Exact solutions for a two-electron quantum dot model in a magnetic field and application to more complex systems

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November 12, 2009

Abstract

We discussed exact solutions of the Schrödinger equation for a two-dimensional parabolic confinement potential in a homogeneous external magnetic field. It turns out that the two-electron system is exactly solvable in the sense, that the problem can be reduced to numerically solving one radial Schrödinger equation. For a denumerably infinite set of values of the effective oscillator frequency \( \tilde{\omega} = \sqrt{\omega_0^2 + (\omega_c/2)^2} \) (where \( \omega_0 \) is the frequency of the harmonic confinement potential and \( \omega_c \) is the cyclotron frequency of the magnetic field) even analytical solutions can be given. Our solutions for three electrons are exact in the strong- and the weak correlation limit. For quantum dot lattices with Coulomb-correlations between the electrons in different dots exact solutions are given, provided the lattice constant is large compared with the dot diameters. We are investigating basic physical properties of these solutions like the formation and distortion of Wigner molecules, the dependence of the correlation strength from \( \omega_0 \) and \( \omega_c \), and we show that in general there is no exact Kohn-Sham system for the semi-relativistic Current-Density-Functional Theory.

keywords: quantum dots, exact solutions of Schrödinger equation, Wigner molecules, Current-Density-Functional Theory
1 Introduction

Exact (and sometimes analytical) solutions of the Schrödinger equation for realistic few-electron models of the quantum-dot-type provide a lot of unique opportunities. The physical essence of basic physical notions like the formation and distortion of Wigner molecules (WMs) and the consequences of inter-dot electron correlations in dot lattices can be understood more easily than with numerical brute-force approaches, which provide no formulas but only data. Moreover, these phenomena can be monitored over a wide range of external parameter values, which allows us to tune the system continuously between the weakly and strongly correlated regime. Intermediate and strong correlations are of particular interest, because for weak correlations there are a lot of mean-field approaches available. In particular we can easily see what the basic difference between strong correlated systems with low density (Wigner crystal) and high magnetic fields (fractional quantum Hall systems) is. Further, exact solutions allow us to check the precision of approximations like Hartree-Fock and Density Functional approaches and to reveal their weak and strong points. Unlike the comparison of approximate solutions for real systems with experiments, this approach has the advantage that all physical quantities (including those which are not experimentally accessible) can be considered, there are no experimental side effects, which obscure the comparison, and there are no discrepancies due to differences between the model and the real system. Last but not least, basic mathematical assumptions about the structure of solutions (like non-interacting \( v \)-representability in current density functional theory), which cannot be proven for general systems, can sometimes be rejected for special systems.

This paper is not a comprehensive review on quantum dots and quantum dot molecules and lattices. In particular it does not describe the approaches and the results from numerical diagonalizations in a complete set of basis functions, quasi-classical approaches for the Wigner limit, as well as quantum Monte Carlo \( \to \), density matrix renormalization group \( \to \), current density functional \( \to \), and Hartree-Fock approaches. Each of these methods warrants a separate review (see e.g. Ref.s [1–4] and references therein). Instead, this paper is focused on those systems which can be solved exactly or analytically, albeit the more complex systems only in some limits for the external parameters.

A problem with some exactly solvable models is that they have to be sufficiently simple and the question is whether all their features are shared by real systems of greater complexity. Therefore, all approaches complement one another and they should be pursued in parallel. Apart from this aspect, our models for the two and three-electron quantum dots and lattices from two-electron dots are already interesting on its own.
2 Specification of the model and exact solutions

2.1 Model Hamiltonian

We consider a two-dimensional (2D) two-electron system (with Coulomb interaction) in a harmonic scalar potential \( v_{\text{ext}}(r) = \frac{1}{2} \omega_0^2 r^2 \) and a magnetic field \( \mathbf{B} = B_0 \mathbf{e}_z \) represented by the vector potential (in symmetric gauge) \( \mathbf{A}_{\text{ext}}(r) = \frac{1}{2} B_0 \times r = \frac{1}{2} B_0 r \mathbf{e}_z \). We introduced cylinder coordinates \((r, \alpha, z)\) with the cylinder axis perpendicular to the plane, to which the electron motion is confined. The Hamiltonian reads

\[
H = 2 \sum_{i=1}^{2} \left\{ \frac{1}{2} \left( \mathbf{p}_i + \frac{1}{c} \mathbf{A}_{\text{ext}}(r_i) \right)^2 + \frac{1}{2} \omega_0^2 r_i^2 \right\} + \frac{1}{|r_2 - r_1|} + H_{\text{spin}}, \tag{1}
\]

where \( H_{\text{spin}} = g^* \sum_{i=1}^{3} s_i \cdot \mathbf{B} \), and atomic units \( \hbar = m = e = 1 \) are used throughout. This is a widely used effective Hamiltonian model for a two-electron quantum dot.

2.2 Exact solutions of the Schrödinger equation

The Schrödinger equation with the Hamiltonian \( H \) can be solved not only by reduction to the numerical solution of an (ordinary) radial Schrödinger equation \([20]\), but even analytically for a discrete, but infinite set of effective frequencies \( \tilde{\omega} = \sqrt{\omega_0^2 + (\omega_c/2)^2} \) \([5]\), where we introduced the cyclotron frequency \( \omega_c = B/c \).

If we introduce relative and center of mass (c.m.) coordinates

\[
r = r_2 - r_1, \quad R = \frac{1}{2}(r_1 + r_2) \tag{2}
\]

the Hamiltonian \( H \) decouples exactly:

\[
H = 2 H_r + \frac{1}{2} H_R + H_{\text{spin}} \tag{3}
\]

The Hamiltonian for the c.m. motion agrees with the Hamiltonian of a non-interacting particle in a magnetic field

\[
H_R = \frac{1}{2} \left[ \mathbf{P} + \frac{1}{c} \mathbf{A}_R \right]^2 + \frac{1}{2} \omega_R^2 R^2 \tag{4}
\]

and only the relative Hamiltonian contains the electron-electron interaction

\[
H_r = \frac{1}{2} \left[ \mathbf{P} + \frac{1}{c} \mathbf{A}_r \right]^2 + \frac{1}{2} \omega_r^2 r^2 + \frac{1}{2} r, \tag{5}
\]

where we introduced rescaled parameters \( \omega_R = 2\omega_0, \mathbf{A}_R = 2\mathbf{A}(R), \omega_r = \frac{1}{2} \omega_0, \mathbf{A}_r = \frac{1}{2} \mathbf{A}(r) \) (the indices ‘r’ and ‘R’ refer to the relative and c.m. coordinate systems, respectively). The decoupling of \( H \) allows the ansatz

\[
\Phi = \xi(R) \varphi(r) \chi(s_1, s_2), \tag{6}
\]
where $\chi(s_1, s_2)$ is the singlet or triplet spin eigen-function.

The eigen-functions of the c.m. Hamiltonian have the form

$$\xi = \frac{e^{iMA}}{\sqrt{2\pi}} \frac{U_M(R)}{R^{1/2}} = \frac{e^{iMA}}{\sqrt{2\pi}} R_M(R),$$

$$M = 0, \pm 1, \pm 2, \ldots,$$

where the polar coordinates of the c.m. vector are denoted by $(R, A)$ and the radial functions $U_M(R)$ and $R_M(R)$ can be found in standard textbooks.

With the following ansatz for the relative motion

$$\varphi = \frac{e^{ima}}{\sqrt{2\pi}} \frac{u_m(r)}{r^{1/2}}, \quad m = 0, \pm 1, \pm 2, \ldots$$

the Schrödinger equation $H_r \varphi(r) = \epsilon_r \varphi(r)$ gives rise to a radial Schrödinger equation for $u(r)$

$$\left\{-\frac{1}{2} \frac{d^2}{dr^2} + \frac{1}{2} \left(m^2 - \frac{1}{4}\right) \frac{1}{r^2} + \frac{1}{2} \bar{\omega}_r^2 r^2 + \frac{1}{2r}\right\} u(r) = \bar{\epsilon}_r u(r),$$

where the polar coordinates for the relative vector are denoted by $(r, \alpha)$, $\bar{\omega}_r = \frac{1}{2} \tilde{\omega}$, $\bar{\epsilon}_r = \epsilon_r - \frac{1}{4} m \omega_c$, and $\omega_c = B/c$. The solutions are subject to the normalization condition $\int_0^\infty dr |u(r)|^2 = 1$. The Pauli principle demands that (because of the different particle exchange symmetry of the spin eigen-functions) the relative angular momentum $m$ has to be even and odd in the singlet and triplet state, respectively. There is no constraint for the c.m. angular momentum $M$ following from the Pauli principle. Because of the orthogonality of the coordinate transformation, the above described solutions are eigenfunctions of the total orbital angular momentum with the eigenvalue $M_L = M + m$.

Fig. 1 shows that the modulus of the orbital angular momentum of the ground state (GS) grows stepwise with increasing magnetic field. This implies that the spin state oscillates between singlet and triplet [21]. The Zeeman term and quenching of the singlet state for higher magnetic fields is not included in Fig. 1. The c.m. excitations are not included as well, because they have no impact on the character of the ground state.

In Fig. 2, the magnetic field and the e-e-interaction are successively added to the levels in the confinement only. We observe that the magnetic field removes the degeneracy with respect to the sign of $M_L$ and breaks the symmetry with respect to up and downward directed fields. Angular momenta which are parallel to the field (positive) produce an magnetic moment which is anti-parallel to the field. They have a large interaction energy with the external field which shifts the levels upwards. In the opposite case the shift due to this contribution is downwards. Without e-e-interaction the GS has always $M_L = 0$. The shift due to the e-e-interaction is positive definite and it decreases with increasing $|M_L|$. This can be explained with the radial equation (9), which determines the contribution of the relative motion to the total energy. For large $M_L = m$ and small $r$ the last (e-e-interaction) term is dwarfed by the second (centrifugal potential) term. For large $r$ the
Figure 1: Total energy for fixed confinement frequency $\omega_0 = 1$ versus cyclotron frequency $\omega_c$ (i.e. magnetic field). The c.m. system is always in the ground state with $M = 0$. The relative angular momentum $m$ is varied. The vertical lines show where the total orbital angular momentum $M_L = M + m$ of the ground state changes. S and T indicates whether the ground state is singlet or triplet. Thick lines indicate states which can be NIVR.

Figure 2: Energy levels for fixed external fields versus total orbital angular momentum. The level of the GS is indicated. We started with noninteracting electrons in the confinement only, added the magnetic field and the e-e-interaction. (In the energy unit $\tilde{\omega}$ we used $\omega_c = 2.5$ for all three cases.)
third term (effective confinement) is dominating in all cases. In a classical picture this means that two electrons rotating with a high angular momentum are separated by the centrifugal force, so that the job of the e-e-interaction is already largely done and the addition of the e-e-interaction does not change much. It is this $M_L$-dependence of the e-e-interaction shift which moves the GS to smaller $M_L$ with increasing $\omega_c$.

2.3 Analytical solutions

In [5, 6] it has been shown that the radial Schrödinger equation (9) has simple analytical solutions for a discrete, but infinite set of effective oscillator frequencies $\bar{\omega}$, the pattern of which for $|m| = 1$ can be seen in Fig.3. The patterns for all $|m|$ look qualitatively similar. All solutions have the following form:

$$u(r) = r^{|m|+\frac{1}{2}} p(r) e^{-\frac{1}{4} \bar{\omega} r^2}$$

(10)

where $p(r)$ is a finite polynomial of degree $(n - 1)$. For ‘non-soluble’ systems, the polynomial has an infinite number of terms.

Figure 3: Reduced energies (energy over effective oscillator frequency) versus inverse effective oscillator frequency for relative angular momentum $|m| = 1$. The crosses indicate solvable states. The lines are just a guide for the eye and they connect states with the same node number $k$. $n$ is the same for all horizontal rows of crosses with the same ordinate.

In this review we only provide the results for the simplest analytical solutions. For $n = 1$ there is only a solution for infinite $\bar{\omega}$, which we call an asymptotic solution, because
it is exact for $\tilde{\omega} \to \infty$
\[ \frac{1}{\tilde{\omega}} = 0 , \quad p(r) = 1 \] (11)
This solution agrees not only with the Laughlin model wave function (WF), if the latter is applied to $N = 2$ and expressed in terms of the coordinates used here, but it is also the exact solution for non-interacting electrons (electrons without Coulomb interaction) in relative- and c.m. coordinates. The corresponding WF has no node and is a ground state.
For $n = 2$ there is one finite-field solution
\[ \frac{1}{\tilde{\omega}} = (2 \mid m \mid + 1) , \quad p(r) = 1 + \frac{r}{(2 \mid m \mid + 1)} \] (12)
which is a ground state as well.
For $n = 3$ there is one asymptotic solution, which is a first excited state,
\[ \frac{1}{\tilde{\omega}} = 0 , \quad p(r) = 1 - \frac{r^2}{(\mid m \mid + 1)} \] (13)
and one finite field solution, which is a ground state.
\[ \frac{1}{\tilde{\omega}} = 2 \left( 4 \mid m \mid + 3 \right) , \quad p(r) = 1 + \frac{r}{(2 \mid m \mid + 1)} + \frac{r^2}{2(2 \mid m \mid + 1)(4 \mid m \mid + 3)} \] (14)
The exact energies $\epsilon$ of the relative coordinate systems corresponding to these eigenfunctions can be obtained from one compact formula.
\[ (\epsilon - \frac{1}{2} m \omega_c) = (\mid m \mid + n) \tilde{\omega} \] (15)
If we compare this result with the spectrum of a single electron in a quantum dot $\left( \epsilon - \frac{1}{2} m \omega_c \right) = (\mid m \mid + 2k + 1) \tilde{\omega}$, where $k$ is the node number or degree of excitation, then it becomes clear that in both cases $\left( \epsilon - \frac{1}{2} m \omega_c \right)$ is a integer multiple of $\tilde{\omega}$. We can also say that an analytical solution exists for those value of $\mid m \mid$ and $\tilde{\omega}$, for which one state of the interacting system is degenerate with one state of the non-interacting system.
A great deal of approaches for the 2D electron gas in external fields is based on model wave functions (WF). For inspirations and checks in the limit $N=2$ it would be desirable to have analytical solutions of the two-electron problem for a wide range of external field values. One idea is to use the special analytical solutions [10] with one of the exactly solvable polynomials given in (11-14) as discussed in Ref. [6]. If we use a special exact solution for a finite interval of external potential values we assume that the polynomial is independent of $\tilde{\omega}$ in this interval and depends only on $\mid m \mid$. Each of the choices [11-14] provides a different approximation to the exact solution. Now we check, what the precision of these choices over a wide range of external fields is.
Figure 4: Projection of analytical model wave functions with polynomials of degree \( n \) onto the exact WF. The logarithm of the deviation of the squared matrix element from unity is on the ordinate. Full, dashed and dash-dotted curves belong to \( \log(\omega_0) = -2, 0, \) and \(+2\), respectively (see also first number in the legend). Thick, medium and thin lines belong to \( n=1, 2, \) and \( 3 \), respectively.
Fig. 4 compares the precision of model WFs with different $n$. The negative poles in the curves for $\log(\omega_0) = +2$ and $n=2$ and 3 indicate the vicinity of those $\omega$, which provide exact solutions. It is seen that the solution for $n > 1$ is everywhere better than the solution for $n = 1$ (the latter is exact for infinite fields), and that all solutions become exact for $\omega \to \infty$. This means that the ansatz for the N-electron system proposed in [6] is definitely more precise than the Laughlin ansatz, if both are applied to the 2-electron system. We want to mention that the logarithm of the relative error in the energies calculated with the model WFs shows qualitatively the same behavior as the projection. It is only smaller in magnitude.

### 2.4 Exact densities

With (7) and (8), we obtain for the total density

$$n(r) = 2 \int dr' |\Phi(r, r')|^2$$

the general expression

$$n(r) = \frac{1}{2\pi^2} \int_0^{2\pi} d\alpha \int_0^\infty dr' \left[ R_M(\sqrt{r^2 + \frac{1}{4}r'^2 + rr'\cos\alpha}) \right]^2 [u_m(r')]^2$$

Because we are interested in the ground state only, we can safely use the c.m. state for $M = 0$: $R_0(R) = 2\sqrt{\omega} \exp(-\omega R^2)$ which allows to do one integration analytically leaving us with

$$n(r) = \frac{4\omega}{\pi} e^{-2\omega r^2} \int_0^\infty dr' e^{-\omega/2) r'^2} I_0(2\omega rr') [u_m(r')]^2$$

where $I_n(x)$ are the modified Bessel functions.

The general expression for the paramagnetic current density

$$j^p(r) = -i \int dr' \left[ \Phi^*(r, r') \nabla \Phi(r, r') - \Phi(r, r') \nabla \Phi^*(r, r') \right]$$

is somewhat complicated. Therefore, we give here only the formula for $M = 0$

$$j^p(r) = e_\alpha m \frac{4\omega}{\pi} e^{-2\omega r^2} \int_0^\infty dr' e^{-\omega/2) r'^2} \frac{I_1(2\omega rr')}{r'} [u_m(r')]^2 = e_\alpha j^p(r)$$

As to be expected, the paramagnetic current density is proportional to the total angular momentum, points in azimuthal direction $e_\alpha$, and the scalar $j^p(r)$ depends only on the distance $r$ from the center and not from the azimuthal angle.

Although both formulas (18) and (20) rely on the functions $u_m(r)$, which are solutions of (9), the analytical behavior for $r \to 0$ can be expressed in terms of two positive definite integrals.

$$A_0 = \int_0^\infty dr e^{-\omega/2) r^2} [u_m(r)]^2$$

$$A_2 = \int_0^\infty dr r^2 e^{-\omega/2) r^2} [u_m(r)]^2$$
After power series expansion of $I_n(x)$, we obtain

$$n(r) \rightarrow \frac{4\tilde{\omega}}{\pi}e^{-2\tilde{\omega}r^2}\left[ A_0 + A_2 \tilde{\omega}^2 r^2 + \cdots \right], \quad (23)$$

$$j^p(r) \rightarrow m\frac{4\tilde{\omega}^2}{\pi}e^{-2\tilde{\omega}r^2}r\left[ A_0 + \frac{1}{2}A_2 \tilde{\omega}^2 r^2 + \cdots \right]. \quad (24)$$

For the origin this means that $n(0) = 4\tilde{\omega} A_0/\pi$ is always finite and $j_p(0) = 0$ always vanishes. On the other hand, the derivative of the density at the origin $\frac{dn}{dr}(0) = 0$ vanishes, but the derivative of the paramagnetic current density $\frac{dj}{dr}(0) = m(4\tilde{\omega}^2/\pi)A_0$ is finite, unless $m = 0$. Besides, there is a relation which does not involve the radial WFs explicitly.

$$\frac{d j_p}{dr}(0) = m \tilde{\omega} n(0) \quad (26)$$

The exact vorticity, which has the form $\gamma(r) = e_z \gamma(r)$ reads in this limit

$$\gamma(r) \rightarrow m 2 \tilde{\omega} \left( 1 - \tilde{\omega}^2 \frac{A_2}{A_0} r^2 + \cdots \right). \quad (27)$$

As will be seen in Sect.4, the limit $r \rightarrow 0$ is decisive for our proof of the violation of non-interacting $v$ representability.

### 3 Formation of Wigner molecules and correlation strength

A illustrative classical picture for a WM in an environment with rotational symmetry is a rotating and vibrating electron molecule. For a two-electron system this is a dumbbell-like object. We are going to show that this configuration is a manifestation of strong e-e-correlations and it is formed in the limit of small $\omega_0$ or large $\omega_c$. The issue is: why is small $\omega_0$ equivalent to large $\omega_c$, although the exact WF and consequently all distribution functions depend only on the effective confinement frequency $\tilde{\omega} = \sqrt{\omega_0^2 + (\omega_c/2)^2}$ where both $\omega_0$ and $\omega_c$ have qualitatively the same influence. In particular, we will point out, how strong magnetic fields can cause strong correlations. This is not the same mechanism as for weak confinement (see also Ref. [8]).

For illustration we use the density (16), which provides the distribution of the electrons in space, and the pair correlation function

$$g(r) = \langle \psi | \sum_{i<j} \delta(r_i - r_j - r) | \psi \rangle \quad (28)$$

which determines the distribution of the distance between two electrons. Both quantities depend only from the modulus: $n(r) = n(r)$ and $g(r) = g(r)$. In our system the latter is given by the radial part of the relative WF alone.

$$g(r) = |\varphi(r)|^2 = \frac{|u(r)|^2}{2\pi r} \quad (29)$$
Figure 5: Density (upper) and pair correlation function (lower) for several correlation strength. $\omega_0, \omega_c,$ and the angular momentum of the ground state are given in the legend. The scaling parameters are: $\bar{r}=0.0901(A), 1.0192(B), 0.6345(C), 14.5022(D),$ and $13.6472(E)$
In Fig. 5 both quantities are shown for a few typical parameter sets. We have chosen scaled axes (tilted quantities) which allow us to show and compare different extreme cases in the same picture. On the abscissas the $r$-coordinate is scaled $\tilde{r} = r/\bar{r}$ with the average radius of the dot $\bar{r} = (1/2) \int \! d^2 r \, r \, n(r)$ and the ordinates are scaled in such a way that the norms are conserved: $\int \! d^2 \tilde{r} \, \tilde{n}(\tilde{r}) = 2$ and $\int \! d^2 \tilde{r} \, \tilde{g}(\tilde{r}) = 1$. For weak correlations $n(r)$ is peaked in the region of lowest potential energy (center of the dot) and $g(r)$ is spread out over the whole range of non-vanishing density, allowing in particular small distances between the electrons. This regime is realized in curves A and B applying to strong ($\omega_0$ large) or medium confinement and small and medium $\omega_c$. Strong correlations are connected with sharply peaked densities at non-zero $r$ confining the electrons on a ring with radius $\bar{r}$. The pair correlation function is sharply peaked at a distance $2\bar{r}$ which is the diameter of the ring. This means that the electrons are localized at a ring and have virtually antipodal positions $[?, \text{Taut-2einB}]$ that agrees with the above mentioned classical picture of a WM. This minimizes the e-e-interaction energy in the limits allowed by the potential confinement energy without enhancing the kinetic energy. In terms of external parameters this can be realized in two scenarios.

i) If $\omega_c$ is small (or zero), the confinement has to be weak ($\omega_0$ small). This can be concluded from the comparison of curve B and D. For weak confinement the state is spread out widely and the density is low. Low density implies the dominance of the the e-e-interaction over the kinetic energy (last term in radial Schrödinger equation (9) versus the first term) and a state which minimizes the e-e-interaction. The condensed matter analog to this state is the Wigner crystal. All in all, strong correlations in systems with low densities are produced by the dominance of the the e-e-interaction over the kinetic energy.

ii) If $\omega_c$ is medium or large (and the confinement not too strong), then the angular momentum of the GS is strongly negative (see curve C and E). Large (modulus of) angular momentum means strong centrifugal potential (second term in radial Schrödinger equation (9)) which drives the electrons away from the center and produces the ring structure in the density. At the same time the remaining e-e-term maximizes the e-e-distance within the limits set by the density. This is most pronounced in curves C and E. The case of small $\omega_0$ and large $\omega_c$ (which is not shown because of its numerical difficulties caused by of the extremely strong angular momentum) is even more strongly correlated. The condensed matter analog to this state is the fractional quantum Hall state. The state of curve C shows strong correlations as well, but does not have a large diameter ($\bar{r} = 0.6345$) and consequently a low density. This proves that low density is not necessary for strong correlation, but a magnetic field can do the job alone. All in all, strong correlations in high magnetic fields are mainly produced by the high modulus of the angular momentum.
of the ground state.

From these considerations it follows that in our family of systems a suitable dimensionless quantitative definition of the correlation strength can be set up by the mean square radius of the pair correlation function \( r^2 = \int d^2 r r^2 g(r) \) and its half width \( \Delta^2 r = \int d^2 r (r - \bar{r})^2 g(r) \), where \( \bar{r} = \int d^2 r r g(r) \), according to

\[
 s_{corr} = \frac{r^2}{\Delta^2 r} .
\]  

(30)

This means, small half width and a peak at large \( r \) produce strong correlations. Fig.6 shows this quantity as a function of the external field parameters. The steps are caused by a change in the angular momentum of the GS. It is obvious that for small \( \omega_c \) a weakening of the confinement increases \( s_{corr} \), but an increase of the magnetic field is much more effective, if it is connected to an increase of the modulus of the angular momentum of the GS, what happens in the region where the steps are found.

Matulis and Peeters [8] investigated the same issue using qualitative asymptotic expressions for the wave function instead of exact solutions. Nevertheless the resulting trends are the same, although their visual picture is different.

4 Violation of non-interacting \( \nu \)-representability of the exact solutions of the Schrödinger equation

The exact solutions of the special system considered in this review can be used to show that (unlike generally assumed) an exact Kohn-Sham (KS) system in the framework of semi–relativistic Current Density Functional Theory (CDF T) can exist only in special cases.

In Density Functional Theory (DFT) it can be shown that for the GS the external potential is a functional of the density [14] (see also textbooks [15, 16] with more modern approaches)

\[
v^{ext}(\mathbf{r}) \overset{\mathcal{C}}{\leftarrow} \Psi \overset{\mathcal{D}}{\leftrightarrow} n(\mathbf{r})
\]

(31)

which would imply non-interacting \( \nu \)-representability (NIRV) or the existence of an exact Kohn-Sham system for the GSs, if the interacting and the non-interacting systems would have a common set of ground state densities.

In the presence of a magnetic field and for (semi-relativistic) Current Density Functional Theory (CDFT), the generalization of \( \mathcal{D}^{-1} \) for the ground state still exists, but Vignale and Rasolt [10, 11] just presupposed the existence of the generalization of \( \mathcal{C} \) [17]

1Unlike in common quantum chemistry language, the correlation strength defined here comprises all effects beyond the Hartree approximation, in particular it includes the effect of exchange.
Figure 6: Correlation strength versus external field parameters in log-scales for all axes. The steps, corresponding to parameters where the angular momentum of the GS changes (see Fig.1), are fully resolved only in the lower panel, which shows curves for 3 discrete $\omega_0$. 
implying that NIVR and the existence of a KS scheme has not been proven. Capelle and Vignale [17], on the other hand, have shown that there can be several external potentials $V_{\text{ext}}$ which provide the same WFs and densities

$$
\begin{align*}
V_{\text{ext}}(r) &\rightarrow \Psi \equiv \mathcal{N}(r) \\
\vdots &
\end{align*}
$$

where $V_{\text{ext}}(r)$ and $\mathcal{N}(r)$ represent both external potentials ($v_{\text{ext}}(r)$ and $A_{\text{ext}}(r)$) and both densities ($n(r)$ and $j^p(r)$), respectively. Hence, $C$ cannot exist anymore as an unique mapping and the question of NIVR cannot be answered in this way. However, the exact solutions of the special system considered in this review can be used to show that an exact Kohn-Sham system or NIVR can exist only in the following special cases.

All those states at non-zero $B$ can be NIVR, which are continuously connected to the singlet and triplet ground states at $B = 0$ (see also Fig.1). In more detail:

If the GS is a singlet (total orbital angular momentum $M_L$ is even) both densities can be NIVR if the vorticity $\gamma(r) = \nabla \times \left(\frac{j^p(r)}{n(r)}\right)$ of the exact solution vanishes. For $M_L = 0$ this is trivially guaranteed because the paramagnetic current density vanishes. The vorticity based on the exact solutions for the higher $M_L$ does not vanish, in particular for small $r$. In the limit $r \rightarrow 0$ this can even be shown analytically.

If the GS is a triplet ($M_L$ is odd) and we assume circular symmetry for the KS system (the same symmetry as the real system) then only the exact states with $|M_L| = 1$ can be NIVR with KS states having angular momenta $m_1 = 0$ and $|m_2| = 1$.

Without specification of the symmetry of the KS system the condition for NIVR is that the small-$r$-exponents of the KS states are 0 and 1.

The proof of the statement for the singlet state is extremely simple and will be given here. The other proofs and more detailed information can be found in [9]. The question is if the (in this case doubly occupied) KS-WF $\varphi(r) = R(r) e^{i\zeta(r)}$ can be chosen in such a way that the density and the gauge invariant vorticity of the non-interacting KS system and the exact solution agree.

$$
n_{\text{exact}}(r) = n_{KS}(r) = 2 |R(r)|^2 \quad (33)
$$

$$
\gamma_{\text{exact}}(r) = \gamma_{KS}(r) = 0 \quad (34)
$$

Eq. (33) defines the real part of the KS-WF. On the other hand, the vorticity of a two-electron singlet KS state vanishes exactly irrespective of the special form of $R(r)$ and $\zeta(r)$. Therefore, equation (34) can only be satisfied if the vorticity of the corresponding exact solution vanishes as well. Fig.7 shows that this is not the case, in particular for small $r$, the violation is massive. Eq. (27) provides $\gamma_{\text{exact}}(0) = 2 M_L \bar{\omega}$ which shows that the
Figure 7: The vorticities for $\omega_0 = 1$ and a few typical cyclotron frequencies $\omega_c$ where the state with negative $M_L$ is the ground state. The sign of $\gamma_{\text{exact}}(r)$ agrees with the sign of $M_L$.

‘degree of violation’ grows with growing $\tilde{\omega}$. The exact vorticity vanishes only for the state with zero angular momentum, which is the GS for small magnetic fields (see also Fig.1).

5 Distortion of the three-electron Wigner molecule

As shown above, the two-electron system is the simplest system which exhibits the phenomenon of the formation of WMs in finite systems. For three electrons there is another effect, namely a Jahn-Teller-like distortion of the WM [7] shown schematically in Fig.8, which can be investigated using the solutions described above. The point is that in the strong correlation limit the three-electron system can be decoupled into three independent pairs, the Schrödinger equation for which agrees (apart from a renormalisation of the interaction parameters) with the Schrödinger equation for the relative coordinates in the two-electron system [6, 7].

The Hamiltonian of the three-electron system reads

$$H = \sum_{i=1}^{3} \left[ \frac{1}{2} \left( \frac{1}{i} \nabla_i + \frac{1}{c} A(r_i) \right)^2 + \frac{1}{2} \omega_0^2 r_i^2 \right] + \sum_{i<k} \frac{1}{|r_i - r_k|}$$

(35)

where the Zeeman term is disregarded because it has no influence on the spatial distribution of the electrons, but shifts only the energies. We consider the unitary coordinate
transformation from the original position vectors \( r_i \) to new ones \( x_i \):

\[
\begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3
\end{bmatrix} = \begin{bmatrix}
  1/3 & a & b \\
  b & 1/3 & a \\
  a & b & 1/3
\end{bmatrix} \begin{bmatrix}
  r_1 \\
  r_2 \\
  r_3
\end{bmatrix}
\]

where \( a = 1/3 - 1/\sqrt{3} \) and \( b = 1/3 + 1/\sqrt{3} \). The corresponding inverse transformation provides for the difference coordinates in the e-e-interaction terms

\[
r_i - r_j = \sqrt{3} \left( X - x_k \right)
\]

where \((i, j, k) = (1, 2, 3)\) and cyclic permutations, and \( X \equiv \frac{1}{3} \sum_{i=1}^{3} x_i \) is the center of mass (c.m.) in the new coordinates. It is a special feature of this transformation that the latter agrees with the c.m. \( R \) in the original coordinates. This transformation provides the equivalent Hamiltonian

\[
H = \sum_{i=1}^{3} \left[ \frac{1}{2} \left( \frac{1}{i} \nabla_i + \frac{1}{c} A(x_i) \right)^2 + \frac{1}{2} \omega_o^2 x_i^2 + \frac{1}{\sqrt{3}} \frac{1}{|x_i - X|} \right]
\]

Next we have to observe that in the strong correlation limit the uncertainty of the c.m. \( X \) is small compared with the expectation value of the new coordinates \( x_i \) (see the appendix of Ref. [7]). Therefore \( X \) can be considered as a small perturbation and in zero order in \( X \) the Hamiltonian (38) decouples into a sum of independent quasi-particle Hamiltonians

\[
H^{(0)} = \sum_{i=1}^{3} h_i
\]

The Schrödinger equation for the quasi-particles

\[
h \varphi_q(x) = \varepsilon_q \varphi_q(x)
\]

is similar to the Schrödinger equation for the Hamiltonian in the relative coordinates (5) and therefore it can be solved exactly. In terms of these solutions, the total energy is a sum
of quasi-particle energies and the total orbital eigenfunction is a product of quasi-particle functions.

\[ E_{q_1,q_2,q_3} = \varepsilon_{q_1} + \varepsilon_{q_2} + \varepsilon_{q_3} \] (41)

\[ \Phi_{q_1,q_2,q_3}(x_1,x_2,x_3) = \varphi_{q_1}(x_1) \cdot \varphi_{q_2}(x_2) \cdot \varphi_{q_3}(x_3) \] (42)

where \( q_i \) comprises all quantum numbers. We can consider the quasi-particles as electron pairs, whereby their WFs \( \varphi_q(x_k) \) describe the distance \( x_k \) between two electrons (see Eq. [37]). The crucial point in explaining the distortion of the WM is the generalised Pauli exclusion principle for the quasi-particles states, i.e., the rules which determine the allowed combination of quantum numbers in Eqs. (41) and (42) in order to guarantee the antisymmetry of the WF under electron transposition. These rules depend on the total spin \( S \) and orbital angular momentum \( M_L \) and they rule for some configurations the agreement of all three quantum numbers \( q_i \) out (see [6]). This means that the electron distances in all three electron pairs cannot agree giving rise to a distortion of the WM.

The final result is the following [7]:

In the ground state the electrons in an WM form an equilateral triangle (as might be expected from naive reasoning) only, if the state is a quartet \( (S = 3/2) \) and the orbital angular momentum is a magic quantum number \( (M_L = 3m; m = \text{integer}) \). Otherwise the triangle in the ground state is isosceles. For \( M_L = (3m + 1) \) one of the sides is longer and for \( M_L = (3m - 1) \) one of the sides is shorter than the other two.

6 Coulomb correlations between Quantum dots

Other systems where the above described two-electron solutions play a crucial role are two-electron quantum dot molecules and quantum dot lattices, where the Coulomb correlation between electrons in different dots is taken into account in the Van der Waals approximation [22]. This means that the diameter of the dots must be small compared with the distance between the dots and that the overlap between WFs of different dots should be negligible. Then the Coulomb interaction between the electrons at \( r_{nk} = R_n^0 + u_{nk} \) and \( r_{n'k'} = R_{n'}^0 + u_{n'k'} \) in different dots centered at \( R_n^0 \) and \( R_{n'}^0 \) with \( (n \neq n') \) can be expanded in second order (dipole approximation) as

\[
\frac{1}{|r_{nk} - r_{n'k'}|} = \frac{1}{|R_n^0 - R_{n'}^0 + (u_{nk} - u_{n'k'})|} = \\
\frac{1}{|R_n^0 - R_{n'}^0|} + \frac{1}{2} (u_{nk} - u_{n'k'}) \cdot T(R_n^0 - R_{n'}^0) \cdot (u_{nk} - u_{n'k'}) + \ldots
\]

where the dipole tensor \( T(R) = (1/R^3)[3 R \cdot R - R^2 I] \) has been introduced.

In the following the arrangement and number of dots is arbitrary, but for simpler notations we consider only dots with two electrons each. The bare confinement potential
can vary from dot to dot. If we introduce for each dot a c.m. coordinate $R_n = R^0_n + U_n$ with $U_n = (1/2)(u_{n1} + u_{n2})$ and a relative coordinate $r_n = r_{n2} - r_{n1} = u_{n2} - u_{n1}$, then the total Hamiltonian decouples

$$H = H_{cm}(\{R_n\}) + \sum_n H_{rel,n}(r_n) \quad (43)$$

into a collective Hamiltonian

$$H_{cm} = \frac{1}{2} \left\{ \sum_n \frac{1}{2} \left[ p_n + \frac{2}{c} A(U_n) \right]^2 + 2 \sum_{n,n'} U_n \cdot C_{n,n'} \cdot U_{n'} \right\} \quad (44)$$

and a sum of individual intradot Hamiltonians

$$H_{rel,n} = 2 \left\{ \frac{1}{2} \left[ p + \frac{1}{2c} A(r) \right]^2 + \frac{1}{2} r \cdot D_n \cdot r + \frac{1}{2} r \right\} \quad (45)$$

The force constant tensor $C_{n,n'}$ of the collective Hamiltonian and the effective confinement tensor

The spectrum of the intradot excitations from (45) can be obtained with the methods for single quantum dots and its general features have been described in the previous sections. The Hamiltonian (44) describes magneto-phonon excitations. If the strength of...
the interdot interaction reaches a critical value, a magneto-phonon mode can become soft
indicating a lattice instability. Such a case is shown in Fig.9 for a rectangular periodic
lattice. Solutions for a selection of dot dimers and periodic lattices are given and discussed
in some detail in Ref. [22].

Acknowledgement This work was supported by the German Research Foundation (DFG) in the Priority Program SPP 1145.

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