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LETTER TO THE EDITOR

Correlation energies of quantum dot electrons with harmonic model interactions

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Abstract. The correlation energies of quantum dot electrons with harmonic model interactions in a large magnetic field are studied by comparing the Hartree–Fock (HF) ground state energies with the exact values. The results for GaAs quantum dots show that the correlation corrections to the ground state energies are very small, only 0.1–0.8% for $N = 2$–7 electrons. The changes of the correlation energies with the electron–electron interaction strength Ω^2 are also studied. It is shown that the correlation energies increase rapidly with Ω^2 for larger N, but are limited by the condition $\Omega^2 < \omega_0^2/N$ for a stable dot. The comparison of the HF and the exact energies, varying with the total angular momentum, reveals that the correlation energies take their minima at the so-called 'magic' angular momenta that exist in the cases of Coulomb interactions.

It is well known that correlation interactions are important to determine the energy spectra of quantum dot electrons [1]. So, a reliable theoretical approach to treat this problem should include the correlation effects. The existing approaches mainly include the Hartree or Hartree–Fock (HF) approximation and the direct numerical diagonalization. In the calculations using the Hartree approximation for electron numbers $N < 10$ the exchange and correlation effects were neglected [2–4]. The important role of the exchange and correlation effects has been investigated for the ground state of a two-electron quantum dot by comparison of a Hartree, a Hartree–Fock (HF) and an exact treatment [5]. It was found that the HF approximation, including the exchange interaction but neglecting the electron correlation, could give qualitatively incorrect results about the spin singlet–triplet transition [6–8]. Though the correlation effects can be completely included in the exact numerical diagonalization treatment, which has been performed for systems with electron numbers $N \leqslant 4$ [9, 10], it is computationally extensive and exceedingly difficult for more than six electrons. So it is not a good choice to resort to the exact numerical diagonalization method to treat a greater number of electron quantum dots. Indeed, if the correlation corrections are considered properly the HF approximation can still be a useful method for these systems. The problem is how to get the information about the role of the correlation effects in determining the energy spectra of quantum dots. The most direct way to do this is to compare the results from the HF approximation and the exact treatment, as was done for two electrons by Pfannkuche *et al* [5] and for three electrons by Wang and Mao [11, 12]. Though results obtained in this way could be useful in treating the problems with a greater number of electrons, we still expect to get more direct results for them.

In this letter, however, we shall use another way to investigate the correlation interactions of quantum dot electrons. Instead of treating the quantum dot of N electrons with Coulomb

interactions, we treat a quantum dot of N electrons with harmonic model interactions. Since this model can be solved analytically for any N and the solution has been given by Johnson and Payne [13], it is rather easy to calculate the correlation energies for any N. Despite the simplicity of the model electron–electron interaction, the basic features of the energy spectrum of this model still resemble those with Coulomb interactions [10]. Thus, it is natural to expect that the roles of the correlation interactions in both cases are similar.

The model Hamiltonian for an isolated, quasi-two-dimensional quantum dot in a perpendicular magnetic field is

$$H = \frac{1}{2m^*}\sum_i (\boldsymbol{p}_i + e\boldsymbol{A}_i)^2 + \frac{1}{2}m^*\omega_o^2\sum_i |\boldsymbol{r}_i|^2 + \sum_{i<j} V(\boldsymbol{r}_i, \boldsymbol{r}_j) - g^*\mu_B B\sum_i s_{i,z}. \tag{1}$$

The dot lies in the x-y plane and contains N interacting electrons with effective mass m^*, negative charge $-e$, effective g-factor g^*, spatial coordinates $\boldsymbol{r}_i = (x_i, y_i)$ and spin components $s_{i,z}$ along the z-axis. The quantity $\boldsymbol{A}_i = \frac{B}{2}(-y_i, x_i, 0)$ is the vector potential in the symmetric gauge and μ_B is the Bohr magneton. The model interaction potential is given by [13]

$$V(\boldsymbol{r}_i, \boldsymbol{r}_j) = 2V_0 - \frac{1}{2}m^*\Omega^2\left|\boldsymbol{r}_i - \boldsymbol{r}_j\right| \tag{2}$$

where V_0 and Ω are positive parameters.

Generally, the correlation energy is defined as the difference between the exact and the HF ground state energies, that is

$$E_c = E_g^{exact} - E_g^{HF}. \tag{3}$$

In a large magnetic field (typically, several tesla is large enough [14]), the lower-energy eigenstates of the total Hamiltonian H will be completely spin polarized, yielding a total spin $S_z = N\overline{h}/2$. In this case, the exact ground state energies are then given by [13]

$$E_g^{exact} = \overline{h}\left[\omega_0(B) + \frac{1}{2}(N-1)(N+2)\Omega_0(B) - \frac{1}{4}N\left[N - 1 + \frac{g^*m^*}{m_0}\right]\omega_c\right] + N(N-1)V_0 \tag{4}$$

where $\omega_o(B) = (\omega_0^2 + \omega_c^2/4)^{1/2}$, $\omega_c = eB/m^*$ and $\Omega_0(B) = \left[\omega_0^2(B) - N\Omega^2\right]^{1/2}$.

In the HF calculations, after replacing the Coulomb interactions with the harmonic interactions, the whole process is the same as for the former case [11, 12]. If the occupied single-electron orbitals are $(n_1, m_1), (n_2, m_2), \ldots, (n_N, m_N)$, then the corresponding total energy state is labelled as $\{n_1m_1, n_2m_2, \ldots, n_Nm_N\}$. Since all the low-lying energy states considered here correspond to the lowest Landau level, that is, $n_1 = n_2 = \ldots = 0$, so the energy state can be labelled as $\{m_1, m_2, \ldots, m_N\}$ for short. If the N occupied orbitals are those with the lowest orbital energies, then the total state is the ground state of the system with energy E_g^{HF}.

For a given value of N, the exact ground state energy is easily obtained by equation (4), while the HF value of the ground state energy is obtained by setting the occupied single-electron orbitals to be $(0, 0), (0, 1), \ldots, (0, N-1)$. Choosing $\overline{h}\Omega = 5.6$ meV, $V_0 = 10$ meV and $\overline{h}\omega_0 = 15$ meV for GaAs quantum dots [14], the ground state energies for $N = 2, 3, \ldots, 7$ ($N > 7$ is unstable for the chosen dot parameters) are calculated and the results are shown in figure 1. In this and the following figures, the energies are given in units of $\overline{h}\omega_0$. It is clear that the correlation corrections to the ground state energies are very small for all the cases discussed here. For $N = 2$, the correlation energy $E_c = -0.043\overline{h}\omega_0$ is 0.1% of the total energy. Even for $N = 7$, the correlation energy $E_c = -0.27\overline{h}\omega_0$ is only 0.8% of the total one. It should be mentioned that in the HF calculation only five Gaussian functions are taken into account in the expansions of single-electron wave functions, just as in the case of Coulomb

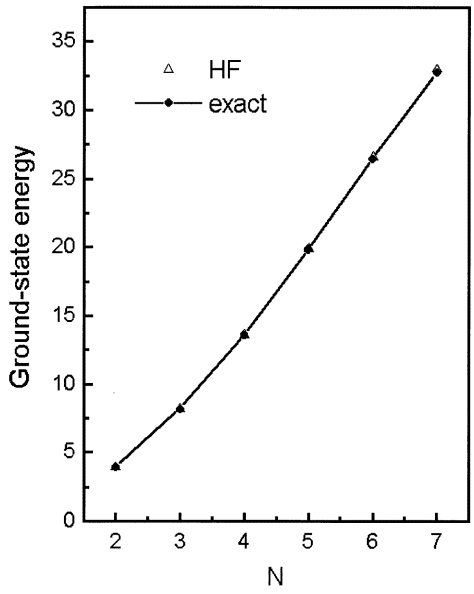

Figure 1. Comparison of the HF and the exact ground state energies for quantum dots with $N = 2$–7 electrons. The energies are in units of $\hbar\omega_0$, the dot parameters are appropriate to GaAs and $\omega_c/\omega_0 = 1$.

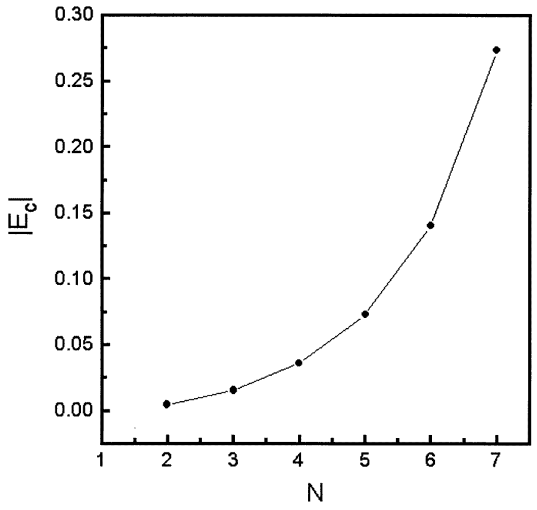

Figure 2. The absolute values of correlation energies for quantum dots with $N = 2$–7 electrons. The energy unit and the dot parameters are the same as in figure 1.

interactions, where this truncation caused an error of about 0.1% [11]. But for the case of harmonic interactions, the numerical results converge much more quickly than for the case of Coulumb interactions, and the estimated error is less than 0.02% . So, even if the numerical error is considered, the present results of the correlation energy E_c are still reliable. To see the change of the correlation energy E_c with the number of electrons N more clearly, the curve of $|E_c|$ versus N is plotted in figure 2.

In order to investigate the relation between the electron correlations and the electron interaction strength, the absolute values of correlation energies $|E_c|$ as functions of electron interaction strength Ω^2 are plotted in figure 3. Here the electron interaction strength Ω^2 is limited in the regime $\Omega^2 < \omega_0^2/N$ in order that all the electrons remain in the dot. It is shown that the larger N is, the faster $|E_c|$ grows with Ω^2. If Ω^2 continues to increase after reaching the value ω_0^2/N, the Nth electron will leave the dot to keep the other $N-1$ electrons confined in the dot [14]. So, the upper end of each curve at the limit $\Omega^2 = \omega_0^2/N$ corresponds to the largest value of $|E_c|$ permitted for a stable dot with the given number of electrons. This phenomenon does not exist in a dot with electron–electron interactions of Coulombic form.

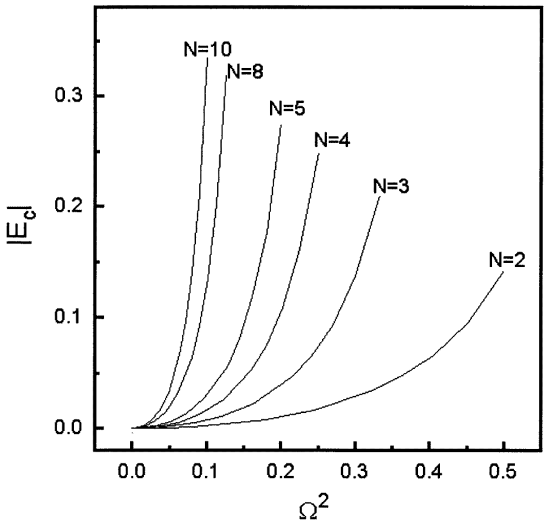

Figure 3. The absolute values of correlation energies as functions of electron–electron interaction strength $\Omega^2 (< \omega_0^2/N)$ for quantum dots with $N = 2$–5, 8 and 10 electrons. The energies are in units of $\hbar\omega_0$ and $\omega_c/\omega_0 = 1$.

The 'magic' ground-state angular momentum sequence is well known for the Coulomb interactions [1, 10]. But for the harmonic interactions the ground state of the dot does not show such angular momenta transitions so clearly, even for $N = 2$ electrons. To get a fuller comprehension of this case and to show the role of electron correlations, the exact and the HF lowest energy levels for given values of ΔM above the ground state value $M_g = N(N-1)/2$ are compared in figure 4. For a given total angular momentum $M = M_g + \Delta M$, the exact energy values of possible states above the ground state are given by [14]

$$\Delta E = (\Delta M - n)\hbar(\omega_0(B) - \omega_c/2) + n\hbar(\Omega_0(B) - \omega_c/2) \tag{5}$$

where n is the relative mode quantum number and $\Delta M - n$ is the centre-of-mass mode quantum number. Due to the antisymmetric requirement on the total N-electron wave function, for $N = 2$, n can take only even numbers less than or equal to ΔM, and for $N > 2$, n can take any numbers less than or equal to ΔM except $n = 1$. The lowest energy level for a given ΔM corresponds to the largest permitted n.

In the case of $N = 2$, both the exact and HF energies oscillate with ΔM in period of 2. But in the cases of $N > 2$, only the HF energies oscillate with ΔM in period of N, while the exact ones vary linearly except at the point $\Delta M = 1$. The difference between the cases of $N = 2$ and $N > 2$ is caused by the different limitations to n for $N = 2$ and $N > 2$. In all cases, we

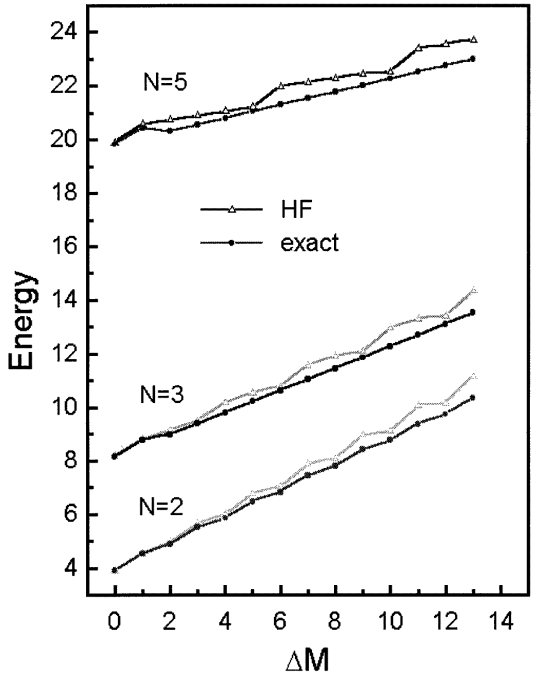

Figure 4. The lowest state energies as functions of the additional angular momentum above the ground states for quantum dots with $N = 2$, 3 and 5 electrons. The energy unit and the dot parameters are the same as in figure 1.

note that in the 'magic' angular momentum states the HF levels lie more closely to the exact ones. It is reasonable to explain this as due to the fact that the electron correlation interactions in the 'magic' angular momentum states are smaller than in the other states. Indeed, this is also the case for the dots with Coulomb interactions [11].

In summary, we have studied the correlation energies of quantum dot electrons with harmonic interactions in a magnetic field by comparing the HF ground state energies with the corresponding exact values. The results show that the correlation corrections to the ground state energies are not more than 1% for all the cases with given dot parameters appropriate to GaAs. Though the role of correlation interactions becomes more important with the increase of the number of electrons N and the electron–electron interaction strength Ω^2, it is limited by the condition $\Omega^2 < \omega_0^2/N$ for a stable dot. The calculated results also show that the correlation energies oscillate with the angular momentum M in periods of N. At the so called 'magic' angular momenta for Coulomb interactions, the correlation energies always take their minima. This characteristic of correlation interactions for the harmonic model is similar to that for the Coulombic model.

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