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Electron–electron correlation in quantum dots

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Abstract

The problem of correlation has been studied for two-electron systems in semiconductor quantum dots with harmonic-oscillator confinement potentials of both the spherical and cylindrical symmetry. The eigenvalue problems have been solved by the iterative extraction-orthogonalization method, which provides the exact results for the harmonic-oscillator potential with arbitrary frequency. It is shown that — on the contrary to the previous results — in the absence of external magnetic field, the ground state is the spin singlet for quantum dots of arbitrary size, i.e., a singlet–triplet spontaneous “phase transition” does not occur. We have performed the comparative calculations using the Hartree–Fock method and shown that the previously predicted singlet–triplet “phase transition” results from the neglect of the electron–electron correlation. We have found that for sufficiently large quantum dots the singlet ground state becomes degenerate with the first excited triplet state and pair-correlation functions for these states are almost identical. © 2000 Elsevier Science B.V. All rights reserved.

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1. Introduction

Bound atom-like states (artificial atoms) [1,2] can be created in a system of excess electrons confined in a semiconductor quantum dot if the “quantum capacity” [3] of the dot is sufficiently large. The properties of few-electron artificial atoms have been investigated in both the experimental [4–7] and theoretical papers [3,8–17]. The excess electrons in quantum dots are subjected to confinement potentials,

which result from either heterojunction band offsets or potentials applied to external microelectrodes. In the theoretical papers, the confinement potentials are usually approximated by the following two model potentials: harmonic-oscillator potential and rectangular potential well. In our recent papers [3,17], we have studied the properties of few-electron [3] and many-electron [17] artificial atoms with the confinement potential assumed to be the spherical potential well of finite depth.

In the majority of the papers on quantum dots (for a review, see Ref. [18]), the confinement potential was assumed in the form of the two-dimensional harmonic-oscillator potential. An application of this

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potential [8,11,14–16] to an interpretation of experimental data for cylindrical quantum dots is based on the assumption that the electrons are “frozen” in the ground state, which results from the size quantization of their motion in the growth (z) direction. However, this assumption neglects a finite extent of the electronic wave function in the z direction and requires an approximate treatment of the three-dimensional electron–electron Coulomb interaction [10]. In the present paper, in order to avoid these drawbacks we apply the three-dimensional model of the quantum dot. The many-electron system in the three-dimensional anisotropic harmonic-oscillator potential was studied with the use of the Hartree–Fock (HF) method by Fujito et al. [12], who argued that the many-electron ground state is completely spin polarized for large quantum dots. In particular, the results [12] suggest that for the two electrons a spontaneous singlet–triplet “phase transition” appears for some critical size of the dot. Such phase transition would be an analog to the density-induced para-ferromagnetic phase transition studied by the Hartree–Fock [22,23] and Monte Carlo [24,25] methods for the electron gas with the uniform neutralizing background. The problem of two electrons in a spherically symmetric harmonic-oscillator potential was studied in papers [19–21]. For a particular set of oscillator frequencies the analytical solutions were found [19]. The singlet–triplet splitting between the two-electron energy levels was calculated [21] for the fixed oscillator frequency $\omega = \frac{1}{2}$, which admits the analytical solutions [19]. However, the authors [21] did not study the singlet–triplet splitting in the weak-confinement regime, i.e., for large quantum dots, for which the density-induced phase transition was supposed [12].

The purpose of the present paper is to perform a systematic study of the influence of electron–electron correlation on a presumed singlet–triplet phase transition for quantum dots of arbitrary size. We assume the three-dimensional confinement of the electrons in the quantum dot and employ the harmonic-oscillator confinement potentials of both the spherical and cylindrical symmetry. We show that the previously predicted triplet ground state results from the omission of the correlation in the HF approximation. We have found a new property of two-electron quantum dots, namely, we predict that in large quantum dots the singlet and triplet states are nearly degenerate, i.e., their

energy levels lie very close, but do not cross each other.

The paper is organized as follows: Section 2 consists of a theoretical model and basic analytical results, the numerical results are presented in Section 3, the discussion and conclusions are in Section 4, and the summary is in Section 5.

2. Theory

We consider the two-electron systems in quantum dots with the confinement potentials assumed to be the harmonic-oscillator potentials of either the spherical or cylindrical symmetry. The basic properties of the two electrons confined in the spherically symmetric harmonic-oscillator potential have been discussed in papers [19,20]. We present here in more detail the problem of the electronic pair confined in the anisotropic harmonic-oscillator potential of the cylindrical symmetry. The Hamiltonian of this system has the form

$$\mathcal{H} = -\frac{\hbar^2}{2m_e}(\nabla_1^2 + \nabla_2^2) + \frac{m_e\omega_x^2}{2}(x_1^2 + x_2^2 + y_1^2 + y_2^2) + \frac{m_e\omega_z^2}{2}(z_1^2 + z_2^2) + \frac{\kappa e^2}{\epsilon_s|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (1)$$

where m_e is the band electron mass, ω_x and ω_z are the anisotropic harmonic-oscillator frequencies, $\kappa = 1/4\pi\epsilon_0$, ϵ_0 is the permittivity of vacuum, and ϵ_s is the static dielectric constant. We introduce the center-of-mass position vector $\mathbf{R} = (X, Y, Z) = (\mathbf{r}_1 + \mathbf{r}_2)/2$, relative-position vector $\mathbf{r} = (x, y, z) = \mathbf{r}_1 - \mathbf{r}_2$, the donor rydberg $R_D = m_e\kappa^2 e^4 / 2\hbar^2 \epsilon_s^2$ as the unit of energy, and the donor Bohr radius $a_D = \epsilon_s \hbar^2 / m_e \kappa e^2$ as the unit of length. Then, Hamiltonian (1) takes on the form

$$\mathcal{H} = H_{CM} + H_{rel}, \quad (2)$$

where

$$H_{CM} = -\frac{1}{2}\nabla_{\mathbf{R}}^2 + 2\gamma_x^2(X^2 + Y^2) + 2\gamma_z^2 Z^2 \quad (3)$$

is the center-of-mass Hamiltonian and

$$H_{rel} = -2\nabla_{\mathbf{r}}^2 + \frac{\gamma_x^2}{2}\rho^2 + \frac{\gamma_z^2}{2}z^2 + \frac{2}{r} \quad (4)$$

is the relative-motion Hamiltonian. In Eqs. (3) and (4), $\rho^2 = x^2 + y^2$, $r = \sqrt{\rho^2 + z^2}$, $\gamma_x = \hbar\omega_x/2R_D$, and $\gamma_z = \hbar\omega_z/2R_D$. Since Hamiltonian (4) commutes

with the operator L_z^{op} of z -component of angular momentum, we can project it onto a subspace of states with the definite eigenvalues of L_z^{op} and write it down in the cylindrical coordinates. We obtain

$$H = 2 \left(-\frac{\partial^2}{\partial \rho^2} - \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{M^2}{\rho^2} - \frac{\partial^2}{\partial z^2} + \frac{\gamma_x^2}{4} \rho^2 + \frac{\gamma_z^2}{4} z^2 + \frac{1}{r} \right), \quad (5)$$

where M is the quantum number of z -component of angular momentum.

For the three-dimensional spherical harmonic-oscillator potential, the corresponding relative-motion Hamiltonian projected onto the subspace of states with the definite angular momentum has the form

$$H_{\text{spher}} = 2 \left(-\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{L(L+1)}{r^2} + \frac{\gamma^2}{4} r^2 + \frac{1}{r} \right), \quad (6)$$

where $r = (x^2 + y^2 + z^2)^{1/2}$, L is the angular momentum quantum number, $\gamma = \hbar\omega/2R_D$, and ω is the frequency of the isotropic harmonic oscillator. If we omit the electron–electron interaction, the energy eigenvalues of relative-motion Hamiltonians (5) and (6) are given by

$$E_{nMn_z}^0 = 2\gamma_x(2n + |M| + 1) + \gamma_z(2n_z + 1) \quad (7)$$

for Hamiltonian (5) and

$$E_{nL}^0 = \gamma(4n + 2L + 3) \quad (8)$$

for Hamiltonian (6), where n is the radial quantum number and n_z is the oscillator quantum number.

Let us consider the basic physical properties of the two-electron system in the harmonic-oscillator potential. We are interested in an influence of the electron–electron correlation on the lowest-energy eigenstates. Therefore, we will only discuss the eigenvalue problems for the relative-motion Hamiltonians (5) and (6), since the energy spectrum of the center-of-mass Hamiltonian (3) is independent of the electron–electron interaction. Moreover, due to the symmetry of the center-of-mass Hamiltonian (3) (and its spherically symmetric analog), the wave function describing the center-of-mass motion is symmetric against the interchange of the electrons and both the singlet and triplet states of the lowest energy are associated with the ground state of the center-of-mass motion. Wave function $\Psi(\mathbf{r}, \sigma_1, \sigma_2)$, describing the

relative motion of electrons, can be factorized as follows: $\Psi(\mathbf{r}, \sigma_1, \sigma_2) = \psi(\mathbf{r})\chi(\sigma_1, \sigma_2)$, where $\psi(\mathbf{r})$ is the eigenfunction of Hamiltonian (5) [or Hamiltonian (6) for the isotropic harmonic oscillator] and $\chi(\sigma_1, \sigma_2)$ is the spin wave function of spin variables σ_1 and σ_2 . Two-electron wave function $\Psi(\mathbf{r}, \sigma_1, \sigma_2)$ has to be antisymmetric with respect to the exchange of electrons. For the two electrons, the total spin can be either 0 or 1 (in units \hbar), i.e., the spin states χ are either the antisymmetric singlet or symmetric triplet states, respectively. The symmetry of spatial wave function $\psi(\mathbf{r})$ with respect to the electron permutation is determined by the quantum numbers M and L for Hamiltonians (5) and (6), respectively. In particular, the states with $M = 0$ or $L = 0$ (S -like states) are symmetric against the exchange of electrons, i.e., they are the spin singlet states, and the states with $M = 1$ or $L = 1$ (P -like states) are antisymmetric against the exchange of electrons, i.e., they are the spin-triplet states. For the states with $M \neq 0$ and $L > 0$, the positive definite operators M^2/ρ^2 in Hamiltonian (5) and $L(L+1)/r^2$ in Hamiltonian (6) yield positive contributions to the energy of the considered states. According to the comparison theorem [26], the energy levels of the states with $M \neq 0$ and $L > 0$ are shifted upwards with respect to those of the corresponding states with $M = 0$ and $L = 0$. We conclude that for both the harmonic-oscillator confinement potentials the two-electron ground state is the singlet state with the energy $E_{\text{GS}}^{\text{singlet}}$, which is lower than the minimum energy $E_{\text{min}}^{\text{triplet}}$ of the first excited triplet state, i.e.,

$$E_{\text{GS}}^{\text{singlet}} < E_{\text{min}}^{\text{triplet}}. \quad (9)$$

This inequality is valid for the lowest energy levels only. The order of the higher energy levels can be different.

3. Results

We have solved the eigenvalue problems for the following lowest energy states: the spin-singlet states, that correspond to the orbital states with $M = 0$ for Hamiltonian (5) and $L = 0$ for Hamiltonian (6), and the spin-triplet states, that correspond to the orbital states with $M = 1$ for Hamiltonian (5) and $L = 1$ for Hamiltonian (6). We remind that the singlet and triplet states considered in the present paper are associated

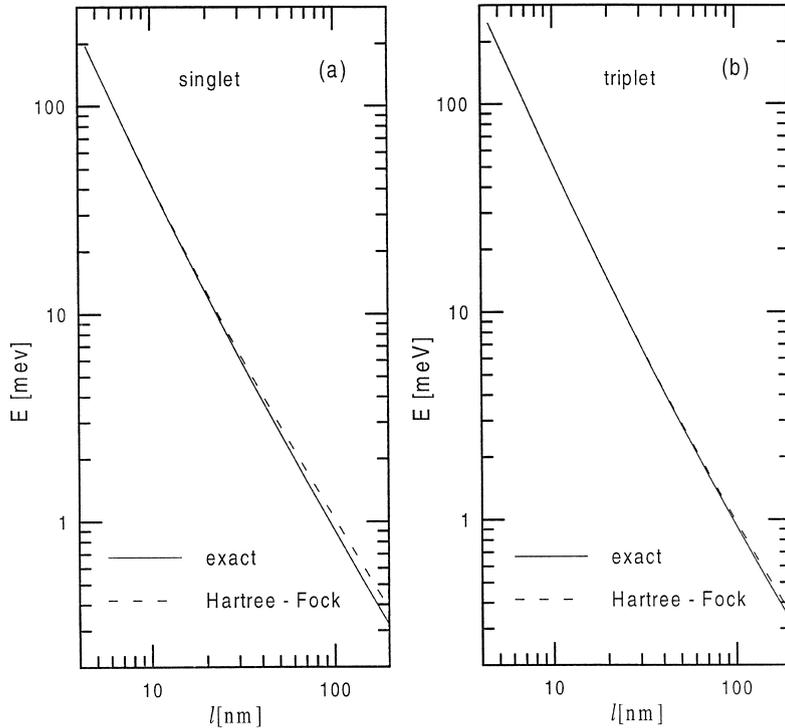


Fig. 1. The lowest singlet (a) and triplet (b) energy levels of two electrons in spherically symmetric harmonic-oscillator potential as functions of characteristic length $l = \gamma^{-1/2}$. Solid curves show the exact results obtained by the iterative extraction-orthogonalization method and dashed curves the results of the unrestricted HF method.

with the same quantum state of the center-of-mass Hamiltonian.

In order to find exact solutions, which are valid for arbitrary confinement potential, we have applied the modified version of the iterative extraction-orthogonalization method [27,28]. Here, we briefly discuss the present implementation of this method to the eigenvalue problem dependent on two variables. The wave function is determined on a two-dimensional grid $(i\Delta\rho, j\Delta z)$, where $\Delta\rho = \rho_{\max}/N$, $\Delta z = z_{\max}/N$, i and j are integers, $i \in [0, N]$, and $j \in [-N, N]$. We have checked that the sufficiently high precision for the purposes of the present work is achieved if we take on the number of mesh points, which corresponds to $N = 200$. The discretized form of Hamiltonian H is obtained by replacing the derivatives in the kinetic-energy operator by their finite difference approximations. We put the following boundary conditions: the wave function has to vanish at $\rho = \rho_{\max}$ and $|z| = z_{\max}$.

The values of ρ_{\max} and z_{\max} , which determine the size of the computational box, are optimized to give the lowest energy eigenvalue. The iteration procedure runs as follows: in the k th iteration step, the values ψ_{ij}^k of the wave function on the mesh points are evaluated according to the formula

$$\psi_{ij}^k = \exp(-\lambda H)\psi_{ij}^{k-1} \simeq (1 - \lambda H)\psi_{ij}^{k-1}. \quad (10)$$

One can prove [28] that – independently of starting values – the above iteration procedure converges to the exact wave function, which corresponds to the lowest energy eigenstate of the required symmetry, if the iteration parameter λ is small enough. After each iteration step, the new wave function is normalized and the Rayleigh quotient $\langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle$ is evaluated. If the convergence is reached, the value of the Rayleigh quotient provides a very accurate estimate of the energy eigenvalue, which allows us to obtain the results with the required precision, i.e., these

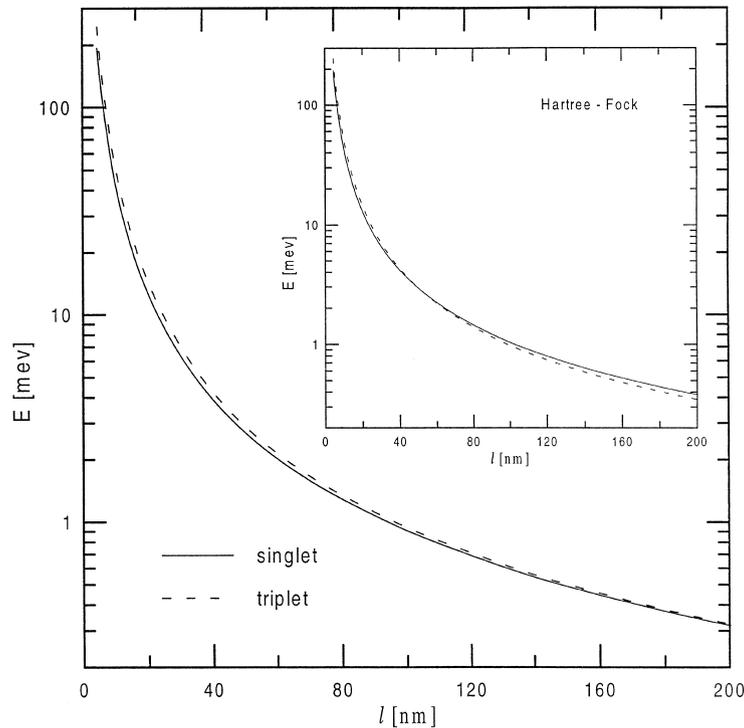


Fig. 2. Singlet–triplet splitting for the two-electron system in isotropic harmonic-oscillator potential as a function of quantum-dot size l . Solid (dashed) curves correspond to spin-singlet (triplet) states. Inset: the corresponding results obtained by the HF method.

numerical results can be regarded to be exact. We have solved the Schrödinger equation with Hamiltonian (5) by this method. When solving the radial Schrödinger equation with Hamiltonian (6) the one-dimensional grid has been applied. In order to study the influence of electron–electron correlation on the properties of the two-electron quantum dots, we have also performed the comparative calculations by the unrestricted HF method with the use of the Gaussian basis of both the spherical [17] and cylindrical [29] symmetry. The HF approximation neglects the correlation. Therefore, a comparison of the results obtained by the exact method and HF method allows us to draw conclusions about a contribution of the correlation to the results.

Throughout the present paper, we take on the values $R_D = 5.8$ meV and $a_D = 9.9$ nm, which correspond to GaAs quantum dots and are the same as in Ref. [12]. Fig. 1 shows the lowest energy levels associated with the spin-singlet (a) and spin-triplet (b) states of Hamiltonian (1) with the isotropic harmonic-oscillator po-

tential. The characteristic length $l = \gamma^{-1/2}$ determines the size of the quantum dot. We obtain a very good agreement of the HF results with the exact results for quantum dots of small and intermediate size, i.e., in the strong- and intermediate-confinement regimes, respectively. Small deviations of the HF results from the exact results are visible only for large quantum dots, i.e., in the weak-confinement regime. We note that the deviations for the triplet states are smaller than those for the singlet states. A direct comparison of the singlet and triplet energy levels is depicted in Fig. 2, which shows that – for all values of l – the energy level of the singlet state is located below the lowest energy level of the triplet state. This is a numerical confirmation of conclusion (9) and means that – independently of the dot size – the spin-singlet state is the ground state of the electron pair confined in the quantum dot with the isotropic harmonic-oscillator potential. Fig. 2 also shows that both the states become degenerate for the dots of large size ($l > 160$ nm). For comparison, the singlet–triplet splitting

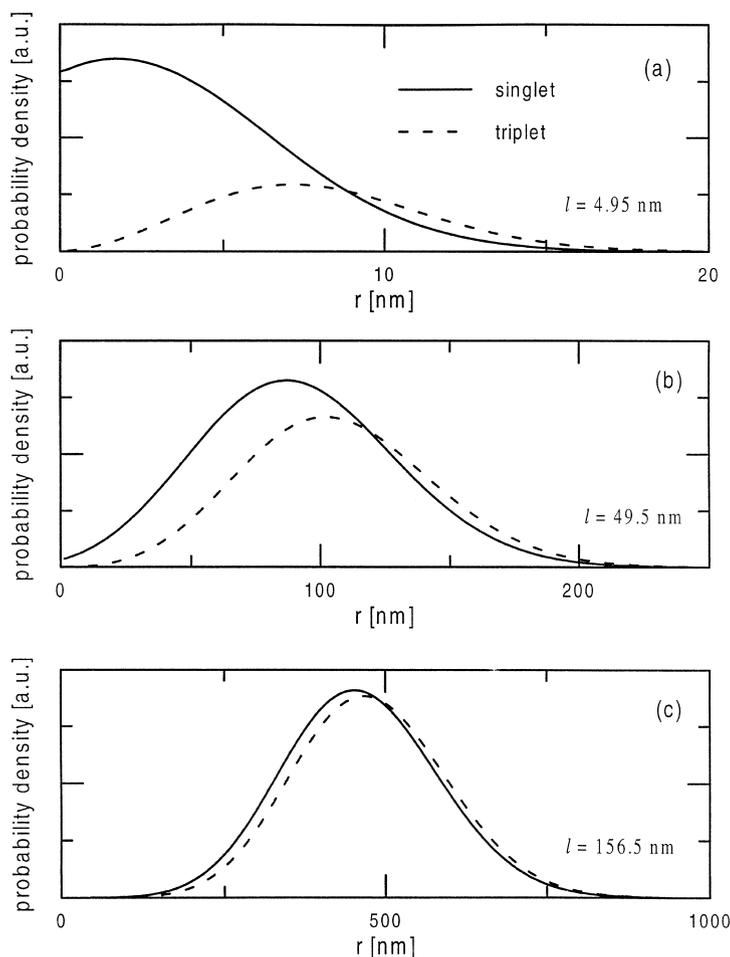


Fig. 3. Probability density $|\psi(r)|^2$ (equal to the pair-correlation function) in arbitrary units for singlet (solid curves) and triplet (dashed curves) states of two electrons confined in the spherical harmonic-oscillator potential for $l = 4.95$ nm (a), 49.5 nm (b), and 156.5 nm (c).

obtained by the HF method is displayed in the inset of Fig. 2. We see that for $l > 50$ nm the HF triplet energy level is located below the corresponding singlet energy level. This means that – in a contradiction to the exact results – the HF approach leads to a fictitious singlet-triplet “phase transition”.

The numerical values of errors of the HF method can be estimated from the results displayed in Fig. 1. The differences between the HF and exact results for $l = 12.5$ and 100 nm are equal to 0.41 and 0.13 meV, respectively, for the singlet states (0.07 and 0.04 meV for the triplet states). The corresponding relative errors are 1.44% and 14.2% for the singlet (0.21% and 0.40% for the triplet).

The electron–electron correlation can be studied with the help of a pair-correlation function, which for the electron pair in the harmonic-oscillator potential is equal to [19] a two-electron probability density, i.e., $|\psi(r)|^2$. The results of the present numerical calculations of the two-electron probability density for the singlet and triplet states are displayed in Fig. 3. The cusp for the singlet state near $r = 0$ [Fig. 3(a)] is a signature of a Coulomb hole, which results from the coulombic electron–electron repulsion, and can also be obtained from the analytical solution, which is valid for $r \rightarrow 0$ (cusp condition). If the dot size increases, the probability densities of singlet and triplet states approach each other and coincide with themselves almost

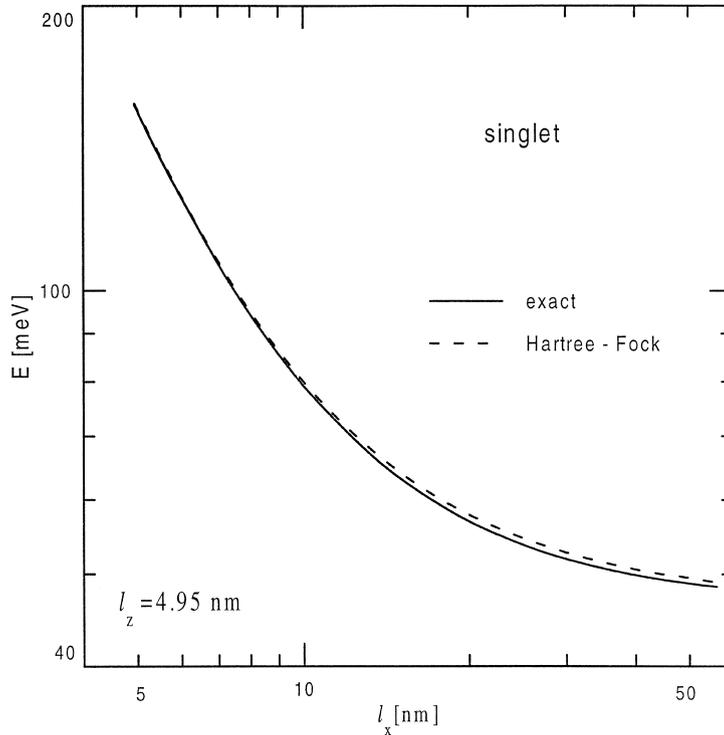


Fig. 4. Ground-state energy of singlet two-electron states in the anisotropic harmonic-oscillator potential with fixed $l_z = \gamma_z^{-1/2} = 4.95$ nm as a function of $l_x = \gamma_x^{-1/2}$. Solid (dashed) curve shows the exact (Hartree–Fock) results.

exactly [Fig. 3(c)] in the weak-confinement regime, in which both the states are nearly degenerate.

The anisotropic harmonic-oscillator potential, which can be used to a description of cylindrical quantum dots, is characterized by two parameters γ_x and γ_z [Eq. (4)]. We have performed the calculations for several values of characteristic length $l_x = \gamma_x^{-1/2}$ and a fixed value of $l_z = \gamma_z^{-1/2}$. We have taken $l_z = 4.95$ nm in accordance with Ref. [12]. The calculated energy of the singlet state is depicted in Fig. 4. Similarly as for the isotropic harmonic-oscillator potential, the exact and HF results coincide with themselves for small- and intermediate-size quantum dots, and slightly differ for large dots. For the triplet states (not shown in Fig. 4), we obtain an almost perfect coincidence of the exact and HF results for the dots of the size $l_x \leq 50$ nm. The comparison of the singlet and triplet energy levels is displayed in Fig. 5, which shows that – in accordance with inequality (9) – the singlet energy level is located below the

lowest triplet level for the dots of arbitrary radial extension. The singlet–triplet degeneracy is achieved for the cylindrical quantum dots of smaller size than for the spherical dots (cf. Figs. 2 and 5). Inset of Fig. 5 shows that the HF approach leads to the fictitious singlet–triplet “phase transition” at $l_x \simeq 25$ nm.

For the anisotropic oscillator potential characterized by $l_z = 4.95$ nm and $l_x = 7$ and 56 nm, the errors of the HF approximation for the singlet states are estimated to be 0.65 and 0.55 meV, respectively (0.12 and 0.08 meV for the triplet states). The corresponding relative errors are 0.6% and 1.1% for the singlet (0.10% and 0.15% for the triplet).

Fig. 6 reports the calculated electron probability density for cylindrical quantum dots in the plane $z = 0$ as a function of radius ρ . Again we see that the probability densities of the singlet and triplet states approach each other for the large dots [Fig. 6(c)] and this effect is associated with the degeneracy of the corresponding energy levels.

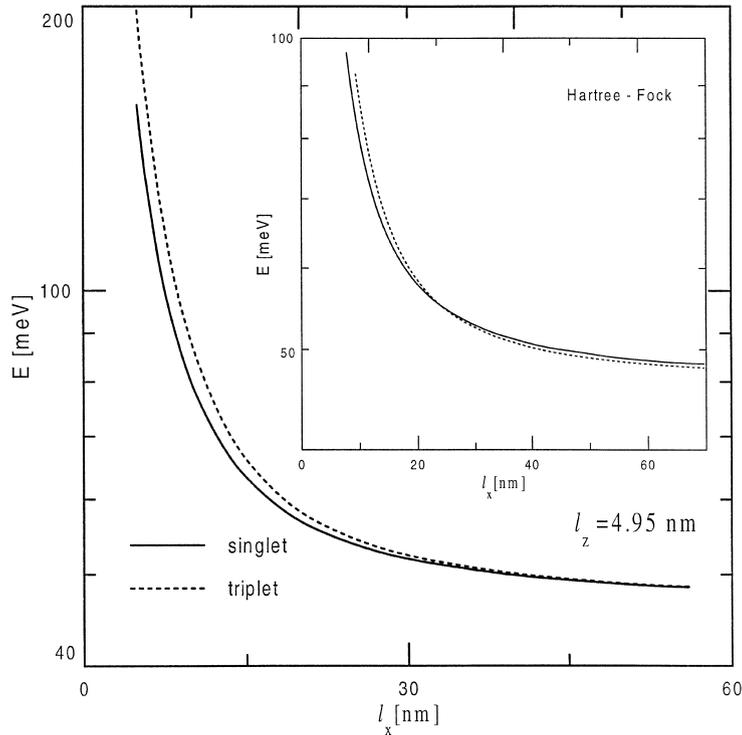


Fig. 5. Singlet–triplet splitting for the two-electron system in anisotropic harmonic-oscillator potential as a function of quantum-dot radial size l_x for fixed $l_z = 4.95$ nm. Solid (dashed) curves correspond to spin singlet (triplet) states. Inset: the corresponding results obtained by the HF method.

4. Discussion and conclusions

The results of the present paper show that the ground state of the two-electron quantum dot of arbitrary size is the spin-singlet state if the confinement potential is the harmonic-oscillator potential of the spherical or cylindrical symmetry. For the considered systems, no singlet–triplet phase transition takes place. This statement is supported by the analytical proof given in Section 2 as well as numerical results reported in Section 3. In the case of the anisotropic harmonic-oscillator confinement, our conclusion is in contradiction with the results of Fujito et al. [12], who used the HF method and obtained the spin-polarized ground state for large quantum dots. However, the results of Fujito et al. [12] agree with the present HF results (cf. inset of Fig. 5). This shows that the HF approximation leads to small systematic errors, which are caused by the neglect of the electron–electron

correlation. These errors are usually smaller for the triplet states than for the singlet states and slightly affect the results for the large quantum dots, i.e., in the weak-confinement regime. We note that in this regime all the calculated triplet–singlet energy differences are very small. Nevertheless, the small systematic error of the HF method can result in a fictitious spin-polarized ground state. On the other hand, the present results, that are exact for the two-electron states only, do not allow us to reject or confirm a spin polarization of the many-electron ground state. According to the HF results [12], the N -electron ground state with $N \leq 12$ electrons is spin polarized for large enough quantum dots. It is known that the HF method works better for many-electron systems.

The electron pair in the spherical harmonic-oscillator potential has been used [20] as a test system for studying the applicability of the HF method and few versions of the local spin density approximation.

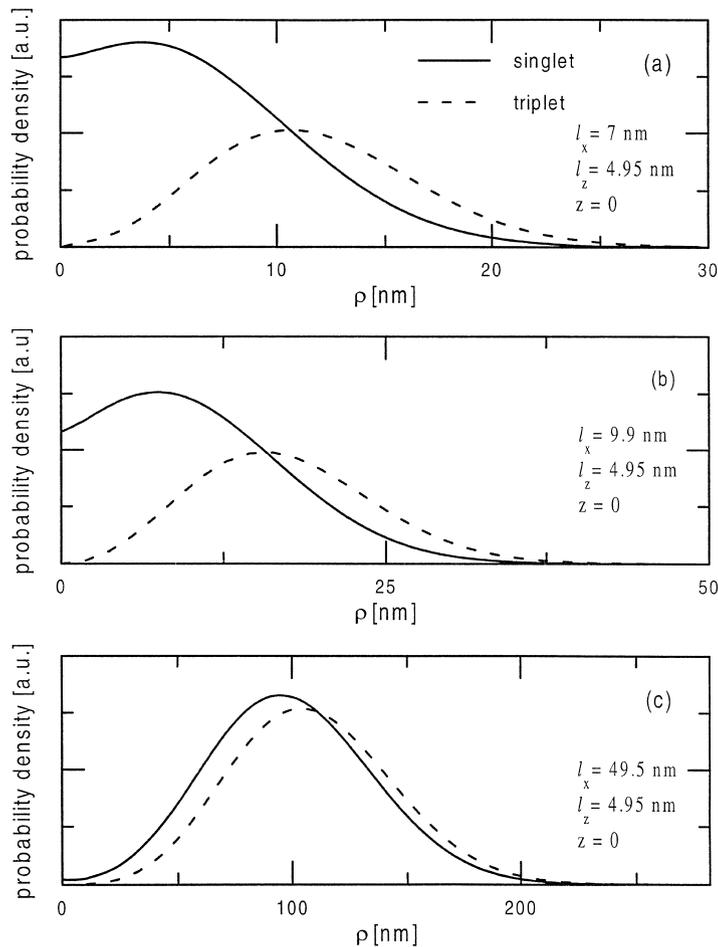


Fig. 6. Probability density $|\psi(\rho)|^2$ displayed in $z = 0$ plane in arbitrary units for singlet (solid curves) and triplet (dashed curves) states of two electrons confined in anisotropic harmonic-oscillator potential with fixed $l_z = 4.95$ nm and $l_x = 7$ nm (a), 9.9 nm (b), and 49.5 nm (c).

Taut et al. [20] discussed the errors introduced by these approximations in the weak-, intermediate-, and strong-confinement regimes. The conclusions of Ref. [20] about the applicability of the HF method to the isotropic harmonic-oscillator potential agree with our conclusions.

In our previous paper [3] on the two- and three-electron quantum dots we assumed the confinement potential in the form of the spherically symmetric potential well of finite depth. We predicted [3] a “phase transitions” from the low-spin to high-spin states if the radius of the dot was sufficiently large. These results were obtained with the help of the extended HF approach, which partially included

the electron–electron correlation. The estimated [3] energy differences between the spin-polarized and spin-unpolarized states were very small (of the order of $0.01R_D$). There arises a question if these “phase transitions” could result from a partial neglect of the correlation. Unfortunately, for the electronic system confined in the spherical potential well of finite depth it is impossible to separate out the center-of-mass motion and the eigenvalue problem depends on more than two variables. The problem [3] is more complicated than those considered in the present paper and the iterative extraction-orthogonalization method cannot be applied to check the results of Ref. [3]. We cannot exclude that the extended HF approach [3]

also prefers the fictitious spin-triplet ground state for large quantum dots. Nevertheless, the calculated [3] singlet and triplet energy levels lie in close proximity to each other and may be treated as nearly degenerate. Possible corrections to the results [3] would be very small and do not remove this near degeneracy, which determines the physical properties of the ground state of two electrons in large quantum dots.

We note that – due to the singlet–triplet degeneracy in large quantum dots – the presumed singlet–triplet “phase transition” cannot be verified experimentally in the absence of external fields. Such “phase transition” could only be detected under application of an external perturbation, e.g., a magnetic field, which lifts the degeneracy and splits the energy levels.

According to the results shown in Section 3, the pair-correlation function, which – for the systems considered in the present paper – is equal to the two-electron probability density, is nearly the same for the degenerate singlet and triplet states, i.e., for large quantum dots. This means that the influence of the orbital angular momentum on the electron distribution is suppressed in the weak-confinement regime. Therefore, for large quantum dots the singlet and triplet states possess (nearly) the same energy and (nearly) the same pair-correlation function.

In very large quantum dots, the electrons exhibit a Wigner-type localization [10], i.e., they behave similarly as classical point charges. This limit corresponds to the completely correlated electrons and cannot be obtained by the HF method. For the very large quantum dot, the two-electron probability density exhibits an enormous Coulomb hole in the vicinity of $r = 0$. Therefore, the influence of the centrifugal potential is negligibly small and the singlet and triplet states become degenerate. The HF method is less accurate for the singlet than for the triplet states (cf. Ref. [9]), since it neglects the vanishing two-electron probability density for the singlet states. The different accuracy of the HF method for both the states is responsible for the fictitious singlet–triplet “phase transition”.

5. Summary

We have shown that – in the absence of external magnetic field – the ground state is the spin singlet for the electron pair in the quantum dot of arbitrary size

for the harmonic-oscillator confinement potentials of spherical and cylindrical symmetry. We have found that for large quantum dots (in the weak-confinement regime) the singlet and triplet states become degenerate with almost coinciding pair-correlation functions. However, the lowest singlet energy level lies slightly below the lowest triplet level. This close proximity of singlet and triplet energy levels, when reproduced without adequate computational accuracy, can lead to a fictitious singlet–triplet “phase transition”. The previously predicted spin polarization of the ground state results from small systematic errors introduced by the HF approximation, which slightly underestimates the energy of the singlet states, but provides rather accurate estimates for the triplet states. This leads to the spin-triplet state to be preferred by the HF method as the lowest energy state in the weak-confinement regime. The small error of the HF approach is a result of the neglected electron–electron correlation. It can be noticeable for large quantum dots, i.e., for electron systems of low density. However, if we consider the quantum state of the given symmetry, e.g., singlet state, and if we are not interested in very subtle energy differences between the considered state and the first excited triplet state, then the HF method is very useful in determining the ground-state properties of the artificial atoms. The results of the present paper allow us to estimate the reliability of the HF method when applied to the quantum dots. We have pointed out that the HF approach provides reliable results for the quantum dots of small and intermediate size, i.e., in the strong- and intermediate-confinement regimes.

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