Quantum dots

A survey of rigorous results

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1 Introduction

Modern semiconductor technology has in recent years made it possible to fabricate ultrasmall structures that confine electrons on scales comparable to their de Broglie wavelength. If the confinement is only in one spatial direction such systems are called *quantum wells.* In *quantum wires* the electrons can move freely in one dimension but are restricted in the other two. Structures that restrict the motion of the electrons in all directions are called *quantum dots.* The number of electrons, N, in a quantum dot can range from zero to several thousand. The confinement length scales R_1, R_2, R_3 can be different in the three spatial dimensions, but typically $R_3 \ll R_1 \approx R_2 \approx 100$ nm. In models of such dots R_3 is often taken to be strictly zero and the confinement in the other two dimensions is described by a potential V with $V(x) \to \infty$ for $|x| \to \infty$, $x = (x^1, x^2) \in \mathbf{R}^2$. A parabolic potential, $V = \frac{1}{2}\omega|x|^2$, is often used as a realistic and at the same time computationally convenient approximation.

Quantum dots have potential applications in microelectronics and have been extensively studied both experimentally and theoretically. Apart from possible practical uses they are of great interest for basic quantum physics. Their parameters (strength and shape of the confining potential, magnetic field strength, number of electrons) can be varied in a controlled way and their properties can be studied by clever experimental techniques. This offers many possibilities to confront theoretical predictions with experimental findings. There exist by now many excellent reviews on the physics of quantum dots, e.g. [1]–[8]. In the present contribution the focus will be on some theoretical aspects that are only partly covered by these reviews, in particular on rigorous limit theorems [9], [10] which apply to dots in high magnetic fields and/or with high electron density.

A quantum dot with N electrons is usually modeled by a Hamiltonian of the

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following form, acting on the Hilbert space

$$\mathcal{H}_N = \bigwedge_1^N L^2(\mathbf{R}^2; \mathbf{C}^2) \tag{1}$$

appropriate for two dimensional Fermions of spin 1/2:

$$H_N = \sum_{j=1}^N H_1^{(j)} + \sum_{1\leq i<j\leq N} W(x_i - x_j), \tag{2}$$

where $x_i \in \mathbf{R}^2$, $i = 1, \ldots, N$ and $H_1^{(j)} = 1 \otimes \cdots \otimes H_1 \otimes \cdots \otimes 1$ (H_1 in the j-th place) with the one-body hamiltonian

$$H_1 = \frac{\hbar^2}{2m_*}\left(\mathrm{i}\nabla - \frac{e}{\hbar c}A(x)\right)^2 + V(x) + g_*\left(\frac{\hbar e}{2m_\mathrm{e}c}\right) S_3 B - CB. \tag{3}$$

Here $A(x) = \frac{1}{2}(-Bx^2, Bx^1)$ is the vector potential of a homogeneous magnetic field of strength B in the x^3-direction, V is the confining potential, assumed to be continuous with $V(x) \to \infty$ for $|x| \to \infty$, and S_3 is the spin operator in x^3-direction. The parameters m_* and g_* are respectively the effective mass and the effective g-factor of the electrons, while m_e and e are the bare values of the electron mass and electric charge, and $\hbar$ and c have their usual meanings. The constant

$$C = \left(\frac{\hbar e}{2m_\mathrm{e}c}\right)\left(\frac{m_\mathrm{e}}{m_*} - \frac{|g_*|}{2}\right) \tag{4}$$

has been introduced in (3) for convenience: Subtraction of CB has the effect that the spectrum of the kinetic energy operator (including spin) $H_1^{\mathrm{kin}} = H_1 - V$ starts at zero for all B, even if $m_* \neq m_\mathrm{e}$ and $g_* \neq 2$.

The interaction potential W represents the Coulomb repulsion between the electrons, modified by the properties of the surrounding medium. Usually it is simply taken to be

$$W(x_i - x_j) = e_*^2 |x_i - x_j|^{-1} \tag{5}$$

where $e_* = e/\sqrt{\epsilon}$ with ϵ the dielectric constant, but some regularization of the bare Coulomb potential, e.g.,

$$W(x_i - x_j) = e_*^2\left[(|x_i - x_j|^2 + \delta_+^2)^{-1/2} - (|x_i - x_j|^2 + \delta_-^2)^{-1/2}\right] \tag{6}$$

with $\delta_- > \delta_+ > 0$ [11], or even a potential that depends not just on the differences $x_i - x_j$, may sometimes fit the effective interaction better. For the proof of some of the theorems below the important property of (5) is that W is repulsive, of positive type and tends to zero at infinity; these features are shared by (6).

Writing the Hamiltonian in the above form is, of course, an approximation, because the effect of the medium on the electrons is only taken into account through the modification of the parameters from their bare values. The size of a quantum dot ($\approx$ 100 nm) is however usually much larger than the lattice constant of the medium where it resides (< 0.5 nm), so this approximation is usually a good one.

Quantum dots, especially such with few electrons, are sometimes referred to as *artificial atoms* with V playing the role of the attractive nuclear potential in real atoms. The analogy is not perfect, however, because V is regular around the origin in contrast to the potential from an atomic nucleus, and also because the electron interaction is the three dimensional Coulomb potential (5) (or modified Coulomb potential (6)), while the motion is (essentially) restricted to two dimensions. But in many respects quantum dots can indeed be regarded as artificial atoms, with an important additional aspect: The effective parameters are to a certain extent tunable and may differ appreciably form their counterparts in real atoms.

In a quantum dot the natural atomic unit of length is $a_* = \epsilon\hbar^2/(m_* e^2)$. Compared with the usual Bohr radius, $a_0 = \hbar^2/(m_\mathrm{e} e^2) = 0.53 \times 10^{-1}$ nm, the length a_* is typically large, e.g., $a_* \approx 185\ a_0 \approx 10$ nm in GaAs. The natural energy unit is $E_* = e_*^2/a_* = e_*^4 m_*/\hbar^2$, and in GaAs $E_* \approx 12$ meV, which should be compared with $E_0 = e^2/a_0 = e^4 m_\mathrm{e}/\hbar^2 = 27.2$ eV, i.e., $E_* \approx 4 \times 10^{-4} E_0$.

The natural unit, B_*, for magnetic field strength is the field at which the magnetic length $\ell_B = \hbar e/(B^{1/2}c)$ equals a_*, or equivalently, at which the cyclotron energy $\hbar e B_*/m_* c$ equals E_*. Hence $B_* = (a_0/a_*)^2 B_0$, where $B_0 = e^3 m_\mathrm{e}^2 c/\hbar^3 = 2.35 \times 10^5$ T is the value corresponding to free electrons. If a_0/a_* is small, B_* can be much smaller than B_0. Thus $B_* \approx 7$ T in GaAs. This opens the very interesting possibility to study in the laboratory magnetic effects, whose analog for real atoms require field strengths prevailing only on neutron stars.

On the experimental side the main techniques for studying quantum dots are *charge transport and capacitance spectroscopy* ([12], [6], [13]) and *optical far infrared spectroscopy* ([14], [15]). The former is in particular suited for measuring the N dependence of ground state energies, but excited states can be investigated as well. The applicability of optical spectroscopy is to a certain extent limited by Kohn's theorem, to be discussed below, but refined techniques allow also to infer many properties by this method. Altogether it is fair to say that the energy spectrum of quantum dots and even some aspects of the corresponding wave functions are experimentally accessible with considerable precision. See also [16] for recently discovered effects in charge transport spectroscopy that wait for an adequate explanation.

On the theoretical side the spectral properties of the Hamiltonian (2) have been studied by a variety of methods, which can be roughly divided into the following categories:

- Exact analytic solutions
- Rigorous limit theorems
- Numerical diagonalizations

- Hartree and Hartree-Fock approximations
- Variational calculations
- Density functional methods

In the condensed matter literature the last four categories are by far the most prominent, but the present survey is mostly concerned with the first two, which lie within the realm of mathematical physics. It is impossible here to do any justice to the extensive physics literature on the theory of quantum dots, but an annotated bibliography of some representative references will be given in the last section.

2 Exact solutions

2.1 The Fock-Darwin spectrum

From now on units are chosen such that $\hbar = e_* = m_* = B_* = 1$. The Hamiltonian (3) can then be written

$$H_1 = \frac{1}{2}\left(\mathrm{i}\nabla - A(x)\right)^2 + V(x) + \gamma S_3 B - \tfrac{1}{2}(1-|\gamma|)B \tag{7}$$

with $\gamma = g_* m_*/(2m_\mathrm{e})$. For a confining potential of the harmonic oscillator form

$$V(x) = \tfrac{1}{2}\omega|x|^2, \tag{8}$$

the eigenvalues and eigenfunctions of

$$H_1^{\mathrm{orb}} = \tfrac{1}{2}\left(\mathrm{i}\nabla - A(x)\right)^2 + \tfrac{1}{2}\omega^2|x|^2 \tag{9}$$

were determined by Fock already in 1928 [17], and also by Darwin in 1930 [18]. The Fock-Darwin spectrum of (9) consists of the eigenvalues

$$\varepsilon_{k,l}^{\mathrm{FD}} = (2k + |l| + 1)\Omega - \tfrac{1}{2}lB \tag{10}$$

with

$$\Omega = \left(\tfrac{1}{4}B^2 + \omega^2\right)^{1/2}, \tag{11}$$

$k = 0, 1, 2 \ldots, l = 0, \pm 1, \pm 2, \ldots$. The corresponding eigenfunctions are

$$\psi_{k,l}^{\mathrm{FD}}(x) = (\mathrm{const.}) \exp(\mathrm{i}l\varphi) r^{|l|} \exp(-\Omega r^2/2) L_k^{|l|}(\Omega r^2) \tag{12}$$

where $x = (r\cos\varphi, r\sin\varphi)$ and $L_k^{|l|}$ is an associated Laguerre polynomial. These functions are also eigenfunctions of the angular momentum L_3 in the x^3-direction with eigenvalue l. Eigenfunctions with the same value of

$$n = k + \tfrac{1}{2}(|l| - l) \tag{13}$$

are grouped together in a *Fock-Darwin level* (FDL). In the limit $\omega/B \to 0$ the eigenvalues in a FDL coalesce and a FDL becomes identical to a *Landau level* (LL) with the eigenvalues

$$\varepsilon_n^{\mathrm{L}} = (n + \tfrac{1}{2})B \tag{14}$$

and eigenfunctions

$$\psi_{k,l}^{\mathrm{L}}(x) = (\mathrm{const.}) \exp(\mathrm{i}l\varphi) r^{|l|} \exp(-Br^2) L_k^{|l|}(2Br^2) \tag{15}$$

The degeneracy of a LL per unit area is $B/(2\pi)$.

If the interaction W between the electrons is ignored the FD spectrum together with the Pauli principle, taking spin into account, completely solves the eigenvalue problem for H_N in the case of the quadratic potential (8). This approximation even fits some experimental data quite well [1], [2]. When the interaction W is taken into account this picture has to be modified, of course. For a quadratic confining potential, however, the FD spectrum continues to apply to the motion of the center of mass, independently of the interaction. This simple, but important fact [19], [20] goes under the heading *Kohn's theorem.* The proof is essentially contained in the identity

$$N \sum_{j=1}^{N} x_j^2 = \left(\sum_{j=1}^{N} x_j \right)^2 + \sum_{i<j} (x_i - x_j)^2, \tag{16}$$

for it implies that H_N can be written

$$H_N = H_N^{\mathrm{CM}} + H_N^{\mathrm{spin}} + H_N^{\mathrm{rel}} \tag{17}$$

where H_N^{rel} operates only on the relative coordinates $x_i - x_j$, while all dependence on the center of mass coordinate $X = (x_1 + \cdots + x_N)/N$ is contained in

$$H_N^{\mathrm{CM}} = \tfrac{1}{2N} \left(\mathrm{i}\nabla_X - NA(X) \right)^2 + \tfrac{N}{2}\omega^2 |X|^2. \tag{18}$$

The spectrum of H_N^{CM} is exactly the same as that of H_1^{orb}, independent of N and W. In the dipole approximation the radiation field couples only to X and in this approximation optical FIR spectroscopy thus probes only the FD spectrum.

There is a further instance where the FD eigenfunctions play a role even for $W \neq 0$. Let Π_0^{FD} denote the projector on the subspace of $\mathcal{H}_N$ generated by eigenfunctions with FD index $n = 0$ and complete polarization, i.e., spin magnetic moment in the direction of the field. Consider the operator

$$H_N' = \Pi_0^{\mathrm{FD}} H_N \Pi_0^{\mathrm{FD}}. \tag{19}$$

For large B the spectral properties of this operator can be expected to approximate those of H_N. If $W = 0$ the ground state of this operator has the orbital wave function

$$\Psi^{\mathrm{mdd}} = \psi_{0,0}^{\mathrm{FD}} \wedge \psi_{0,1}^{\mathrm{FD}} \wedge \ldots \wedge \psi_{0,N-1}^{\mathrm{FD}}. \tag{20}$$

This eigenfunction is called the *maximum density droplet* [21] because the electrons are as "tightly packed" as possible around the origin. It is an amusing observation that Ψ^{mdd} remains an *exact eigenfunction* of H'_N also for $W \neq 0$. The proof is very simple: H'_N and the angular momentum operator L_3 on $\mathcal{H}_N$ commute and have discrete spectrum. Hence for every eigenvalue of L_3 there is a corresponding eigenfunction that is simultaneously an eigenfunction of H'_N. But the lowest eigenvalue, $N(N-1)/2$, of L_3 in the subspace of $\mathcal{H}_N$ generated by the FD functions with $n = 0$ is nondegenerate, and the corresponding eigenfunction Ψ^{mdd} must hence also be an eigenfunction of H'_N. There is numerical ([21], [22], [23]) and even experimental [24] evidence that Ψ^{mdd} is a ground state of H'_N for some range of values of B.

2.2 Analytic solutions for $N > 1$

For $N = 2$ the Hamiltonian for the relative coordinate $x = x_1 - x_2$ is

$$H_2^{\mathrm{rel}} = (\mathrm{i}\nabla - \tfrac{1}{2}A(x))^2 + \tfrac{1}{4}\omega^2|x|^2 + W(x) \tag{21}$$

In the case of a pure Coulomb interaction, $W(x) = 1/|x|$, explicit formulas for eigenfunctions and eigenvalues of (21) have been found by Taut [25]. His approach is based on an ansatz for the wave functions of the form

$$\psi(x) = \exp(\mathrm{i}m\varphi)\exp(-\rho^2/2)\rho^{|m|}P(\rho) \tag{22}$$

where P is a polynomial in $\rho = (\Omega/2)^{1/2}r$, with $\Omega = \left(\frac{1}{4}B^2 + \omega^2\right)^{1/2}$, φ is the angular variable and $m \in \mathbf{Z}$. Solutions of the form (22) with P a polynomial do not exist for arbitrary values of B, but Taut's method produces at least eigenfunctions and eigenvalues for a countable infinity of values of Ω which accumulate at 0. In fact, an ansatz like (22) in the eigenvalue equation $H_2^{\mathrm{rel}}\psi = E\psi$ with P a power series,

$$P(\rho) = \sum_{\nu=0} a_\nu \rho^\nu, \tag{23}$$

leads to

$$a_\nu = F(|m|, \nu, E')a_0 \tag{24}$$

with a certain recursively computable function F and where E' is related to E by

$$E = \tfrac{1}{4}\Omega E' - \tfrac{1}{2}mB. \tag{25}$$

The condition that a_ν vanishes for all ν larger than some positive integer n is equivalent to the two equations

$$F(|m|, n, E', \Omega) = 0 \tag{26}$$

and

$$E' = 2(|m| + n). \tag{27}$$

For given n and m this gives one or more acceptable values for Ω and corresponding energy values

$$E = \tfrac{1}{2}(n + |m|)\Omega - \tfrac{1}{2}mB. \tag{28}$$

The solutions found in this way are not necessarily ground states of (21) but the position of E in the spectrum can be inferred from the number of nodes of the corresponding wave function.

The solutions of Taut seem so far to be the only known exact solutions for $N = 2$ and the Coulomb interaction (5). They are limited to the special values of Ω defined by (26) and (27). For W of the inverse square form

$$W(x) = \alpha|x|^{-2} \tag{29}$$

on the other hand, the Hamiltonian (21) can be exactly diagonalized fo all B [26]. In fact, addition of (29) merely modifies the centrifugal term in the radial part of the FD Hamiltonian (9) and we obtain as eigenvalues of (21)

$$E = [2n + \mu + 1]\Omega - \tfrac{1}{2}mB \tag{30}$$

with $\mu = (m^2 + \alpha)^{1/2}$ not necessarily an integer, and the eigenfunctions

$$\psi(x) = \exp(\mathrm{i}m\varphi)\exp(-\rho^2/2)\rho^\mu L_n^\mu(\rho^2). \tag{31}$$

It should be noted that the inverse square form (29) for the effective interaction between the electrons is not necessarily less realistic than the pure Coulomb repulsion (5). In fact, the form (6) of the interaction, that is motivated by the situation in real dots [11], has an inverse square decrease for large separation. At small separation, on the other hand, the effective interaction may be less singular than (5). It is therefore not entirely academic to consider also a harmonic interaction [27] of the form

$$W(x_i - x_j) = 2W_0 - \tfrac{1}{2}\beta|x_i - x_j|^2 \tag{32}$$

with positive parameters W_0 and β. For this case one can even solve the problem for *all* N exactly, using (16) to decouple the oscillators. The result for the ground state energy $E^{\mathrm{Q}}(N,B)$ of H_N with $N \geq 2$ and $\gamma = 0$ (for simplicity) is [27]

$$E^{\mathrm{Q}}(N,B) = \Omega + \tfrac{1}{2}(N-1)(N-2)\Omega_0(N) - \tfrac{1}{4}N(N+1)B + N(N-1)W_0 \tag{33}$$

with $\Omega_0(N) = (\Omega^2 - N\beta^2)^{1/2}$. It is assumed that $\omega \geq N^{1/2}\beta$, so $\Omega_0(N) \in \mathbf{R}_+$ for all B. The corresponding wave function for the relative motion is

$$\psi(x) = \prod_{i<j}[z_{ij}\exp(-\Omega_0|z_{ij}|^2/2N)] \tag{34}$$

where $z_{ij} = (x_i^1 - x_j^1) - \mathrm{i}(x_i^2 - x_j^2)$ are the relative coordinates regarded as points in $\mathbf{C}$. The form (32) of the repulsion, of course, quite wrong for large separation, but this error is to some extent counterbalanced by the confining potential. For a comparison of the solutions for different W's and their confrontation with numerical calculations and experiments we refer to [4].

3 Rigorous limit theorems

While exact solutions of the eigenvalue problem for H_N with W of the form (5) or (6) are not available for $N > 2$, it is possible to analyze at least the ground state properties for large large B or large N by minimizing simple functionals of the electron density. In this analysis, which implies a drastic reduction of the quantum mechanical N-body problem, it is not necessary that the confining potential V has the quadratic form (8). From now on V will stand for an arbitrary continuous function of $x \in \mathbf{R}^2$ tending to ∞ for $|x| \to \infty$; when additional properties are required these will be explicitly stated. It is no restriction to assume that $V \geq 0$. To be able to consider variations of the strength of the potential at fixed shape, we write

$$V(x) = Kv(x) \tag{35}$$

with a coupling constant K. The interaction W will for definiteness be assumed to be pure Coulomb with $e_* = 1$, i.e.,

$$W(x-y) = |x-y|^{-1}, \tag{36}$$

but other repulsive potentials of positive type could be treated similarly. The quantum mechanical ground state energy is

$$E^{\mathrm{Q}}(N,B,K) = \langle \Psi_0, H_N \Psi \rangle, \tag{37}$$

where Ψ_0 is a normalized ground state of H_N. The corresponding ground state electron density is

$$\rho^{\mathrm{Q}}_{N,B,K}(x) = \sum_{\text{spins } \sigma_k = \pm 1/2} \int |\Psi_0(x,\sigma_1; x_2,\sigma_2; \ldots, x_N, \sigma_N)|^2 dx_2 \cdots dx_N. \tag{38}$$

We are concerned with the asymptotics of these quantities when one or more of the parameters N, K and B tends to ∞ with v fixed.

The large B limit at fixed N and K is easiest and will be considered first.

3.1 High field limit

In the lowest Landau level (i.e., for $n = 0$) the wave functions (15) are essentially localized on scale $B^{-1/2}$, and the quantum mechanical kinetic energy vanishes after the spin contribution and the subtraction of $\frac{1}{2}(1-|\gamma|)$ in (7) have been taken into account. In the limit $B \to \infty$ it can therefore be expected that a classical model of N point particles with the energy function

$$\mathcal{E}^{\mathrm{P}}[x_1, \ldots, x_N] = \sum_{i=1}^{N} V(x_i) + \sum_{i<j} |x_i - x_j|^{-1} \tag{39}$$

describes the ground state energy correctly. This is indeed the case: Defining

$$E^{\mathrm{P}}(N,K) = \inf \mathcal{E}^{\mathrm{P}}[x_1,\ldots,x_N] \tag{40}$$

we have

Theorem 3.1 (High field limit.) *For N and K fixed,*

$$\lim_{B\to\infty} E^{\mathrm{Q}}(N,B,K) = E^{\mathrm{P}}(N,K). \tag{41}$$

Proof: The lower bound for E^{Q} in the proof of this theorem is trivial: Since the kinetic energy part of (2) is ≥ 0, $E^{\mathrm{P}} \leq E^{\mathrm{Q}}$. The upper bound is a simple variational calculation: Since $V(x)$ tends to ∞ for $|x| \to \infty$ and $|x_i - x_j|^{-1} \to \infty$ for $|x_i - x_j| \to 0$, the infimum of $\mathcal{E}^{\mathrm{P}}$ is obtained at some point $(\bar{x}_1,\ldots,\bar{x}_N) \in \mathbf{R}^{2N}$ with $\bar{x}_i \neq \bar{x}_j$ for $i \neq j$. We test the Hamiltonian with the wave function

$$\Psi(x_1\ldots,x_N) = \exp(\mathrm{i}x_1\times\bar{x}_1/B)\psi^{\mathrm{L}}_{0,0}(x_1-\bar{x}_1)\wedge\ldots\wedge\exp(\mathrm{i}x_N\times\bar{x}_N/B)\psi^{\mathrm{L}}_{0,0}(x_N-\bar{x}_N) \tag{42}$$

$\wedge$ indicates antisymmetrization in the coordinates $(x_1,\ldots,x_N)$, and the vector product $\times$ of two points in $\mathbf{R}^2$ is regarded as $\mathbf{R}$ valued. The spins are totally aligned and are therefore omitted in the notation. The kinetic energy of Ψ is zero, because the wave functions $\exp(\mathrm{i}x\times\bar{x}_j/B)\psi^{\mathrm{L}}_{0,0}(x-\bar{x}_j)$ belong to the lowest Landau level. The potential energy part approximates $\mathcal{E}^{\mathrm{P}}[\bar{x}_1,\ldots,\bar{x}_N]$ arbitrarily well as $B\to\infty$, because $|\psi^{\mathrm{L}}_{0,0}(x-\bar{x}_j)|^2$ is essentially localized within a radius $\sim B^{-1/2}$ around $\bar{x}_j$ and tends to a delta function as $B\to\infty$.

3.2 Large N limits

Before stating the limit theorems formally let us briefly discuss their heuristic basis.

For $B = 0$ each of the N electrons in a dot of radius R occupies a "private room" of spatial extension $R/N^{1/2}$, because of the Pauli principle. Hence the kinetic energy of an electron is $\varepsilon_{\mathrm{kin}} \sim N/R^2$. The potential energy due to the confining potential is $\varepsilon_{\mathrm{conf}} \sim Kv(R)$ and the repulsive energy due to the other electrons $\varepsilon_{\mathrm{rep}} \sim N/R$. The radius R can be estimated by minimizing the sum $\varepsilon_{\mathrm{kin}}+\varepsilon_{\mathrm{conf}}+\varepsilon_{\mathrm{rep}}$. If K/N is kept fixed while $N\to\infty$, all these terms are proportional to N. The radius is therefore *independent of* N an the mean distance between the electrons is $\sim RN^{-1/2}$. In this limit the density tends to infinity. The ground state energy of the dot, i.e., the total energy E^{Q} of the N electrons, is $\sim N^2$, and this is large compared to the exchange/correlation energy $\sim N\cdot(N^{-1/2})^{-1} = N^{3/2}$. One may therefore expect that a Thomas-Fermi theory [28] captures the leading asymptotics for $N,K\to\infty$ with K/N fixed.

A magnetic field B will not influence the asymptotics as long as $B \ll N$, because the energy differences between Landau levels are much smaller than the other energy contributions. If $B \sim N$, on the other hand, all Landau levels have to be taken into account, and the Thomas-Fermi theory has to be modified ([11], [29]). For $B \gg N$ the electrons will essentially all sit in the lowest Landau level and the kinetic energy contribution vanishes. The radius is essentially independent of B and N (as long as $B \gg N$) and slightly smaller than in the $B = 0$ case, because the positive kinetic energy term $\varepsilon_{\mathrm{kin}} \sim N/R^2$ is now missing. The ground state energy is $\sim N^2$ as before. Theorem 3.1 applies, but the large N limit leads to an additional simplification: The point charges can be replaced by a continuous distribution [28], because the interelectronic distance $\sim RN^{-1/2}$ tends to zero. The asymptotics is described by the energy functional of a charged fluid in the confining potential V.

For a homogeneous potential V of degree $s \geq 1$, i.e., $V(\lambda x) = \lambda^s V(x)$, this last mentioned "classical" energy functional describes also the large N limit for arbitrary B if $K/N \to 0$, in particular if K is fixed while $N \to \infty$. The radius $R \sim (N/K)^{1/(s+1)}$ tends in this case to ∞. The density may go to zero or to infinity. The kinetic energy per particle $\sim N/R^2 \sim N(K/N)^{2/(s+1)}$ is in both cases small compared to the other contributions $\sim KR^s \sim K(N/K)^{s/(s+1)}$. Smearing out the point charges brings in an error $\sim N^{1/2}/R$ per particle, but it is small compared to the total Coulomb repulsion $\sim N/R$.

These heuristic considerations will now be turned into precise statements. We define three functionals of the electron density $\rho \in L_1(\mathbf{R}^2, dx)$, $\rho \geq 0$ as follows.

The **2D Thomas-Fermi functional** is

$$\mathcal{E}^{\mathrm{TF}}[\rho; K] = \pi \int \rho(x)^2 dx + \int V(x)\rho(x)dx + D(\rho,\rho) \tag{43}$$

with $D(\rho,\rho) = \frac{1}{2}\int\int \rho(x)|x-y|^{-1}\rho(y)dxdy$. All integrals are over $\mathbf{R}^2$. The $\pi\rho^2$ in the first term is just the kinetic energy density of a two dimensional noninteracting electron gas of density ρ at $B = 0$.

The **2D magnetic Thomas-Fermi functional** is defined as

$$\mathcal{E}^{\mathrm{MTF}}[\rho; B, K] = \int j_B(\rho(x))dx + \int V(x)\rho(x)dx + D(\rho,\rho) \tag{44}$$

where j_B is a piece wise linear function representing the kinetic energy density of the electrons in a magnetic field B, taking all Landau levels (including spin) into account. If γ in (7) were 0, the derivative $j_B' = dj_B/d\rho$ would just be the step function

$$j_B'(\rho) = B[2\pi\rho/B] \tag{45}$$

where $[t]$ denotes the integer part of a real number t. This, together with $j_B(0) = 0$ fixes $j_B(\rho)$. As $B \to 0$, $j_B(\rho) \to \pi\rho^2$. If $\gamma \neq 0$, then j_B is a slightly more complicated step function, cf. Eq. (2.3) in [9], but since the explicit form is not significant we refrain form stating it here. When a concrete j_B is needed for discussion purposes we shall stick to the simplest case (45).

Finally, the **classical energy functional** is defined as

$$\mathcal{E}^{\mathrm{C}}[\rho;K]=\int V(x)\rho(x)dx+D(\rho,\rho). \tag{46}$$

All three functionals are convex, and for each there is a unique nonnegative density that minimizes the functional under the constraint $\int \rho(x)dx=N$; this is discussed in [9].

We denotes the minimizing densities and the corresponding energies by $\rho^{\mathrm{TF}}_{N,K}$ and $E^{\mathrm{TF}}(N,K)$ for the TF functional (43), by $\rho^{\mathrm{MTF}}_{N,B,K}$ and $E^{\mathrm{MTF}}(N,B,K)$ for the magnetic TF functional (44), and by $\rho^{\mathrm{C}}_{N,K}$ and $E^{\mathrm{C}}(N,K)$ for the classical functional (46). In the last case some regularity of V is needed in order to ensure that $\rho^{\mathrm{C}}_{N,K}$ is a function and not just a positive measure; a sufficient conditions is that V satisfies locally an estimate of the form

$$|\nabla V(x)-\nabla V(y)|\leq(\mathrm{const.})\,|x-y|^{\alpha} \tag{47}$$

with some $\alpha>0$.

The TF functional (43) and the classical functional (46) are both limiting cases of the MTF functional (44), for $B\to 0$ and $\to\infty$ respectively. More precisely,

$$\begin{aligned}\lim_{B\to 0} E^{\mathrm{MTF}}(N,B,K) &= E^{\mathrm{TF}}(N,K) &(48)\\ \lim_{B\to 0}\rho^{\mathrm{MTF}}_{N,B,K} &= \rho^{\mathrm{TF}}_{N,K} &(49)\end{aligned}$$

and

$$\begin{aligned}\lim_{B\to \infty} E^{\mathrm{MTF}}(N,B,K) &= E^{\mathrm{C}}(N,K) &(50)\\ \lim_{B\to \infty}\rho^{\mathrm{MTF}}_{N,B,K} &= \rho^{\mathrm{C}}_{N,K}. &(51)\end{aligned}$$

The limit for the densities should be understood in the weak L_1 sense, but for special V much stronger convergence may hold. For instance, if V is monotonically increasing with $|x|$, $\rho^{\mathrm{C}}_{N,K}$ is a bounded function, and $\rho^{\mathrm{C}}_{N,K}=\rho^{\mathrm{MTF}}_{N,B,K}$ for sufficiently large B, because $j_B(\rho^{\mathrm{C}}_{N,K})=0$ for $B>2\pi\|\rho^{\mathrm{C}}\|_\infty$.

The MTF theory has two nontrivial parameters because of the **scaling relations**

$$\begin{aligned}E^{\mathrm{MTF}}(N,B,K) &= N^2E^{\mathrm{MTF}}(1,B/N,K/N) &(52)\\ \rho^{\mathrm{MTF}}_{N,B,K}(x) &= N\rho^{\mathrm{MTF}}_{1,B/N,K/N}(x). &(53)\end{aligned}$$

Corresponding relations (without B) hold for the TF theory and the classical theory, and also for E^{P}.

A further important property of the densities is their compact support: For fixed K/N the minimizers of $\mathcal{E}^{\mathrm{TF}}$, $\mathcal{E}^{\mathrm{MTF}}$, $\mathcal{E}^{\mathrm{C}}$ and also of $\mathcal{E}^{\mathrm{P}}$ have support in a disc whose radius is uniformly bounded in N and B (Lemma A.1 in [9]).

Each minimizer satisfies a variational equation, which in the case of the MTF theory has an unusual form, since it consists really of inequalities. To state it compactly it is convenient to modify the definition (45) slightly and regard j'_B as an *interval valued* function if $2\pi\rho/B$ is an integer, namely, if $2\pi\rho/B = n$, then j'_B is the closed interval $[(n-1)B, nB]$. The **MTF equation** that is satisfied by ρ^{MTF} can then be written

$$\mu - V(x) - \rho * |x|^{-1} \begin{cases} \in j'_B(\rho(x)) & \text{if} \quad \rho(x) > 0 \\ \leq 0 & \text{if} \quad \rho(x) = 0 \end{cases} \tag{54}$$

with a unique $\mu = \mu(N, B, K)$. Such generalized variational equations have been studied by Lieb and Loss [30].

If the potential is quadratic, $V(x) = K|x|^2$, there is an explicit formula ([28], [9]) for the minimizer for $\mathcal{E}^{\mathrm{C}}$, which is equal to ρ^{MTF} for B sufficiently large:

$$\rho^{\mathrm{C}}_{N,K}(x) = \begin{cases} \frac{3}{2\pi} N\lambda\sqrt{1-\lambda|x|^2} & \text{if} \quad |x| \leq \lambda^{-1} \\ 0 & \text{if} \quad |x| > \lambda^{-1} \end{cases} \tag{55}$$

with $\lambda = (8K/3\pi N)^{2/3}$. The density profile has the shape of a half ellipsoid with a maximum at $x = 0$. Note the difference between the two dimensional case considered here, and three dimensional electrostatics: In three dimensions the density would be homogeneously distributed in a ball.

The criterion for $\rho^{\mathrm{MTF}} = \rho^{\mathrm{C}}$ is that $j_B(\rho^{\mathrm{C}}(0)) = 0$, which holds if

$$B \geq (6/3^{2/3}\pi^{5/3})K^{2/3}N^{1/3}. \tag{56}$$

Numerically computed profiles of the minimizers ρ^{MTF} and the corresponding effective potentials

$$V_{\mathrm{eff}}(x) = V(x) + \rho^{\mathrm{MTF}} * |x|^{-1} \tag{57}$$

with $V(x) = K|x|^2$ are shown in Fig. 1. The computations were carried out by Kristinn Johnsen.

At the highest value of the field (Fig. 1(a)) condition (56) is fulfilled and ρ^{MTF} has the form (55). On the support of $\rho^{\mathrm{MTF}} = \rho^{\mathrm{C}}$ we have $V_{\mathrm{eff}}(x)$ =constant= μ.

When the field is gradually turned down the maximal density $B/(2\pi)$ of electrons that can be accommodated in the lowest Landau level goes down also. Condition (56) no longer holds, i.e., the density ρ^{C} near the center is higher than $B/(2\pi)$ and charges have to be moved into other states in phase space. If B is only slightly smaller than the value given by (56) (Fig. 1(b)) it would cost too much energy to bring the electrons near the origin into the next Landau level and it pays to move them spatially away from the center, because the potential energy increase is less than B. Hence in a certain range of B values, the density near the center is locked at the value $B/(2\pi)$ ("incompressible" domain). The effective potential is no longer constant in this domain. In the complementary "compressible" domain, on the other hand, the density is below the critical value $B/(2\pi)$, and tends to zero in such a way that the effective potential stays constant. Reducing the field strength

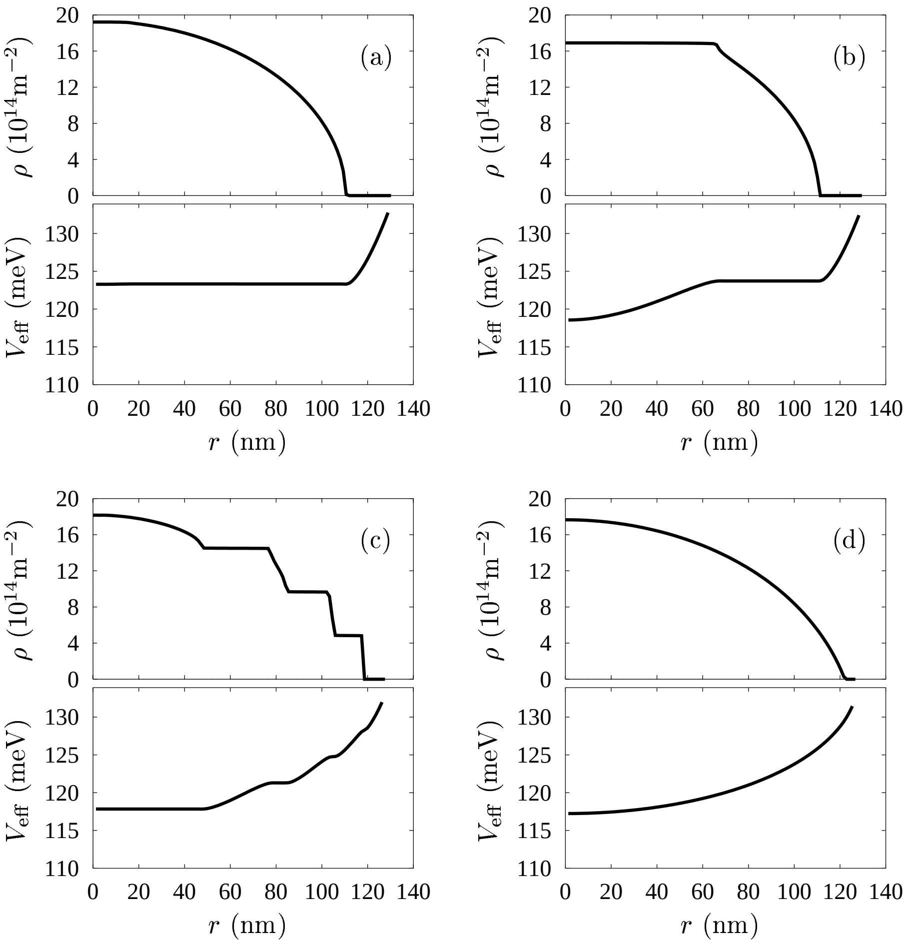

Figure 1: Density profiles and effective potentials for the MTF theory at different magnetic field strengths, calculated for $N = 50$ and $V(x) = K|x|^2$ with $K = 1,7$ meV and the material parameters of GaAs. (a) $B = 8$ T, (b) $B = 7$ T, (c) $B = 2$ T, (d) $B = 0$ T.

further brings more Landau levels into play (Fig. 1(c)). Incompressible domains, where the density is an integer multiple of $B/(2\pi)$, alternate with compressible domains, where the effective potential has a constant value. When $B \to 0$ the profile becomes indistinguishable from the smooth profile of $\rho^{\rm TF}$ (Fig. 1(d)). It is interesting to note that the alternation of compressible and incompressible domains in moderate magnetic fields may account for some fine structure in the charge transport spectroscopy of quantum dots with a large number of electrons [31].

The basic **limit theorem** [9] that relates the energy functionals (43)-(46) to the quantum mechanical ground state of H_N is as follows:

Theorem 3.2 (High density limit.) *Let $N \to \infty$ with K/N fixed. Then, uniformly in B/N,*

$$E^{Q}(N,B,K)/E^{\rm MTF}(N,B,K) \to 1 \tag{58}$$

and

$$N^{-1}\rho^{Q}_{N,B,K}(x) \to \rho^{\rm MTF}_{1,B/N,K/N}(x) \tag{59}$$

in weak L^1 sense. Moreover, if $B/N \to 0$, then

$$E^{Q}(N,B,K)/E^{\rm TF}(N,B,K) \to 1 \tag{60}$$

$$N^{-1}\rho^{Q}_{N,B,K}(x) \to \rho^{\rm TF}_{1,B/N,K/N}(x), \tag{61}$$

and if $B/N \to \infty$, then

$$E^{Q}(N,B,K)/E^{\rm C}(N,B,K) \to 1 \tag{62}$$

$$N^{-1}\rho^{Q}_{N,B,K}(x) \to \rho^{\rm C}_{1,B/N,K/N}(x). \tag{63}$$

According to this theorem there are thus three asymptotic regimes for quantum dots as N and K tend to ∞ with K/N fixed: $B \ll N$, $B \sim N$ and $N \ll B$. This should be compared with the more complex situation for three dimensional natural atoms in strong magnetic field, where there are five regimes [32], [33] for $N \to \infty$ with Z/N fixed (Z = nuclear charge): $B \ll N^{4/3}$, $B \sim N^{4/3}$, $N^{4/3} \ll B \ll N^3$, $B \sim N^3$, $N^3 \ll B$.

For homogeneous potentials a stronger asymptotic result holds, for K/N may tend to zero as $N \to \infty$.

Theorem 3.3 (Homogeneous potentials.) *Assume that V is homogeneous of degree $s \geq 1$, i.e.,*

$$V(\lambda x) = \lambda^s V(x). \tag{64}$$

Then

$$\lim_{N\to\infty} E^{\rm Q}(N,B,K)/E^{\rm MTF}(N,B,K) = 1 \tag{65}$$

uniformly in B and in K as long as K/N is bounded above. Moreover, if $K/N \to 0$ as $N \to \infty$, then

$$\lim_{N\to\infty} E^{\rm Q}(N,B,K)/E^{\rm C}(N,K) = 1 \tag{66}$$

uniformly in B.

We shall now discuss briefly the main techniques used for the proof of these theorems. As usual it is sufficient to prove the limit theorems for the energy, because the corresponding results for the density can be obtained by variation with respect to the potential V. The basic result is thus Eq. (58); the other limit theorems follow by (48)–(51). One has to prove upper and lower bounds for the quantum mechanical energy $E^{\rm Q}$ in terms of the energy $E^{\rm MTF}$, with controllable errors.

The upper bound is obtained, using the variational principle of [34], by testing H_N with a suitable one particle density operator. Its kernel in the space and spin variables x, σ has the form

$$\mathcal{K}(x,\sigma;x',\sigma') = \sum_{\nu} f_\nu(u)\Pi_{\nu u}(x,\sigma;x',\sigma')d^2u \tag{67}$$

where the sum is over all Landau levels and $f_\nu(u)$ is the filling factor of the ν-th Landau level at point u when the density is $\rho^{\rm MTF}(u)$. The kernel $\Pi_{\nu u}(x,\sigma;x',\sigma')$ is obtained from the kernel $\Pi_\nu(x,\sigma;x',\sigma')$ of the projector on the ν-th Landau level by localizing around u with a smooth function g of compact support, i.e.,

$$\Pi_{\nu u}(x,\sigma;x',\sigma') = g(x-u)\Pi_\nu(x,\sigma;x',\sigma')g(x'-u). \tag{68}$$

This operator is positive and approximately a projector, localizing simultaneously in space, i.e., around u, and in the Landau level index ν. By letting the support of g shrink with N more slowly that the average electron spacing $N^{-1/2}$, the error terms in the estimate above for $E^{\rm Q} - E^{\rm MTF}$ are of lower order than N^2, which is the order of $E^{\rm MTF}$.

The lower bound for $E^{\rm Q}$ is proved separately for large B and for small B. For large B, i.e., $B \gg N$, one starts with the obvious estimate $E^{\rm Q} \geq E^{\rm P}$. One then has to compare $E^{\rm P}$ with $E^{\rm C}$, i.e., the energy of point charges with those of smeared charges. Since the electron distance is $\sim N^{-1/2}$ the self energy of a smeared unit charge is $\sim N^{1/2}$. Hence an estimate

$$E^{\rm P}(N,K) \geq E^{\rm C}(N,K) - bN^{3/2} \tag{69}$$

with b depending only on K/N is to be expected, and this can indeed be proved, using an electrostatic lemma of Lieb and Yau [35].

The lower bound for small B, i.e., $B \ll N$ or $B \sim N$, requires an estimate on the indirect Coulomb energy, that is derived in essentially the same way as a corresponding inequality in [38], using the positive definiteness of the Coulomb interaction 5, cf. also [39].

Lemma 3.1 (Exchange inequality in 2 dimensions.)

$$\sum_{\rm spins} \int_{\mathbf{R}^{2N}} |\Psi|^2 \sum_{i<j} |x_i - x_j|^{-1} \geq D(\rho_\Psi,\rho_\Psi) - 192(2\pi)^{1/2} \int_{\mathbf{R}^2} \rho_\Psi^{3/2}. \tag{70}$$

In order to control negative term $\sim \int \rho_\Psi^{3/2}$ on the right side of (70) a lower bound on the kinetic energy is needed. This in turn is derived from a two dimensional magnetic Lieb-Thirring inequality, which has to be proved in a slightly different way from the corresponding inequality in [33], because there is no kinetic energy associated with a motion in the x^3 direction. The following inequality is adequate for the present purpose, but sharper Lieb-Thirring type inequalities that hold even for inhomogeneous fields have been derived by Erdős and Solovej [36], [37].

Theorem 3.4 (Lieb-Thirring inequality in 2 dimensions.) *Let U be locally integrable and let $e_1(U), e_2(U), \ldots$ denote the negative eigenvalues (if any) of the Hamiltonian $\frac{1}{2}(\mathrm{i}\nabla - \mathbf{A})^2 + S_3 B - U$. Define $|U|_+(x) = \frac{1}{2}[|U(x)| + U(x)]$. For all $0 < \lambda < 1$ we have the estimate*

$$\sum_j |e_j(U)| \leq \lambda^{-1} \frac{B}{2\pi} \int_{\mathbf{R}^2} |U|_+(x)dx + \tfrac{3}{4}(1-\lambda)^{-2} \int_{\mathbf{R}^2} |U|_+^2(x)dx. \tag{71}$$

By a Legendre transformation with respect to U it follows from (71) that for all $0 < \lambda < 1$ the kinetic energy T_Ψ of a state Ψ is bounded below by $\frac{1}{3}(1 - \lambda)^2 \int [\rho_\Psi - \lambda^{-1} B/2\pi]_+^2$. It is then possible, for B/N smaller than a certain critical value depending on v, to chose an N dependent $\varepsilon > 0$ in such a way that $\varepsilon \to 0$ as $N \to \infty$, but $\varepsilon T_\psi -$ (const) $\int \rho_\Psi^{3/2} \geq 0$ for all N-particle states Ψ.

4 Other approaches

The rigorous results presented above concern mainly (but not exclusively) the extreme cases of very few ($N = 1$ or $N = 2$) or very many ($N \to \infty$) electrons. These cases play a similar role as the hydrogen atom and the Thomas-Fermi atom do in ordinary atomic physics, i.e., they set a standard that can be used as a starting point of various approximation schemes, or as a test for such schemes whose connection with the original Hamiltonian (2) may not be entirely clear. The physics literature on quantum dots is by now quite extensive, and many approaches have been used for gaining insight where rigorous results are not yet available. Here it is only possible to mention the main methods and give a list of some references that are representative for the approaches of condensed matter physicists to these problems and from it further sources can be traced. See also [8] for a more comprehensive list.

For small N a direct numerical diagonalization of H_N is possible and has been carried out, e.g., in [40], [41], [42], [44], [45], for various values of $N \leq 8$. It is, of course, necessary to restrict H_N to a finite dimensional subspace of the full Hilbert space, and the error made in this step is seldom estimated rigorously. By the mini-max principle, however, the computed values give at least upper bounds to the true eigenvalues. One of the features studied by this method is the orbital angular momentum and spin of the ground state, and analogs of Hund's rules from atomic physics, as well as oscillations between triplet and singlet states for $N = 2$ as B is varied have been seen in the calculations [1], [41].

For $N > 10$ numerical diagonalization of the Hamiltonian is at present hardly feasible and resource is taken to other techniques of many body theory like Hartree and Hartree-Fock approximations (e.g., [42], [43], [22], [15]), perturbation theory [46], variational methods (e.g. [47]), quantum Monte Carlo methods ([48], [49]), and (current) density functional theory ([50], [23], [51], [52]). In quantum dots with a moderate electron number correlations play a much greater role than in natural atoms because the confining potential is usually quite shallow around the origin and the density may be low. (By contrast, one of the main steps in the proof of Theorem 3.2 is to show that exchange and correlation effects vanish in the high density limit for arbitrary magnetic fields.) Strong corelations together with strong dependence on magnetic fields make up much of the special flavor of quantum dot physics and it remains a challenge for mathematical physics to capture these effects in a rigorous way.

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