QUANTUM DOTS

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Abstract: Atomic-like systems in which electronic motion is two dimensional are now realizable as "quantum dots". In place of the attraction of a nucleus there is a confining potential, usually assumed to be quadratic. Additionally, a perpendicular magnetic field B may be present. We review some recent rigorous results for these systems. We have shown that a Thomas-Fermi type theory for the ground state is asymptotically correct when N and B tend to infinity. There are several mathematically and physically novel features. 1. The derivation of the appropriate Lieb-Thirring inequality requires some added effort. 2. When B is appropriately large the TF "kinetic energy" term disappears and a peculiar "classical" continuum electrostatic theory emerges. This is a two dimensional problem, but with a three dimensional Coulomb potential. 3. Corresponding to this continuum theory is a discrete "classical" electrostatic theory. The former provides an upper bound and the latter a lower bound to the true quantum energy; the problem of relating the two classical energies offers an amusing exercise in electrostatics.

* Work partially supported by U.S. National Science Foundation grant PHY90-19433 A03

** Work partially supported by U.S. National Science Foundation grant DMS 92-03829

*** Work partially supported by the Icelandic Science Foundation.

To appear in the proceedings of the conference on partial differential equations and mathematical physics held at the University of Alabama, Birmingham, March 1994, International Press

I. INTRODUCTION

Recent developments in semiconductor technology have produced remarkably small pieces of matter that behave like two-dimensional atoms. These “dots” are part of the world of mesoscopic physics which contains objects that are large compared to atoms but small enough to demonstrate typical quantum effects such as discrete energy levels and interference phenomena.

The simplest quantum dot consists of an insulator, e.g. AlGaAs, and a semiconductor, e.g. GaAs. Between these two materials is a potential difference that confines injected electrons to a thin layer at the interface. The thickness of the layer ranges from 30 to 100 angstroms while the diameter of the dot, typically of the order 300 to 8000 angstroms, is controlled by a metal gate on top of the insulator, or by edging a pattern through the insulator and the interface. (Recall that $a_{\mathrm{Bohr}} := \hbar^2/(me^2)$, the radius of a hydrogen atom, is about half an angstrom, i.e. 0.5×10^{-8} cm). The number of injected electrons, N can conveniently be from zero to several thousand.

Perpendicular to the dot a uniform magnetic field, B, can be introduced, thereby making it possible to investigate the quantum mechanics of motion in a magnetic field. The quantized Landau levels can then become prominent.

Although this system is very quantum mechanical, its parameters are sufficiently different from ordinary atoms and molecules that it is possible to demonstrate in the laboratory effects that would otherwise require the magnetic field of a neutron star ($10^9 - 10^{12}$ gauss).

- Energies are typically in units of meV (millielectron volts), not eV.
- Large magnetic fields need only be several teslas (one tesla $= 10^4$ gauss). By a “large” field is meant one for which the effective Landau radius is comparable to the effective Bohr radius or smaller.

- The system is effectively two-dimensional because the electronic motion in the direction perpendicular to the sandwich is essentially "frozen out". The thickness, $L_\perp$, is so small that each electron remains in the ground state, $\phi(x_\perp) = (\sqrt{2}/L_\perp)\sin(\pi x_\perp/L_\perp)$. It costs a large kinetic energy to promote an electron to the next state $(\sqrt{2}/L_\perp)\sin(2\pi x_\perp/L_\perp)$.

Whether or not such transitions can be totally disregarded remains to be proved, but this is the customary assumption and we shall make it here. From the mathematical point of view, the assumption of two-dimensional motion is the most interesting feature of this model. Some of our results here contrast markedly with those in our earlier work on conventional atoms in large magnetic fields [LSY1-3]. In this paper we present some recent work; details will appear elsewhere.

Our N-body system can be modeled by the following Hamiltonian, H_N.

$$H_N = \sum_{j=1}^{N} H_j^1 + e_*^2 \sum_{1\le i<j\le N} |x_i - x_j|^{-1}, \tag{1.1}$$

with $x_i \in \mathbf{R}^2$ and where H^1 is the one-body Hamiltonian

$$H^1 = \frac{\hbar^2}{2m_*}\left(i\nabla - \frac{e}{\hbar c}A\right)^2 + g_*\left(\frac{\hbar e}{2m_* c}\right)S^z B - \left(\frac{\hbar e}{2m_* c}\right)\left(1 - \frac{|g_*|}{2}\right)B + V(x), \tag{1.2}$$

with the following notation.

The magnetic vector potential is $A = \frac{1}{2}B(-y, x)$.

The potential $V(x)$ is confining, which is to say that $V(x) \to \infty$ as $|x| \to \infty$, and it is assumed to be continuous. For convenience in computations it is usually taken to be of the form $V(x) = \frac{1}{2}m_*\omega^2 x^2$, but this is somewhat phenomenological and arbitrary. It is created by an external gate and it is therefore adjustable to a certain extent. This V replaces the Coulomb attraction to the nucleus, $-Z/|x|$, in a conventional atom. We write the potential generally as

$$V(x) = Kv(x)$$

and let the coupling constant K and the magnetic field be N dependent,

$$K = \kappa N \quad \text{and} \quad B = \beta N$$

with β and κ fixed. In this way the ground state energy, E^Q, will scale as N^2 as $N \to \infty$. (This contrasts with $N^{7/3}$ for a natural atom.)

The operator S^z is the perpendicular component of the spin and takes the values $\pm 1/2$ for each electron. It commutes with H.

The constant term in (1.2), $-(\hbar e/(2m_* c))(1 - |g_*|/2)B$, is included in order that the "kinetic energy" operator, $H^1 - V(x)$, has a spectrum starting at zero.

The Hilbert space is that appropriate for fermions, the antisymmetric tensor product $\bigwedge_1^N L^2(\mathbf{R}^2; \mathbf{C}^2)$.

The numbers m_*, e_*, g_* are "effective" values that differ from the usual ones because of the electron's interaction with the crystal in which it finds itself. The values for GaAs are

$m_* =$ effective mass $= 0.07\ m_{\text{electron}}$

$e_* =$ effective charge $= e\cdot$ (dielectric constant)$^{-1/2} = 0.3\ e$

$g_* = -.03$

Corresponding to these values there are respectively a natural length, energy and magnetic field strength:

$a_* = \hbar^2/m_* e_*^2 = 185\ a_{\text{Bohr}} = 10^{-6}$ cm

$E_* = e_*^4 m_*/\hbar^2 = 9 \times 10^{-4}\,\text{Ry} = 12$ meV

$B_* = e_*^4 m_*^2 c/e\hbar^3 = 6.7 \times 10^4\,\text{G} = 6.7$ T

Henceforth, we choose units such that $\hbar = e_* = 2m_* = 1$. The energy unit is then $2E_*$, and if we moreover measure the magnetic field in units of $4B_*$, the numerical factors in (1.1) and (1.2), except g_*, can be dropped. The eigenvalues of $(i\nabla - A)^2$ are the Landau levels

$B, 3B, 5B$ in these units. The g-factor for normal electrons is 2, which is what appears in the Pauli operator, and which leads to eigenvalues $0, 2B, 4B, 6B, \ldots$ of $(i\nabla - A)^2 + 2S^z B$, with the first being singly degenerate and the others doubly degenerate (as far as spin is concerned). In our case $g_* \neq 2$. In fact, it is slightly negative in GaAs! This merely makes the bookkeeping a bit more complicated, but has no essential effect. A derivation of the effective g-factor in a solid is given in [KC, pp. 282-286].

We draw attention to the fact that the Coulomb repulsion in (1.1) is the *three-dimensional* potential, $|x|^{-1}$, even though our system is two-dimensional. The absence of Newton's theorem makes our job a little harder.

If the repulsion is omitted, and if V is quadratic, $V(x) = \frac{1}{4}\omega^2 x^2$, the problem is solvable. The spectrum of H^1 was determined by Fock [FV] in 1928, two years before Landau's paper. For $(i\nabla - A)^2 + \frac{1}{4}\omega^2 x^2$ the spectrum is given by

$$E = (n_1 - n_2)B + (n_1 + n_2 + 1)[\omega^2 + B^2]^{1/2} \tag{1.3}$$

with $n_1, n_2 = 0, 1, 2, \ldots$. It is remarkable that the simple spectrum, (1.3), gives a qualitatively good fit to some of the data [KM, KLS].

One of the most important physically measurable quantities is the spectrum of H. Here we concentrate on the ground state energy E^Q and will demonstrate that the Thomas-Fermi (TF) energy, which scales precisely as N^2, is asymptotically exact as $N \to \infty$ with κ and β fixed. The $N \to \infty$ limit of E^Q turns out to be *uniform* in β, i.e. given any $\varepsilon > 0$ we can find N large enough, but independent of β, so that $N^{-2}|E^{\mathrm{TF}} - E^Q| < \varepsilon$.

II. THOMAS-FERMI THEORY

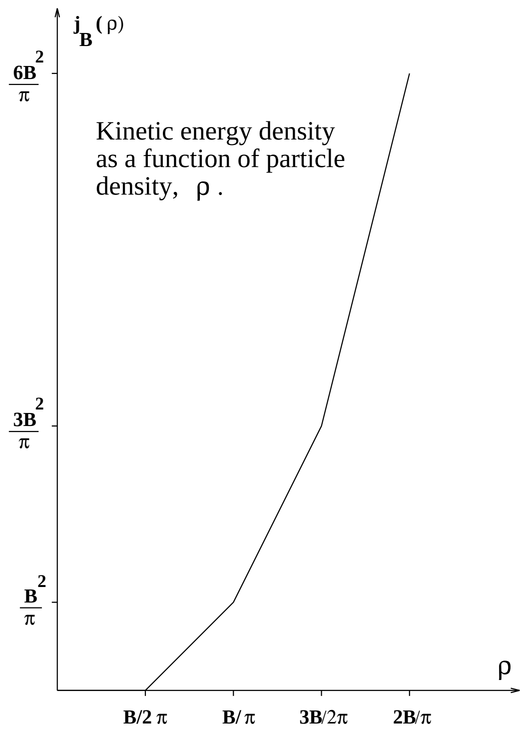
TF theory is defined by the following functional, $\mathcal{E}^{\mathrm{TF}}$, of a nonnegative "density" function $\rho = \mathbf{R}^2 \to [0, \infty)$.

$$\mathcal{E}^{\mathrm{TF}}(\rho) = \int\limits_{\mathbf{R}^2} j_B(\rho(x))\mathrm{d}x + \int\limits_{\mathbf{R}^2} V(x)\rho(x)\mathrm{d}x + D(\rho,\rho) \tag{2.1}$$

with

$$D(f,g) = \tfrac{1}{2}\int\limits_{\mathbf{R}^2}\int\limits_{\mathbf{R}^2} f(x)g(y)|x-y|^{-1}\mathrm{d}x\mathrm{d}y. \tag{2.2}$$

The function $j_B(\rho)$ imitates the kinetic energy, $(i\nabla - A)^2 + g_* S^z B - (1-|g_*|/2)B$. It is the smallest kinetic energy density for electrons in a 2-dimensional box with particle density ρ. For simplicity we give explicit formulas for spinless fermions. For electrons (with spin) this would correspond to having $g_* = 0$ (which is close to the value for GaAs) except for the trivial fact that one must replace $j_B(\rho)$ by $2j_B(\rho/2)$ due to the spin degeneracy. Everything goes through, however, with obvious modifications, for electrons with $g_* \neq 0$. If spin is ignored we have $j_B(0) = 0$ and $j_B(\rho)$ has slope $2nB$ for $n(B/2\pi) \leq \rho \leq (n+1)(B/2\pi)$, with $n = 0, 1, 2, \ldots$. See the graph.



The function j_B satisfies $j_B(\rho) = B^2 j_1(\rho/B)$. It has the upper bound $j_B(\rho) \leq 2\pi\rho^2$, and $j_B(\rho) \to j_0(\rho) := 2\pi\rho^2$ as $B \to 0$. The functional $\mathcal{E}^{\mathrm{TF}}$ was first stated by McEuen *et al* [M] but it was not analyzed completely and it was not proved to give the asymptotic limit of E^Q as $N \to \infty$. They call it the self-consistent (SC) model. Actually their repulsion term is slightly different from our $D(\rho,\rho)$. They replace the Coulomb repulsion $|x-y|^{-1}$ by

$$W(x-y) := [|x-y|^2 + \delta z^2]^{1/2} - [|x-y|^2 + 4d^2]^{1/2}, \tag{2.3}$$

where $\delta z \sim 100$ angstroms is the thickness of the dot and $d \sim 1000$ angstroms is the distance to an external gate. This W has a short-distance and a long-distance cutoff. It is, however, positive definite as a kernel. Our methods can easily be adapted to prove the analogues of Theorems 1 and 2 with $|x-y|^{-1}$ replaced by W everywhere.

The TF energy is defined with $V(x) = Kv(x)$, $K = \kappa N$ and $B = \beta N$ by

$$E^{\rm TF}(\kappa, \beta, N) = \inf\left\{\mathcal{E}^{\rm TF}(\rho) : \rho(x) \geq 0, \int \rho = N, K = \kappa N, B = \beta N\right\} \tag{2.3}$$

and it is evident that

$$E^{\rm TF}(\kappa, \beta, N) = N^2 e^{\rm TF}(\kappa, \beta) \quad \textit{and} \quad \rho^{\rm TF}(x) = N\rho_1^{\rm TF}(x) \tag{2.4}$$

where ρ_1 and $e^{\rm TF}$ are ρ and $E^{\rm TF}$ in the special case $N = 1$.

The functional $\mathcal{E}^{\rm TF}$ is convex in ρ and it is strictly convex since the kernel $|x-y|^{-1}$ is strictly convex. Standard methods yield

1. THEOREM. *For each $N \geq 0$ and any g_* there is a unique minimizer, i.e., a ρ such that $\mathcal{E}^{\rm TF}(\rho) = N^2 e^{\rm TF}(\kappa, \beta)$ and $\int \rho = N$.*

The only novel feature here is the existence of a minimizer for *all* N, which is a consequence of the fact that $V(x) \to \infty$ as $|x| \to \infty$ instead of $V(x) \to 0$ as $|x| \to \infty$.

The minimizer satisfies a TF equation, which we illustrate for the particular j_B defined above. Since $j_B(\rho)$ is not differentiable at the points $\rho = n(B/2\pi)$, we first have to define the *set valued* function for $\rho \geq 0$ and $n \geq 0$ given by

$$\begin{aligned} j'_B(\rho) &= \{2nB\} && \text{if} \quad n(B/2\pi) < \rho < (n+1)(B/2\pi) \\ j'_B(\rho) &= [2nB, (2n+2)/B] && \text{if} \quad \rho = (n+1)(B/2\pi) \end{aligned} \tag{2.5}$$

where $\{x\}$ denotes a single point x and $[a, b]$ is the closed interval. The TF equation can now be written as

$$-Kv(x) - |x|^{-1} * \rho + \mu \begin{cases} \in j'_B(\rho(x)) & \text{if } \rho(x) > 0 \\ \leq 0 & \text{if } \rho(x) = 0 \end{cases} . \tag{2.6}$$

This holds also for arbitrary g_* with a suitably modified j'_B. The quantity μ is the physical chemical potential, i.e.

$$\mu = \frac{\partial E(K, B, N)}{\partial N} \tag{2.7}$$

with K and B fixed.

Not only is it true that ρ satisfies (2.6), but it is also true that *any* (nonnegative) solution pair (μ, ρ) to (2.6) is a minimizing pair, i.e. ρ is necessarily a minimizer for $\mathcal{E}^{\mathrm{TF}}$ for some N and μ is the chemical potential (2.7) at that N. Previously, such an assertion was proved [LS] for j a continuously differentiable function. The proof when j' is not C^1 is a bit trickier and was carried out by Lieb and Loss [LL].

Our main theorem is the following

2. THEOREM (Convergence of energy and density). *Fix κ, β and $v(x)$. Then the quantum and TF energies converge in the sense that*

$$N^{-2}|E^{\mathrm{TF}}(\kappa, \beta, N) - E^{Q}(\kappa, \beta, N)| \to 0$$

as $N \to \infty$. The convergence is uniform in β. The densities also converge as $N \to \infty$:

$$N^{-1}\rho^{Q}(x) \to \rho_1^{\mathrm{TF}}(x)$$

in the weak L^1 sense.

Customary techniques, such as coherent states based on Landau orbitals [LSY2,3], are employed to prove this theorem, but they are insufficient for the following important reason. The function j_B in (2.1) is zero in the interval $0 \leq \rho \leq B/2\pi$. Correspondingly, the quantum-mechanical kinetic energy operator $(i\nabla - A)^2 + g_* S^z B - (1 - |g_*|/2)B$ has a whole *band* of zero modes. (Note: It makes no difference if $g_* \neq 0$ because that will merely entail a shift of the chemical potential.) These zero modes cause several problems which we turn to in Sect. III.

Before doing so, however, let us comment on several unusual features of the TF density $\rho(x)$. For one thing, it always has compact support. This is perhaps not surprising since the usual atomic TF density has compact support except when $N = Z$. A more interesting feature is that when B is large, $0 < \rho(x) < B/2\pi$ for all x and hence $j_B(\rho(x)) \equiv 0$. This is not surprising. When B decreases, however, $\rho(x)$ develops a flat spot because (2.6) causes $\rho(x)$ to be anchored at $B/2\pi$ for a set of positive measure in $\mathbf{R}^2$. The first situation for $v(x) = x^2$, $\kappa = 10^{-4}$ and $B = 8$ tesla (with $N = 50$, so $\beta = 6 \times 10^{-3}$ in our units) is shown in Fig. 1. The upper part of the picture shows the density and the lower part the effective potential $V_{\text{eff}} = V + |x|^{-1} * \rho$ (lower part) are shown. The second situation ($B =$ 7 tesla) is shown in Fig. 2. As B is decreased further the second Landau level starts to be occupied and the flat spot, caused by the anchoring at B, moves further out (Fig. 3, $B = 5$ tesla). For a still lower field two flat spots appear because $2\pi\rho$ is anchored at B and at $2B$. Eventually more and more flat spots appear. Fig. 4 shows three flat spots at 2 tesla. From the point of view of the Schrödinger kinetic energy, we are seeing the filling of successive Landau bands. Also shown on these figures, for comparison, is a dotted curve representing the solution to a Hartree calculation of the quantum density for $N = 50$. The curves for the TF theory were computed by Kristinn Johnsen while the Hartree calculations are due to Vidar Gudmundsson (see [PGM] for details about Hartree calculations for quantum dots).

III. TWO-DIMENSIONAL LIEB-THIRRING INEQUALITY WITH A MAGNETIC FIELD

Here we consider spinless fermions to simplify the discussion. Given any normalized fermionic wave function $\psi(x_1, \ldots, x_N)$, with $x_i \in \mathbf{R}^d$ we can form the density

$$\rho_\psi(x) = N \int\limits_{\mathbf{R}^{d(N-1)}} |\psi(x_1, x_2, \ldots, x_N)|^2 \mathrm{d}x_2 \ldots \mathrm{d}x_N, \tag{3.1}$$

so that $\int\limits_{\mathbf{R}^d} \rho_\psi(x)\mathrm{d}x = N$. The Lieb-Thirring inequality relates T_ψ, the kinetic energy of ψ defined by

$$T_\psi = \left\langle \psi \middle| \sum_{i=1}^{N} (i\nabla - A)^2 - B \middle| \psi \right\rangle \tag{3.2}$$

to some integral of ρ_ψ. If $B = 0$ the original bound was $T_\psi \geq K_d \int \rho_\psi^{(1+2/d)}$, with K_d being a universal constant that is positive for all $d \geq 1$.

If we omit the $-B$ term in (3.2) then this original inequality continues to hold for all vector potentials A. If the $-B$ term is retained, however, the situation is much more delicate because of the possibility of zero modes (which certainly exist for $d = 2$, for example, when $B(x)$ has nonzero total flux). For $d = 3$ we proved [LSY3] that for some $C_1 > 0$

$$T_\psi \geq C_1 \int j_B^{(3)}(\rho_\psi(x))\mathrm{d}x \tag{3.3}$$

where $j_B^{(3)}(\rho)$ is the function that appears in the $d = 3$ TF theory with a constant magnetic field.

In two dimensions we would like to have a similar inequality, but the fact that $j_B(\rho) = 0$ for $\rho \leq B/2\pi$ in two-dimensions causes difficulties. The following is adequate, however.

3. LEMMA ($d = 2$ kinetic energy inequality). *With T_ψ and ρ_ψ defined as above, with B constant in space and with j_B the kinetic energy function defined in Sect. II (i.e.,* *the energy per unit volume of spinless particles at density ρ), there is a constant $C_\varepsilon > 0$, for every $0 < \varepsilon < 1$, such that*

$$T_\psi \geq C_\varepsilon \int j_B(\varepsilon\rho_\psi(x))\mathrm{d}x. \tag{3.4}$$

Inequality (3.4) is equivalent to an assertion about the negative eigenvalues $e_1 \leq e_2 \leq \ldots < 0$ of $H_B = (i\nabla - A)^2 - B - U(x)$ for an arbitrary nonnegative potential $U(x)$. One shows that

$$\sum_i |e_i| \leq \int f(U(x))\mathrm{d}x$$

from which it follows that $T_\psi \geq \int w(\rho_\psi(x))\mathrm{d}x$ with w being the Legendre transform of f. We are able to show that for every $0 < \lambda < 1$

$$\sum |e_i| \leq \lambda^{-1}\frac{B}{2\pi}\int U + \tfrac{3}{8}(1-\lambda)^{-2}\int U^2, \tag{3.5}$$

and (3.4) follows easily from this.

Our proof uses, as usual, the Birman-Schwinger kernel $U^{1/2}[(i\nabla - A)^2 - B + E]^{-1}U^{1/2}$. The hard part is to control the zero modes of $h = (i\nabla - A)^2 - B$, i.e., the lowest Landau level. Two-dimensions is very different from three where the energy in the z-direction precludes having a macroscopically degenerate level of zero energy states. We are able to isolate this lowest level with the aid of Ky Fan's inequality on singular values of sums of operators; the effect of this level is to produce the $B\int U$ term in (3.5).

Technicalities aside, (3.4) presents a nontrivial mathematical problem. T_ψ can, indeed, be zero; this is easily accomplished, even for positive density, by making use of all the lowest Landau level eigenfunctions. If we want to bound T_ψ from below by the integral of a *nonnegative*, but nontrivial function of ρ, such as $j_B(\rho)$, we have to be sure that the function is zero for low density. The function j_B, which is zero for $0 \leq \rho \leq B/2\pi$, precisely accomodates the maximum density in the lowest Landau band that is allowed by the Pauli principle.

IV. EXCHANGE-CORRELATION ENERGY AND THE TWO CLASSICAL ELECTROSTATICS PROBLEMS

The exchange-correlation energy of a normalized state ψ is defined to be

$$E_{\rm ex}(\psi) = \left\langle \psi \left| \sum_{1\le i<j\le N} |x_i - x_j|^{-1} \right| \psi \right\rangle - D(\rho_\psi, \rho_\psi), \tag{4.1}$$

with ρ_ψ defined as in (3.1) (but with a sum over spin states) and $D(f,g)$ defined as in (3.2). By imitating the original proof in [LE1], i.e., using the "maximal function", we can prove

4. LEMMA (Exchange inequality in 2 dimensions). *There is a constant $C > 0$ such that*

$$E_{\rm ex}(\psi) \ge -C \int_{\mathbf{R}^2} \rho_\psi(x)^{3/2} dx. \tag{4.2}$$

This inequality is quite adequate for small and moderate $B = \beta N$, for the simple reason that it can be controlled by $\int j_B(\rho_\psi)$ as follows.

$$\begin{aligned}\int \rho_\psi^{3/2} &= \int\limits_{\rho_\psi \le B/\pi} \rho_\psi^{3/2} + \int\limits_{\rho_\psi > B/\pi} \rho_\psi^{3/2} \\ &\le N\sqrt{B/\pi} + \left\{ \int\limits_{\rho_\psi > B/\pi} \rho_\psi^2 \right\}^{1/2} \left\{ \int \rho_\psi \right\}^{1/2} \le \left\{ \sqrt{\frac{\beta}{\pi}} + (\text{const.}) \frac{\sqrt{T_\psi}}{N} \right\} N^{3/2}. \end{aligned} \tag{4.3}$$

The last line is $O(N^{3/2})$ in the ground state, which is small compared to the total energy (which is $O(N^2)$) provided one can prove the "obvious" fact that $T_\psi = O(N^2)$; this is easy to do.

For large β (4.3) is not optimal because it asserts that the error is $\beta^{1/2}N^{3/2}$. While this is $O(N^{-1/2})$ relative to E^Q, it is not uniform in β and it is certainly not optimal. The source of the difficulty, once again, is the zero modes of the kinetic energy operator. We can do better by introducing the **Classical Particle Energy**, E_K^P, defined as follows. First define the function on $\mathbf{R}^{2N}$ by

$$\mathcal{E}_K^P(x_1,\ldots,x_N) = K\sum_{i=1}^N v(x_i) + \sum_{1\le i<j\le N} |x_i - x_j|^{-1}. \tag{4.4}$$

Then E_K^P is defined by

$$E_K^P(N) = \inf\{\mathcal{E}_K^P(x_1,\ldots,x_N) : x_i \in \mathbf{R}^2\}. \tag{4.5}$$

Corresponding to this particle energy is the **Classical Continuous Energy**:

$$\mathcal{E}_K^C(\rho) = K\int_{\mathbf{R}^2} \rho(x)v(x)\mathrm{d}x + D(\rho,\rho) \tag{4.6}$$

$$E_K^C(N) = \inf\{\mathcal{E}_K^C(\rho) : \rho(x)\ge 0, \int \rho = N\}. \tag{4.7}$$

The classical continuous problem is the same as the TF problem, but without the kinetic energy $j_B(\rho)$ term and hence, in particular, it does not involve B. As a result of the lack of a $\int \rho^2$ control, the minimizer, which one can show always exists (since $V(x)\to\infty$ as $|x|\to\infty$) and is unique, might turn out to be a measure! Since V is continuous, this makes sense, but we question whether this actually happens. (Note: There are Hausdorff measures in two-dimensions that have finite energy $D(\rho,\rho)$.) However, as discussed just before Lemma 7, measures to not occur when $V\in C^{1,\alpha}$.

The classical continuous problem has the same simple scaling property as the TF problem, namely

$$E_K^C(N) = N^2 E_\kappa^C(1) \quad \textit{and} \quad \rho_N(x) = N\rho_1(x), \tag{4.8}$$

where ρ_N is the minimizer (with κ fixed) for $\int \rho = N$ and $K = \kappa N$.

The minimization problem (4.7) leads, of course, to the following Euler-Lagrange equation for ρ that parallels the TF equation (2.6). For $N = 1, K = \kappa$

$$V_{\text{eff}}(x) := \kappa v(x) + [|x|^{-1} * \rho](x) = \begin{cases} \mu & \text{if } \rho(x) > 0 \\ \geq \mu & \text{if } \rho(x) = 0 \end{cases} \tag{4.9}$$

with μ being the chemical potential. [Note: if ρ is a measure the left side of (4.9) should be $\geq \mu$ everywhere and $= \mu$ ρ-almost everywhere.

Eq. (4.9) states that the potential generated by ρ plus the confining potential V add up to a constant when $\rho > 0$. *If* we were in three-dimensions instead of two, the solution is easy. Just apply $-\Delta$ to both sides. If $v(x) = x^2$ one has that ρ is a constant, C, inside some ball of radius R (with $C = 3\kappa/(2\pi),\ 2\kappa R^3 = 1,\ \mu = 1/R + \kappa R^2$).

The solution to (4.9) in two-dimensions is much more difficult. However, when $v(x) = x^2$ it can be solved:

$$\rho(x) = \begin{cases} C\sqrt{R^2 - x^2} & |x| \leq R \\ 0 & |x| \geq R \end{cases} \tag{4.10}$$

for suitable constants C and R. The computation of the convolution $|x|^{-1} *$ (right side of (4.10)) is an amusing exercise!

We have three non-quantum energies before us, $E^{\text{TF}}(\kappa, \beta, N), E^P_K(N), E^C_K(N)$. In order to discuss their relationship we first need a technical lemma

5. LEMMA (Finite radius). *Fix κ and set $K = \kappa N$.*

There is a radius $R_v(\kappa)$, independent of N, such that for every N the infimum for E^{TF}, E^P, E^C can be sought among densities (in the case of E^{TF} and E^C), or particle coordinates (in the case of E^P) that have support in the ball of radius $R_v(\kappa)$ centered at the origin in $\mathbf{R}^2$.

The proof of Lemma 5 is fairly simple. If there is some charge outside some large ball, $R_v(\kappa)$, then there is some location inside the ball of unit radius to which this charge can be moved in such a way that the energy is lowered. Here, we make use of the fact that $V(x) \to \infty$ as $|x| \to \infty$.

In the remainder of this section we discuss the relationship between the two classical energies $E_K^P(N)$ and $E_K^C(N)$. In the next section we discuss the relationship of these classical energies to $E^{\rm TF}$. We first point out that Lemma 4 cannot be used in order to compare E_K^P and E_K^C. In fact, what corresponds to the minimizing "density" ρ_ψ for the $\mathcal{E}_K^P$ problem is a sum of delta functions and thus $\int \rho_\psi^{3/2}$ is meaningless (if we approximate the delta functions by continuous functions this error term will go to infinity).

Using an electrostatics inequality of Lieb and Yau [LY] we are able to prove that $E_K^C(N)$ is indeed a good approximation to the particle energy $E_K^P(N)$. That electrostatics inequality generalizes (4.2) in a certain sense. It is the following

6. LEMMA (The interaction of points and densities). *Given points $x_1, \dots, x_N$ in $\mathbf{R}^2$, we define Voronoi cells $\Gamma_1, \dots, \Gamma_N \subset \mathbf{R}^2$ by*

$$\Gamma_j = \{ y \in \mathbf{R}^2 : |y - x_j| \le |y - x_k| \ \ \textit{for all} \ \ k \ne j \} \quad .$$

These Γ_j have disjoint interiors and their union covers $\mathbf{R}^2$. We also define R_j to be the distance from x_j to the boundary of Γ_j, i.e., R_j is half the distance of x_j to its nearest neighbor. Let ρ be any (not necessarily positive) function on $\mathbf{R}^2$. (In general, ρ can be replaced by a measure, but it is not necessary for us to do so.) Then

$$\begin{aligned} \sum_{1 \le i < j \le N} |x_i - x_j|^{-1} \ge &- D(\rho, \rho) + \sum_{j=1}^N \int_{\mathbf{R}^2} \rho(y) |y - x_j|^{-1} dy \\ &+ \tfrac{1}{8} \sum_{j=1}^N R_j^{-1} - \sum_{j=1}^N \int_{\Gamma_j} \rho(y) |y - x_j|^{-1} dy \quad . \end{aligned} \tag{4.11}$$

This comparison of $E_K^C(N)$ and $E_K^P(N)$ requires that the minimizing density for the continuous energy $\mathcal{E}_K^C$ has some regularity. A-priori the minimizing density for $\mathcal{E}_K^C$ *could* *be* a singular measure and if this is the case we cannot expect to get a good estimate of the difference between E_K^C and E_K^P. To ensure that the minimizer for $\mathcal{E}_K^C$ is neither a measure not too singular a function we need the confining potential V to be sufficiently regular. Although we do not believe this to be optimal, we find it convenient to assume that V is in $C^{1,\alpha}$ (Hölder continuous first derivative with exponent $\alpha > 0$). We prove that ρ is then in $L^q(\mathbf{R}^2)$ for some exponent $q > 2$ that depends on α. With this in hand, we are then able to prove

7. LEMMA (Classical correlation estimate). *Assume that V is a potential in $C^{1,\alpha}$. For all N we have*

$$E_K^C(N) - b(\kappa)N^{3/2} \leq E_K^P(N) \leq E_K^C(N) - a(\kappa)N^{3/2}, \tag{4.12}$$

where $a(\kappa)$ and $b(\kappa)$ are positive constants independent of N that depend on the radius $R_v(\kappa)$ of Lemma 5 and on the exponent q (and its dual $p = q/(q-1)$).

$$\begin{aligned} a(\kappa) &= (8R_v(\kappa))^{-1} \\ b(\kappa) &= \tfrac{4}{3}\sqrt{\tfrac{2}{3}} \int \rho_1(x)^{3/2} \mathrm{d}x + \left(\frac{2\pi}{2-p}\right)^{1/p} (2R_v(\kappa))^{-1+2/p} \|\rho_1\|_q, \end{aligned}$$

with ρ_1 being the minimizer for $\mathcal{E}_K^C$ for $N = 1$, i.e., the minimizer for $\mathcal{E}_\kappa^C$.

V. OUTLINE OF THE PROOF OF THE LIMIT THEOREM

We now give a very sketchy outline of the proof of Theorem 2. We shall mainly emphasize the steps in the proof that do not use standard techniques. In particular, we shall stress the use of the estimates given in the two previous sections.

The aim is to prove that for a given $\varepsilon > 0$ we can find an electron number $N(\varepsilon, \kappa)$, depending on ε and κ but *independent of* β, such that $N \geq N(\varepsilon, \kappa)$ implies

$$N^{-2}|E^{\mathrm{TF}}(\kappa, \beta, N) - E^{\mathrm{Q}}(\kappa, \beta, N)| < \varepsilon \tag{5.1}$$

for all β. To prove this we have to treat small and large β differently. We therefore choose β_ε (to be specified below) and consider $\beta \leq \beta_\varepsilon$ and $\beta > \beta_\varepsilon$. In both cases the proof consists of finding upper and lower bounds to $E^Q(\kappa, \beta, N)$. As usual, the upper bound is a relatively simple variational argument. In both cases we construct a trial wave function using magnetic coherent states similar to the ones used in [YJ] and [LSY1-3]. The lower bounds are more difficult; the case of large β, in particular, requires new ideas—again due to the presence of a large number of zero modes. We discuss this large β case first.

Case 1. (Lower bound on E^Q for $\beta > \beta_\varepsilon$): By simply ignoring the kinetic energy operator, which we had normalized to be positive, we have the obvious inequality $E^Q(\kappa, \beta, N) \geq E_K^P(N)$.

From Lemma 7 we can therefore conclude that

$$E^Q(\kappa, \beta, N) \geq E_K^C(N) - b(\kappa)N^{3/2}. \tag{5.2}$$

The final step in the proof is to relate $E_K^C(N)$ to $E^{\mathrm{TF}}(\kappa, \beta, N)$. In order to do this we choose a *bounded* density $\widetilde{\rho}_1$ with $\int \widetilde{\rho}_1 = 1$ such that $\mathcal{E}_\kappa^C(\widetilde{\rho}_1) \leq E_K^C(1) + \varepsilon/2$. Note that $\mathcal{E}_\kappa^C$ does not depend on β. We may then assume that β_ε is so large that $\widetilde{\rho}_1(x) \leq \beta_\varepsilon/2\pi$ for all x. For all $\beta > \beta_\varepsilon$ we therefore have $j_{\beta N}(N\widetilde{\rho}) = 0$ (for simplicity we are here again ignoring spin).

Consequently, using $\widetilde{\rho} = N\widetilde{\rho}_1$ as a trial density in the TF functional we find that

$$E^{\mathrm{TF}}(\kappa, \beta, N) \leq \mathcal{E}^{\mathrm{TF}}(\widetilde{\rho}) = \mathcal{E}_K^C(\widetilde{\rho}) = N^2[E_K^C(1) + \varepsilon/2] \leq E_K^C(N) + \frac{\varepsilon}{2}N^2. \tag{5.3}$$

Comparing (5.2) and (5.3) we immediately see that $N(\varepsilon, \kappa)$ can be chosen so that (5.1) holds.

In the special case of $v(x) = x^2$ we know that the minimizer ρ_1 of $\mathcal{E}_\kappa^C$ given by (4.10) is continuous and bounded. In this case we can therefore choose $\widetilde{\rho}_1 = \rho_1$ and we can make the explicit choice $\beta_\varepsilon = \sup_x 2\pi\rho_1(x) = 2\pi\rho_1(0) = CR$.

Case 2. (Lower bound on E^Q for $\beta \leq \beta_\varepsilon$): In this case we follow the standard route of using inequalities (4.2) and (4.3) to reduce the many-body problem to a one-body problem. Combining (1.1), (4.1-3) we obtain

$$\langle\psi|H_N|\psi\rangle = \sum_{j=1}^{N}\langle\psi|H_j^1|\psi\rangle + D(\rho_\psi,\rho_\psi) - C(\kappa,\varepsilon)N^{3/2}, \tag{5.4}$$

where $C(\kappa,\varepsilon)$ is chosen as an estimate on the factor in $\{\ \ \}$ on the right side of (4.3), i.e., $\sqrt{\beta\varepsilon/\pi} + (\text{const.})\sqrt{T_\psi/N} \leq C(\kappa,\varepsilon)$.

To relate (5.4) to the Thomas-Fermi problem we use the inequality

$$0 \leq D(\rho_\psi - \rho^{\mathrm{TF}}, \rho_\psi - \rho^{\mathrm{TF}}) = -\left\langle\psi\middle|\sum_{j=1}^{N}\rho^{\mathrm{TF}} * |x_j|^{-1}\middle|\psi\right\rangle + D(\rho_\psi,\rho_\psi) + D(\rho^{\mathrm{TF}},\rho^{\mathrm{TF}}),$$

which is a consequence of the positive definiteness of the kernel $|x-y|^{-1}$. Inserting this in (5.4) gives

$$\langle\psi|H_N|\psi\rangle \geq \sum_{j=1}^{N}\left\langle\psi\middle|H_j^1 + \sum_{j=1}^{N}\rho^{\mathrm{TF}} * |x_j|^{-1}\middle|\psi\right\rangle - D(\rho^{\mathrm{TF}},\rho^{\mathrm{TF}}) - C(\kappa,\varepsilon)N^{3/2}. \tag{5.5}$$

The importance of (5.5) is that the quantum energy, $\langle\psi|H_N|\psi\rangle$, is bounded below by the expectation of the one-body operator $H^1 + \rho^{\mathrm{TF}} * |x|^{-1}$.

To prove Theorem 2 it remains to do a semiclassical analysis (with $N^{-1/2}$ playing the role of an effective Planck's constant) of the sum of the negative eigenvalues of this one-body operator. This semiclassical analysis again uses the magnetic coherent states and is very similar to the analysis in [LSY3].

Acknowledgements We thank Kristinn Johnsen and Dr. Vidar Gudmundsson for valuable comments and for allowing us to use the pictures of densities and effective potentials that they prepared.

REFERENCES

[FV] V. Fock, *Bemerkung zur Quantelung des harmonischen Oszillators in Magnetfeld*, Z. Phys. **47**, 446-448 (1928).

[KC] C. Kittel, *Quantum Theory of Solids*, Wiley (1963).

[KLS] A. Kumar, S.E. Laux and F. Stern, *Electron states in a GaAs quantum dot in a magnetic field*, Phys. Rev. B. **42**, 5166-5175 (1990).

[KM] M.A. Kastner, *Artificial atoms*, Physics Today **46**, 24-31 (1993).

[LE1] E.H. Lieb, *A lower bound for Coulomb energies*, Phys. Lett. **70A**, 444-446 (1979).

[LL] E.H. Lieb and M. Loss, unpublished section of a book on stability of matter.

[LS] E.H. Lieb and B. Simon, *Thomas-Fermi theory of atoms, molecules and solids*, Adv. in Math. **23**, 22-116 (1977).

[LSY1] 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).

[LSY2] E.H. Lieb, J.P. Solovej and J. Yngvason, *Asymptotics of heavy atoms in high magnetic fields: I. Lowest Landau band region*, Commun. Pure Appl. Math. (in press).

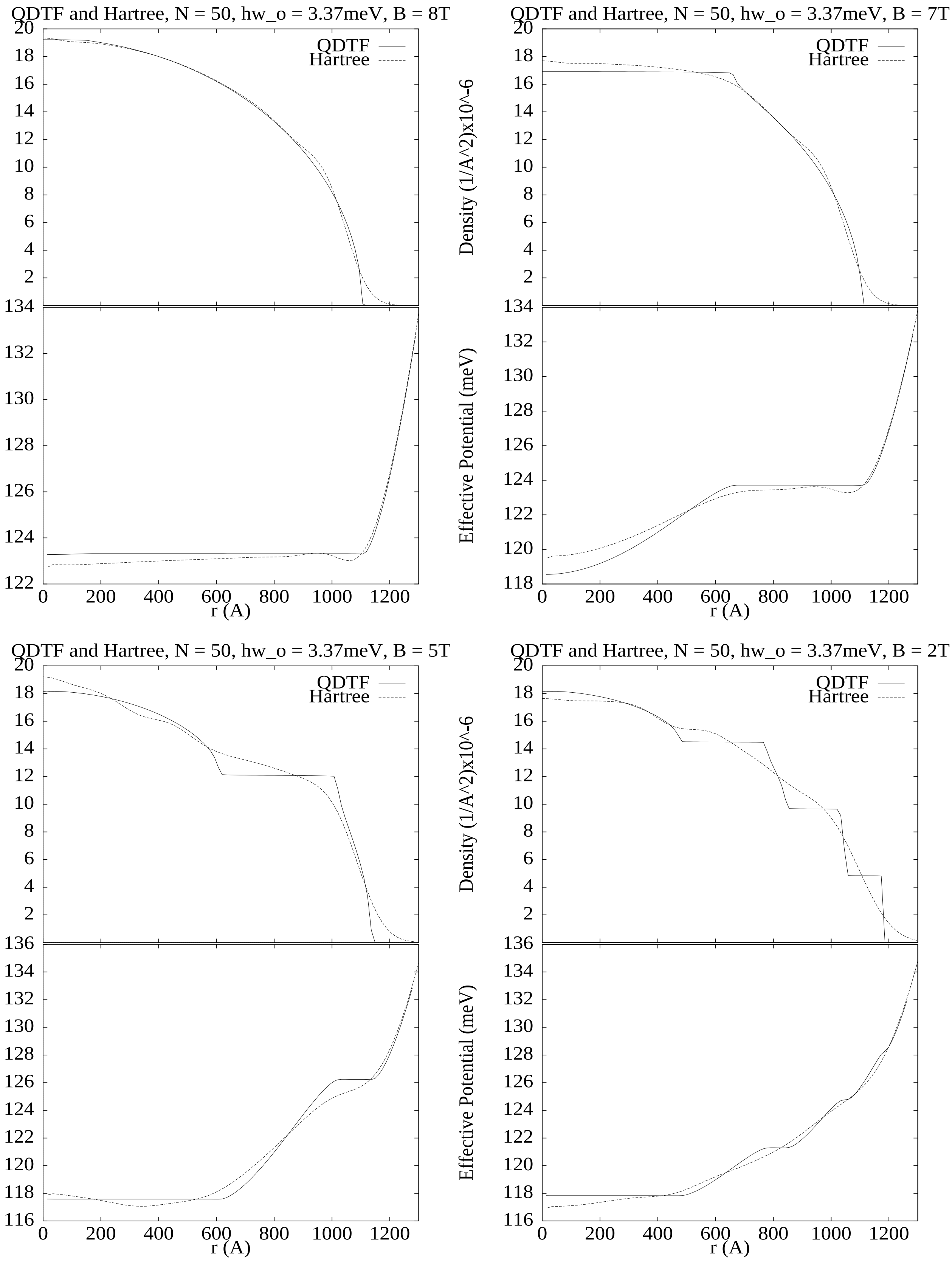
[LSY3] E.H. Lieb, J.P. Solovej and J. Yngvason, *Asymptotics of heavy atoms in high magnetic fields: II. Semiclassical regions*, Commun. Math. Phys. **161**, 77-124 (1994).

[LY] E.H. Lieb and H.-T. Yau, *The stability and instability of relativistic matter*, Commun. Math. Phys. **118**, 177-213 (1988).

[M] P.L. McEuen, E.B. Foxman, J. Kinaret, U. Meirav, M.A. Kastner, N.S. Wingreen and S.J. Wind, *Self consistent addition spectrum of a Coulomb, island in the quantum Hall regime*, Phys. Rev. B, **45**, 11419-11422 (1992). Cf. eqn. (3).

[PGM] D. Pfannkuche, V. Gudmundsson, P.A. Maksym, *Comparison of a Hartree, a Hartree-Fock, and an exact treatment of quantum dot helium*, Phys. Rev. B, **47**, 2244-2250 (1993).

[YJ] J. Yngvason, *Thomas-Fermi theory for matter in a magnetic field as a limit of quantum mechanics*, Lett. Math. Phys. **22**, 107-117 (1991).



QDTF and Hartree, N = 50, hw_o = 3.37meV, B = 8T
QDTF and Hartree, N = 50, hw_o = 3.37meV, B = 7T
QDTF and Hartree, N = 50, hw_o = 3.37meV, B = 5T
QDTF and Hartree, N = 50, hw_o = 3.37meV, B = 2T
QDTF
Hartree
Density (1/A^2)x10^-6
Effective Potential (meV)
r (A)