Bounds on One–Dimensional Exchange Energies with Application to Lowest Landau Band Quantum Mechanics

Christian Hainzl
Robert Seiringer

Vienna, Preprint ESI 990 (2001) February 12, 2001

Supported by Federal Ministry of Science and Transport, Austria
Available via http://www.esi.ac.at

Bounds on one-dimensional exchange energies with application to lowest Landau band quantum mechanics

Christian Hainzl[1] and Robert Seiringer[2]

Institut für Theoretische Physik, Universität Wien
Boltzmanngasse 5, A-1090 Vienna, Austria

February 7, 2001

Abstract

By means of a generalization of the Fefferman-de la Llave decomposition we derive a general lower bound on the interaction energy of one-dimensional quantum systems. We apply this result to a specific class of lowest Landau band wave functions.

An important issue in the quantum mechanics of many interacting particles is the description of the energy of the system in terms of the particle density. In particular, a lower bound to the difference of the interaction energy and its "direct" part is of interest. For the three-dimensional Coulomb potential it is known that for any N-particle wave function Ψ the so-called Lieb-Oxford inequality [LO81]

$$\langle\Psi|\sum_{i<j}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}\Psi\rangle \geq D(\rho_\Psi,\rho_\Psi) - 1.68\int_{\mathbb{R}^3}\rho_\Psi(\mathbf{x})^{4/3}d^3\mathbf{x} \tag{1}$$

holds, where $D(\rho,\rho)=\frac{1}{2}\int_{\mathbb{R}^6}\rho(\mathbf{x})\rho(\mathbf{y})|\mathbf{x}-\mathbf{y}|^{-1}d^3\mathbf{x}d^3\mathbf{y}$ is the direct part of the energy, and ρ_Ψ is the density of Ψ. This inequality is very useful for many electron systems, e.g. large atoms, where the "exchange term" $\int\rho_\Psi^{4/3}$ really captures the correct order of magnitude. However, for states Ψ describing particles in strong magnetic fields, $\int\rho_\Psi^{4/3}$ is generally much too large, and (1), although valid for all Ψ, is not very useful in this case.

In the presence of a strong, homogeneous magnetic field, the particles are confined to the lowest Landau band, which determines their motion perpendicular to the magnetic field and makes them behave essentially like a one-dimensional system. Therefore we study the one-dimensional analogue of (1) for arbitrary convex interaction potentials. For short, we shall call the indirect part of the interaction energy the "exchange energy"; it is defined by

$$\mathrm{Ex}_\psi = \langle\psi|\sum_{i<j}V(|x_i-x_j|)\psi\rangle - \tfrac{1}{2}\int_{\mathbb{R}^2}\rho_\psi(x)\rho_\psi(y)V(|x-y|)dxdy. \tag{2}$$

[1] E-Mail: hainzl@thp.univie.ac.at
[2] E-Mail: rseiring@ap.univie.ac.at

In the following, we derive a general lower bound to Ex_ψ. Our method follows closely the proof of the Lieb-Oxford inequality given in [S95]. The following Lemma replaces the Fefferman-de la Llave decomposition of the Coulomb potential. We will then apply this general bound to special potentials of interest in the study of systems in magnetic fields.

1 LEMMA (Decomposition of V). *Let $V : \mathbb{R}_+ \to \mathbb{R}$ be twice continuously differentiable, with $\lim_{x\to\infty} V(x) = \lim_{x\to\infty} xV'(x) = 0$. Then*

$$V(x) = 2\int_0^\infty V''(2r)\chi_r * \chi_r(x)dr, \tag{3}$$

where $\chi_r(x) = \Theta(r - |x|)$.

Proof. A simple computation, using partial integration and the fact that $\chi_r * \chi_r(x) = \max\{0, 2r - x\}$. □

Although stated only for differentiable potentials, Lemma 1 holds more generally if the derivatives are interpreted in the sense of distributions. In particular, if V is convex and tends to zero at infinity, V'' defines a Borel measure and (3) holds. Note also that (3) implies that a convex V is positive definite.

We now consider N-particle wave functions $\psi \in \mathcal{L}^2(\mathbb{R}^N, d^N x)$. A vector in $\mathbb{R}^N$ will be denoted by $(x_1, \ldots, x_N)$. Corresponding to ψ its density ρ_ψ is defined as

$$\rho_\psi(x) = \sum_{i=1}^N \int_{\mathbb{R}^{N-1}} |\psi(x_1, \ldots, x_{i-1}, x, x_{i+1}, \ldots, x_N)|^2 dx_1 \ldots dx_{i-1} dx_{i+1} \ldots dx_N. \tag{4}$$

Note that $\int \rho = N$. Assuming that ψ has finite kinetic energy, i.e.,

$$\langle\psi| \sum_{i=1}^N -\frac{\partial^2}{\partial x_i^2} |\psi\rangle < \infty, \tag{5}$$

$\sqrt{\rho_\psi}$ is in $\mathcal{H}^1(\mathbb{R})$ by the Hoffmann-Ostenhof inequality [HH77], so it is a bounded and continuous function. In particular, $\rho_\psi \in \mathcal{L}^2(\mathbb{R})$, so we can define a *mean density* $\bar{\rho}_\psi$ by

$$\bar{\rho}_\psi = \frac{1}{N}\int_{-\infty}^\infty \rho_\psi(x)^2 dx. \tag{6}$$

Given a function $f \in \mathcal{L}^p(\mathbb{R})$, its Hardy-Littlewood maximal function f^* is defined as

$$f^*(x) = \sup_{r>0} \frac{1}{2r}\int_{x-r}^{x+r} |f(y)|dy. \tag{7}$$

For $p > 1$ the inequality

$$\|f^*\|_p \leq 2\left(\frac{2p}{p-1}\right)^{1/p} \|f\|_p \tag{8}$$

holds for all $f \in \mathcal{L}^p(\mathbb{R})$ [SW71].

2 LEMMA (General bound on the exchange energy). *Let $V : \mathbb{R}_+ \to \mathbb{R}_+$ be a convex function, with $\lim_{r\to\infty} V(r) = 0$. Let $\psi \in \mathcal{L}^2(\mathbb{R}^N)$. Then, for all $\beta(z) \geq 0$,*

$$\mathrm{Ex}_\psi \geq -\tfrac{1}{2}\int_{-\infty}^{\infty} dz \left(\rho_\psi^{*2}(z)\int_0^{\beta(z)} V''(r)r^2dr + \rho_\psi^*(z)\int_{\beta(z)}^{\infty} V''(r)rdr\right). \tag{9}$$

Proof. With the aid of Lemma 1 we can write

$$\sum_{i<j} V(|x_i - x_j|) = 2\int_{-\infty}^{\infty} dz \int_0^{\infty} drV''(2r)\sum_{i<j}\chi_r(x_i - z)\chi_r(x_j - z). \tag{10}$$

Denote

$$\alpha_{r,z} = \langle\psi|\sum_{i=1}^{N}\chi_r(x_i - z)\psi\rangle = \int_{z-r}^{z+r}\rho_\psi(x)dx. \tag{11}$$

Since V is convex by assumption, we get, for each positive function $\beta(z)$,

$$\begin{aligned} 0 &\leq \langle\psi|\int_{-\infty}^{\infty} dz \int_{\frac{1}{2}\beta(z)}^{\infty} drV''(2r)\left(\sum_{i=1}^{N}\chi_r(x_i - z) - \alpha_{r,z}\right)^2\psi\rangle \\ &\leq \mathrm{Ex}_\psi + \int_{-\infty}^{\infty} dz \int_0^{\frac{1}{2}\beta(z)} drV''(2r)\alpha_{r,z}^2 + \int_{-\infty}^{\infty} dz \int_{\frac{1}{2}\beta(z)}^{\infty} drV''(2r)\alpha_{r,z}, \end{aligned} \tag{12}$$

where we used the fact that $\chi_r(x)^2 = \chi_r(x)$ and

$$\int_{-\infty}^{\infty} dz \int_0^{\infty} drV''(2r)\alpha_{r,z}^2 = \tfrac{1}{2}\int_{\mathbb{R}^2} dxdyV(|x-y|)\rho_\psi(x)\rho_\psi(y) \tag{13}$$

by (3) and (11). The definition of the maximal function (7) implies $\alpha_{r,z} \leq 2r\rho_\psi^*(z)$, so we arrive at (9). □

Of particular interest in the study of particles interacting with Coulomb forces in the presence of a strong magnetic field are the potentials (see e.g. [HS00] and references therein)

$$V_{m,n}(z) = \int_{\mathbb{R}^4}\frac{|\phi_m(\mathbf{x}^\perp)|^2|\phi_n(\mathbf{y}^\perp)|^2}{\sqrt{|\mathbf{x}^\perp - \mathbf{y}^\perp|^2 + z^2}}d^2\mathbf{x}^\perp d^2\mathbf{y}^\perp, \tag{14}$$

where $\mathbf{x}^\perp \in \mathbb{R}^2$ and ϕ_m denotes the function in the lowest Landau band with angular momentum $-m \leq 0$, i.e., using polar coordinates (r,φ),

$$\phi_m(\mathbf{x}^\perp) = \sqrt{\frac{B}{2\pi}}\frac{1}{\sqrt{m!}}\left(\frac{Br^2}{2}\right)^{m/2} e^{-im\varphi}e^{-Br^2/4}. \tag{15}$$

Here $B > 0$ is the magnetic field strength. We are in particular interested in the strong field case, where $B \gg \bar{\rho}_\psi^2$.

Using the relation

$$B^{-1/2}V_{m,m}(B^{-1/2}z) = \int_0^{\infty} dqe^{-q|z|}e^{-q^2}L_m(q^2/2)^2 \equiv W_m(z) \tag{16}$$

(see [V76]), where L_m are the Laguerre polynomials, one easily sees that the potentials $V_{m,m}$ are smooth convex functions away from $z = 0$, for all $m \in \mathbb{N}_0$. Hence we can use Lemma 2 to get a lower bound on the exchange energy for these potentials. In the following, we will use the estimate

$$W_m(0) \leq W_0(0) = \sqrt{\frac{\pi}{4}} < 1. \tag{17}$$

We do not try to give the best possible constants in the bound stated below, but concentrate on the asymptotic behavior of Ex_ψ for large $B/\bar{\rho}_\psi^2$.

3 THEOREM (Exchange energy for $V_{m,m}$). *Let $V = V_{m,m}$ be given by (14), for some $m \in \mathbb{N}_0$ and $B > 0$. Then, for all $\psi \in \mathcal{L}^2(\mathbb{R}^N)$ with $\rho_\psi \in \mathcal{L}^2(\mathbb{R})$,*

$$\mathrm{Ex}_\psi \geq -16N\bar{\rho}_\psi \left(\ln\left[e^3 + \frac{B^{1/2}}{\bar{\rho}_\psi} \right] + 2 \right). \tag{18}$$

Proof. From (14) and (16) one easily verifies the estimates

$$W_m''(r) \leq \frac{2}{r^2} W_m(r) \quad \text{and} \quad W_m(r) \leq \min\left\{ \frac{1}{r}, W_m(0) \right\}. \tag{19}$$

Using this and (17) we get

$$\int_\beta^\infty V''(r) r dr \leq \frac{2}{\beta} \tag{20}$$

and

$$\int_0^\beta V''(r) r^2 dr \leq 2\left(1 + \left[\ln \beta B^{1/2} \right]_+ \right), \tag{21}$$

where $[t]_+ = \max\{t, 0\}$. Choosing $\beta = \beta(z) = \rho_\psi^*(z)^{-1}$ Lemma 2 implies that

$$\mathrm{Ex}_\psi \geq -\int_{-\infty}^\infty \rho_\psi^*(z)^2 \left(2 + \left[\ln B^{1/2}/\rho_\psi^*(z) \right]_+ \right) dz. \tag{22}$$

Next we use that for $a > 0$

$$[\ln a]_+ = \inf_{s>0} \frac{1}{se} a^s \leq \inf_{0<s<\frac{1}{3}} \frac{1}{se} a^s. \tag{23}$$

Using (8) and the fact that $2^{p+1}p/(p-1) \leq 16$ for $5/3 \leq p \leq 2$ this implies

$$\begin{aligned} \mathrm{Ex}_\psi &\geq -\int_{-\infty}^\infty \rho_\psi^*(z)^2 \left(2 + \inf_{0<s<\frac{1}{3}} \frac{1}{se} \left(\frac{B^{1/2}}{\rho_\psi^*(z)} \right)^s \right) dz \\ &\geq -32 \int_{-\infty}^\infty \rho_\psi(z)^2 dz - 16 \inf_{0<s<\frac{1}{3}} \frac{1}{se} B^{s/2} \int_{-\infty}^\infty \rho_\psi(z)^{2-s} dz \\ &\geq -16N\bar{\rho}_\psi \left(2 + \inf_{0<s<\frac{1}{3}} \frac{1}{se} \left(\frac{B^{1/2}}{\bar{\rho}_\psi} \right)^s \right), \end{aligned} \tag{24}$$

where we have used that, for $0 \leq s \leq 1$, $\int \rho^{2-s} \leq (\int \rho^2)^{1-s} (\int \rho)^s$ by Hölder's inequality. Now

$$\inf_{0<s<\frac{1}{3}} \frac{1}{se} a^s \leq \inf_{0<s<\frac{1}{3}} \frac{1}{se} (e^3 + a)^s = \ln(e^3 + a), \tag{25}$$

which, inserted into (24), proves the Theorem. □

A lower bound on the exchange energy useful for small fields, i.e., for $B \ll \bar{\rho}_\psi^2$, can be obtained much easier. A general inequality, exploiting the positive definiteness of the potential, gives [T94]

$$\mathrm{Ex}_\psi \geq -\frac{N}{2} V(0) \geq -\frac{N}{2} B^{1/2}. \tag{26}$$

We remark that the bound on the exchange energy given in Theorem 3 is indeed nearly optimal for large $B/\bar{\rho}_\psi^2$. Namely, if we take for ψ the Slater determinant of φ_i, $1 \leq i \leq N$, with $\varphi_1(x) = (2R)^{-1/2} \Theta(R - |x|)$ and $\varphi_i(x) = \varphi_1(x + 2R(i-1))$ for some $R > 0$, the exchange energy is easily calculated to be

$$\mathrm{Ex}_\psi = -N \bar{\rho}_\psi \int_0^{B^{1/2}/\bar{\rho}_\psi} W_m(r) \left(1 - \frac{\bar{\rho}_\psi}{B^{1/2}} r\right) dr, \tag{27}$$

which is precisely of the order $N \bar{\rho}_\psi \ln[B^{1/2}/\bar{\rho}_\psi]$ for $B \gg \bar{\rho}_\psi^2$. The same holds for the bosonic case, i.e., for ψ the totally symmetric product of the φ_i's.

We now apply our results to a model described by the Hamiltonian

$$H_m = \sum_{i=1}^N \left(-\hbar^2 \frac{\partial^2}{\partial x_i^2} - Z V_m(x_i) \right) + \sum_{i<j} V_{m,m}(x_i - x_j), \tag{28}$$

where V_m is defined similarly to (14), namely

$$V_m(z) = \int_{\mathbb{R}^2} \frac{|\phi_m(\mathbf{x}^\perp)|^2}{\sqrt{|\mathbf{x}^\perp|^2 + z^2}} d^2\mathbf{x}^\perp. \tag{29}$$

This Hamiltonian is the projection of the full three-dimensional Hamiltonian for N electrons in the Coulomb field of a nucleus of charge Z and in a homogeneous magnetic field B onto the space of functions in the lowest Landau band with fixed angular momentum m. It acts on the totally antisymmetric functions in $\mathcal{L}^2(\mathbb{R}^N)$. We first estimate the ground state energy $E_m(N, Z, B, \hbar) = \inf \operatorname{spec} H_m$. Neglecting the positive interaction term the one-dimensional Lieb-Thirring inequality ([LT76]; the constant is taken from [HLW00]) yields, with $\bar{m} = \max\{1/4, m\}$,

$$\begin{aligned} E_m(N, Z, B, \hbar) &\geq -\frac{4}{3\pi} \frac{1}{\hbar} Z^{3/2} \int_{\mathbb{R}} V_m^{3/2} \\ &\geq -\frac{16}{3\sqrt{\pi}} \frac{1}{\hbar \bar{m}^{1/4}} \frac{\Gamma(5/4)}{\Gamma(3/4)} \frac{1}{\hbar} Z^{3/2} B^{1/4} \end{aligned} \tag{30}$$

independently of N, where we used that $V_m(x) \leq (\bar{m}/B + x^2)^{1/2}$ ([RW00], Sect. 1.2; the bound for $m = 0$ follows easily from Thm. 20 there). However, for $B \gg Z^2$, this is a very crude estimate, but can be improved using Lemma 2.1 of [LSY94a] instead. The result is

$$E_m(N, Z, B, \hbar) \geq -\frac{Z^2}{\hbar^2} \left(\left[\sinh^{-1}(\hbar^2 B^{1/2} / Z \bar{m}^{1/2}) \right]^2 + 1 + \frac{\pi^2}{12} \right). \tag{31}$$

By appropriate variational upper bounds one can show that these lower bounds indeed capture the correct leading order of the ground state energy for large Z and N.

We are interested in the exchange energy in a state close to the ground state of H_m. In the following, we will assume that $\langle\psi|H_m\psi\rangle \leq 0$. The kinetic energy is then bounded by

$$T_\psi = \langle\psi|\sum_i -\hbar^2\frac{\partial^2}{\partial x_i^2}\psi\rangle \leq \frac{1}{1-\lambda}|E_m(N,Z,B,\lambda^{1/2}\hbar)| \tag{32}$$

for all $0<\lambda<1$. Moreover, again by the Lieb-Thirring inequality, $\int\rho_\psi^3 \leq 12\pi^{-2}\hbar^{-2}T_\psi$, so this gives a bound on $\bar\rho_\psi$ by Hölders inequality, namely $\bar\rho_\psi \leq (\int\rho_\psi^3)^{1/2}(\int\rho_\psi)^{-1/2}$. Using the fact that the bound on the exchange energy given in Theorem 3 is monotonically increasing in $\bar\rho_\psi$, we arrive at an explicit bound on Ex_ψ, which is of the order

$$\mathrm{Ex}_\psi \gtrsim -\left\{\begin{array}{l} N^{1/2}Z\left(\frac{B}{Z^2\bar m}\right)^{1/8}\ln\left[N^{4/3}BZ^{-2}\bar m^{1/3}\right] \\ N^{1/2}Z\ln\left[B/Z^2\bar m\right]\ln\left[NBZ^{-2}\right]\end{array}\right. \tag{33}$$

as long as $\langle\psi|H_m\psi\rangle\leq 0$. Note that $B\gg\bar\rho_\psi^2$ is equivalent to $B\gg Z^2N^{-4/3}\bar m^{-1/3}$.

Our method of estimating the exchange energy also applies to the three-dimensional Coulomb interaction case, if we restrict ourselves to considering wave functions Ψ that are the total antisymmetrization of tensor products of functions of the form

$$\psi_m(z_1,\dots,z_{n_m})\prod_{i=1}^{n_m}\phi_m(\mathbf{x}_i^\perp), \tag{34}$$

where the ψ_m's are antisymmetric in all variables, with one-particle density matrix γ_m, density ρ_m, and $\sum_m n_m = N$. In the following, we will be concerned with the potentials

$$\hat V_{m,n}(z) = \int_{\mathbb{R}^4}\frac{\phi_m(\mathbf{x}^\perp)\overline{\phi_n(\mathbf{x}^\perp)}\phi_n(\mathbf{y}^\perp)\overline{\phi_m(\mathbf{y}^\perp)}}{\sqrt{|\mathbf{x}^\perp-\mathbf{y}^\perp|^2+z^2}}d^2\mathbf{x}^\perp d^2\mathbf{y}^\perp. \tag{35}$$

Analogously to (16) there is the relation

$$B^{-1/2}\hat V_{m,n}(B^{-1/2}z) = \int_0^\infty dq e^{-q|z|}e^{-q^2}\frac{m!}{n!}\left(\tfrac12 q^2\right)^{n-m}L_m^{n-m}(q^2/2)^2 \tag{36}$$

(see [V76]), where the L_m^n are the associated Laguerre polynomials. From this decomposition we deduce the important property

$$\sum_{n=0}^\infty B^{-1/2}\hat V_{m,n}(B^{-1/2}z) = \int_0^\infty dq e^{-q|z|}e^{-q^2/2} = B^{-1/2}V_0(B^{-1/2}z) \leq \min\left\{\sqrt{\frac{\pi}{2}},\frac{1}{|z|}\right\}, \tag{37}$$

where V_0 is defined in (29) and the last identity follows again from [V76].

For Ψ as above, we now estimate the exchange energy. We have

$$\begin{aligned}\langle\Psi|\sum_{i<j}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}\Psi\rangle &= \sum_m\langle\psi_m|\sum_{i<j}^{n_m}V_{m,m}(z_i-z_j)\psi_m\rangle \\ &+\tfrac12\sum_{n\neq m}\int_{\mathbb{R}^2}\left(V_{m,n}(z-z')\rho_m(z)\rho_n(z')-\hat V_{m,n}(z-z')\overline{\gamma_m(z,z')}\gamma_n(z,z')\right)dzdz'. \end{aligned}\tag{38}$$

For the last term in (38) we use (37) and $|\gamma_m(z,z')|^2 \le \rho_m(z)\rho_m(z')$ to estimate

$$\sum_{n\neq m}\int_{\mathbb{R}^2} \hat{V}_{m,n}(z-z')\overline{\gamma_m(z,z')}\gamma_n(z,z')dzdz' \le \sum_m \int_{\mathbb{R}^2} V_0(z-z')|\gamma_m(z,z')|^2 dzdz'$$
$$\le \sum_m \int_{|z-z'|\le\bar\rho_m^{-1}} V_0(z-z')\rho_m(z)\rho_m(z')dzdz' + \sum_m \int_{|z-z'|\ge\bar\rho_m^{-1}} V_0(z-z')|\gamma_m(z,z')|^2 dzdz'$$
$$\le \sum_m n_m\bar\rho_m \left(2 + \left[\ln\sqrt{\frac{\pi}{2}}\frac{B^{1/2}}{\bar\rho_m}\right]_+\right), \tag{39}$$

where we used the Cauchy-Schwarz inequality for the first part the fact that $\int|\gamma_m|^2 = \mathrm{Tr}[\gamma_m^2] \le \mathrm{Tr}[\gamma_m] = n_m$ for the second. For the first term in (38) we apply Thm. 3 (and the fact that by an analogous estimate as above this theorem holds also for $N=1$, where the interaction energy is zero). Therefore

$$\langle\Psi|\sum_{i<j}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}\Psi\rangle \ge D(\rho_\Psi,\rho_\Psi) - \sum_m n_m\bar\rho_m\left(\frac{33}{2}\ln\left[e^3+\frac{B^{1/2}}{\bar\rho_m}\right] + 33 + \frac{1}{4}\ln[\pi/2]\right). \tag{40}$$

Now using Hölder's inequality for $\bar\rho_m$ and concavity and monotonicity of $x^{1/2}\ln[e^3+x^{-1/2}]$ in x we conclude

$$\langle\Psi|\sum_{i<j}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}\Psi\rangle \ge D(\rho_\Psi,\rho_\Psi)$$
$$-N^{1/2}\sqrt{\sum_m\int_{\mathbb{R}}\rho_m^3}\left(\frac{33}{2}\ln\left[e^3+\sqrt{BN/\sum_m\int_{\mathbb{R}}\rho_m^3}\right] + 33 + \frac{1}{4}\ln[\pi/2]\right). \tag{41}$$

The Lieb-Thirring inequality implies that

$$\sum_m\int_{\mathbb{R}}\rho_m^3 \le \frac{12}{\pi^2}\sum_m\langle\psi_m|\sum_{j=1}^{n_m}-\frac{\partial^2}{\partial z_j^2}|\psi_m\rangle = \frac{12}{\pi^2}\langle\Psi|\sum_{j=1}^{N}-\frac{\partial^2}{\partial z_j^2}|\Psi\rangle, \tag{42}$$

which can be bound as in (32), as long as Ψ has negative energy. Explicit bounds on the total energy of an atom in a magnetic field are given in [LSY94b], (2.42) and (2.43), which imply

$$\mathrm{Ex}_\Psi \gtrsim -\begin{cases} Z^{3/5}N^{4/5}B^{1/5}\ln[BN^{2/3}/Z^2] & \text{for} \quad B \gg Z^2N^{-2/3} \\ NZ\ln[B/Z^2]\ln[B/Z^2N] & \text{for} \quad B \gg Z^2N \end{cases} \tag{43}$$

for this system.

The result in (43) agrees excellently with the expected order of magnitude of the exchange energy of wave functions close to the ground state of large atoms in strong magnetic fields ([LSY94a]; see also [HS00], Remark 6.1). Although our considerations neglect correlations between particles with different angular momentum, we strongly conjecture that their contribution is of the same or of lower order, so it can be expected that (43) gives the correct order of the exchange energy in the ground state. The bound (43) in particular applies to all Slater determinants of angular momentum eigenfunctions in the lowest Landau band.

Note that since in the lowest Landau band the density orthogonal to the magnetic field is bounded by $B/2\pi$, the quantity $(\sum_m\int\rho_m^3/N)^{1/2}$ is of the order of $\bar\rho_{3D}/B$, where $\bar\rho_{3D}$ is the mean three-dimensional density. Therefore the result stated above is in total agreement with investigations on the homogeneous electron gas in a strong magnetic field [DG71, FGPY92], where an exchange energy of the order $NB^{-1}\bar\rho_{3D}\ln[B^{3/2}/\bar\rho_{3D}]$ was obtained.

References

[DG71] R.W. Danz and M.L. Glasser, *Exchange Energy of an Electron Gas in a Magnetic Field*, Phys. Rev. B **4**, 94–99 (1971)

[FGPY92] I. Fushiki, E.H. Gudmundsson, C.J. Pethick, and J. Yngvason, *Matter in a Magnetic Field in the Thomas-Fermi and Related Theories*, Ann. Physics **216**, 29–72 (1992)

[HH77] M. Hoffmann-Ostenhof and T. Hoffmann-Ostenhof, *"Schrödinger inequalities" and asymptotic behavior of the electron density of atoms and molecules*, Phys. Rev. A **16**, 1782–85 (1977)

[HLW00] D. Hundertmark, A. Laptev, and T. Weidl, *New bounds on the Lieb-Thirring constants*, Inventiones Math. **140**, 693–704 (2000)

[HS00] C. Hainzl and R. Seiringer, *A discrete density matrix theory for atoms in strong magnetic fields*, arXiv:math-ph/0010005, to appear in Commun. Math. Phys.

[LO81] E.H. Lieb and S. Oxford, *Improved Lower Bound on the Indirect Coulomb Energy*, Int. J. Quant. Chem. **19**, 427–439 (1981)

[LSY94a] E.H. Lieb, J.P. Solovej, and J. Yngvason, *Asymptotics of Heavy Atoms in High Magnetic Fields: I. Lowest Landau Band Regions*, Commun. Pure Appl. Math. **47**, 513–591 (1994)

[LSY94b] E.H. Lieb, J.P. Solovej, and J. Yngvason, *Asymptotics of Heavy Atoms in High Magnetic Fields: II. Semiclassical Regions*, Commun. Math. Phys. **161**, 77–124 (1994)

[LT76] E.H. Lieb and W. Thirring, *A bound on the moments of the eigenvalues of the Schrödinger Hamiltonian and their relation to Sobolev inequalities*, in: *Studies in Mathematical Physics*, 269–303, Princeton University Press (1976)

[RW00] M.B. Ruskai and E. Werner, *Study of a Class of Regularizations of* $1/|x|$ *using Gaussian Integrals*, SIAM J. Math. Anal. **32**, 435–463 (2000)

[S95] I.M. Sigal, *Lectures on Large Coulomb Systems*, in: *Mathematical Quantum Theory II: Schrödinger Operators*, CRM Proceedings & Lecture Notes, J. Feldman, R. Froese, L.M. Rosen, eds., 73–107 (1995)

[SW71] E.M. Stein and G. Weiss, *Introduction to Fourier analysis on Euclidean Spaces*, Princeton Mathematical Series No. 32, Princeton University Press, Princeton, N.J. (1971)

[T94] W. Thirring, *Quantenmechanik von Atomen und Molekülen*, 2nd ed., Springer (1994)

[V76] J. Virtamo, *Hartree-Fock calculation of the ground state energies of two-electron atoms in an intense magnetic field*, J. Phys. B **9**, 751–60 (1976)