Int J Theor Phys (2010) 49: 1187–1194
DOI 10.1007/s10773-010-0298-1

Ordering of Ground State Energy Levels of Two-Electron Quantum Dot in a Magnetic Field

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Received: 23 December 2009 / Accepted: 25 February 2010 / Published online: 19 March 2010

Abstract The energy levels structure of two interacting electrons in a parabolic quantum dot under an external magnetic field of arbitrary strength is studied via the asymptotic iteration method. The method gives accurate results over the full range of quantum dot parameters. A crossings between spin-singlet and spin-triplet ground states energies as a function of the magnetic field is predicted.

Keywords Quantum dot · Asymptotic iteration method

1 Introduction

Advances in semiconductor technology have made it possible to fabricate nano-structures called quantum dots (QDs) [1–3]. Currently, the size and the shape of these nano-structures and therefore the number of electrons they contain, can be precisely controlled and a small number of electrons per dot has been achieved experimentally [4, 5].

In most experiments, the electrons are tightly bound in the z-direction and has no freedom to move in this direction, so the dots can be viewed as two-dimensional disks, and the electrons to be bound laterally in the x–y plane by a harmonic oscillator potential [6].

The presence of discrete energy levels and even the manifestations of the shell structure which was predicted and experimentally observed for QDs give grounds for treating them as artificial atoms. The two-electron QD is the simplest example which turn out to be a useful system to trace the peculiarities of even intricate complexes. Effectively, it is possible to describe the typical features of transport processes, spin oscillations and correlation effects in the ground state of a two-electron QDs under the effect of applied magnetic field. In particular, transitions which never observed in the spectra of real atoms even at high applied magnetic field are readily seen for artificial ones. Moreover, the electrons in artificial atoms act lethargically, reluctant to displace themselves to make way for another electron, even on a timescale of milliseconds. Most strangely, the large Coulomb repulsion can make it seem

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that electrons attract one another. Thus, several experimental [7–11] and theoretical [12–20] methods were invested for the study of spectroscopic structure of interacting electrons in a harmonic QD under the effect of applied magnetic field. In particular, the spectral properties of a two-electron QD for any ratio of the electron–electron strength to the harmonic confinement provoke special interest [21–27]. In this work, we aim to show that the asymptotic iteration method (AIM) [28] which has been investigated by others [29–35] could give the spectroscopic structure of the relative motion of two interacting electrons at an arbitrary values of an applied magnetic field in a parabolic quantum dot, and could provide energy eigenvalues for potentials that have no analytical solutions for any quantum states.

With this in mind, this paper is organized as follows. In Sect. 2 we formulate the AIM for two interacting electrons in a two-dimensional harmonic QD under external magnetic field with Coulomb interaction. The analytical expressions for AIM are cast in such a way that allows the reader to use them without proceeding into their derivation. In Sect. 3 we explained how to obtain from AIM the energy eigenvalues numerically for any quantum dot state, and therein we present our results and give explanation for the ground state spin oscillations and ordering. Finally, the paper ends with a brief summary and concluding remarks on the method and our findings.

2 Formalism of the Problem

The Hamiltonian for two interacting electrons of charge $-e$ and effective mass m^* in a plane with a perpendicular magnetic field $\mathbf{B} = B\hat{\mathbf{u}}_z$ and a confining harmonic potential of length $\ell_0 = \sqrt{\hbar/(m^*\omega_0)}$ is

$$H = \sum_{i=1}^{2}\left[\frac{1}{2m^*}(\mathbf{p}_i + e\mathbf{A}_i)^2 + \frac{1}{2}m^*\omega_0^2 r_i^2\right] + \frac{e^2}{4\pi\epsilon\epsilon_0}\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}, \tag{1}$$

where $\mathbf{A}_i = \frac{\mathbf{B}}{2}(\mathbf{y}_i\hat{\mathbf{u}}_x - \mathbf{x}_i\hat{\mathbf{u}}_y)$ is the magnetic vector potential in the symmetric gauge.

By introducing the center-of-mass coordinates $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$, the total mass $M = 2m^*$, and charge $Q = 2e$, as well as the relative coordinates $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, $\mathbf{p} = (\mathbf{p}_1 - \mathbf{p}_2)/2$, the reduced mass $\mu = m^*/2$, and charge $q = e/2$ the above Hamiltonian can be separated into center-of-mass and the relative-motion terms as

$$H = \frac{[\mathbf{P} + Q\mathbf{A}(\mathbf{R})]^2}{2M} + \frac{1}{2}M\omega_0^2 R^2 + \frac{[\mathbf{p} + q\mathbf{A}(\mathbf{r})]^2}{2\mu} + \frac{1}{2}\mu\omega_0^2 r^2 + \frac{e^2}{4\pi\epsilon\epsilon_0}\frac{1}{r}. \tag{2}$$

The energy eigenvalues of (2) are the sum of the center-of-mass-energy and the energy of the relative motion. The solution of the former is very well known and is given by [12]

$$E_{N,M_\ell} = \hbar\tilde{\omega}(2N + |M_\ell| + 1) + \frac{\hbar\omega_c}{2}M_\ell, \tag{3}$$

where $\tilde{\omega} = \sqrt{\omega_0^2 + \omega_c^2/4}$ is the effective frequency, and $\omega_c = eB/m^*$ is the cyclotron frequency. $(N = 0, 1, 2, \ldots,)$ and $(M_\ell = 0, \pm1, \pm2, \ldots)$ are the radial and azimuthal quantum numbers, respectively.

On the other hand, the energy of the relative motion has quantum numbers n and m_ℓ and includes the electron–electron interaction. The corresponding Schrödinger equation for the relative motion is $H_r\Psi(r,\phi) = E_{n,m_\ell}\Psi(r,\phi)$, where

$$H_r = -\frac{1}{2\mu}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2}\right] + \frac{1}{2}\mu\tilde{\omega}^2 r^2 - \frac{i}{2}\omega_c\frac{\partial}{\partial\phi} + \frac{e^2}{4\pi\epsilon\epsilon_0}\frac{1}{r}. \tag{4}$$

This separability and the cylindrical symmetry of the problem allow us to write the two-particle wave function in plane polar coordinates $r = (r,\phi)$ in the form $\xi(r)e^{(im_\ell\phi)}$. The spatial part of the total wave function is symmetric or antisymmetric with respect to particle permutation ($\phi \to \phi + \pi$) for even, and odd azimuthal quantum number m_ℓ. Hence, upon the substitution of $\Psi(r,\phi) = r^{-1/2}\xi(r)e^{im_\ell\phi}$ and letting $r = \sqrt{2}\ell x$, the Schrödinger equation for the relative motion becomes

$$\frac{d^2\xi_{n,m_\ell}(x)}{dx^2} + \left(\varepsilon_{n,m_\ell} - x^2 - \frac{\gamma}{x} - \frac{m_\ell^2 - 1/4}{x^2}\right)\xi_{n,m_\ell}(x) = 0, \tag{5}$$

where $\varepsilon_{n,m_\ell} = (2E_{n,m_\ell} - \hbar m_\ell\omega_c)/\hbar\tilde{\omega}$ is the reduced energy, and $\ell^2 = (\hbar/m^*\tilde{\omega})$ is the effective length of the harmonic confinement. $\gamma = \sqrt{2}\ell/a^*$ is introduced to measure the ratio of the coulomb strength to the harmonic confinement, and $a^* = (4\pi\epsilon\epsilon_0\hbar^2/m^*e^2)$ is the effective Bohr radius.

To calculate the energy eigenvalues ε_{n,m_ℓ}, we insert the ansatz

$$\xi_{n,m_\ell}(x) = x^{(\frac{1}{2}-m_\ell)}e^{-x^2/2}f_{n,m_\ell}(x), \tag{6}$$

into (5). In this case, a new second-order homogeneous linear differential equation

$$f''_{n,m_\ell}(x) = 2\left(x - \frac{\frac{1}{2} - m_\ell}{x}\right)f'_{n,m_\ell}(x) + \left(\frac{\gamma}{x} + 2 - 2m_\ell - \varepsilon_{n,m_\ell}\right)f_{n,m_\ell}(x), \tag{7}$$

for $f_{n,m_\ell}(x)$ is obtained which is suitable for AIM application [28–35]. The systematic procedure of the AIM begins now rewriting (7) in the following form

$$f''_{n,m_\ell}(x) = \lambda_0(x)f'_{n,m_\ell}(x) + s_0(x)f_{n,m_\ell}(x), \tag{8}$$

where

$$\lambda_0(x) = 2\left(x - \frac{\frac{1}{2} - m_\ell}{x}\right), \quad \text{and} \quad s_0(x) = \left(\frac{\gamma}{x} + 2 - 2m_\ell - \varepsilon_{n,m_\ell}\right). \tag{9}$$

To find a general solution to this equation we rely on the symmetric structure of the right hand side of (8). Thus, if we differentiate (8) with respect to x, we obtain

$$f'''_{n,m_\ell}(x) = \lambda_1(x)f'_{n,m_\ell}(x) + s_1(x)f_{n,m_\ell}(x), \tag{10}$$

where $\lambda_1(x) = \lambda'_0(x) + s_0(x) + \lambda_0^2(x)$, and $s_1(x) = s'_0(x) + s_0(x)\lambda_0(x)$.

Likewise, the calculations of the $(k+1)^{th}$, and $(k+2)^{th}$ derivatives, $k = 1, 2, \ldots$, of (8) yield

$$f^{(k+1)}_{n,m_\ell}(x) = \lambda_{k-1}(x)f'_{n,m_\ell}(x) + s_{k-1}(x)f_{n,m_\ell}(x), \tag{11}$$

and

$$f_{n,m_\ell}^{(k+2)}(x) = \lambda_k(x) f'_{n,m_\ell}(x) + s_k(x) f_{n,m_\ell}(x), \tag{12}$$

respectively, where

$$\begin{aligned} \lambda_k(x) &= \lambda'_{k-1}(x) + s_{k-1}(x) + \lambda_0(x)\lambda_{k-1}(x), \quad \text{and} \\ s_k(x) &= s'_{k-1}(x) + s_0(x)\lambda_{k-1}(x). \end{aligned} \tag{13}$$

The ratio of the $(k+2)$th, and $(k+1)$th derivatives, can be expressed as

$$\frac{d}{dx}\ln\big(f_{n,m_\ell}^{(k+1)}(x)\big) = \frac{f_{n,m_\ell}^{(k+2)}(x)}{f_{n,m_\ell}^{(k+1)}(x)} = \frac{\lambda_k(f'_{n,m_\ell}(x) + \frac{s_k(x)}{\lambda_k(x)} f_{n,m_\ell}(x))}{\lambda_{k-1}(f'_{n,m_\ell}(x) + \frac{s_{k-1}(x)}{\lambda_{k-1}(x)} f_{n,m_\ell}(x))}, \tag{14}$$

and for sufficiently large k, one can now introduce the "asymptotic" aspect of the method, that is

$$\frac{s_k(x)}{\lambda_k(x)} = \frac{s_{k-1}(x)}{\lambda_{k-1}(x)} \equiv \varrho(x). \tag{15}$$

3 Numerical Results for the Energy Eigenvalues of Two Interacting Electrons in a Parabolic Quantum Dot

Within the framework of the AIM mentioned in the above section, the energy eigenvalues of two interacting electrons in a parabolic quantum dot ε_{n,m_ℓ} are calculated by means of (15). To obtain the energy eigenvalues the iterations should be terminated by imposing a condition $\delta_k(\varepsilon_{n,m_\ell}, x)= 0$ as an approximation to (15). With several symbolic mathematical programs available (Maple, or Mathematica), the computation of the energy eigenvalues by means of (15) is merely a straightforward calculation, even for the higher iteration steps. On the other hand, for each iteration, the expression $\delta_k(\varepsilon_{n,m_\ell}, x) = s_k(\varepsilon, x)\lambda_{k-1}(x) - s_{k-1}(\varepsilon, x)\lambda_k(x)$ depends on two variables namely ε_{n,m_ℓ}, and x. The calculated energy eigenvalues ε_{n,m_ℓ} by means of this condition should, however, be independent of the choice of x. Nevertheless, the right choice of x usually accelerates the rate of convergence to the eigenvalues within a reasonable number of iterations, as well as for the stability of the process. For this purpose, the inflection point of the total potential is chosen to be the value of $x = 3.0$ [35].

The results of the $\varepsilon_{n,m_\ell}(AIM)$ of two interacting electrons in a parabolic quantum dot with different values of γ, and m_ℓ are reported in Tables 1, 2, 3 and 4. In the tables, for comparison purposes, the energy eigenvalues for the ground state and excited states are displayed together with the ones which comes out from direct numerical integration $\varepsilon_{n,m_\ell}(exact)$ [23], the WKB-approximation [21–23], and shifted $1/N$ expansion technique [20] results.

Usually, the spin of the two electrons leads to an additional Zeeman energy

$$E_{spin} = g^*\mu_B B S_z = g^*\frac{m^*}{m_e}\frac{\hbar\omega_c}{2}S_z, \tag{16}$$

with $S_z = (1-(-1)^{m_\ell})/2$, g^* is the effective Landé factor, and μ_B is the Bohr magneton. Thus triplet states split into three distinct levels, while singlet states remain unchanged. However, in this work we ignore the contribution of the two electrons spin.

Table 1 The ground state energy eigenvalues for two interacting electrons confined in a quantum dot with different values of parameter γ, calculated by different methods; direct numerical integration method (exact) [23], $1/N$ expansion method [20], WKB approximation [21] compared with AIM results for different quantum states $|n;m\rangle$ expressed in units of $\hbar\omega_0/2$

$\|n,m\rangle$	Exact	$1/N$	WKB	AIM
$\gamma = 1$				
$\|0,0\rangle$	3.49652	3.4234	3.6898	3.49652
$\|0,-1\rangle$	4.8553	4.8524	4.8720	4.85534
$\|0,-2\rangle$	6.6538	6.6535	6.6583	6.65384
$\|0,-3\rangle$	8.5485	8.5484	8.5503	8.54846
$\|0,-4\rangle$	10.4814	10.4814	10.4824	10.4814
$\|0,-5\rangle$	12.4340	12.4340	12.4346	12.4340
$\|0,-6\rangle$	14.3983	14.3983	14.3986	14.3983
$\|0,-7\rangle$	16.3701	16.3701	16.3704	16.3701
$\|0,-8\rangle$	18.3472	18.3472	18.3473	18.3472
$\|0,-9\rangle$	20.3280	20.3280	20.3282	20.3280
$\gamma = 10$				
$\|0,0\rangle$	10.4816	10.4398	10.5220	10.4816
$\|0,-1\rangle$	10.8495	10.8341	10.8797	10.8495
$\|0,-2\rangle$	11.7903	11.7860	11.8078	11.7903
$\|0,-3\rangle$	13.0720	13.0717	13.0823	13.0720
$\|0,-4\rangle$	14.5546	14.5544	14.5611	14.5546
$\|0,-5\rangle$	16.1628	16.1629	16.1672	16.1628
$\|0,-6\rangle$	17.8543	17.8541	17.8573	17.8543
$\|0,-7\rangle$	19.6037	19.6037	19.6059	19.6037
$\|0,-8\rangle$	21.3954	21.3954	21.5342	21.3954
$\|0,-9\rangle$	23.2188	23.2188	23.2200	23.2188

Table 2 The first excited state energy eigenvalues for two interacting electrons confined in a quantum dot with different values of parameter γ, calculated by the direct numerical integration method (exact) [23] compared with AIM results for different quantum states $|n;m\rangle$ expressed in units of $\hbar\omega_0/2$

$\gamma = 1$			$\gamma = 10$		
$\|n,m\rangle$	Exact	AIM	$\|n,m\rangle$	Exact	AIM
$\|1,0\rangle$	7.2340	7.2340	$\|1,0\rangle$	14.0379	14.0380
$\|1,-1\rangle$	8.7594	8.75938	$\|1,-1\rangle$	14.4622	14.4622
$\|1,-2\rangle$	10.6024	10.6024	$\|1,-2\rangle$	15.4916	15.4916
$\|1,-3\rangle$	12.5154	12.5154	$\|1,-3\rangle$	16.8431	16.8431
$\|1,-4\rangle$	14.4579	14.4579	$\|1,-4\rangle$	18.3753	18.3753
$\|1,-5\rangle$	16.4163	16.4163	$\|1,-5\rangle$	20.0186	20.0186
$\|1,-6\rangle$	18.3843	18.3843	$\|1,-6\rangle$	21.7355	21.7355
$\|1,-7\rangle$	20.3587	20.3587	$\|1,-7\rangle$	23.5040	23.5040

Moreover, we investigate the ground state of two interacting electrons as a function of an arbitrary magnetic field strength. Since the center-of-mass quantum numbers N, M_ℓ and the quantum number m_ℓ are conserved by the Coulomb interaction, the ground state has the quantum numbers $N = 0$, $M_\ell = 0$, $n = 0$, $m_\ell \leq 0$, and only m_ℓ is to be determined. The important feature of the ground state to be discussed here is that its angular momentum $\hbar m_\ell$ does depend on the Coulomb interaction. Therefore, in Figs. 1 and 2 we have plotted the energy of the states $N = 0$, $M_\ell = 0$, $n = 0$, $m_\ell \leq 0$ for vanishing Landé factor $g^* = 0$ as a function of the ratio ω_c/ω_0 of cyclotron and oscillator frequency. In Fig. 1 we

Table 3 The excited state energy eigenvalues for two interacting electrons confined in a quantum dot with different values of parameter γ, calculated by the direct numerical integration method (exact) [23] compared with AIM results for different quantum states $|n;m\rangle$ expressed in units of $\hbar\omega_0/2$

$\gamma = 1$			$\gamma = 10$		
$\|n,m\rangle$	Exact	AIM	$\|n,m\rangle$	Exact	AIM
$\|2,0\rangle$	11.0848	11.0848	$\|2,0\rangle$	17.6671	17.6672
$\|2,-1\rangle$	12.6961	12.6961	$\|2,-1\rangle$	18.1420	18.1420
$\|2,-2\rangle$	14.5646	14.5646	$\|2,-2\rangle$	19.2438	19.2438
$\|2,-3\rangle$	16.4895	16.4895	$\|2,-3\rangle$	20.6504	20.6504
$\|2,-4\rangle$	18.4388	18.4388	$\|2,-4\rangle$	22.2217	22.2217
$\|3,0\rangle$	14.9850	14.9850	$\|3,0\rangle$	21.3513	21.3514
$\|3,-1\rangle$	16.6498	16.6498	$\|3,-1\rangle$	21.8721	21.8721
$\|3,-2\rangle$	18.5351	18.5351	$\|3,-2\rangle$	23.0339	23.0339

Table 4 The ground state energy eigenvalues $|0;0\rangle$ for two interacting electrons confined in a quantum dot with different values of parameter γ, calculated by $1/N$ expansion method [20], compared with AIM results expressed in units of $\hbar\omega_0/2$

γ	$1/N$	AIM
0.5	2.7654	2.80923
1.0	3.4234	3.49652
1.5	4.0088	4.09837
2.0	4.5421	4.63909
2.5	5.0360	5.13475
3.0	5.4998	5.59607
3.5	5.9361	6.03041
4.0	6.3544	6.44293
4.5	6.7527	6.83740
5.0	7.1343	7.21660

neglect the Coulomb interaction, $\gamma = 0$, and the $m_\ell = 0$ state is always the ground state. If however, we include the Coulomb interaction $\gamma \neq 0$ as in Fig. 2, the state $m_\ell = 0$ remains as a ground state only for low magnetic fields. Whenever, the magnetic field strength increases, the ground state shifts to the states with higher angular momentum while the states $m_\ell = -1, -2, -3, \ldots$ drop, thus leading to a sequence of different ground states $m_\ell = 0, -1, -2, -3, \ldots$ as the magnetic field is swept. Since the total spin of the two electrons is $S_z = (1-(-1)^{m_\ell})/2$, this entails an alternating sequence of singlet and triplet states. These changes are necessary to keep the total wave function of the fictitious particle state totally antisymmetric in accordance with the Pauli exclusion principle. For example, the first level crossing occurs at $\omega_c/\omega_0 \approx 1.0$. At this point, the ground state of the QD change from $m_\ell = 0$, $S_z = 0$ state to $m_\ell = -1$, and $S_z = 1$ state. The second crossing occurs at $\omega_c/\omega_0 \approx 1.5$ and the state (m_ℓ, S_z) quantum numbers change from $(-1, 1)$ to $(-2, 0)$ and so on. The spin changes from $S_z = 0$ to 1 and from $S_z = 1$ to 0 are known as spin oscillations. Thus, the spin of the quantum dot states oscillates between singlet ($S_z = 0$) and triplet ($S_z = 1$) states as the applied magnetic field B increases.

In conclusion, this work shows that the AIM is very easy to implement for calculating the energy eigenvalues of two interacting electrons in a parabolic quantum dot, and it is quite flexible in the sense that it works very well over the full range of parameter values. The spin oscillations and the ordering of ground state energy levels are easily predicted. Moreover, the obtained eigenvalues are not limited by the magnitude of n or m_ℓ, and they

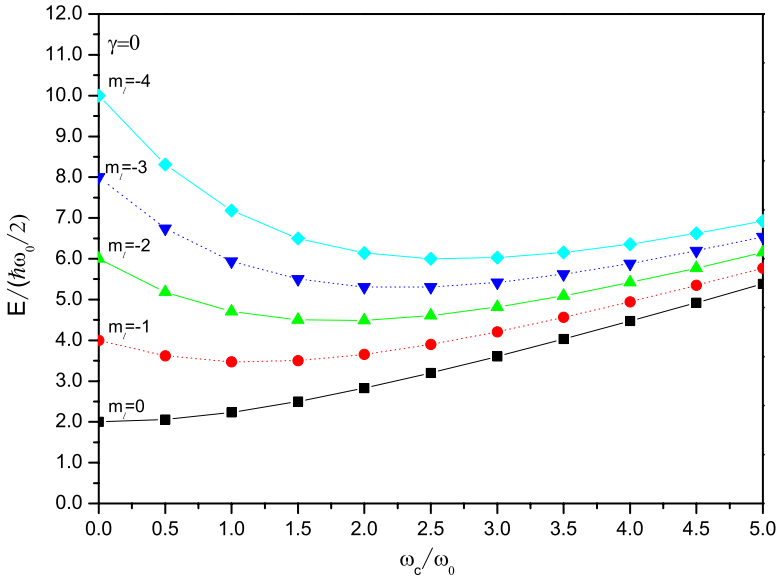

Fig. 1 The ground state energy eigenvalues for two interacting electrons confined in a quantum dot with $\gamma = 0$ vs the ratio ω_c/ω_0, calculated by AIM for quantum states $|0, m\rangle$, $m = 0, -1, -2, -3, -4$. *Solid lines* are singlet ($S_z = 0$) and *dot lines* are triplet ($S_z = 1$) states

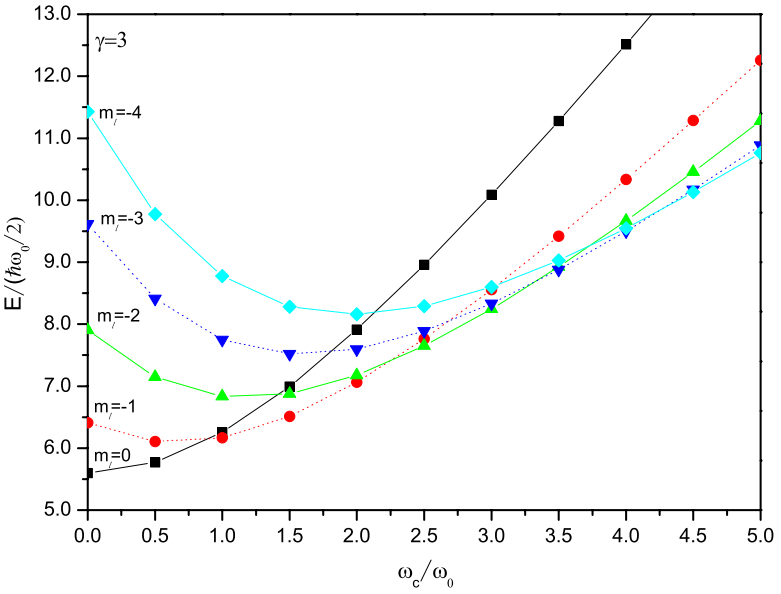

Fig. 2 The ground state energy eigenvalues for two interacting electrons confined in a quantum dot with $\gamma = 3$ vs the ratio ω_c/ω_0, calculated by AIM for quantum states $|0, m\rangle$, $m = 0, -1, -2, -3, -4$. *Solid lines* are singlet ($S_z = 0$) and *dot lines* are triplet ($S_z = 1$) states

are satisfying a simple ordering relation. Therefore, we can unambiguously select the correct starting energy eigenvalues.

Acknowledgement This work is supported by King Saud University, College of Science-Research center project No. (PHYS/2007/52).

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