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Generalized description of few-electron quantum dots at zero and nonzero magnetic fields

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Abstract

We introduce a generalized ground state variational wavefunction for parabolically confined two-dimensional quantum dots that equally applies to both cases of weak (or zero) and strong magnetic field. The wavefunction has a Laughlin-like form in the limit of infinite magnetic field, but transforms into a Jastrow–Slater wavefunction at zero magnetic field. At intermediate magnetic fields (where a fraction of electrons is spin-reversed) it resembles Halperin's spin-reversed wavefunction for the fractional quantum Hall effect. The properties of this variational wavefunction are illustrated for the case of two-dimensional quantum dot helium (a system of two interacting electrons in a parabolic confinement potential) where we find the description to be an excellent representation of the true ground state for the whole range of magnetic fields.

Quantum dots are fabricated semiconductor nanostructures in which charge carriers, such as electrons, are confined in a small region of space [1–8], usually in two dimensions (2D). In particular, the case of few-electron quantum dots subject to a perpendicular magnetic field is of great interest, because, under all experimental conditions, single-electron confinement energy, cyclotron energy and the strength of electronic correlations are of the same order of magnitude, producing very rich physics. The application of a perpendicular magnetic field to a quantum dot plays a fundamental role in changing the nature of single-electron levels from those for the 2D harmonic oscillator to Landau levels in which electronic correlations are strongly enhanced, resulting in behaviour as seen in the fractional quantum Hall effect (FQHE) regime [9–12].

The Hamiltonian for a 2D quantum dot system consisting of N electrons confined by a parabolic potential and subject to a magnetic field, B_z, perpendicular to the dot plane is written as:

$$\hat{H} = \sum_{i=1}^{N} \left\{ \frac{1}{2m} [\hat{\vec{p}}_i + e\vec{A}(\vec{\rho}_i)]^2 + \frac{m}{2}\omega_0^2 \rho_i^2 \right\} + \frac{1}{4\pi\epsilon_0\epsilon_r} \sum_{i>j}^{N} \frac{e^2}{|\vec{\rho}_i - \vec{\rho}_j|} + g\,\mu_B\,B_z\,S_z, \tag{1}$$

where the first term is a one-electron term, the second is the Coulomb potential energy and the last term is the Zeeman energy. In a symmetric gauge, $\vec{A}(\vec{\rho}) = B_z/2(-y, x, 0)$ is the

vector potential, $\vec{\rho} = (x, y)$ is the 2D position vector, $-e(e > 0)$ is electron's charge, m is the electron's mass, g is the electron's g-factor, μ_B is the Bohr magneton, ϵ_r is the dielectric constant, $\hbar\omega_0$ is the parabolic confinement energy and S_z is the z-component of the total spin.

Depending on the strength of the magnetic field, we can identify two main regimes of distinct behaviour for a 2D quantum dot. The regime of strong magnetic field, where all electrons are fully spin polarized, corresponds to the crossover regime between microscopic quantum dots and macroscopic 2D electronic systems of FQHE liquid type (at relatively high density) and Wigner solid type (at low density). The regime of weak or zero magnetic field [13–17] is also very interesting. In the low-density (strong interaction) limit, classical arguments suggest the stabilization of a Wigner solid. In the high-density limit, a Fermi liquid description is expected to be more apropriate. The cross-over regime between the two limits is closely related to the metal–insulator transition problem in 2D [18].

Despite many studies [19–36], a common description of quantum dots for the whole range of magnetic fields is still far from being complete. Proposed models treat the weak (or zero) magnetic field regime [37, 38] separately from the strong magnetic field regime [29] and generally have a limited domain of applicability. Routinely, a wavefunction that describes the strong magnetic field regime well [29] does not apply to the weak (or zero) magnetic field limit, and vice versa [31].

The purpose of this work is to present a unifying framework for the study of 2D quantum dots at any magnetic field by introducing a general ground state wavefunction that applies to both regimes of weak (or zero) and strong magnetic fields. We place only two constraints on the form of the wavefunction: (i) that it is Laughlin-like in the strong magnetic field limit; (ii) that it is of Jastrow–Slater form in the zero magnetic field limit (where, depending on localization/correlation strengths, Fermi liquid or Wigner solid states may emerge).

To illustrate the main properties of this wavefunction, we first concentrate our study on a simple two-electron ($N = 2$) quantum dot system, known as the *2D quantum dot helium*. Even for this case, a unique field-dependent ground state wavefunction for arbitrary magnetic fields ranging from zero to infinity is not yet available. Despite its simplicity, this system shows many characteristic features which persist to larger systems [24, 26, 39–42], therefore it provides a challenging test to gauge the accuracy of any treatment. In the next phase we focus our attention on 2D quantum dots with any number of electrons. We introduce a very general variational wavefunction that applies to both cases of strong and weak (or zero) magnetic field, and clarify how the properties of the generalized approach are reflected in the succesful treatment of *2D quantum dot helium*.

We start the study of *2D quantum dot helium* in a perpendicular magnetic field by considering the following trial wavefunction:

$$\Psi = J(\rho_{12}) \times (z_1 - z_2)^{|m_z|} \exp\left(-\frac{\rho_1^2 + \rho_2^2}{4\, l_\Omega^2}\right) \chi(s_1, s_2), \tag{2}$$

where $\chi(s_1, s_2)$ is the spin function and the Jastrow factor, $J(\rho_{12})$, is given by:

$$J(\rho_{12}) = \exp\left(-\frac{b^2}{2}\, \rho_{12}^2 + c\, b\, \rho_{12}\right), \tag{3}$$

where $z_j = x_j - \mathrm{i} y_j$ ($j = 1, 2$) is the electron's 2D position in complex notation, $\rho_{12} = |\vec{\rho}_1 - \vec{\rho}_2|$ is the inter-electron distance, b and c are non-negative variational parameters to be optimized and $m_z = |m_z| = 0, 1, \ldots$ is the angular momentum quantum number. For a perpendicular magnetic field in the z-direction, we have $l_\Omega = \sqrt{\hbar/(2m\Omega)}$ and $\Omega^2 = \omega_0^2 + (\omega_c/2)^2$. The parity of the space wavefunction depends on the value of $|m_z|$. For even values, $|m_z| = 0, 2, 4, \ldots$, the space wavefunction is symmetric, so the spin function, $\chi(s_1, s_2)$, corresponds to a spin-

singlet state ($S = 0$), while for odd values, $|m_z| = 1, 3, 5, \ldots$, the space wavefunction is antisymmetric, therefore $\chi(s_1, s_2)$ corresponds to a spin-triplet ($S = 1$).

The correlation factor, $J(\rho_{12})$, is a displaced Gaussian (that is centred at nonzero ρ_{12} values) and constitutes a novel choice of electronic correlations in a quantum dot. As we will shortly see, it does an outstanding job in optimizing the separation between a pair of electrons, both at zero and nonzero magnetic field. It also differs from earlier choices in the literature, such as: $J(\rho_{12}) \propto \exp\left(\frac{a\rho_{12}}{1+b\rho_{12}}\right)$, where a and b are two variational parameters [39]; a generalized version of the above form [37, 38]; or a simpler version $J(\rho_{12}) = 1$ used by Bolton [29].

We have previously shown [43] that, at zero magnetic field, the wavefunction equation (2) (for $|m_z| = 0$) is of exceptional quality. Now we study its properties for a nonzero arbitrary perpendicular magnetic field, noting that the Zeeman energy is not included in our calculations (it can always be included afterwards, if a need arises, since the Hamiltonian is spin-free without the Zeeman term).

To simplify calculations, the energy is measured in units of the oscillator energy, $\hbar\omega_0$, and two dimensionless parameters are introduced, $\lambda = (1/4\pi\epsilon_0\epsilon_r)(e^2\alpha/\hbar\omega_0)$ and $\gamma = \omega_c/\omega_0$. The first parameter, λ, measures the strength of the Coulomb interaction (repulsion) with respect to the confinement energy, where $\alpha = \sqrt{m\omega_0/\hbar}$ is the inverse oscillator length. The second parameter, γ, gauges the strength of the magnetic field relative to the confinement energy and is proportional to the magnetic field, with $\omega_c = eB_z/m$ being the cyclotron frequency. Note that $\lambda = l/a_B$, where $l = 1/\alpha$ is the oscillator's length and $a_B = (4\pi\epsilon_0\epsilon_r\hbar^2)/(me^2)$ is interpreted as an effective Bohr radius of the quantum dot. At zero magnetic field, the ground state always has angular momentum $|m_z| = 0$, a result that suggests that only $J(\rho_{12})$ has any effect on optimizing electronic correlations. A nonzero magnetic field changes the whole scenario by bringing the electrons closer to each other. In response to that, at particular values of the magnetic field, the electrons find it energetically more favourable to jump to higher angular momentum ($|m_z| \neq 0$) orbits. When this occurs, the Laughlin factor, $(z_1 - z_2)^{|m_z|}$, which contributes only for $|m_z| \neq 0$ values, adds up to the effect of $J(\rho_{12})$ on optimizing the separation between electrons.

A calculation of the trial energy $E = \langle\Psi|\hat{H}|\Psi\rangle/\langle\Psi|\Psi\rangle$ is straightforward and standard optimization procedures are implemented. A plot of the variational energy, $\epsilon = E/(\hbar\omega_0)$, as a function of $\gamma = \omega_c/\omega_0$ for values of $\lambda = 0, 1, 2, \ldots 10$ is given in figure 1. In figure 2 we show the excellent agreement between variational and numerical diagonalization energies, which holds for the whole range of λ-s and γ-s considered in this work. The exact numerical diagonalization method gives the exact eigenvalues and eigenstates (in the numerical sense) of Schrödinger's equation for the Hamiltonian under consideration (which can be simplified by separating centre-of-mass motion from relative motion). One starts the procedure by expanding the (unknown) wavefunction in a given basis set consisting of a finite number of states. The minimization of the energy functional, $\langle\hat{H}\rangle$, with respect to the expansion coefficients, reduces to a Hamiltonian matrix eigenvalue–eigenvector problem. The matrix to be diagonalized has $N_{max} \times N_{max}$ elements, where N_{max} is the dimensionality of the truncated (finite) basis set. Diagonalization of the Hamiltonian matrix produces a set of energy eigenvalues and expansion coefficients (from where the eigenfunctions can be obtained). The energy eigenvalues obtained for a series of finite values of N_{max} are extrapolated to the $N_{max} \to \infty$ limit (when large basis sets are considered, a linear fit (in $1/N_{max}$) function best fits the data). The values extrapolated in the $N_{max} \to \infty$ limit represent the exact numerical solution of the energy eigenvalue problem (ground and excited state energies).

In the strong magnetic field regime, variational energies are practically identical to exact numerical diagonalization results (within the range of a very small statistical error, associated with the use of a finite matrix in the diagonalization scheme). The relative deviation of the

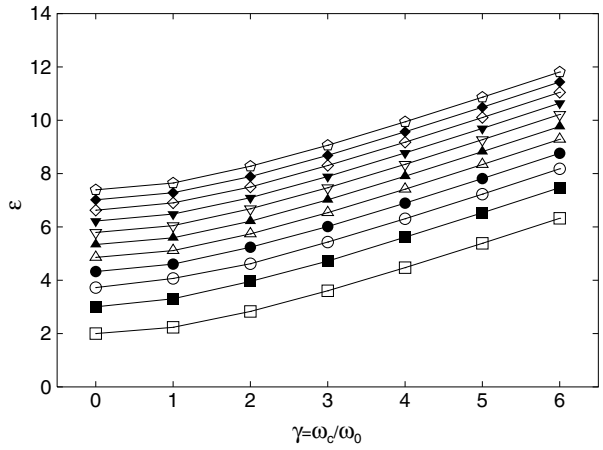

Figure 1. Plot of variational energy, $\epsilon = E/(\hbar\omega_0)$, for *2D quantum dot helium* as a function of $\gamma = \omega_c/\omega_0$ for values of $\lambda = 0, 1, 2, \ldots 10$. The lowest curve corresponds to $\lambda = 0$ and, in increasing order, the top curve corresponds to $\lambda = 10$.

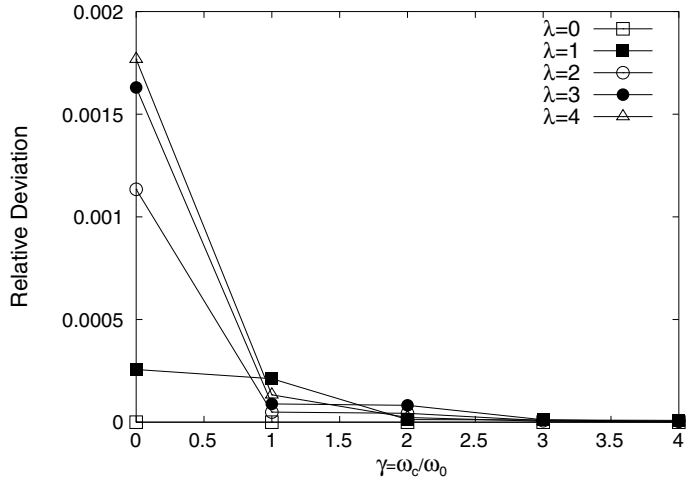

Figure 2. Plot of the relative deviation of the variational ground state energy from the exact numerical diagonalization value, $|\epsilon(\text{Var}) - \epsilon(\text{Exact Diag})|/\epsilon(\text{Exact Diag})$, for *2D quantum dot helium* as a function of $\gamma = \omega_c/\omega_0$ for values of $\lambda = 0, 1, 2, 3, 4$. The exact numerical diagonalization energy eigenvalues are obtained by expanding the (unknown) wavefunction in a finite basis set of $N_{\max}$ functions and then calculating the eigenvalues and eigenstates of the resulting Hamiltonian matrix. The reported results are obtained by extrapolating the energy eigenvalues as a function of $1/N_{\max}$ in the $N_{\max} \to \infty$ limit (see text for more details).

variational ground state energy from the exact numerical diagonalization value, $|\epsilon(\text{Var}) - \epsilon(\text{Exact Diag})|/\epsilon(\text{Exact Diag})$, is always smaller than 0.002 for all values, $0 \leqslant \lambda \leqslant 10$, considered in this work. Only for $\lambda = 4$ and at zero magnetic field ($\gamma = 0$), the relative deviation approaches 0.002, while for all other λ s $(5, \ldots, 10)$ we checked that such a deviation is always smaller than that of $\lambda = 4$ in zero magnetic field. The very good agreement between variational and exact numerical diagonalization energies only improves as the magnetic field increases. It is clear that the Jastrow factor, $J(\rho_{12})$, plays a major contribution in improving the

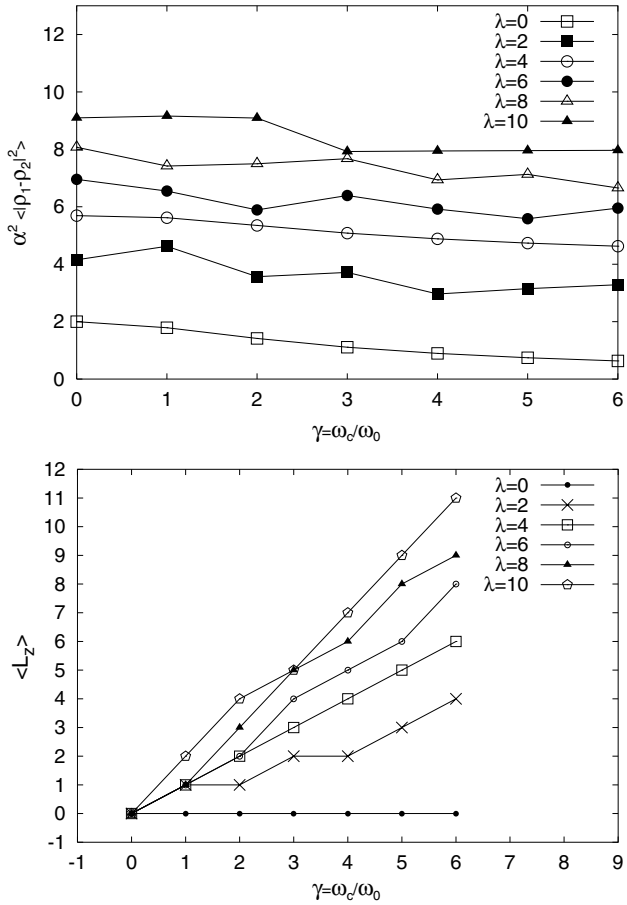

Figure 3. Plot of $\alpha^2 \langle|\vec{\rho}_1 - \vec{\rho}_2|^2\rangle$ for *2D quantum dot helium* calculated from the optimal variational wavefunction as a function of $\gamma = \omega_c/\omega_0$ for values of $\lambda = 0, 2, 4, 6, 8$ and 10. The parameter $\alpha = \sqrt{m\omega_0/\hbar}$ has the dimensionality of an inverse length (top). Plot of ground state angular momentum, $\langle L_z\rangle$ (in units of $\hbar$), as a function of $\gamma = \omega_c/\omega_0 = 0, 1, 2, 3, 4, 5$ and 6 for values of $\lambda = 0, 2, 4, 6, 8$ and 10 (bottom). In both cases, the solid lines joining the data points serve as a guide to the eye.

wavefunction at weak (or zero) magnetic fields, although we noted that, for large magnetic fields, the variational parameter, b, tends to decrease, suggesting that $J(\rho_{12}) \simeq 1$ in the $B_z \rightarrow \infty$ limit. In figure 3 we plot the mean square distance between two electrons, $\alpha^2 \langle|\vec{\rho}_1 - \vec{\rho}_2|^2\rangle$ as a function of ω_c/ω_0 for values of $\lambda = 0, 2, 4, 6, 8$ and 10 (top) and the corresponding values of the angular momentum quantum number (bottom).

The following variational ground state wavefunction serves as a generalization of the approach and is proposed to describe 2D quantum dots with any number of electrons, both at zero and nonzero magnetic fields:

$$\Psi_\gamma = \prod_{i<j}^{N} J(\rho_{ij}) \prod_{i<j}^{N} (z_i - z_j)^n D_\uparrow(\varphi_{\rm FD}) D_\downarrow(\varphi_{\rm FD})\, \chi(S), \tag{4}$$

where, in a short-hand notation, $S = \{s_1, s_2, \ldots, s_N\}$ represents all spin coordinates and the space wavefunction corresponds to a spin function, $\chi(S) = \chi(s_1, s_2, \ldots s_N)$, in which the first

$N_\uparrow$ electrons are spin-up and the remaining electrons, $N_\downarrow = N - N_\uparrow$, are spin-down. The Slater determinants for spin-up, $D_\uparrow(\varphi_{\rm FD})$, and spin-down, $D_\downarrow(\varphi_{\rm FD})$, electrons are built out of Fock–Darwin (FD) states [44, 45] of the form: $\varphi_{\rm FD} \propto (z/l_\Omega)^{|m_z|} \exp(-|z|^2/(4l_\Omega^2))\, L_{n_\rho}^{|m_z|}(|z|^2/(2l_\Omega^2))$, where the $L_{n_\rho}^{|m_z|}$ s are associated Laguerre polynomials, $n_\rho = 0, 1, \ldots$, and $m_z = 0, \pm 1, \ldots$.

The parity of the space wavefunction crucially depends on the value of the integer number, $n = 0, 1, 2, \ldots$, which is even/odd for respectively antisymmetric/symmetric spin functions, $\chi(S)$, in agreement with Pauli's principle.

In the strong magnetic field limit ($B_z \to \infty$), which corresponds to $\gamma \to \infty$, the wavefunction, Ψ_γ reduces to a Laughlin-like wavefunction:

$$\Psi_{\gamma=\infty} = \prod_{i<j}^{N} J(\rho_{ij}) \prod_{i<j}^{N} (z_i - z_j)^{n+1} \exp\left(-\sum_{i=1}^{N} \frac{|z_i|^2}{4l_\Omega^2}\right) \chi(S), \tag{5}$$

where the spin function, $\chi(S)$, corresponds to a fully spin-polarized state. The overall antisymmetry of the wavefunction requires n to be even, with $J(\rho_{ij}) \simeq 1$ eventually becoming a minor correction in this limit. This result is explained by noting that, for a fully spin-polarized system ($N_\uparrow = N$), only $D_\uparrow(\varphi_{\rm FD})$ exists (the other Slater determinant, $D_\downarrow(\varphi_{\rm FD})$, can be formally set to 1) and in this limit FD states transform into Landau states where $D_\uparrow(\varphi_{\rm FD}) = \prod_{i<j}^{N}(z_i - z_j) \exp\left(-\sum_{i=1}^{N} \frac{|z_i|^2}{4l_\Omega^2}\right)$.

In the weak (or zero) magnetic field limit ($B_z \to 0$), which corresponds to $\gamma \to 0$, the variational wavefunction reduces to a standard Jastrow–Slater wavefunction of the form:

$$\Psi_{\gamma=0} = \prod_{i<j}^{N} J(\rho_{ij})\, D_\uparrow(\varphi_{\rm HO})\, D_\downarrow(\varphi_{\rm HO})\, \chi(S), \tag{6}$$

where the spin function, $\chi(S)$, is expected to be antisymmetric (like a spin-unpolarized state) and the FD states have become 2D harmonic oscillator (HO) states of the form:

$$\varphi_{\rm HO} \propto (\alpha\rho)^{|m_z|} \exp(-\alpha^2\rho^2/2)\, L_{n_\rho}^{|m_z|}(\alpha^2\rho^2) \exp(\mathrm{i}m_z\varphi).$$

Pauli's principle imposes the choice $n = 0$ for the polynomial $\prod_{i<j}^{N}(z_i - z_j)^n$, although in a more general setting one can consider any even value, $n = 2, 4, \ldots$, and treat n as a variational parameter.

The general wavefunction in equation (4) should apply to any quantum dot with N electrons in zero or nonzero magnetic fields, and clearly we can see that, for $N = 2$, it reduces to the wavefunction in equation (2), where $n = |m_z|$.

For weak (or zero) confinement and for intermediate values of the magnetic field (when a fraction of electrons is spin-reversed) the wavefunction becomes:

$$\Psi_\gamma \approx \prod_{i<j}^{N} J(\rho_{ij}) \prod_{i<j}^{N_\uparrow} (z_i - z_j)^{n+1} \prod_{i<j}^{N_\downarrow} (z_i - z_j)^{n+1} \prod_{i=1}^{N_\uparrow}\prod_{j=1}^{N_\downarrow} (z_i - z_j)^n \times \exp\left(-\sum_{i=1}^{N_\uparrow} \frac{\rho_i^2}{4\,l_\Omega^2}\right) \exp\left(-\sum_{i=1}^{N_\downarrow} \frac{\rho_i^2}{4\,l_\Omega^2}\right) \chi(S),$$

which is a form reminiscent of Halperin's spin-reversed wavefunction [46] for FQHE, with the $J(\rho_{ij})$ s acting as additional correction factors.

To conclude, we propose a unifying framework to describe 2D quantum dots at zero and nonzero perpendicular magnetic fields, by introducing a general ground state wavefunction that applies to both regimes of weak (or zero) and strong magnetic field. We demonstrate the quality of this wavefunction for the special case of *2D quantum dot helium* and discuss general outcomes for zero, intermediate and strong magnetic fields. Efforts are underway to extend this treatment to larger 2D quantum dots.

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