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Mohammad EL-SAID

M. Abu SAA

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Mohammad EL-SAID & M. ABU SAA
Department of Physics,
Eastern Mediterranean University,
Gazi Magosa, N. Cyprus,
10 Mersin - TURKEY

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Abstract

The energy expressions for QD presented in high- and low-magnetic fields are calculated. An interpolation formula between the energies of the quantum dot in both limits is proposed. The formula is implemented to produce the energy spectra of the parabolic quantum dot in the presence of a magnetic field of arbitrary strength. The transitions in the angular momenta of the ground state energy of interacting electrons confined in the quantum dot as a function of magnetic field strength is studied. A good agreement is obtained when our results are tested against exact numerical work.

1. Introduction

Nanostructure technologies allow the lateral confinement of electrons in all three spatial dimensions in semiconductor structures called quantum dots (QDs). In such away, the electrons are 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 QDs may be regarded as artificial atoms with disk-like shapes.

The growing interest in this field is motivated by the physical effects and the potential device applications, to which many experimental [1-9] and theoretical [10-30] works have been devoted. The effects of the magnetic field, on the states of the interacting electrons, have been extensively studied. Maksym and Chakraborty [10] have studied the eigenstates of the interacting electrons, parabolically confined in the QDs, in a magnetic field perpendicular to the plane of the QD, and they found that the coulomb interaction energy has significant effect on the magnetic field dependence of the energy spectrum. Wagner et.al. [11] have also studied the same problem in addition to the spin, and predict

the oscillations between spin-singlet and spin-triplet ground states. Pfannkuche and collaborators [12] and Merkt [13] have studied the magneto-optical response to far-infrared radiation (FIR) of QD-Helium. De Groote, Hornos and Chaplik [14] have investigated the thermodynamic properties of QDs, such as heat capacity and magnetization, as a sensitive probe to the ground state transitions. Taut [15, 16] obtained exact analytical results for the energy spectrum of a system of two electrons interacting via a Coulomb force for specific values of the magnetic field. He also produced the eigenenergies of the interacting system in high- and low-magnetic field limits and suggested an eigenenergy formula to interpolate between both limits.

In this work, we propose an accurate interpolation formula to reproduce the spectrum of the interacting system and then use this formula to study the energy level-crossing and show the transitions in the orbital momenta of the ground state energy of two interacting electrons confined in a parabolic quantum dot presented in a magnetic field of arbitrary strength.

2. The Model

The effective-mass Hamiltonian for two interacting electrons, confined in a QD by a parabolic potential of the form $m^*\omega_0^2 r^2/2$, in a magnetic field applied parallel to the z-direction, and perpendicular to the plane where the electrons are restricted to move, is written as

$$H = \sum_{i=1}^{2} \left\{ \frac{1}{2m_i^*}(\vec{P}_i + e\vec{A}(\vec{r}_i))^2 + \frac{1}{2}m_i^*\omega_0^2 r_i^2 \right\} + \frac{e^2}{4\pi K\epsilon_0|\vec{r}_2 - \vec{r}_1|} + H_{spin}, \tag{1}$$

where the two-dimensional vectors $\vec{r}_1$ and $\vec{r}_2$ describe the positions of the first and the second electron in the xy-plane, respectively, and m^*, ω_0 and K are the electron effective mass, confinement frequency and dielectric constant of the medium, GaAs, respectively.

Applying the coordinates $\vec{r} = \vec{r}_2 - \vec{r}_1$, $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$ and the corresponding momenta transformations, the total Hamiltonian can be decoupled to center-of-mass and relative Hamiltonians as

$$H_R = \frac{1}{2M}(\vec{P} + Q\vec{A}(\vec{R}))^2 + \frac{1}{2}M\omega_0^2 R^2 \tag{2}$$

$$H_r = \frac{1}{2\mu}(\vec{p} + q\vec{A}(\vec{r}))^2 + \frac{1}{2}\mu\omega_0^2 r^2 + \frac{e^2}{4\pi\epsilon_0 K r} \tag{3}$$

$$H_{spin} = g^*\mu_B B \sum_i S_{i,z},$$

where $M = 2m^*$, $\mu = \frac{m^*}{2}$, $q = \frac{e}{2}$ and $Q = 2e \cdot \mu_s$ and $S_{i,z}$ are the Bohr magneton and the z-component for each electron. In writing Eqs. 2 and 3 the symmetric gauge $\vec{A} = \frac{1}{2}(\vec{B} \times \vec{r})$ is used and the vector potential is assumed to be linear function.

Equation 3 represents the Hamiltonian of the harmonic oscillator with well-known eigenvalues,

$$E_R = \hbar(2n_{cm} + |m_{cm}| + 1)\omega + m_{cm}\frac{\hbar\omega_c}{2}, \tag{4}$$

where $\omega_c = \frac{eB}{m^*}$ is the cyclotron frequency and $\omega = \left(\omega_0^2 + \left(\frac{\omega_c}{2}\right)^2\right)^{\frac{1}{2}}$ is the effective frequency. $n_{cm} = 0, 1, 2, \ldots$ is the radial and $m_{cm} = 0 \pm 1 \pm 2, \ldots$ is the azimuthal quantum numbers which label CM-spectra.

The corresponding eigenstates are

$$\xi(\vec{R}) = \sqrt{\frac{n_{cm}!}{\pi(n_{cm} + |m_{CM}!)}} \omega_R^{\frac{(|m_{cm}|+1)}{2}} R^{|m_{cm}|} e^{-\omega_R R^2/2} e^{im_{cm}\phi} L_{n_{cm}}^{|m_{cm}|}(\omega_R R^2), \tag{5}$$

where $\omega_R = \frac{m_{cm}}{\hbar}\omega$ and $L_{n_{cm}}^{|m_{cm}|}(\omega_R R^2)$ are the associated Laguerre polynomials. Thus the problems is reduced to obtaining eigenenergies $E_{n_r,m}$ of the relative motion Hamiltonian. Antisymmetric of the two electron wavefunction requires that even m are singlets and odd m are triplets with the Zeeman energy term $E_{spin} = g^*\mu_B B S_z$ and the total spin $S_z = \frac{[1-(-1)^m]}{2}$ represents a good quantum number for the system. The total energy of the Hamiltonian, $E = E_R\ (n_{cm}, m_{cm}) + E_r(n_r, m) + E_{spin}(S_z)$, are labeled by the CM and relative quantum numbers $|n_{cm}m_{cm}; n_r m\rangle$. The coexistence of the electron-electron and the oscillator potential terms makes the exact analytic solution not possible and one has to resort to approximate methods.

3. High- and Low-Field Limits

In the limit of high $\omega_r = \frac{\mu}{\hbar}\omega$ the electron-electron interaction Hamiltonian

$$H_1 = \frac{e^2}{4\pi K \epsilon_0 r} \tag{6}$$

can be considered small compared to the magneto-confinement Hamiltonian. The Hamiltonian of the non-interacting system has the form

$$H_0 = \frac{1}{2\mu}(\vec{p} + q\vec{A}(\vec{r}))^2 + \frac{1}{2}\mu\omega_0^2 r^2. \tag{7}$$

H_0 again is the Hamiltonian for the Harmonic oscillator. For the states $(n_r = 0, m \leq 0)$ the eigenenergies have the form

$$E_0 = \hbar(|m| + 1)\omega + m\frac{\hbar\omega_c}{2} \tag{8}$$

and the corresponding eigenstates are

$$\Phi(r) = \frac{1}{\sqrt{\pi|m|!}} \omega_r^{\frac{(|m|+1)}{2}} e^{im_{cm}\phi} e^{\frac{-\omega_r^2 r^2}{2}}. \tag{9}$$

The perturbation theory is reliable. The first order energy correction E_1 to the states $(n_r = 0, m \leq 0)$ can be calculated using the wavefunctions given by Eq. (9). The eigenenergies corresponding to H_1 read as

$$E_1 = \frac{e^2}{4\pi K \epsilon_0} \frac{\Gamma(|m| + \frac{1}{2})}{|m|!} \sqrt{\omega_r}, \tag{10}$$

and thus the energy spectra of the relative part Hamiltonian reads as

$$E_r = \hbar(|m|+1)\omega + m\frac{\hbar\omega_c}{2} + \frac{e^2}{4\pi K\epsilon_0}\frac{\Gamma(|m|+\frac{1}{2})}{|m|!}\sqrt{\omega_r}. \tag{11}$$

The relative Hamiltonian, Eq. (3), can be written as

$$\left\{-\frac{1}{2}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2} + \omega_r^2 r^2 + \frac{\mu\omega_c}{4i\hbar}\frac{\partial}{\partial\phi} + \frac{\mu e^2}{2\pi\hbar^2 K\epsilon_0 r}\right\}\Phi(r) = \frac{2\mu E_r}{\hbar^2}\Phi(r) \tag{12}$$

where $\omega_r = \frac{\mu}{\hbar}\omega$.

The first term in Eq. (12) can be expressed as

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\Phi(r)}{\partial r}\right) = r^{-\frac{1}{2}}\frac{\partial^2}{\partial r^2}\left(r^{\frac{1}{2}}\Phi(r)\right) + \frac{\Phi(r)}{4r^2} \tag{13}$$

and Eq. (12) takes the form

$$\left\{-r^{-\frac{1}{2}}\frac{\partial^2}{\partial r^2}\left(r^{\frac{1}{2}}\right) - \frac{1}{4r^2} - \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2} + \omega_r^2 r^2 + \frac{\mu\omega_c}{4i\hbar}\frac{\partial}{\partial\phi} + \frac{\mu e^2}{2\pi\hbar^2 K\epsilon_0 r}\right\}\Phi(r) = \frac{2\mu E_r}{\hbar^2}\Phi(r). \tag{14}$$

Eq. (14) is separable in the coordinates r and ϕ and upon substituting the ansatz

$$\Phi(r) = \frac{e^{im\phi}u(r)}{\sqrt{2\pi}r^{\frac{1}{2}}}, \tag{15}$$

Eq. (14) reads as

$$\left\{-\frac{1}{2}\frac{d^2}{dr^2} + \frac{1}{2}\left(m^2 - \frac{1}{4}\right)\frac{1}{r^2} + \frac{1}{2}\omega_r^2 r^2 + \frac{\alpha}{2r}\right\}u(r) = E_r'\,u(r), \tag{16}$$

where

$$E_r' = \frac{\mu E_r}{\hbar^2} - \frac{\mu m\omega_c}{2\hbar} \tag{17}$$

and

$$\alpha = \frac{\mu e^2}{2\pi\hbar^2 K\epsilon_0}. \tag{18}$$

We can write Eq. (16) as follows:

$$\left\{-\frac{1}{2}\frac{d^2}{dr^2} + V_{eff}(r)\right\}u(r) = E_r' u(r), \tag{19}$$

where

$$V_{eff}(r) = \frac{1}{2}\omega_r^2 r^2 + \frac{1}{2}\left(m^2 - \frac{1}{4}\right)\frac{1}{r^2} + \frac{\alpha}{2r}. \tag{20}$$

For small ω_r. Eq. (19) can be solved approximately by expanding the $V_{eff}(r)$ around its local minimum [15]. The eigenenergies are calculated to be

$$\begin{aligned} E_r &= \hbar\omega_0 \left\{ 0.945 \left(\frac{\hbar\alpha^2}{\mu\omega_0}\right)^{\frac{1}{3}} \omega_{eff}^{2/3} + 0.794 \left(m^2 - \frac{1}{4}\right) \left(\frac{\mu\omega_0}{\hbar\alpha^2}\right)^{1/3} \omega_{eff}^{4/3} \right. \\ &\left. +0.866\omega_{eff} + 0.364 \left(m^2 - \frac{1}{4}\right) \left(\frac{\mu\omega_0}{\hbar\alpha^2}\right)^{2/3} \omega_{eff}^{5/3} + \frac{m\omega_c}{2\omega_0} \right\} \end{aligned} \tag{21}$$

where

$$\omega_{eff} = \left[1 + \left(\frac{\omega_c}{2\omega_0}\right)^2\right]^{1/2}. \tag{22}$$

4. Interpolation

The energy spectrum of the relative Hamiltonian is calculated only in the high- and low-field limits. To obtain the spectra of the interacting system in a magnetic field of arbitrary strength, we interpolate between both field limits by proposing the following formula:

$$E_r = \frac{E_\ell G + E_s G^{-1}}{G + G^{-1}}, \tag{23}$$

where

$$G = \frac{(|m| + 1)\omega_{eff}}{2} \tag{24}$$

and E_ℓ and E_s are the eigenenergies in strong-field Eq. (11) and the low-field limits of Eq. (21), respectively.

We would like to mention that our proposed interpolation formula Eq. (23) is an improved version of the one which has been suggested recently by Taut [15]. The only difference, yet very important, between our formula and Taut's is in the form of G-function. Taut considered G as a function of the effective frequency ω_{eff}, while ours is a function of the azimuthal quantum number m in addition to ω_{eff}. We find that including the m-dependence significantly improves the eigenenergies. We will use this proposed interpolation formula to study the properties of the interacting electrons confined in the parabolic quantum dot. The accuracy of the quantum dot spectra produced by Eq. (23) will be tested against the exact results.

5. Results and Conclusions

Our numerical results are presented for QD made of GaAs. The material parameters are: electron effective mass $m^* = 0.067m_e$ and dielectric constant $K = 12.5$. With these parameters the effective Bohr radius $a^* = 98.7A^0$ and effective Rydberg $R^* = 5.83meV$. We have used the interpolation formula Eq. (23) to produce the eigenenergy states $|00; 0m>, m = 0, -1, -2, \ldots$ for interacting electrons parabolically confined in the quantum dot of size $\ell_0 = 3a^*$. The results are listed in Table 1 and also displayed in Fig.

1 (a). It is clear that the spectra of the interacting system exhibits energy level crossings. As the magnetic field strength increases the energy of the state $m = 0$ increases while the states with non-vanishing azimuthal quantum number m decrease leading to a sequence of different ground states. The first transition in the orbital momentum of the ground state, $m : 0 \rightarrow -1$, occurs at $\omega_c/\omega_0 \approx 0.6$. This is consistent with the exact results of Wagner et.al. [7] as shown in Figure 1 (b). In Table 2 we have calculated the energies taking into account the spin effect, $g^* = -0.44$. The Zeeman energy lowers the total energies of the states $|00 : 0m >$ with odd m-values while leaving the even-m states unchanged. Additional energy $\mu(N)$ is the energy required to add one more electron to the quantum dot, raising it from an $(N-1)$-electron ground state to an N-electron ground state. That is, we define $\mu(N) = E_N - E_{N-1}$, where E_N is the ground state energy of N-electron system [9, 19]. The addition spectrum of a QD in a magnetic field using capacitance spectroscopy technique is measured by Ashoori et.al. [6].

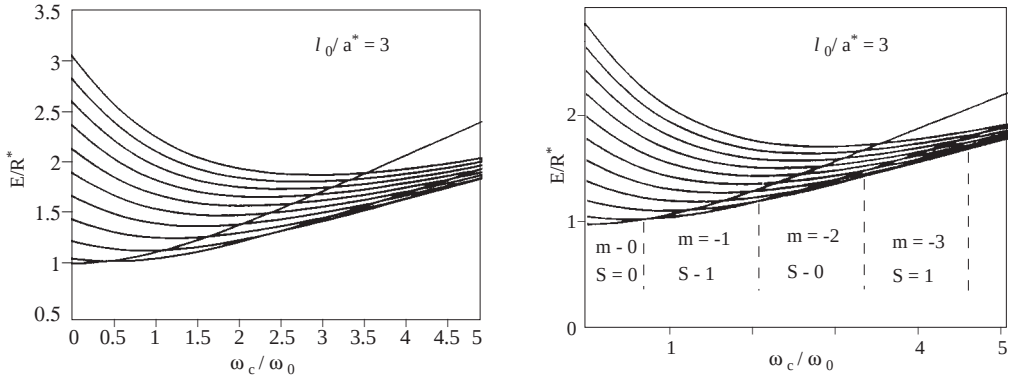

Figure 1. The eigenenergies of the states $|00; 0m >$, for interacting electrons parabolically confined in the quantum dot of size $\ell_0 = 3a^*$ and $g^* = 0.0$. a) Present work ($m = 0, -1, -2, \ldots, -9$) and b) Wagner's et.al., Ref. (7), ($m = 0, -1, -2, \ldots, -10$)

The cusps, which appeared, in the addition spectrum of the QD is due to the transitions in the spin and to the transitions in the relative motion for the quantum dot [18]. More discussion and experimental results can be found in a very recent review article by Ashoor and references there in [7]. Table 3 shows the spectra of the quantum dot using Taut's interpolation and for $g^* = 0.0$.

To test the accuracy of our interpolation scheme, we have compared our results with exact ones [11, 30]. In addition to the obvious agreement between our results, displayed in Fig. (1a) and Wagner's et.al., shown in Fig. (1b), we have listed in Table 4 the energies for $m = 0, -1, -4$ and -9 using different works. For state $m = 0$, Taut's interpolation gives results which are in exact agreement with ours. This results is expected, since for

$m = 0$ case, the G-function Eq. (24) and the interpolation formula Eq. (23) reduce to Taut's interpolation. However, as m increases i.e., $m = -9$, Taut's result deviate significantly from the numerical ones while our interpolation formula gives good results. This accuracy can be clearly seen from Table 4. For example, the energies of the state $|00; 0-9>$, calculated at $\omega_c/\omega_0 = 5$, are 1.83, 1.95 and 9.18 produced by numerical work, Eq. (23) and Taut's formula, respectively.

Table 1. The eigenenergies (in units of R^*) for the states $|00; 0m>, m = 0, -1, \ldots, -10$, for two interacting electrons confined parabolically in the QD with size $\ell_0 = 3a^*$ and effective Lande' factor $g^* = 0$. The eigenenergies are obtained by using the interpolation formula, Eq. (23)

ω_c/ω_0	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
0	1.01	1.04	1.11	1.23	1.37	1.53	1.70	1.87	2.05	2.22	2.40
-1	1.05	1.02	1.05	1.11	1.19	1.30	1.41	1.53	1.66	1.79	1.91
-2	1.22	1.14	1.12	1.15	1.21	1.29	1.38	1.48	1.59	1.70	1.82
-3	1.43	1.30	1.24	1.24	1.27	1.33	1.41	1.50	1.59	1.70	1.80
-4	1.65	1.47	1.37	1.34	1.35	1.39	1.45	1.53	1.52	1.71	1.81
-5	1.88	1.65	1.51	1.45	1.44	1.46	1.51	1.57	1.65	1.74	1.83
-6	2.10	1.83	1.65	1.56	1.53	1.53	1.57	1.62	1.69	1.77	1.85
-7	2.33	2.00	1.79	1.67	1.62	1.61	1.63	1.67	1.73	1.80	1.88
-8	2.56	2.18	1.93	1.78	1.71	1.68	1.70	1.72	1.78	1.84	1.92
-9	2.78	2.36	2.07	1.89	1.80	1.76	1.75	1.78	1.82	1.88	1.95
-10	3.01	2.53	2.21	2.00	1.89	1.83	1.82	1.83	1.87	1.92	1.98

Table 2. The eigenenergies (in units of R^*) for the states $|00; 0m>, m = 0, -1, \ldots, -10$, for two interacting electrons confined parabolically in the QD with size $\ell_0 = 3a^*$ and effective Lande' factor $g^* = -0.44$. The eigenenergies are obtained by using the interpolation formula, Eq. (23)

ω_c/ω_0	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
0	1.01	1.04	1.11	1.23	1.37	1.53	1.70	1.87	2.05	2.22	2.40
-1	1.05	1.02	1.04	1.10	1.19	1.29	1.40	1.52	1.64	1.77	1.90
-2	1.22	1.14	1.12	1.15	1.21	1.29	1.38	1.48	1.59	1.70	1.82
-3	1.43	1.30	1.24	1.23	1.26	1.32	1.40	1.48	1.58	1.68	1.79
-4	1.65	1.47	1.37	1.34	1.35	1.39	1.45	1.53	1.62	1.71	1.81
-5	1.88	1.65	1.51	1.44	1.43	1.45	1.50	1.56	1.64	1.72	1.81
-6	2.10	1.83	1.65	1.56	1.53	1.53	1.57	1.62	1.69	1.77	1.85
-7	2.33	2.00	1.79	1.67	1.61	1.60	1.62	1.66	1.72	1.79	1.87
-8	2.56	2.18	1.93	1.78	1.71	1.68	1.69	1.72	1.78	1.84	1.92
-9	2.78	2.35	2.07	1.89	1.79	1.75	1.74	1.77	1.81	1.86	1.93
-10	3.01	2.53	2.21	2.00	1.89	1.83	1.82	1.83	1.87	1.92	1.98

In conclusion, we have proposed a formula to interpolate between the energies of the quantum dot in high- and low-field limits. The formula is implemented to obtain

the energy spectra of the quantum dot and show the transitions in the orbital angular momenta of the ground state as a function of a magnetic field of arbitrary strength. Our interpolation gives good results compared to the exact numerical works.

Table 3. The eigenenergies (in units of R^*) for the states $|00;0m>, m = 0, -1, \ldots, -10$, for two interacting confined parabolically in the QD with size $\ell_0 = 3a^*$ and for $g^* = 0.0$. The eigenenergies are obtained by using Taut's formula [12]

ω_c/ω_0	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0
0	1.01	1.04	1.11	1.23	1.37	1.53	1.70	1.87	2.05	2.22	2.40
-1	1.03	1.01	1.03	1.09	1.17	1.28	1.39	1.51	1.64	1.77	1.90
-2	1.25	1.17	1.16	1.20	1.27	1.36	1.47	1.59	1.71	1.83	1.95
-3	1.60	1.48	1.45	1.48	1.56	1.66	1.78	1.90	2.03	2.168	2.29
-4	2.08	1.92	1.88	1.92	2.02	2.15	2.30	2.44	2.56	2.73	2.86
-5	2.69	2.49	2.45	2.52	2.66	2.83	3.02	3.20	3.37	3.53	3.67
-6	3.42	3.20	3.17	3.28	3.47	3.71	3.94	4.16	4.37	4.55	4.71
-7	4.29	4.03	4.03	4.19	4.46	4.76	5.06	5.34	5.58	5.79	5.97
-8	5.28	5.00	5.02	5.26	5.61	6.01	6.38	6.73	7.02	7.26	7.46
-9	6.39	6.10	6.16	6.49	6.94	7.43	7.90	8.32	8.67	8.95	9.18
-10	7.64	7.33	7.45	7.87	8.44	9.05	9.62	10.1	10.5	10.8	11.1
								2	4	7	2

Table 4. The eigenenergies (in units of R^*) for two interacting electrons confined in the quantum dot of size $\ell_0 = 3a^*$ and for $g^* = 0.0$

m	0			-1			-4			-9		
ω_c/ω_0	a	b	c	a	b	c	a	b	c	a	b	c
0.5	0.97	1.04	1.04	1.01	1.02	1.01	1.38	1.47	1.92	2.17	2.36	6.10
1.0	1.04	1.11	1.11	1.00	1.05	1.03	1.28	1.37	1.88	1.90	2.07	6.16
2.0	1.26	1.37	1.37	1.16	1.19	1.17	1.26	1.35	2.02	1.64	1.80	6.94
4	1.83	1.70	1.70	1.61	1.53	1.64	1.54	1.62	2.56	1.69	1.82	8.67
5	2.13	2.40	2.40	1.87	1.91	1.90	1.73	1.81	1.86	1.83	1.95	9.18

a ≡ Numerical Results, Ref. [24]
b ≡ Present Interpolation
c ≡ Taut's Interpolation

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