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Energy spectrum of D^- centres in spherical quantum dots

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Abstract. The properties of negatively charged D^- donor centres have been studied for semiconductor quantum dots with the finite spherically symmetric confinement potential. The energy levels of the ground state (1^1S) and the excited states of both the spin-singlet (1^1P , 1^1D , 2^1S) and spin-triplet (1^3P , 1^3D , 2^3S) configurations have been calculated by variational means. It has been shown that the excited states of the D^- centre in quantum dots are bound for sufficiently strong confinement potential. The conditions of binding for the excited states have been determined as functions of the potential-well depth and quantum-dot radius. The formation of the bound excited states of the D^- centre is a new property, which results from the confinement of electrons in the quantum dot. A possible application of the present results to the H^- ion trapped in a microcavity is discussed.

1. Introduction

The D^- donor centres in semiconductor nanostructures have recently been investigated from both the experimental [1–6] and theoretical [7–12] points of view. The experimental evidence for the D^- centre has been found in multiple-quantum-well structures [1]. A possible experimental observation of D^- centres has been discussed [2] for GaAs/ $Al_xGa_{1-x}As$ quantum dots. In bulk materials, the weakly localized, shallow-level donor centre D^- can be treated in the framework of the effective-mass approximation as a solid-state analogue of a H^- ion. According to the Hill theorem [13], the H^- ion in an infinite space and the hydrogen-like D^- centre in a bulk crystal possess only one bound state with the spin-singlet configuration. The applied external magnetic field leads to a formation of bound excited states of the H^- ion and D^- centre [14]. Transitions to the excited states have been identified [3, 9] for the D^- centres in multiple quantum wells in the external magnetic field.

A quantum dot (QD) is a semiconductor nanostructure with a three-dimensional confinement of electrons [15]. Recently the QDs have been fabricated in different shapes, for example, disk-like (cylindrical) shape [2] and spherical [15, 16] shape. The spherically-shaped QDs are formed from semiconductor nanocrystals embedded in either an isolating [16] or a semiconducting matrix [15]. The conduction-band discontinuity between the QD and surrounding material leads to an appearance of the effective confinement potential for electrons. This potential can be approximated by a step function with the potential-well region inside the QD and the potential-barrier region outside the QD. The confinement potential essentially modifies the properties of electronic and impurity states in the QD. We consider the influence of the confinement potential on the properties of the D^- centre. As in the bulk crystal, the ground state of the D^- centre in the QD is always bound. There

arises a problem of the existence of bound excited states of the D^- centre in the QD. We expect that the confinement potential can lead to a creation of bound excited states of the D^- centre.

The ground-state energy of the D^- centre was estimated by variational means [17, 18] for the QD with the confinement potential of finite depth. Using the results of the second-order perturbation theory for the infinitely deep potential-well, Büsser and Proetto [19] put the hypothesis that—as for the H^- ion—only one bound state of D^- exists in the QD of the finite potential well.

The present paper provides a proof of the opposite statement for the excited states. We show that several excited states can be bound for the D^- centre in the QD with the finite confinement potential. We have considered the S, P and D states with both the singlet and triplet spin configuration and determined the conditions of binding for the excited states. We have also calculated the dipole-allowed transition energies and the expectation values of interparticle distances. Preliminary results of this work were announced in [20]. The present paper consists of the complete results with a detailed discussion.

2. Theory

The D^- centre in a semiconductor spherical quantum dot can be described as a system composed of two electrons and a positively charged donor impurity located at the centre of the spherical potential-well region. We consider a single quantum dot embedded in a matrix material. We assume the validity of the effective-mass approximation and neglect the difference of the electron band masses and dielectric constants between the QD region and the surrounding medium. The Hamiltonian of the system has the form

$$H = -\nabla_1^2 - \nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{2}{r_{12}} + V(r_1) + V(r_2) \quad (1)$$

where $r_i = |\mathbf{r}_i|$ ($i = 1, 2$) are the electron–donor centre distances, $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ is the electron–electron separation, the donor Rydberg $R_D = m_e e^4 / 2\hbar^2 \varepsilon^2$ is the unit of energy, the donor Bohr radius $a_D = \hbar^2 \varepsilon / m_e e^2$ is the unit of length, m_e is the conduction-band electron effective mass, and ε is the static dielectric constant. The confinement potential for electrons in the QD is assumed to be a spherically symmetric potential well of finite depth, i.e.

$$V(r) = \begin{cases} 0 & \text{for } r < R \\ V_0 & \text{for } r \geq R \end{cases} \quad (2)$$

where R is the radius of the QD.

In order to find solutions of the eigenproblem for Hamiltonian (1), we apply the variational method and propose the trial wavefunction in the form

$$\Psi_{\pm}^L(\mathbf{r}_1, \mathbf{r}_2) = \exp[-\alpha(r_1 + r_2)] \sum_{mnp} c_{mnp}^L (1 \pm \mathcal{P}_{12}) r_1^m r_2^n r_{12}^p P_L(\cos \theta_1) \quad (3)$$

where the sign $+(-)$ corresponds to the spin singlet (triplet) state, L is the total-angular momentum quantum number, \mathcal{P}_{12} is the permutation operator, which interchanges the electron indices, i.e. $1 \rightleftharpoons 2$, c_{mnp}^L and α are the linear and non-linear variational parameters, respectively, $P_L(\cos \theta_i)$ is the Legendre polynomial of order L , and θ_i is the angle between the z -axis and vector \mathbf{r}_i . We consider the S, P and D states with $L = 0, 1$ and 2 , respectively. The sums in (3) run over integral values of parameters m, n and p , which are chosen as follows: $m = m_1, \dots, 12$, where $m_1 = 0$ for the singlet S states, $m_1 = 1$ for the triplet S

states and the P states and $m_1 = 2$ for the D states; $n = 0, \dots, n_2$, where $n_2 = m$ and $m - 1$ for the singlet and triplet S states, respectively, and $n_2 = 12$ for the P and D states; $p = 0$ and 1 for the S states, and $p = 0$ for the P and D states. We have omitted the dependence of the trial wavefunction on r_{12} for the P and D states, since the electron–electron correlation plays a minor role for the excited states with $L \neq 0$. The numbers of terms in expansion (3) applied in the present calculations were the following: 181 for the singlet S states, 156 for the P states and triplet S states, and 143 for the D states.

The exact wavefunction for the electronic system in the spherical potential well of finite depth obeys the following boundary conditions for $r = R$, i.e. at the QD boundary: the wavefunction and its first derivative are continuous, but the second derivative possesses a finite jump and changes its sign, which results from the finite jump of the potential energy. This means that the wavefunction changes its curvature at the QD boundary. Owing to the presence of the polynomial terms, the proposed trial wavefunction (3) is flexible enough and fulfills this boundary condition. Moreover, the application of trial wavefunction (3) enables us to calculate all the matrix elements of Hamiltonian (1) analytically. A more detailed discussion of the properties of the proposed variational wavefunction is given in section 3.

In order to solve the problem of existence of bound excited states for the D^- centre in the QD, we have to determine the binding energy of the system. The binding energy of the ν th quantum state of the D^- centre is defined as the difference between the continuum-threshold energy and the energy of the considered state of the D^- centre, i.e.

$$W_\nu = E_0^0 + E_b^e - E_\nu^- \quad (4)$$

where E_0^0 is the ground-state energy of the D^0 donor centre, E_b^e is the lowest energy of the electron in the potential-barrier region, and E_ν^- is the energy of the ν th state of the D^- centre, i.e. the corresponding eigenvalue of Hamiltonian (1). For the confinement potential (2), $E_b^e = V_0$. The continuum threshold corresponds to the system composed of the one electron bound in the ground state of the neutral D^0 donor centre in the QD and the second—occupying the lowest-energy conduction-band state in the barrier region. The binding energy defined by (4) possesses the following physical interpretation: this is the minimum energy, which is required to liberate one electron from the bound state of the D^- centre located in a single QD and transfer it into the barrier region. After this dissociation process, the second electron is bound in the ground state of the D^0 centre. The considered ν th state of the D^- centre is bound if $W_\nu > 0$.

We mention that another definition of the binding energy was used in papers [17–19], namely

$$\tilde{W}_\nu = E_0^0 + E_w^e - E_\nu^- \quad (5)$$

where E_w^e is the ground-state energy of the electron bound in the quantum-dot potential well. Let us note that in formulae (4) and (5) two different electron energies are used: the energy E_b^e in (4) is associated with the conduction-band state of the barrier region, while E_w^e in (5) corresponds to the bound state of the electron confined in the QD potential-well region. The physical meanings of W_ν and \tilde{W}_ν are different. The quantity \tilde{W}_ν (5) can be interpreted as the energy needed to liberate one electron from the D^- centre and move it into the lowest-energy state of the electron confined within the another QD. This process cannot occur for the single isolated QD. If the liberated electron were confined in the same QD, the attractive potential of the D^0 centre would immediately bind it into the D^- state. The ‘binding energy’ [17–19] defined by (5) corresponds to a process of tunnelling of the liberated electron into the second QD without an impurity centre. However, the authors [17–19] neglected a coupling between different quantum dots, which means that the probability

of this tunnelling was taken to be zero. Therefore, unlike W_v , the physical meaning of \tilde{W}_v is not quite clear for the single QD. Moreover the negative value of \tilde{W}_v (5) does not mean that the considered state is unbound.

3. Results

Before performing the calculations for the two-electron D^- centre, we checked the applicability of our variational approach to the simple one-electron problems, i.e. the electron and D^0 centre in the finite spherically symmetric potential well, for which the analytical solutions are known. We have applied to these systems the following trial wavefunction

$$\psi(r) = \sum_{n=0}^{12} c_n r^n \exp(-\alpha r) \quad (6)$$

which is a simple one-dimensional version of that given by (3). The shape of wavefunction (6) received from the variational calculation is shown and compared with the exact results in figure 1(a) (for the one electron in the QD) and figure 1(b) (for the D^0 centre in the QD). We see that the variational and exact wavefunctions coincide with each other. In particular, we note that the variational wavefunction of type (6) correctly reproduces the change of curvature for $r = R$. The ground-state energy of the D^0 centre calculated with the help of trial wavefunction (6) is also in very good agreement with the results obtained by analytical methods by Zhu [21] and Buczko and Bassani [22].

The two-electron trial wavefunction (3) has also been tested by applying it to the He atom and H^- ion. Table 1 provides the comparison of the present results with the exact eigenvalues [23, 24] for the ground and excited states of the He atom. For the ground state of the D^- centre in the QD, we can also compare our results with those of the other authors [17–19]. For this purpose, we have calculated the ground-state ‘binding energy’ defined by (5). Here we give the exemplary results, for example, for $V_0 = 40R_D$ and $R = 0.1$ and $0.3a_D$, we obtain 0.0573 and $2.36R_D$, respectively, while the corresponding values taken from [17, 18] are 0.0526 and $2.36R_D$. For all other values of the QD parameters, the present results for the ‘binding energy’ (5) are usually larger than those of Zhu *et al* [17, 18], which is caused by a larger flexibility of the trial wavefunction used in the present work. Let us note that the present approach is also suitable for the excited states.

Table 1. Energy levels of the He atom in atomic Rydbergs. The ‘exact’ results are taken from [23, 24].

State	Present	‘Exact’
1^1S	–5.8074	–5.8074
2^3S	–4.3503	–4.3504
2^1S	–4.2906	–4.2919
1^3P	–4.2647	–4.2663
1^1P	–4.2452	–4.2477

Recently the problem of a H^- ion constrained in a microcavity has been of interest in atomic physics [25]. We have calculated the ground-state energy of the H^- ion in a spherical potential well of finite depth. The present results are listed in table 2. Table 2 also shows the results for the H^- ion in the infinitely deep potential well obtained by the quantum Monte Carlo method [25]. We can observe that the confinement potential of finite

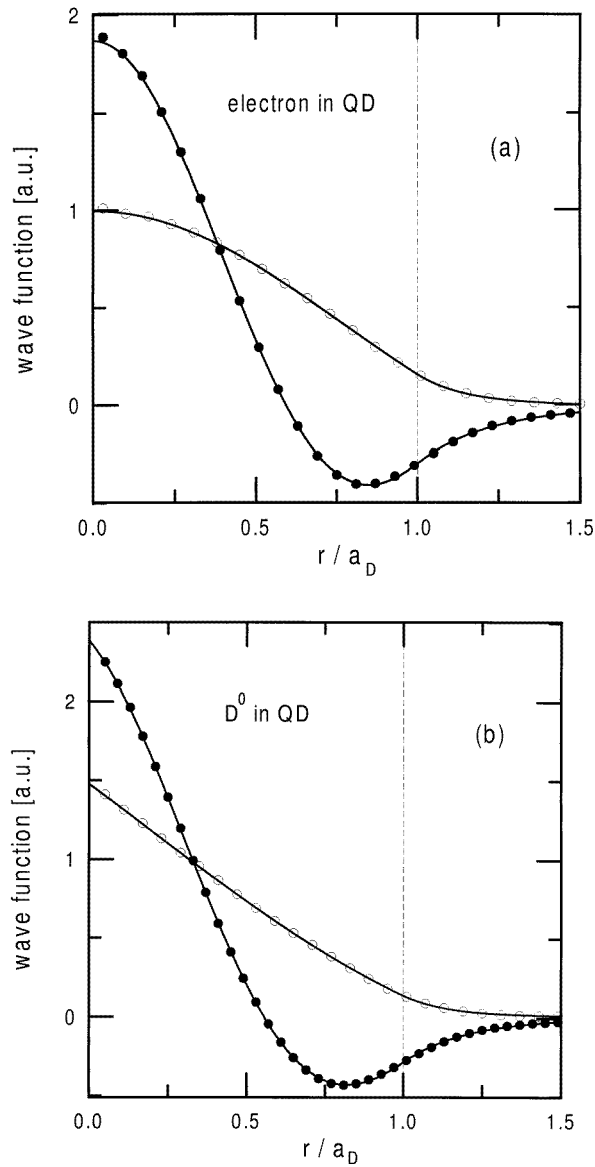


Figure 1. (a) Wavefunctions of 1s (open symbols) and 2s (full symbols) states for the electron in the QD with $V_0 = 40R_D$, $R = 1.0a_D$ as functions of r (electron-QD centre distance). Full curves correspond to the exact wavefunctions and circles, trial wavefunctions (6). The wavefunctions are unnormalized and plotted in arbitrary units, a_D is the donor Bohr radius. (b) Wavefunctions of 1s and 2s states for the D^0 centre in the same QD.

depth leads to a lowering of the ground-state energy. For large R , the effect of confinement decreases and both the energy eigenvalues approach each other. In particular, for $R = \infty$, we deal with the H^- ion in an infinite space. The results of tables 1 and 2 also show that trial wavefunction (3) is sufficiently flexible and yields reliable results for the two-electron systems in the infinite space as well as in the microcavity.

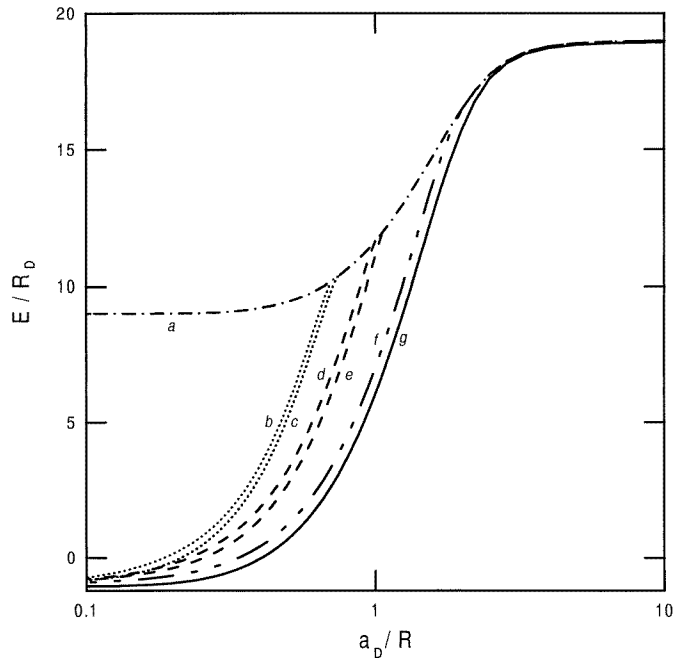


Figure 2. Energy levels of D^- states in a QD as functions of radius R for the potential-well depth $V_0 = 10R_D$. Curves (a) and (b), (c), (d) and (e) correspond to the continuum threshold and 2^1S , 2^3S , 1^1P and 1^3P excited states, respectively, curve (f) shows the sum of ground-state energies of a D^0 centre and an electron in the QD, curve (g) displays the ground-state energy of the D^- centre. The donor Rydberg R_D is the unit of energy, the donor Bohr radius a_D is the unit of length.

For the D^- centre in the QD, we have performed the calculations for the ground state (1^1S) and the following excited states: 1^1P , 1^3P , 1^1D , 1^3D , 2^1S and 2^3S . Figure 2 shows the energy eigenvalues as functions of QD radius for the fixed potential-well depth $V_0 = 10R_D$. We see that for the sufficiently large R the energy levels of all the considered states are located below the continuum-threshold energy. Therefore the excited states of the D^- centre are bound. Moreover we have received the correct bulk-crystal limits, i.e. for $R \rightarrow 0$, the ground-state energy $E(1^1S) \rightarrow 2V_0 - 1.055R_D$ and for $R \rightarrow \infty$, $E(1^1S) \rightarrow -1.055R_D$ and all the excited-state energy levels $E_v \rightarrow -R_D$. The energy levels of the 1^1D and 1^3D states are located above (but very close to) those of the 2^1S and 2^3S , respectively, and are not shown in figure 2. The corresponding numerical results for all the states considered are listed in table 3. Curve (f) in figure 2 shows the sum of the ground-state energies of the D^0 centre and the electron in the spherical potential well. The excited-state energy levels are located above this curve, which is in agreement with the suggestion of Büsser and Proetto [19]. However, according to the discussion in section 2, this does not mean a lack of binding of the excited states.

Table 3 shows a comparison of the calculated two-electron energy levels for the spherical QD without and with the donor centre. In both the cases, trial wavefunction (3) has been applied. For the excited states of two electrons ($2e$) with the same spin, we obtain the same order of energy levels as that for the one electron in the spherical potential well, i.e. $E_{1P} < E_{1D} < E_{2S}$. The influence of the attractive donor centre shifts all the energy

Table 2. Ground-state energy of the H^- ion at a centre of a spherical microcavity as a function of radius R . The present results are given for $V_0 = 40R_D$, QMC denotes the quantum Monte Carlo results [25] for $V_0 = \infty$. The last number in the third row (for $R = \infty$) is the exact value [23]. The unit of energy is the atomic Rydberg, the unit of length is the atomic Bohr radius.

R	2	4	6	8	10	12	15	∞
Present	0.8998	-0.7784	-0.9926	-1.0364	-1.0487	-1.0529	-1.0548	-1.0554
QMC	1.4462	-0.7588	-0.9916	-1.0360	-1.0478	-1.0514	-1.0522	-1.0555

Table 3. Energy levels of two-electron QDs without ($2e$) and with (D^-) the donor centre for the QD parameters: $V_0 = 40R_D$ and $R = 2.5a_D$. The donor Rydberg R_D is the unit of energy.

State	1^1S	1^3P	1^1P	1^3D	1^1D	2^3S	2^1S
$2e$	3.692	4.698	5.192	6.316	6.707	7.188	7.385
D^-	-0.098	1.435	1.871	3.198	3.480	3.014	3.396

Table 4. Critical values of the parameters C_ν (7) determining the binding of the excited states of the D^- centre in the QD (in units $R_D a_D^2$).

1^3P	1^1P	2^3S	2^1S	1^3D	1^1D
9.084	10.21	19.82	21.02	20.63	21.18

levels downwards. In particular, both the singlet and triplet 2S levels are shifted below the corresponding 1D levels.

It is well known that for a spherical potential well of finite depth the one-electron states become bound if the ‘effective capacity’ of the potential well, i.e. $V_0 R^2$, exceeds certain critical values, for example, $\pi^2/4$, π^2 , $2\pi^2$ and $9\pi^2/4$ (in units of $R_D a_D^2$) for the states $1s$, $1p$, $1d$ and $2s$, respectively. We have found that the conditions of binding for the excited states of the D^- centre in the QD can be parametrized in a similar way, i.e.

$$V_0 R^2 > C_\nu \quad (7)$$

which means that the ν th state of the D^- centre is bound if the effective capacity of the QD exceeds the critical value C_ν . The values of C_ν , estimated in the present paper, are quoted in table 4. According to table 4, the number of bound excited states of the D^- centre increases with the increasing effective capacity of the QD, which is consistent with the similar property of the one-electron states.

We have also calculated the experimentally accessible transition energies. Figure 3 shows the ground-state binding energy and the $1^1S \rightarrow 1^1P$ transition energy as functions of the QD radius and potential-well depth. The results for the confinement potential of the infinite depth are also shown. If the 1^1P state is bound, i.e. inequality (7) is filled, the dipole-allowed $1^1S \rightarrow 1^1P$ radiative transitions can take place. The transition energy increases with the decreasing dot size and reaches the maximum value of about half of the potential-well depth for the QD radius, at which the 1^1P state ceases to be bound. Then, the $1^1S \rightarrow 1^1P$ transition energy becomes equal to the 1^1S binding energy, i.e. the energy of the transition of the electron into the barrier region.

Table 5 shows the values of transition energy calculated for the QD nanostructure made from the GaAs nanocrystal embedded in $Al_xGa_{1-x}As$ matrix. For $x = 0.2$, the

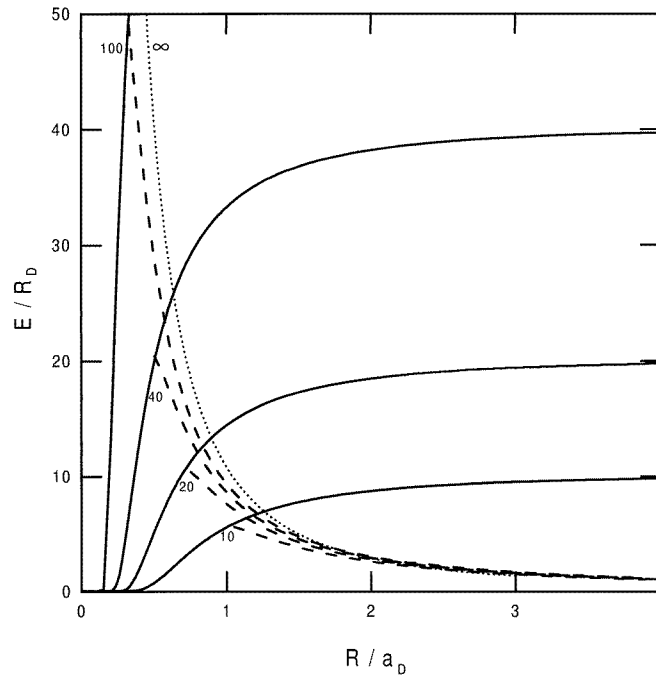


Figure 3. Ground-state binding energy (full curves) and $1^1S \rightarrow 1^1P$ transition energy (broken curves) as functions of quantum-dot radius R for the potential-well depth $V_0 = 10, 20, 40$ and $100R_D$. The dotted curve shows the transition energy for the infinitely deep potential well. The units are the same as in figure 2.

following values of the parameters have been taken on: $V_0 = 0.212$ eV, $R_D = 5.3$ meV and $a_D = 10$ nm. For comparison, we have also listed in table 5 the energies of dipole-allowed radiative transitions between the corresponding states of one- and two-electron systems confined in the QD as well as D^0 donor centre in the QD. We notice that the transition energies for the one ($1e$) and two ($2e$) confined electrons as well as for the D^0 and D^- donor centres in the QD are in pairs close to each other, which means that the corresponding radiative transitions could be hardly distinguishable.

Table 5. Calculated energy of dipole-allowed radiative transitions between the states with $L = 0$ and $L = 1$ of one electron ($1e$), two electrons ($2e$), D^0 and D^- donor centres and binding energy W for the D^- ground state in the GaAs/Al_{0.2}Ga_{0.8}As quantum dot of radius R . The results for $1e$ and D^0 correspond to the $1s \rightarrow 1p$ transitions and those for $2e$ and $D^- - 1^1S \rightarrow 1^1P$ transitions. The dash (—) means that the 1^1P state is unbound. The radius is expressed in nm, the energy in meV.

R	$1e$	$2e$	D^0	D^-	W
5	97.0	—	112.5	—	106.5
10	40.0	42.1	46.3	45.5	176.3
20	11.7	13.3	16.0	15.4	202.5
30	5.5	6.8	9.1	8.5	208.3

Having at our disposal the optimized trial wavefunction, we have also calculated the expectation values of electron–donor ($\langle r_1 \rangle$) and electron–electron ($\langle r_{12} \rangle$) distances. Figure 4 shows the results for the ground state (1^1S) and the excited state (2^1S) as functions of the QD radius. The ground-state interparticle distances equal to those for the H^- ion [24] in the bulk-crystal limit, i.e. for $R = 0$, possess a minimum for small R , and next increase reaching again the bulk-crystal values for large R . For the excited 2^1S state, the curves in figure 4 begin at this value of R , which corresponds to the critical binding for this state. The interparticle distances for the excited state increase almost linearly with R , which is a manifestation of a physical nature of binding of the excited state in the QD. This binding mainly results from the confinement of electrons in the QD. Therefore, the interparticle separations grow proportionally to R , but remain smaller than the QD radius. We have obtained similar results for the average distances for the other excited states.

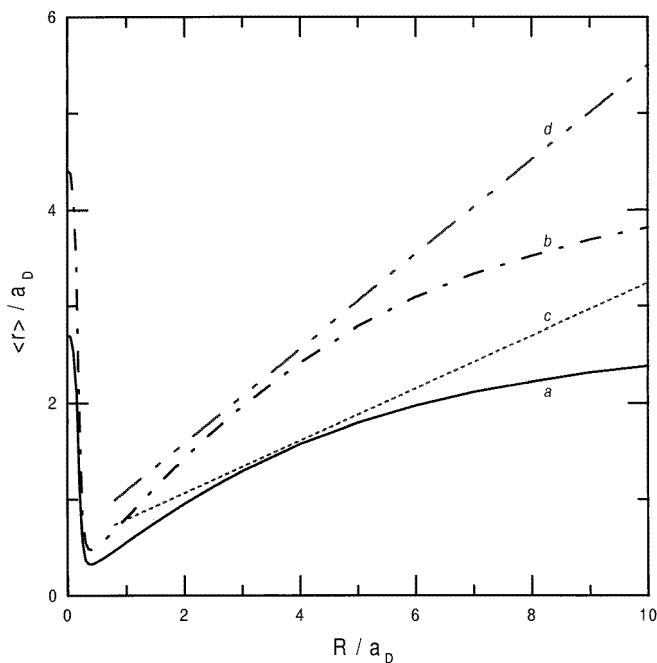


Figure 4. Expectation values of interparticle distances for the D^- centre in the QD with $V_0 = 40R_D$ as functions of radius R . Curves (a) and (b) show the results for the ground state (1^1S): electron–donor $\langle r_1 \rangle$ and electron–electron $\langle r_{12} \rangle$ distances, and curves (c) and (d) the excited-state (2^1S): $\langle r_1 \rangle$ and $\langle r_{12} \rangle$, respectively. The donor Bohr radius a_D is the unit of length.

4. Discussion

The present calculations show that the energy spectrum of the D^- centre in the QD exhibits the following characteristic properties: (i) the spin-triplet states possess lower energy than the corresponding spin-singlet states; (ii) the energy levels of the $2S$ states are located above those of the $1P$ states, i.e. the Lamb shift ($2S-1P$ energy difference) is positive; (iii) the $2S$ states possess lower energy than the corresponding $1D$ states with the same spin. Property (i) corresponds to the same order of energy levels for the He atom in the infinite space (cf

table 1), i.e. it results from the bulk-like behaviour of the D^- centre. However, the positive Lamb shift (property (ii)) is opposite the negative Lamb shift observed for the He atom (cf table 1), but is compatible with the order of the 2S and 1P energy levels of one electron in the spherical potential well. Moreover, the same order of the 2S and 2P energy levels has been obtained for the electron pair confined in the QD (cf table 3). The 2S–1D energy-level order (property (iii)) is caused by the non-vanishing probability of finding the electron at the Coulomb centre in the S state. Therefore, the bound states of the D^- centre in the QD possess a mixed bulk-like/well-like character.

The properties of the D^- states discussed above have been obtained by the variational method, which yields reliable upper bounds on the total energy, i.e. lower bounds on the binding energy (provided that the ground-state energies of the electron and D^0 centre in the QD are exact, which is true in our case). In turn, the lower bounds to the binding energy lead to the lower bounds to the critical effective capacity of the QD (7). This means that the bound excited states of the D^- centre can appear in a broader class of QD nanostructures than these determined by the values given in table 4.

In the present work we have considered the six excited states of the D^- centre in the QD. For these states we have determined the conditions of binding in the form of inequality (7). We expect that the criteria of binding in form (7) are also valid for the higher excited states of the D^- centre in the QD. A possibility of binding of a larger number of the D^- excited states can be inferred from the following argument. The subsystems of D^- centre, i.e. the hydrogen-like D^0 centre and the electron in the QD, possess infinite and finite numbers of bound states, respectively. The quantum states of the D^- centre in the QD are constructed from the corresponding quantum states of both the subsystems. As a result, the D^- centre always forms one bound state and can form bound excited states for the sufficiently strong confinement potential. The number of these states should be finite and increases with the increasing radius and potential-well depth.

We would like to comment about the question how the present results can be applied to the GaAs/ $\text{Al}_x\text{Ga}_{1-x}\text{As}$ nanostructure (table 5) despite the change of the electron band mass at the boundary of this QD, which is neglected in the present work. In order to answer this question we have estimated the two-electron probability density for the 1^1S and 2^1S states (cf figure 2b in [20]), which provides a measure of the penetration of electrons into the barrier region. For the QD radius $R > \sim a_D$, this penetration appears to be negligibly small [20], which is caused by the presence of the potential barrier of the height $V_0 = 40R_D$.

The effect of spatially variable electron band mass can be taken into account by modifying the kinetic-energy operator in (1) according to the BenDaniel–Duke model [26]. Such a modification is equivalent to the explicit incorporation of the jump of the electron band mass into the kinetic-energy operator in (1) together with the requirement that the envelope wavefunction f for electrons in the spherical QD fulfills the boundary condition

$$\frac{1}{m_e^w} \frac{df}{dr} \Big|_{r \rightarrow R^-} = \frac{1}{m_e^b} \frac{df}{dr} \Big|_{r \rightarrow R^+} \quad (8)$$

where m_e^w (m_e^b) is the electron band mass of the potential-well (potential-barrier) region. Taking on $m_e^w = 0.067m_{e0}$ and $m_e^b = 0.084m_{e0}$, where m_{e0} is the electron rest mass, we have solved the Schrödinger equation for the electron and D^0 centre in the spherical QD by a finite-difference method, which allows us to include the jump of the electron band mass and boundary condition (8) explicitly. The results (figure 5) show that taking into account the change of the electron band mass at the GaAs/ $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ boundary leads to a slight lowering of the ground-state energy, i.e. increase of the binding energy. This effect is negligibly small for $R > a_D$, since the electron penetration into the barrier region

additionally decreases owing to the increase of the electron band mass in $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$. These results provide the quantitative arguments for the neglect of the change of the electron band mass at the QD boundary.

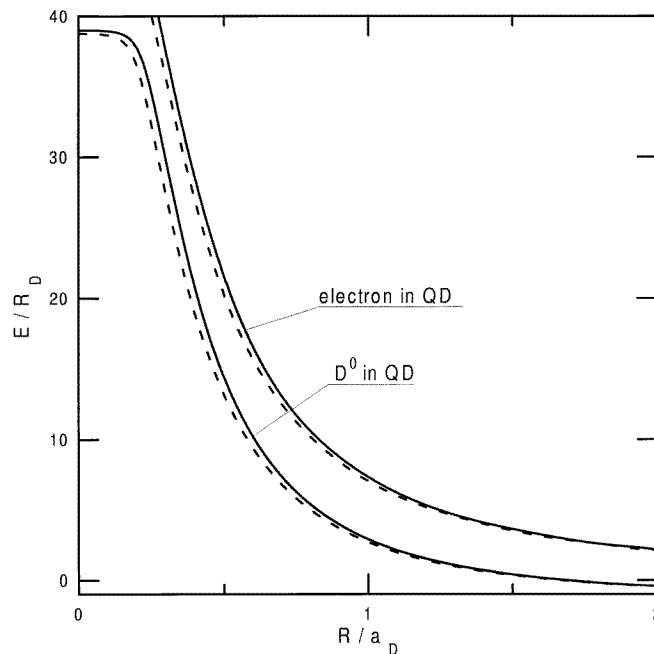


Figure 5. Ground-state energy of the electron and D^0 centre in the spherical QD of radius R calculated with the change of the electron band mass at the QD boundary included (broken curves) and excluded (full curves). The values of material parameters correspond to the GaAs/ $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$ nanostructure.

As mentioned in section 3, an ion trapped in a microcavity [27] should exhibit properties similar to those studied in the present work for charged donor centres in semiconductor QDs. The present results could be applied to the H^- ion confined in an ionic trap provided that the confining potential was approximated by the spherical potential well. Based on the results of the present paper, we expect that the bound excited states can exist for the H^- ion trapped in an ultra-high vacuum microcavity by external electric fields. Therefore the spectroscopic experiments with these ions could reveal the transitions between the excited and ground states considered in the present work.

5. Summary

The present paper provides the proof of binding for the excited states of the D^- centre and H^- ion, which are confined in a spherical microcavity. Such a microcavity can be formed either in a solid material as a semiconductor quantum-dot nanostructure or in a vacuum as an ionic trap. It has been shown that several excited states of the D^- and H^- ions are bound if the confinement potential is sufficiently strong. The criteria of the binding have been determined in the simple analytical form.

The following physical interpretation can be given to an origin of binding of these excited states: this property results from the confinement of electrons in the microcavity

and the bound excited states of the two-electron systems correspond to those of the single electron confined in the spherical potential well. We expect that the present results will be helpful in planning future experiments for possible evidence of the excited states of the D^- centre in a semiconductor quantum dot and H^- ion in an ionic trap.

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