Author(s): Harju, A. & Sverdlov, V. A. & Nieminen, Risto M. & Halonen, V.

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Many-body wave function for a quantum dot in a weak magnetic field

A. Harju,* V. A. Sverdlov,† and R. M. Nieminen
Laboratory of Physics, Helsinki University of Technology, FIN-02150 Espoo, Finland

V. Halonen
Theoretical Physics, University of Oulu, FIN-90570 Oulu, Finland

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The ground states of parabolically confined electrons in a quantum dot are studied by both direct numerical diagonalization and quantum Monte Carlo (QMC) methods. We present a simple but accurate variational many-body wave function for the dot in the limit of a weak magnetic field. The wave function has the center-of-mass motion restricted to the lowest-energy state and the electron-electron interaction is taken into account by a Jastrow two-body correlation factor. The optimized wave function has an accuracy very close to the state-of-the-art numerical diagonalization calculations. The results and the computational efficiency indicate that the presented wave function combined with the QMC method suits ideally for studies of large quantum dots. [S0163-1829(99)07907-2]

I. INTRODUCTION

The progress in the fabrication of semiconductor quantum dots (QD) has stimulated an increasing interest in investigating the properties of such systems.[1] From the theoretical point of view, a QD is an ideal many-electron object for studying fundamental physical properties of correlated electron systems. One of the theoretical goals is to understand the nature of the many-body ground states for various magnetic-field strengths. As the experiments are mainly performed in the magnetic-field strengths of few tesla, we concentrate on the limit of weak magnetic field.

In principle, the most accurate theoretical method for studying QD's is the direct numerical diagonalization of the many-body Hamiltonian.[2] The method is, however, restricted to rather small electron numbers. For the zero-magnetic-field case, it is applicable to less than ten electrons. Moreover, being purely numerical, the method does not give much physical insight. From the mean-field approaches, the density-functional theory and its generalization for a nonzero magnetic field, the current-density-functional theory (CDFT),[3] approximatively include the correlation effects and are thus good candidates for studying systems of larger electron numbers. The comparison of CDFT to numerical diagonalization results[4] shows reasonable (a few percent) agreement in energies for a three-electron dot, but its general applicability for strongly correlated cases is questionable.

In this paper, we show that a simple trial wave function combined with a quantum Monte Carlo method (QMC) can solve the ground states of the parabolic QD in the weak magnetic fields nearly exactly. We show that the agreement with the diagonalization method is extremely good and that the scheme presented here can be easily extended to a much larger number of electrons than is possible to handle accurately by diagonalization. In this way, the scheme is nearly as accurate as the diagonalization method, but its computational cost is comparable to the cost of CDFT or other mean-field methods.

II. VARIATIONAL WAVE FUNCTION

In the usual model for a quantum dot, electrons with an effective mass m^* are moving in two dimensions and are confined by a parabolic potential $\frac{1}{2}\omega_0^2 r^2$.[5] The one-body problem is similar to the harmonic oscillator one (with frequency $\omega^2=\omega_0^2+\frac{1}{4}\omega_c^2$, where $\omega_c=eH/m^*c$) and is easily solved for an arbitrary magnetic field H.[6] The single-particle wave functions are in scaled units,[7]

$$\psi_{n,\pm|m|}\propto(x\pm iy)^{|m|}L_{n'}^{|m|}(r^2)\exp\left(-\frac{r^2}{2}\right), \tag{1}$$

where m is the angular momentum quantum number, n is the shell index and $n'=(n-|m|)/2$. The normalization is not needed, because it drops away in the QMC approach. For the interaction between electrons, the normal $1/r_{ij}$ potential is used.

As a consequence of the parabolic potential, the center-of-mass (CM) motion can be separated from the relative motion for any number of particles. If one is interested only in the ground state, one should ensure that the CM motion has been restricted to the lowest-energy state. In practice, this requirement is most easily fulfilled by the following coordinate replacement:[8]

$$x\pm iy\rightarrow\hat{x}\pm i\hat{y}\equiv(x-x_{\rm cm})\pm i(y-y_{\rm cm}), \tag{2}$$

where $x_{\rm cm}$ and $y_{\rm cm}$ are the coordinates of the CM. Note that this replacement is done only in the phase part of the single-particle wave function.

The variational many-body wave function is built from the single-particle basis given above. If one is to solve the many-body problem in a mean-field sense, the one-body wave functions would be used to build Slater determinants for spin-up and for spin-down electrons. Then one would modify the one-body wave functions to account for the effect of other electrons in some ''self-consistent–mean-field'' way. This is not, however, done here. On the contrary, we assume that the effect of the electron-electron interaction on

TABLE I. Numerical diagonalization (Ref. 12) and variational energies for a three-electron QD. The parameter values $m^*/m_0 = 0.067$, $\epsilon = 12.4$ have been used, and the confinement is $\hbar\omega_0 = 3.37$ meV. The magnetic field is zero. The energies are in meV.

State	Exact energy	QMC energy
1	26.82	26.88
2	28.27	28.35
3	30.02	30.03

the many-body wave function can be separated from the Slater determinants discussed above. We will see later that this is really a reasonable approximation. Doing so, the variational many-body wave function reads

$$\Psi = \det_{\uparrow}[\{\psi_{n,m}\}]\det_{\downarrow}[\{\psi_{n,m}\}] \times F(\{\mathrm{r_i}\}), \tag{3}$$

where only the function F is unknown. The function F depends on the coordinates of all electrons. One should also note that each one-body wave function containing x or y depends on *all* other states via the CM coordinates. In this way, the one-body orbitals are already ''correlated.'' But the one-body orbitals do not have any variational parameters, as is the case in the usual QMC treatment of, for example, atoms and molecules. More details on good quantum numbers and the spin contamination of the present form can be found in Ref. 9.

A great simplification is obtained for the variational wave function if we assume that the main effect in F is the two-body correlation, as is the case in the strong-magnetic-field limit.[10] In that limit, up to 98% of the Landau-level mixing is captured by two-body correlation factors, without modifying the multiconfigurational many-body wave function built from the lowest-Landau-level functions. Using this approximation for F, it can be written as

$$F(\{\mathrm{r_i}\}) = \prod_{i<j}^{N} J(r_{ij}), \tag{4}$$

where the product is over all pairs of electrons and J is a two-body correlation factor. For it we use the Jastrow form $J(r_{ij}) = \exp[ar_{ij}/(1+br_{ij})]$, where a and b are variational parameters. We use different a and b for pairs of parallel and opposite spins. Our many-body wave function has thus only four variational parameters. These are easily found by the stochastic gradient approximation[11] (SGA) technique.

The explicit rule for building the variational wave function has thus two important parts. The first one is the restriction of the CM motion to ensure that it is in the lowest-energy state. The second ingredient is the inclusion of the two-body correlation factor that reflects the simple idea that the electrons avoid each other and their relative motion is correlated. Next, we will show that these two simple ideas are enough to explain a great deal of the many-body physics in QD's.

III. RESULTS

A good test for the variational wave function given above is to compare the energies obtained with it with the ones from the direct numerical diagonalization. In Table I, we compare the QMC energies for a three-electron QD with the diagonalization ones.[12] The three states presented are the first three lowest-energy states in the limit of weak magnetic field.[13] We can see that the agreement is very good, the error being approximately 0.3% in the worst case. For comparison, the CDFT error is larger by an order of magnitude.[4]

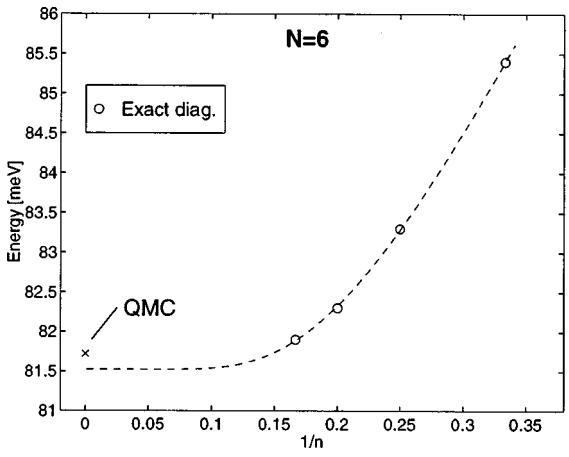

FIG. 1. The two-particle density $\rho^{(2)}(r_1, r_2)$ from diagonalization (full line) and from QMC (dashed line) for the state Ψ_1 of Eq. (5). Lengths in nm. On the left (right) panel, electron with spin down (up) is fixed to 20 nm from the center and the density of opposite spins are plotted.

The determinant parts of the states given in Table I are

$$\Psi_1 = \det_{\downarrow}[\psi_{0,0}]\det_{\uparrow}[\psi_{0,0}, \psi_{1,1}], \tag{5}$$

$$\Psi_2 = \det_{\downarrow}[\psi_{1,1}]\det_{\uparrow}[\psi_{0,0}, \psi_{1,1}], \tag{6}$$

$$\Psi_3 = \det_{\uparrow}[\psi_{0,0}, \psi_{1,1}\psi_{2,2}]. \tag{7}$$

One can analyze the phase structure of these wave functions by explicitly writing down the determinants. The common exponential part of the one-body wave functions does not change the phase structure of the many-body wave function. One should note that the same is true for the form of F used in the present work. Having this in mind, the phase structures of the three lowest states can be written as

$$\Psi_1 \propto (z_2 - z_3), \tag{8}$$

$$\Psi_2 \propto (z_1 - z_{\mathrm{cm}})(z_2 - z_3), \tag{9}$$

$$\Psi_3 \propto (z_1 - z_2)(z_2 - z_3)(z_3 - z_1), \tag{10}$$

where we have used $z = x + iy$. It is very interesting to compare this with the work of Bolton.[14] It turns out that his trial wave function has exactly the same phase structure. Further evidence for the correctness of these phase structures is given by the fixed-phase Monte Carlo energies of Bolton.[14] He has shown that having these phase structures *fixed*, the exact energies are within the error bars of his Monte Carlo simulations. We can thus speculate that the small error in the energies above is due to the form used for the function F, and is mainly a three-body correlation effect. In addition, if other forms of F are used, these should also leave the phase structure of the wave function the same.

In Fig. 1, we compare the two-particle densities

TABLE II. Exact and variational energies for a four-electron QD. The magnetic field is zero. The parameter values are $m^*/m_0 = 0.067$, $\epsilon = 13$, and $\hbar\omega_0 = 1.0$ meV. The energies are in meV. The error estimate for the last digit is in the parentheses.

State	Exact energy	QMC energy
1	17.22(2)	17.27(1)
2	17.36(0)	17.44(1)

$\rho^{(2)}(r_1, r_2)$ from diagonalization and from QMC for the state Ψ_1, with one of the electron coordinates fixed. The agreement is excellent.

The one-electron picture has a second candidate for the determinant part of the Ψ_2, namely,

$$\tilde{\Psi}_2 = \det_\downarrow[\psi_{0,0}]\det_\uparrow[\psi_{0,0}, \psi_{2,2}]. \tag{11}$$

This has the same angular momentum as state Ψ_2. The states corresponding to Ψ_2 and $\tilde{\Psi}_2$ (without restricting the CM motion) are the two important configurations for the second ground state of a three-electron QD (Ref. 1) as the magnetic field increases from zero. The phases of these two states *without* restricting the CM motion are

$$\Psi_2' \propto z_1(z_2 - z_3), \tag{12}$$

$$\tilde{\Psi}_2' \propto (z_2^2 - z_3^2), \tag{13}$$

and the two wave functions are clearly linearly independent. If, however, one restricts the CM motion to the lowest level in these two states, their phases change. The phase obtained for Ψ_2 is given in Eq. (9), and for $\tilde{\Psi}_2$, the use of Eq. (2) leads to an identical phase structure. Thus the total many-body wave functions are the same for these two modified states. This is a satisfactory feature of the presented construction of the many-body wave function. In addition, the problem of identifying the experimentally observed second ground state using a one-particle description can be solved.[1]

One should note that we have not used any analytical tricks for the construction of the variational wave function as was done, for example, in Ref. 14 to obtain the phase structures given above. These kinds of tricks are only applicable for small particle numbers and the generalization to larger particle numbers is difficult to find. In this respect, the variational basis presented here should work equally well for QD's containing any number of particles.

For four electrons, we compare the following two states with the diagonalization method. The determinant parts of the wave functions for the states are given by

$$\Psi_1 = \det_\downarrow[\psi_{0,0}]\det_\uparrow[\psi_{0,0}, \psi_{1,1}, \psi_{1,-1}], \tag{14}$$

$$\Psi_2 = \det_\downarrow[\psi_{0,0}, \psi_{1,1}]\det_\uparrow[\psi_{0,0}, \psi_{1,1}]. \tag{15}$$

These states are the two ground states for small magnetic field values. In Table II, we compare the QMC results with the diagonalization ones. We can see that the agreement is again very good. The errors are around 0.3% and 0.5%. We can also see that the state number one is lower in energy, in good agreement with the experimental finding of Ref. 1 and Hund's rule.

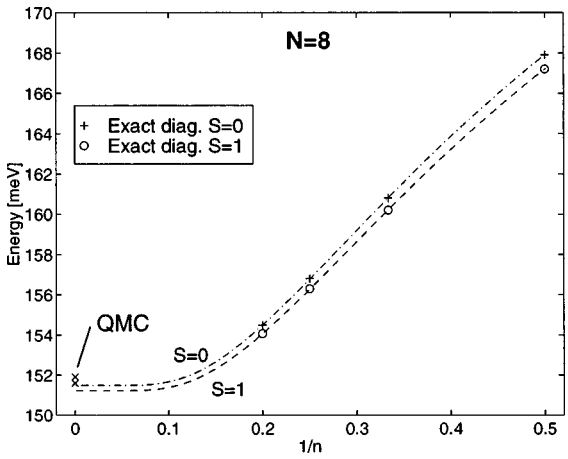

FIG. 2. Total energy as a function of the inverse of the number of shells used in the numerical diagonalization for six electrons. The parameter values are $m^*/m_0 = 0.067$, $\epsilon = 13.0$, $\hbar\omega_0 = 3.0$ meV, and H=0. The QMC energy is marked with $\times$. The fit presented is discussed in the text.

For larger particle numbers, the number of states that can be used in the direct numerical diagonalization restricts more seriously the accuracy obtained. In Fig. 2, we present our numerical diagonalization energies for various numbers of basis states together with our QMC energy for six electrons. The extrapolation to an infinite basis in the diagonalization predicts the energy ~ 81.5 meV. This is, however, only an estimate, obtained by a least-squares fit using a function $E_0 + \alpha \exp[-\beta n]$, where n is the number of the lowest many-body shells included in the basis of the numerical diagonalization and E_0, α, and β are the fitted parameters. The convergence of the diagonalization does not, in general, follow exactly the form used, and it is not even as smooth a function of n as we assume in the present form, but the accuracy of the energy estimate is sufficient for the present comparison. The QMC energy is in good agreement with the extrapolated value, being only approximately 0.2 meV higher. One should note that the QMC energy is clearly more accurate than the diagonalization using six lowest shells. On the other hand, even the use of five lowest shells is enough to obtain semiquantitative agreement with experiments.[15]

The last comparison with the numerical diagonalization is for an eight-electron QD. For it only five lowest many-body shells can be used in the diagonalization. We compare two states with total spins $S=1$ and $S=0$. The results can be seen in Fig. 3. The difference of the QMC energies from the extrapolated ones is again very small, only around 0.3%. The error of the five-shell diagonalization is six times larger.

The recent experiments of Refs. 1 and 16 provide a good test for the theoretical methods. In Fig. 4 we compare the experimental transition points with the QMC ones for $N = 6$ case. One can see that the agreement is very good. The finite thickness of the real QD and the long-range screening of the electron-electron interaction are treated using a scaled Coulomb strength in the calculation, which is only a crude approximation for these effects. The confinement strength and the scaling of the Coulomb interaction cannot be obtained from the experiments and are thus free parameters for theory. The confinement value used $\hbar\omega_0 = 4.5$ meV is in a reasonable range with experimental value $\hbar\omega_0 \approx 5$ meV for

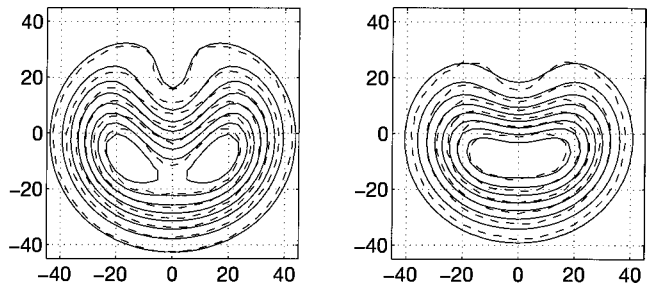

FIG. 3. Total energies as a function of the inverse of the number of shells used in the numerical diagonalization for eight electrons. The higher energies are for $S=0$ and lower for $S=1$, respectively. The parameter values are $m^*/m_0=0.067$, $\epsilon=13.0$, $\hbar\omega_0=3.457$ meV, and H=0. The QMC energies are marked with $\times$. The fits are discussed in the text.

one electron dot, as the confinement is weaker for larger electron numbers. The scaling of the Coulomb interaction value $\alpha=0.7$ is obtained from the experimental transition point for the $N=2$ case,[1] assuming that the confinement strength is nearly the same as for $N=1$.

IV. CONCLUSION

The results reported above clearly show that the presented variational many-body wave function is extremely efficient. The energies obtained are, in every case, in excellent agreement with the diagonalization energies. The error is of the same order for all the cases. Because the number of variational parameters is independent of the electron number, we can conclude that the presented variational wave function combined with the quantum Monte Carlo method is a very promising technique to study larger quantum dots, too.

Perhaps the most important aspect of the variational many-body wave function presented in this paper is that it is easy to construct and it can be easily interpreted. There are two explicit rules in the construction, namely that the CM motion must be in the lowest level and that the electrons avoid each other. The practical implementation is straightforward, as was shown above. These simple rules lead to an accuracy that has previously been obtained only by the direct numerical diagonalization technique. In the diagonalization method, the topology of the total many-body wave function is, however, hidden in the enormous set of the expansion coefficients. The wave function presented here really gives insight into the topology of the many-body wave function for electrons in a parabolic QD. Also the experimentally observed states can be identified using simple free-electron determinants with certain good quantum numbers, if the two important ingredients of the construction presented here are kept in mind.

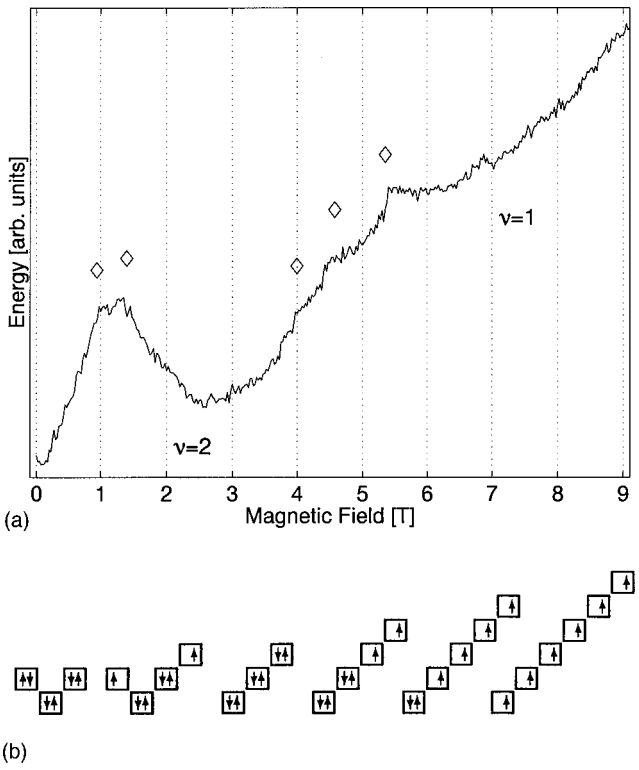

FIG. 4. Upper panel: Experimental energy for $N=6$ QD (Ref. 16). The kinks show the transition points where the lowest energy state changes. The QMC transition points are marked with $\diamond$. QMC parameters used are $m^*/m_0=0.067$, $\epsilon=12.9$, $\hbar\omega_0=4.5$ meV, $g^*=-0.44$. $V_{ee}=\alpha e^2/\epsilon r_{ij}$, with $\alpha=0.7$. Lower panel: Electron occupations of the lowest energy states.

In summary, we have built a simple variational many-body wave function for a parabolic quantum dot. The wave function leads to an accuracy comparable with the direct numerical diagonalization. It has much better computational scaling as a function of the electron number. The wave function proposed has a very intuitive structure, which is useful in understanding the many-body physics of electrons in quantum dots. In addition, the good scaling of the computational cost of the quantum Monte Carlo method combined with the proposed variational wave function indicates that the method outlined here is a perfect tool for studying the electronic properties of quantum dots.

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*Electronic address: Ari.Harju@hut.fi

†Permanent address: Department of Theoretical Physics, University of St. Petersburg, Universitetskaya 7/9, 199034 St. Petersburg, Russia.

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