Turk J Phys
32 (2008) , 79 – 84.

The Energy Spectrum of Two-Electron Semiconductor Quantum Dots

Mohammad K. ELSAID
Department of Physics, College of Sciences, University of Hail (UOH)
P.O.Box 2440, Hail, SAUDI ARABIA
e-mail: mkelsaid@uoh.edu.sa

Received 05.12.2007

Abstract

The ground-state properties of a two-dimensional quantum-dot are studied. We have used the shifted 1/N expansion method to solve the relative part Hamiltonian of two electrons confined in a quantum in the presence of an applied uniform magnetic field. The spin singlet-triplet transition in the ground state of the QD is shown. We have also displayed the singlet-triplet energy gap, $J = \Delta = E_T - E_S$, against the strength of the magnetic field for two electron quantum dot. Based on comparisons, the eigenenergies obtained by the shifted method are in excellent agreement with exact, variational, Hartree-Fock (HF) and Full-Configuration Interaction (FCI) methods.

Key Words: Quantum dots, Magnetic Field, Eigenenergies, Energy Gap Splitting.

PACS numbers: 73.21La,71.70Gm,03.65Ge

1. Introduction

Quantum dots (QDs), or artificial atoms, have been the subject of intense research studies over the last years for their potential applications in quantum information in which the spin is used as a qubit. These man-made quantum dots, fabricated in semiconductor quantum materials have attracted a great attention as a laboratory for investigations of few-body systems with high controllable parameters such as the electron number, confinement strength, and interaction repulsion. Different methods [1-3] have been used to investigate the energy spectrum and the correlation effects of the interacting electrons confined in a quantum dot under the effect of an applied magnetic field [4]. One of the most interesting features of electron correlation is the change of the spin and angular momenta structure in the ground state of the QD system in the presence of the magnetic field. The QD has the potential to serve as a qubit of a quantum computer since the magnetic field can be used to tune the transition in the spin of the ground state of the quantum dot from singlet ($S = 0$) to triplet ($S = 1$) state. Motivated by the accuracy of 1/N expansion method, we shall use in this work the shifted technique to compute the eigenenergies of the relative part Hamiltonian of two interacting electron quantum dot in zero and non-zero applied magnetic field. The singlet-triplet energy splitting J is also calculated. We have compared our computed results with the corresponding ones obtained by various techniques like: exact diagonalization method, variational method, Full-Configuration Interaction method, Hartree-Fock method and Laughlin-type variational wavefunction method [5-10].

Method of Solution

The effective-mass Hamiltonian for an interacting pair of electrons confined in a quantum-dot by a parabolic potential in a uniform magnetic field of strength B is given as,

$$H=\sum_{i=1}^{2}\left\{\frac{P_i^2}{2m^*}+\frac{1}{2}m\left[\omega_0^2+\frac{\omega_c^2}{4}\right]\rho_i^2+\frac{\omega_c}{2}L_i\right\}+\frac{e^2}{\kappa\left|\vec{\rho}_2-\vec{\rho}_1\right|}+g\mu_B BS_z, \tag{1}$$

where ω_0 is the confinement frequency, μ_B is the Bohr magneton and κ is the dielectric constant. The energy E is measured in units of $\hbar\omega_0\cdot$ λ is the dimensionless parameter defined as the ratio of the coulomb strength to the confining energy, $\lambda={}^{e^2\alpha}/_{\hbar\omega_0}$, where $\alpha=\sqrt{\frac{m\omega_0}{\hbar}}$ has the dimension of inverse length and $\gamma=\frac{\omega_c}{\omega_0}$. Upon introducing the standard coordinates and momenta transformation the Hamiltonian (H) can be decoupled to center-of-mass (H_R) and relative H_r parts. The Hamiltonian H_R is of a harmonic oscillator type with a well-known eigenenergies $E_{n_{cm}m_{cm}}=(2n_{cm}+|m_{cm}|+1)\hbar\omega_0$, $n_{cm}=0,1,2,....$, and $m_{cm}=0\pm1,\pm2,....$ The main issue in the present work is to solve the relative-part Hamiltonian H_r,

$$H_r=\frac{p^2}{2\mu}+\frac{1}{2}\mu\left[\omega_0^2+\frac{\omega_c^2}{4}\right]\rho^2+m\frac{\hbar\omega_0}{2}+\frac{e^2}{k\rho}+g\mu_B BS_z \tag{2}$$

by using the shifted 1/N expansion method. The steps to produce the eigenenergies by the shifted method are clearly presented in references [11-14] and will not be repeated here. Only the necessary expressions to compute the energies will be given. The energy eigenvalues in powers of ${}^{1}/_{\bar{k}}$ (up to third order) read as:

$$E_{n,m}=\frac{\lambda}{\rho_0}+\frac{1}{4}\left[1+\frac{\gamma^2}{4}\right]\rho_0^2-\frac{1}{2}\gamma\left|m_z\right|+\frac{\bar{k}^2}{4\rho_0}+\frac{1}{\rho_0^2}\left[\frac{(1-a)(3-a)}{4}+\alpha_1\right]+\frac{\alpha_2}{\bar{k}\rho_0^2}. \tag{3}$$

Parameters α_1 and α_2 are expressed in terms of Q,ϖ and quantum numbers n_r and m, given in reference [11]; $\bar{k}=N+2\left|m\right|-a$, where N is the spatial dimension, shift parameter $a=2-(2n_r+1)\varpi$ and $\varpi=\left[3+\frac{V''(\rho_0)}{V'(\rho_0)}\right]^{1}/_{2}$. The roots ρ_0 (where the effective potential has a minimum) are determined for particular quantum state $\left|n_r m\right\rangle$, ω_0 and ω_c through the relation

$$\left[2\rho_0^3V'(\rho_o)\right]^{\frac{1}{2}}=Q^{\frac{1}{2}}=\bar{k}=(2+2\left|m\right|-a). \tag{4}$$

After obtaining the roots,ρ_0, the eigenenergies can be computed using equation (3). n_r is the radial quantum number related to the principle (n) one by the standard relation: $n_r=n-|m|-1$.

Results and Discussion

Our computed results for quantum dot in zero and non-zero applied magnetic fields are presented in Tables 1 to 3 and Figures 1 and 2. We have listed, in Table 1, the ground state energies, in units of $\hbar\omega_0$, calculated by exact, variation, Laughlin-type variational wavefunction and shifted methods for various values of magnetic field strength ($\gamma=0,1,...,5$) and ratio parameter ($\lambda=0,1,...,5$). The angular momentum quantum number $(m)\,m_z$ is also mentioned. The energy results produced by 1/N method are given against various methods: exact, variational and Laughlin-type variation wavefunction. The calculated results show that the ground state energy of the system for $\gamma=0$ and $\lambda=0$ has, as usual, zero angular momentum, $m_z=0$. As we sweep the parameters γ and/or λ the angular momentum changes from $m_z=0$ to higher values indicating a spin singlet-triplet transition in the ground state of the quantum dot. An example, is for$\lambda=1$, the angular momentum changes from $m_z=0$ to $m_z=1$ as γ changes from 1 to 2. For high magnetic field range the angular momentum of the ground state jumps to higher values : $|m_z|=6$ at $\lambda=\gamma=5$. To make a comparison between our produced results and the recent ones given by Ciftja and

Table 1. The ground eigenenergies, in units of $\hbar\omega_0$, of the 2D quantum-dot helium as a function of a magnetic field strength γ and various coulomb to confining ratio parameter λcalculated by shifted 1/N methods against: exact, variational and Laughlin-type trial wave function [8].

$m_z = 0\lambda = 1\gamma = 0$		$m_z = 1\lambda = 2\gamma = 1$	$m_z = 1\lambda = 3\gamma = 1$	
Exact	3.00097	4.06684	4.60594	
Var.	3.00174	4.06704	4.60635	
1/N	2.9562	4.0626	4.6002	
Laughlin	3.25331	4.17932	4.84193	
$m_z = 1\lambda = 1\gamma = 2$		$m_z = 1\lambda = 2\gamma = 2$	$m_z = 2\lambda = 4\gamma = 2$	
Exact	3.95732	4.61879	5.73642	
Var.	3.95737	4.61899	5.73655	
1/N	3.9549	4.6138	5.7349	
Laughlin	3.98787	4.73309	5.89253	
$m_z = 1\lambda = 1\gamma = 3$		$m_z = 2\lambda = 2\gamma = 3$	$m_z = 3\lambda = 4\gamma = 3$	$m_z = 4\lambda = 6\gamma = 3$
Exact	4.71894	5.43123	6.53522	7.46782
Var.	4.71899	5.43127	6.53525	7.46785
1/N	4.7162	5.4305	6.5350	7.4901
Laughlin	4.74972	5.47320	6.61737	7.57749
$m_z = 1\lambda = 1\gamma = 4$		$m_z = 2\lambda = 2\gamma = 4$	$m_z = 3\lambda = 3\gamma = 4$	$m_z = 4\lambda = 4\gamma = 4$
Exact	5.61430	6.30766	6.89002	7.41600
Var.	5.61435	6.30769	6.89004	7.41601
1/N	5.6122	6.3068	6.8898	7.4159
Laughlin	5.64527	6.34988	6.93735	7.46625
$m_z = 5\lambda = 6\gamma = 4$		$m_z = 0\lambda = 0\gamma = 5$	$m_z = 2\lambda = 1\gamma = 5$	$m_z = 3\lambda = 2\gamma = 5$
Exact	8.34530	5.38516	6.53067	7.22681
Var.	8.34532	5.38516	6.53068	7.22683
1/N	8.3833	5.3852	6.5303	7.2267
Laughlin	8.41976	5.38516	6.54155	7.24827
$m_z = 4\lambda = 3\gamma = 5$		$m_z = 5\lambda = 4\gamma = 5$	$m_z = 6\lambda = 5\gamma = 5$	
Exact	7.81384	8.33874	8.82281	
Var.	7.81385	8.33875	8.82282	
1/N	7.8139	8.3387	8.8828	
Laughlin	7.84253	8.37252	8.86033	

Faruk in reference [8], we have displayed in Figure 1 the roots (ρ_0) of the QD-ground states as a function of λ for $\gamma = 0$ and 1. The authors in reference [8] have plotted the mean square distance between the electrons in the QD against λ for the same values of γ. In fact both figures have shown the same crossing behaviour. This type of crossing between $\gamma = 0$ and $\gamma = 1$ curves can be attributed to the transitions in the QD ground state and thus to the jump in the corresponding angular momentum quantum number. For example, at the overlapping value $\lambda \approx 2$ in our curve, the transition occurs and the angular momentum of the QD-ground state jumps from $m_z = 0$ at $\gamma = 0$ to $m_z = 1$ at $\gamma = 1$. The exact values of the roots are 1.9720 at $\gamma = 0$ and 2.1610 at $\gamma = 1$. Thus, the roots in our calculations give information a bout the transitions in the angular momentum of the QD ground state like the mean-square values in reference [8]. In Figure 2, we have also plotted the singlet-triplet splitting J $=\Delta = E_T - E_S$ as a function of magnetic field strength B for quantum dot system and for confinement energy $\hbar\omega_0 = 3meV$. We can obviously see the changes in the sign of J at different values of B. The sign change of J from positive to negative value at some

magnetic field is an essential feature for the quantum dot to serve as a quantum-gate in quantum computing. To check further the accuracy of 1/N shifted method, we have compared in Tables 2 and 3 our calculated results against the results computed by various methods. The results produced by exact, variational and Full-Configuration interaction methods are in very good agreement with the corresponding ones obtained by the shifted technique. On the other hand, the results produced by Hartree-Fock show a little deviation from the rest of all given methods [7-10].

Table 2. The ground state energies (in units of Hartree, 1H = $\hbar\omega_0$ = 11.857 meV) for four different methods: Perturbation E_0^p, analytical (variation) E_0^A, numerical E_0^N and shifted $E_0^{I/N}$ methods. The confining energy strength $\hbar\omega_\bullet = \hbar\omega_0 = 3.32$ meV (see reference [9]).

B(T)	E_0^p	E_0^A	E_0^N	$E_0^{I/N}$
0.0	1.22319	1.03223	1.02214	1.0354
0.5	1.23071	1.03930	1.02928	1.0417
1.0	1.25281	1.06012	1.05029	1.0605
1.5	1.28831	1.09361	1.08408	1.0909
2.0	1.33551	1.13821	1.12909	1.1310
2.5	1.39252	1.19223	1.18360	1.1791
3.0	1.45753	1.25396	1.24589	1.2341
3.5	1.52890	1.32193	1.31446	1.2937
4.0	1.60526	1.39485	1.38800	1.3576
4.5	1.68551	1.47168	1.46547	1.4245
5.0	1.76876	1.55158	1.54601	1.4934

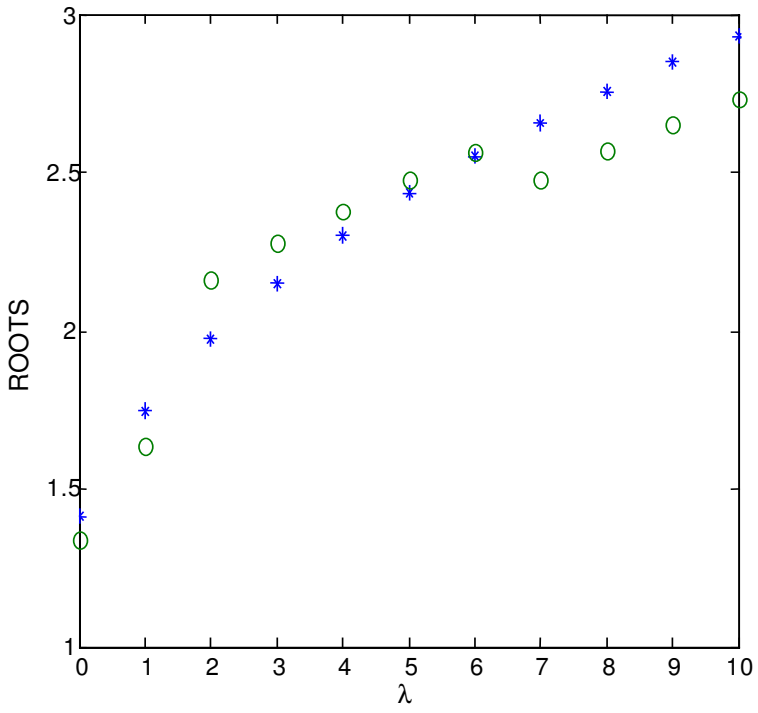

Figure 1. The roots (ρ_0) of the ground state energies against the coulomb ratio λ and field strength γ, (***: $\gamma = 0$; °°°: $\gamma = 1$).

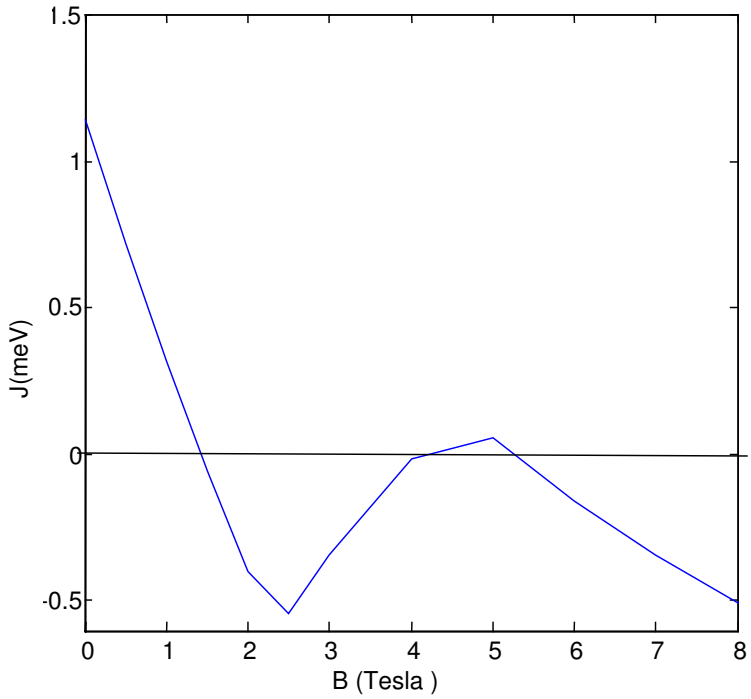

Figure 2. The triplet-singlet energy splitting (J in meV) for two electron quantum dot against the magnetic field (B in Tesla) for confinement strength $\hbar\omega_0 = 3$ meV. [Material parameters for GaAs are: $m^* = 0.067$ m_e, $\kappa = 12.4$, $R^* = 5.93$ meV, $a^* = 9.8$ nm, $g^* = -0.44$].

Table 3. The ground state energies $|00;00\rangle$ of the quantum-dot helium system are calculated for various range of ratio parameter λ. The results are computed by: perturbation theory, variational, exact diagonalization, full configuration interaction [10], Hartree-Fock [7] and 1/N methods.

λ	$\overset{(1)}{E}(\lambda)$	E(var.3)	E(diag.)	E(FCI)	E(HF)	E(1/N)
0	2.00000	2.00000	2.00000			2.0000
1	3.25331	3.00174	3.00097			2.9556
2	4.50663	3.72565	3.72143	3.7295	4.034	3.6706
3	5.75994	4.32576	4.31872			4.2739
4	7.01326	4.85637	4.84780	4.8502	5.182	4.8114
5	8.26657	5.34141	5.33224			5.3016
6	9.51988	5.79354	5.78429	5.7850	6.107	5.7580
7	10.7732	6.22032	6.21129			6.2069
8	12.0265	6.62674	6.61804	6.6185	6.930	6.6000
9	13.2798	7.01626	7.00795			7.0084
10	14.5331	7.39141	7.38351	7.3840	7.686	7.3700

Conclusions

In conclusion, we have studied the spectral properties of $2e$ QD-system in presence of an applied uniform magnetic field using the shifted 1/N expansion method. The ground state energies of the QD-helium are calculated for various values of magnetic field γ, and the wide range of ratio parameter λ. The spin singlet-triplet transition in the ground state of the QD system is also investigated. We have also computed the

singlet-triplet energy as a function of magnetic field strength. Based on comparisons with exact, numerical, variational and full-configuration interaction methods, the shifted 1/N expansion method gives excellent results for all ranges of magnetic field strength γ and ratio parameter λ of the QD system.

References

[1] P. A. Maksym, H. Imamura, G. P. Mallon and H. Aoki, *J. Physics: Condens. Matter*, **12**, (2000), R299**.**

[2] L. P. Kouwenhoven, D. G. Austing and T. Tarucha, *Rep. Prog. Phys.*, **64**, (2001), 701.

[3] S. M. Reimann and M. Manninen, *Rev. Mod. Phys.*, **74**, (2002), 1283.

[4] M. Wagner, U. Merkt, and A. V. Chapllik, *Phys. Rev.*, **B45**, (1992), 1951**.**

[5] G. Burkard, D. Loss and D. P. DiVincenzo, *Phys. Rev.*, **B59**, (1999), 2070.

[6] D. Loss and D. P. Di Vincenzo, *Phys. Rev.*, **A57**, (1998), 120.

[7] O. Ciftja and A. A. Kumar, *Phys. Rev.*, **B70**, (2004), 205326.

[8] O. Gifta and G. Faruk, *Phys. Rev.*, **B72**, (2005), 205334.

[9] B. Kandemir, *Phys. Rev.*, **B72**, (2005), 165350.

[10] M. Rotani, C. Cavazzoni, D. Beluucci and G. Goldoni, *J. Chem. Physics*, **124**, (2006), 124102.

[11] M. El-Said, *Semicond. Scien. Technol.*, **10**, (1995), 1310.

[12] T. Imbo and U. Sukhatme, *Phys. Rev.*, **D28**, (1983), 418; ibid, **31**, (1985), 2655.

[13] R. Dutt, Mukherji and Y. P. Varshni, *J. Phys.*, **B19**, (1986), 3411.

[14] M. El-Said, *Turk J Phys*, **26**, (2002), 331.