Quantum dots in high magnetic fields: Calculation of ground-state properties

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We present a variational method for calculating ground-state properties of quantum dots in high magnetic fields. Assuming a perfect spin alignment, we construct a many-body trial wave function in the form of a single Slater determinant of overlapping oscillator functions from the lowest Landau level centered around some points $\mathbf{R}_i$ inside the dot. The points $\mathbf{R}_i$ either coincide with the classical equilibrium positions or are considered as variational parameters to minimize the total energy of the system. Using these trial wave functions, we analytically calculate the ground-state properties. We present ground-state energies for up to $N=40$ electrons, compare them with available exact results for up to $N=10$, and give a transparent interpretation of the results.

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I. INTRODUCTION

Quantum dots are nanoscale structures realized in semiconductor heterosystems in which electrons are confined in all three spatial directions. Because of their discrete energy spectra and shell structure, they are frequently referred to as artificial atoms.[1] However in contrast to natural atoms, their properties (size and shape of the confining potential, number N, and effective mass m^* of the electrons) can be varied. This has made them an attractive system for studying effects of electronic correlations, which has been done with emphases placed on ground-state properties both experimentally[2,3] and theoretically.[4–26] More recently quantum dots have also gained increasing interest in view of future applications.[27–30]

The possibility to measure addition spectra of quantum dots (i.e. the energy necessary to charge an additional electron into the dot) by single electron capacitance[2] or transport spectroscopy[3] stimulated many ground-state calculations based on quite different concepts. The most rigorous one is exact diagonalization (ED),[4–9] which has the additional advantage of providing whole spectra, but is typically restricted to $N<10$ because of demands in computation time. There are different types of quantum Monte Carlo (QMC) calculations,[10–16] which can be considered to be exact, but require less computation time at the price of being restricted to ground-state energies. The largest electron numbers can be dealt with so far within calculations basing on the density-functional theory (DFT).[17–19] The practical limitations of these methods come from the not exactly known exchange-correlation potential, but general experience is that DFT results are quite reliable. They contributed substantially to an understanding of addition spectra. Finally we mention the stochastic variational approach[23] and Hartree-Fock calculations,[8,24,25] where the range of the latter method is comparable to that of DFT, but which does not consider correlation effects.

In this paper we present a concept to calculate ground-state properties of quantum dots in high magnetic fields, with application to systems with up to 40 electrons. The method, originally developed to describe quantum Hall systems,[31] is modified here for the case of quantum dots. This approach is motivated by the evidence that in high magnetic fields B quantum dot electrons tend to form a Wigner cluster.[10,12] The ground-state many-body variational wave function is therefore searched for by using a Slater determinant formed from single-particle wave functions centered at or near equilibrium positions of classical point particles. The classical configurations are calculated either analytically (for $N\leqslant 8$) or using the Monte Carlo minimization. The energy and other physical properties of the trial many-body states are then calculated analytically using our method, which is applicable at an arbitrary (not necessarily small) overlap of the neighboring single-particle wave functions.

In Sec. II we describe the Hamiltonian used to model the quantum dot, and review the calculation of classical equilibrium positions. Section III explains the construction of the trial wave function, and how to calculate expectation values of physical properties. Finally, we present our results in Sec. IV, and compare with other methods.

II. MODEL HAMILTONIAN

We consider quantum dots obtained by applying a lateral confining potential to a two-dimensional electron gas, which forms at the interface of a semiconductor heterostructure. The typical situation of the lateral confining potential being much weaker than the confinement at the interface allows us to define the system by the effective two-dimensional Hamiltonian

$$\hat{H}=\sum_{i=1}^{N}\left[\frac{[\mathbf{p}_i+e\mathbf{A}(\mathbf{r}_i)]^2}{2m^*}+V(\mathbf{r}_i)\right]+E_Z+V_C, \qquad (1)$$

where $\mathbf{p}_i$ and $\mathbf{r}_i$ are vectors in the (x,y) plane. The vector potential in symmetric gauge $\mathbf{A}(\mathbf{r})=(B/2)(-y,x)$ takes into account the magnetic field B perpendicular to the plane of the interface. The lateral confining potential $V(\mathbf{r})$ is assumed to be harmonic:

$$V(\mathbf{r})=\tfrac{1}{2}m^*\omega_0^2 r^2. \qquad (2)$$

This choice is generally accepted in the literature,[32] and is in agreement with experimental results (see, e.g., Ref. 33). The electrons in the quantum dot interact via Coulomb interaction with a screening given by the relative dielectric constant ε_r:

$$V_C=\frac{1}{2}\frac{e^2}{4\pi\varepsilon_0\varepsilon_r}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}. \tag{3}$$

In addition, the Zeeman energy $E_Z=\Sigma_{i=1}^{N}g^*\mu_B B\sigma_i$ is taken into account, where σ_i is the projection of the ith electron spin upon the direction of the magnetic field, g^* is the effective g factor and $\mu_B=e\hbar/2m_e$ is the Bohr magneton.

In the following we use the normalized solutions of the single-particle problem given by[26]

$$\psi_{n,l}(r,\varphi)=\frac{1}{\lambda}\sqrt{\frac{n!}{\pi(n+|l|)!}}\,\mathrm{e}^{\mathrm{i}l\varphi}r^{|l|}\mathrm{e}^{-r^2/2}L_n^{|l|}(r^2), \tag{4}$$

where $r=\sqrt{x^2+y^2}/\lambda$ is a polar coordinate scaled with the hybrid length $\lambda=\sqrt{\hbar/m^*}(\omega_0^2+\omega_c^2/4)^{-1/4}$, $\omega_c=eB/m^*$ is the cyclotron frequency, and $L_n^{|l|}(r^2)$ are associated Laguerre polynomials. This so-called Fock-Darwin (FD) solution depends on two quantum numbers n and l, where $n\in\mathbb{N}_0$ counts the number of nodes and $l\in\mathbb{Z}$ is the quantum number of angular momentum. The single-particle energy eigenvalues (without Zeeman energy) are

$$E_{n,l}^{\mathrm{FD}}=l\hbar\omega_c/2+(2n+|l|+1)\hbar\sqrt{\omega_0^2+(\omega_c/2)^2}. \tag{5}$$

In order to construct the trial many-body wave function (Sec. III), we will need to know the classical equilibrium configurations of N electrons in a dot. A classical system of N point charges in the parabolic potential [Eq. (2)] is described by the Hamiltonian $E_N^{\mathrm{class}}(\mathbf{r}_1,\ldots,\mathbf{r}_N)=\Sigma_i V(\mathbf{r}_i)+V_C$. Its equilibrium configuration $(\mathbf{r}_1^0,\ldots,\mathbf{r}_N^0)$ can be found by minimizing E_N^{class} with respect to the particle positions. For few electrons symmetry considerations, Monte Carlo minimization[10] as well as analytical calculations show that the charges occupy the corners of a regular polygon without electrons (for $N\leqslant 5$) and with one electron (for $5<N\leqslant 8$) in the center. For higher electron numbers ($N>8$) the classical equilibrium configuration is a more complex shell structure, which can be found using Monte Carlo minimization.[10,34]

Due to the rotational symmetry of the confining potential, all classical configurations are energetically degenerate with respect to the arbitrary rotation. As our approach takes account of only one arbitrarily chosen classical configuration, a problem concerning the rotational symmetry of the constructed trial wave function occurs (see Sec. IV B).

III. APPROACH

In strong magnetic fields, electrons tend to be localized around the classical equilibrium positions with their spins aligned along the magnetic field. Following Ref. 31 we write the trial many-body wave function Ψ_L in the form of a Slater determinant

$$\Psi_L=\frac{1}{\sqrt{N!}}\begin{vmatrix}\chi_{11}^{(L)} & \chi_{12}^{(L)} & \cdots & \chi_{1N}^{(L)}\\ \chi_{21}^{(L)} & \chi_{22}^{(L)} & \cdots & \chi_{2N}^{(L)}\\ \vdots & & \ddots & \vdots\\ \chi_{N1}^{(L)} & \chi_{N2}^{(L)} & \cdots & \chi_{NN}^{(L)}\end{vmatrix},\quad L\in\mathbb{N}_0, \tag{6}$$

where

$$\chi_{ij}^{(L)}=\psi_{0,-L}(\mathbf{r}_i-\mathbf{R}_j)\exp\left(-\frac{\mathrm{i}e}{2\hbar}(\mathbf{B}\times\mathbf{R}_j)\cdot\mathbf{r}_i\right) \tag{7}$$

are Fock-Darwin wave functions [see Eq. (4)] with an additional phase factor caused by the magnetic translation operator[35] when shifting the electron i from the origin to $\mathbf{R}_j$. The integer L (negative quantum number of single-particle angular momentum) and the vectors $\mathbf{R}_1,\ldots,\mathbf{R}_N$ are *free* parameters of the theory. They will be varied below in order to obtain the minimal estimate of the ground-state energy.

The main difference between the approach presented here and the Hartree-Fock method is the nonorthogonality of our single-particle wave functions $\chi_{ij}^{(L)}$. It will result in three- and four-particle contributions when calculating expectations values with respect to the constructed trial wave function Ψ_L, and thus include correlation.

The function Ψ_L is an eigenfunction of the operator $\hat{H}-\hat{V}$ with the eigenvalue $NE_{0,-L}^{\mathrm{FD}}$, where

$$\hat{V}=\sum_{i=1}^{N}\frac{m^*\omega_0^2}{2}(2\mathbf{r}_i\cdot\mathbf{R}_i-R_i^2)+V_C. \tag{8}$$

Thus the ground-state energy of Hamiltonian (1) can be approached by minimizing

$$E_{L,\mathbf{R}_i}=\frac{\langle\Psi_L|\hat{H}|\Psi_L\rangle}{\langle\Psi_L|\Psi_L\rangle}=NE_{0,-L}^{\mathrm{FD}}+\frac{\langle\Psi_L|\hat{V}|\Psi_L\rangle}{\langle\Psi_L|\Psi_L\rangle}. \tag{9}$$

For calculating the normalization factor $\langle\Psi_L|\Psi_L\rangle$, it is sufficient to know the single-particle overlap integrals $\langle\chi_{ak}^{(L)}|\chi_{al}^{(L)}\rangle$ for $k,\ l=1,\ldots,N$. In a similar way,[31] expectation values of powers of the single-particle operator $\mathbf{r}_a$ appearing in the harmonic potential can be reduced to calculating $\langle\chi_{ak}^{(L)}|\mathbf{r}_a|\chi_{al}^{(L)}\rangle$.

A more demanding task is the calculation of the Coulomb interaction energy, which requires evaluating the matrix elements

$$V_{ijkl}^{(L)}=\langle\chi_{ai}^{(L)}\chi_{bk}^{(L)}|\frac{1}{|\mathbf{r}_a-\mathbf{r}_b|}|\chi_{aj}^{(L)}\chi_{bl}^{(L)}\rangle. \tag{10}$$

This is carried out separately for the five cases: (i) $V_{iijj}^{(L)}$ (Hartree terms), (ii) $V_{ijji}^{(L)}$ (exchange terms), (iii) $V_{iikl}^{(L)}$ (three-site terms, type I), (iv) $V_{ijki}^{(L)}$ (three-site-terms, type II), and (v) $V_{ijkl}^{(L)}$ (four-site-terms). For each of these an exact analytical expression has been calculated. In a similar way expectation values of other observables can be formulated analytically. As one further example, we refer to the single-particle density

$$\rho(\mathbf{r})=\frac{\langle\Psi_L|\sum_{i=1}^{N}\delta(\mathbf{r}-\mathbf{r}_i)|\Psi_L\rangle}{\langle\Psi_L|\Psi_L\rangle}. \tag{11}$$

The obtained analytical expressions are rather complex, and were calculated in Ref. 36. Their evaluation has to be

done numerically. In Sec. IV, we present results for ground-state expectation values of the energy and density, and compare with exact results.

IV. RESULTS

Our calculated ground state energies (in units of $\hbar\omega_0$) are considered to be functions of two dimensionless parameters, l_0/a_B^* and ω_c/ω_0, where $l_0=(\hbar/m^*\omega_0)^{1/2}$ is the oscillator length, $a_B^*=4\pi\varepsilon_0\varepsilon_r\hbar^2/m^*e^2$ is the effective Bohr radius, and

$$\frac{l_0}{a_B^*}\approx\sqrt{\frac{m^*/m_e}{\hbar\omega_0/(\mathrm{meV})}}\frac{1}{\varepsilon_r}\times 1.650\times 10^2, \tag{12}$$

$$\frac{\omega_c}{\omega_0}\approx\frac{\left(\frac{m^*}{m_e}\right)^{-1}\times 1.158\times 10^{-1}}{\hbar\omega_0/(\mathrm{meV})}\frac{B}{(\mathrm{T})}. \tag{13}$$

For typical GaAs parameters ($m^*/m_e=0.067$, $\varepsilon_r=12.9$) with a confinement strength $\hbar\omega_0=3$ meV, we obtain $l_0/a_B^*\approx 1.91$ and $\omega_c/\omega_0\approx 0.58\ B/(\mathrm{T})$.

A. Quantum dot helium

The two-electron quantum dot, also referred to as quantum dot helium, is the simplest non-trivial problem and the first test for our approach. Merkt *et al.*[4] calculated energies for ground and excited states for this system using the exact diagonalization approach. As in Ref. 4, only results for a small range of total angular momenta ($L^z_{\mathrm{tot}}\leqslant 3$) were published, we repeated this calculation (using a slightly modified program of Ref. 18) with extension to larger values of L^z_{tot}. As a test we reproduced the data of Ref. 4. Calculating the expectation value [Eq. (9)] for $L=0$, with $\mathbf{R}_i$ defined by the classical equilibrium positions, we find, for the special choice of parameters $l_0/a_B^*=2$, $g^*=-0.44$, and $m^*/m_e=0.067$, that the relative deviation of the total energy calculated with our approach from the exact results drops from 2.5% at $\omega_c/\omega_0=3.6$ to 0.8% at $\omega_c/\omega_0=10$. This result, which could be improved by optimizing with respect to the positions $\mathbf{R}_i$, demonstrates the capability of our method for $N=2$.

B. Results for $N\leqslant 10$

Extending our tests to higher electron numbers, we show first, in Fig. 1, the calculated results for the addition energy $\mu_6=E_6-E_5$ of the sixth electron in comparison with exact results[6] obtained with ED. The relative deviation from exact results is less than 1% everywhere in the range of $\omega_c/\omega_0\geqslant 4$, and only 0.2% at $\omega_c/\omega_0=6$. It should be noted that, despite this general agreement, our method cannot describe crossings between eigenstates of angular momentum, and is therefore not capable to reproduce the cusps seen in the exact results.

Results for a ground-state energy of 3–10 electrons are shown in Fig. 2, in comparison with QMC results from Ref. 10, which were obtained using lowest Landau-level trial wave functions. One sees that our results are very close to (and sometimes even lower than) the QMC results at $\omega_c/\omega_0\gtrsim 2$. In this range typical relative deviations of the total energy are 2% and less. Figure 2 shows the general trend of an increasing accuracy of our results with increasing N and/or B. At the highest magnetic fields (where comparison is possible) the relative deviation is about 1% for N

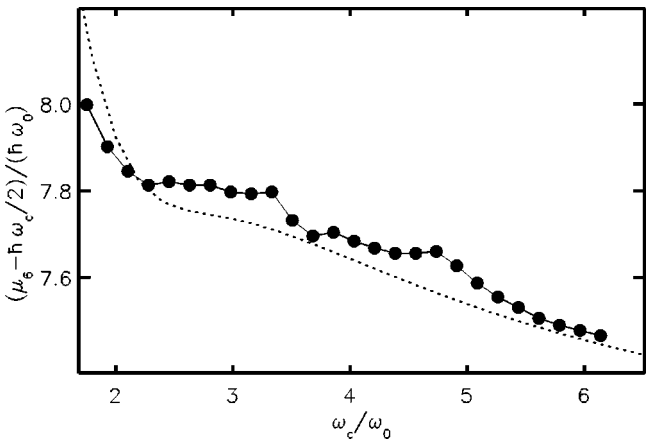

FIG. 1. Addition energy for the sixth electron obtained with our method (dotted) and corresponding exact values (full dots) from exact diagonalization (Ref. 6). Both the five- and six-electron ground states are spin polarized for $\omega_c/\omega_0\gtrsim 4$. The parameters are $l_0/a_B^*=2.32$, and $g^*=-0.44$.

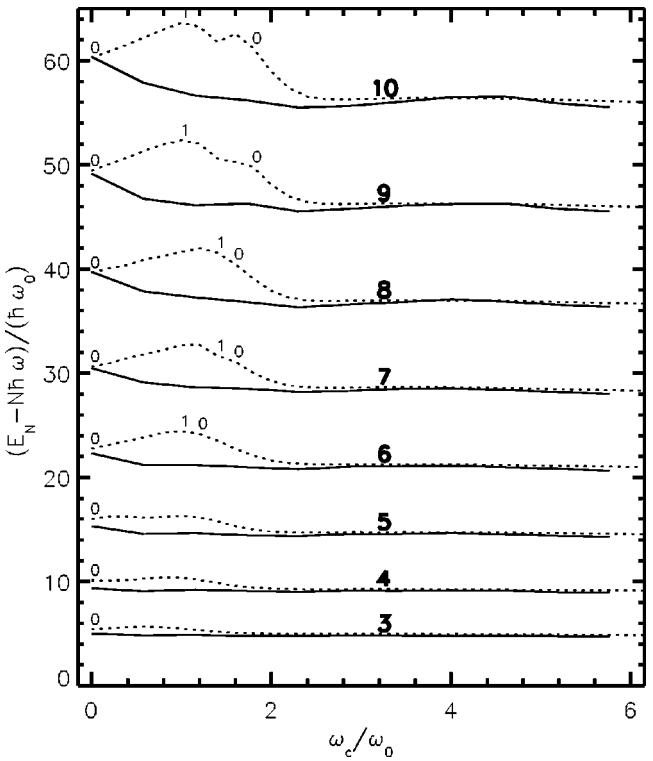

FIG. 2. Ground-state energies [reduced by N times the hybrid energy $\hbar\omega=\hbar(\omega_0^2+\omega_c^2/4)^{1/2}$] for dots with 3–10 electrons obtained with our method (dotted lines) and from the QMC method (Ref. 10) (full lines). The small numbers (0,1) at the dotted lines mark the value of ω_c/ω_0 beyond which the ground-state energy is obtained with Ψ_L ($L=0,1$). The parameters for GaAs are as given at the beginning of Sec. IV.

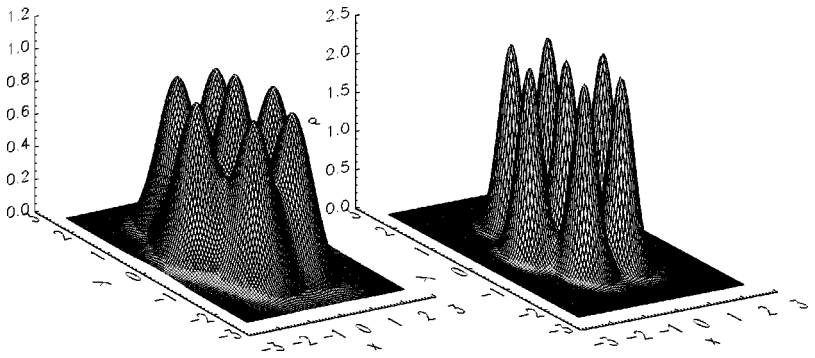

FIG. 3. Electron densities ρ (in units of R_{class}^{-2}) of the seven-electron system calculated for $\omega_c/\omega_0=0$ (left) and 6 (right) using the trial wave function Ψ_0. The length scale of the axes is $R_{\mathrm{class}}=(2l_0^4/a_B^*)^{1/3}$ and l_0/a_B^* as in Fig. 2.

$\leqslant 6$ and even less for higher N. We take this quantitative agreement (obtained without making use of the freedom to vary the positions $\mathbf{R}_i$) as a clear demonstration of the usefulness of our method, and as a promise that it will also yield reliable results for higher N, for which exact data do not (yet) exist.

Figure 3 shows electron densities calculated from the trial wave function Ψ_0 for two different values of the magnetic field. As is clearly seen, the magnetic field shrinks the density peaks around the assumed positions, and reduces the overlap of the single-particle wave functions. This ultimately leads to the expected Wigner cluster as the limiting case for very high magnetic fields. We should mention, however, that the densities shown in Fig. 3 correspond to a charge-density wave lacking the axial symmetry expected for the true ground state.[12]

C. Variation of parameters

Our trial wave function Ψ_L depends on the set of (free) parameters $\{L,\mathbf{R}_1,\ldots,\mathbf{R}_N\}$. The small numbers 0 and 1 over the dotted lines on Fig. 2 indicate that, starting from the corresponding points, the trial wave functions $\Psi_{L=0}$ or $\Psi_{L=1}$ give the lowest energy. For up to five electrons Ψ_0 always gives the lowest energy over the whole range of magnetic field. For higher electron numbers Ψ_1 gives lower energies in a small range of (weak) magnetic fields. We calculated energies for $L=2$ and partially for $L=3$. These energies were never minimal.

Thus the essential behavior of the system is already described quite well, if only Ψ_0 is used; however, the use of a more complicated trial wave function, e.g., of a linear combination of $\psi_{0,0}$ and $\psi_{0,1}$ in $\chi_{ij}^{(L)}$, may improve the estimate of the ground-state energy at low fields. Taking into account Ψ_1 frequently gives a substantially better approximation for low fields.

Up to now the parameters $\mathbf{R}_1,\ldots,\mathbf{R}_N$ were chosen according to a classical equilibrium configuration. For $N\leqslant 8$ we minimized the expression for the ground-state energy by varying the radius R of the outer shell. In the range $0.6\lesssim\omega_c/\omega_0\lesssim 2.4$, a significantly lower energy was achieved by optimizing the radius R. For higher fields the energies calculated using the classical equilibrium radius are already very close to the exact ground state, and the variation of R did not significantly change the results. The optimized shell radius $R^{\min}$ was found to be larger (''stretched'' configurations) than the classical radius R_0: it varied from $R^{\min}/R_0\approx 1.2$ in small fields to $R^{\min}/R_0\approx 1.015$ in higher fields.

D. Results and interpretation for $10\leqslant N\leqslant 40$

Figure 4 gives calculated ground-state energies E_N for up to $N=40$ (a quantum dot zirconium), where suitable exact reference values were not available. With increasing magnetic field we find a clear convergence of $E_N-N\hbar\omega$ toward E_N^{class} (indicated by the dashed lines in Fig. 4), so that we can write

$$E_N=E_N^{\mathrm{class}}+N\hbar\sqrt{\omega_0^2+(\omega_c/2)^2}+N\hbar\,\delta\Omega(B). \qquad (14)$$

The frequency $\delta\Omega(B)$ is positive, almost independent of N, and tends to zero at $B\to\infty$. The relative correction due to the third term in Eq. (14) is smaller than 2% at $\omega_c/\omega_0>6$ and smaller than 0.6% at $\omega_c/\omega_0>18$ for $10\leqslant N\leqslant 40$. Equation

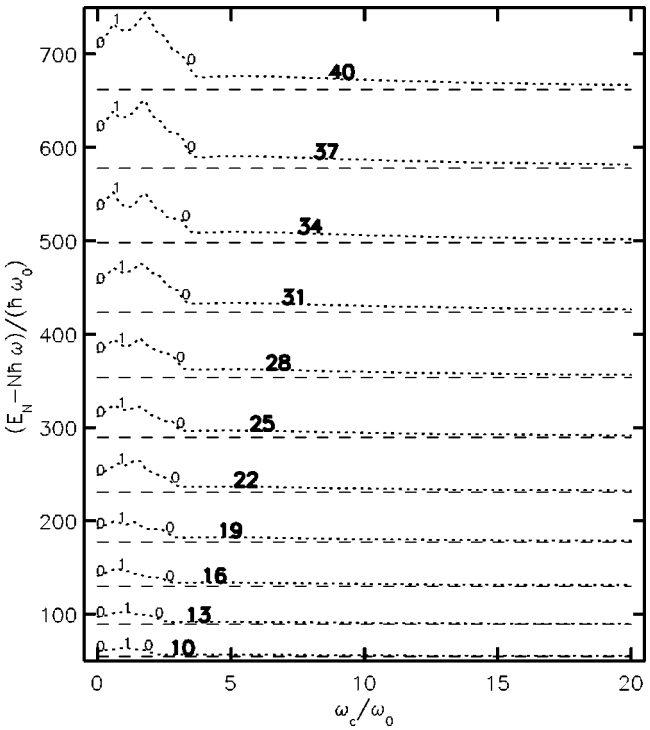

FIG. 4. Calculated ground-state energies for 10–40 electrons (dotted lines). The horizontal dashed lines indicate the value of classical ground-state energy $E_N^{\mathrm{class}}/\hbar\omega_0$. The meaning of the numbers in the plot and the parameter l_0/a_B^* are as in Fig. 2, except that $g^*=0$ here.

(14) refines the rigorous mathematical result of Ref. 22, that $E_N \sim E_N^{\text{class}} + N\hbar\omega_c/2$ at $B \to \infty$, and has a transparent physical meaning: The quantum-mechanical ground-state energy of the dot is a sum of the classical potential energy, the quantum-mechanical kinetic energy, and the small rest energy $\propto \delta\Omega(B)$, which decreases with increasing B.

V. CONCLUSION

We have presented a variational method for calculating ground-state properties of parabolic quantum dots in (high) magnetic fields. A specially designed trial many-body wave function takes into account the classical equilibrium positions of the quantum dot electrons, and has the correct symmetry for a fermion system with fully polarized spins. The expectation values of all observables can then be analytically calculated with this trial wave function.

Our results for the ground-state energy are upper bounds to the exact values, and compare favorably with reference data, but are much less demanding in terms of computation time. As the accuracy even seems to increase with the increasing size of the system, an extension to higher electron numbers becomes possible, which we demonstrate by showing results for up to 40 electrons. The extension of our approach to other observables was demonstrated by giving results for the density, which reflects the localization in strong magnetic fields.

We put forward a simple interpretation of our results, stating that the quantum mechanical ground-state energy is approximately the sum of the classical potential energy and the single-particle kinetic energy. This estimate is made exact by adding a rest energy term, for which we gave an upper estimate in the studied range of N and magnetic field.

Further work in this field might be directed upon inclusion of non spin-polarized states or the treatment of more general (nonparabolic, anisotropic) confining potentials, where the latter problem is quite straightforward. Another aim is to develop a method which could treat functions Ψ_L with angular averaging over positions of vectors $\mathbf{R}_j$ [Eq. (6)], so that the density shows the axial symmetry to be expected for the ground state.

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