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STUDY OF THE ENERGY LEVEL-CROSSINGS IN GaAs/Al$_x$Ga$_{1-x}$As QUANTUM DOTS

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The energy spectra of two interacting electrons, confined by a parabolic potential, in a magnetic field applied perpendicular to the plane of the quantum dot are obtained. The electron–electron interaction and the energy level-crossings are discussed. Comparison shows that our calculated spectra of the quantum dot states are in good agreement with those of Wagner *et al.*

1. INTRODUCTION

WITH RECENT progress in nanofabrication technology, it has been possible to confine electrons in all three spatial dimensions in semiconductor structures called quantum dots (QDs). In such small structures the electrons are fully quantized into a discrete spectrum of energy levels. The confinement in z-direction, which is the growth direction, is assumed to be stronger than that in the xy-plane, so that the dots can be viewed as two dimensional disks. The growing interest in this field is motivated by the physical effects and the potential device applications, both as electronic memories as well as optoelectronic devices [1] to which many experimental [1–5] and theoretical [6–18] works have been devoted. The effects of the magnetic field, which plays a useful role in identifying the absorption features, on the states of interacting electrons, impurity and excitons confined in the QD have been extensively studied. Maksym and Chakraborty [6] have studied the eigenstates of interacting electrons, parabolically confined in QD, in a magnetic field perpendicular to the plane of the QD and found that the Coulomb interaction energy has an important effect on the magnetic field dependence of the energy spectrum. When the potential is quadratic, far-infrared (FIR) spectroscopy is unable to detect the Coulomb interaction by the virtue of the generalized Kohn's theorem. Wagner *et al.* [7] have also considered two interacting electrons, parabolically confined in a perpendicular magnetic field in addition to the spin and they predict the oscillations between the

spin–singlet and the spin–triplet ground state. Pfannkuche and Gerhardts [8] have made a theoretical study of the magneto-optical response to far-infrared radiation of quantum dot helium. De Groote, Hornos and Chaplik [9] have investigated thermodynamic properties of quantum dots, such as heat capacity and magnetization, as sensitive probes to the ground-state transitions. The purpose of this work is to show the level-crossings and the transitions in the ground-state energy of the interacting system against the magnetic field strength.

In this work, we shall use the shifted $1/N$ expansion method to solve the effective-mass Hamiltonian of two electrons and obtain the energy spectra of this interacting system.

2. THEORY

Within the effective-mass approximation (EMA), the Hamiltonian of an interacting pair of electrons confined in a quantum dot by a parabolic potential of the form $m^* \omega_0^2 r^2 / 2$ in a magnetic field applied parallel to the z-axis (and perpendicular to the plane where the electrons are restricted to move) in the symmetric gauge is written as follows,

$$H = \sum_{i=1}^{2} \left[-\frac{\hbar^2 \nabla_i^2}{2m^*} + \frac{1}{2} m^* \omega^2 r_i^2 + \frac{\hbar \omega_c}{2} L_i^z \right] + \frac{e^2}{\epsilon |r_1 - r_2|},$$

(1)

where the two-dimensional vectors r_1 and r_2 describe the positions of the first and the second electron in the x–y plane, respectively. L_i^z stands for the z-component

of the orbital angular momentum for each electron and $\omega_c = eB/m^*c$, m^* and ϵ are the cyclotron frequency, effective mass and dielectric constant of the medium, respectively. The frequency ω depends on both the magnetic field B and the confinement frequency ω_o and is given by

$$\omega = \left(\omega_o^2 + \frac{\omega_c^2}{4}\right)^{1/2}. \tag{2}$$

The natural units of length and energy to be used are the effective Bohr radius $a^* = \epsilon\hbar^2/m^*e^2$ and effective Rydberg $R^* = \hbar^2/2m^*a^{*2}$. The dimensionless constant $\gamma = \hbar\omega_c/2R^*$ plays the role of effective magnetic field strength.

Upon introducing the center-of-mass $R = (r_1 + r_2)/\sqrt{2}$ and the relative coordinates $r = (r_1 - r_2)/\sqrt{2}$, the Hamiltonian [9] in Equation (1) can be written as a sum of two separable parts that represent the center-of-mass motion Hamiltonian,

$$H_R = -\frac{\hbar^2}{2m^*}\nabla_R^2 + \frac{m^*}{2}\omega^2 R^2 + \frac{\hbar\omega_c}{2}L_z^R, \tag{3}$$

and the relative motion Hamiltonian,

$$H_r = -\frac{\hbar^2}{2m^*}\nabla_r^2 + \frac{m^*}{2}\omega^2 r^2 + \frac{\hbar\omega_c}{2}L_z^r + \frac{e^2}{\sqrt{2}r}. \tag{4}$$

Equation (3) describes the Hamiltonian of the harmonic oscillator with the well-known eigenenergies,

$$E_{n_{cm},m_{cm}} = (2n_{cm} + |m_{cm}| + 1)\hbar\omega + \frac{\hbar\omega_c}{2}m_{cm}, \tag{5}$$

labeled by the radial $(n_{cm} = 0, 1, 2, \ldots)$ and azimuthal $(m_{cm} = 0, \pm1, \pm2, \pm3, \ldots)$ quantum numbers. The problem is reduced to obtaining eigenenergies $E_{n,m}$ of the relative motion Hamiltonian. The energy states of the total Hamiltonian are labeled by the CM and relative quantum numbers, $|n_{cm}m_{cm}; n,m\rangle$. The coexistence of the electron–electron and the oscillator terms makes an exact analytic solution, using available special functions, not possible.

3. THE SHIFTED 1/N EXPANSION METHOD

The shifted $1/N$ expansion method, N being the spatial dimension, is a pseudoperturbative technique in the sense that it proposes a perturbation parameter that is not directly related to the coupling constant [19–21]. The aspect of this method has been clearly stated by Imbo et al. [19, 20] who had given step-by-step calculations relevant to this method. Following their work, we present here only the analytic expressions which are required to determine the energy states.

The method starts by writing the radial Schrödinger equation, for an arbitrary cylindrically symmetric potential, in an N-dimensional space as,

$$\left[-\frac{d^2}{dr^2} + \frac{(k-1)(k-3)}{4r^2} + V(r)\right]\psi(r) = E_r\psi(r), \tag{6}$$

where $k = N + 2m$.

In order to get useful results from $1/\bar{k}$ expansion, where $\bar{k} = k - a$ and a is a suitable shift parameter, the large $\bar{k}$-limit of the potential must be suitably defined [16]. Since the angular momentum barrier term behaves like $\bar{k}^2$ at large $\bar{k}$, so the potential should behave similarly. This will give rise to an effective potential which does not vary with $\bar{k}$ at large values of $\bar{k}$, resulting in a sensible zeroth-order classical result. Hence Equation (6) in terms of the shift parameter becomes,

$$\left[-\frac{d^2}{dr^2} + \frac{\bar{k}^2[1 - (1-a)/\bar{k}][1 - (3-a)/\bar{k}]}{4r^2}\right]\psi(r)$$
$$= E_r\psi(r), \tag{7}$$

where

$$V(r) = \frac{\sqrt{2}}{r} + \frac{1}{4}\omega^2 r^2 + m\frac{\omega_c}{2}, \tag{8}$$

and Q is a scaling constant to be specified from Equation (10). The shifted $1/N$ expansion method consists of solving Equation (7) systematically in terms of the expansion parameter $1/\bar{k}$. The leading contribution term to the energy comes from

$$\bar{k}^2 V_{eff}(r) = \frac{\bar{k}^2}{r_o^2}\left(\frac{1}{4} + \frac{r_o^2 V(r_o)}{Q}\right), \tag{9}$$

where r_o is the minimum of the effective potential, given by

$$2r_o^3 V'(r_o) = Q. \tag{10}$$

It is convenient to shift the origin to r_o by the definition

$$x = \bar{k}^{1/2}(r - r_o)/r_o, \tag{11}$$

and to expand Equation (7) about $x = 0$ in powers of x. Comparing the coefficients of powers of x in the series with the corresponding ones of the same order in the Schrödinger equation for a one-dimensional anharmonic oscillator, we determine the anharmonic oscillator frequency, the energy eigenvalue and the scaling constant in terms of $\bar{k}, Q, r_o$ and the potential derivatives. The anharmonic frequency parameter is

$$\bar{\omega} = \left[3 + \frac{V''(r_o)}{V'(r_o)}\right]^{1/2}, \tag{12}$$

and the energy eigenvalues in powers of $1/\bar{k}$ (up to

third order) read as

$$E_{n_r,m} = \frac{\sqrt{2}}{r_0} + \frac{1}{4}\omega^2 r_0^2 + m\frac{\omega_c}{2} + \frac{\bar{k}^2}{4r_0} + \frac{1}{r_0^3}$$

$$\times \left[\frac{(1-a)(3-a)}{4} + \gamma_1\right] + \frac{\gamma_2}{\bar{k}r_0^2}, \qquad (13)$$

where the γ_1 and γ_2 parameters can be expressed in terms of $Q, a, \bar{\omega}$ and n_r. The shift parameter a, which introduces an additional degree of freedom, is chosen so as to make the first term in the energy series of order $\bar{k}$ to vanish, namely,

$$\frac{\bar{k}}{r_0^2}\left[(n_r + \tfrac{1}{2})\bar{\omega} - \frac{(2-a)}{2}\right] = 0, \qquad (14)$$

to obtain

$$a = 2 - (2n_r + 1)\bar{\omega}, \qquad (15)$$

where n_r is the radial quantum number related to the principal (n) and magnetic (m) quantum numbers by the relation $n_r = n - |m| - 1$. Energies and lengths in Equations (6)–(15) are expressed in units of R^* and a^*, respectively.

For the two-dimensional case, $N = 2$, Equation (10) takes the following form,

$$\sqrt{2r_0^3 V'(r_0)} = 2 + 2m - a = Q^{1/2}. \qquad (16)$$

Once r_0 (for a particular quantum state and confining frequency) is determined, the task of computing the energy is relatively simple.
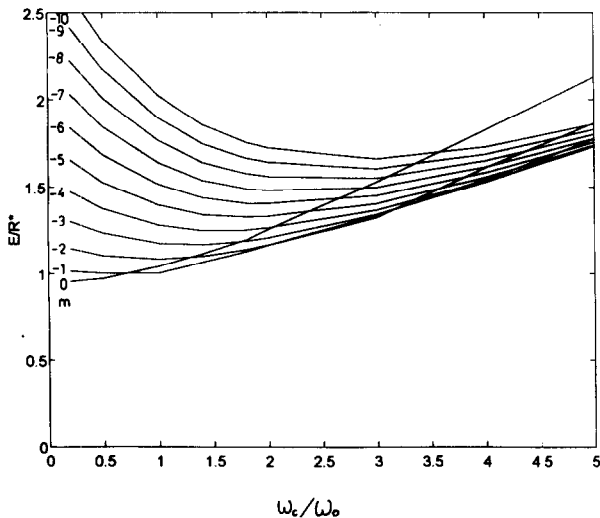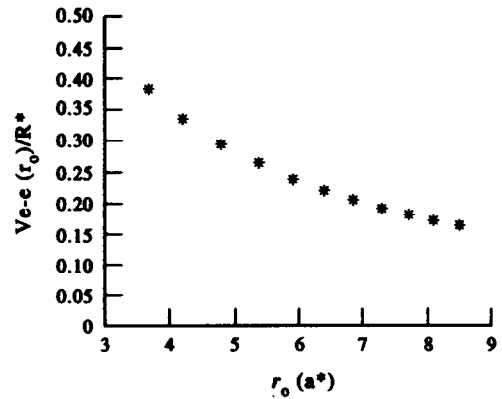

Fig. 2. The Coulomb interaction energy as a function of the roots calculated for quantum states $|0, m\rangle$, $m = 0, -1, -2, \ldots, -10, \omega_c/\omega_o = 2$ and $l_o = 3a^*$.

4. RESULTS AND CONCLUSIONS

Our results for QDs made of GaAs/AlGaAs are presented in Figs 1–3 and Tables 1 and 2. The energy level-crossings are shown in Fig. 1. We have displayed the eigenenergies of the states $|00; 0m\rangle$, $m = 0, -1, -2, \ldots, -10$, for two interacting electrons parabolically confined in the quantum dot of size $l_o = 3a^*$ as a function of the ratio ω_c/ω_o. As the magnetic field strength increases, the energy of the state $m = 0$ increases while the energy of the states with non-vanishing quantum number m decreases, thus leading to a sequence of different ground states. The reduction in the eigenenergies of the interacting system states with non-vanishing quantum number m is attributed to the behavior of the electron–electron Coulomb interaction.
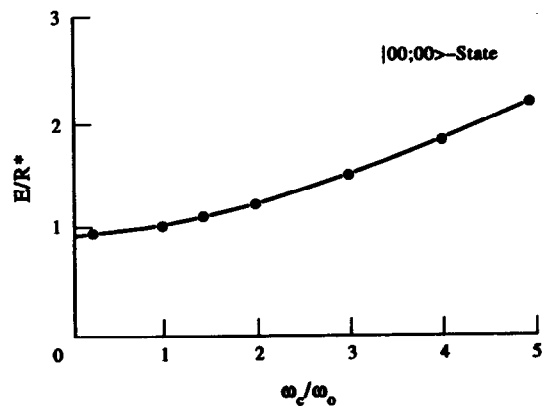

Fig. 1. The total eigenenergies of the states $|00; 0m\rangle$, $m = 0, -1, -2, \ldots, -10$, for two interacting electrons parabolically confined in the quantum dot of size $l_o = 3a^*$, as a function of the ratio ω_c/ω_o. $\epsilon = 12.4$ and $m^* = 0.067m_e$ for GaAs.

Fig. 3. The total ground-state energy $|00; 00\rangle$ for two interacting electrons in a quantum dot of size $l_o = 3a^*$ against the ratio ω_c/ω_o. (...) present results, (——) Ref. (7).

Table 1. The values of the Coulomb interaction energy and the roots for quantum dot states with non-vanishing azimuthal quantum numbers (m) *calculated at* $l_o = 3a^*$ *and* $\omega_c/\omega_o = 2$

m	0	−1	−2	−3	−4	−5	−6	−7	−8	−9	−10
r_o	3.692	4.222	4.801	5.363	5.890	6.384	6.847	7.285	7.700	8.096	8.473
$V_{e-e}(r_o)$	0.383	0.335	0.295	0.264	0.240	0.222	0.207	0.194	0.184	0.175	0.167

Table 2. The ground state energy $|00; 00\rangle$ *of two interacting electrons calculated by* $1/N$ *expansion for quantum dot of size* $l_o = 3a^*$

ω_c/ω_o	0.2	1.0	1.4	2	3	4	5
E/R^*	0.953	1.040	1.115	1.256	1.531	1.827	2.130

In Fig. 2, we have plotted the Coulomb interaction energy term $V_{e-e}(r_o) \approx \sqrt{2}/r_o$, the dominant interaction term in the energy series expression Equation (13), against the roots r_o, evaluated using Equation (9), for particular values of ω_c/ω_o $n_r = 0$ and $m = 0, -1, -2, \ldots, -10$. As the figure shows, the interaction energy decreases as the roots increase, or equivalently, as the azimuthal quantum number m increases. The numerical values of the Coulomb interaction energy and roots are listed in Table 1. On the other hand, the confining energy, $V_c(r_o) \approx \frac{1}{4}\omega^2 r_o^2$, increases as the roots increase. The interplay between the electron-electron energy term and the confining energy term leads to a system with different ground states. The transitions in the ground state of the interacting system depends on the strength of the applied magnetic field.

To test the accuracy of the $1/N$ expansion method, we have compared in Fig. 3 our results for the ground-state energy $|00; 00\rangle$ of the total Hamiltonian against the ratio ω_c/ω_o with the results of Wagner *et al.* [7]. The present results ($\ldots$) obviously show an excellent agreement with the numerical results of Ref. (7) (solid line). In Table 2 we have listed the energies for the ground state for the sake of completeness.

In conclusion, we have obtained the energy spectra of two interacting electrons as a function of field strength for a quantum dot of a particular size. We have discussed the effect of the electron–electron term and its significance on the energy level-crossings in states with different azimuthal quantum numbers. The $1/N$ expansion gives accurate results without putting constraints on the Hamiltonian of the system.

REFERENCES

1. H. Drexler, D. Leonard, W. Hansen, J.P. Kotthaus & P.M. Petroff, *Phys. Rev. Lett.* **73**, 2252 (1994).
2. C. Sikorski & U. Merkt, *Phys. Rev. Lett.* **62**, 2164 (1989).
3. T. Demel, D. Heitmann, P. Grambow & K. Ploog, *Phys. Rev. Lett.* **64**, 788 (1990).
4. A. Lorke, J.P. Kothaus & K. Ploog, *Phys. Rev. Lett.* **64**, 2559 (1990).
5. A. Wixforth *et al.*, *Semicond. Science and Technol.* **9**, 215 (1994).
6. P.A. Maksym & T.T. Chakraborty, *Phys. Rev. Lett.* **65**, 108 (1990).
7. M. Wagner, U. Merkt & A.V. Chaplik, *Phys. Rev.* **B45**, 1951 (1992).
8. D. Pfannkuche & R.R. Gerhardts, *Physica* **B189**, 6 (1993).
9. J.J.S. De Groote, J.E.M. Honos & A.V. Chaplik, *Phys. Rev.* **B46**, 12773 (1992).
10. U. Merkt, J. Huser & M. Wagner, *Phys. Rev.* **B43**, 7320 (1991).
11. Pfannkuche & R.R. Gerhardts, *Phys. Rev.* **B44**, 13132 (1991).
12. K.D. Zhu & S.W. Gu, *Phys. Lett.* **A172**, 296 (1993).
13. N.F. Johnson & M.C. Payne, *Phys. Rev. Lett.* **67**, 1157 (1991).
14. W. Que, *Phys. Rev.* **B45**, 11036 (1992).
15. V. Halonen, T. Chakraborty & M. Pietalainen, *Phys. Rev.* **B45**, 5980 (1992).
16. G.T. Einevoll, *Phys. Rev.* **B45**, 3410 (1992).
17. Y. Kayanuma, *Phys. Rev.* **B38**, 9797 (1990).
18. G.W. Bryant, *Phys. Rev. Lett.* **59**, 1140 (1987); *Phys. Rev.* **B37**, 8763 (1988).
19. T. Imbo, A. Pagnamento & U. Sukhatme, *Phys. Rev.* **D29**, 8763 (1984).
20. T. Imbo & U. Sukhatme, *Phys. Rev.* **D28**, 418 (1983); **31**, 2655 (1985).
21. R. Dutt, Mukherji & Y.P. Varshni, *J. Phys.* **B19**, 3411 (1986).