On the ordering of energy levels in homogeneous magnetic fields

Bernhard Baumgartner[1] and Robert Seiringer[2]

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

November 17, 2000

Abstract

We study the energy levels of a single particle in a homogeneous magnetic field and in an axially symmetric external potential. For potentials that are superharmonic off the central axis, we find a general "pseudoconcave" ordering of the ground state energies of the Hamiltonian restricted to the sectors with fixed angular momentum. The physical applications include atoms and ions in strong magnetic fields. There the energies are monotone increasing and concave in angular momentum. In the case of a periodic chain of atoms the pseudoconcavity extends to the entire lowest band of Bloch functions.

1 Introduction

We consider the non-relativistic quantum mechanical theory of a single particle in a homogeneous magnetic field and in an external potential. The study of such systems is currently of interest in the context of theories of atoms in strong magnetic fields. In the way of describing the atoms as an assembly of electrons in an effective potential, an essential question is where the electrons are located. In the case of a very strong magnetic field this problem is connected with the comparison of individual energy levels, as the atom is not to be described with a completely semiclassical theory. See [LSY94, BSY00, HS00]. In all these studies the superharmonicity of the potential off the nucleus turned out to be the right property to deduce theorems on the localization of the electrons and on level ordering. It is precisely this property, superharmonicity off a certain axis, which is also used in our extension of the present knowledge presented in this paper.

[1]E-Mail: `baumgart@ap.univie.ac.at`
[2]E-Mail: `rseiring@ap.univie.ac.at`

The potential is assumed to be invariant under rotations around the z-axis, the magnetic field in z-direction, so that the eigenvalue m of L_z, the z-component of the angular momentum, is a "good quantum number". We may ignore spin and intrinsic magnetic moment, since this degree of freedom decouples in this case from the spatial behavior. Assuming appropriate gauging and appropriate units, either with a positive charge of the particle and the magnetic field pointing into the positive z-direction, or with a negative charge of the particle and the magnetic field pointing into the negative z-direction, the Hamiltonian acts in $\mathcal{L}^2(\mathbb{R}^3, d^3\mathbf{x})$ as

$$H = -\Delta - B\,L_z + \frac{B^2}{4} r_\perp^2 + V(r_\perp, z), \tag{1}$$

where $B > 0$ denotes the absolute value of the strength of the magnetic field, $r_\perp = \sqrt{x^2 + y^2}$, $\mathbf{x} = (x, y, z)$. See [AHS78] for details on the definition of H.

The Hamiltonian can be considered as a direct sum of H_m, where each H_m acts in the subspace of eigenfunctions of L_z with $L_z = m$. We compare the spectra of the operators H_m, denoting

$$E_m = \inf \operatorname{spec} H_m. \tag{2}$$

Since each H_{-m} is unitarily equivalent to $H_m + 2mB$, we can restrict the investigation to non-negative m. (Note that, for $V = 0$, $E_m = B$ for all $m \geq 0$.)

If $V(r_\perp, z) = V_\perp(r_\perp) + V_z(z)$, the three-dimensional system splits into a one-dimensional z-dependent and a two-dimensional $r_\perp$-dependent system, and all the level comparison theorems concerning comparison with a two-dimensional oscillator can be applied, with obvious modifications. See [BGM85], the Subsections 4.7 and 6.4 of [B85], and [B91] for a simpler proof; see also Theorem B in [GS95].

But here we are interested in general cases without a splitting into $r_\perp$-dependent and z-dependent systems. What is known up to now in these general situations is:

(i) There are examples, where $\inf\{E_m\}$ is attained as a minimum, but not at $m = 0$, [LC77, AHS78].

(ii) For all $m \geq 0$ we have $E_m \leq E_{m+1} + B$, with strict inequality if the E_m's are eigenvalues.

(iii) If E_m and E_{m+1} are eigenvalues, $V(r_\perp, z)$ not constant in $r_\perp$, then $\partial V/\partial r_\perp \geq 0$ implies $E_{m+1} > E_m$, and $\partial V/\partial r_\perp \leq 0$ implies $E_{m+1} < E_m$, as shown by Grosse and Stubbe in [GS95].

(iv) If $\inf \operatorname{spec} H$ is an eigenvalue, $\Delta V \leq 0$ (in the sense of distributions) and $\Delta V \neq 0$, both at $r_\perp > 0$, the corresponding eigenvector is unique and has angular momentum $m = 0$, [BS00].

The general bound (ii), which holds also for higher eigenvalues, is shown in Lemma 13 in the Appendix, where also a short version of the proof of (iii) is given.

1. Remark (On proving (iv)). In [BS00] we considered $V = -\frac{1}{|\mathbf{x}|} + \frac{1}{|\mathbf{x}|} * \rho$, with ρ a nice axially symmetric positive function. But the proof can be extended, without any change, to the more general case, where negative electric charges are located on the z-axis, and where ρ is any repulsive axially symmetric distribution which is not zero everywhere away from the z-axis. Actually, this theorem will be a corollary of the central mathematical result of this paper, Theorem 4 (at least if inf spec H is a discrete eigenvalue).

Posing conditions on the potential V in Section 2, we try to allow for a wide variety of physical applications. One of special importance is dealing with the energies of a charged particle in the electric field generated by attractive charges situated on the z-axis and by an axially symmetric repulsive charge-distribution. It is

2. THEOREM (Monotonicity and concavity for finite charges). *Let*

$$V(r_\perp, z) = -\int_{-\infty}^{\infty} \frac{1}{|\mathbf{x} - (0,0,z')|}\sigma(z')dz' + \int_{\mathbb{R}^3} \frac{1}{|\mathbf{x} - \mathbf{x}'|}\rho(r'_\perp, z')d^3\mathbf{x}', \qquad (3)$$

with $\sigma(z)dz$ a positive finite Borel measure on $\mathbb{R}$, and $\rho(r_\perp, z)d^3\mathbf{x}$ a non-negative finite Borel measure on $\mathbb{R}^3$. In these cases the sequence E_m is non-decreasing, concave, and $\lim_{m\to\infty} E_m = B$. Moreover, if $\int \rho(r_\perp, z)d^3\mathbf{x} < \int \sigma(z)dz$, the sequence E_m is strictly monotone increasing and strictly concave.

The proof will be given at the end of Section 2.

Another physical application deals with the entire lowest band of energies in an infinite periodic system. It will be stated in Theorem 10.

2 Ordering in external potentials

Consider the "annihilation operator"

$$a = \frac{1}{2}\left(\sqrt{\frac{2}{B}}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right) + \sqrt{\frac{B}{2}}\,(x - iy)\right), \qquad (4)$$

and its adjoint, the "creation operator" $a^\dagger$. These operators obey the commutation relation

$$[a, a^\dagger] = 1, \qquad (5)$$

and the operator a lowers the angular momentum,

$$[L_z, a] = -a. \qquad (6)$$

In absence of external potentials both a and $a^\dagger$ commute with the Hamiltonian

$$H_B = -\Delta - B\,L_z + \frac{B^2}{4} r_\perp^2. \tag{7}$$

Given any multiplication operator V, a straightforward calculation shows the formal equation

$$[a^\dagger, [a, V]] = [[V, a^\dagger], a] = \frac{1}{2B}\left(-\frac{\partial^2 V}{\partial x^2} - \frac{\partial^2 V}{\partial y^2}\right). \tag{8}$$

It holds in the sense of distributions, if $V \in \mathcal{L}^1_{\mathrm{loc}}$, and this condition will be fulfilled as a consequence of the following

Technical condition on V:

For fixed angular momentum $L_z = m$, V is relatively bounded with respect to H_B, with some bound less than 1; i.e., for some $b_1 < 1$ and b_2, depending on m,

$$\|V\psi\| \le b_1 \|H_B \psi\| + b_2 \|\psi\| \tag{9}$$

for all ψ with $L_z \psi = m\psi$. Note that this condition implies in particular that $V \in \mathcal{L}^2_{\mathrm{loc}}$.

The condition (9) guarantees that each H_m is semibounded and essentially self-adjoint on $\mathcal{C}_0^\infty$, and H is well defined by $H = \bigoplus_m H_m$, without having to assume the semiboundedness of H.

The following proposition provides a large class of examples of potentials that fulfill the technical condition stated above, and is applicable for most practical purposes.

3. PROPOSITION. *Assume that $V(\mathbf{x})$ is locally $\mathcal{L}^2$, and there exists a constant, which we denote as $\|V\|_{2,\mathrm{loc}}$, such that for all n and some $R > 0$*

$$\int_n^{n+1} dz \int_{r_\perp < R} dx\, dy\, |V(\mathbf{x})|^2 \le \|V\|^2_{2,\mathrm{loc}}. \tag{10}$$

Moreover, we assume that there exist constants C and $C_V < B^2/4$, such that

$$|V(r_\perp, z)| \le C + C_V\, r_\perp^2 \quad \text{for all} \quad r_\perp > R. \tag{11}$$

Then V fulfills the condition (9).

Proof. Note that for operators $A \ge 0$ and $D^* = D$ the inequality

$$\begin{aligned}(A + D^2)^2 &= A^2 + D^4 + 2DAD - [[D, A], D] \\ &\ge A^2 + D^4 - [[D, A], D] \end{aligned} \tag{12}$$

holds. Using this with $A=-\Delta$ and $D=Br_\perp/2$ we get, for any ψ,

$$\|\Delta\psi\|^2+\left(\frac{B}{2}\right)^4\|r_\perp^2\psi\|^2\le\|\left(-\Delta+\frac{B^2}{4}r_\perp^2\right)\psi\|^2+B^2\|\psi\|^2. \qquad (13)$$

Denoting $V_1(\mathbf{x})=V(\mathbf{x})\theta(R-r_\perp)$ and $V_2=V-V_1$, we can estimate

$$\begin{aligned}\|V\psi\| &\le \|V_1\psi\|+\|V_2\psi\|\\ &\le \|V_1\psi\|+\frac{4C_V}{B^2}\|H_B\psi\|+\left(\frac{4C_V}{B}(|m|+1)+C\right)\|\psi\|, \end{aligned}\qquad (14)$$

where we used $L_z\psi=m\psi$. Now V_1 is relatively $-\Delta$-bounded with arbitrary small bound ([RS78], Thm. XIII.96), and by (13) the same holds with $-\Delta$ replaced by H_B. □

For $m\ge 0$ let now ψ_m denote the ground state wave function of H_m, if it exists. Writing

$$\psi_m(\mathbf{x})=e^{im\varphi}r_\perp^m f(r_\perp,z), \qquad (15)$$

where $(r_\perp,\varphi)$ denote polar coordinates for (x,y), we see that f is a ground state for

$$\widetilde{H}_m=-\frac{\partial^2}{\partial r_\perp^2}-\frac{2m+1}{r_\perp}\frac{\partial}{\partial r_\perp}-\frac{\partial^2}{\partial z^2}+\frac{B^2}{4}r_\perp^2-m\,B+V(r_\perp,z) \qquad (16)$$

on $\mathcal{L}^2(\mathbb{R}^3,r_\perp^{2m}d^3\mathbf{x})$. If $\widetilde{H}_m$ has a ground state, it is unique and strictly positive. So ψ_m is unique. Moreover, f is a bounded Hölder continuous function, so ψ_m behaves like $r_\perp^m$ for small $r_\perp$; i.e. $|\psi_m(\mathbf{x})|\le C|r_\perp|^m$.

We now have the necessary prerequisites to prove

4. THEOREM (Pseudoconcavity in angular momentum). *If $V(r_\perp,z)$ fulfills the technical condition stated above, and if the Laplacian of the potential off the z-axis is non-positive, the ground state energies E_m of the restricted Hamiltonians H_m obey the following inequalities, if $m\ge 1$:*

$$E_m\ge\min\{E_{m-1},E_{m+1}\}, \qquad (17)$$

$$E_m\ge\frac{1}{2}(E_{m-1}+E_{m+1}) \qquad \text{if} \quad E_m\ge E_{m-1}, \qquad (18)$$

$$E_m\ge\frac{1}{2m+1}(mE_{m-1}+(m+1)E_{m+1}) \qquad \text{if} \quad E_m\ge E_{m+1}. \qquad (19)$$

If ΔV is not vanishing everywhere off the z-axis, and if E_m is a discrete eigenvalue, the inequalities (17), (18) and (19) are strict.

Proof. We add $H_B - E_m$ to V in (8), use $[H_B, a] = 0$, note that $H = H_B + V$, take the expectation value with $\varphi \in \mathcal{C}_0^\infty$ and expand the double commutator. We get, using moreover $\partial^2/\partial x^2 + \partial^2/\partial y^2 = \Delta - \partial^2/\partial z^2$,

$$\langle\varphi|a^\dagger(H - E_m)a + a(H - E_m)a^\dagger|\varphi\rangle = \frac{1}{2B}\langle\varphi|\Delta V|\varphi\rangle - \frac{1}{2B}\langle\varphi|\frac{\partial^2 V}{\partial z^2}|\varphi\rangle + \langle\varphi|a^\dagger a(H - E_m) + (H - E_m)aa^\dagger|\varphi\rangle. \tag{20}$$

Now assume that E_m is a discrete eigenvalue and let ψ_m be the corresponding ground state. Since H is a closed operator and $\mathcal{C}_0^\infty$ is a core of H, there exist sequences of wave functions $\varphi_k \in \mathcal{C}_0^\infty$ with $\|\varphi_k\| = 1$ and angular momentum m, converging in norm to ψ_m such that also $H\varphi_k \to H\psi_m = E_m\psi_m$ in norm. Since

$$2Ba^\dagger a = H_B + \frac{\partial^2}{\partial z^2} + 2BL_z - B, \tag{21}$$

condition (9) on V guarantees that the operators $a^\dagger a$ and $aa^\dagger$ are bounded relative to H_m on $\mathcal{H}_m$, the subspace of $\mathcal{H}$ where $L_z = m$. It follows that, as $k \to \infty$, also $a^\dagger a\varphi_k$ and $aa^\dagger\varphi_k$ converge and are bounded in norm, and the second line in (20), with $\varphi = \varphi_k$, converges to 0.

Set $\mathbf{a} = (0, 0, a)$. We claim that it is no restriction to assume that the functions

$$f_k(a) \equiv \int |\varphi_k(\mathbf{x} + \mathbf{a})|^2 V(\mathbf{x}) d^3\mathbf{x} \tag{22}$$

have their minimum at $a = 0$. To see this, let $\tilde{\varphi}_k(\mathbf{x}) = \varphi_k(\mathbf{x} - \mathbf{a}_k)$, where $\mathbf{a}_k = (0, 0, a_k)$ is chosen such that $f_k(a_k) \leq f_k(a)$ for all a. This is possible since by assumption E_m is a discrete eigenvalue, so one can not attain any expectation value in the gap above E_m by shifting φ_k to infinity. Now

$$\langle\tilde{\varphi}_k|H|\tilde{\varphi}_k\rangle \leq \langle\varphi_k|H|\varphi_k\rangle \longrightarrow E_m, \tag{23}$$

so there exists a subsequence, again denoted by $\tilde{\varphi}_k$, such that $\tilde{\varphi}_k \rightharpoonup \psi_m$ weakly in $\mathcal{L}^2$. Since also the norms converge, there is even strong convergence. In particular, $a_k \to 0$ as $k \to \infty$. Therefore, since H_B is translation invariant in z-direction, and since V is relatively bounded,

$$\|H(\tilde{\varphi}_k - \psi_m)\| \longrightarrow 0. \tag{24}$$

Now denote $\tilde{\varphi}_k$ by φ_k, which proves our claim. With φ_k chosen as above, we have

$$\int |\varphi_k|^2 \frac{\partial^2 V}{\partial z^2} = \frac{\partial^2}{\partial a^2} f_k(a)\bigg|_{a=0} \geq 0. \tag{25}$$

Concerning $\langle\varphi_k|\Delta V|\varphi_k\rangle$, the Hölder continuity of ψ_m ([LL97], Theorem 11.7) and the fact that $\psi_m(r_\perp = 0, z) = 0$ if $m \geq 1$ allows us to integrate $|\psi_m|^2\Delta V$ and apply Fatou's Lemma to conclude that

$$\limsup_{k\to\infty} \frac{1}{2B}\langle\varphi_k|\Delta V|\varphi_k\rangle \leq \frac{1}{2B}\langle\psi_m|\Delta V|\psi_m\rangle, \tag{26}$$

where we used that $\varphi_k(\mathbf{x}) \to \psi_m(\mathbf{x})$ pointwise. (The convergence is even uniform in $\mathbf{x}$, since $\|\Delta\varphi_k\|$ is uniformly bounded by (13).) If $\Delta V < 0$ somewhere away from the z-axis, the fact that $|\psi_m| > 0$ away from $r_\perp = 0$ implies that the right hand side of (26) is strictly negative. Using this and (25) in (20) we can conclude that

$$\limsup_{k\to\infty} \langle \varphi_k | a^\dagger (H - E_m) a + a (H - E_m) a^\dagger | \varphi_k \rangle < 0. \tag{27}$$

Now, since $a^\dagger|\varphi_k\rangle$ has angular momentum $L_z = m+1$, and $a|\varphi_k\rangle$ has angular momentum $L_z = m-1$, this implies that the spectrum of either H_{m+1} or H_{m-1} must reach below E_m, that is

$$E_m > \min\{E_{m-1}, E_{m+1}\} \qquad \text{if} \quad m \geq 1. \tag{28}$$

To prove the relations (18) and (19) in their strict form we use the commutation relation (5) and observe that $\|a^\dagger\varphi_k\|^2 = \|a\varphi_k\|^2 + 1$. So the inequality (27) tells us moreover that

$$\limsup_{k\to\infty} \big((E_{m-1} - E_m)\|a\varphi_k\|^2 + (E_{m+1} - E_m)(\|a\varphi_k\|^2 + 1) \big) < 0. \tag{29}$$

In the case $E_m \geq E_{m-1}$, we note that the strict form of (18) holds trivially, if $E_m > E_{m+1}$. Otherwise, if $E_m \leq E_{m+1}$, (29) gives

$$\limsup_{k\to\infty} \|a\varphi_k\|^2 (E_{m-1} + E_{m+1} - 2E_m) < E_m - E_{m+1} \leq 0. \tag{30}$$

In the case $E_m \geq E_{m+1}$ we use $\|a\varphi_k\|^2 \geq m > 0$, which is a consequence of $a^\dagger a \geq L_z$. Using $1/m \geq 1/\|a\varphi_k\|^2$, the inequality (29) gives

$$\limsup_{k\to\infty} \|a\varphi_k\|^2 \left((E_{m-1} - E_m) + (E_{m+1} - E_m)(1 + \frac{1}{m}) \right) < 0. \tag{31}$$

So our assertions on the strict inequalities follow.

If H_m does not have a discrete eigenvalue at the bottom of its spectrum, or if ΔV happens to be zero everywhere off the z-axis, add εW to the potential, with the superharmonic function $W(r_\perp, z) = (z^2 - r_\perp^2)$, and ε small enough (more precisely, $0 < \varepsilon < B^2(1 - b_1)/4$, with b_1 as in (9)). The Hamiltonians $H_m(\varepsilon) = H_m + \varepsilon W$ do have discrete ground states for each m ([RS78], Theorem XIII.67), and (28), as well as (30) and (31) hold for the corresponding energies $E_m(\varepsilon)$. Strictly speaking, the potentials $V + \varepsilon W$ are not relatively bounded with respect to H_B on $\mathcal{H}_m$, but it is not difficult to see, using boundedness relative to $H_B + \varepsilon z^2$ instead, that the conclusions above remain valid. Now taking the limit $\varepsilon \to 0$ leads to the inequalities (17), (18) and (19). $\square$

5. Remark (Change of the conditions). Theorem 4 and the following corollaries hold also when the condition $\Delta V \leq 0$ off the z-axis is replaced by $\partial^2 V/\partial x^2 + \partial^2 V/\partial y^2 \leq 0$ off the z-axis. The proof is essentially the same as above, but without any involvement of $\partial^2 V/\partial z^2$, and discreteness of the ground state is not needed.

Considering the entire sequence E_m, the relation (17) obviously implies that an increase of E_m in m can turn into a decrease, but not vice versa. We state this and the global forms of the other relations as

6. COROLLARY (Global pseudoconcavity). *Under the same conditions on V as above, there is an M, possibly 0 or ∞, such that the sequence $\{E_m\}$ is strictly increasing and concave for $0 \le m \le M$ and non-increasing for $m \ge M$. Moreover, the ground state energies of two neighboring values of angular momentum, $\ell, \ell+1$, determine upper bounds on all of $\{E_m\}$ by a tangential sequence: For all $\ell \ge 0$ and $m \ge 0$,*

$$E_m \le E_\ell + (m-\ell)(E_{\ell+1} - E_\ell) \qquad \text{if} \quad E_\ell \le E_{\ell+1}, \tag{32}$$

$$E_m \le E_\ell + (S_m - S_\ell)(\ell+1)(E_{\ell+1} - E_\ell) \qquad \text{if} \quad E_\ell \ge E_{\ell+1}, \tag{33}$$

where

$$S_m = \sum_{\mu=1}^{m} \frac{1}{\mu}. \tag{34}$$

These inequalities are strict, if some E_μ for $m \le \mu \le \ell$ or $\ell+1 \le \mu \le m$ is a discrete eigenvalue, if $m \notin \{\ell, \ell+1\}$ and if the Laplacian of the potential is not identically zero off the z-axis.

Proof. For E_m in the increasing part of the sequence $\{E_m\}$, the inequality (32) is the standard statement that a tangent line lies above a concave sequence. Since the linear tangential sequence is increasing, it is trivial to extend this inequality to the E_m in the decreasing part.

To prove (33), consider $\Delta_m = (E_m - E_{m-1})$ and observe that (19) can be written as a monotonicity relation for $m\Delta_m$,

$$(m+1)\Delta_{m+1} \le m\Delta_m \qquad \text{if} \quad E_m \ge E_{m+1}. \tag{35}$$

Starting with $\Delta_{\ell+1}$, which is not positive, this means $\Delta_\mu \le \frac{\ell+1}{\mu}\Delta_{\ell+1}$ if $\mu \ge \ell+1$, and $\Delta_\mu \ge \frac{\ell+1}{\mu}\Delta_{\ell+1}$ if $\mu \le \ell$. The extension of the latter inequality to the increasing part of $\{E_\mu\}$ is trivial. Summing these inequalities for Δ_μ, either for $m+1 \le \mu \le \ell$ or $\ell+1 \le \mu \le m$, gives (33). Moreover, any strict inequality for one of the Δ_μ gives (33) as a strict inequality. $\square$

We remark that the asymptotic behavior of the decreasing tangential sequence, $S_m \sim \ln m$, is optimal. This is demonstrated on the example with the infinite charged tube in Section 3.

An immediate consequence of this logarithmic divergence is

7. COROLLARY (Either no decrease or infinite decrease). *The sequence $\{E_m\}$ is either not decreasing at all or it is decreasing to $-\infty$ as $m \to \infty$.*

Moreover, we have the generalization of the theorem on the ground state stated in [BS00].

8. COROLLARY (The ground state has zero angular momentum). *If V fulfills the conditions as in Theorem 4, and if* inf spec H *is a discrete eigenvalue, the corresponding eigenvector is unique and has zero angular momentum.*

Proof. Corollaries 6 and 7 imply that either $E_0 < E_m$ or $E_0 = E_m$ for all m. Since inf spec H is a discrete eigenvalue by assumption, it cannot be infinitely degenerate, so our assertion is proved. □

9. Remark (The hydrogen atom). Corollary 8 applies also to the hydrogen atom in a constant magnetic field, and provides a simple proof of $L_z = 0$ in the ground state; the third proof following [AHS81] and [GS95].

We now have the tools to prove Theorem 2.

Proof of Theorem 2. The potential V is relatively bounded with respect to $-\Delta$ with relative bound 0 on the *entire* Hilbert space. This implies that V fulfills the technical condition which is necessary to apply Theorem 4 and Corollary 7, and moreover that the Hamiltonian is bounded below. So the sequence E_m is non-decreasing and concave, and $\lim E_m = B$. Since the asymptotic behavior of the potential, as $r_\perp \to \infty$, is $V(\mathbf{x}) \sim -(Z-C)/|\mathbf{x}|$, where $Z = \int \sigma dz$, $C = \int \rho\, d^3\mathbf{x}$, it is easy, if $C < Z$, to construct trial functions for large m, such that the expectation value of H_m is lower than the edge of its essential spectrum, which is at B. Such trial wave functions are of the form $\Phi_m(x,y)\varepsilon\varphi(\varepsilon z)$, where Φ_m is the wave function in $\mathcal{L}^2(\mathbb{R}^2)$ with $L_z = m$ in the lowest Landau band, and ε has to be small enough. So each E_m is a discrete eigenvalue, and increase and concavity are strict. □

3 Physical applications and extensions

The mean field model of a positively charged ion
Consider

$$V = -\frac{1}{|\mathbf{x}|} + \rho * \frac{1}{|\mathbf{x}|} \tag{36}$$

with $\rho = \rho(r_\perp, z) \geq 0$ and $C = \int \rho < 1$. We can apply Theorem 2, and infer that the E_m's are monotone increasing eigenvalues.

The mean field model of a negatively charged ion
The potential is as in (36), but now with $C > 1$. Since $V(\mathbf{x}) \sim (C-1)/|\mathbf{x}|$ as $r_\perp \to \infty$, and since the angular momentum barrier shields the nucleus, there are no bound states for large m. The energies E_m may be increasing up to some finite M, and will all be equal to B for $m \geq M$.

Attractive point charge in a repulsive homogeneously charged hollow tube

Consider the potential

$$V = -\frac{1}{|\mathbf{x}|} - \tau\theta(r_\perp - R)\ln(r_\perp/R) \tag{37}$$

where τ and R are positive constants. The second part of V is the "renormalized" potential of an infinite hollow tube with radius R. It is unbounded below as $r_\perp \to \infty$, and this implies $E_m \to -\infty$ as $m \to \infty$. On the other hand, the ground states with angular momentum m are localized near $r_\perp \sim \sqrt{2m/B}$, and will not really "feel" the hollow tube, if they are inside. The E_m will increase like the corresponding states of the free hydrogen atom, at least up to $m \sim R^2B/2$. So there is an increase of ground state energies followed by a decrease. Moreover, since the E_m are varying continuously as functions of the parameters τ and R, there will be cases, where the maximum of the E_m is attained twice, at two neighboring angular momenta simultaneously. The asymptotics of $\{E_m\}$ as $m \to \infty$ is, to leading order,

$$E_m \sim -\frac{\tau}{2}\ln m. \tag{38}$$

An infinite periodic chain of atoms

Let $\mathbf{a}$ be the vector $(0,0,a)$, defining the periodicity in z-direction. Consider

$$V(r_\perp, z) = \sum_{n\in\mathbb{Z},\mathrm{ren}} \left(-\frac{1}{|\mathbf{x}-n\mathbf{a}|} + \rho * \frac{1}{|\mathbf{x}-n\mathbf{a}|} \right), \tag{39}$$

where the axially symmetric positive charge density ρ is localized in the elementary slice $0 \le z < a$, and $\int \rho$ is assumed to be finite. If $\int \rho \neq 1$, the infinite sum has to be coupled with a renormalization: Let $D = 1 - \int \rho$.

$$\sum_{n\in\mathbb{Z},\mathrm{ren}} \ldots \equiv \lim_{N\to\infty} \left(\sum_{-N}^{N} \ldots + 2D\ln N \right). \tag{40}$$

(Convergence is guaranteed at least for ρ with compact support.) This potential is e.g. of interest for the study of chains of atoms in strong magnetic fields within the DM theory of [LSY94], as will be discussed in [JRY00]. Finiteness of $\int \rho$ guarantees that V can be split into the sum of two parts, one of them uniformly locally $\mathcal{L}^2$, the other diverging only logarithmically as $r_\perp \to \infty$. So Proposition 3 applies and V fulfills the technical condition.

Since the Hamiltonian commutes with a group of discrete translations in z-direction, the Hilbert space can be decomposed into the direct integral of $\mathcal{H}_\alpha$, $0 \le \alpha < 2\pi$, such that the Hamiltonian H is represented as a direct integral of H_α, where the domain of definition of H_α contains the Bloch-functions, continuous functions with the property

$$\psi(x,y,z+a) = e^{i\alpha}\psi(x,y,z), \tag{41}$$

normalized by $\|\psi\|^2 = \int_{\mathbb{R}^2} dx\, dy \int_0^a |\psi|^2 dz$. The ground state energies E_m are attained in the space $\mathcal{H}_0$, but we can extend our results to all of the lowest band, to the $E_m(\alpha)$, the ground state energies of H_m restricted to $\mathcal{H}_\alpha$.

10. THEOREM (Pseudoconcavity of Bloch function energies). *Consider potentials which are symmetric under a group of discrete z-translations, i.e. $V(r_\perp, z+a) = V(r_\perp, z)$ for some $a > 0$, and fulfill the conditions of Prop. 3. Let H_α and $H_{\alpha,m}$ be the restrictions of H and H_m onto the space of Bloch functions, and denote $E_m(\alpha) = \inf \operatorname{spec} H_{\alpha,m}$. Theorem 4 and the Corollaries 6, 7 and 8 hold also for each of the $E_m(\alpha)$ instead of the E_m. The pseudoconcavity is moreover strict if ΔV is not identically zero off the z-axis.*

Proof. One can mimic the proof of Theorem 4. All the operations we made there commute with the z-translation. Since each $H_{\alpha,m}$ has discrete spectrum, as we show in Proposition 12 in the Appendix, the inequalities (17) – (19) hold in strict form if $\Delta V \neq 0$. □

Appendix

11. LEMMA. *Let Δ be the Laplacian with Neumann boundary conditions on*

$$\mathcal{G}_n = \{\mathbf{x}, n \leq z < n+1\}. \tag{42}$$

Then, for $p > 3/2$ and for some constant depending on p,

$$-\Delta + V(\mathbf{x}) \geq -1 - C(p)\|V_-\|_p^{2p/(2p-3)}, \tag{43}$$

where $V_- = min\{V, 0\}$, and the norm is for the restriction of V_- onto $\mathcal{G}_n$.

Proof. By the Sobolev inequality on $\mathcal{G}_n$ there is a constant $C > 0$ such that

$$\|\nabla f\|_2^2 + \|f\|_2^2 \geq C\|f\|_6^2 \tag{44}$$

for all $f \in \mathcal{H}^1(\mathcal{G}_n)$ (cf. [A75], Thm. 5.4). Therefore we can estimate, for $\|\psi\|_2 = 1$,

$$\langle\psi| - \Delta + V|\psi\rangle \geq -1 + C(R)\|\psi\|_6^2 - \|V_-\|_p\|\psi\|_6^{3/p}, \tag{45}$$

where we used Hölders inequality, with $p^{-1} + q^{-1} = 1$, twice:

$$\begin{aligned} |\langle\psi|V_-|\psi\rangle| &\leq \|V_-\|_p\|\psi^2\|_q, & (46)\\ \|\psi^2\|_q &\leq \|\psi\|_6^{3/p}\|\psi\|_2^{2-3/p}. & (47)\end{aligned}$$

Optimizing (45) with respect to $\|\psi\|_6$ yields the desired result. □

12. PROPOSITION (Discrete spectrum). *Each operator $H_{\alpha,m}$ defined in Theorem 10 has discrete spectrum.*

Proof. We split the potential V into

$$\begin{aligned} V_{\mathrm{loc}} &= \theta(R-r_\perp)V \\ \text{and} \qquad V_\infty &= \theta(r_\perp - R)V. \end{aligned}$$

Then we split the Hamiltonian H into

$$\begin{aligned} H_{\mathrm{loc}} &= \delta H_B + V_{\mathrm{loc}} \\ \text{and} \qquad H_\infty &= (1-\delta)H_B + V_\infty, \end{aligned}$$

where $\delta = \frac{1}{2}(1-4C_V/B^2)$, C_V as defined in Prop. 3. We do the same splittings for all the $H_{\alpha,m}$. We use that inf spec $H_{\alpha,m,\mathrm{loc}} \geq$ inf spec $H_{N,m,\mathrm{loc}}$, where N denotes the Neumann boundary conditions, use Lemma 11 and the condition (10) to find a lower bound to $H_{\alpha,m,\mathrm{loc}}$ by a constant operator,

$$H_{\alpha,m,\mathrm{loc}} \geq -\mathrm{const.}(1 + \|V\|^4_{2,\mathrm{loc}}) \equiv -C(V). \tag{48}$$

Now we add $H_{\alpha,m,\mathrm{loc}}$ and $H_{\alpha,m,\infty}$ and use the condition (11):

$$H_{\alpha,m} \geq -C(V) - (1-\delta)(\Delta + Bm) - C + \frac{1}{2}(\frac{B^2}{4} - C_V)r_\perp^2. \tag{49}$$

The operator on the right side obviously has discrete spectrum, and the min-max principle implies that the same is true for $H_{\alpha,m}$. $\square$

We add a short version of the proof of the Grosse-Stubbe inequality. We need the following

13. LEMMA (General bound on the decrease). *Let $E_{m,n}$ be the n'th eigenvalue (counted from below) of H_m, or the edge of its essential spectrum, if there are less than n discrete eigenvalues. Then, if $m \geq 0$,*

$$E_{m,n} \leq E_{m+1,n} + B. \tag{50}$$

Proof. We map each subspace $\mathcal{H}_m$ unitarily onto $\mathcal{L}^2(\mathbb{R}_+ \times \mathbb{R}, 2\pi r_\perp dr_\perp\, dz)$, by writing, for $\psi \in \mathcal{H}_m$,

$$\psi(\mathbf{x}) = e^{im\varphi}\chi(r_\perp, z), \tag{51}$$

and mapping $\psi \to \chi$.

The Hamiltonian H_m is then unitarily equivalent to

$$\hat{H}_m = -\frac{\partial^2}{\partial r_\perp^2} - \frac{1}{r_\perp}\frac{\partial}{\partial r_\perp} - \frac{\partial^2}{\partial z^2} + \frac{B^2}{4}r_\perp^2 + \frac{m^2}{r_\perp^2} - m\,B + V(r_\perp, z), \tag{52}$$

and the right side of (50) is the n'th eigenvalue of

$$\hat{H}_{m+1} + B = \hat{H}_m + \frac{2m+1}{r_\perp^2}. \tag{53}$$

This means that $\hat{H}_{m+1} + B \geq \hat{H}_m$, so (50) follows with the help of the min-max principle. □

Proof of the Grosse-Stubbe inequality. The following formula can be interpreted as calculating the acceleration of the particle, subtracting the effect of the Lorentz force, and then taking a linear combination of the x- and y-components, denoted as $x_+ = x + iy$:

$$[H,[H,x_+]] + 2B[H,x_+] = 2\frac{x_+}{r_\perp}\frac{\partial V}{\partial r_\perp}. \tag{54}$$

Now we take the matrix elements between ψ_{m+1} and ψ_m,

$$\left((E_{m+1}-E_m)^2 + 2B(E_{m+1}-E_m)\right)\langle\psi_{m+1}|x_+|\psi_m\rangle = 2\langle\psi_{m+1}|\frac{x_+}{r_\perp}\frac{\partial V}{\partial r_\perp}|\psi_m\rangle, \tag{55}$$

and choose the phases appropriately, so that we can write $\psi_m = (x_+/r_\perp)^m\chi_m$ with $\chi_m \geq 0$. We get

$$(E_{m+1}-E_m)(E_{m+1}-E_m+2B)\langle\chi_{m+1}|r_\perp|\chi_m\rangle = 2\langle\chi_{m+1}|\frac{\partial V}{\partial r_\perp}|\chi_m\rangle. \tag{56}$$

The matrix element on the left side is positive, and by Lemma 13 we know that $E_{m+1} - E_m + 2B \geq B > 0$. So the sign of $\frac{\partial V}{\partial r_\perp}$, which determines the sign of the right side, determines also the sign of $(E_{m+1} - E_m)$ on the left side. □

The Grosse-Stubbe inequality can be extended in a weakened form to cases where the E_m are not necessarily eigenvalues. To see this, we approximate $V(r_\perp, z)$ by $V_R(r_\perp, z) \equiv V(\min\{r_\perp, R\}, z) + z^2/R$. With this potential the ground state energies $E_{R,m}$ have to be eigenvalues, and are strictly ordered. Then we consider the limit $R \to \infty$. Since $E_{R,m} \to E_m$, it follows that the monotonicities of V in $r_\perp$ imply monotonicities of the E_m in m, which don't have to be strict if they are not eigenvalues.

References

[LSY94] Elliott H. Lieb, Jan Philip Solovej, and Jakob Yngvason: *Asymptotics of Heavy Atoms in High Magnetic Fields: I. Lowest Landau Band Regions*, Commun. Pure Appl. Math. **XLVII**, 513–591 (1994)

[BSY00] Bernhard Baumgartner, Jan Philip Solovej, and Jakob Yngvason: *Atoms in strong magnetic fields: The high field limit at fixed nuclear charge*, Commun. Math. Phys. **212**, 703–724 (2000)

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

[AHS78] J. Avron, I. Herbst, B. Simon, *Schrödinger Operators with Magnetic Fields. I. General Interaction*, Duke Math. J. **45**, 847-883 (1978)

[BGM85] Bernhard Baumgartner, Harald Grosse, André Martin, *Order of Levels in Potential Models*, Nucl. Phys. B**254**, 528-42 (1985)

[B85] Bernhard Baumgartner, *Level Comparison Theorems*, Ann. Phys. (NY) **168**, 484-526 (1985)

[B91] Bernhard Baumgartner, *Perturbation of Supersymmetric Systems in Quantum Mechanics*, in *Recent Developments in Quantum Mechanics*, A. Boutet de Monvel et al. (eds.), pp195-208, Kluwer Acad. Publ., Netherlands, 1991

[GS95] Harald Grosse, Joachim Stubbe, *Splitting of Landau Levels in the Presence of External Potentials*, Lett. Math. Phys. **34**, 59-68 (1995)

[LC77] Richard Lavine, Michael O'Carroll, *Ground state properties and lower bounds for energy levels of a particle in a uniform magnetic field and external potential*, J. Math. Phys. **18**, 1908-12 (1977)

[BS00] Bernhard Baumgartner, Robert Seiringer, *Atoms with bosonic "electrons" in strong magnetic fields*, arXiv:math-ph/0007007, to be published in Annales Henri Poincaré.

[AHS81] J.E. Avron, Ira W. Herbst, and Barry Simon, *Schrödinger Operators with Magnetic Fields III. Atoms in Homogeneous Magnetic Field*, Commun. Math. Phys. **79**, 529-572 (1981)

[RS78] M. Reed, B. Simon, *Methods of Modern Mathematical Physics IV*, Acad. Press, NY (1978)

[LL97] E.H. Lieb, M. Loss, *Analysis*, Amer. Math. Society (1997)

[JRY00] K. Johnsen, Ö. Rögnvaldsson, J. Yngvason, in preparation

[A75] R.A. Adams, *Sobolev Spaces*, Acad. Press, NY (1975)