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## Exact solutions of two electrons in a quantum dot

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**Abstract.** Making use of the expansion in a power series, the exact eigensolutions of two electrons in a parabolic quantum dot are obtained. The quantum-size effects on the energy spectra of two electrons are shown for the first time.

Advances in nanofabrication technology have made it possible to manufacture quantum dots (QDs) containing one, two and more electrons, which are investigated experimentally and theoretically. The experimental study of quasi-two-dimensional quantum dots is expanding rapidly [1–6], and exchange and correlation effects are shown to be of great importance [7–9] in such systems. Therefore, it is very important to have reliable methods to calculate the electronic structures and showing the physical properties in QDs. Approaches to the problem mainly include the ‘exact’ numerical diagonalization [7–8], numerical simulations based on quantum Monte Carlo techniques [10] and Hartree–Fock calculations [7, 11–13]. Recently, convergent renormalized perturbation series in powers of the electron–electron interaction were proposed for calculating the energy of a quantum dot consisting of two electrons [9]. In this paper, we propose a method making use of the expansion in a power series in wavefunctions of the relative motion of two electrons to obtain exact spectra in a quantum dot. Based on the present results, the quantum-size effects on the spectra of two electrons are shown for the first time.

In experimentally realized dots, the motion in the  $z$  direction is always frozen out into the lowest subband. Since the corresponding extent of the wavefunction is much less than the one in  $x$ – $y$  plane, we can treat the dots in the two-dimensional limit of thin disks. For most dots, a harmonic oscillator is a very good approximation to describe the lateral confinement of the electrons [1, 11]. Hence, it is reasonable to write the Hamiltonian of two electrons in such a parabolic quantum dot as follows:

$$H = -\nabla_1^2 - \nabla_2^2 + \frac{1}{4}\gamma^2\rho_1^2 + \frac{1}{4}\gamma^2\rho_2^2 + \frac{2}{|\rho_1 - \rho_2|} \quad (1)$$

where the effective atomic units are used. The effective Rydberg  $Ry^*$  and the effective Bohr radius  $a^*$  are taken to be the energy and length units, respectively. It is easy to see that  $\gamma^{-1/2}$  is related to the confinement region of electrons in the dot.

The Hamiltonian of (1) can be separated into centre-of-mass and relative-motion terms as

$$H = H_R + H_r \quad (2)$$

with

$$H_R = -\frac{\nabla_R^2}{2} + \frac{1}{2}\gamma^2 R^2 \quad (3)$$

and

$$H_r = -2\nabla_r^2 + \frac{1}{8}\gamma^2 r^2 + \frac{2}{r} \quad (4)$$

where  $\mathbf{R} = (\boldsymbol{\rho}_1 + \boldsymbol{\rho}_2)/2$ ,  $\nabla_R = \nabla_1 + \nabla_2$ ,  $\mathbf{r} = \boldsymbol{\rho}_1 - \boldsymbol{\rho}_2$  and  $\nabla_r = (\nabla_1 - \nabla_2)/2$ . This separability and the cylindrical symmetry of the problem allow us to write the two-particle wavefunctions in plane polar coordinates  $\mathbf{r} = (r, \varphi)$  in the form  $\Phi(R)\phi(r)\exp(im\varphi)$ . The spatial part of the total wavefunction is symmetric (antisymmetric) with respect to particle permutation ( $\varphi \rightarrow \varphi + \pi$ ) for even (odd) azimuthal quantum numbers  $m$ . Since the Pauli exclusion principle requires the total wavefunction to be antisymmetric, we therefore have spin singlet ( $s = 0$ ) and triplet ( $s = 1$ ) states for even and odd  $m$  [14], respectively. The energy eigenvalues of (3) are given by

$$E(N_R, M) = (2N_R + |M| + 1)\gamma \quad (5)$$

with radial ( $N_R = 0, 1, 2, \dots$ ) and azimuthal ( $M = 0, \pm 1, \pm 2, \dots$ ) quantum numbers. The eigenvalues of the relative motion excluding the electron–electron interaction are also given by

$$E_0(n_r, m) = (2n_r + |m| + 1)\gamma \quad (6)$$

with the corresponding radial and azimuthal quantum numbers  $n_r = 0, 1, 2, \dots$  and  $m = 0, \pm 1, \pm 2, \dots$ . However, we should solve the Schrödinger-like equation

$$H_r [\phi(r)\exp(im\varphi)] = E(m) [\phi(r)\exp(im\varphi)] \quad (7)$$

to get the energy of the relative motion including the electron–electron interaction. It is easy to find the equation satisfied by the function  $\phi(r)$ :

$$\frac{d^2\phi}{dr^2} + \frac{1}{r} \frac{d\phi}{dr} + \left( \frac{E(m)}{2} - \frac{1}{r} - \frac{m^2}{r^2} - \frac{1}{16}\gamma^2 r^2 \right) \phi = 0. \quad (8)$$

Now, we are prevented from analytically obtaining exact solutions of the eigenvalue problem because (8) with suitable boundary conditions is beyond the analytical problem of confluent hypergeometric equations. In this paper, we use the method of series expansion [15] to obtain exact series forms in different regions of (8) and the exact values of  $E(m)$  and, then, the exact solutions of two electrons in the quantum dot.

It should be noted that zero and infinity are regular and irregular points of (8), respectively. In the region  $0 < r$ , we have a series solution, which has a finite value at  $r = 0$ , as follows:

$$\phi(r) = Ar^{|m|} \sum_{n=0}^{\infty} a_n r^n \quad (9)$$

where  $A$  is a constant and  $a_0$  is equal to 1. Noting that  $a_n$  are equal to zero as  $n$  is equal to a negative integer, the other  $a_n$  can be determined by the following recurrence relation:

$$a_n = \left( 2a_{n-1} - E(m)a_{n-2} + \frac{1}{8}\gamma^2 a_{n-4} \right) / (4|m| + 2n)n \quad \text{for } n = 1, 2, 3, \dots \quad (10)$$

In the region  $r < \infty$ , we can obtain a normal solution. It approaches zero at  $r = \infty$  and is found in the form

$$\phi(r) = B \exp\left(-\frac{1}{8}\gamma r^2\right) r^s \sum_{n=0}^N b_n r^{-n} \quad (11)$$

where

$$s = E(m)/\gamma - 1 \quad (12)$$

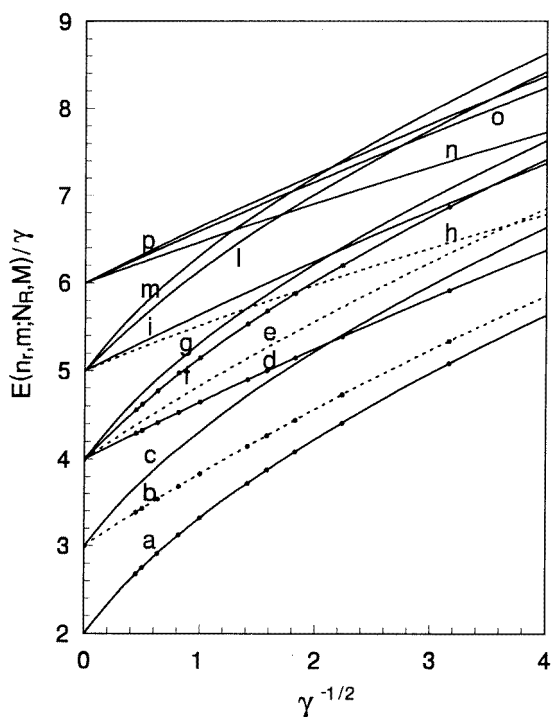
$$\begin{cases} b_0 = b_1 = 1 \\ b_n = 2b_{n-1} - [(s - n + 2)^2 - m^2]b_{n-2} \end{cases} \quad \text{for } n = 2, 3, 4 \dots \quad (13)$$

and  $B$  is a constant. We should point out that (9) and (11) are suitable for numerical calculations in a regions of small and large  $r$ , respectively.

In order to match the solution of (9) with that of (11), we give  $T$  solutions around  $R_1, R_2 \dots$  and  $R_T$ , which are the proper points for solving (8) exactly. The solution of uniformly convergent Taylor series around  $R_i (i = 1, 2 \dots T)$  is written as follows:

$$\phi(r) = C_i \sum_{n=0}^{\infty} c_{in}(r - R_i)^n + D_i \sum_{n=0}^{\infty} d_{in}(r - R_i)^n \quad (14)$$

where  $C_i$  and  $D_i$  are constants,  $c_{i0}$  and  $d_{i1}$  are equal to 1, and  $c_{i1}$  and  $d_{i0}$  are equal to 0. The  $c_{in}$  and  $d_{in}$  can be determined by recurrence relations.



**Figure 1.**  $E(n_r, m; N_R, M)$  normalized by  $\gamma$  versus  $\gamma^{-1/2}$  for a, b, c, d, e, f, g, h, i, l, m, n, o and p states with the quantum numbers indicated in table 1. The solid circles represent those obtained by using the ‘exact’ diagonalization method.

Using the matching conditions at  $r = R_i (i = 1, 2 \dots T)$ , and the  $2 \times 2$  transfer matrices, we can get the equation for eigenenergies  $E(n_r, m)$  easily. The values of  $E(n_r, m)$  and  $\phi_{n,m}(r)$  are obtained numerically. For the sake of convenience, we define  $E_r(n_r, m)$  as the difference between  $E(n_r, m)$  and  $E_0(n_r, m)$ , i.e.,

$$E_r(n_r, m) = E(n_r, m) - E_0(n_r, m). \quad (15)$$

Then, the energy eigenvalues of the Hamiltonian in (1) are the sum of the centre-of-mass energy and the energy of the relative motion as follows

$$E(n_r, m; N_R, M) = E(n_r, m) + E(N_R, M) = [2(N_R + n_r) + |M| + |m| + 2]\gamma + E_r(n_r, m). \quad (16)$$

Before the present results are shown and discussed, it is worthwhile to note the way to indicate the quantum levels of two electrons in QDs. As shown in (16), the levels  $E(n_r, m; N_R, M)$  can be indicated by four symbols  $n_r, m, N_R$  and  $M$ . The even and odd  $m$  correspond to the spin singlet ( $s = 0$ ) and triplet ( $s = 1$ ) states, respectively because of the Pauli exclusion principle as mentioned above. We have states 1s, 2p, 2s, 3d, 3p (1S, 2P, 2S, 3D, 3P) and so on if the principal quantum numbers  $n = n_r + |m| + 1$  ( $N = N_R + |M| + 1$ ) are used instead of  $n_r$  ( $N_R$ ) and the notation s, p, d... (S, P, D...) is used for  $|m|$  ( $|M|$ ) = 0, 1, 2, ...

**Table 1.** Exact quantum levels of two electrons in QDs with different  $\gamma$ . The level sequences are in order of increasing magnitude. For the sake of convenience, the short notation, i.e., a, b, c and so on, is used to indicate the quantum numbers ( $n_r, m; N_R, M; s$ ) and to show the changes of the level order. The energy unit is  $R\gamma^*$ .

$\gamma(\gamma^{-1/2})$	1.0(1.0)	0.2(2.2361)	0.05(4.4721)
a: (0,0;0,0:0)	(a) 3.3196	(a) 0.8816	(a) 0.2962
b: (0,1;0,0:1)	(b) 3.8278	(b) 0.9450	(b) 0.3062
c: (0,0;0,1:0)	(c) 4.3196	(d) 1.0776	(d) 0.3310
d: (0,2;0,0:0)	(d) 4.6436	(c) 1.0816	(c) 0.3462
e: (0,1;0,1:1)	(e) 4.8278	(e) 1.1450	(h) 0.3476
f: (1,0;0,0:0)	(f) 5.1472	(h) 1.2156	(e) 0.3562
g: (0,0;1,0:0)	(g) 5.3196	(f) 1.2402	(i) 0.3810
h: (0,3;0,0:1)	(h) 5.5174	(i) 1.2776	(f) 0.3854
i: (0,2;0,1:0)	(i) 5.6436	(g) 1.2816	(g) 0.3962
j: (1,1;0,0:1)	(j) 5.7438	(j) 1.3170	(j) 0.3968
k: (0,1;1,0:1)	(k) 5.8278	(k) 1.3450	(k) 0.4062
l: (1,0;0,1:0)	(l) 6.1472	(n) 1.4053	(n) 0.4066
m: (0,0;1,1:0)	(m) 6.3196	(l) 1.4402	(o) 0.4240
n: (0,4;0,0:0)	(n) 6.4693	(o) 1.4594	(p) 0.4310
o: (1,2;0,0:0)	(o) 6.5956	(p) 1.4776	(l) 0.4354
p: (0,2;1,0:0)	(p) 6.6436	(m) 1.4816	(m) 0.4462

We have performed numerical calculations for energy levels of two electrons in QDs with  $\gamma$  between 0.05 and 5. As shown in table 1, the two-electron spectra vary not only in the values but also in the level ordering as  $\gamma$  changes from 0.05 to 1. In order to better show the quantum-size effects and compare with others, we have plotted most of them normalized by  $\gamma$  as functions of  $\gamma^{-1/2}$  in figure 1. It is readily seen that the results are in good agreement with others [7, 9] and that the energy-level structure is dramatically changed as the  $\gamma^{-1/2}$  changes from 0 to 4. As illustrated in figure 1 and table 1, an important aspect of the quantum-size effects is the changes of the level-ordering and the level differences, and then, the crossover of two levels can appear as  $\gamma^{-1/2}$  ( $\gamma$ ) is larger (less) than one.

For a better understanding of the quantum-size effects, it is interesting to study the  $E_r(n_r, m)$  defined by (15). In figure 2, the  $E_r(n_r, m)$  is plotted as a function of  $\gamma$ . As shown in the figure, the  $E_r(n_r, m)$  increases with  $\gamma$  and the ordering is as follows:  $E_r(0, 0) > E_r(1, 0) > E_r(2, 0) > E_r(0, 1) > E_r(1, 1) > E_r(0, 2) > E_r(1, 2) \dots$

It is accurate enough to calculate the  $E_r(n_r, m)$  with the use of the first-order perturbation as  $\gamma$  is sufficiently large compared with electron-electron interaction. Then,  $E_r(n_r, m)$  is

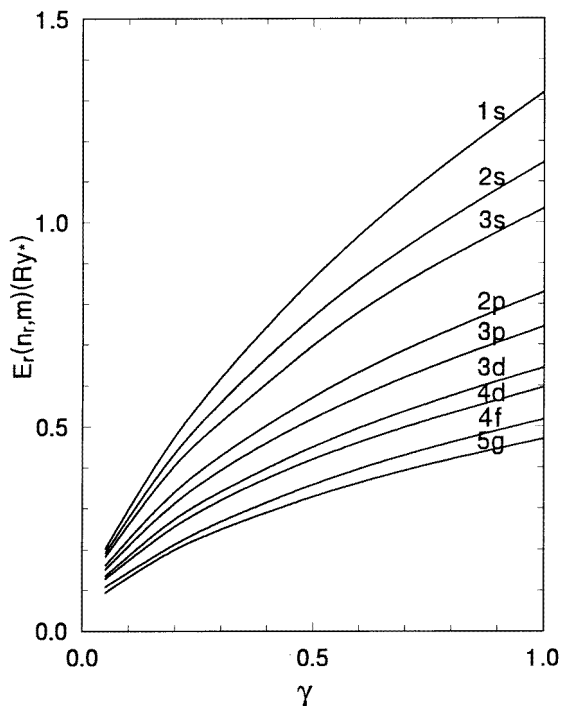


Figure 2.  $E_r(n_r, m)$  versus  $\gamma$  for 1s, 2s, 3s, 2p, 3p, 3d, 4d, 4f and 5g states.

given by

$$E_r(n_r, m) = \langle \phi_{n_r, m}(r) \left| \frac{2}{r} \right| \phi_{n_r, m}(r) \rangle \quad (17)$$

where  $\phi_{n_r, m}(r)$  is a normalized radial wavefunction of (8) without the electron–electron interaction term. Using (17), we can easily find the ordering mentioned above. The values of  $E_r(n_r, m)$  are proportional to  $\gamma^{1/2}$ . However, both  $E(N_R, M)$  and  $E_0(n_r, m)$  shown in (5) and (6) are proportional to  $\gamma$ . As  $\gamma^{-1/2}$  ( $\gamma$ ) is less (larger) than one, the level-ordering is mainly determined by the sum of  $E_0(n_r, m)$  and  $E(N_R, M)$ . It can be strongly changed by  $E_r(n_r, m)$  if  $\gamma^{-1/2}$  ( $\gamma$ ) is much larger (less) than one. This is the reason why the quantum-size effects appear.

In conclusion, we have used different series solutions in different regions for the radial equation of the relative motion of two electrons to obtain the exact solutions. Calculated results are in good agreement with those obtained by using the ‘exact’ diagonalization method [7, 9]. Based on the results, the quantum-size effects are clearly shown.

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