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Low-energy states in a quantum dot obtained by the orbital integration method

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Abstract

The ground-state energy of two electrons in a harmonic quantum dot is obtained by using the recently developed orbital integration method. Compared to other analytical methods previously used to study this system, this method is much simpler and the result is more accurate. However, in this method we can directly calculate the ground-state energy without solving for the corresponding wavefunction. The ground-state energy is represented as a systematic series in an analytic form and it converges very fast in the range of experimental interest. We find that without a magnetic field the ground state always has the azimuthal quantum number $m_\phi = 0$; this result is at variance with a previous work. The critical magnetic field for spin-singlet–triplet crossing for a quantum dot made of GaAs is also obtained. In addition, on the basis of this method a new trial wavefunction for the ground state is also examined.

1. Introduction

The rapid progress in nanostructure technology has made solving the few-electron problems more urgent. In the last decade the energy levels of N electrons confined in a bulk of a solid with a magnetic field have been measured by various experimental approaches and a variety of new phenomena have been observed [1–8]. For theoretical studies, one of the most important problems is the two-electron quantum dot problem. Although there are only two electrons in the system with a confinement potential, it is not yet possible to find an exact analytical solution due to the presence of Coulomb interaction. Although accurate results could easily be obtained by numerical approaches like exact diagonalization [10–12], the series expansion method [13, 14], and the quantum Monte Carlo technique [18, 19], many groups are interested in finding a simple but accurate analytical method to gain insight into the competition between the confinement potential and the Coulomb repulsion. In addition to the conventional analytical methods such as Hartree approximation [9, 11], dimensional perturbation theory [15], and WKB treatment [16, 17], a new method was used by Dineykhon and Nazmitdinov [20, 21]. It provides a systematic approach. However, their method is rather complicated and one of

the conclusions—that even without a magnetic field the ground state may change from the state with azimuthal quantum number m_ϕ equal to zero to a state with a non-zero one just on changing the confinement potential—is quite counterintuitive, and it disagrees with our result presented below.

In this paper we use a newly developed method, the orbital integration method (OIM) [22], to study this problem. The method is shown to be quite simple and straightforward, representing the energy as a series in the inverse of potential strength. The series is shown to converge fast. Furthermore, the critical magnetic field for a singlet–triplet transition of the ground state [2, 4, 10, 23] is also calculated and is shown to be in good agreement with exact numerical calculations. In addition, a trial wavefunction for this system is also presented. We also applied this method to a three-dimensional harmonic quantum dot to demonstrate the simplicity and generality of the method.

2. Introduction to the orbital integration method

The OIM invented by Friedberg *et al* [22, 25] proposed a set of relations between the low-lying state wavefunction, the potential, and the energy. This method is applicable to a system with potential V satisfying the condition $V \geq 0$ throughout the entire space. There is at least one r_0 such that $V(r_0) = 0$. The method could also treat a potential with degenerate minima. We shall only consider the non-degenerate case. Here we will only briefly sketch the method. Details can be found in [22] and [25].

Suppose that we have a system satisfying these requirements; the Schrödinger equation is

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi = E\Psi. \quad (1)$$

We may assume that

$$V(\vec{r}) = g^2 v(\vec{r}). \quad (2)$$

The ground-state wavefunction can be expanded as

$$\Psi(\vec{r}) = e^{-S(\vec{r})} \quad (3)$$

where

$$S(\vec{r}) = gS_0(\vec{r}) + S_1(\vec{r}) + g^{-1}S_2(\vec{r}) + \dots \quad (4)$$

The ground-state energy can also be expanded in a similar form as

$$E = gE_0 + E_1 + g^{-1}E_2 + \dots \quad (5)$$

In an appendix we show that the particular choice of the series of values of g for equations (4) and (5) might be understood in terms of a dimensional argument. Substituting equations (2)–(5) into equation (1), and equating the coefficients of g^{-n} on both sides, we have

$$g^2: \quad (\vec{\nabla}S_0) \cdot (\vec{\nabla}S_0) = \frac{2m}{\hbar^2}v \quad (6)$$

$$g^1: \quad \frac{\hbar^2}{m}(\vec{\nabla}S_0) \cdot (\vec{\nabla}S_1) = \frac{\hbar^2}{2m}\nabla^2 S_0 - E_0 \quad (7)$$

$$g^0: \quad \frac{\hbar^2}{m}(\vec{\nabla}S_0) \cdot (\vec{\nabla}S_2) = \frac{\hbar^2}{2m}(\nabla^2 S_1 - (\vec{\nabla}S_1)^2) - E_1 \quad (8)$$

$$g^{-1}: \quad \frac{\hbar^2}{m}(\vec{\nabla}S_0) \cdot (\vec{\nabla}S_3) = \frac{\hbar^2}{2m}(\nabla^2 S_2 - 2(\vec{\nabla}S_1) \cdot (\vec{\nabla}S_2)) - E_2. \quad (9)$$

If S_0 depends only on one variable, equation (6) becomes $\nabla S_0 = \pm\sqrt{(2m/\hbar^2)v}$, where the sign is defined as + for $r > r_0$ and - for $r < r_0$. Because $\nabla S_0|_{r=r_0} = 0$, E_0 is chosen to make the right-hand side of equation (7) vanishing at $r = r_0$; otherwise, ∇S_1 will diverge at $r = r_0$, which is unsuitable for the ground state. Therefore we have

$$E_0 = \frac{\hbar^2}{2m} \nabla^2 S_0|_{r=r_0}. \quad (10)$$

Once E_0 and ∇S_0 are known, $\vec{\nabla} S_1$ can be obtained from equation (7). Consequently, we can determine E_1 from the relation $E_1 = (\hbar^2/2m)(\nabla^2 S_1 - (\vec{\nabla} S_1)^2)|_{r=r_0}$. By repeating the same steps, all E_n and $\vec{\nabla} S_n$ can be determined uniquely. As a result, we obtain not only the ground-state energy but also the wavefunction, if $\{\vec{\nabla} S_n\}$ can be integrated. In the following sections we will apply this method to a quantum dot problem.

3. The two-dimensional quantum dot

The Hamiltonian of two electrons in a two-dimensional parabolic confinement potential can be written as

$$H(\vec{r}_1, \vec{r}_2) = -\frac{\hbar^2}{2m^*} (\nabla_1^2 + \nabla_2^2) + \frac{m^* \omega_0^2}{2} (r_1^2 + r_2^2) + \frac{e^2}{\epsilon|\vec{r}_1 - \vec{r}_2|} \quad (11)$$

where ϵ is the effective dielectric constant, m^* and e are the effective mass and the charge of an electron respectively. We define the effective Bohr radius $a^* = \epsilon\hbar^2/m^*e^2$, the dot size $\ell_0 = \sqrt{\hbar/m^*\omega_0}$, and the effective Rydberg energy $R^* = e^2/2\epsilon a^*$. Then we may rewrite equation (11) in a simpler form with energy in units of the effective Rydberg energy R^* , length in units of the effective Bohr radius a^* , and the confinement potential described by the ratio of a^* to the dot size ℓ_0 : $\gamma = 2(a^*/\ell_0)^2 = \hbar\omega_0/R^*$ [15]:

$$H(\vec{r}_1, \vec{r}_2) = -(\vec{\nabla}_1^2 + \vec{\nabla}_2^2) + \frac{1}{4}\gamma^2(r_1^2 + r_2^2) + \frac{2}{|\vec{r}_1 - \vec{r}_2|}. \quad (12)$$

It can be separated into centre-of-mass (CM) and relative-mass (RM) coordinates as follows:

$$H_{\text{CM}}(\vec{R}) = -\frac{1}{2}\nabla_{\text{CM}}^2 + \frac{1}{2}\gamma^2 R^2 \quad (13)$$

$$H_{\text{RM}}(\vec{r}) = -2\nabla_{\text{RM}}^2 + \frac{1}{8}\gamma^2 r^2 + \frac{2}{r} \quad (14)$$

where the CM and RM coordinates are defined as $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$ and $\vec{r} = \vec{r}_1 - \vec{r}_2$ respectively. Since the equation for the CM part is exactly solvable, we will focus our attention on the RM part in this paper. The potential in equation (14) is $V(r) = \frac{1}{8}\gamma^2 r^2 + 2/r$. It is easy to find its minimum value $3/r_0$ at $r = r_0 = (8/\gamma^2)^{1/3}$. r_0 could be roughly considered as a mean separation distance between two electrons. Substituting r_0 into $V(r)$ and shifting the minimum of the potential by $-3/r_0$, we obtain a new potential $V'(r) = r^2/r_0^3 + 2/r - 3/r_0$. Thus the new equation that we want to solve is

$$(-2\nabla_{\text{RM}}^2 + V'(r))\Phi = E_{r'}\Phi \quad (15)$$

where $E_{r'} = E_{\text{RM}} - 3/r_0$. Now this equation satisfies the requirement of the OIM. Using planar polar coordinates and setting $v(r) = r^2/r_0^3 + 2/r - 3/r_0$ in equation (6), we have

$$\nabla_r S_0 = \sqrt{2r_0 r^2 + 4r_0^2 r} \frac{r - r_0}{2r_0^2 r} \quad (16)$$

$$\nabla_r S_1 = \frac{r^3 + 3r_0 r^2 + 3r_0^2 r - r_0^3}{2r(r + 2r_0)(2r^2 + 2r_0 r - r_0^2 + r\sqrt{3(r^2 + 2r_0 r)})} \quad (17)$$

and $E_0 = \sqrt{6}(1/r_0)^{3/2}$, $E_1 = (-1/9)(1/r_0)^2, \dots$. Substituting them into equation (5) and setting $g = 1$, we have

$$E_{\text{RM}} = 3 \left(\frac{1}{r_0} \right) \left(1 + \frac{\sqrt{6}}{3} \left(\frac{1}{r_0} \right)^{1/2} + \frac{-1}{27} \left(\frac{1}{r_0} \right) + \dots \right). \quad (18)$$

The ground-state energy is presented in a nice power series in $(1/r_0)^{1/2}$. Usually, in realistic quantum dots [2], the confinement potential is slightly less than the effective Rydberg energy, so γ is less than 1 and r_0 is greater than 2. Moreover, the coefficient C_n is also well behaved; thus E_{RM} converges very fast in the range of experimental interest. As a result, we can calculate the ground-state energy by iterative steps and obtain accurate answers with few terms.

Comparing equation (18) with the harmonic approximation used by Klama and Mishchenko [16], we find the first two terms to be the same in both methods. This is because the OIM also starts with a harmonic potential. But using the harmonic approximation, they will need to calculate higher-order perturbation terms to obtain the same accuracy as our method. This will be made clear later. Another advantage of this method is that most of the calculations here only involve simple integrations and algebra; coefficients in the series (equation (18)) could be obtained analytically. The formulation is also quite general and thus it could be easily extended to other cases such as inclusion of the magnetic field, and the three-dimensional quantum dot.

Next we consider the same system in the presence of a magnetic field. If the magnetic field is perpendicular to the xy -plane ($\vec{B} = B\vec{z}$) and the motion in the z -direction is frozen, the Hamiltonian can be written in terms of CM, RM coordinates and the Zeeman energy for spin:

$$H_{\text{CM}}(\vec{R}) = \frac{1}{2M} \left(-i\hbar \vec{\nabla}_{\text{CM}} + \frac{Q}{c} \vec{A} \right)^2 + m^* \omega_0^2 R^2 \quad (19)$$

$$H_{\text{RM}}(\vec{r}) = \frac{1}{2\mu} \left(-i\hbar \vec{\nabla}_{\text{RM}} + \frac{q}{c} \vec{A} \right)^2 + \frac{1}{4} m^* \omega_0^2 r^2 + \frac{e^2}{\epsilon r} \quad (20)$$

where $Q = 2e$, $q = e/2$, $M = 2m^*$, and $\mu = m^*/2$. Other symbols are defined as before. We choose the Coulomb gauge and the same units as were used in the previous section, so that equations (21) and (22) become

$$H_{\text{CM}}(\vec{r}) = -\frac{1}{2} \vec{\nabla}_{\text{CM}}^2 - \frac{i\gamma_m}{2} \frac{\partial}{\partial \phi_{\text{CM}}} + \frac{1}{2} \gamma'^2 R^2 \quad (21)$$

$$H_{\text{RM}}(\vec{r}) = -2\vec{\nabla}_{\text{RM}}^2 - \frac{i\gamma_m}{2} \frac{\partial}{\partial \phi_{\text{RM}}} + \frac{1}{8} \gamma'^2 r^2 + \frac{2}{r} \quad (22)$$

$$\gamma' = \sqrt{\gamma^2 + \frac{\gamma_m^2}{4}} \quad \gamma_m = \frac{\hbar\omega_c}{R^*}. \quad (23)$$

For the CM part, the exact eigenstates have been found to be

$$E_{\text{CM}} = (2N + |M_\phi| + 1)\gamma' + \frac{\gamma_m}{2} M_\phi \quad (24)$$

where N and M_ϕ are the radial and the azimuthal quantum numbers respectively for CM coordinates. For the relative coordinates, we also introduce the azimuthal quantum number m_ϕ , so the wavefunction is

$$\Phi(r, \phi) = e^{im_\phi \phi} \psi(r). \quad (25)$$

With this definition, we know that m_ϕ is associated with the spin state of the system. The system is in the triplet (singlet) state if m_ϕ is odd (even). Operating with H_{RM} on $\Phi(r, \phi)$ we get

$$(-2\vec{\nabla}_{\text{RM}}^2 + V(r))\psi(r) = \left(E_{\text{RM}} - \frac{\gamma_m}{2} m_\phi \right) \psi \quad (26)$$

$$V(r) = \frac{1}{8} \gamma'^2 r^2 + \frac{2}{r} + \frac{2m_\phi^2}{r^2} \quad (27)$$

Table 1. A list of the low-lying energy states with $\gamma = 1$ for a set of quantum numbers (m_ϕ, N, M_ϕ) obtained by our calculations up to fourth order, and exact numerical calculation and dimensional perturbation theory up to sixth order in [15] for a two-dimensional quantum dot without a magnetic field. The energy is in units of the effective Rydberg energy.

(N, M, m)	Ours	Reference [15]	Exact
(0, 0, 0)	3.3198	3.3188	3.3242
(0, 0, 1)	3.8280	3.8279	3.8279
(0, 1, 0)	4.3198	4.3188	4.3242
(0, 0, 2)	4.6436	4.6436	4.6437
(0, 1, 1)	4.8280	4.8278	4.8279
(1, 0, 0)	5.3198	5.3188	5.3242
(0, 0, 3)	5.5432	5.5432	5.5432
(0, 1, 2)	5.6436	5.6436	5.6436
(1, 0, 1)	5.8280	5.8279	5.8279
(1, 1, 0)	6.3198	6.3188	6.3242
(0, 0, 4)	6.4782	6.4782	6.4782
(1, 0, 2)	6.6436	6.6436	6.6436

Following the same method as in the previous section, we find

$$E_{RM} = \frac{\gamma_m}{2} m_\phi + \left(\frac{1}{4} \gamma^2 r_0^3 + 1 \right) r_0^{-1} + \sqrt{\gamma^2 r_0^3 - 2} r_0^{-3/2} + \frac{\gamma^2 r_0^3 - 24}{4(\gamma^2 r_0^3 - 2)^2} r_0^{-2} + \dots \quad (28)$$

where r_0 is the real and positive solution of the following equation:

$$\frac{1}{4} \gamma^2 r_0^4 - 2r_0 - 4m_\phi^2 = 0. \quad (29)$$

Including the additional Zeeman energy induced by spin, we obtain the total energy as

$$E = E_{CM} + E_{RM} + E_s \quad (30)$$

$$E_{CM} = (2N + |M_\phi| + 1)\gamma' + \frac{\gamma_m}{2} M_\phi \quad (31)$$

$$E_{RM} = \frac{\gamma_m}{2} m_\phi + \left(\frac{1}{4} \gamma^2 r_0^3 + 1 \right) r_0^{-1} + \sqrt{\gamma^2 r_0^3 - 2} r_0^{-3/2} + \frac{\gamma^2 r_0^3 - 24}{4(\gamma^2 r_0^3 - 2)^2} r_0^{-2} + \dots \quad (32)$$

$$E_s = \frac{g^* \gamma_m m^*}{4 m_e} (1 - (-1)^{m_\phi}) m_s \quad (33)$$

$$r_0 = \frac{\alpha + \sqrt{16/(\alpha \gamma^2) - \alpha^2}}{2}$$

$$\alpha = \sqrt{\left(\frac{32}{\gamma'^4} + 32 \sqrt{\frac{1}{\gamma'^8} + \frac{256m_\phi^6}{27\gamma'^6}} \right)^{1/3} + \left(\frac{32}{\gamma'^4} - 32 \sqrt{\frac{1}{\gamma'^8} + \frac{256m_\phi^6}{27\gamma'^6}} \right)^{1/3}} \quad (34)$$

$$E_s = \frac{g^* m^*}{4 m_e} (1 - (-1)^{m_\phi}) m_s \gamma_m \quad (35)$$

where g^* is the effective Landé factor, m_s is the magnetic spin quantum number, and $m_s = 0$ for singlet states, $m_s = -1, 0, 1$ for triplet states. Note that the spectrum considered here does not include the excited states with radial quantum numbers of RM $n \neq 0$. The method of treating this part by the OIM is under development [25].

Tables 1 and 2 list the low-lying energy states with two different γ -values for a set of quantum numbers (m_ϕ, N, M_ϕ) obtained by our calculations up to fourth order, exact numerical calculations, and the dimensional perturbation theory used in [15] for zero magnetic field. We found for $\gamma = 0.05$ that both sets of results are very accurate, while for $\gamma = 1$ our result

Table 2. As table 1, except that here $\gamma = 0.05$.

(N, M, m)	Ours	Reference [15]	Exact
(0, 0, 0)	0.2963	0.2963	0.2963
(0, 0, 1)	0.3062	0.3062	0.3062
(0, 1, 0)	0.3463	0.3463	0.3463
(0, 0, 2)	0.3311	0.3311	0.3311
(0, 1, 1)	0.3562	0.3562	0.3562
(1, 0, 0)	0.3963	0.3963	0.3963
(0, 0, 3)	0.3644	0.3644	0.3644
(0, 1, 2)	0.3811	0.3811	0.3811
(1, 0, 1)	0.4062	0.4062	0.4062
(1, 1, 0)	0.4463	0.4463	0.4463
(0, 0, 4)	0.4025	0.4025	0.4025
(1, 0, 2)	0.4311	0.4311	0.4311

slightly deviates from the exact numerical calculation for $m_\phi = 0$. This deviation results from the small ratio of r_0 to a^* for $m_\phi = 0$ and we may reduce it by including the next-order correction. The typical experimental value of γ is usually less than 1, and even for $\gamma = 1$ our energy deviates from the exact result by less than 0.6%. Given the simplicity of the method, the result is already surprisingly accurate.

Next we discuss the energy spectrum in the presence of a magnetic field. Since non-zero M_ϕ will always increase E_{CM} , the ground state must have the quantum number $M_\phi = 0$. According to equations (32)–(37), we found that if the magnetic field is absent, the ground state always has $m_\phi = 0$. If the magnetic field is applied, the ground state may no longer have $m_\phi = 0$. The energy of states with $N = M_\phi = n = 0$, $m_\phi \leq 0$ as a function of magnetic field without considering the additional Zeeman energy (i.e. setting $g^* = 0$) is plotted in figure 1 for $\ell_0/a^* = 2$ and $\ell_0/a^* = 4$ up to fourth order. As we have seen, the ground state is oscillating between singlet and triplet states as a function of field strength. If the additional Zeeman energy is considered and g^* is large enough, the ground state clearly favours more states with $m_\phi = -1, -3, \dots$. When the magnetic field is strong enough, the spins of the two electrons will tend to be antiparallel to the magnetic field, and the triplet state is favoured. Figure 2 shows the resulting spectrum with $g^* = 2$ for $\ell_0/a^* = 2$ and $\ell_0/a^* = 4$ up to fourth order. These results are in good agreement with numerical analysis [7, 18]. For a typical experiment, the magnitude of the confinement potential is about $\hbar\omega_0 = 5.4$ meV and the effective parameters for GaAs conduction band electrons are $R^* = 5.8$ meV, $g^* = -0.44$. The spectrum for this case is plotted in figure 3, and we found that the singlet–triplet crossing occurs at $\omega_c/\omega_0 = 1.085$, which corresponds to $B = 3.383$ T. This result is in good agreement with exact numerical calculation [2].

4. The three-dimensional quantum dot

Recently the three-dimensional quantum dot has been fabricated successfully [24]. Hence it is useful to obtain the energy spectrum. All the formalisms are still valid here except that we use spherical polar coordinates instead of planar coordinates. Using the same definition as before, we obtained the energy spectrum:

$$E_{CM} = (2N + |L| + \frac{3}{2})\gamma \quad (36)$$

$$E_{RM} = \left(\frac{1}{4}\gamma^2 r_0^3 + 1 \right) r_0^{-1} + \sqrt{\gamma^2 r_0^3 - 2} r_0^{-3/2} + \frac{(2\gamma^4 r_0^6 - 7\gamma^2 r_0^3 - 16)}{4(\gamma^2 r_0^3 - 2)^2} r_0^{-2} + \dots \quad (37)$$

$$r_0 = \frac{\beta + \sqrt{16/(\beta\gamma^2) - \beta^2}}{2} \quad (38)$$

$$\beta = \sqrt{\left(\frac{32}{\gamma^4} + 32\sqrt{\frac{1}{\gamma^8} + \frac{256\ell^3(\ell+1)^3}{27\gamma^6}}\right)^{1/3} + \left(\frac{32}{\gamma^4} - 32\sqrt{\frac{1}{\gamma^8} + \frac{256\ell^3(\ell+1)^3}{27\gamma^6}}\right)^{1/3}} \quad (39)$$

$$\gamma = 2\left(\frac{a^*}{\ell_0}\right)^2 = \frac{\hbar\omega_0}{R^*} \quad \ell_0 = \sqrt{\frac{\hbar}{m^*\omega_0}} \quad (40)$$

where L is the orbital angular quantum number of CM motion and ℓ is that of RM motion. Table 3 lists the energy spectrum with $\gamma = 1$ and 0.05. The radial excitations in the relative coordinates are not included here.

5. The variational wavefunction

From equation (16), we found $\nabla_r S_0$ to be integrable:

$$S_0(r) = \frac{\sqrt{2}}{4}r_0^{-3/2}\sqrt{(r^2+2r_0r)}(r-r_0) - \frac{3\sqrt{2}}{2}r_0^{1/2}\ln\left(\sqrt{\frac{r}{r_0}} + \sqrt{\frac{r}{r_0}+2}\right) + \frac{3\sqrt{2}}{2}r_0^{1/2}\ln(1+\sqrt{3}). \quad (41)$$

According to the formalism of the OIM, the maximum of e^{-S_0} occurs at $r = r_0$, which is also the position of minimum potential energy. However, this cannot be correct for the true ground state of this system as the potential is asymmetrical. Thus it is reasonable to take r_0 as a variational parameter and introduce another parameter a to adjust the weight. Thus we propose a trial wavefunction $e^{-S(r)}$ with variational parameters a, b and the following functional form of $S(r)$:

$$S(r) = a\left(\frac{\sqrt{2}}{4}b^{-3/2}\sqrt{(r^2+2br)}(r-b) - \frac{3\sqrt{2}}{2}b^{1/2}\ln\left(\sqrt{\frac{r}{b}} + \sqrt{\frac{r}{b}+2}\right) + \frac{3\sqrt{2}}{2}b^{1/2}\ln(1+\sqrt{3})\right). \quad (42)$$

Table 4 lists the optimized variational energies for $\gamma = 1$ and 0.05. We find the result to be closer to the exact energy for small γ . We believe that the larger deviation for $\gamma = 1$ is due to the large weight at small r in this trial wavefunction. When γ is closer to 1, r_0 is only about 2 and the two electrons have a larger probability of being fairly near to each other. This trial wavefunction is not quite correct for small r ; the cusp condition at $r = 0$ is not satisfied for equations (43). We could probably correct this error by introducing new variational parameters. For practical purposes, the result obtained is already quite satisfactory.

6. Conclusions

As pointed out by Friedberg *et al* [22], an important advantage of this OIM is that it is an analytical method. It provides new insights that are difficult to obtain from numerical approaches. For example, without including the Zeeman energy the switching of the ground state from a singlet to a triplet state when the magnetic field increases is not quite obvious. Here we have a simple way to understand it. In our approach, energy is expressed as a series in $(1/r_0)^{1/2}$. As the magnetic field is absent, non-zero m_ϕ will always increase the minimum

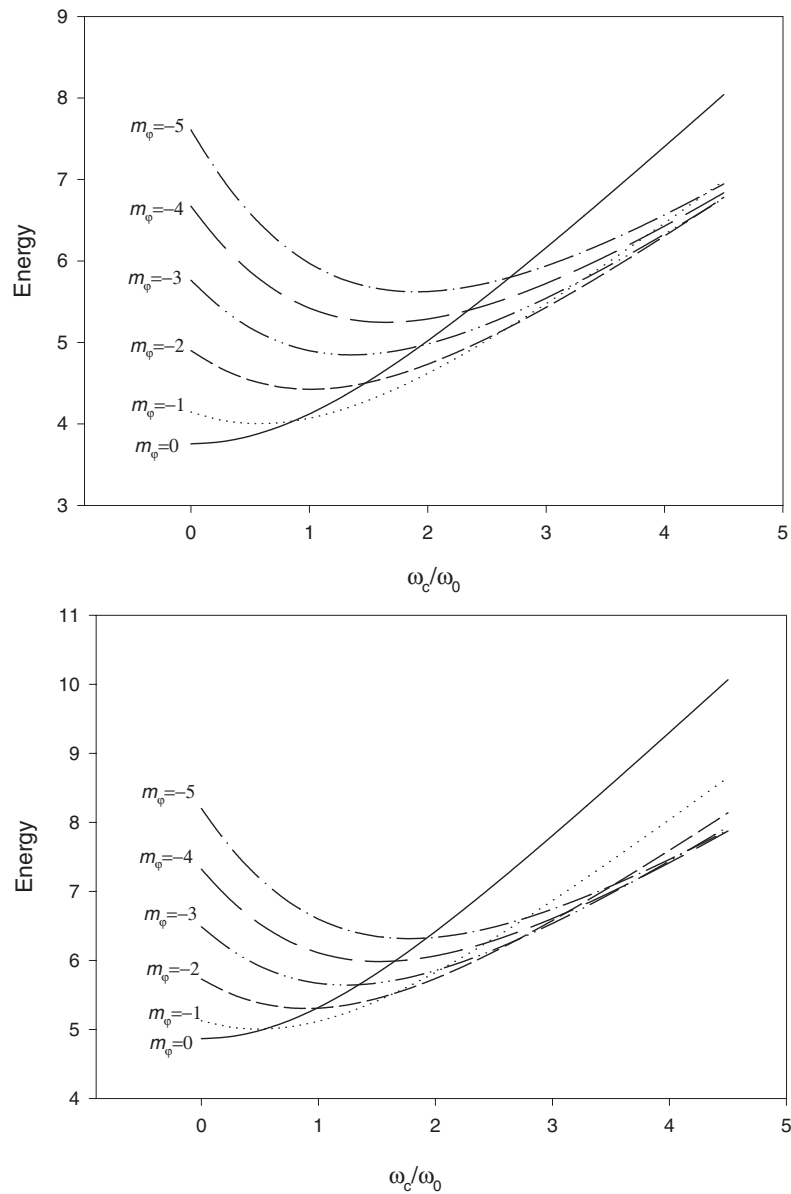


Figure 1. The energy spectrum of a two-dimensional quantum dot as a function of magnetic field strength without Zeeman energy of the spin is shown for (upper) $\ell_0/a^* = 2$, (lower) $\ell_0/a^* = 4$, and $N = M_\phi = n = 0$, $m_\phi \leq 0$. Energies are in units of $\hbar\omega_0$ and calculated up to fourth order. The ground state is oscillating between singlet and triplet states.

and decrease the width of the potential energy (appendix B); thus the ground state must be always at the $m_\phi = 0$ state. If the magnetic field is applied, however, then due to the term $(\gamma_m/2)m_\phi$ in equation (32), the total energy of the states with negative m_ϕ is lowered. At the same time, other terms in equation (32) will increase the total energy due to larger confinement potential γ' and smaller r_0 . Thus, for a suitable magnetic field strength, negative- m_ϕ states can have lower total energy than the zero- m_ϕ state, so the singlet–triplet crossing occurs. It

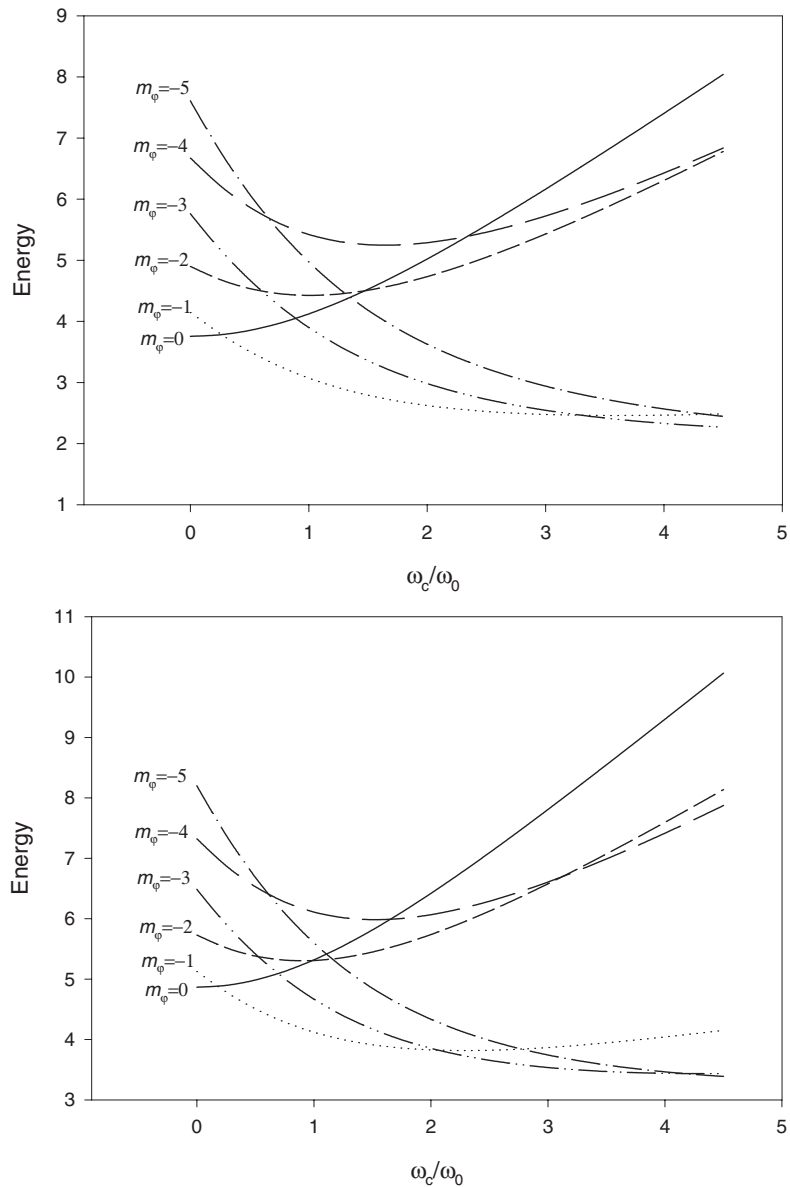


Figure 2. The energy spectrum of a two-dimensional quantum dot as a function of magnetic field strength with Zeeman energy of the spin is shown for (upper) $\ell_0/a^* = 2$, (lower) $\ell_0/a^* = 4$, and $N = M_\phi = n = 0$, $m_\phi \leq 0$, $g^* = 2$. Energies are in units of $\hbar\omega_0$ and calculated up to fourth order. The ground state tends to be a triplet state as the magnetic field increases.

can be easily shown that the crossing does not occur without Coulomb interaction because the increase of total energy due to non-zero m_ϕ is always larger than $(\gamma_m/2)m_\phi$. However, the presence of Coulomb interaction can reduce the differences in total energy between non-zero- and zero- m_ϕ states which, together with the term $(\gamma_m/2)m_\phi$ from the magnetic field, make the singlet–triplet crossing possible. This is also why the ground state always has either negative m_ϕ or $m_\phi = 0$. Thus our result shows that without a magnetic field the ground state always has $m_\phi = 0$. This disagrees with the results reported in [21]. For a dot

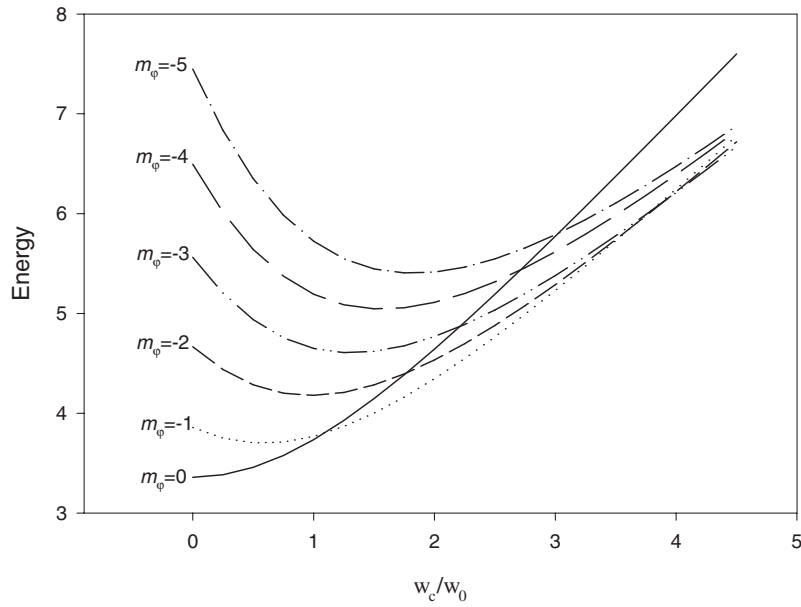


Figure 3. The energy spectrum of a two-dimensional quantum dot made from GaAs with quantum numbers $N = M_\phi = n = 0$, $m_\phi \leq 0$. The effective Rydberg energy $R^* = 5.8$ meV, and the confinement potential is $\hbar\omega_0 = 5.4$ meV. Energies are in units of $\hbar\omega_0$ and calculated up to fourth order. The singlet–triplet crossing occurs at $\omega_c/\omega_0 = 1.085$, which corresponds to $B = 3.383$ T.

Table 3. A list of the low-lying energy states with $\gamma = 1$ and 0.05 for a set of quantum numbers (m_ϕ, N, M_ϕ) obtained by our calculations up to second order for a three-dimensional quantum dot. The energy is in units of the effective Rydberg energy.

$\gamma = 1$		$\gamma = 0.05$	
(N, L, ℓ)	Energy	(N, L, ℓ)	Energy
(0, 0, 0)	3.9632	(0, 0, 0)	0.3237
(0, 0, 1)	4.7167	(0, 0, 1)	0.3421
(0, 1, 0)	4.6932	(0, 0, 2)	0.3719
(0, 0, 2)	5.5867	(0, 1, 0)	0.3737
(0, 1, 1)	5.7167	(0, 1, 1)	0.3921
(1, 0, 0)	5.9632	(0, 0, 3)	0.4079
(0, 0, 3)	6.5075	(0, 1, 2)	0.4219
(0, 1, 2)	6.5867	(1, 0, 0)	0.4237
(1, 0, 1)	6.7167	(1, 0, 1)	0.4421
(1, 1, 0)	6.9632	(0, 0, 4)	0.4477
(0, 0, 4)	7.4532	(1, 0, 2)	0.4719
(1, 0, 2)	7.5867	(1, 1, 0)	0.4737

with size $\ell_0/a^* = 4$, they obtained a ground state with $m_\phi = -1$ even in the absence of magnetic field. We note that if their results is correct, the state with $m_\phi = 1$ should also be the ground state in the absence of magnetic field, because the Hamiltonian depends only on m_ϕ^2 .

In summary, we have studied the low-energy eigenstates of the two-electron quantum dots in two and three dimensions with and without magnetic field present by using the recently developed OIM. Our result agrees very well with that from numerical approaches. However,

Table 4. A list of the optimized values found using the trial wavefunction in equation (A1) for a two-dimensional quantum dot. The optimized energy for small γ is close to the exact energy listed in table 2.

γ	(a, b)	Variational energy	Exact energy
1	(0.4, 1.16)	3.5015	3.3242
0.05	(0.735, 12.44)	0.2989	0.2963

this method is very different from other methods. We are able to obtain very accurate energies for the low-lying states directly without ever solving for the wavefunctions; nor do we need to expand our wavefunctions in a certain basis. In addition, the process of calculating energies is only related to simple differentials, and it can be done easily and precisely. We also pointed out that the singlet–triplet crossing is mainly a result of the magnetic field. The effect of Coulomb interaction is to reduce the difference in energy level spacing as the magnetic field increases, so with the additional term $(\gamma_m/2)m_\phi$, a negative- m_ϕ state can be the ground state as long as the magnetic field is strong enough. We also emphasized and argued that without a magnetic field the ground state is always the $m_\phi = 0$ state.

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Appendix A

Here we would like to present a dimensional argument as to why the particular series of g are chosen for equations (4) and (5). For a harmonic oscillator, the potential is $V = \frac{1}{2}g^2r^2$. If we use units where $\hbar = m = 1$, the dimension of energy is length^{-2} . Consequently, the dimension of g is also length^{-2} . The OIM is a strong-coupling expansion, it emphasizes small- r behaviour. Both the energy and wavefunction are expanded in decreasing power series in g . Since energy is also of dimension length^{-2} , very naturally, the first term in the energy series should be set to be proportional to g . Thus equation (5) follows. Once the expansion for the energy is determined, the choice of expansion for the wavefunction is limited. Since there is no g^2 -term in the expansions for the energy and potential, the term with the highest power of g generated from the wavefunction must be g^2 in order to be related to the potential. Thus the function S in the wavefunction must have its leading order proportional to g as in equation (4).

The same argument can be generalized to other potentials. For a hydrogen atom, the potential is $V = -g^2/r$. Hence g^2 has dimension length^{-1} . Since the energy has dimension length^{-2} , the leading term in the energy series must be proportional to g^4 ; it is given by

$$E = g^4 E_0 + g^2 E_1 + E_2 + g^{-2} E_3 + \dots \quad (43)$$

Then the function S must have the leading term in g^2 . Consequently we must have

$$S(\vec{r}) = g^2 S_0(\vec{r}) + S_1(\vec{r}) + g^{-2} S_2(\vec{r}) + g^{-4} S_3(\vec{r}) + \dots \quad (44)$$

It has been shown that these two expansions are applicable to the hydrogen-atom problem. Excellent results for the Stark effect [25] have already been reported.

Appendix B

In this appendix we will show that, in the absence of a magnetic field, states with non-zero m_ϕ have higher energy than the state with $m_\phi = 0$. If this were not correct, the most likely candidates to consider would be states with $|m_\phi| = 1$. The argument given below can be easily extended to larger- m_ϕ states.

According to equation (27), the potentials for states with $m_\phi = 0$ (V_0) and $|m_\phi| = 1$ (V_1) are

$$V_0(r) = \frac{1}{8}\gamma^2 r^2 + \frac{2}{r} \quad (45)$$

$$V_1(r) = \frac{1}{8}\gamma^2 r^2 + \frac{2}{r} + \frac{2}{r^2}. \quad (46)$$

We note that both $V_0(r)$ and $V_1(r)$ are convex. The minimum value of $V_0(r)$ is $V_0(r = r_0) = 3/r_0$ where r_0 is given by equation (34) with $m_\phi = 0$, and the minimum value of $V_1(r)$ is $V_1(r = r_1) = 3/r_1 + 4/r_1^2$ where r_1 is given by equation (34) with $|m_\phi| = 1$. It is easy to show that r_1 is greater than r_0 ; in fact,

$$\frac{r_1^3}{r_0^3} = 1 + \frac{2}{r_1}. \quad (47)$$

Using equations (B1)–(B3) and equation (34), and after some algebra, we obtain

$$V_1^3(r_1) - V_0^3(r_0) = \frac{27}{r_1^3} \left(\frac{2}{r_1} + \frac{16}{3r_1^2} + \frac{64}{27r_1^3} \right) > 0. \quad (48)$$

Since $V_1(r_1) > V_0(r_0)$, the ground-state energy for the potential $V_1(r)$ is likely to have higher energy than the ground-state energy for $V_0(r)$. But this is not sufficient. After we discount the difference in potential minimum by considering the potentials

$$V'_0(r) = V_0(r) - V_0(r_0) \quad (49)$$

and

$$V'_1(r) = V_1(r) - V_1(r_1) \quad (50)$$

we need to show that the potential $V'_1(r)$ is narrower than $V'_0(r)$ at the same energy E . According to the uncertainty principle, a potential with less width or smaller uncertainty in position must have larger uncertainty in momentum, and hence a higher ground-state energy. Thus the ground-state energy of $V'_1(r)$ must be greater than that of $V'_0(r)$. Consequently the ground-state energy of $V_1(r) = V'_1(r) + V_1(r_1)$ is greater than that of $V_0(r) = V'_0(r) + V_0(r_0)$, and states with $|m_\phi| = 1$ must have higher energy than $m_\phi = 0$ states.

$V'_1(r)$ and $V'_0(r)$ are plotted in figure B.1 for a dot with size $\ell_0/a^* = 4$. In order to compare the width, $V'_1(r)$ is shifted so that its minimum position r_1 coincides with r_0 , the minimum position of $V'_0(r)$. To show that $V'_1(r)$ has a smaller width than $V'_0(r)$ at the same energy E , we will first compare the potentials on the right-hand side of the minimum ($r > r_0$ for $V'_0(r)$ and $r > r_1$ for $V'_1(r)$) and then consider the left-hand side of the minimum.

As shown in figure B.2, for any positive E , $V'_0(r) = E$ has two positive solutions r_a and r_b , where $r_a > r_0 > r_b$; similarly, for $V'_1(r) = E$, there are two solutions r'_a and r'_b , where $r'_a > r_1 > r'_b$. Let $x_a = r_a - r_0$ and $x_b = r_0 - r_b$. It is straightforward to derive

$$V'_1(r_1 + x_a) - E = \frac{2r_0^2}{r_1^2(r_1 + x_a)} \left(\frac{1}{(r_1 + x_a)} + \frac{(r_1 - r_0)x_a r_1^2}{r_a r_0^3} \right) > 0. \quad (51)$$

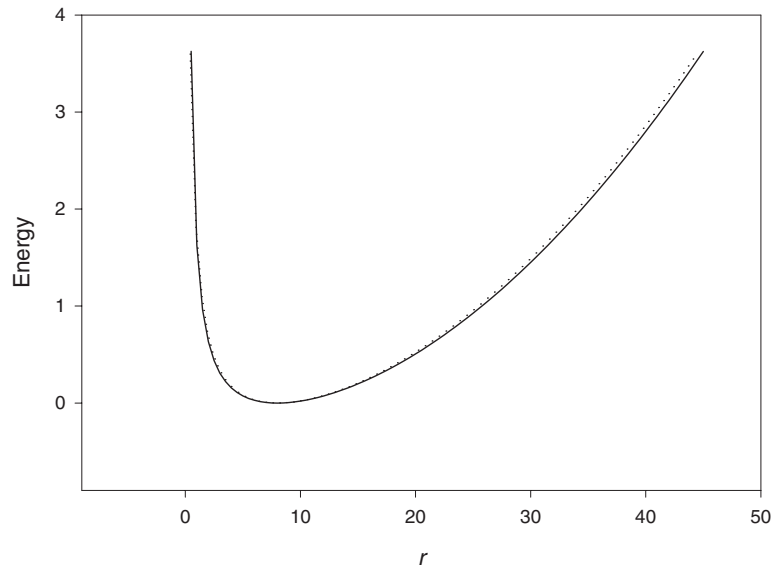


Figure B.1. The potentials $V'_0(r)$ for $m_\phi = 0$ (solid) and $V'_1(r)$ for $m_\phi = 1$ (dotted) are plotted for a dot with size $\ell_0/a^* = 4$. In order to compare the width, we have shifted the potential V'_1 so that the minima of both are located at $V(r = 8) = 0$. For $r > 8$, $V_1(r)$ or $V'_1(r)$ rises faster than $V_0(r)$ or $V'_0(r)$. For $r < 8$, the dotted curve crossed the solid curve at an energy around 2. Energy is in units of R^* and r is in units of a^* .

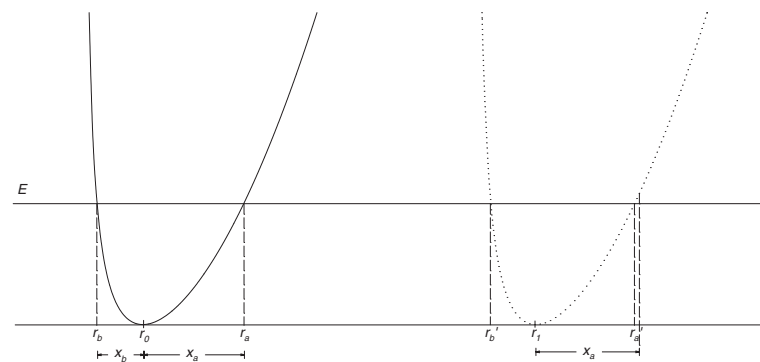


Figure B.2. A schematic illustration of the relationship between $r_a, r_b, r'_a,$ and r'_b . The solid curve is for $V'_0(r)$ and the dotted curve is for $V'_1(r)$. If $V'_1(r_1 + x_a) > E = V'_0(r_0 + x_a)$, then $r'_a - r_1 < x_a$. See appendix B for details.

Because $r_1 > r_0$, the above quantity is always positive, which means $V'_1(r_1 + x_a) > V'_1(r'_a) = V'_0(r_0 + x_a) = E$. The potential $V'_1(r)$ for $r > r_1$ rises faster than $V'_0(r)$ for $r > r_0$; hence $r_1 + x_a > r'_a$, as shown in figure B.1. Figure B.2 gives a schematic illustration of the relationship between $r_0, r_1,$ and x_a .

Use similar arguments, we consider the left-hand side of the minimum ($r < r_0$ for $V'_0(r)$ and $r < r_1$ for $V'_1(r)$):

$$V'_1(r_1 - x_b) - E = \frac{2x_b^2}{r_0 r_1^2 (r_1 - x_b)} \left(\frac{1}{(r_1 - x_b)} - \frac{(r_1 - r_0)x_b r_1^2}{r_b r_0^3} \right). \quad (52)$$

This quantity becomes negative when E lies between E_{c1} and E_{c2} , where $E_{c1} < E_{c2}$. For

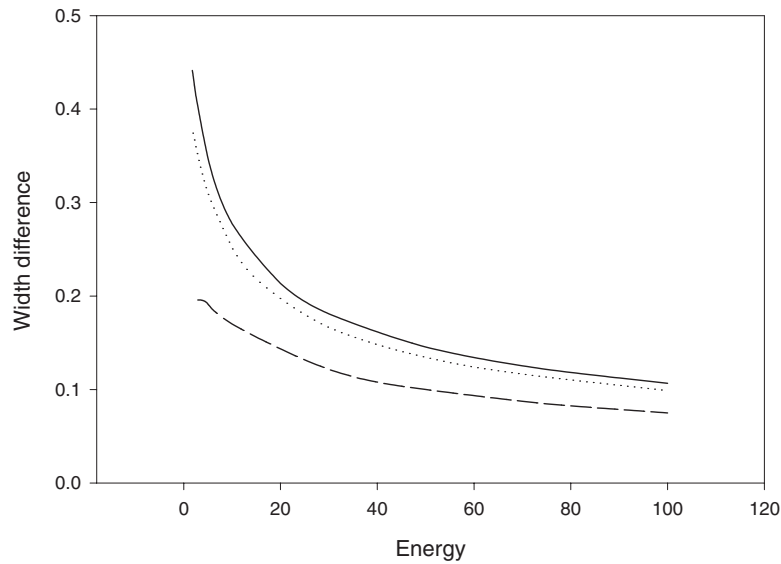


Figure B.3. The width difference (width of V_0 – width of V_1) versus energy is plotted for (solid) $\gamma = 0.05$, $E_c = 1.78$, (dotted) $\gamma = 0.125$, $E_c = 1.89$, and (dashed) $\gamma = 1.0$, $E_c = 2.91$. Notice that the width difference is always positive. Energy is in units of R^* and width difference is in units of a^* .

$E \leq E_{c1}$, $V_1'(r_1 - x_b) > V_1'(r'_b) = E$; hence $r_1 - x_b < r'_b$ and $r'_a - r'_b < x_a + x_b = r_a - r_b$. Thus the width of $V_1'(r)$ is smaller than that of $V_0'(r)$. A similar conclusion holds for $E \geq E_{c2}$. However, for $E_{c2} \geq E \geq E_{c1}$, $r_1 - x_b > r'_b$. Thus we are not able to use the above argument to show that the width of $V_1'(r)$ is smaller than that of $V_0'(r)$. Instead, we try to find two solutions for $V_0'(r) = E$ and $V_1'(r) = E$ directly and compare $(r_a - r_b)$ and $r'_a - r'_b$. The analytical form of $(r_a - r_b) - (r'_a - r'_b)$ is quite complicated; hence we will use numerical methods. Figure B.3 shows the numerical data for three typical γ -values. We can see that even for $E \geq E_{c1}$, the width of $V_1'(r)$ is still smaller than that of $V_0'(r)$ over a wide range of E . Thus we conclude that the width of $V_1'(r)$, which is the same as the width of $V_1(r)$, is always smaller than that of $V_0'(r)$ or $V_0(r)$. Notice that the dashed curve in figure B.3 has the same parameters as were used in [20] and [21] but with the different result that $m_\phi = -1$ is not the ground state.

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