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1998 J. Phys.: Condens. Matter 10 11025

(http://iopscience.iop.org/0953-8984/10/48/022)

J. Phys.: Condens. Matter **10** (1998) 11025–11031. Printed in the UK PII: S0953-8984(98)95466-2

Many-body effects on the low-lying energy levels of three-electron quantum dots in a magnetic field

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Received 30 June 1998, in final form 10 September 1998

Abstract. The low-lying energy levels of three-electron quantum dots in a magnetic field are calculated by both the Hartree–Fock (HF) and the numerical diagonalization methods. Many-body effects on the energy level structure are investigated by comparing the results from these two approaches. It is found that many-body interactions can apparently change the relative positions of the low-lying energy levels, especially at larger angular momentum quantum numbers, and the relative changes of the levels almost have nothing to do with the external magnetic field, but linearly depend on the dot size.

1. Introduction

With the recent progress in semiconductor technology the experimental study of quantum dots in which only a few electrons are bound at semiconductor interfaces is expanding rapidly [1–6]. Due to the low effective density and the restriction of electron motion to only two dimensions, the electrons in such systems are usually highly correlated. A full understanding of the experimental results needs an analysis of many-body effects. Theoretical calculations using the Hartree approximation for electron numbers $N < 10$ neglected the exchange and correlation effects [7–9]. 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 [10]. It was found that the HF approximation, including the exchange interaction but neglecting the electron correlation, can even give qualitatively incorrect results about the spin singlet–triplet transition [6, 11, 12]. Though the many-body effects can be completely included in the exact numerical diagonalization treatment, which has been performed for systems with electron numbers $N \leqslant 4$ [13, 14], 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 quantum dots with more electrons. Indeed, if the correlation effects are treated properly the HF approximation still can be a useful method for these systems. The problem is how we can obtain the information about the role of the correlation effects in determining the energy spectra of quantum dots. The most direct way to do so is to compare the results from the HF approximation and the exact treatment as done for two electrons [10]. Though this way is not suitable for systems with more than six electrons, it still can give us some valuable information about the electron correlations and is expected to give a guide to treat the problems for more electrons. To our knowledge, there has been no such a study on quantum dots with more than two electrons. As a first

0953-8984/98/4811025+07$19.50

step to future study on many-electron quantum dots, we shall treat only the three-electron case in the present work.

The main purpose of this paper is to present a detailed study of the many-body effects in three-electron quantum dots in a magnetic field. To fully understand the influence of many-body interactions on the properties of the dots, we shall not only investigate the effects on their ground states but also on their low-lying exciting states which are also important to determine the properties of the systems.

In section 2, the methods used to calculate the low-lying energy levels of the systems are briefly described. The HF and the numerical diagonalization results are compared and discussed in section 3. Finally, a summary is given in section 4.

2. Methods to calculate the energy levels

Throughout this paper we assume we are dealing with the case of ideally two-dimensional electrons, in a circular dot, confined by a parabolic potential with a magnetic field B perpendicular to the plane of the dot, and B is supposed to be strong enough to keep the electrons spin polarized. In this case the constant Zeeman term can be ignored, so the total Hamiltonian is [13]

$$H = \sum_{i=1}^{3} h(i) + \frac{e^2}{4\pi\varepsilon\varepsilon_0} \sum_{i<j} \frac{1}{r_{ij}} \tag{1}$$

where

$$h(i) = \frac{1}{2m^*}(\boldsymbol{p}_i + e\boldsymbol{A}_i)^2 + \frac{1}{2}m^*\omega_0^2 r_i^2 \tag{2}$$

is the single-electron Hamiltonian. Here m^* is the electron effective mass, and $\boldsymbol{A}_i = (B/2)(-y_i, x_i, 0)$, the vector potential in the symmetric gauge. In the way mentioned in the introduction, to investigate many-body effects in the dots we shall calculate their low-lying energy levels by both the HF approximation and direct numerical diagonalization. So, in the following these two methods are briefly described first.

2.1. Numerical diagonalization

To numerically diagonalize the Hamiltonian matrix corresponding to H, a suitable set of basis functions must be chosen first. Here the basis functions Φ_α are chosen to be the eigenfunctions of the free-electron Hamiltonian $H^0 = \sum_{i=1}^{3} h(i)$, which are the Slater determinants composed by the eigenfunctions of the single-electron Hamiltonian $h(i)$ with the form [15]

$$\phi_{nm}(\boldsymbol{r}) = N_{nm} r^{|m|}\, \mathrm{e}^{-\mathrm{i}m\varphi} L_n^{|m|}\left(\frac{r^2}{2a^2}\right) \mathrm{e}^{-(r^2/4a^2)} \tag{3}$$

where N_{nm} is the normalization constant, $a^2 = (\hbar/m^*)(\omega_c^2 + 4\omega_0^2)^{-1/2}$, $\omega_c = eB/m^*$ and $L_n^{|m|}(x)$ is a Laguerre polynomial. The spin function is omitted from equation (3) since only the spin-polarized state is considered.

In this basis set the eigenfunctions of H are expanded as

$$\Psi = \sum_{\alpha} C_\alpha \Phi_\alpha \tag{4}$$

where the multiple index $\alpha = (n_1 m_1, n_2 m_2, n_3 m_3)$, n_i and m_i denote the radial and the angular quantum numbers of electron i. For the state with total angular momentum $-M\hbar$,

which is conserved due to the rotational symmetry of the interaction, the sum is over all indices α limited by the conditions $m_1+m_2+m_3 = M$ and $(n_1, m_1) \neq (n_2, m_2) \neq (n_3, m_3)$.

In practical calculations, only a finite set of indices α can be used in equation (4). For the systems we treat here, because of the large separations between different Landau levels the contribution of the Landau-level mixing to the many-body effects is relatively small, especially in a large magnetic field. It does not give a significant influence on the energy spectra of the dots [13] and can be ignored in the process of numerical diagonalization. Though this procedure may cause certain errors, the accuracy of the results can be estimated and improved as necessary. In this sense we still think that the method is exact.

2.2. Hartree–Fock approximation

In the HF approximation the many-electron problem is reduced to a single-electron problem. Following the usual procedure, we also expand the single-electron wavefunctions in a set of basis functions. Instead of choosing the eigenfunctions of $h(i)$ to be the basis set as Pfannkuche *et al* did [10], here we use the simple Gaussian functions as the basis set, which are more convenient for mathematical treatment. This choice is indeed similar to the cases in atomic structure calculations where the Slater functions, not the hydrogen-like wavefunctions, are usually used. Thus, in terms of Gaussian functions the HF single-electron wavefunctions are expanded as

$$\Phi_{nm}^{HF}(\boldsymbol{r}) = \sum_p C_{nmp}\chi_{mp}(\boldsymbol{r}) \tag{5}$$

where

$$\chi_{mp}(\boldsymbol{r}) = \frac{2^{(|m|+2)/2}\alpha_p^{(|m|+1)/2}}{(|m|!)^{1/2}} r^{|m|}\,\mathrm{e}^{-\alpha_p r^2}\frac{1}{\sqrt{2\pi}}\,\mathrm{e}^{-\mathrm{i}m\varphi}. \tag{6}$$

By choosing some finite basis set size to minimize the Hamiltonian integral and varying the expansion coefficients C_{nmp} for a fixed set of exponents α_p, we obtain the HF secular equations [16]:

$$\mathbf{FC} = \varepsilon\mathbf{SC} \tag{7}$$

where the overlap matrix $\mathbf{S}$ and the Fock matrix $\mathbf{F}$ are defined by

$$S_{mpq} = \langle\chi_{mp}|\chi_{mq}\rangle \tag{8}$$

$$F_{mpq} = h_{mpq} + G_{mpq} \tag{9}$$

$$h_{mpq} = \langle\chi_{mp}|h|\chi_{mp}\rangle \tag{10}$$

$$G_{mpq} = \sum_{n',m'}^{occ}\sum_{r,s} C^*_{n'm'r}C_{n'm's}[(mp\,mq|m'r\,m's) - (mp\,m's|m'r\,mq)] \tag{11}$$

with

$$(mp\,mq|m'r\,m's) = \frac{e^2}{4\pi\varepsilon\varepsilon_0}\left\langle\chi_{mp}(1)\chi_{m'r}(2)\left|\frac{1}{r_{12}}\right|\chi_{mq}(1)\chi_{m's}(2)\right\rangle. \tag{12}$$

The orbital energies ε_{nm} are related to the total energy E^{HF} by

$$E^{HF} = \frac{1}{2}\left[\sum_{n,m}^{occ}\varepsilon_m + \sum_{n,m}^{occ}\sum_{p,q} C^*_{nmp}C_{nmq}h_{mpq}\right]. \tag{13}$$

The summation $\sum_{n,m}^{occ}$ in equations (11) and (13) is over all occupied orbitals. If the three occupied single-electron orbitals are (n_1, m_1), (n_2, m_2) and (n_3, m_3), then the corresponding total energy state is labelled as $\{n_1m_1, n_2m_2, n_3m_3\}$.

3. Results and discussion

In the numerical diagonalization, since the mixing of the Landau levels is neglected the low-lying energy states with a given value of M are determined by using a finite set of basis functions Φ_α corresponding to the lowest Landau level where $\alpha = (0m_1, 0m_2, 0m_3)$ or (m_1, m_2, m_3) with the limitations $m_1 \neq m_2 \neq m_3$ and $m_1 + m_2 + m_3 = M$. For example, if $M = 6$, then $\alpha = (1, 2, 3)$, $(0, 2, 4)$ and $(0, 1, 5)$. In the HF calculation, for a given value of M the three occupied single-electron orbitals are $(0, m_1)$, $(0, m_2)$ and $(0, m_3)$ with the same limitations as for α and the energy levels are labelled as $\{m_1, m_2, m_3\}$. The low-lying energy levels at the magic numbers $M = 6$, 9 and 12 of a three-electron quantum dot with parameters $\omega_c/\omega_0 = 3$ and $l_0/a^* = 3$ ($l_0 = (\hbar/m^*\omega_0)^{1/2}$ is the oscillator length and a^* the effective Bohr radius) are calculated by both the HF and the numerical diagonalization methods. The results are illustrated in figure 1. For the HF calculation five Gaussian functions are taken into account in equation (5). This corresponds to an accuracy of the results of about 0.1%. The errors caused by neglecting the mixing of the Landau levels in the numerical diagonalization are believed not to influence the physics especially for the cases of few electrons in a large magnetic field [13].

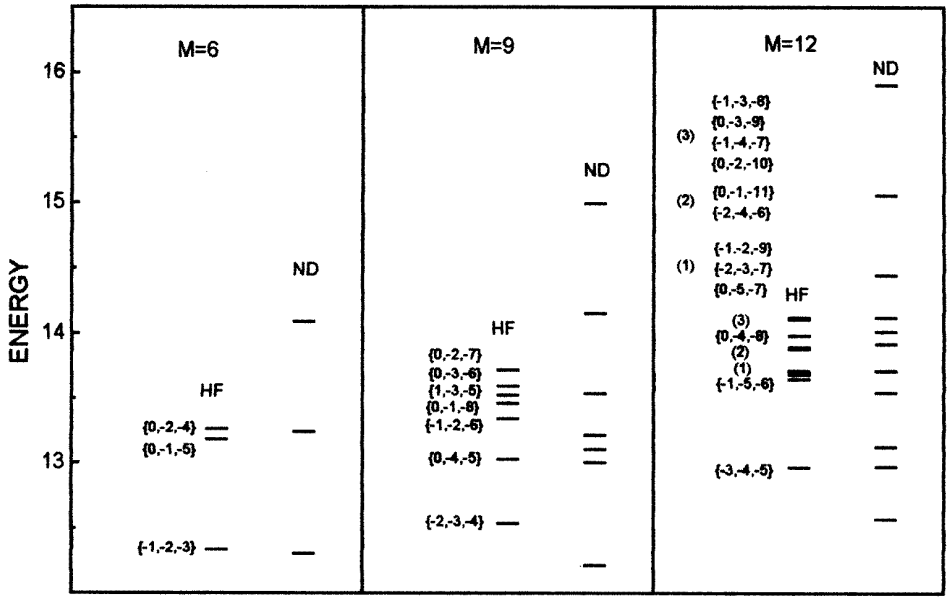

Figure 1. The low-lying energy level structures in the HF approximation and the numerical diagonalization (ND) at $M = 6$, 9 and 12. The energies are in units of $\hbar\omega_0$ and the dot parameters are set as $\omega_c/\omega_0 = 3$ and $l_0/a^* = 3$.

Many-body effects on the low-lying energy levels of the dot are clearly shown in figure 1. Because of the many-body interactions the relative positions of the energy levels are rearranged. In the HF approximation, the low-lying energy levels at any M lie close together except for the lowest one. When the many-body effects are included, however, the distribution of the corresponding levels is more scattered. At $M = 6$, for example, the HF levels $\{0, 1, 5\}$ and $\{0, 2, 4\}$ lie close together and have a relatively larger spacing with the

lowest one $\{1, 2, 3\}$, but when the many-body interactions are included the two close-lying levels are pushed away from each other and these three levels are almost equally separated. At larger M, where there are more close-lying energy states corresponding to the first Landau level, the role of the many-body interactions is more apparent. As shown in figure 1, at $M = 12$ there are three groups of HF energy levels lying very close together. Group (1) includes levels $\{0, 5, 7\}$, $\{2, 3, 7\}$ and $\{1, 2, 9\}$, group (2) includes $\{2, 4, 6\}$ and $\{0, 1, 11\}$ and group (3) includes $\{0, 2, 10\}$, $\{1, 4, 7\}$, $\{0, 3, 9\}$ and $\{1, 3, 8\}$. After the many-body interactions are considered, this phenomenon disappears.

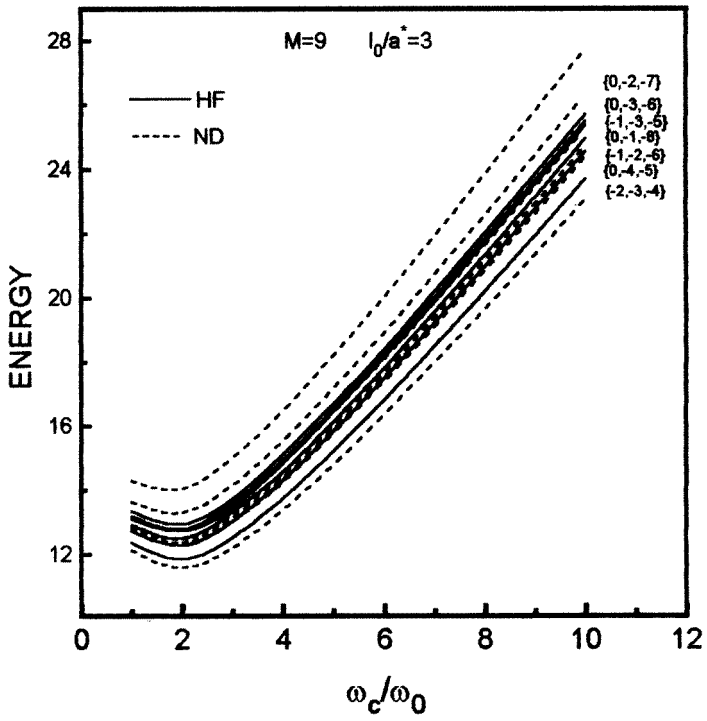

Figure 2. The low-lying energy levels at $M = 9$ as a function of the relative magnetic field. The energy unit is the same as in figure 1 and $l_0/a^* = 3$.

To fully understand the role of many-body interactions, the low-lying energy levels as functions of the relative magnetic strength ω_c/ω_0 and the relative dot size l_0/a^* are also studied, and the results at $M = 9$ are shown in figures 2 and 3, respectively. From figure 2 we can see that the two sets of energy levels keep parallel as the magnetic field is changed. This illustrates that the influence of the many-body interactions on the relative positions of the energy levels almost does not change with the relative magnetic strength ω_c/ω_0. So, in the present problem the role of the external magnetic field, besides keeping the electrons spin polarized (typically, a field of several tesla is large enough to do so), is just to move the energy levels of a given M upward or downward as a whole. As shown in figure 3, the energy levels vary linearly with the relative dot size l_0/a^*, but the slopes of the levels are different. The HF levels have smaller slopes than those from the numerical diagonalization. This means that for the larger size the role of the many-body interactions is more important.

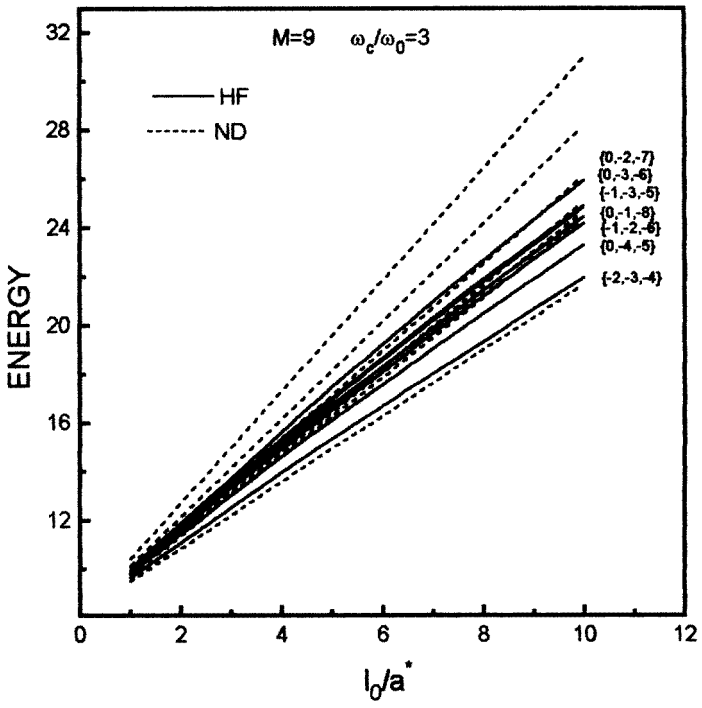

Figure 3. The low-lying energy levels at $M = 9$ as a function of the relative dot size. The energy unit is the same as in figure 1 and $\omega_c/\omega_0 = 3$.

4. Summary

We have compared the low-lying energy levels at $M = 6$, 9 and 12 of three-electron quantum dots calculated in the HF approximation with those from the numerical diagonalization. Many-body effects on the energy level structure are analysed. It is shown that because of the absence of the many-body interactions some of the HF levels lie very close together, especially at larger M, but when the many-body interactions are included the close-lying energy levels are pushed away from each other and the level structure is apparently changed. It is also shown that the changes of the relative positions of the energy levels caused by many-body interactions almost have nothing to do with the external magnetic field, but linearly depend on the dot size. Though present study is only for three-electron quantum dots, the results could be expected useful for other few-electron quantum dots.

Acknowledgments

We would like to thank Professor Q Q Shu for his encouragement to this research. One of us (XQW) also thanks him for his kind hospitality during a visit to Shenzhen University. This research is partly supported by the Basic Research Foundation of Chongqing University.

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