\right) \\
&\quad + \mathcal{F}_{h_\tau,\mathbf{B}_\tau}\left([V_\tau]_- * \theta_\lambda^2 - [V_\tau]_-\right) + \mathcal{F}_{h_\tau,\mathbf{B}_\tau}\left(c\delta_1^{-1}h_\tau^2\lambda^{-2}(\Theta_\varrho^*)^2\right)\Big\} \\
&\leq C\delta_1^{-5/2}\Big\{\mathcal{F}_{h_\tau,\mathbf{B}_\tau}\left([V_\tau\chi_\varrho]_- - [V_\tau]_-\right) \\
&\quad + \mathcal{F}_{h_\tau,\mathbf{B}_\tau}\left([V_\tau]_- * \theta_\lambda^2 - [V_\tau]_-\right) + \mathcal{F}_{h_\tau,\mathbf{B}_\tau}\left(c\delta_1^{-1}h_\tau^2\lambda^{-2}(\Theta_\varrho^*)^2\right)\Big\},
\end{aligned}$$

where we used Jensen's inequality. Note that Jensen also imples that

$$\mathcal{F}_{h_\tau,\mathbf{B}_\tau}\left([V_\tau]_- * \theta_\lambda^2 - [V_\tau]_-\right) \leq \int \mathcal{F}_{h_\tau,\mathbf{B}_\tau}([V_\tau]_- - [V_\tau(\cdot - y)]_-)\theta_\lambda(y)^2\mathrm{d}y.$$

The integrand vanishes unless $|y| \leq \lambda$. Since $\lambda = \tilde{\lambda}(\tau) \to 0$ as $\tau \to 0$ it follows from (4.4-4.8), (4.10) and dominated convergence that this term tends to zero relative to $|E_{scl}(h_\tau, \mathbf{B}_\tau, V_\tau)|$ as $\tau \to 0$. If we also use condition (4.9) and the definition of $\lambda = \tilde{\lambda}(\tau) = \lambda(\kappa(\tau), \mu(\tau), h_\tau)$ (see (4.18)), after a short computation, using $h_\tau d_\tau^{-1} = \max\{\kappa(\tau)^{1/4}, \mu(\tau)\} \leq 1$ (if τ is small enough), we see that

$$\begin{aligned}
&\frac{\mathcal{F}_{h_\tau,\mathbf{B}_\tau}\left(\delta_1^{-1}W_{err,\tau}\right)}{|E_{scl}(h_\tau,\mathbf{B}_\tau,V_\tau)|} \qquad\qquad (4.56)\\
&\leq c\delta_1^{-5/2}C_-(\tau)^{-1}\Bigg(\varepsilon_2(\tau,\varrho) + \sup_{|y|\leq\tilde{\lambda}(\tau)} \varepsilon_-(\tau,y) \\
&\quad + \left(R_\tau^{5/2} + R_\tau^{3/2} + R_\tau + R_\tau\tilde{\lambda}(\tau)^{-1}h_\tau\right)(\varrho + 3\tilde{\lambda}(\tau))^3\Bigg) \\
&\leq c\delta_1^{-5}C_-(\tau)^{-1}\left(\varepsilon_2(\tau,\varrho) + \sup_{|y|\leq\tilde{\lambda}(\tau)} \varepsilon_-(\tau,y) + \tilde{\varepsilon}(\tau)(\varrho + 3\tilde{\lambda}(\tau))^3\right) \qquad (4.57)
\end{aligned}$$

with $R_\tau := \delta_1^{-1} h_\tau^2 \tilde\lambda(\tau)^{-2}$ and using $h_\tau^2 \tilde\lambda^{-2}(\tau) \le \tilde\varepsilon(\tau) \le 1/2$ (see (4.49) and $|\nabla \Theta_\varrho^*| \le c\tilde\lambda(\tau)^{-1}$.

Let $f_1, f_2, \dots f_N$ be a family of compactly supported smooth orthonormal spinors and we want to estimate

$$\sum_{j=1}^N \langle f_j | H_\tau | f_j \rangle \ge \sum_{j=1}^N \int \langle f_j \theta_{u,\lambda} | \tilde H_{u,\tau} | \theta_{u,\lambda} f_j \rangle \mathrm{d}u + \sum_{j=1}^N \langle f_j | H_{err,\tau} | f_j \rangle \tag{4.58}$$

uniformly in N.

By the Lieb-Thirring inequality we have

$$\sum_{j=1}^N \langle f_j | H_{err,\tau} | f_j \rangle \ge -c\delta_1 \mathcal{F}_{h_\tau, \mathbf{B}_\tau} \left(\delta_1^{-1} W_{err,\tau} \right) \tag{4.59}$$

which will be controlled using (4.56).

For the main term, we use

$$\sum_{j=1}^N \langle f_j \theta_{u,\lambda} | \tilde H_{u,\tau} | \theta_{u,\lambda} f_j \rangle \tag{4.60}$$

$$\ge \sum_{j=1}^N \int \left[(1-2\delta_1) |\boldsymbol{\sigma} \cdot (h_\tau \mathbf{p} + \mathbf{A}_\tau)(\Theta_\varrho \theta_{u,\lambda} f_j)(x)|^2 - \int \left\{ [V_\tau \chi_\varrho(u)]_- |(\theta_{u,\lambda} \eta_v^u \Theta_\varrho f_j)(x)|^2 \right\} \mathrm{d}v \right] \mathrm{d}x,$$

where η^u is defined in Section 4.1 (note that we could insert Θ_ϱ for free in the potential term thanks to the supports of $\chi_\varrho(u)$ and $\theta_{u,\lambda}(x)$).

For each $\nu \in \mathbf{N}$, $u \in \mathbf{R}^3$, $v \in B(u_{\perp(u)}, 2\lambda)$, $p \in \mathbf{R}$ we define the following positive operators via their kernel

$$\Pi_\tau^\pm(\nu, u, v, p)(x, y) \tag{4.61}$$

$$:= \theta_\lambda(x-u) \eta^u (x_{\perp(u)} - v) e^{-i\phi_{u,v}(x)} \Pi_{u,v}^{\nu,\pm}(x_{\perp(u)}, y_{\perp(u)}) e^{ip(x_{3(u)} - y_{3(u)})} e^{i\phi_{u,v}(y)} \eta^u(y_{\perp(u)} - v) \theta_\lambda(y-u)$$

where we used the notations from Section 4.1, and $\Pi_{u,v}^{\nu,\pm}$ is the two dimensional ν^{th} Landau level projection corresponding to the constant field $\hat{\mathbf{B}}_{u,v}^\pm$ and to the gauge $\hat{\mathbf{A}}_{u,v}^\pm$, obtained in Proposition 4.2 (all these objects naturally depend on τ, but we omit this fact from the notation). Note that $\Pi_\tau^\pm(\nu, u, v, p) = 0$ unless $|v - u_{\perp(u)}| \le 2\lambda = 2\tilde\lambda(\tau)$. In this section we shall use $\Pi_\tau^+(\nu, u, v, p)$ only, the other operator will be useful in Section 4.3.

Since $\theta_{u,\lambda}$ has support in $B(u, \lambda)$, we see from (4.19) (carefully keeping track of the u-dependences which we neglected in the previous section)

$$\sum_j \langle f_j \theta_{u,\lambda} | \tilde H_{u,\tau} | \theta_{u,\lambda} f_j \rangle \tag{4.62}$$

$$
\begin{aligned}
&\geq \sum_j \int_{\mathbf{R}^2} \int \Big[(1-2\delta_1)(1-\tilde{\varepsilon}(\tau)) |\boldsymbol{\sigma}\cdot(h_\tau \mathbf{p} + \hat{\mathbf{A}}^+_{u,v})(e^{i\phi_{u,v}}\eta^u_v \theta_{u,\lambda}\Theta_\varrho f_j)(x)|^2 \\
&\quad -([V_\tau(u)]_- + \tilde{\varepsilon}(\tau))|(e^{i\phi_{u,v}}\eta^u_v\theta_{u,\lambda}\Theta_\varrho f_j)(x)|^2 \Big] \mathrm{d}x\, \mathrm{d}v \\
&= (1-\delta_2(\tau)) \sum_j \sum_{\nu=0}^{\infty} \int_{\mathbf{R}^2}\int_{\mathbf{R}} \Big\{ h_\tau^2(p_3^2 + 2\nu h_\tau^{-1}\hat{B}^+_{u,v}) - (1-\delta_2(\tau))^{-1}([V_\tau(u)]_- + \tilde{\varepsilon}(\tau)) \Big\} \\
&\quad \times \langle f_j | \Theta_\varrho \Pi^+_\tau(\nu,u,v,p_3)\Theta_\varrho | f_j\rangle \mathrm{d}p_3\, \mathrm{d}v. \qquad (4.63)
\end{aligned}
$$

Here

$$
(1-\delta_2(\tau)) := (1-2\delta_1)(1-\tilde{\varepsilon}(\tau)). \qquad (4.64)
$$

Observe now that for each $\nu \in \mathbf{N}$ we have from (4.17) that

$$
\Pi^{\nu,\pm}_{u,v}(x_\perp, x_\perp) = d_\nu h_\tau^{-1}\hat{B}^\pm_{u,v} \leq d_\nu h_\tau^{-1}(1+\tilde{\varepsilon}(\tau))B_\tau(u). \qquad (4.65)
$$

if $|v-u_\perp| \leq 2\lambda = 2\tilde{\lambda}(\tau)$.

Therefore

$$
\begin{aligned}
&\int \sum_j \langle f_j|\Theta_\varrho \Pi^+_\tau(\nu,u,v,p_3)\Theta_\varrho|f_j\rangle \mathrm{d}v \\
&\leq \int \mathrm{Tr}[\Theta_\varrho \Pi^+_\tau(\nu,u,v,p_3)\Theta_\varrho]\mathrm{d}v \leq \int \mathrm{Tr}\Pi^+_\tau(\nu,u,v,p_3)\mathrm{d}v \leq d_\nu h_\tau^{-1}(1+\tilde{\varepsilon}(\tau))B_\tau(u), \qquad (4.66)
\end{aligned}
$$

where d_ν was defined in (1.4).

Thus, combining (4.66) with (4.60), (4.62), both the upper and lower bounds of (4.17), and the definition (1.4) of P, after performing the dp_3-integral we have

$$
\begin{aligned}
&\sum_{j=1}^N \int \langle f_j\theta_{u,\lambda}|\tilde{H}_{u,\tau}|\theta_{u,\lambda}f_j\rangle \mathrm{d}u \\
&\geq -h_\tau^{-3}(1-\tilde{\varepsilon}(\tau)^2)(1-\tilde{\varepsilon}(\tau))^{1/2}(1-\delta_2(\tau)) \int_{|u|\leq \varrho+3\lambda} P\left(h_\tau B_\tau(u), \frac{[V_\tau(u)]_- + \tilde{\varepsilon}(\tau)}{1-\delta_3(\tau)}\right) \mathrm{d}u \\
&\geq -h_\tau^{-3} \int_{|u|\leq\varrho+3\lambda} P\left(h_\tau B_\tau(u), \frac{[V_\tau(u)]_- + \tilde{\varepsilon}(\tau)}{1-\delta_3(\tau)}\right) \mathrm{d}u \qquad (4.67)
\end{aligned}
$$

independently of N, with

$$
(1-\delta_3(\tau)) := (1-\delta_2(\tau))(1-\tilde{\varepsilon}(\tau)) = (1-2\delta_1)(1-\tilde{\varepsilon}(\tau))^2. \qquad (4.68)
$$

We used that the integral on the left side of (4.67) vanished unless $|u| \leq \varrho + 3\lambda$.

Putting together (4.58), (4.59) and (4.67), we see that

$$\sum_j \langle f_j | H_\tau | f_j \rangle \tag{4.69}$$

$$\geq -h_\tau^{-3} \int_{|u|\leq \varrho+3\lambda} P\left(h_\tau B_\tau(u), \frac{[V_\tau(u)]_- + \tilde{\varepsilon}(\tau)}{1-\delta_3(\tau)}\right) \mathrm{d}u - c\delta_1 \mathcal{F}_{h_\tau, \mathbf{B}_\tau}\left(\delta_1^{-1} W_{err,\tau}\right).$$

Clearly

$$0 \geq \partial_2 P(B,W) := \frac{\partial}{\partial W} P(B,W) = \pi^{-1} \sum_{\nu=0}^{\infty} d_\nu B [2\nu B - W]_-^{1/2} \leq cBW^{1/2} + cW^{3/2}. \tag{4.70}$$

Therefore, using $0 \leq P(B, W+V) - P(B,W) \leq V \partial_2 P(B, W+V)$ for any $V \geq 0$, Hölder's inequality and (1.7), we obtain if $\tilde{\varepsilon}(\tau) \leq 1$, and $\delta_3 \leq 1/2$ that

$$\begin{aligned} 0 &\leq h_\tau^{-3} \int_{|u|<\varrho+3\lambda} \left[P\left(h_\tau B_\tau(u), \frac{[V_\tau(u)]_- + \tilde{\varepsilon}(\tau)}{1-\delta_3(\tau)}\right) - P(h_\tau B_\tau(u), [V_\tau(u)]_-) \right] \mathrm{d}u \\ &\leq ch_\tau^{-3} \int_{|u|<\varrho+3\lambda} (\tilde{\varepsilon}(\tau) + \delta_3(\tau)[V_\tau(v)]_-) \left[h_\tau \|B_\tau\| ([V_\tau(u)]_- + \tilde{\varepsilon}(\tau))^{1/2} + ([V_\tau(u)]_- + \tilde{\varepsilon}(\tau))^{3/2} \right] \mathrm{d}u \\ &\leq c\left[\tilde{\varepsilon}(\tau)(\varrho + 3\lambda)^3 [\|B_\tau\| h_\tau^{-2} + h_\tau^{-3}] + (\tilde{\varepsilon}(\tau) + \delta_3(\tau)) \mathcal{E}_{h_\tau, \mathbf{B}_\tau}([V_\tau]_-) \right]. \end{aligned} \tag{4.71}$$

Using (1.3), (4.69), (4.71), (4.4–4.5), (4.56) and (4.10), and recalling that $\lambda = \tilde{\lambda}(\tau)$ we get

$$\frac{\sum_j \langle f_j | H_\tau | f_j \rangle}{E_{scl}(h_\tau, \mathbf{B}_\tau, V_\tau)} \leq 1 + cC_-(\tau)^{-1} \Big[\tilde{\varepsilon}(\tau)(\varrho + 3\tilde{\lambda}(\tau))^3 + (\tilde{\varepsilon}(\tau) + \delta_3(\tau)) C_+(\tau) \tag{4.72}$$

$$+ \delta_1^{-5} \Big\{ \varepsilon_2(\tau, \varrho) + \sup_{|y|\leq \tilde{\lambda}(\tau)} \varepsilon_-(\tau, y) + \tilde{\varepsilon}(\tau)(\varrho + 3\tilde{\lambda}(\tau))^3 \Big\} \Big]. \tag{4.73}$$

This estimate is valid independently of N, therefore the ratio of the sum of the negative eigenvalues $\sum_k e_k(H_\tau)$ of $H_\tau = H(h_\tau, \mathbf{A}_\tau, V_\tau)$, to $E_{scl}(h_\tau, \mathbf{B}_\tau, V_\tau)$ is therefore estimated above by the right side of (4.72).

It is clear that we can choose δ_1 and ϱ as functions of τ such that the error in (4.72) tends to 0 as $\tau \to 0$ using (4.8), (4.9) and that $\tau \to 0$ implies $\tilde{\varepsilon}(\tau), \tilde{\lambda}(\tau) \to 0$. This yields (4.50).

4.3 Upper bound

In this section we shall show the opposite asymptotic bound

$$\liminf_{\tau\to 0}\frac{\sum_k e_k(H_\tau)}{E_{scl}(h_\tau,\mathbf{B}_\tau,V_\tau)}\geq 1, \tag{4.74}$$

in Theorem 4.1. We shall construct a suitable trial density matrix and use the variational principle.

As in Section 4.2, we define $\kappa(\tau):=h_\tau^3\|\mathbf{B}_\tau\|l(\mathbf{B}_\tau)^{-2}$, $\mu(\tau):=h_\tau\max\{L(\mathbf{B}_\tau)^{-1},l(\mathbf{B}_\tau)^{-1}\}$, $\lambda:=\tilde{\lambda}(\tau):=\lambda(\kappa(\tau),\mu(\tau),h_\tau)$, $\tilde{\varepsilon}(\tau):=\varepsilon(\kappa(\tau),\mu(\tau),h_\tau)$. We shall also need the coherent state operators $\Pi_\tau^-(\nu,u,v,p)$ defined in (4.61), and recall that $\Pi_\tau^-(\nu,u,v,p)=0$ unless $|v-u_{\perp(u)}|\leq 2\lambda$.

For any $\varrho>0$ let $M_{\tau,\varrho}(\nu,u,p)$ be the characteristic function of the set

$$\{(\nu,u,p)\ :\ h_\tau^2(p^2+2\nu h_\tau^{-1}B_\tau(u))<[V_\tau(u)]_-,|u|\leq\varrho\}.$$

Note that $M_{\tau,\varrho}(\nu,u,p)=0$ if $V_\tau(u)\geq 0$. Define the operator $\gamma_{\tau,\varrho}$ on $L^2(\mathbf{R}^3,\mathbf{C}^2)$ by

$$\gamma_{\tau,\varrho}=(2\pi)^{-1}\sum_{\nu=0}^{\infty}\iint_{\mathbf{R}}M_{\tau,\varrho}(\nu,u,p)\int_{\mathbf{R}^2}\Pi_\tau^-(\nu,u,v,p)\mathrm{d}v\mathrm{d}p\mathrm{d}u.$$

Theorem 4.3 *With the notations above, for any $\varrho>0$, the operator $\gamma_{\tau,\varrho}$ satisfies the density matrix condition $0\leq\gamma_{\tau,\varrho}\leq 1_{L^2(\mathbf{R}^3,\mathbf{C}^2)}$, its density function, $\rho_{\gamma_{\tau,\varrho}}(x):=Tr_{\mathbf{C}^2}(\gamma_{\tau,\varrho}(x,x))$ satisfies the estimate*

$$(1-\tilde{\varepsilon}(\tau))\leq\frac{\rho_{\gamma_{\tau,\varrho}}(x)}{h_\tau^{-3}\int_{|u|\leq\varrho}\partial_2P(h_\tau,B_\tau(u),[V_\tau(u)]_-)\theta_\lambda(x-u)^2\mathrm{d}u}\leq(1+\tilde{\varepsilon}(\tau)), \tag{4.75}$$

(it should be understood such that we allow both the nominator and the denominator be simultaneously zero), and, as a trial density matrix, $\gamma_{\tau,\varrho}$ gives the exact semiclassical upper bound to the energy asymptotics, i.e. for any $\varrho>0$

$$\liminf_{\tau\to 0}\frac{Tr[H_\tau\gamma_{\tau,\varrho}]}{E_{scl}(h_\tau,\mathbf{B}_\tau,V_\tau)}\geq 1-\limsup_{\tau\to 0}\frac{\varepsilon_2(\tau,\varrho)}{C_-(\tau)}. \tag{4.76}$$

Letting $\varrho\to\infty$, (4.76), (4.4) and (4.6) obviously imply (4.74) by using the variational principle: $\sum_k e_k(H_\tau)\leq\mathrm{Tr}[H_\tau\gamma_{\tau,\varrho}]$.

Proof: The following relations are immediate to check

$$(2\pi)^{-1}\sum_{\nu=0}^{\infty}\iint_{\mathbf{R}}\int_{\mathbf{R}^2}\Pi_\tau^-(\nu,u,v,p)\mathrm{d}v\mathrm{d}p\mathrm{d}u \;=\; 1_{L^2(\mathbf{R}^3,\mathbf{C}^2)}, \tag{4.77}$$

$$\mathrm{Tr}_{\mathbf{C}^2}[\Pi_\tau^-(\nu,u,v,p)(x,x)] \;=\; d_\nu h^{-1}\hat{B}^-_{u,v}(\theta_\lambda(x-u)\eta^u(x_{\perp(u)}-v))^2. \tag{4.78}$$

In particular (4.77) implies that $\gamma_{\tau,\varrho}$ satisfies the density matrix condition. The relation

$$(2\pi)^{-1}\sum_\nu d_\nu h_\tau^{-1}B_\tau(u)\int_{\mathbf{R}}M_{\tau,\varrho}(\nu,u,p)\mathrm{d}p = h_\tau^{-3}\partial_2 P(h_\tau B_\tau(u),[V_\tau(u)]_-), \tag{4.79}$$

for $|u|\leq\varrho$ and (4.78) immediately give (4.75).

For $\mathrm{Tr}[H_\tau\gamma_{\tau,\varrho}]$ we shall need

$$\mathrm{Tr}\Pi_\tau^-(\nu,u,v,p) := \mathrm{Tr}_{L^2(\mathbf{R}^3,\mathbf{C}^2)}\Pi_\tau^-(\nu,u,v,p) = d_\nu h^{-1}\hat{B}^-_{u,v}\Phi(u,v) \tag{4.80}$$

with

$$\Phi(u,v) := \int(\theta_\lambda(x-u)^2\eta^u(x_{\perp(u)}-v))^2\mathrm{d}x,$$

and

$$\int_{\mathbf{R}^2}\mathrm{Tr}[V_\tau\Pi_\tau^-(\nu,u,v,p)]\mathrm{d}v \leq d_\nu h_\tau^{-1}B_\tau(u)\left(\{(1+\tilde{\varepsilon}(\tau))[V_\tau]_+ - (1-\tilde{\varepsilon}(\tau))[V_\tau]_-\} * (\theta_\lambda)^2\right)(u) \tag{4.81}$$

obtained from (4.17).

In order to calculate the kinetic energy we note, similarly to the two dimensional case, that $\Pi_\tau^-(\nu,u,v,p)=\Xi_\tau(\nu,u,v,p)\Xi_\tau(\nu,u,v,p)^*$, where $\Xi_\tau(\nu,u,v,p)$ has an integral kernel

$$\Xi_\tau(\nu,u,v,p)(x,y) = \theta_\lambda(x-u)\eta^u(x_{\perp(u)}-v)e^{-i\phi_{u,v}(x)}\Pi^{\nu,-}_{u,v}(x_{\perp(u)},y_{\perp(u)})e^{ip(x_{3(u)}-y_{(3)})}.$$

Let, furthermore, $\Gamma^\nu_{u,v,p}$ be the positive operator with kernel

$$\Gamma^\nu_{u,v,p}(x,y) := \Pi^{\nu,-}_{u,v}(x_{\perp(u)},y_{\perp(u)})e^{ip(x_{3(u)}-y_{(3)})}.$$

We therefore have

$$\begin{aligned}
&\int_{\mathbf{R}^2}\mathrm{Tr}\left([\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\mathbf{A}_\tau)]^2\Pi_\tau^-(\nu,u,v,p)\right)\mathrm{d}v\\
&= \int_{\mathbf{R}^2}\mathrm{Tr}\left[(\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\mathbf{A}_\tau)\Xi_\tau(\nu,u,v,p))^*\left(\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\mathbf{A}_\tau)\Xi_\tau(\nu,u,v,p)\right)\right]\mathrm{d}v\\
&= \int_{\mathbf{R}^2}\iint|[\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\mathbf{A}_\tau)\Xi_\tau(\nu,u,v,p)](x,y)|^2\mathrm{d}x\mathrm{d}y\mathrm{d}v.
\end{aligned} \tag{4.82}$$

To estimate this, we use (4.20) for each fixed y, with for $g := \theta_{u,\lambda}$ and $f^v(x) = \Gamma^\nu_{u,v,p}(x,y)$.

We begin by examining the error terms. Exactly as in the two dimensional case, from the spectral density expression (4.65), the moment estimate (4.16), the field comparison (4.17) and the normalization of $\theta_{\lambda,u}$ we find

$$\begin{aligned}
&\int (\eta^u_v\theta_{\lambda,u})^2(x)W_{u,v}(x_\perp)|\Pi^{\nu,-}_{u,v}(x_\perp,y_\perp)|^2\mathrm{d}y\mathrm{d}x\mathrm{d}v && (4.83)\\
&= \int \left(w_u^{-4}(x-v)^4 + w_u^{-2}(x-v)^2+1\right)(\eta^u_v(x))^2\theta^2_{\lambda,u}(x)|\Pi^{\nu,-}_{u,v}(x_\perp,x_\perp)|\mathrm{d}x\mathrm{d}v\\
&\leq cd_\nu h_\tau^{-1}(1+\tilde\varepsilon(\tau))B_\tau(u), && (4.84)
\end{aligned}$$

where the first identity follows since $\Pi^{\nu,-}_{u,v}$ is a projection.

Likewise, for the second error term we get

$$\begin{aligned}
\int (\eta^u_v\theta_{\lambda,u})^2(x)W^+_{u,v}(x_\perp)|P_+\Pi^{\nu,-}_{u,v}(x_\perp,y_\perp)|^2\mathrm{d}y\mathrm{d}x\mathrm{d}v &\leq \nu h_\tau B^\#_\tau(u)d_\nu h_\tau^{-1}(1+\tilde\varepsilon(\tau))B_\tau(u)\\
&\leq c\nu(h_\tau B_\tau(u))d_\nu h_\tau^{-1}(1+\tilde\varepsilon(\tau))B_\tau(u). \quad (4.85)
\end{aligned}$$

In the last line we used (4.15) to estimate $B^\#_\tau(u)$ in terms of $B_\tau(u)$. Note that we inserted a ν in the estimate. This is clearly allowed for $\nu\geq 1$. For $\nu = 0$ it follows simply because $P_+\Pi^{0,-}_{u,v} = 0$ (i.e., the lowest Landau level contains only spinors with spin down).

For the last error term in (4.20) we just have to recall that $\int_{\mathrm{supp}\,\zeta}(\eta^{(0),u})^2 < c$ to conclude that

$$\int |\nabla(\zeta_v\theta_{\lambda,u})(x)|^2(\eta^{(0),u}_v)^2(x)|\Pi^{\nu,-}_{u,v}(x_\perp,y_\perp)|^2\mathrm{d}x\mathrm{d}y\mathrm{d}v \leq c\tilde\lambda(\tau)^{-2}d_\nu h_\tau^{-1}(1+\tilde\varepsilon(\tau))B_\tau(u). \quad (4.86)$$

If we insert (4.82–4.86) into (4.20) we arrive at

$$\begin{aligned}
&\int \mathrm{Tr}\left([\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\mathbf{A}_\tau)]^2\Pi^-_\tau(\nu,u,v,p)\right)\mathrm{d}v\\
&\leq (1+\tilde\varepsilon(\tau))\iiint \eta^u_v(x)^2\theta_{\lambda,u}(x)^2\left|\left[\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\hat{\mathbf{A}}^-_{u,v})\Gamma^\nu_{u,v,p}\right](x,y)\right|^2\mathrm{d}x\mathrm{d}y\mathrm{d}v\\
&\quad + cd_\nu h_\tau^{-1}(1+\tilde\varepsilon(\tau))B_\tau(u)\Big[\tilde\varepsilon(\tau)+\nu(h_\tau B_\tau(u))\tilde\varepsilon(\tau)+h_\tau^2\tilde\lambda(\tau)^{-2}\Big].
\end{aligned}$$

To compute the first term we observe that since $\Gamma^\nu_{u,v,p}$ is an eigenprojection for $[\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\hat{\mathbf{A}}^-_{u,v})]^2$ it commutes with $\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\hat{\mathbf{A}}^-_{u,v})$. Hence, using again the spectral density expression (4.65), we get

$$\begin{aligned}
&\int \left|\left[\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\hat{\mathbf{A}}^-_{u,v})\Gamma^\nu_{u,v,p}\right](x,y)\right|^2\mathrm{d}y = \left[\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\hat{\mathbf{A}}^-_{u,v})\Gamma^\nu_{u,v,p}\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\hat{\mathbf{A}}^-_{u,v})\right](x,x)\\
&= \left[[\boldsymbol{\sigma}\cdot(h_\tau\mathbf{p}+\hat{\mathbf{A}}^-_{u,v})]^2\Gamma^\nu_{u,v,p}\right](x,x) = (h_\tau^2p^2+2\nu h_\tau\hat{B}^-_{u,v})\Pi^{\nu,-}_{u,v}(x_\perp,x_\perp)\\
&= (h_\tau^2p^2+2\nu h_\tau\hat{B}^-_{u,v})(d_\nu h_\tau^{-1}\hat{B}^-_{u,v}).
\end{aligned}$$

If we insert this identity into the estimate above we conclude, again using the field comparison (4.17) that

$$\int \operatorname{Tr}\Big([\boldsymbol{\sigma}\cdot(h_\tau \mathbf{p}+\mathbf{A})]^2\Pi_\tau^-(\nu,u,v,p)\Big)\,\mathrm{d}v \tag{4.87}$$

$$\leq \; d_\nu h_\tau^{-1}(1+\tilde{\varepsilon}(\tau))B_\tau(u)\Big[\int_{\mathbf{R}^2}\Big\{(1+c\tilde{\varepsilon}(\tau))h_\tau^2(p^2+2\nu h_\tau^{-1}B_\tau(u))\Phi(u,v)\Big\}+c\tilde{\varepsilon}(\tau)+ch_\tau^2\tilde{\lambda}(\tau)^{-2}\Big] \tag{4.88}$$

From (4.87) and (4.81) we have

$$\operatorname{Tr}[H_\tau\gamma_{\tau,\varrho}] \leq (2\pi)^{-1}\sum_\nu \iint_{\mathbf{R}} M_{\tau,\varrho}(\nu,u,p)d_\nu h_\tau^{-1}(1+\tilde{\varepsilon}(\tau))B_\tau(u) \tag{4.89}$$

$$\times\Big\{\int_{\mathbf{R}^2}\Big(\Phi(u,v)(1+c\tilde{\varepsilon}(\tau))^2h_\tau^2(p^2+2\nu h_\tau^{-1}B_\tau(u))\Big)\,\mathrm{d}v$$

$$+c\tilde{\varepsilon}(\tau)+ch_\tau^2\tilde{\lambda}^{-2}(\tau)+\left(\left\{[V_\tau]_+-\frac{1-\tilde{\varepsilon}(\tau)}{1+\tilde{\varepsilon}(\tau)}[V_\tau]_-\right\}*(\theta_\lambda)^2\right)(u)\Big\}\,\mathrm{d}p\,\mathrm{d}u.$$

Using (4.79) we can continue the estimate (4.89) by performing first the dv-integral (note that $\int_{\mathbf{R}^2}\Phi(u,v)\mathrm{d}v=1$) then the d$p$-integral

$$\operatorname{Tr}[H_\tau\gamma_{\tau,\varrho}] \leq (1+c\tilde{\varepsilon}(\tau))^2h_\tau^{-3}\int_{|u|\leq\varrho}P(h_\tau B_\tau(u),[V_\tau(u)]_-)\mathrm{d}u+\mathrm{Error}(\tau,\varrho)$$

$$\leq -h_\tau^{-3}\int_{|u|\leq\varrho}P(h_\tau B_\tau(u),[V_\tau(u)]_-)\mathrm{d}u+\mathrm{Error}(\tau,\varrho)$$

with

$$\mathrm{Error}(\tau,\varrho) := h_\tau^{-3}\int_{\substack{|u|\leq\varrho\\ V_\tau(u)<0}}(1+\tilde{\varepsilon}(\tau))\partial_2P\left(h_\tau B_\tau(u),[V_\tau(u)]_-\right) \tag{4.90}$$

$$\times\left((1+c\tilde{\varepsilon}(\tau))^2[V_\tau(u)]_-+\left(\left\{[V_\tau]_+-\frac{1-\tilde{\varepsilon}(\tau)}{1+\tilde{\varepsilon}(\tau)}[V_\tau]_-\right\}*(\theta_\lambda)^2\right)(u)+c\tilde{\varepsilon}(\tau)\right)\mathrm{d}u.$$

Therefore, using (4.70), we have (if $\tilde{\varepsilon}(\tau)\leq 1$, $\lambda=\tilde{\lambda}(\tau)\leq 1$ which we can assume)

$$\mathrm{Error}(\tau,\varrho) \leq h_\tau^{-3}\int_{|u|\leq\varrho}c(h_\tau\|\mathbf{B}_\tau\|[V_\tau(u)]_-^{1/2}+[V_\tau(u)]_-^{3/2})\Big[\Big|[V_\tau]_- - [V_\tau]_-*(\theta_\lambda)^2\Big|(u) \tag{4.91}$$

$$+\Big|[V_\tau]_+*\theta_\lambda^2-[V_\tau]_+\Big|(u)+\tilde{\varepsilon}(\tau)[V_\tau(u)]_-+\tilde{\varepsilon}(\tau)\Big]\mathrm{d}u$$

$$\leq c\Big\{\tilde{\varepsilon}(\tau)[h_\tau^{-2}\|\mathbf{B}_\tau\|+h_\tau^{-3}](\varrho+1)^3+\tilde{\varepsilon}(\tau)\mathcal{E}_{h_\tau,\mathbf{B}_\tau}([V_\tau]_-)$$

$$+\sum_{\pm}\left(\mathcal{E}_{h_\tau,\mathbf{B}_\tau}\left([V_\tau]_\pm - [V_\tau]_\pm * (\theta_\lambda)^2\right)^{2/3}\mathcal{E}_{h_\tau,\mathbf{B}_\tau}([V_\tau]_-)^{1/3}\right.$$

$$\left.+\mathcal{E}_{h_\tau,\mathbf{B}_\tau}\left([V_\tau]_\pm - [V_\tau]_\pm * (\theta_\lambda)^2\right)^{2/5}\mathcal{E}_{h_\tau,\mathbf{B}_\tau}([V_\tau]_-)^{3/5}\right)\Bigg\}$$

where we used Hölder's inequality.

Considering (4.4)-(4.8) and (4.10), recalling that $\mathcal{E}_{h_\tau,\mathbf{B}_\tau} \le \mathcal{F}_{h_\tau,\mathbf{B}_\tau}$, and $\lambda = \tilde{\lambda}(\tau) \to 0$ we get, using Jensen's inequality and dominated convergence, as in the lower bound, that

$$\frac{\mathrm{Error}(\tau)}{|E_{scl}(h_\tau,\mathbf{B}_\tau,V_\tau)|} \to 0$$

as $\tau \to 0$, uniformly in $\varrho > 0$. Hence for all $\varrho > 0$ we have

$$\liminf_{\tau\to 0}\frac{\mathrm{Tr}[H_\tau\gamma_\tau])}{E_{scl}(h_\tau,\mathbf{B}_\tau,V_\tau)} \ge \left(1 - \limsup_{\tau\to 0}\frac{h_\tau^{-3}\int_{|u|\ge\varrho} P(h_\tau B_\tau(u),[V_\tau(u)]_-)\mathrm{d}u}{|E_{scl}(h_\tau,\mathbf{B}_\tau,V_\tau)|}\right). \tag{4.92}$$

By the definition of $C_-(\tau)$ (see (4.4)) and (4.9)

$$h_\tau^{-3}\int_{|u|\ge\varrho} P(h_\tau B_\tau(u),[V_\tau(u)]_-)\mathrm{d}u = h_\tau^{-3}\int P(h_\tau B_\tau(u),[V_\tau(1-\chi_\varrho)(u)]_-)\mathrm{d}u$$

$$\le \mathcal{E}_{h_\tau,\mathbf{B}_\tau}([V_\tau - V_\tau\chi_\varrho]_-) = \mathcal{E}_{h_\tau,\mathbf{B}_\tau}([V_\tau\chi_\varrho]_- - [V_\tau]_-) \le \varepsilon_2(\tau,\varrho)|E_{scl}(h_\tau,\mathbf{B}_\tau,V_\tau)|/C_-(\tau),$$

hence we obtain (4.76). $\square$

5 Magnetic Thomas-Fermi theory

In Section 1.2 of the introduction we stated our simplest theorem on the asymptotic validity of the magnetic Thomas-Fermi (MTF) theory as the limit of quantum mechanics and we also introduced the basic notations. Here we recall some further results on the MTF theory, obtained in [LSY-II].

The first important result (Proposition 4.3 of [LSY-II]) is that the MTF energy $E^{\mathrm{MTF}}(N,B,Z)$ (defined in (1.18)) is always finite, $E^{\mathrm{MTF}}(N,B,Z) > -\infty$, as long as B is a locally bounded function. Furthermore, it was proved in Theorems 4.5–4.7 that there is a unique minimizer ρ^{MTF}, which satisfies the Thomas-Fermi equation (see [LSY-II] equation (4.27))

$$\rho^{\mathrm{MTF}}(x) = \partial_2 P(B(x),[V^{\mathrm{MTF}}(x)]_-), \tag{5.1}$$

where

$$V^{\mathrm{MTF}}(x) = -Z|x|^{-1} + \rho^{\mathrm{MTF}}(x) * |x|^{-1} + \mu \tag{5.2}$$

with $\mu := \mu(N,B,Z) := -\partial E^{\mathrm{MTF}}(N,B,Z)/\partial N \geq 0$ being the chemical potential (see [LSY-II] Theorem 4.8). Conversely, if the pair (ρ,μ) satisfies (5.1) and (5.2) (with ρ instead of ρ^{MTF}) then there exists N such that ρ is the minimizer of $\mathcal{E}$ with $\int \rho \leq N$ and $\mu = \mu(N,B,Z)$.

Note that according to [LSY-II] Proposition 4.2 the minimizer ρ^{MTF} is in $L^{5/3}_{\mathrm{loc}}(\mathbf{R}^3) \cap L^1(\mathbf{R})$. The convolution integral $\rho^{\mathrm{MTF}} * |x|^{-1}$ therefore makes sense and for $x \neq 0$ we have

$$-(4\pi)^{-1}\Delta V^{\mathrm{MTF}}(x) = \rho^{\mathrm{MTF}}(x). \tag{5.3}$$

From Theorem 4.8 in [LSY-II] we see that

$$\int \rho^{\mathrm{MTF}} < N \Rightarrow \mu(N,B,Z) = 0.$$

We therefore have

$$\mu \int \rho^{\mathrm{MTF}} = \mu N. \tag{5.4}$$

Note that (5.1) and the definiton (1.17) of τ as a Legendre transform imply that

$$\tau(B(x), \rho^{\mathrm{MTF}}(x)) = \rho^{\mathrm{MTF}}(x)[V^{\mathrm{MTF}}(x)]_- - P(B(x), [V^{\mathrm{MTF}}(x)]_-). \tag{5.5}$$

We can now use (5.5) and (5.4) to express the energy as follows

$$\begin{aligned} E^{\mathrm{MTF}}(N,B,Z) = \mathcal{E}[\rho^{\mathrm{MTF}}; B, Z] &= -\int P(B(x), [V^{\mathrm{MTF}}(x)]_-)dx \\ &\quad - \tfrac{1}{2}\iint \rho^{\mathrm{MTF}}(x)|x-y|^{-1}\rho^{\mathrm{MTF}}(y)\mathrm{d}x\mathrm{d}y - \mu N. \end{aligned} \tag{5.6}$$

Our main result on the energy of large atoms was given in the introduction, in Theorem 1.3. There only the the strength of the magnetic field was rescaled. One could also have asked whether the field can be allowed to vary on a scale depending the parameters Z and b. This is of some interest since the atomic scale, in fact, decreases with increasing Z and b, at least asymptotically.

We shall see that the size of the atom is of order

$$s := s(b,Z) := Z^{-1/3}(1 + bZ^{-4/3})^{-2/5}. \tag{5.7}$$

Concerning the shortest allowed length scales of $\mathbf{B}$ we have the following version of the limit theorem.

Theorem 5.1 *Let $\mathbf{B} = \nabla \times \mathbf{A} : \mathbf{R}^3 \to \mathbf{R}^3$ be a fixed magnetic field satisfying (1.7–1.9). There exists a constant $K > 0$ depending on $\mathbf{B}$ such that if we define a rescaled field by $\mathbf{B}_{Z,b}(x) := b\mathbf{B}(x/[s(b,Z)K])$ then the following result holds. Assume that $Z, N \to \infty$ with N/Z fixed and $b/Z^2 \to 0$, then*

$$E(N, b\mathbf{B}_{Z,b}, Z)/E^{\mathrm{MTF}}(N, bB_{Z,b}, Z) \to 1.$$

We see therefore that the scale on which we allow the magnetic field to vary is greater than the size of the atom if $B(0) \gg Z^2$. It is an open question to allow the magnetic field to vary on the scale of the atom if $B(0) \gg Z^2$.

Both Theorem 1.3 and Theorem 5.1 are simple consequences of the following stronger result.

Theorem 5.2 *Consider sequences N_n of positive integers and Z_n of positive real numbers with $N_n, Z_n \to \infty$ as $n \to \infty$ and N_n/Z_n bounded above and below away from zero. If $k > 0$ is a constant then there exists a constant $K > 0$ such that if, $\mathbf{B}_n := \nabla \times \mathbf{A}_n : \mathbf{R}^3 \to \mathbf{R}^3$ is a sequence of magnetic fields satisfying $B_n(0) \geq k\|B_n\|$ and*

$$L(\mathbf{B}_n) \geq Ks(\|B_n\|, Z_n) \tag{5.8}$$

for all n,

$$l(\mathbf{B}_n)^{-1} s(\|B_n\|, Z_n) \max\left\{s(\|B_n\|, Z_n)^{-1/2} Z_n^{-1/2}, \|B_n\|^{1/2} Z_n^{-1}\right\} \to 0 \quad \text{as } n \to \infty, \tag{5.9}$$

and

$$\|B_n\| Z_n^{-3} \to 0 \tag{5.10}$$

as $n \to \infty$, then

$$\lim_{n\to\infty} E(N_n, \mathbf{B}_n, Z_n)/E^{\mathrm{MTF}}(N_n, B_n, Z_n) \to 1 \tag{5.11}$$

as $n \to \infty$.

The roles of the constants K and k may seem mysterious and the corresponding conditions could possibly be weakened. The constant k ensures that we are not considering a magnetic field which is much weaker in the center than its maximum. If this were the case, s, as defined here would not be the correct scale of the atom, since it presumably should involve also the typical field strength around the nucleus. The constant K ensures that the field does not change too fast on the scale of the atom. If this happened the atom could actually have two different relevant scales, one where B is large, another where B is small. In the following all positive constants, denoted by capital C or C_1 etc. , may depend on k. Constants that are universal will be denoted by the common symbol c. It is of no importance to the proof whether a constant is universal or depends on k.

We devote the rest of this chapter to the proof of Theorem 5.2. For simplicity we omit the subscript n.

5.1 Rescaling

We rescale the Hamiltonian (1.14) using the unitary

$$(U_s\psi)(x_1,\ldots,x_N) = s^{-3N/2}\psi(s^{-1}x_1,\ldots,s^{-1}x_N),$$

where $s = s(\|B\|, Z)$ is given in (5.7). We obtain that $Z^{-1}sE(N,\mathbf{B},Z)$ is the bottom of the spectrum of the operator

$$H_{\text{eff}} := \sum_{i=1}^{N}\left\{[\boldsymbol{\sigma}_i\cdot(h\mathbf{p}_i+\mathbf{A}_{\text{eff}}(x_i))]^2 - |x_i|^{-1}\right\} + Z^{-1}\sum_{i<j}^{N}|x_i-x_j|^{-1}, \tag{5.12}$$

where

$$\mathbf{B}_{\text{eff}}(x) := \nabla\times\mathbf{A}_{\text{eff}}(x) := s^{3/2}Z^{-1/2}\mathbf{B}(sx) \tag{5.13}$$

and

$$h := s^{-1/2}Z^{-1/2}. \tag{5.14}$$

Note that the assumptions (5.8)–(5.10) imply that we are considering a limit such that

$$h\to 0,\quad L(\mathbf{B}_{\text{eff}})\geq K,\quad l(\mathbf{B}_{\text{eff}})^{-1}h\to 0,\quad h^3\|B_{\text{eff}}\|l(\mathbf{B}_{\text{eff}})^{-2}\to 0 \tag{5.15}$$

We shall now perform the same rescaling of the MTF theory. We obtain from (5.6) and the scaling relation $\alpha^{-5/2}P(\alpha B,\alpha W) = P(B,W)$ that

$$\begin{aligned} Z^{-1}sE^{\text{MTF}}(N,B,Z) \;&=\; E_{scl}(h,\mathbf{B}_{\text{eff}},V_{\text{eff}}) \\ &\quad -\tfrac{1}{2}Z^{-1}\iint \rho_{\text{eff}}(x)|x-y|^{-1}\rho_{\text{eff}}(y)\mathrm{d}x\mathrm{d}y - s\mu N Z^{-1}, \end{aligned} \tag{5.16}$$

where we have used the definition (1.3) of E_{scl} and

$$\rho_{\text{eff}}(x) := s^3\rho^{\text{MTF}}(sx) \tag{5.17}$$

$$V_{\text{eff}}(x) := sZ^{-1}V^{\text{MTF}}(sx) = -|x|^{-1} + Z^{-1}\rho_{\text{eff}} * |x|^{-1} + sZ^{-1}\mu. \tag{5.18}$$

5.2 Reduction to a one-body problem

We shall here explain how to relate the many-body operator H_{eff} to a one-body operator, which can be analyzed by the semiclassical methods of the previous sections. As always this is done separately for the upper and the lower bound. Before we begin this analysis we want to note what error terms will be allowed. Since we are aiming at using the results of Section 4 we allow errors that are small in comparison to $\|B_{\text{eff}}\|h^{-2} + h^{-3}$. Using the definitions of s, $\mathbf{B}_{\text{eff}}$ and h in (5.7), (5.13) and (5.14) we see that

$$Z \leq \|B_{\text{eff}}\|h^{-2} + h^{-3} \leq 2Z. \tag{5.19}$$

We can therefore allow errors that are lower order than Z. Note that on the original scale we are aiming at proving that the energy is of order $Zs^{-1}(\|B_{\text{eff}}\|h^{-2} + h^{-3})$, i.e., of order Z^2s^{-1}.

5.2.1 Reducing the lower bound

In [LSY-II] this was done using the Lieb-Oxford inequality [LO] and the fact that the Lieb-Thirring inequality in [LSY-II] could be written as a kinetic energy inequality (see Corollary 2.2 in [LSY-II]). The standard way of transforming an estimate on the sum of eigenvalues of a one-body operator into a kinetic energy inequality is to use a Legendre transform. This requires, however, that the eigenvalue sum is estimated by the integral of a function of V. In our Lieb-Thirring inequality we have a term that depends on the gradient of V and we can therefore not transform it into a kinetic energy bound.

Instead of the Lieb-Oxford inequality we use another well known technique for reducing to a one-body problem. Choose a function $\varphi \in C_0^\infty(\mathbf{R}^3)$ which is spherically symmetric, non-negative and satisfies $\int \varphi = 1$. Let for all $a > 0$, $\varphi_a(x) = a^{-3}\varphi(x/a)$ we then have for all $\tilde{\rho} : \mathbf{R}^3 \to \mathbf{R}$

$$\begin{aligned}
&\sum_{1\leq i<j\leq N} |x_i - x_j|^{-1} \geq \sum_{1\leq i<j\leq N} \iint \varphi_a(x-x_i)\varphi_a(y-x_j)|x-y|^{-1}\mathrm{d}x\mathrm{d}y \\
&= \tfrac{1}{2}\sum_{i,j} \iint \varphi_a(x-x_i)\varphi_a(y-x_j)|x-y|^{-1}\mathrm{d}x\mathrm{d}y - \tfrac{1}{2}N \iint \varphi_a(x)\varphi_a(y)|x-y|^{-1}\mathrm{d}x\mathrm{d}y \\
&= \sum_{i=1}^N \int \tilde{\rho}(y)\varphi_a(x_i - x)|x-y|^{-1}\mathrm{d}x\mathrm{d}y - \tfrac{1}{2}\iint \tilde{\rho}(x)|x-y|^{-1}\tilde{\rho}(y)\mathrm{d}x\mathrm{d}y - c_\varphi N a^{-1} \\
&\quad + \tfrac{1}{2}\iint \left(\sum_i \varphi_a(x-x_i) - \tilde{\rho}(x)\right)\left(\sum_i \varphi_a(y-x_i) - \tilde{\rho}(y)\right)|x-y|^{-1}\mathrm{d}x\mathrm{d}y \\
&\geq \sum_i \int \tilde{\rho}(y)\varphi_a(x_i - x)|x-y|^{-1}\mathrm{d}x\mathrm{d}y - \tfrac{1}{2}\iint \tilde{\rho}(x)|x-y|^{-1}\tilde{\rho}(y)\mathrm{d}x\mathrm{d}y - c_\varphi N a^{-1},
\end{aligned}$$

where in the last inequality we used that $|x-y|^{-1}$ is of positive type (a positive kernel) and c_φ depends on φ, but not on a. From this inequality, with $\tilde{\rho} = \rho_{\text{eff}}$, and the definition (5.12) of H_{eff} we get the operator inequality

$$\begin{aligned} H_{\text{eff}} \;\; &\geq \;\; \sum_{i=1}^{N} \Big\{ [\boldsymbol{\sigma}_i \cdot (h\mathbf{p}_i + \mathbf{A}_{\text{eff}}(x_i))]^2 - |x_i|^{-1} + Z^{-1}\rho_{\text{eff}} * \varphi_a * |x_i|^{-1} \Big\} \\ &\quad -\tfrac{1}{2}Z^{-1} \iint \rho_{\text{eff}}(x)|x-y|^{-1}\rho_{\text{eff}}(y)\mathrm{d}x\mathrm{d}y - c_\varphi Z^{-1} N a^{-1}. \end{aligned}$$

Thus

$$\begin{aligned} H_{\text{eff}} \;\; &\geq \;\; \sum_{i=1}^{N} \Big\{ [\boldsymbol{\sigma}_i \cdot (h\mathbf{p}_i + \mathbf{A}_{\text{eff}}(x_i))]^2 + V_{a,R}^{-}(x_i) \Big\} \\ &\quad -\tfrac{1}{2}Z^{-1} \iint \rho_{\text{eff}}(x)|x-y|^{-1}\rho_{\text{eff}}(y)\mathrm{d}x\mathrm{d}y - s\mu N Z^{-1} - NR^{-1} - c_\varphi Z^{-1} N a^{-1}, \end{aligned} \tag{5.20}$$

where

$$V_{a,R}^{-}(x) := \Big(-|x|^{-1} + Z^{-1}\rho_{\text{eff}} * \varphi_a * |x|^{-1} + s\mu Z^{-1} \Big)\, \Theta_R(x)$$

with $\Theta_R(x) = \Theta(x/R)$ and Θ a smooth compactly supported function on $\mathbf{R}^3$ with $0 \leq \Theta \leq 1$ and satisfying $\Theta(x) = 1$ for $|x| \leq 1$ and $\Theta(x) = 0$ for $|x| \geq 2$.

We define the one-body operator

$$H_{a,R} := [\boldsymbol{\sigma} \cdot (h\mathbf{p} + \mathbf{A}_{\text{eff}}(x))]^2 + V_{a,R}^{-}(x). \tag{5.21}$$

Then with $e_1(H_{a,R}), e_2(H_{a,R}), \ldots$ being the negative eigenvalues of this operator we have

$$\begin{aligned} H_{\text{eff}} \;\; &\geq \;\; \sum_k e_k(H_{a,R}) - \tfrac{1}{2}Z^{-1} \iint \rho_{\text{eff}}(x)|x-y|^{-1}\rho_{\text{eff}}(x)\mathrm{d}x\mathrm{d}y \\ &\quad - s\mu N Z^{-1} - NR^{-1} - c_\varphi Z^{-1} N a^{-1}. \end{aligned} \tag{5.22}$$

Comparing this with (5.16) it should be clear that we intend to analyze the limits $h \to 0$, $R \to \infty$, and $a \to 0$ (but $aZ \to \infty$).

5.2.2 Reducing the upper bound

Here we use Lieb's variational principle (see [L-1981]), which states that if γ is an admissible density matrix on $L^2(\mathbf{R}^3;\mathbf{C}^2)$, i.e., an operator satisfying $0 \leq \gamma \leq 1$ and $\mathrm{Tr}[\gamma] \leq N$, then

$$\begin{aligned} Z^{-1}sE(N,\mathbf{B},Z) \;\; &\leq \;\; \mathrm{Tr}\Big[\gamma\Big([\boldsymbol{\sigma}\cdot(h\mathbf{p} + \mathbf{A}_{\text{eff}}(x))]^2 - |x|^{-1}\Big)\Big] \\ &\quad + \tfrac{1}{2}Z^{-1} \iint \rho_\gamma(x)|x-y|^{-1}\rho_\gamma(y)\mathrm{d}x\mathrm{d}y, \end{aligned} \tag{5.23}$$

where $\rho_\gamma(x,x) = \mathrm{Tr}_{\mathbf{C}^2}[\gamma(x,x)]$ is a function in $L^1(\mathbf{R}^3)$ with $\int \rho_\gamma \le N$. [Note that if we allow the value $+\infty$ we can consider the above expression as being defined for all admissible γ (not only those with range in $H^2(\mathbf{R}^3;\mathbf{C}^2)$).]

We shall choose as our γ the trial density matrix described in Theorem 4.3 corresponding to the potential $V_{\mathrm{eff}}\Theta_R$, where Θ_R is as above, and the magnetic field B_{eff}. (We may ignore ϱ in the definition of γ since we can assume that $\varrho > R$). We then have from (4.75) that

$$(1-\tilde{\varepsilon}(h,\mathbf{B}_{\mathrm{eff}})) \le \frac{\rho_\gamma(x)}{\int h^{-3}\partial_2 P(hB_{\mathrm{eff}}(u), [(\Theta_R V_{\mathrm{eff}})(u)]_-)\theta_\lambda(x-u)^2 \mathrm{d}u} \le (1+\tilde{\varepsilon}(h,\mathbf{B}_{\mathrm{eff}}))$$

where according to (5.15) we may assume that $\tilde{\varepsilon}(h,\mathbf{B}_{\mathrm{eff}}) \to 0$ in the limit we consider. If we now use the rescaled form of (5.1) we see that

$$(1-\tilde{\varepsilon}(h,\mathbf{B}_{\mathrm{eff}}))(\chi_R\rho_{\mathrm{eff}}) * \theta_\lambda^2(x) \le \rho_\gamma(x) \le (1+\tilde{\varepsilon}(h,\mathbf{B}_{\mathrm{eff}}))(\chi_{2R}\rho_{\mathrm{eff}}) * \theta_\lambda^2(x) \tag{5.24}$$

where χ_R is the characteristic function of the ball of radius R. Since,

$$\iint \theta_\lambda(x-z)^2|z-w|^{-1}\theta_\lambda(y-w)^2 \mathrm{d}z\mathrm{d}w \le |x-y|^{-1}$$

we have that

$$\tfrac{1}{2}\iint \rho_\gamma(x)|x-y|^{-1}\rho_\gamma(y)\mathrm{d}x\mathrm{d}y \le \tfrac{1}{2}(1+\tilde{\varepsilon}(h,\mathbf{B}_{\mathrm{eff}}))^2 \iint \rho_{\mathrm{eff}}(x)|x-y|^{-1}\rho_{\mathrm{eff}}(y)\mathrm{d}x\mathrm{d}y.$$

We therefore get from (5.4) and (5.23) that

$$\begin{aligned} Z^{-1}sE(N,\mathbf{B},Z) \le{}& \mathrm{Tr}\left[\gamma\left([\boldsymbol{\sigma}\cdot(h\mathbf{p}+\mathbf{A}_{\mathrm{eff}})]^2 + V_{\mathrm{eff}}\Theta_R\right)\right] - s\mu N Z^{-1} \\ & - \tfrac{1}{2}Z^{-1}\iint \rho_{\mathrm{eff}}(x)|x-y|^{-1}\rho_{\mathrm{eff}}(y)\mathrm{d}x\mathrm{d}y + \Delta^+E_1 + \Delta^+E_2, \end{aligned} \tag{5.25}$$

where according to (5.24) and assuming $R > 2\lambda$

$$\Delta^+E_1 := \Delta^+E_1(R) := \mu s Z^{-1}\int(\rho_{\mathrm{eff}} - \Theta_R\rho_\gamma) \le \mu s Z^{-1}\int\left(\rho_{\mathrm{eff}} - (1-\tilde{\varepsilon}(h,\mathbf{B}_{\mathrm{eff}}))(\chi_{R/2}\rho_{\mathrm{eff}})\right), \tag{5.26}$$

and (again assuming $R > 2\lambda$)

$$\begin{aligned} \Delta^+E_2 := \Delta^+E_1(R) \;:=\;& Z^{-1}(1+\tilde{\varepsilon}(h,\mathbf{B}_{\mathrm{eff}}))^2 \iint \rho_{\mathrm{eff}}(x)|x-y|^{-1}\rho_{\mathrm{eff}}(y)\mathrm{d}x\mathrm{d}y \\ & -Z^{-1}\iint \rho_{\mathrm{eff}}(x)|x-y|^{-1}(\Theta_R\rho_\gamma)(y)\mathrm{d}x\mathrm{d}y \\ \le\;& Z^{-1}\iint \rho_{\mathrm{eff}}(x)|x-y|^{-1}\left(\rho_{\mathrm{eff}}(y) - (\chi_{R/2}\rho_{\mathrm{eff}}) * \theta_\lambda^2(y)\right)\mathrm{d}x\mathrm{d}y \qquad (5.27) \\ & +c\left(\tilde{\varepsilon}(h,\mathbf{B}_{\mathrm{eff}}) + \tilde{\varepsilon}(h,\mathbf{B}_{\mathrm{eff}})^2\right)Z^{-1}\iint \rho_{\mathrm{eff}}(x)|x-y|^{-1}\rho_{\mathrm{eff}}(y)\mathrm{d}x\mathrm{d}y \end{aligned}$$

5.3 Properties of the potentials

In proving our main result we shall apply Theorem 4.1 with V replaced by $V_{a,R}^-$ for the lower bound and with $\Theta_R V_{\text{eff}}$ for the upper bound. In order to do this we must show that these potentials satisfy the necessary conditions of Theorem 4.1.

Lemma 5.3 *If $B(0) \geq k\|B\|$ then there exists constans $C_0 > 0$ and $K > 0$ (depending on k) such that if* $\mathbf{B}$ *satisfies (5.8) (with this constant K) we have*

$$[V_{\text{eff}}(x)]_- \leq C_0 \min\{|x|^{-1}, |x|^{-4}\}, \tag{5.28}$$

$$Z^{-1}\rho_{\text{eff}}(x) \leq C_0 \min\{|x|^{-3/2}, |x|^{-2}\} \tag{5.29}$$

$$Z^{-1}s\mu \leq C_0(Z/N), \tag{5.30}$$

where $s = s(\|B\|, Z)$.

Proof. It is clear from (5.18) that $[V_{\text{eff}}(x)]_- \leq |x|^{-1}$.
We consider $|x| \leq r$ for some $r > 0$. Using (5.8) we obtain that on this set

$$B_0 := k\|B\|e^{-K^{-1}s^{-1}r} \leq B(0)e^{-L^{-1}r} \leq B(x).$$

Consider now the magnetic function $\tilde{B}_r : \mathbf{R}^3 \to \mathbf{R}^3$ which is equal to $B(x)$ for $|x| \leq r$ and which is constantly equal to B_0 if $|x| > r$. We may now study the MTF theory of atoms in this 'magnetic' field. (The reader may worry that we have not defined a magnetic field, but only a scalar function. The observation is that, although this was not explicit in [LSY-II], MTF theory makes sense for any locally bounded scalar function $B(x)$.) It now follows from Theorem 4.11 in [LSY-II] that the support of this new MTF atom is bounded above by (see (4.32) in [LSY-II])

$$r_{\max} \leq c \max\left\{ZB_0^{-1}, Z^{1/5}B_0^{-2/5}\right\},$$

where $c > 0$ is a universal constant. This means that the new density and the negative part of the new effective potential vanish outside this radius (recall the MTF equation (5.1) relating the density and the effective potential). Since B and $\tilde{B}_r$ agree for $|x| \leq r$ we conclude by uniqueness of the minimizer to the MTF equations (5.1) and (5.2) that the original atom has radius $r_{\max}$ if

$$r_{\max} \leq r. \tag{5.31}$$

We shall now show that we may choose r such that this condition is satisfied.

We shall attempt to make a choice consistent with

$$e^{K^{-1}s^{-1}r} \leq 2. \tag{5.32}$$

Then $k\|B\|/2 \le B_0 \le \|B\|$ and

$$r_{\max} \le C_1 s(\|B\|, Z)$$

if $\|B\| > CZ^{4/3}$ for some $C, C_1 > 0$ depending on k. If we choose $r = C_1 s$ we have satisfied (5.31) and it is clear that if K is large enough then (5.32) is also satisified.

We have thus proved that if $\|B\| > CZ^{4/3}$ then

$$[V^{\mathrm{MTF}}(x)]_- = 0$$

if $|x| \ge C_1 s$. Recalling the definition (5.18) of V_{eff} this identity implies (5.28) if $\|B\| > CZ^{4/3}$.

We now turn to the case $\|B\| \le CZ^{4/3}$. Since $\partial_2 P(B, W) \ge cW^{3/2}$, we see from (5.3) and (5.1) that for $x \ne 0$, $V^{\mathrm{MTF}}(x)$ satisfies

$$-(4\pi)^{-1}\Delta V^{\mathrm{MTF}}(x) = \rho^{\mathrm{MTF}}(x) = \partial_2 P(B(x), [V^{\mathrm{MTF}}(x)]_-) \ge c[V^{\mathrm{MTF}}(x)]_-^{3/2}.$$

Since $\Delta|x|^{-4} = c(|x|^{-4})^{3/2}$ it follows from a simple comparison argument, using that $V^{\mathrm{MTF}}(x) \ge -c|x|^{-4}$ for small enough $|x|$ and that $V^{\mathrm{MTF}}(x) \ge -Z|x|^{-1} \to 0$ as $|x| \to \infty$, that $V^{\mathrm{MTF}}(x) \ge -c|x|^{-4}$ for all $x \ne 0$. This is true for all B. If we now use that $\|B\| \le CZ^{4/3}$ and hence $s \ge CZ^{-1/3}$ it then also follows that $V_{\mathrm{eff}}(x) \ge -C|x|^{-4}$. We have thus proved (5.28).

The Thomas-Fermi equation (5.1) implies that

$$\rho^{\mathrm{MTF}}(x) = \partial_2 P(B(x), [V^{\mathrm{MTF}}(x)]_-) \le c\|B\|[V^{\mathrm{MTF}}(x)]_-^{1/2} + c[V^{\mathrm{MTF}}(x)]_-^{3/2}.$$

If we insert the bound $[V^{\mathrm{MTF}}(x)]_- \le c|x|^{-4}$ we obtain

$$\rho_{\mathrm{eff}}(x) = s^3\rho^{\mathrm{MTF}}(sx) \le cs\|B\||x|^{-2} + cs^{-3}|x|^{-6}, \tag{5.33}$$

while the bound $[V^{\mathrm{MTF}}(x)]_- \le Z|x|^{-1}$ gives

$$\rho_{\mathrm{eff}}(x) \le cs^{5/2}\|B\|Z^{1/2}|x|^{-1/2} + cs^{3/2}Z^{3/2}|x|^{-3/2}. \tag{5.34}$$

If $\|B\| \le CZ^{4/3}$ we arrive at (5.29) using the bound (5.33) for large $|x|$ and (5.34) for small $|x|$. If $\|B\| \ge CZ^{4/3}$ we prove (5.29) using (5.34) and that, as proved above, $\rho_{\mathrm{eff}}(x) = 0$ if $|x| \ge C$.

In order to prove the bound on μ we observe from (5.1) and (5.2) that $\rho^{\mathrm{MTF}}(x) = 0$ if $Z|x|^{-1} \le \mu$. Thus from (5.29) we find that if $\mu \ne 0$ then

$$N = \int \rho^{\mathrm{eff}} \le cZ \int_{|x|\le\mu^{-1}Zs^{-1}} |x|^{-2}\mathrm{d}x = c\mu^{-1}Z^2 s^{-1},$$

which implies (5.30). □

We note that the bound in Lemma 5.3 on $\rho_{\rm eff}$ is not integrable. It follows, however, from Theorem 4.9 in [LSY-II] that $Z^{-1}\int\rho_{\rm eff}(x){\rm d}x \le 1$. In fact, it follows from the proof of that theorem that

$$Z^{-1}\rho_{\rm eff} * |x|^{-1} \le |x|^{-1}. \tag{5.35}$$

We shall now prove a stronger bound than (5.35) for small $|x|$.

Lemma 5.4 *With the same assumptions as in Lemma 5.3 and if $a>0$, we obtain the estimates*

$$Z^{-1}\rho_{\rm eff} * |x|^{-1} \le C\min\{1, |x|^{-1}\} \tag{5.36}$$

and

$$\int\left|\nabla(Z^{-1}\Theta_R(x)\rho_{\rm eff} * \varphi_a * |x|^{-1})\right|{\rm d}x \le CR^2 \quad \textit{and} \quad \int\left|\nabla(Z^{-1}\Theta_R(x)\rho_{\rm eff} * |x|^{-1})\right|{\rm d}x \le CR^2. \tag{5.37}$$

Proof: Considering (5.35) it is enough, in order to prove (5.36), to show that $Z^{-1}\rho_{\rm eff} * |x|^{-1} \le C$ for $|x|\le 1$. Using (5.29) and $\int\rho_{\rm eff} \le N$ we find for $|x|\le 1$

$$Z^{-1}\rho_{\rm eff} * |x|^{-1} \le C\int_{|y|\le 2}|y|^{-3/2}|x-y|^{-1}{\rm d}y + N/Z \le C.$$

To prove (5.37) we write

$$\int\left|\nabla(Z^{-1}\Theta_R(x)\rho_{\rm eff} * |x|^{-1})\right|{\rm d}x \le R^{-1}Z^{-1}\int_{|x|<2R}\rho_{\rm eff} * |x|^{-1}{\rm d}x + Z^{-1}\int_{|x|<2R}\rho_{\rm eff} * |x|^{-2}{\rm d}x.$$

Inserting the bounds (5.29) and (5.36) we obtain (5.37). Note that bounds similar to (5.29) and (5.36), possibly with different constants, hold also if $\rho_{\rm eff}$ is replaced by $\rho_{\rm eff}*\varphi_a$. In fact, to prove (5.36) for $\rho_{\rm eff}*\varphi_a$ (with the same constant) simply note that $\rho_{\rm eff}*|x|^{-1}$ is superharmonic. To prove (5.29) for $\rho_{\rm eff}*\varphi_a$ one simply computes the convolution on both sides of (5.29). $\square$

We are now ready to control the quantities in (4.4–4.7).

Lemma 5.5 *There exists a constant $C>0$ (depending on only k) such that if $R>1$ and $a<1$ we have the estimates*

$$|E_{scl}(h, B_{\rm eff}, V^-_{a,R})| \ \ge\ C(\|B_{\rm eff}\|h^{-2}+h^{-3}) \tag{5.38}$$

$$|E_{scl}(h, B_{\rm eff}, \Theta_R V_{\rm eff})| \ \ge\ C(\|B_{\rm eff}\|h^{-2}+h^{-3}) \tag{5.39}$$

$$\mathcal{E}_{h,\mathbf{B}_{\rm eff}}([V^-_{a,R}]_-) \ \le\ C(\|B_{\rm eff}\|h^{-2}+h^{-3}) \tag{5.40}$$

and

$$\mathcal{E}_{h,\mathbf{B}_{\rm eff}}([\Theta_R V_{\rm eff}]_-) \le \mathcal{E}_{h,\mathbf{B}_{\rm eff}}([V_{\rm eff}]_-) \ \le\ C(\|B_{\rm eff}\|h^{-2}+h^{-3}). \tag{5.41}$$

Proof: Since $\rho_{\text{eff}} * |x|^{-1}$ is superharmonic we have $\rho_{\text{eff}} * \varphi_a * |x|^{-1} \leq \rho_{\text{eff}} * |x|^{-1}$. Hence $[V_{a,R}^-]_- \geq [V_{\text{eff}}]_- \Theta_R$. Using (5.36) and (5.30) and recalling that N/Z is bounded away from zero we see that for $|x| < C$, $[V_{\text{eff}}]_- \Theta_R \geq C|x|^{-1}$. The estimates (5.38) and (5.39) easily follow from this together with the assumptions $B(0) \geq k\|B\|$ and $L(B_{\text{eff}}) \geq K$ from (5.15).

The estimate (5.41) is an immediate consequence of (5.28). In order to prove (5.40) observe that

$$V_{a,R}^-(x) = \left(V_{\text{eff}} * \varphi_a(x) - |x|^{-1} + \varphi_a * |x|^{-1}\right)\Theta_R(x) \geq -[V_{\text{eff}} * \varphi_a(x)]_- - \left||x|^{-1} - \varphi_a * |x|^{-1}\right|.$$

From Jensen's inequality (note that $t \mapsto [t]_-$ is convex) we conclude that

$$\mathcal{E}_{h,\mathbf{B}_{\text{eff}}}([V_{a,R}^-]_-) \leq \mathcal{E}_{h,\mathbf{B}_{\text{eff}}}([V_{\text{eff}}]_-) + \mathcal{E}_{h,\mathbf{B}_{\text{eff}}}(|x|^{-1} - \varphi_a * |x|^{-1}).$$

Since φ_a is supported for $|x| < ca$, is spherically symmetric, and has integral 1 it follows from Newton's Theorem that $|x|^{-1} - \varphi_a * |x|^{-1} = 0$ if $|x| > ca$. Since $0 < |x|^{-1} - \varphi_a * |x|^{-1} \leq |x|^{-1}$ the estimate (5.40) follows immediately. □

Lemma 5.6 *If $R > 1$ and $a < 1$ then both for $V = V_{a,R}^-$ and $V = V_{\text{eff}}\Theta_R$ we have*

$$\frac{\mathcal{E}_{h,\mathbf{B}_{\text{eff}}}([V]_\pm - [V(\cdot - y)]_\pm)}{\|B_{\text{eff}}\|h^{-2} + h^{-3}} \leq C\left(|y|^{1/2} + |y|^{3/2}\left(1 + |\ln(|y|/R)|\right)\right). \tag{5.42}$$

Likewise,

$$\frac{\mathcal{F}_{h,\mathbf{B}_{\text{eff}}}([V]_\pm - [V(\cdot - y)]_\pm)}{\|B_{\text{eff}}\|h^{-2} + h^{-3}} \leq C\Big(|y|^{1/2} + |y|^{3/2}\left(1 + |\ln(|y|/R)|\right) + |y|R + hR^2\Big). \tag{5.43}$$

Proof: Note that for all V, $|[V(x)]_\pm - [V(x-y)]_\pm| \leq |V(x) - V(x-y)|$. Using the simple case, $\|u * v\|_p \leq \|u\|_1\|v\|_p$, of Young's inequality for $p = 1$, $p = 3/2$ or $p = 5/2$ we find for both cases $V = V_{a,R}^-$ and $V = \Theta_R V_{\text{eff}}$ that

$$\begin{aligned}
\|V(\cdot) - V(\cdot - y)\|_p^p &\leq (1 + (N/Z))^p\left(\left\|\Theta_R(\cdot)|\cdot|^{-1} - \Theta_R(\cdot - y)|\cdot - y|^{-1}\right\|_p^p\right) \\
&\leq C\begin{cases} |y|R, & \text{if } p = 1 \\ |y|^{1/2}, & \text{if } p = 5/2 \\ |y|^{3/2}\left(1 + |\ln(|y|/R)|\right), & \text{if } p = 3/2 \end{cases}.
\end{aligned} \tag{5.44}$$

This gives (5.42).

We next turn to the estimates on $\mathcal{F}_{h,\mathbf{B}_{\text{eff}}}$. First we note that the requirements (5.15) on $\mathbf{B}_{\text{eff}}$, $l(\mathbf{B}_{\text{eff}})$ and $L(\mathbf{B}_{\text{eff}})$ imply that $d(h,\mathbf{B}_{\text{eff}})^{-1} \leq Ch^{-1}$. Thus for all W

$$\mathcal{F}_{h,\mathbf{B}_{\text{eff}}}(W) \leq C\left(\mathcal{E}_{h,\mathbf{B}_{\text{eff}}}(W) + (\|B_{\text{eff}}\|h^{-2}+h^{-3})\int |W| + (\|B_{\text{eff}}\|h^{-2}+h^{-3})h\int |\nabla W|\right).$$

In order to prove (5.43) it therefore remains to control $\int |V(x)-V(x-y)|\mathrm{d}x$ and $\int |\nabla V(x) - \nabla V(x-y)|\mathrm{d}x$ for the two cases $V = V_{a,R}^{-}$ and $V = \Theta_R V_{\text{eff}}$. The first integral was controlled in (5.44). For the gradient we use (5.37) and the trivial estimate $\int_{|x|\leq 2R} |\nabla |x|^{-1}|\mathrm{d}x \leq CR^2$ to arrive at

$$\int |\nabla V(x) - \nabla V(x-y)|\,\mathrm{d}x \leq \int (|\nabla V(x)| + |\nabla V(x-y)|)\,\mathrm{d}x \leq CR^2,$$

in both cases. □

Corollary 5.7 *There exist constants $C_{\pm} > 0$ (depending only on k) such that the MTF energy satisfies*

$$-C_{-}\left(\|B_{\text{eff}}\|h^{-2}+h^{-3}\right) \geq Z^{-1}sE^{\text{MTF}}(N,B,Z) \geq -C_{+}\left(\|B_{\text{eff}}\|h^{-2}+h^{-3}\right). \tag{5.45}$$

Note, in particular, that $E^{\text{MTF}}(N,B,Z)$ is negative.

Proof: Recall that according to (5.19), $\|B_{\text{eff}}\|h^{-2}+h^{-3} \sim Z$. We shall use the expression (5.16) for E^{MTF}. From (5.28) and (5.39) we find that

$$0 < CZ \leq |E_{scl}(h, B_{\text{eff}}, \Theta_R V_{\text{eff}})| \leq |E_{scl}(h, B_{\text{eff}}, V_{\text{eff}})| \leq C^{-1}Z.$$

We also see from (5.36) that

$$0 \leq Z^{-1}\iint \rho_{\text{eff}}(x)|x-y|^{-1}\rho_{\text{eff}}(y)\mathrm{d}x\mathrm{d}y \leq C\int \rho_{\text{eff}}(x)\mathrm{d}x \leq CN.$$

Inserting these two bounds together with (5.30) into (5.16) proves the corollary. □

5.4 Completing the proof of the MTF Theorem

We shall now put together the results of the previous sections to complete the proof of the main result, Theorem 5.2. We begin by proving an asymptotic lower bound on $E(N,\mathbf{B},Z)$.

Proof of the lower bound: From (5.22) and (5.16) we conclude that

$$Z^{-1}sE(N,\mathbf{B},Z) \geq Z^{-1}sE^{\text{MTF}}(N,B,Z) - \Delta_1^{-}E - \Delta_2^{-}E - \Delta_3^{-}E$$

where we have divided the error into three separate terms

$$\Delta_1^- E := \Delta_1^- E(a,R) := \left|\sum_k e_k(H_{a,R}) - E_{scl}(h, B_{\text{eff}}, V_{a,R}^-)\right|$$

$$\Delta_2^- E := \Delta_2^- E(a,R) := \left|E_{scl}(h, B_{\text{eff}}, V_{a,R}^-) - E_{scl}(h, B_{\text{eff}}, V_{\text{eff}})\right|$$

and

$$\Delta_3^- E := \Delta_3^- E(a,R) := NR^{-1} + c_\varphi Z^{-1} N a^{-1}.$$

We shall study these error terms in the limit as $n \to \infty$. Recall, that we are omitting the subscript n on Z, N, and $\mathbf{B}$. We shall prove that the three error terms satisfy

$$\lim_{R\to\infty} \lim_{a\to 0} \limsup_{n\to\infty} \frac{\Delta_j^- E}{\|B_{\text{eff}}\| h^{-2} + h^{-3}} = 0. \tag{5.46}$$

It then follows from Corollary 5.7 that

$$\limsup_{n\to\infty} \frac{E(N,\mathbf{B},Z)}{E^{\text{MTF}}(N,B,Z)} \leq 1, \tag{5.47}$$

(recall that the energies are negative) which is what we want to prove.

That (5.46) holds for $\Delta_3^- E$, i.e., for $j=3$, is trivial.

It follows from (5.15) that we consider a limit where $\mathbf{B}$ and h satisfy the conditions needed for Theorem 4.1. Finally, Lemmas 5.5 and 5.6 show that the conditions on the potential $V_{a,R}^-$ are satisfied. Note that condition (4.9) is trivially satisfied for fixed R. We conclude that

$$\limsup_{n\to\infty} \frac{\Delta_1^- E}{\|B_{\text{eff}}\| h^{-2} + h^{-3}} = \limsup_{n\to\infty} \frac{\Delta_1^- E}{|E_{scl}(h, B_{\text{eff}}, V_{a,R}^-)|} = 0.$$

It remains to prove (5.46) for $\Delta_2^- E$. We observe that

$$\frac{\Delta_2^- E}{\|B_{\text{eff}}\| h^{-2} + h^{-3}} \leq C \sum_{\substack{p=3/2\\p=5/2}} \left(\|[V_{\text{eff}}]_- - \Theta_R[V_{\text{eff}}]_-\|_p^p + \|Z^{-1}\rho_{\text{eff}} * \varphi_a * |x|^{-1} - Z^{-1}\rho_{\text{eff}} * |x|^{-1}\|_p^p \right).$$

Using the bound (5.28) on V_{eff} it is obvious that

$$\lim_{R\to\infty} \lim_{a\to 0} \limsup_{n\to\infty} \|[V_{\text{eff}}]_- - \Theta_R[V_{\text{eff}}]_-\|_p^p = 0$$

for both $p = 3/2$ and $p = 5/2$. Here there really is no dependence on the parameter a.

Finally, we have

$$\left\| Z^{-1}\rho_{\text{eff}} * \left(|x|^{-1} - \varphi_a * |x|^{-1}\right)\right\|_p \leq \|Z^{-1}\rho_{\text{eff}}\|_1 \||x|^{-1} - \varphi_a * |x|^{-1}\|_p \leq c(N/Z)a^{(3-p)/p},$$

where we used Newton's Theorem as in the proof of Lemma 5.5. This proves the limit (5.46) for $\Delta_2^- E$. □

Proof of the upper bound: We proceed analogously to the lower bound. From (5.25) and (5.16) we have

$$Z^{-1}sE(N, \mathbf{B}, Z) \leq Z^{-1}sE^{\text{MTF}}(N, B, Z) + \Delta_1^+ E + \Delta_2^+ E + \Delta_3^+ E + \Delta_4^+ E,$$

where $\Delta_1^+ E$ and $\Delta_2^+ E$ were defined in (5.26)–(5.27) and

$$\Delta_3^+ E := \Delta_3^+ E(R) := \left| \text{Tr}\left[\gamma\left([\boldsymbol{\sigma}\cdot(h\mathbf{p} + \mathbf{A}_{\text{eff}})]^2 + V_{\text{eff}}\Theta_R\right)\right] - E_{scl}(h, B_{\text{eff}}, \Theta_R V_{\text{eff}})\right|$$

and

$$\Delta_4^+ E := \Delta_4^+ E(R) := \left|E_{scl}(h, B_{\text{eff}}, \Theta_R V_{\text{eff}}) - E_{scl}(h, B_{\text{eff}}, V_{\text{eff}})\right|.$$

As for the lower bound the goal is to prove that the four error terms satisfy

$$\lim_{R\to\infty} \limsup_{n\to\infty} \frac{\Delta_j^+ E}{\|B_{\text{eff}}\| h^{-2} + h^{-3}} = 0. \tag{5.48}$$

It then follows that

$$\liminf_{n\to\infty} \frac{E(N, \mathbf{B}, Z)}{E^{\text{MTF}}(N, B, Z)} \geq 1 \tag{5.49}$$

which together with (5.47) proves Theorem 5.2.

As for the lower bound we conclude from the results of the previous sections that we can apply Theorem 4.3 to conclude that (5.48) holds for $\Delta_3^+ E$, i.e., for $j = 3$.

That (5.48) holds for $\Delta_4^+ E$, is a simple consequence of (5.28).

We turn now to $\Delta_1^+ E$. From (5.1) and (5.2) it is clear that $\rho^{\text{MTF}}(x) = 0$ if $Z|x|^{-1} \leq \mu$. Thus $\rho_{\text{eff}}(x) = 0$ if $|x| > Zs^{-1}\mu^{-1}$. Thus if $R/2 \geq Zs^{-1}\mu^{-1}$ we get from (5.30)

$$\Delta_1^+ E \leq \tilde{\varepsilon}(h, \mathbf{B}_{\text{eff}}) Z^{-1} s\mu \int \rho_{\text{eff}} \leq \tilde{\varepsilon}(h, \mathbf{B}_{\text{eff}}) C_0(Z/N) \int \rho_{\text{eff}} \leq C\tilde{\varepsilon}(h, \mathbf{B}_{\text{eff}}) Z,$$

where in the last inequality we used that $\int \rho_{\text{eff}} \leq Z$ and the assumption that N/Z is bounded below. On the other hand if $R/2 \leq Zs^{-1}\mu^{-1}$, i.e., if $\mu s Z^{-1} \leq 2R^{-1}$ then (assuming $\tilde{\varepsilon}(h, \mathbf{B}_{\text{eff}}) \leq 1$) $\Delta_1^+ E \leq 2R^{-1}Z$. Thus we have proved that

$$\Delta_1^+ E \leq CZ \min\left\{\tilde{\varepsilon}(h, \mathbf{B}_{\text{eff}}), R^{-1}\right\}.$$

Recalling (5.19) and $\tilde{\varepsilon}(h, \mathbf{B}_{\rm eff}) \to 0$ as $n \to \infty$ we conclude (5.48) for $\Delta_1^+ E$.

It remains to consider $\Delta_2^+ E$. Assuming that $\tilde{\varepsilon}(h, \mathbf{B}_{\rm eff}) < 1$ and $\lambda \leq R/2$

$$\begin{aligned} \Delta_2^+ E \ \leq\ & Z^{-1} \iint_{|y| \geq R/2} \rho_{\rm eff}(x)|x-y|^{-1}\rho_{\rm eff}(y) {\rm d}x{\rm d}y \\ & + Z^{-1} \left| \iint \rho_{\rm eff}(x)|x-y|^{-1} \Big((\chi_{R/2}\rho_{\rm eff})(y) - (\chi_{R/2}\rho_{\rm eff}) * \theta_\lambda^2(y) \Big) {\rm d}x{\rm d}y \right| + C\tilde{\varepsilon}(h, \mathbf{B}_{\rm eff})Z, \end{aligned}$$

where we estimated the last term in $\Delta_2^+ E$ using (5.36) and $\int \rho_{\rm eff} \leq Z$. From (5.36) and $\int \rho_{\rm eff} \leq Z$ we also see that

$$Z^{-1} \iint_{|y| \geq R/2} \rho_{\rm eff}(x)|x-y|^{-1}\rho_{\rm eff}(y) {\rm d}x{\rm d}y \leq CZR^{-1}.$$

Finally, using (5.29) we see that $\|Z^{-1}\rho_{\rm eff}\|_p < C$ for $3/2 < p < 2$. Thus using Hölder and Young's inequalities we obtain

$$\begin{aligned} & Z^{-1} \left| \iint \rho_{\rm eff}(x)|x-y|^{-1} \Big((\chi_{R/2}\rho_{\rm eff})(y) - (\chi_{R/2}\rho_{\rm eff}) * \theta_\lambda^2(y) \Big) {\rm d}x{\rm d}y \right| \\ \leq\ & \|Z^{-1}\rho_{\rm eff}\|_p \|(\chi_{R/2}\rho_{\rm eff}) * \Big(|x|^{-1} - \theta_\lambda^2 * |x|^{-1} \Big) \|_q \\ \leq\ & C \left\| \chi_{R/2}\rho_{\rm eff} \right\|_1 \left\| |x|^{-1} - \theta_\lambda^2 * |x|^{-1} \right\|_q \leq CZ\lambda^{(3-q)/q}, \end{aligned}$$

where $p^{-1} + q^{-1} = 1$, so that $2 < q < 3$. As before we used Newton's Theorem to conclude that since θ_λ is supported on $|x| \leq 2\lambda$, is spherically symmetric and has integral one then $|x|^{-1} - \theta_\lambda^2 * |x|^{-1}$ vanishes for $|x| > 2\lambda$ and is bounded by $|x|^{-1}$ for $|x| \leq 2\lambda$.

Putting these estimates together gives

$$\Delta_2^+ E \leq CZ \Big(R^{-1} + \lambda^2 + \tilde{\varepsilon}(h, \mathbf{B}_{\rm eff}) \Big).$$

Since $\tilde{\varepsilon}(h, \mathbf{B}_{\rm eff}) \to 0$ and $\lambda \to 0$ as $n \to 0$ we see from (5.19) that (5.48) holds also for $\Delta_2^+ E$.
□

A The geometry of the three dimensional magnetic field

In this Appendix we recall two results from [ES-I] related to the geometry of a non-homogeneous three dimensional magnetic field. Here we just give the statements and the necessary notations for the reader's convenience, the proofs are found in [ES-I].

The following proposition will be used to approximate a general magnetic field by a *constant direction* field. We recall the definitions $l(\mathbf{B})^{-1} = \|\nabla(\mathbf{B}/B)\|$ and $L(\mathbf{B})^{-1} = \||\nabla B|/B\|$.

Proposition A.1 *Consider an arbitrary cube $\Omega \subset \mathbf{R}^3$ with center Q and edge length λ and a nonvanishing C^1 magnetic (divergence free) field $\mathbf{B} : \mathbf{R}^3 \to \mathbf{R}^3$. Assume that*

$$(6 + 3\sqrt{3})\lambda l(\mathbf{B})^{-1} \leq 1. \tag{A.1}$$

Then there exists a magnetic (divergence free) field $\tilde{\mathbf{B}}$, with constant direction parallel to the field at the center Q of Ω, such that for all $x \in \Omega$

$$|\mathbf{B}(x) - \tilde{\mathbf{B}}(x)| \leq \lambda l(\mathbf{B})^{-1} \left\{ \sup_{|x-Q| \leq 5\lambda} B(x) \right\} \left(\frac{\sqrt{3} + 4\sqrt{6}}{\sqrt{2}} + \frac{6 + 3\sqrt{3}}{2} \lambda \left(l(\mathbf{B})^{-1} + L(\mathbf{B})^{-1} \right) \right) \tag{A.2}$$

and

$$|\nabla \tilde{\mathbf{B}}(x)| \leq |\nabla \mathbf{B}(x)| \leq \left\{ \sup_{|x-Q| \leq 5\lambda} B(x) \right\} (L(\mathbf{B})^{-1} + l(\mathbf{B})^{-1}). \tag{A.3}$$

Remarks. (i) The assumption (A.1) is a geometric condition, which states that the field lines of the field $\mathbf{B}$ should not vary too fast over the scale of the cube.

(ii) In our application, where typically $l \gg \lambda$, the approximation in (A.2) will be better than the straightforward choice $\tilde{\mathbf{B}}(x) := \mathbf{B}(Q)$ (constant field), since that would yield only $|\mathbf{B}(x) - \mathbf{B}(Q)| \leq (\sqrt{3}/2)\lambda \sup |\nabla \mathbf{B}|$, which is of order $\sup |B| \lambda (l^{-1} + L^{-1})$. This is worse by a factor of $l\lambda^{-1} \gg 1$ than the similar term in (A.2).

We shall, indeed, also need approximations of the magnetic field by a constant field and not just a constant direction field. In order to keep the same accuracy in the approximation we must restrict to a smaller region. It turns out that we can cover the cube by parallel cylinders such that within each of these we, without losing in the approximation, can approximate the magnetic field by a constant field along the cylinder axis.

To formulate this more precisely we choose an orthonormal coordinate system $\{\xi_i\}_{i=1}^3$ in $\mathbf{R}^3$, such that the center Q of the cube Ω is the origin and that $\mathbf{B}(Q) = \mathbf{B}(0)$ points in the positive third direction. Note that the sides of Ω need not be parallel with the coordinate planes in this new coordinate system. We shall refer to the plane $\mathcal{P} := \{ \xi \, : \, \xi_3 = 0\}$ as the base plane of the cube. We consider cylinders, C_P, given in this new coordinate system by

$$C_P = \{ \xi \, : \, |\xi_\perp - P| \leq w \ \ |\xi_3| \leq \sqrt{3}\lambda/2\}, \tag{A.4}$$

where $P \in \mathcal{P}$ and $w > 0$ (here $\xi_\perp := (\xi_1, \xi_2, 0)$). The point P is called the center of the cylinder.

Note that the cylinders are aligned along $\mathbf{B}(Q)$, the magnetic field at the center of the cube Ω and that the union of all these cylinders covers Ω. Moreover, all the cylinders C_P

such that $C_P \cap \Omega \neq \emptyset$ are subsets of the larger cube Ω', that, in the new coordinate system, is defined by $[-w - \sqrt{3}\lambda/2, w + \sqrt{3}\lambda/2]^3$.

Corollary A.2 *Let Ω, Ω' and C_P, for $P \in \mathcal{P}$ be as defined above. Assume that the magnetic field $\mathbf{B}$ satisfies*

$$(6 + 3\sqrt{3})(2w + \sqrt{3}\lambda)l(\mathbf{B})^{-1} \leq 1. \tag{A.5}$$

Then within each C_P such that $C_P \cap \Omega \neq \emptyset$, one can approximate the magnetic field $\mathbf{B}$ by a constant field, $\tilde{\mathbf{B}}_P$ pointing along the axis of the cylinder, with the following precision

$$|\mathbf{B}(x) - \tilde{\mathbf{B}}_P| \leq \tag{A.6}$$

$$(2w+\sqrt{3}\lambda)l(\mathbf{B})^{-1}\left\{\sup_{|x-Q|<5(\sqrt{3}\lambda+2w)} B(x)\right\}\left(\frac{\sqrt{3}+4\sqrt{6}}{\sqrt{2}}+\frac{6+3\sqrt{3}}{2}(2w+\sqrt{3}\lambda)\left(l(\mathbf{B})^{-1}+L(\mathbf{B})^{-1}\right)\right)$$

$$+w\left\{\sup_{|x-Q|<5(\sqrt{3}\lambda+2w)} B(x)\right\}\left(l(\mathbf{B})^{-1}+L(\mathbf{B})^{-1}\right),$$

for $x \in C_P$.

Remark. Note that it is only the radius of the cylinder that appears in the last term in (A.6). This is important since in our applications, typically $w \ll \lambda$, i.e., the cylinder is very thin compared to the cube. The size λ of the cube appears only together with $l(\mathbf{B})^{-1}$ which, in our setup, will typically be small. It is in this way that we will achieve that the constant field approximation within C_P is as good as the constant direction field approximation within Ω.

The corollary of the previous proposition will provide us with a good approximating constant field within a cylinder (see (A.4)). Here we show that the difference field (which is supposed to be small) can be generated by a small vector potential within this cylinder. In general, if one is given a magnetic field within a domain, then there exists a vector potential bounded by the supremum of the field times the largest linear size of the domain (see (A.9) below). For instance, one can choose the gauge given by the Poincaré formula (see below). This gives a very crude bound for domains which are elongated cylinders.

The crucial fact is that, assuming some bound on the first derivative of the field in addition to its supremum bound, one can choose a gauge independent of the longest linear size of the domain. In particular, we can choose a gauge within our cylinder which is bounded by a constant independent of the length of the cylinder.

Proposition A.3 *Given a C^1 magnetic field $\beta : \mathbf{R}^3 \to \mathbf{R}^3$ and consider a cylinder C with radius w. Then there exists a vector potential $\alpha : \mathbf{R}^3 \to \mathbf{R}^3$, such that $\nabla \times \alpha = \beta$ and*

$$\sup_C \|\alpha\| \leq 4(w \sup_C \|\beta\| + w^2 \sup_C \|\nabla \beta\|). \tag{A.7}$$

The bound is uniform in the length of the cylinder.

Remark. For comparison, the Poincaré formula

$$\alpha(y) = \int_0^1 t(\beta(ty) \times y) \mathrm{d}t \tag{A.8}$$

obviously yields a gauge α, for any domain D, satisfying the bound

$$\sup_D \|\alpha\| \leq \sqrt{3} \sup_D \|\beta\| \cdot \mathrm{diam}(D). \tag{A.9}$$

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