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The ground-state electronic properties of a quantum dot with a magnetic field

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Abstract
The ground-state energies of two interacting electrons, confined in a quantum dot (QD), are calculated. We have used the shifted $1/N$ expansion method to solve the relative part Hamiltonian of a QD presented in a uniform magnetic field. An energy expression for QD states in a magnetic field of arbitrary strength is given. The transitions in the angular momentum and spin of the QD ground state are also shown. Based on comparisons with the eigenenergies produced by various computational methods like: exact, Hartree–Fock (HF), local spin density approximation (LSDA), variational Monte Carlo (VMC) and diffusion Monte Carlo (DMC) methods, the shifted expansion method gives very good results.

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Quantum dots (QDs), or artificial atom, have been the subject of intense research studies over the last few years. The growing interests are motivated by the physical effects and potential device applications. In particular, the effects of an applied magnetic field on the states of the interacting electrons confined in QDs have been extensively studied. Different methods [1–31] have been used to investigate the energy spectrum and the correlation effects of the interacting electrons confined in a QD in the presence of an applied uniform magnetic field. Maksym and Chakraborty [6] have considered the eigenstates of interacting electrons, parabolically confined, in a QD in a magnetic field and show the transitions in the angular momentum of the ground states. They have used the heat capacity and magnetization as sensitive probes to these ground state transitions. Wagner *et al* [7] have also studied the same problem in addition to the spin and predict oscillations between spin-singlet (S) and spin-triplet (T) ground states. Taut [27] managed to obtain exact analytical results for the energy spectrum of two electrons interacting via coulomb force, confined in a QD, for specific values of the magnetic field. El-Said [28] have used the $1/N$ expansion technique to solve the QD-Hamiltonian and calculate the spectra of two interacting electrons for any arbitrary ratio of coulomb to confinement energies and gave an explanation to the phenomena of level crossings. Ciftja and Golam Faruk [29] and Kandemir [30] introduced trial wavefunction for two-dimensional QD helium and calculated variationally the energies of the ground state for all values of the magnetic field. The exact analytical solution of the two interacting electrons via coulomb force under the influence of parabolic potential is not attainable and thus the corresponding entire energy spectra is not possible. This QD-Hamiltonian belongs to a quasi-exactly solvable quantum mechanical type where only several eigenvalues and associated eigenstates are possible to calculate analytically. In a very recent study [31], Kandemir found the general closed-form expression for the eigenstates of the problem and its corresponding eigenenergies for particular values of the magnetic field and spatial confinement length. 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, in this case, 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 QD from singlet ($S = 0$) to triplet ($S = 1$) state, [29, 32]. The accuracy of the $1/N$ method obtained in our previous work [28] and its ability to explain the level ordering spectra in the QD greatly motivated us to use the shifted $1/N$ expansion method in order to solve the relative Hamiltonian part of two interacting electron QD-helium under the effect of an applied magnetic field. We shall compare our results against the corresponding ones produced by various computational methods like: exact, Hartree–Fock (HF), local spin density approximation (LSDA), variational Monte Carlo (VMC) and diffusion Monte Carlo (DMC), given very recently by Kandemir in [30].

The effective-mass Hamiltonian for two interacting electrons confined in a QD-helium by a parabolic potential in a uniform magnetic field of strength B, applied along z-axis, is given as

$$H = \sum_{i=1}^{2}\left\{\frac{p_i^2}{2m^*} + \frac{1}{2}m^*\left[\omega_0^2 + \frac{\omega_c^2}{4}\right]r_i^2 + \frac{\omega_c}{2}\hat{L}_{i_z}\right\} + \frac{e^2}{\kappa\,|\vec{r}_2 - \vec{r}_1|}, \tag{1}$$

where ω_0 is the confining frequency and κ is the dielectric constant for the GaAs medium. $\vec{r}_2$ and $\vec{r}_1$ describe the positions of the first and second electron in the xy-plane. $\omega_c = eB/m^*c$ is the cyclotron frequency and the symmetric gauge $\vec{A}_i = \frac{1}{2}\vec{B}\times\vec{r}_i$ is used in equation (1). Upon introducing the centre-of-mass (cm) $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$ and the relative coordinates $\vec{r} = \vec{r}_1 - \vec{r}_2$, the Hamiltonian in equation (1) can be decoupled to a centre-of-mass H_R and relative H_r parts. The cm-part is a harmonic oscillator type with well-known eigenenergies

$$E_{cm} = (2n_{cm} + |m_{cm}| + 1)\hbar\left[\omega_0^2 + \frac{\omega_c^2}{4}\right]^{1/2} + m_{cm}\frac{\hbar\omega_c}{2}, \tag{2}$$

where $n_{cm} = 0, 1, 2, \ldots$ and $m_{cm} = 0 \pm 1, \pm 2, \ldots$.

The main task in this study is to solve the relative Hamiltonian part

$$H_r = \frac{p^2}{2\mu} + \frac{1}{4}\left[\omega_0^2 + \frac{\omega_c^2}{4}\right]r^2 + \frac{e^2}{\kappa\,|\vec{r}|} + m\frac{\hbar\omega_c}{2}, \tag{3}$$

by using the shifted $1/N$ expansion method. The energy states of the Hamiltonian are labelled by the CM and the relative quantum numbers $|n_{cm}\, m_{cm};\, n_r\, m\rangle$. The steps to produce the eigenenergies by the shifted method are given in [33–35] and will not be repeated here. Only the necessary expressions to compute the energies will be presented. The energy eigenvalues in powers of $1/\bar{k}$ (up to third order) read as

$$E_{n,m} = E_0 + \frac{\bar{k}^2}{4r_0} + \frac{1}{r_0^2}\left[\frac{(1-a)(3-a)}{4} + \alpha_1\right] + \frac{\alpha_2}{\bar{k}r_0^2}, \tag{4}$$

where

$$E_0 = \frac{1}{r_0} + \frac{1}{4}\left[\omega_0^2 + \frac{\omega_c^2}{4}\right]r_0^2 + m\frac{\omega_c}{2}, \tag{5}$$

α_1 and α_2 are parameters expressed in terms of Q, ϖ and quantum numbers n_r and m, given in [28]. $\bar{k} = N + 2|m| - a$, where N is the spatial dimension, shift parameter $a = 2 - (2n_r + 1)\varpi$ and $\varpi = \left[3 + \left(V''(r_0)/V'(r_0)\right)\right]^{1/2}$. The roots r_0 (where the effective potential has a minimum) are determined for particular quantum state $|n_r\, m\rangle, \omega_0$ and ω_c, through the relation,

$$\left[2r_0^3 V'(r_0)\right]^{1/2} = Q^{1/2} = \bar{k} = (2 + 2|m| - a). \tag{6}$$

After obtaining the roots r_0, the eigenenergies can be computed using equation (4). n_r is the radial quantum number related to the principle (n) one by the standard relation: $n_r = n - |m| - 1$.

Our computed results for 2e QD are presented in tables 1–3. In table 1, we have listed the ground state energies, in units of $\hbar\omega_0 = 11.857$ meV for GaAs, for various values of magnetic field from zero to 5 T. The confining energy $\hbar\omega_0 = 3.32$ meV value has been used. Our energies produced by the shifted method are given against perturbation, variation and numerical methods. The comparison clearly shows very good agreement between the methods. In table 2, we have also compared the results of the ground state energy produced by various methods: HF, LSDA, VMC, DMC, variation, numerical and $1/N$. In addition to these comparisons we have tested, in table 3, our shifted method against exact and variational ones, published very recently by Ciftja and Golam Faruk [29], by computing the ground state energies for various values of field strength $\gamma = \omega_c/\omega_0$ and ratio parameter $\lambda = e^2\alpha/\hbar\omega_0$, where $\alpha = \sqrt{m\omega_0/\hbar}$ has the dimension of inverse length. Varying the parameters γ and λ, the angular momentum changes from $m_z = 0$ to higher values indicating a spin singlet–triplet transition in the QD. For fixed value of ratio parameter, $\lambda = 5$, the angular momentum of the

Table 1. The ground state energies (in units of $\hbar\omega_0 = 11.857$ meV) for four different methods: perturbation E_0^P, analytical E_0^A, numerical E_0^N and shifted $E_0^{1/N}$ methods. The confining energy $\hbar\omega_0 = 3.32$ meV [30].

$B(T)$	E_0^P	E_0^A	E_0^N	$E_0^{1/N}$
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	1.03961	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

Table 2. The ground state energy (in units of Hartree, $H^* = \hbar\omega_0 = 11.857$ meV) calculated by different methods taken from [30]: HF, LSDA, VMC, DMC, analytical variational method, numerical solution method and shifted $1/N$ method.

E_{HF}	E_{LSDA}	E_{VMC}	E_{DMC}	E_0^A	E_0^N	$E_0^{1/N}$
1.1420	1.04684	1.02165	1.02164	1.03223	1.02214	1.0354

Table 3. The ground state energies (in units of confining energy $\hbar\omega_0$) : E(exact), E(var.), and $E(1/N)$ of the 2D QD-helium as a function of magnetic field strength $\gamma = 0, 1, \ldots, 5$ and ratio parameter $\lambda = 1$ and 5, calculated by exact numerical diagonalization method, variational and shifted $1/N$ methods. The exact and two-parameters type variational wavefunction results are taken from tables 1 and 2 of [29], respectively. m_z is the angular momentum quantum number of the ground state.

		γ					
λ		0	1	2	3	4	5
1	m_z	0	0	1	1	1	2
	E(exact)	3.00097	3.30508	3.95732	4.71894	5.61430	6.53067
	E(var.)	3.00174	3.30578	3.95737	4.71899	5.61435	6.53068
	$E(1/N)$	2.9562	3.2566	3.9549	4.7162	5.6112	6.55303
5	m_z	0	1	2	3	4	6
	E(exact)	5.33224	5.58995	6.21499	7.01716	7.90109	6.82281
	E(var.)	5.34141	5.59088	6.21518	7.01722	7.90111	8.82282
	$E(1/N)$	5.3016	5.5821	6.2132	7.0167	7.9010	8.8228

ground state (m_z) changes in discrete manner, from $m_z = 0 \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 6$ as we vary the magnetic field strength γ from 0 to 5. These results are in very good agreement with [29].

In conclusion, we have studied the ground state properties of the 2e QD in the presence of an applied uniform magnetic field. The ground state energies of the QD are calculated for various values of field strength and ratio parameter. We have also shown the spin-single-triplet transition in the ground state of the QD. Based on comparisons with exact and variational methods, the shifted method gives very good results for all ranges of magnetic field strength and ratio parameter of the QD system.

References

[1] Drexler H *et al* 1994 *Phys. Rev. Lett.* **73** 2252
[2] Sikorski C and Merks U 1989 *Phys. Rev. Lett.* **62** 2164
[3] Demel T, Hietmann D, Grambow P and Ploog K 1990 *Phys. Rev. Lett.* **64** 788
[4] Lorke A, Kothaus J P and Ploog K 1990 *Phys. Rev. Lett.* **64** 2259
[5] Ashoori R C *et al* 1993 *Phys. Rev. Lett.* **71** 613
[6] Maksym P A and Chakraborty T T 1990 *Phys. Rev. Lett.* **65** 108
[7] Wagner M, Merkt U and Chapllik A V 1992 *Phys. Rev.* B **45** 1951
[8] Pfannkuche D and Gerhardts R R 1993 *Physica* B **189** 6
[9] De Groote J J S, Hornos J E M and Chaplik A V 1992 *Phys. Rev.* B **46** 12773
[10] Merkt U, Huser J and Wagner M 1991 *Phys. Rev.* B **43** 7320
[11] Pfannkuche D and Gerhardts R R 1991 *Phys. Rev.* B **44** 13132
[12] Zhu K D and Gu S W 1993 *Phys. Rev. Lett.* A **172** 296
[13] Jhonson N F and Payne M C 1991 *Phys. Rev. Lett.* **67** 1157
[14] Klama S and Mishchenko E G 1998 *J. Phys. Condens. Matter* **10** 601
[15] Zhu J L *et al* 1997 *Phys. Rev.* B **55** 15819
[16] Dineykhan M and Nazmitdinov R G 1997 *Phys. Rev.* B **55** 133707
[17] Bryant G 1987 *Phys. Rev. Lett.* **59** 1140
[18] Zhu J L, Kawazoe Y and Yao T 1999 *J. Phys.: Condens. Matter* **11** 299
[19] Anisimovas E and Matulis A 1998 *J. Phys.: Condens. Matter* **10** 601
[20] Matulis A and Peeters P M 1994 *J. Phys.: Condens. Matter* **6** 775
[21] Blanter Y M, Kaputkina N E and Lozovik Y E 1996 *Phys. Scri.* **54** 539
[22] Peeters F M and Schweigert V A 1996 *Phys. Rev.* B **53** 1468
[23] Oh J H, Huang K J, Ihm G and Lee S J 1996 *Phys. Rev.* B **53** 13264
[24] El-Said M 1995 *Semicond. Sci. Technol.* **10** 1310
[25] Nazmitdinov R G, Simonovic N S and Rost J M 2002 *Phys. Rev.* B **65** 155307
[26] Drouvelis P S, Schmelcher P and Diakonos F K 2004 *Phys. Rev.* B **69** 155312
[27] Taut M 1994 *J. Math. Phys. A: Math. Gen.* **27** 1045
Taut M *J. Math. Phys. A: Math. Gen.* **27** 4723
[28] El-Said M 2000 *Phys. Rev.* B **61** 13021
[29] Ciftja O and Golam Faruk M 2005 *Phys. Rev.* B **72** 205334
[30] Kandemir B S 2005 *Phys. Rev.* B **72** 165350
[31] Kandemir B S 2005 *J. Math. Phys.* **46** 032110
[32] Burkard G, Loss D and Faruk M G 2005 *Phys. Rev.* B **72** 205334
[33] Imbo T, Pagnamento A and Sukhatme 1984 *Phys. Rev.* D **29** 8763
[34] Imbo T and Sukhatme U 1983 *Phys. Rev.* D **28** 418
Imbo T and Sukhatme U *Phys. Rev.* D **31** 2655
[35] Dutt R, Mukherji U and Varshni Y P 1986 *J. Phys. B: At. Mol. Phys.* **19** 3411