Journal of Statistical Physics, Vol. 116, Nos. 1/4, August 2004 (© 2004)

One-Dimensional Models for Atoms in Strong Magnetic Fields, II: Anti-Symmetry in the Landau Levels[1,2]

Raymond Brummelhuis[3] and Mary Beth Ruskai[4]

Received July 25, 2003; accepted December 3, 2003

Electrons in strong magnetic fields can be described by one-dimensional models in which the Coulomb potential and interactions are replaced by regularizations associated with the lowest Landau band. For a large class of models of this type, we show that the maximum number of electrons that can be bound is less than $aZ+Zf(Z)$. The function $f(Z)$ represents a small non-linear growth which reduces to $A_pZ(\log Z)^2$ when the magnetic field $B=O(Z^p)$ grows polynomially with the nuclear charge Z. In contrast to earlier work, the models considered here include those arising from realistic cases in which the full trial wave function for N-electrons is the product of an N-electron trial function in one-dimension and an antisymmetric product of states in the lowest Landau level.

KEY WORDS: Atoms in strong magnetic fields; maximum negative ionization; one-dimensional models; lowest Landau band.

1. INTRODUCTION

It is well-known that systems in strong magnetic fields behave like systems in one-dimension, i.e., a strong magnetic field confines the particles to Landau orbits orthogonal to the field, leaving only their behavior in the direction of the field subject to significant influence by a static potential. Motivated by this general principle and the work of Lieb, Solovej, and Yngvason[(12)] (LSY) on atoms in extremely strong magnetic fields,

[2] Dedicated to Elliott Lieb on the occasion of his 70th birthday.

[3] School of Economics, Mathematics and Statistics, Birkbeck College–University of London, Mallet Street, London, United Kingdom; e-mail: r.brummelhuis@statistics.bbk.ac.uk

[4] Department of Mathematics, Tufts University, Medford, Massachusetts 02155; e-mail: marybeth.ruskai@tufts.edu

Brummelhuis and Ruskai[5] initiated a study of models of atoms in homogeneous strong magnetic fields in which the 3-dimensional wave-function has the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2,..., \mathbf{r}_n) = \Phi(x_1,..., x_n)\, \Upsilon(y_1, z_1, y_2, z_2,..., y_n, z_n) \tag{1}$$

where Υ lies in the projection onto the lowest Landau band for an N-electron system. We follow the somewhat non-standard convention of choosing the magnetic field in the x-direction, i.e, $\mathbf{B} = (B, 0, 0)$ where B is a constant denoting the fields strength, in order to avoid notational confusion with the nuclear charge Z.

The Hamiltonian for an N electron atom in a magnetic field $\mathbf{B}$ is

$$H(N, Z, B) = \sum_{j=1}^{N} \left[|\mathbf{P}_j + \mathbf{A}|^2 - \frac{Z}{|\mathbf{r}_j|} \right] + \sum_{j<k} \frac{1}{|\mathbf{r}_j - \mathbf{r}_k|} \tag{2}$$

where $\mathbf{A}$ is a vector potential such that $\nabla \times \mathbf{A} = \mathbf{B}$. The ground-state energy of $H(N, Z, B)$ is given by

$$E_0(N, Z, B) = \inf_{\|\Psi\| = 1} \langle \Psi, H(N, Z, B)\, \Psi \rangle. \tag{3}$$

Let $E_0^{\text{conf}}(N, Z, B)$ denote the corresponding infimum restricted to linear combinations of functions of the form (1). For extremely strong fields, it was shown in ref. 12 that $E/E_0^{\text{conf}} \to 1$ as $B/Z^{4/3} \to \infty$ with N/Z fixed.

In this paper we consider $E_0^{\Upsilon}(N, Z, B)$, the infimum when (3) is further restricted to those functions of the form (1) corresponding to a particular choice for Υ. As discussed in ref. 5, is straightforward to show that

$$E_0^{\Upsilon}(N, Z, B) = \sqrt{B} \inf_{\|\Phi\| = 1} \langle \Phi, h(N, Z, B^{-1/2})\, \Phi \rangle + NB \tag{4}$$

where

$$h^{\Upsilon}(N, Z, M) = \sum_{j=1}^{N} \left[-\frac{1}{M} \frac{d^2}{dx_j^2} - Z\tilde{V}_j^{\Upsilon}(x_j) \right] + \sum_{j<k} \tilde{W}_{jk}^{\Upsilon}(x_j - x_k), \tag{5}$$

and we have scaled out the field strength B so that the only remnant of the magnetic field is in the "mass" $M = B^{-1/2}$. The effective one-dimensional potentials $\tilde{V}_j^{\Upsilon}$ and $\tilde{W}_{jk}^{\Upsilon}$ can be written in terms of the functions[5, 7, 17]

$$V_m(x) = \frac{1}{m!} \int_0^{\infty} \frac{s^{2m} e^{-s^2}}{\sqrt{x^2 + s^2}}\, s\, ds, \tag{6}$$

which are discussed in Section 2.1 and studied in detail in ref. 16. The precise form of $\tilde{V}_j^{\Upsilon}$ and $\tilde{W}_{jk}^{\Upsilon}$ depends on the choice of Υ; some special cases are discussed in Section 2. When Υ is a simple product of one-particle Landau states, or a finite linear combination of such products, the effective potentials satisfy $\tilde{V}_j^{\Upsilon}(x) \leqslant V_\mu(x)$ and $\tilde{W}_{jk}^{\Upsilon}(x) \geqslant V_\nu(x)$ for some integers μ and ν which depend upon Υ. We will primarily be interested in the case of symmetrized and anti-symmetrized products of one-particle Landau states. In this case, as discussed in more detail in Section 2.1 and Appendix A, bounds of the form above are readily obtained. For those situations in which $\nu < 2\mu$, a bound on the maximum negative ionization is given in Theorems 1 and 2.

In ref. 5 we considered the simple, but unrealistic, situation in which Υ is a product of Landau states with $m=0$. In this paper we introduce a more realistic model, which we call the "Slater model," in which Υ is an antisymmetrized product of Landau states. As in ref. 5, we concentrate on the question of maximum negative ionization. Define $N_{\max}(Z, B)$ as the maximum number of electrons for which the Hamiltonian (5) has a bound state in the sense $E_0(N, Z, B) < E_0(N-1, Z, B)$.

LSY[12] showed that in extremely strong magnetic fields, atoms bind $2Z$ electrons in the sense

$$\liminf_{Z,\, B/Z^3 \to \infty} \frac{N_{\max}(Z, B)}{Z} \geqslant 2. \tag{7}$$

and conjectured that $2Z$ was also an upper bound to this limit. However, even for the simple model in ref. 5 we were only able to show the weaker bound $N_{\max}(Z, B) < 2Z + 1 + c\sqrt{B}$. Unfortunately, when $B > O(Z^3)$ as required for the limit in (7), the term $c\sqrt{B} = cZ^{3/2}$ dominates so that we can only conclude that $N_{\max}(Z, B) \leqslant 2Z + O(Z^{3/2})$.

In this note we show that for a large class of one-dimensional models, including some in which Υ in (1) is a simple product or a Slater determinant, the bound on $N_{\max}(Z, B)$ can be improved to one of the form $aZ + Zf(Z)$ with $f(Z) = O(\log Z)^2$ when B grows polynomially with Z. Our results were announced earlier in refs. 6 and 7 in the form

$$N_{\max}(Z, B) \leqslant aZ + Zg(Z, B) \tag{8}$$

with $g(Z, B) = (\log Z)^2 + \log Z (\log B)^{1+\omega}$ for some $\omega > 0$. Subsequently, Seiringer[18] gave a similar bound for the full 3-dimensional Hamiltonian. For fermions, Seiringer's bound[18] has the form (8) with $g(Z, B) = \min\{(\frac{B}{Z^3})^{2/5}, (\log \frac{B}{Z^3})^2\}$; it is obtained by applying Lieb's method to the full

3-dimensional Hamiltonian. Hainzl and Seiringer[9] then extended this bound to a density matrix model in which the variable perpendicular to the field is replaced by discrete angular momentum quantum numbers.

Our use of one-dimensional models was motivated by a desire to understand the physics associated with the consequence of the one-dimensional character of atoms in strong magnetic fields, which is well-known and made precise in the work of LSY.[12] Brummelhuis and Duclos[2–4] also showed that, for each fixed total angular momentum in the field direction, the full QM Hamiltonian (2) converges in norm-resolvent sense[5] to the projected Hamiltonian $H_s(N, Z, B) = \Pi_s H(N, Z, B)\, \Pi_s$ where Π_s denotes the orthogonal projection onto the lowest Landau band. In the special case of zero total angular momentum, $\langle \Psi H_s(N, Z, B)\, \Psi \rangle$ has the form (5) when Ψ has the form (1). Full details will be given in ref. 4. In contrast to ref. 12, the strategy in refs. 2 and 3 does not require an *a priori* bound on N in terms of Z, but *does* need to fix the total angular momentum in the direction of the magnetic field.

Despite Seiringer's result[18] and the work in ref. 9, we feel that our argument, which uses the RS localization approach, is of some interest. Because our analyses of the models in ref. 5 showed that electrons are highly delocalized in the direction orthogonal to the field, it may seem surprising that such a localization technique works at all. However, a careful examination of the proof in Section 3, shows that it reflects this delocalization in the sense that the "inner ball" grows with B. Nevertheless, the localization error can be controlled with a modest excess charge as described in the results which follow.

We now state same rather general results. Applications to special cases of particular physical interest are described in Section 2.

Theorem 1. Suppose the potentials in the Hamiltonian (5) satisfy

$$\tilde{V}_j^{\Upsilon}(x) \leqslant V_\mu(x) \qquad \text{and} \qquad \tilde{W}_{jk}^{\Upsilon}(x) \geqslant \frac{1}{\sqrt{2}} V_{\nu-1}\left(\frac{x}{\sqrt{2}}\right), \tag{9}$$

for all j, k and $0 \leqslant \nu \leqslant 2\mu$. Then for every $\alpha > 0$ there is a constant $A_\alpha > 0$ and constants a_1, a_2 (independent of α) such that the Hamiltonian $h^{\Upsilon}(N, Z, B)$ has no bound states provided that

$$N > 2Z + A_\alpha Z^{1+\alpha}, \qquad \text{and} \tag{10a}$$

$$a_1 e^{Z^{\alpha/4}} > B \geqslant a_2 Z^{\gamma_\nu}, \tag{10b}$$

[5] To be precise, let R be the resolvent of H, and R_s that of H_s. Then $\|\Pi_s R \Pi_s - R_s\| = O(B^{-1/2})$ on $\Pi_s \mathscr{H}$, and $\|R\| = O(B^{-1/2})$ on $\Pi_s^{\perp} \mathscr{H}$ at a distance $(\log B)^2$ to the spectrum of H_s.

where the exponent α can be arbitrarily small and the exponent γ_ν depends upon ν. In particular, when $\nu = O(1)$, it suffices to take $\gamma_\nu > 2$; when $\nu = O(N)$ one must choose $\gamma_\nu > 3$.

Although the non-linear term is higher order than $2Z$, it is useful to write the linear term separately. It is due to the relative strength of the potentials near the nucleus, while the non-linear terms are needed to control the localization error. The upper bound on B is needed for technical reasons associated with the fact that the localization error can not be controlled when B grows exponentially. As discussed in Remark 1 of Section 3.4, the requirement $\nu \leqslant 2\mu$ can be relaxed at the expense of replacing $2Z$ by cZ in (10a) with $c > 2$.

The non-linear term in the lower bound (10a) can be improved to one that is logarithmic. We first state it in general and then under the simple, and realistic, assumption that $B = Z^p$ for $p > 3$. The case $\gamma_\nu > 3$ in (11b), corresponds to the superstrong region considered by LSY in ref. 12.

Theorem 2. Assume that the potentials $\tilde{V}_j^\Upsilon$ and $\tilde{W}_{jk}^\Upsilon$ satisfy (9) with $0 \leqslant \nu \leqslant 2\mu$. Then there are positive constants A, a_ϵ, a_2 such that the Hamiltonian $h^\Upsilon(N, Z, B)$ has no bound states provided that

$$N > 3Z + 1 + AZ \log Z \left|\log \frac{Z^2}{B}\right|, \qquad \text{and} \tag{11a}$$

$$a_\epsilon e^{Z^{1/2-\epsilon}} > B \geqslant a_2 Z^{\gamma_\nu}, \tag{11b}$$

where $\epsilon > 0$ can be arbitrarily small and γ_ν is as in Theorem 1.

Corollary 3. Assume that the potentials $\tilde{V}_j^\Upsilon$ and $\tilde{W}_{jk}^\Upsilon$ satisfy (9) with $0 \leqslant \nu \leqslant 2\mu$ and that $B = aZ^p$ for some $a > 0$ and $p > 3$. Then there is a constant A such that the Hamiltonian $h^\Upsilon(N, Z, B)$ has no bound states provided that

$$N > 3Z + AZ(\log Z)^2. \tag{12}$$

Each of these results, immediately yields an upper bound on $N_{\max}(Z, B)$ which we state for ease of comparison with the results in refs. 7, 9, and 18. Under the hypotheses of Theorem 2

$$N_{\max}(Z, B) \leqslant 3Z + A \log Z \left|\log \frac{Z^2}{B}\right|. \tag{13}$$

Under the hypotheses of Corollary 3

$$N_{\max}(Z, B) \leqslant 3Z + AZ(\log Z)^2. \tag{14}$$

Unfortunately, unlike Theorem 1, the $3Z$ in the linear term includes a contribution from the localization error as well as the expected $2Z$ from electrostatics.

2. EFFECTIVE POTENTIALS

2.1. Regularized Coulomb Potentials

The Landau state with energy B and angular momentum $-m$ can be written compactly using the complex variable $\zeta = y + iz$ as

$$\gamma_m^B(y,z) = [\pi m!]^{-1/2}\, B^{(m+1)/2} \bar{\zeta}^m e^{-B|\zeta|^2/2}. \tag{15}$$

The effective one-dimensional potentials in our models can be written using the regularization of the 3-dimensional Coulomb potential with a Landau state, i.e.,

$$\begin{aligned} V_m^B(x) &\equiv \left\langle \gamma_m^B, \frac{1}{|\mathbf{r}|}\gamma_m^B \right\rangle = \int_{\mathbf{R}^2} \frac{|\gamma_m^B|^2}{|\mathbf{r}|}\, dy\, dz \\ &= \frac{B^{m+1}}{m!}\int_0^\infty \frac{s^{2m} e^{-Bs^2}}{\sqrt{x^2+s^2}}\, s\, ds \\ &= \frac{1}{m!}\int_0^\infty \frac{u^m e^{-u}}{\sqrt{x^2+u/B}}\, du \\ &= \frac{2B^{m+1}}{m!}\, e^{Bx^2} \int_{|x|}^\infty (t^2 - x^2)^m\, e^{-Bt^2}\, dt, \end{aligned} \tag{16}$$

where $\mathbf{r}$ in $\mathbf{R}^3$ and $s = y^2 + z^2$. In view of the rescaling in (4), it suffices to consider only the case $B = 1$ for which we drop the superscript, i.e., $V_m(x) \equiv V_m^1(x)$. The properties of $V_m(x)$ were studied in detail in ref. 16 and summarized in ref. 7. Those which we need here are listed below.

$$V_m(x) \text{ is monotonically decreasing for } x \geqslant 0. \tag{17}$$

$$V_{m+1}(x) < V_m(x) < \frac{1}{|x|}. \tag{18}$$

$$\frac{1}{\sqrt{x^2+m}} > V_m(x) > \frac{1}{\sqrt{x^2+m+1}} \tag{19}$$

$$\text{If} \quad V_{\text{av}}(x) \equiv \frac{1}{N}\sum_{j=0}^{N-1} V_j(x), \qquad \text{then} \quad V_{\text{av}}(x) \leqslant 2V_N(x). \tag{20}$$

2.2. Simple Product Landau Model

We restrict to wave functions of the form (1) with $\Upsilon = \prod_{k=1}^{N} \gamma_{m_k}^{B}(y_k, z_k)$ a simple product of Landau states. Then

$$\Psi_{m_1 \cdots m_N} = \Phi(x_1 \cdots x_n) \prod_{k=1}^{N} \gamma_{m_k}^{B}(y_k, z_k), \tag{21}$$

and

$$\langle \Psi_{m_1 \cdots m_N}, H(N, Z, B)\, \Psi_{m_1 \cdots m_N} \rangle = \sqrt{B}\, \langle \Phi, h^{\mathbf{m}}(N, Z, B^{-1/2})\, \Phi \rangle + NB \tag{22}$$

where we rescale as in (4) and $\mathbf{m} = (m_1,..., m_n)$. Then

$$h^{\mathbf{m}}(N, Z, M) = \sum_{j=1}^{N} \left[-\frac{1}{M} \frac{d^2}{dx_j^2} - Z V_{m_j}(x_j) \right] + \sum_{j<k} W_{m_j, m_k}(|x_j - x_k|), \tag{23}$$

V_m is given by (6) (with $B = 1$) and the effective interaction satisfies

$$W_{m, m'}(x - x') = \left\langle \gamma_m \otimes \gamma_{m'}, \frac{1}{|\mathbf{r} - \mathbf{r}'|} \gamma_m \otimes \gamma_{m'} \right\rangle \tag{24}$$

$$= \sum_{j=0}^{m+m'} b_j \frac{1}{\sqrt{2}} V_j \left(\frac{|x - x'|}{\sqrt{2}} \right) \tag{25}$$

$$\geqslant \frac{1}{\sqrt{2}} V_{m+m'} \left(\frac{x - x'|}{\sqrt{2}} \right) \tag{26}$$

for some $b_j \geqslant 0$ with $\sum_j b_j = 1$. That $W_{m, m'}$ can be written as a convex sum as in (25) was shown in ref. 13. For completeness, a proof in the special case $m = m'$ is included in the Appendix. When $m = m' = 0$ (25) reduces to $W_{0,0}(|x - x'|) = \frac{1}{\sqrt{2}} V_0\, (\frac{|x - x'|}{\sqrt{2}})$ as shown in ref. 5.

When all $m_j = m$ are equal, we denote the effective Hamiltonian in (23) by $h^m(N, Z, M)$ and refer to it as the *m-momentum Landau model*. For this model, $\tilde{V}^{\Upsilon}(x) = V_m(x)$ and $\tilde{W}^{\Upsilon}(x) = \frac{1}{\sqrt{2}} V_{2m}(\frac{x}{\sqrt{2}})$. The case $m = 0$ was considered in refs. 5 and 7.

Corollary 4. Let $h^m(N, Z, B^{-1/2})$ be the Hamiltonian described above. Then for any $\alpha > 0$ and any B satisfying $a_1 e^{Z^{\alpha/4}} > B \geqslant a_2 Z^{2+\varepsilon}$ for suitable constants a_1, a_2 and some $\varepsilon > 0$, there exists a constant $A_\alpha > 0$

$$N_{\max}(Z, B) \leqslant 2Z + A_\alpha Z^{1+\alpha}. \tag{27}$$

Moreover, when $B = aZ^p$ for some $p > 3$, one can find a constant A (depending on a, p) such that

$$N_{\max}(Z, B) \leqslant 3Z + AZ(\log Z)^2. \tag{28}$$

The Thomas–Fermi theories introduced by LSY in ref. 12 for the superstrong and hyperstrong regimes have a kinetic energy term typically associated to bosonic systems. It seems therefore reasonable to consider $h^m(N, Z, B^{-1/2})$ with domain in the symmetric wave functions. This is however in clear contradiction with the fact that the electrons described by the original 3-dimensional Hamiltonian (2) are fermions, and (1) should be anti-symmetric. Therefore, in the next section, we introduce a model which reflects the anti-symmetry.

2.3. A Slater Determinant Landau Model

It is reasonable to expect that the electrons will try to satisfy the Pauli principle by going into different orbits in the lowest Landau band, and that any realistic one dimensional model will have similar behavior. We now consider the special case in which Ψ has the form (1) with Υ an anti-symmetrized product constructed using $m = 0, 1, 2, \ldots, N-1$. Thus, we let

$$\Upsilon = \left(\frac{1}{\sqrt{N!}} \gamma_0 \wedge \cdots \wedge \gamma_{N-1} \right), \tag{29}$$

where the wedge $\wedge$ denotes the anti-symmetric product so that Υ is a Slater determinant in the Landau states γ_j for $j = 0, 1, \ldots, N-1$. In this case,

$$\langle H(N, Z, B)\, \Psi, \Psi \rangle = \sqrt{B}\, \langle h^{\det}(N, Z, B^{-1/2})\, \Phi, \Phi \rangle + NB \tag{30}$$

with

$$h^{\det}(N, Z, M) = \sum_{j=1}^{N} \left[-\frac{1}{M} \frac{d^2}{dx_j^2} - Z V_{\mathrm{av}}(x_j) \right] + \sum_{j<k} W_{\det}(|x_j - x_k|), \tag{31}$$

where

$$V_{\mathrm{av}}(x) = \frac{1}{N} \sum_{j=0}^{N-1} V_j(x) \tag{32}$$

and the effective interaction is

$$W_{\det}(x) = \frac{1}{\sqrt{2}} \sum_{j=0}^{N-2} b_{2j+1} V_{2j+1}\left(\frac{x}{\sqrt{2}} \right) \tag{33}$$

with $b_{2j+1} \geqslant 0$ and $\sum_{j=0}^{N-2} b_{2j+1} = 1$. It then follows from (17) that

$$W_{\det}(x) \geqslant \frac{1}{\sqrt{2}} V_{2N-3}\left(\frac{x}{\sqrt{2}}\right). \tag{34}$$

To verify (32) recall that the γ_j's are normalized and mutually orthogonal. Thus

$$\begin{aligned} \frac{1}{N!} &\left\langle \gamma_0 \wedge \cdots \wedge \gamma_{N-1}, \frac{1}{|\mathbf{r}_j|} \gamma_0 \wedge \cdots \wedge \gamma_{N-1} \right\rangle \\ &= \frac{1}{N} \sum_{k=0}^{N-1} \left\langle \gamma_k, \frac{1}{|\mathbf{r}_j|} \gamma_k \right\rangle \\ &= \frac{1}{N} \sum_{k=0}^{N-1} V_k(x) = V_{\mathrm{av}}(x) < 2V_N(x) \end{aligned} \tag{35}$$

where we used (20) in the last line. Expression (33) for $W_{\det}(x)$ is proved in the Appendix.

Corollary 5. Let $h^{\det}(N, Z, B^{-1/2})$ be the Hamiltonian described above. Then for any $\alpha > 0$ and any B satisfying $a_1 e^{Z^{\alpha/4}} > B \geqslant a_2 Z^{3+\varepsilon}$ for suitable constants a_1, a_2 and some $\varepsilon > 0$, there exists a constant $A_\alpha > 0$

$$N_{\max}(Z, B) \leqslant 4Z + A_\alpha Z^{1+\alpha}. \tag{36}$$

Moreover, when $B = aZ^p$ for some $p > 3$, one can find a constant A (depending on a, p) such that

$$N_{\max}(Z, B) \leqslant 6Z + AZ(\log Z)^2. \tag{37}$$

2.4. Other Models

For any fixed choice of Landau functions $\gamma_{m_1} \cdots \gamma_{m_N}$ the effective potentials $\tilde{V}^{\Upsilon}$ and $\tilde{W}^{\Upsilon}$ can be computed explicitly for both the case of a simple product and that of a Slater determinant. However, general formulas[6] are not so easily obtained. Nevertheless, the results in the Appendix hold rather generally in the sense that $\tilde{W}^{\Upsilon}$ is a convex combination of the form $\sum_{i=0}^{J} b_i \frac{1}{\sqrt{2}} V_i(\frac{x}{\sqrt{2}})$ with $J \approx 2 \max_k |m_k|$.

[6] In the special case, $\Upsilon = \prod_{k=1}^{N} \gamma_{m_k}^{B}(y_k, z_k)$ with all m_k odd, $\tilde{W}^{\Upsilon}$ is given by a convex sum which contains only V_{2j} with *even* subscripts as in (74).

Thus, one might hope to obtain bounds on the effective potentials similar to those in (9) but without the constraint $\nu \leqslant 2\mu$. In fact, one easily finds $\tilde{W}^{\Upsilon}(x) \geqslant \frac{1}{\sqrt{2}} V_{\nu-1}(\frac{x}{\sqrt{2}})$ with $\nu = 2 \max |m_k|$. However, bounds better than $\tilde{V}^{\Upsilon}(x) \leqslant V_1(x)$ are not so easily obtained. In situations in which bounds of the form

$$\tilde{V}^{\Upsilon}(x) \leqslant c V_{\mu(N)}(x), \qquad \tilde{W}^{\Upsilon}(x) \geqslant \frac{1}{\sqrt{2}} V_{\nu(N)-1}\left(\frac{x}{\sqrt{2}}\right) \tag{38}$$

hold with the dependence of μ and ν on N known, this would lead to similar bounds on $N_{\max}(Z, B)$ with the contributon of $2Z$ to the linear term replaced by one of the form κZ with κ depending on the relative size of $\mu(N)$ and $\nu(N)$.

3. PROOFS

3.1. Localization

The proof of the main theorem will use the RS localization method which is summarized in ref. 8. The argument used here requires some refinements discussed in more detail in refs. 14 and 15.

Let $G_0, G_1,..., G_N$ denote a partition of unity consisting of functions which are Lipschitz continuous on $\mathbf{R}^N$ and satisfy $\sum_{j=0}^{N} G_\nu^2(x) = 1$ as well as the following additional properties:

(i) $\text{supp}(G_0) \subset \{x: \|x\|_\infty \leqslant (1+\delta)\, \rho\}$,

(ii) $\text{supp}(G_k) \subset \{x: \|x\|_\infty \geqslant \rho, |x_k| > \frac{1}{1+\delta} \|x\|_\infty\}$ for $1 \leqslant k \leqslant N$,

(iii) $\sum_{j=0}^{N} |\nabla G_i|^2 < \lambda \frac{(\log N)^2}{\delta^2 \rho^2}$ on $\text{supp}(G_0)$, and

(iv) $\sum_{j=0}^{N} |\nabla G_i|^2 < \lambda \frac{(\log N)^2}{\delta^2 x_k^2} \leqslant \lambda \frac{(\log N)^2}{\delta^2 \rho\, |x_k|}$ on $\text{supp}(G_k)$,

where λ is a constant and ∇ denotes the gradient in all the variables $x_1,..., x_N$. The existence of a partition with these properties is guaranteed by the constructions in refs. 14 and 15.

In many applications, one wants a "sharp" localization which is achieved by choosing δ so that $\delta \to 0$ as $Z \to \infty$, e.g., $\delta = Z^{-\alpha}$ for some $\alpha > 0$. In such situation, it often suffices if $\|x\|_\infty \leqslant 2\rho$ on $\text{supp}(G_0)$. In this paper, the term "localization" is a bit of a misnomer, as the radius ρ of the "inner ball" will grow with Z. In this case, it can be advantageous to let the localization be far from sharp and even permit δ to grow with Z.

Now let $h(N, Z, B^{-1/2})$ be as in (5), and note that the IMS localization formula[8] implies that for any $\Phi(x_1,..., x_N)$ in the domain of $h = h(N, Z, B^{-1/2})$,

$$\langle \Phi, h\,\Phi\rangle = \sum_{\nu=0}^{N} \langle G_\nu \Phi, h\, G_\nu \Phi\rangle - \langle \Phi, LE(x)\,\Phi\rangle \tag{39}$$

$$= \sum_{\nu=0}^{N} \langle G_\nu \Phi, [h\,(N, Z, B^{-1/2}) - LE(x)]\, G_\nu \Phi\rangle, \tag{40}$$

where $LE(x)$ denotes the localization error

$$LE(x) = \sqrt{B} \sum_{\nu=0}^{N} |\nabla G_\nu(x)|^2. \tag{41}$$

It follows from properties (iii) and (iv) of G_k that the localization error is bounded above by

$$L_0 \equiv \lambda \frac{\sqrt{B}(\log N)^2}{\delta^2 \rho^2} \quad \text{on} \quad \text{supp}(G_0) \tag{42a}$$

$$L_k \equiv \lambda \frac{\sqrt{B}(\log N)^2}{\delta^2 \rho\, |x_k|} \quad \text{on} \quad \text{supp}(G_k), \qquad k = 1,..., N. \tag{42b}$$

To prove Theorem 1 it suffices to show that

$$(G_k \Phi, [h(N, Z, B^{-1/2}) - L_k]\, G_k \Phi\rangle \geqslant e_0(N-1, Z, B)\, \|G_k \Phi^2\| \tag{43}$$

for $k = 0, 1,..., N$ with $e_0(N, Z, B)$ the ground state energy of $h(N, Z, B^{-1/2})$. Since (43) is equivalent to

$$(G_k \Phi, [h(N, Z, B^{-1/2}) - L_k - e_0(N-1, Z, B)]\, G_k \Phi\rangle \geqslant 0, \tag{44}$$

it suffices to show that the quantity in square brackets in (44) is positive on $\text{supp}(G_k)$ for each $k = 0, 1,..., N$. It is useful to handle the cases G_0 (inner ball estimates) and $G_1 \cdots G_N$ (outer estimates) separately.

In the next two sections, we use the convention that c and C denote constants in the sense that some constant exists for which the indicated bound holds.

3.2. Inner Ball Estimates

On the inner ball (i.e., on $\text{supp}(G_0)$) the 1-dimensional Hamiltonian (5) with effective potentials satisfying (9) can be bounded by

$$h(N,Z,B^{-1/2}) \geqslant Ne_0(1,Z,\sqrt{B}) + \frac{N(N-1)}{2\sqrt{2}} V_{\nu-1}\left(\frac{2(1+\delta)\,\rho}{\sqrt{2}}\right) \tag{45}$$

$$\geqslant -CN\frac{Z^2}{\sqrt{B}}\left(\log\frac{Z^2}{B}\right)^2 + \frac{N(N-1)}{2}\frac{1}{\sqrt{4(1+\delta)^2\,\rho^2+2\nu}} \tag{46}$$

where we used $h(N,Z,M) \geqslant Ne_0(1,Z,M) + \sum_{j<k} \tilde{W}^{\Upsilon}_{jk}(|x_j - x_k|)$, $|x_j - x_k| < 2(1+\delta)\,\rho$ on $\operatorname{supp}(G_0)$, property (19) and

$$-\sqrt{B}\frac{d^2}{dx^2} - ZV_\mu(x) \geqslant e_0(1,Z,\sqrt{B}) \geqslant -C\frac{Z^2}{\sqrt{B}}\left(\log\frac{Z^2}{B}\right)^2. \tag{47}$$

The lower bound in (47) above follows from the asymptotic formula in ref. 1 for the ground state energy of the one-electron Hamiltonian on the left in (47). Now (ignoring the difference between N and $N-1$), the right side of (46) will be positive if

$$(1+\delta)^2\,\rho^2 + \frac{\nu}{2} < \frac{1}{C}\frac{N^2 B}{Z^4(\log\frac{Z^2}{B})^4}. \tag{48}$$

Since we can assume $Z \leqslant N$, the right side of (48) will be greater than ν for sufficiently large N, Z if

$$B > \frac{\nu}{N} Z^{3+\varepsilon} \tag{49}$$

for some $\varepsilon > 0$. For bosonic models we are be primarily interested in the case $\nu = O(1)$ for which (49) holds if $B > Z^{2+\varepsilon}$; for anti-symmetric models, $\nu = O(N)$ so that we need $B > Z^{3+\varepsilon}$. For now, we assume that (49) holds, in which case the requirement (48) can be rewritten as

$$(1+\delta)^2\,\rho^2 < \frac{1}{C}\frac{N^2 B}{Z^4(\log\frac{Z^2}{B})^4} - \frac{\nu}{2} < \frac{1}{2C}\frac{N^2 B}{Z^4(\log\frac{Z^2}{B})^4}. \tag{50}$$

Thus we can ensure that the right side of (46) is positive by choosing

$$\rho = c\,\frac{1}{1+\delta}\frac{N\sqrt{B}}{Z^2(\log\frac{Z^2}{B})^2} \tag{51}$$

for some constant c independent of N, Z, B, δ.

Then, since $-e_0(N-1, Z, B) \geqslant 0$, condition (44) will hold for G_0 if

$$-CN\frac{Z^2}{\sqrt{B}}\left(\log\frac{Z^2}{B}\right)^2+\frac{N^2}{2\sqrt{4(1+\delta)^2\,\rho^2+2\nu}}-\lambda\frac{\sqrt{B}\,(\log N)^2}{\delta^2\rho^2}>0. \tag{52}$$

The first two terms in (52) behave like $+CN\frac{Z^2}{\sqrt{B}}(\log\frac{Z^2}{B})^2$ and the third like $-\lambda\,(\frac{\delta+1}{\delta})^2\,\frac{(\log N)^2\,Z^4(\log\frac{Z^2}{B})^4}{\sqrt{B}\,N^2}$. Comparing these expressions, we find that (using the assumption that $N>Z$) control of the localization error requires

$$\lambda\left(\frac{\delta+1}{\delta}\right)^2<\frac{N}{(\log N)^2\,(\log\frac{Z^2}{B})^2}\left(\frac{N}{Z}\right)^2. \tag{53}$$

We consider two cases of small and large δ separately.

(a) When $\delta=Z^{-\alpha}$, the left side of (53) behaves like $\frac{\lambda}{\delta^2}$. In this case (53) holds with ρ given by (51) provided that $N>Z$ is sufficiently large and $B\leqslant Ce^{Z^{1/2-\epsilon}}$ for some $\epsilon>\alpha$.

(b) When $\delta>1$, we can use the fact that $\frac{\delta+1}{\delta}\leqslant 2$ to see that (53) holds for *any* $\delta>1$ if $N>Z$ and $B\leqslant Ce^{Z^{1/2-\epsilon}}$ for some $\epsilon>0$. Alternatively, we can eliminate the upper bound on B by letting N grow with B as well as Z. In particular, (53) holds for any $\delta>1$ if $N>Z\ \log\frac{Z^2}{B}$.

3.3. Outer Ball Estimates

For any k such that $1\leqslant k\leqslant N$, we can write

$$\begin{aligned} h^{\Upsilon}(N, Z, M)=h_k^{\Upsilon}(N-1, Z, M)-\frac{1}{M}\frac{d^2}{dx_k^2}\\ -Z\tilde{V}_k^{\Upsilon}(x_k)+\sum_{j:\,j\neq k}\tilde{W}_{jk}^{\Upsilon}(x_j-x_k)\end{aligned} \tag{54}$$

with the understanding that $h_k^{\Upsilon}(N-1, Z, M)$ is the Hamiltonian obtained by omitting terms in (5) involving x_k, but with potentials defined by the N-particle state Υ. Let $E_0^{\Upsilon,k}(N-1, Z, B)$ denote the corresponding ground state energy. Since $h_k^{\Upsilon}(N-1, Z, M)\geqslant E_0^{\Upsilon,k}(N-1, Z, B)$ and $-\frac{d^2}{dx^2}\geqslant 0$, it follows that

$$(G_k\Phi, [h^{\Upsilon}(N, Z, B^{-1/2})-L_k-E_0^{\Upsilon,k}(N-1, Z, B)]\, G_k\Phi\rangle \tag{55}$$

$$\geqslant\left\langle G_k\Phi, \left[-Z\tilde{V}_k^{\Upsilon}(x_k)+\sum_{j:\,j\neq k}\tilde{W}_{jk}^{\Upsilon}(|x_j-x_k|)-L_k\right]G_k\Phi\right\rangle. \tag{56}$$

For simplicity, we henceforth omit indices j, k on $E_0, \tilde{V}, \tilde{W}$ and assume[7] that Υ is a symmetrized or anti-symmetrized product.

Now for $x \in \operatorname{supp} G_k$ we have that $|x_j - x_k| \leqslant |x_j| + |x_k| \leqslant (2+\delta)\,|x_k|$, so that

$$\begin{aligned}\tilde{W}^{\Upsilon}(|x_j - x_k|) &\geqslant \frac{1}{\sqrt{2}} V_{\nu-1}\left(\frac{|x_j - x_k|}{\sqrt{2}}\right) \geqslant \frac{1}{\sqrt{2}} V_{\nu-1}\left(\frac{(2+\delta)\,|x_k|}{\sqrt{2}}\right) \\ &\geqslant \frac{1}{\sqrt{(2+\delta)^2\, x_k^2 + 2\nu}} = \frac{1}{2} \frac{1}{\sqrt{(1+\frac{\delta}{2})^2\, x_k^2 + \frac{\nu}{2}}},\end{aligned} \tag{57}$$

where we used (17) and (19).

It follows from the upper bound in (19) that

$$\tilde{V}^{\Upsilon}(x_k) \leqslant V_{\mu}(x_k) \leqslant \frac{1}{\sqrt{x_k^2 + \mu}}. \tag{58}$$

Thus

$$-Z\tilde{V}^{\Upsilon}(x_k) + \sum_{j:\, j \neq k} \tilde{W}^{\Upsilon}(x_k) \geqslant -\frac{Z}{\sqrt{x_k^2 + \mu}} + \frac{N-1}{2} \frac{1}{\sqrt{(1+\frac{\delta}{2})^2\, x_k^2 + \frac{\nu}{2}}}. \tag{59}$$

If one ignores δ, the right side of (59) is approximately

$$\frac{-Z}{\sqrt{x_k^2 + \mu}} + \frac{N}{2} \frac{1}{\sqrt{x_k^2 + \frac{\nu}{2}}} \tag{60}$$

which will be positive if $N > 2Z$ and $\nu < 2\mu$.

This explains the origin of the linear term in Theorem 1. It remains to take into account the localization error (42b). When $\delta \to 0$ one need only choose $N - 2Z$ large enough to control (42b). When larger choices of δ are made, one pays the price of an increase of $Z\delta$ in the electrostatic estimates, as shown in (64) below.

Substituting (59) in (56) and using the estimate (42b), one finds that (56) is bounded below by

$$\left\langle G_k\Phi, \frac{T(x_k)}{\sqrt{(1+\frac{\delta}{2})^2\, x_k^2 + \frac{\nu}{2}}}\, G_k\Phi \right\rangle, \tag{61}$$

[7] Since the bounds on $\tilde{V}$ and $\tilde{W}$ are independent of j this is not a significant restriction. In the case of distinguishable particles, one need only compare to $E_0^{\Upsilon,k}(N-1, Z, B)$ for a particular k. When indistinguishable particles are associated with an asymmetric product of Landau states, the full wave function must be a linear combination of states of the form (1) with terms associated with irreducible representations of S_n to yield the appropriate total symmetry; this is a more complex situation than the simple product model considered here.

where

$$T(x) = -Z\sqrt{\frac{(1+\frac{\delta}{2})^2 x^2 + \frac{\nu}{2}}{x^2+\mu}} + \frac{N-1}{2} - \lambda\frac{\sqrt{B}(\log N)^2}{\delta^2\rho}\sqrt{\left(1+\frac{\delta}{2}\right)^2 + \frac{\nu}{2x^2}}. \quad (62)$$

Expression (61) will be positive, ensuring that (44) holds for $k = 1,..., N$, if $T(x) > 0$ for $|x| > \rho$. Since $|x_k| \geqslant \rho$ on $\text{supp}(G_k)$, we find that, with ρ given by (51),

$$\frac{\nu}{2x_k^2} \leqslant \frac{\nu}{2N}\frac{Z^3}{B}\frac{Z}{N}\left(\log\frac{Z^2}{B}\right)^4 \leqslant 1 \quad (63)$$

when $N > Z$ and (49) holds. Thus, we can conclude that

$$\begin{aligned} 2T(x) &\geqslant N-1-2Z\sqrt{\frac{(1+\frac{\delta}{2})^2 x^2+\frac{\nu}{2}}{x^2+\mu}} - 2\lambda\frac{(1+\delta)^2(\log N)^2(\log\frac{Z^2}{B})^2 Z^2}{\delta^2 N} \\ &\geqslant N-1-2Z\left(1+\frac{\delta}{2}\right) - 2\lambda\frac{(\log N)^2(\log\frac{Z^2}{B})^2 Z^2}{N}\frac{(1+\delta)^2}{\delta^2} \end{aligned} \quad (64)$$

where the second inequality used the assumption $\nu < 2\mu$.

Now, we can analyze the N-dependence of the right side of (64) by writing it in the form

$$2T(x) \geqslant N - \frac{(\log N)^2 Q}{N} - R \quad (65)$$

where Q, R are positive and may depend on Z, B, δ but are independent of N. The expression on the right is increasing in N. Hence, for any fixed choice of Z, B, δ, if it is positive for some critical $N = N_c$, then it will be positive for all $N > N_c$.

3.4. Completion of Proofs

To prove Theorem 1, choose $N_c = 2Z + 1 + aZ^{1+2\alpha}$. Then

$$2T(x) \geqslant Z\left[aZ^{2\alpha} - c\frac{[(1+2\alpha)\log Z]^2(2\log Z - \log B)^2}{\delta^2 Z^{2\alpha}} - \delta\right]. \quad (66)$$

Thus if $\delta = O(Z^{-\alpha})$, then for sufficiently large Z,

$$2T(x) \geqslant Z\left[aZ^{2\alpha} - c(\log Z)^2(2\log Z - \log B)^2 - Z^{-\alpha}\right] \quad (67)$$

which can be made positive for sufficiently large Z as long as $\log B < C\frac{Z^\alpha}{\log Z}$, for some suitable constant C. This will be true if $B \leqslant a_1 e^{Z^{\alpha/2}}$ for some constant a_1. Replacing α by $\alpha/2$ yields Theorem 1.

To improve the Z^α growth of N to one involving only logarithmic terms, as in Theorem 2, one can not let $\delta \to 0$. Moreover, the term $\frac{(\delta+1)^2}{\delta^2}$ in (64) implies that one can not decrease the localization error by choosing δ large. Therefore, we simply take $\delta = 1$, in which case (64) becomes

$$2T(x) \geqslant N-1-2Z-Z-c\,\frac{(\log N)^2\,(\log\frac{Z^2}{B})^2\,Z^2}{N}. \tag{68}$$

We now set $N = N_c$ in (68) and write $N_c = 2Z+1+Zf(Z, B)$. Then

$$2T(x) \geqslant Z\left[f(Z, B)-1-c\,\frac{(\log\frac{Z^2}{B})^2\,(\log Z+\log f(Z, B))^2}{f(Z)}\right]. \tag{69}$$

The inner ball estimates in Section 3.2 require $B = O(\exp Z^{1/2-\varepsilon})$. Under this assumption, Theorem 1 implies that $f(Z, B)$ grows more slowly than Z^α for some suitable α, so that $\log f(Z, B) \leqslant \log Z$ for sufficiently large Z. Hence we can find a constant A such that the right side of (69) is positive when $f(Z, B) = A\,|\log\frac{Z^2}{B}|\,\log Z$. (Note that $|\log\frac{Z^2}{B}|$ will stay bounded away from 0, due to the lower bound $B > Z^{\gamma_\nu}$, $\gamma_\nu > 2$, which ensures that $f(Z, B) > 1$ for big Z.) This proves Theorem 2.

Since our hypotheses do not permit B to grow exponentially with Z and the case of greatest interest is polynomial growth, e.g., $B = Z^{3+\varepsilon}$, it is useful to restate our results under the assumption that $B = Z^p$ for some $p > 0$. In that case, we can conclude that there is a constant A, depending on p, such that (69) is positive for $f(Z) = A(\log Z)^2$, which proves Theorem 3. This also gives a bound of $N_{\max}(Z, Z^p) \leqslant 2Z + AZ(\log Z)^2$.

Corollary 3 follows immediately from Theorem 2 and the discussion above.

To prove Corollary 4, it suffices to observe that the hypotheses of Theorems 1 and 2 hold with $\mu = m$, and $\nu = 2m$. Unless m depends upon N, we now have $\nu = O(1)$ so that (49) holds if $B > Z^{2+\varepsilon}$.

To prove Corollary 5 for the Slater model, note that it follows from (20) and (32) that $\tilde{V}^\Upsilon(x) = V_{\text{av}}(x) \leqslant 2V_N(x)$, and from (34) that $\tilde{W}^\Upsilon(x) \geqslant V_{2N-3}(x)$. Thus, $h^{\det}(N, Z, M)$ satisfies the hypotheses of Theorems 1 and 2 with $\mu = N$, $\nu = 2N-2$, but with Z *is replaced by an effective charge* of $2Z$. This has the effect of doubling the coefficient in the linear term and modifying the constant in the non-linear term. Since ν is $O(N)$, (49) requires $B > Z^{3+\varepsilon}$.

Remark. With more technical effort some of the hypotheses can be relaxed and/or estimates improved as sketched below.

1. The condition $\nu \leqslant 2\mu$ is needed only for the bound $\sqrt{((1+\frac{\delta}{2})^2 x^2 + \frac{\nu}{2})/(x^2+\mu)}|_{x\approx 0} \leqslant 1$ implicitly used in (64). However, this is actually used only in analyzing the outer region for which one can assume $|x_k| \geqslant \rho$ is much larger than 0. Hence, with a bit more effort, this condition can probably be dispensed with. At worst, allowing $\nu > 2\mu$ would only change the coefficient of the (lower order) linear term.

2. The upper bound $B \leqslant Ce^{Z^{1/2-\varepsilon}}$ is somewhat artificial. It arises because we have chosen to state our results in a way that emphasizes the dependence of $N_{\max}(Z, B)$ on Z. More rapid growth of B will increase the confinement of the electrons in two dimensions, but make them more delocalized in the direction orthogonal to the field. Hence, it is not surprising that the localization error will be harder to control if B grows exponentially with Z.

In the case of Theorem 2, one can eliminate the need for this upper bound in controlling the localization error on the inner ball by using the fact that $\frac{N}{Z} > \log \frac{Z^2}{B}$. This was noted in remark (b) after (53). However, if B grows exponentially with Z, then the estimate $\log f(Z, B) < \log Z$ used after (69) will no longer be valid. The upper bound can be eliminated by allowing N_c to grow sufficiently with B. The choice $f(Z, B) = (\log Z)^2 + \log Z(\log B)^{1+\omega}$ for some $\omega > 0$ will suffice. This proves the result stated as Theorem 3.1 in ref. 7 and given after (8) in the introduction.

3. The linear term in the Slater model is doubled because we use the estimate $V_{\text{av}}(x) \leqslant 2V_N(X)$ which gives an effective charge of $2Z$ rather than Z. Although this bound is tight near $x \approx 0$, it is used only in the outer ball where $|x_k| > \rho$ and one would expect $V_{\text{av}}(x) \approx V_N(x) \approx V_{N-1}(x)$. (Note that since $\nu = 2(N-1)$ it would suffice to have a bound with $\mu = N-1$.)

In fact, using results in refs. 7 and 16 one can show that

$$V_{\text{av}}(x) = 2V_N(x) - \frac{2x^2}{N}\left(\frac{1}{x} - V_{N-1}(x)\right) \tag{70}$$

$$\approx 2V_N(x) - \frac{1}{\sqrt{x^2+N}} + O\left(\frac{N}{x^2}\right). \tag{71}$$

When $|x| > p$, and $B > Z^3$ this becomes

$$V_{\text{av}}(x) \approx 2V_N(x) - \frac{1}{\sqrt{x^2+N}} + O\left(\frac{(\log Z)^4}{N}\right)$$

$$\leqslant V_N(x) + C\,\frac{1}{Z} \tag{72}$$

for sufficiently large Z and $N > Z^{1+\alpha}$ Thus, one could expect to show that (36) can be replaced by $N_{\max}(Z, B) \leqslant 2Z + A_\alpha Z^{1+\alpha}$ in Corollary 5 by using more refined estimates for $V_{\mathrm{av}}(x)$. This would give the expected behavior of $2Z$ for the linear term when B grows more rapidly than Z^3.

4. DISCUSSION

The first step of the RS method is to divide the system into a small "inner" ball in which binding is precluded because the electrons are confined to a small region, and an "outer" ball in which the localization error becomes negligible as $Z \to \infty$. For bosonic systems, one expects to be able to squeeze the electrons closer together, yielding a smaller cut-off ρ than for fermions. This feature is the *only* factor which precludes extending the proof of asymptotic neutrality in ref. 11 to bosonic atoms. This suggests that the localization error is not simply a technical artifact, but a reflection of a real physical effect. In the one-dimensional models considered here, the anti-symmetry required by the fermionic nature of electrons is achieved entirely within the Landau band. This results in a one dimensional model that is bosonic, with the anti-symmetry reflected only in the effective potentials.

The one-dimensional confinement also delocalizes the electrons. This is reflected by the the effective mass of $M = B^{-1/2}$ in (5) which implies that in strong fields the electrons behave like extremely light particles. The uncertainty principle then implies that trial wave functions which localize the electrons cannot yield bound states. Thus, it may seem rather surprising that localization methods can be applied successfully. For atoms in strong magnetic fields, this terminology may be misleading because the cut-off radius ρ is not small. Instead $\rho \sim N\sqrt{B}\, Z^{-2}(\log \frac{Z^2}{B})^{-2}$ which grows with B. Thus, localization methods can be used to obtain (non-optimal) upper bounds on $N_{\max}$ despite the fact that the electrons are highly delocalized and the size of the "inner" region becomes large as $B \to \infty$.

Lieb's method can be interpreted as a different type of localization in which G_k is essentially the inverse square root of the potential. In three dimensions, the resulting localization error can be completely controlled by the kinetic energy, eliminating the need for an additional inner/outer delocalization provided that the magnetic field goes to zero at infinity. However, as discussed in Section 3 of ref. 5, control of the localization error is more complex in models resulting from the types of magnetic fields considered here.

When Lieb's method was applied to a one-dimensional model in ref. 5 control of the localization error led to a $\sqrt{B}$ growth in N. In ref. 18

Seiringer showed that better bounds can be obtained if one applies Lieb's method to the full 3-dimensional Hamiltonian, yielding results comparable to those obtained here.

One might try to combine Lieb's method with the inner/outer localization used here, i.e., in Section 3.1 use G_0 as in (i) but in (ii) replace G_k by $\sqrt{\frac{1-G_0^2}{\tilde{V}^Y(x_k)}}$ for $k \geqslant 1$. In the case of the simple 0-model, the argument given in Section 4 of ref. 5 can be used in the outer region with the term $\lim_{x \to 0} \frac{|v'(x)|^2}{4v(x)}$ replaced by $\frac{|v'(\rho)|^2}{4v(\rho)}$. With ρ as in Section 3.2, this would, yield a net bound of

$$N_{\max}(Z, B) \leqslant 2Z + AZ \left|\log \frac{Z^2}{B}\right| \tag{73}$$

which is a very slight improvement.[8] To extend this to $m \neq 0$, would require additional work. However, for $|x| > \rho$ one should be able to show that $[V_m(x)]^{-1} \approx \sqrt{x^2+m}$ to obtain a similar bound. In the case of the Slater model, one would also need estimates of the type discussed in Remark 3.

APPENDIX A

We begin by proving a special case of Pröschel, *et al.*'s result[13] that the effective interaction $W_{mm'}(x_1 - x_2)$ can be written as a convex combination of potentials of the form $\frac{1}{\sqrt{2}} V_j(\frac{x_1 - x_2}{\sqrt{2}})$ with $j \leqslant m + m'$. In the special case $m = m'$, only terms with even subscript occur in the convex combination.

Lemma 6. The effective interaction $W_{mm}(x_1 - x_2)$ defined in (25) satisifies

$$W_{mm}(x_1 - x_2) = \sum_{j=0}^{m} b_{2j} \frac{1}{\sqrt{2}} V_{2j}\left(\frac{(x_1 - x_2)}{\sqrt{2}}\right), \tag{74}$$

with $b_{2j} > 0$ and $\sum_{j=0}^{m} b_{2j} = 1$.

Proof. Substituting for γ_m in (24) and writing out the resulting integral yields

$$W_{mm}(x_1 - x_2) = \frac{1}{\pi m!} \int_{\mathbb{C}} \int_{\mathbb{C}} d\zeta_1 \, d\zeta_2 \frac{|\zeta_1|^{2m} |\zeta_2|^{2m} e^{-|\zeta_1|^2} e^{-|\zeta_2|^2}}{\sqrt{(x_1 - x_2)^2 + |\zeta_1 - \zeta_2|^2}}. \tag{75}$$

[8] The change from a quadratic to a linear dependence on log Z is due to the fact that the LE arising from G_0 does not require a $(\log N)^2$ in the numerator in (iii) and (iv), resulting in a net bound of the form $\frac{\lambda}{\rho^2}$.

We now make the complex change of variables to

$$\begin{aligned} \sigma &\equiv \tfrac{1}{\sqrt{2}}(\zeta_1+\zeta_2) & \tau &\equiv \tfrac{1}{\sqrt{2}}(\zeta_1-\zeta_2) \\ s &= |\sigma| = \tfrac{1}{\sqrt{2}}|\zeta_1+\zeta_2| & t &= |\tau| = \tfrac{1}{\sqrt{2}}|\zeta_1-\zeta_2| \end{aligned} \tag{76}$$

and let θ be the angle between σ and τ. Then $|\zeta_1|^2+|\zeta_2|^2=s^2+t^2$ and

$$\begin{aligned} |\zeta_1|^2\,|\zeta_2|^2 &= (s^2+t^2+2st\cos\theta)(s^2+t^2-2st\cos\theta) \\ &= s^4+t^4-s^2t^2\cos 2\theta. \end{aligned} \tag{77}$$

Substituting in (75) yields

$$W_{mm}(x_1-x_2) = \frac{2}{m!}\int_0^\infty e^{-t^2} t\,dt \int_0^\infty e^{-s^2} s\,ds \int_0^{2\pi} d\theta\, \frac{(s^4+t^4-s^2t^2\cos 2\theta)^m}{\sqrt{(x_1-x_2)^2+2t^2}}. \tag{78}$$

Performing the integral over s and θ yields

$$W_{mm}(x_1-x_2) = \int_0^\infty e^{-t^2} t\,dt\, \frac{P(t^2)}{\sqrt{(x_1-x_2)^2+2t^2}} \tag{79}$$

for some polynomial $P(u)$ of degree $2m$. Writing $P(u)=\sum_{i=0}^{2m} b_i u^i$, and substituting in (79) immediately yields

$$W_{mm}(x_1-x_2) = \sum_{i=0}^{2m} b_i \frac{1}{\sqrt{2}} V_i\left(\frac{x_1-x_2}{\sqrt{2}}\right). \tag{80}$$

It remains only to show that the coefficients b_i are even, positive and sum to one. Applying the binomial expansion to the numerator in (78), one easily sees that terms with $i=2j$ have positive coefficients $b_{2j}>0$. When $i=2j+1$ is odd, one has an integral of the form $\int_0^{2\pi}\cos^{2j+1}2\theta\,d\theta=0$ which implies $b_{2j+1}=0$. Thus, only the coefficients with $i=2j$ survive, and these are positive. To see that $\sum_{j=0}^m b_{2j}=1$, it suffices to use the fact that both $W_{mm}(x)$ and all $V_i(x)$ behave like $1/|x|$ at infinity.

When $m\neq m'$ the integrand will contain an additional factor of the form $(s^2+t^2+2st\cos\theta)^{|m-m'|}$. As above, one can show that terms involving $\cos^j\theta$ integrate to zero when j is odd.

One can use a similar strategy to show that any inner product of the form

$$\left\langle \gamma_j(\zeta_1)\,\gamma_k(\zeta_2), \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\,\gamma_j(\zeta_1)\,\gamma_k(\zeta_2)\right\rangle \qquad \text{or} \tag{81a}$$

$$\left\langle \gamma_j(\zeta_1)\,\gamma_k(\zeta_2), \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\,\gamma_k(\zeta_1)\,\gamma_j(\zeta_2)\right\rangle \tag{81b}$$

can be written as a linear combination $\sum_{j=0}^{j+k} c_j \frac{1}{\sqrt{2}} V_j(\frac{(x_1-x_2)}{\sqrt{2}})$ with $\sum_j c_j = 1$. In the case of (81a), as sketched above and shown in ref. 13, the coefficients c_j are positive giving a convex combination. For the exchange integrals (81b), this need not be true. However, for antisymmetric products, the two types of integrals arise together in combinations whose net coefficients are positive, as shown below.

Lemma 7. For any choice of $0 < m_1 < m_2 < \cdots < m_N$,

$$W_{\text{det}}^{m_1 \cdots m_N}(x_1 - x_2) = \frac{1}{N!} \left\langle \gamma_{m_1} \wedge \cdots \wedge \gamma_{m_N}, \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \gamma_{m_1} \wedge \cdots \wedge \gamma_{m_N} \right\rangle$$
$$= \frac{1}{\sqrt{2}} \sum_{j=0}^{J} b_{2j+1} V_{2j+1} \left(\frac{x_1 - x_2}{\sqrt{2}} \right), \tag{82}$$

with $b_{2j+1} \geqslant 0$ and $\sum_j b_{2j+1} = 1$, and $J = m_{N-1} + m_N$.

In the Slater model, we have $m_k = k-1$, from which it follows that $J = 2N-3$.

Corollary 8. For the Slater model, the effective interaction in $h^{\text{det}}(N, Z, B^{-1/2})$ (5) is a convex combination of V_m with odd $m = 1, 3, \ldots, 2N-3$, i.e.,

$$\widetilde{W}^{\Upsilon}(x_1 - x_2) = W_{\text{det}}(x_1 - x_2) = \frac{1}{\sqrt{2}} \sum_{j=0}^{N-2} b_{2j+1} V_{2j+1} \left(\frac{x_1 - x_2}{\sqrt{2}} \right), \tag{83}$$

with $b_{2j+1} > 0$ and $\sum_{j=0}^{N-2} b_{2j+1} = 1$.

Proof. To prove Lemma 7, we first consider the special case $N = 2$. Let j, k be fixed, and write

$$W_{\text{det}}^{j,k}(x_1 - x_2) = 2 \left\langle \gamma_j \wedge \gamma_k(\zeta_1, \zeta_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \gamma_j \wedge \gamma_k(\zeta_1, \zeta_2) \right\rangle$$
$$= \int_{\mathbb{C}} \int_{\mathbb{C}} \frac{|\zeta_1^j \zeta_2^k - \zeta_1^k \zeta_2^j|^2 \, e^{-|\zeta_1|^2 - |\zeta_2|^2}}{\sqrt{(x_1 - x_2)^2 + |\zeta_1 - \zeta_2|^2}} \, d\zeta_1 \, d\zeta_2, \tag{84}$$

where we used (15) and as before, $\mathbf{r}_j = (x_j, y_j, z_j)$ and $\zeta_j = y_j + i z_j$. Now make a change of variables as in (76). Using the binomial expansion, we find

$$\zeta_1^j \zeta_2^k = 2^{-(j+k)/2} \sum_{\nu=0}^{j} \sum_{\mu=0}^{k} (-1)^{\mu} \binom{j}{\nu} \binom{k}{\mu} \tau^{\mu+\nu} \sigma^{j+k-(\mu+\nu)},$$

so that

$$\zeta_1^j \zeta_2^k - \zeta_1^k \zeta_2^j = \sum_{\alpha=0}^{j+k} A_\alpha \tau^\alpha \sigma^{j+k-\alpha}, \tag{85}$$

where

$$A_\alpha = 2^{-(j+k)/2} \sum_{\substack{\nu+\mu=\alpha \\ \nu \leqslant j,\, \mu \leqslant k}} [(-1)^\mu - (-1)^\nu] \binom{j}{\nu} \binom{k}{\mu}$$

and we suppress the dependence of A_α on j, k. When α is even, $(-1)^\mu = (-1)^\nu$ so that $A_\alpha = 0$. Therefore, only terms with α odd survive in the sum (85). Moreover,

$$\begin{aligned} W_{\mathrm{det}}^{j,k}(x_1 - x_2) &= \int_{\mathbf{C}} \int_{\mathbf{C}} \frac{|\zeta_1^j \zeta_2^k - \zeta_1^k \zeta_2^j|^2 \, e^{-|\zeta_1|^2 - |\zeta_2|^2}}{\sqrt{(x_1 - x_2)^2 + |\zeta_1 - \zeta_2|^2}} \, d\zeta_1 \, d\zeta_2 \\ &= \sum_{\alpha \text{ odd}} \sum_{\beta \text{ odd}} A_\alpha \bar{A}_\beta \int_{\mathbf{C}} \int_{\mathbf{C}} \frac{\tau^\alpha \bar{\tau}^\beta \sigma^{j+k-\alpha} \bar{\sigma}^{j+k-\beta}}{\sqrt{(x_1 - x_2)^2 + 2t^2}} \, e^{-s^2 - t^2} \, d\sigma \, d\tau. \end{aligned} \tag{86}$$

Next, write $\tau = te^{i\varphi}$ and use the fact that

$$\int_{\mathbf{C}} \tau^\alpha \bar{\tau}^\beta f(t) \, d\tau = \int_0^\infty t^{\alpha+\beta} f(t) \, dt \int_0^{2\pi} e^{i\varphi(\alpha-\beta)} \, d\varphi$$

is zero if $\alpha \neq \beta$ to see that the integral (86) becomes

$$(2\pi)^2 \sum_{\alpha \text{ odd}} |A_\alpha|^2 \int_0^\infty s^{2(j+k-\alpha)+1} e^{-s^2} \, ds \int_0^\infty \frac{|t|^{2\alpha+1} \, e^{-t^2}}{\sqrt{(x_1 - x_2)^2 + 2t^2}} \, dt. \tag{87}$$

Integrating over s then yields

$$W_{\mathrm{det}}^{j,k}(x_1 - x_2) = \sum_{\alpha \text{ odd}} b_\alpha \frac{1}{\sqrt{2}} V_\alpha \left(\frac{x_1 - x_2}{\sqrt{2}} \right),$$

for suitable constants b_α, of which we only want to note that they are strictly positive when α is odd and in the range $1 \leqslant \alpha \leqslant j+k$. As before, $\sum_j b_j = 1$ follows easily from the fact that both $W_{\mathrm{det}}(x)$ and the $V_j(x)$ behave like $1/|x|$ at infinity. This proves Lemma 7 in the case $N = 2$.

The general case then follows from the fact that an N-particle Slater determinant is a convex combination of two-particle Slater determinants. In fact,

$$
\begin{aligned}
W_{\text{det}}^{m_1\cdots m_N}(x_1-x_2) &= \frac{1}{N!}\left\langle \gamma_{m_1}\wedge\cdots\wedge\gamma_{m_N}, \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\gamma_{m_1}\wedge\cdots\wedge\gamma_{m_N}\right\rangle \\
&= \frac{2}{N(N-1)}\sum_{j<k}\left\langle \gamma_{m_j}\wedge\gamma_{m_k}(\zeta_1,\zeta_2), \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\gamma_{m_j}\wedge\gamma_{m_k}(\zeta_1,\zeta_2)\right\rangle \\
&= \frac{2}{N(N-1)}\sum_{j<k} W_{\text{det}}^{m_j,m_k}(x_1-x_2). \qquad (88)
\end{aligned}
$$

ACKNOWLEDGMENTS

This work was started when R.B. was professor at the University of Reims, France, and M.B.R. a visiting professor there. Some of this work was done while both authors were visiting the Schrödinger Institute at the University of Vienna. The final version was written while M.B.R. was a Walton visitor at the Communications Network Research Institute of Dublin Institute of Technology. It is a pleasure to acknowledge the hospitable environment at these institutions. © by authors. The work of M.B.R. was partially supported by the National Science Foundation under Grants DMS-0074566 and DMS-0314228.

REFERENCES

1. Y. Avron, I. Herbst, and B. Simon, Strongly bound states of hydrogen in intense magnetic field, *Phys. Rev. A* **20**:2287–2296 (1979).
2. R. Brummelhuis and P. Duclos, On the one dimensional behavior of atoms in intense homogenous magnetic fields, in *Operator Theory: Advances and Applications*, Vol. 126 (Birkhaüser, 2001).
3. R. Brummelhuis and P. Duclos, Effective Hamiltonians for atoms in very strong magnetic fields, *Few-Body Systems* **31**:119–124 (2002).
4. R. Brummelhuis and P. Duclos, Norm-resolvent convergence to effective Hamiltonians for atoms in strong magnetic fields (2003), in preparation.
5. R. Brummelhuis and M. B. Ruskai, A one-dimensional model for many electron atoms in extremely strong magnetic fields: Maximum negative ionization, *J. Phys. A* **32**:2567–2582 (1999).
6. R. Brummelhuis and M. B. Ruskai, Talks at the Schrödinger institute in Vienna and the Q-Math 7 conference in Prague (June, 1998).
7. R. Brummelhuis, M. B. Ruskai, and E. Werner, One-dimensional regularizations of the Coulomb potential with applications to atoms in extremely strong magnetic fields, in *Differential Equations and Mathematical Physics*, G. Weinstein and R. Weikard, eds. (International Press, 2000), pp. 43–51.

8. H. L. Cycon, R. J. Froese, W. Kirsch, and B. Simon, *Schrödinger Operators* (Springer-Verlag, 1987).
9. C. Hainzl and R. Seiringer, A discrete density matrix theory for atoms in strong magnetic fields, *Comm. Math. Phys.* **217**:229–248 (2001).
10. E. H. Lieb, Bound on the maximum negative ionization of atoms and molecules, *Phys. Rev. A* **29**:3018–3028 (1984).
11. E. H. Lieb, L. M. Sigal, B. Simon, and W. Thirring, Asymptotic neutrality of large-Z ions, *Commun. Math. Phys.* **116**:635–644 (1988).
12. E. H. Lieb, J. P. Solovej, and J. Yngvason, Heavy atoms in the strong magnetic field of a neutron star, *Phys. Rev. Lett.* **69**:749–752 (1992); and Asymptotics of heavy atoms in high magnetic fields I: Lowest Landau band regions, *Commun. Pure Appl. Math.* **47**:513–591 (1993).
13. P. Pröschel, W. Rösner, G. Wunner, H. Ruder, and H. Herold, Hartree-Fock calacula-tions for atoms in strong magnetic fields I: Energy levels of two electron systems, *J. Phys. B* **15**:1959–1976 (1982).
14. M. B. Ruskai, Improved estimates on the number of bound states of negative bosonic atoms, *Ann. Inst. H. Poincare A: Physique Theorique* **61**:153–162 (1994).
15. M. B. Ruskai, Localization of outer electrons in negative atoms, in *Differential Equations and Mathematical Physics*, R. Lewis and I. Knowles, eds. (International Press, 1995), pp. 187–192.
16. 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).
17. L. Schiff and H. Snyder, Theory of the quadratic Zeeman effect, *Phys. Rev.* **55**:59–63 (1939).
18. R. Seiringer, On the maximum ionization of atoms in strong magnetic fields, *J. Phys. A* **34**:1943–1948 (2001); math-ph/0006002.