Dimensionality and potential-shape effects on D^0 and D^- ground states in quantum dots

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The binding energies $E_B(D^0)$ and $E_B(D^-)$ of neutral and negative donor (D^0 and D^-) centers in quantum dots (QD's) with different dimensionality and potential shape have been obtained by a variational approach with a trial function, which consists of the exact solutions of D^0-like ground states in the dots, includes the electron-correlation effect, and approaches the Chandrasekhar-type trial function at zero barrier height. The dimensionality and potential-shape effects of QD's on $E_B(D^0)$ and $E_B(D^-)$ have been studied in detail. It has been found that the electron-correlation effect on $E_B(D^-)$ depends on the dimensionality and decreases with increasing confinement. The ratio σ of $E_B(D^-)$ to $E_B(D^0)$ approaches a constant value in the limit of strong confinement. It has been shown that the ratio σ and the electron-correlation effect are strongly dependent on the dimensionality of QD's and weakly dependent on the potential shape. Using the value of the σ obtained, calculated results of different quantum-well structures can be checked and compared with others.

I. INTRODUCTION

There is an increasing interest in the electronic structure and properties of neutral[1] and negative[2-14] donor centers in various low-dimensional structures, such as two-dimensional quantum wells (2DQW's), quantum-well wires (QWW's), quantum dots (QD's), and so on. It has been shown that many effects in 2DQW's, such as quantum Hall effects, metal-insulator transitions, and electron localizations, are intimately related to phenomena of high magnetic fields and impurity states. Now, we can believe that the fundamental study of the properties of donor centers not only in 2DQW's but also in QWW's and QD's with and without magnetic fields is important in its own right, as reducing the dimensionality often introduces unexpected physical phenomena.

There have been many investigations of neutral shallow donors D^0 in GaAs-$Ga_{1-x}Al_xAs$ multiple-quantum-well structures with and without doping in strong magnetic fields.[14-17] Recently, negative donor D^- centers (i.e., a D^0 center that binds a second electron) have been shown to form readily in selectively doped multiple quantum wells owing to electron transfer from the $Ga_{1-x}Al_xAs$ barrier to neutral donors located in GaAs well.[3-7] Using far-infrared magnetotransmission and magnetophotoconductivity measurements, Huant, Najda, and Etienne have shown the transition from D^- ground state to the excited states associated with successive Landau levels.[3] Furthermore, D^- centers have been unambiguously identified in GaAs-$Ga_{1-x}Al_xAs$ quantum wells by Mueller, Larsen, Waldman, and Goodhue according to the dependence of the observed photoconductivity spectrum on the applied magnetic field and sample orientation.[4] Very recently, Holmes, Cheng, McCombe, and Schaff have reported a far-infrared magnetospectropic study of the evolution of the intensities of various impurity lines carried out by a photon-dose technique on Si-doped GaAs-$Ga_{1-x}Al_xAs$ multiple-quantum-well samples.[5] The results have clearly demonstrated that the binding energy of the two-electron bound state, i.e., D^- ground state is much smaller than that of the D^0 state and, hence, it should be populated after the D^0 states, but before the free-electron states.

Using the double planar-doping technique and magneto-optical study, Mandray, Huant, and Etienne have shown that for a proper choice of the doping geometry, it is possible to control the D^- concentration, and eventually to convert all neutral donors in the wells to D^- centers.[6] It is worthwhile to point out that having a well-controlled D^- and electron population under equilibrium conditions opens the possibility of studying many interesting phenomena related to negatively charged donors in quantum-well structures, such as many-electron effects on D^0 centers in 2DQW's in high magnetic fields.[7]

The effective-mass model has been applied to the D^0 and D^- centers in a magnetic field in both 2DQW's and bulk semiconductors, and the model has been solved by a diffusion quantum Monte Carlo method.[8] For bulk semiconductors, comparison of the results with the experimental data [18] and other calculations[19,20] shows that electron correlation effects are very important to obtain better results. For 2DQW's, there is a large increase in binding energies over those of bulk semiconductors. It represents that the binding energies of D^- centers in a magnetic field are strongly dependent on confined dimensionality, i.e., the dimensions and the strength of the magnetic field. In order to know the limits of the binding

energies of the pure two-dimensional (2D) D^- centers in a magnetic field and the electron correlation effect on them, the ground states have been studied by use of a variational approach.[11] The calculated results have shown that the binding energies of D^- centers in 2D case are larger than those in 2DQW and three-dimensional (3D) cases, and that the electron-correlation effects are strongly dependent on the confinement. To analyze the dependence of the observed photoconductivity spectrum on the applied magnetic field and sample orientation and identify D^- centers in GaAs-$Ga_{1-x}Al_xAs$ quantum wells, variational calculations have been carried out for the ground states and the singlet $M=0$ and 1 excited states and, then, splitting of the D^- transition due to tilting the sample relative to field has been calculated.[4]

In order to achieve a better understanding of the dimensional characteristics of multielectron systems with less positive ion centers, a D^- center in a spherical quantum dot has been studied by use of a variational approach.[2] The well-radius and barrier-height dependence of the binding energy of the D^- center is obtained. The dimensional characteristics are clearly demonstrated not only for the binding energy and its maximum of the D^- center but also for the ratio of D^- and D^0 binding energy and the electron-correlation effect. However, one effect not addressed by the study mentioned is the effect that the dimensionality and potential shape of the quantum dot microstructure have on the binding energy, the ratio of D^- to D^0 binding energy and the electron correlation. The effect should be considered to obtain the correct quantum levels of a D^- center in a quantum dot because there are different neutral donor wave functions in different QD's and they can cause quite different Coulomb and exchange potentials seen by the other electron. The dimensionality and potential-shape effect of D^- states is related to and different from that on D^0 states, and, therefore, it is interesting to investigate both of them.

This paper explores the effect on binding energies of D^0 and D^- ground states in QD's. It is done by determining the ground states for 3D D^0 and D^{-0} centers in QD's with a spherically rectangular potential well or a 3D isotropic parabolic potential and comparing the results with those for 2D D^0 and D^- centers in QD's with a circularly rectangular potential well or a 2D isotropic parabolic potential. For definiteness let us write down the potential forms for QD's mentioned above. The forms of circularly and spherically rectangular potential wells are given by

$$V(\rho)=\begin{cases}V_0 & \text{if } \rho \geq R_0 \\ 0 & \text{if } \rho < R_0\end{cases} \tag{1}$$

and

$$V(r)=\begin{cases}V_0 & \text{if } r \geq R_0 \\ 0 & \text{if } r < R_0\end{cases}, \tag{2}$$

whereas the 2D and 3D isotropic parabolic potentials have the forms

$$V(\rho)=\tfrac{1}{4}\gamma^2\rho^2 \tag{3}$$

and

$$V(r)=\tfrac{1}{4}\gamma^2 r^2, \tag{4}$$

respectively. In the above equations R_0 is the radius of a QD, ρ and r are electron-QD (donor) center distances in 2D and 3D conditions, respectively. V_0 is a barrier height which can be infinite or finite. In this paper, effective atomic units are used so that all energies are measured in units of the effective Rydberg Ry* and all distances are measured in units of the effective Bohr radius a^*. It is interesting to point out that the parabolic potential introduced by a magnetic field perpendicular to the 2D plane is equal to that shown in Eq. (3) if the dimensionless magnetic-field strength in effective atomic units is equal to γ, which is related to the confinement energies. This is the reason why the forms of Eqs. (3) and (4) are taken. Then, there are three parameters R_0, V_0 and γ in both of 2D and 3D cases which could be correlated with the electronic structures and properties of D^0 and D^- centers in QD's.

It is well known that for a 2D electron in QD's of Eqs. (1) and (3) and a 3D electron in QD's of Eqs. (2) and (4), the quantum levels and eigenfunctions can be obtained analytically.[22] The corresponding states of D^0 centers in the QD's can be solved by using different series forms in different regions of the radial equations.[23] However, the D^- states in the QD's cannot be solved exactly, approximation methods should be used. For determining the ground states (spin singlet states) in the QD's, we use a trial function which includes electron-correlation effect and approaches the Chandrasekhar-type trial function at $V_0=0$ and $\gamma=0$ of Eqs. (1)–(4).[21] It is as follows:

$$\Psi=\begin{cases}A(1+Cr_{12})\{\Psi(\lambda_1,r_1)\Psi(\lambda_2,r_2)+\Psi(\lambda_2,r_1)\Psi(\lambda_1,r_2)\} & \text{for 3D QD's} \\ B(1+C\rho_{12})\{\Psi(\lambda_1,\rho_1)\Psi(\lambda_2,\rho_2)+\Psi(\lambda_2,\rho_1)\Psi(\lambda_1,\rho_2)\} & \text{for 2D QD's},\end{cases} \tag{5}$$

where C, λ_1, and λ_2 are variational parameters, and A and B are the normalization constants. $\Psi(\lambda_i,r_i)$ and $\Psi(\lambda_i,\rho_i)$ are the ground-state eigenfunctions of hydrogenic donor centers with the ion charge λ_i in the 3D and 2D QD's, respectively.

Our study will help show how much difference the dimensions and potential shape of QD's make to the binding energies, the electron-correlation, and the ratio of D^- to D^0 binding energy in different regions of R_0, V_0, and γ. In Sec. II, we present binding energies of D^0 and D^- ground states in different QD's and discuss the dimensionality and potential-shape effects of QD's on them. The electron-correlation effect on the binding energy of D^- center in different QD's is also studied. The ratio of

D^- and D^0 binding energy is shown as a function of γ or V_0 and R_0 of 2D and 3D QD's and the dimensionality and potential-shape effects of QD's on the ratio and its limit or maximum is discussed in Sec. III. A summary of the results and a conclusion are presented in Sec. IV.

II. BINDING ENERGIES

According to hydrogenic-effective-mass theory with neglecting the differences of the electronic effective masses and the dielectric constants between quantum dots and surrounding material, the Hamiltonian for an electron in a QD and a neutral donor at the center of QD is

$$H(W)=\begin{cases}-\Delta_3-\dfrac{2W}{r}+V(r) & \text{for 3D QD's}\\ -\Delta_2-\dfrac{2W}{\rho}+V(\rho) & \text{for 2D QD's}\end{cases}, \tag{6}$$

where Δ_3 and Δ_2 are, respectively, 3D and 2D Laplace operators, $V(r)$ and $V(\rho)$ are 3D and 2D QD potentials as shown in Eqs. (1)–(4), and W is, respectively, equal to zero and one for the electron and the donor in the QD's. The orbital (l) and magnetic (m) quantum number can be well defined for the 3D QD's, whereas the magnetic (m) quantum number can be well defined for the 2D QD's. Therefore, the wave functions of an electron in the spherically and circularly symmetric potentials, which are the QD and Coulomb potentials, are written in the form

$$\psi=\begin{cases}\psi^{(l)}(r)Y_{lm}(\theta,\phi) & \text{for 3D QD's}\\ \psi^{(m)}(\rho)e^{im\phi} & \text{for 2D QD's}\end{cases}, \tag{7}$$

where $\psi^{(l)}(r)$ and $\psi^{(m)}(\rho)$ are the radial wave functions and $Y_{lm}(\theta,\phi)$ is the spherical harmonic function. The radial equations can be solved exactly by using the method as introduced by us,[23] and then for a well-defined orbital quantum number l, the nth electron-level E_n $(l,W=0)$ and donor-level E_n $(l,W=1)$ and the corresponding eigenfunctions $\psi_n^{(l)}(r,W=0)$ and $\psi_n^{(l)}(r,W=1)$, which degenerate with respect to m (magnetic quantum number), can be obtained for the 3D electron and donor in 3D QD's. It is similar to the way to obtain the nth eigenenergies $E_n(m,W=0)$ and E_n $(m,W=1)$ and the corresponding eigenfunctions $\psi^{(m)}(\rho,W=0)$ and $\psi_n^{(m)}(\rho,W=1)$, which degenerate with respect to m and $-m$, for the 2D electron and donor in 2D QD's. Compared with the binding energy of a D^0 center in a three-, two-, or one-dimensional system, the binding energies of the D^0 ground and excited states in QD's can be defined as follows:

$$E_{nB}(l,D^0)=E_n(l,W=0)-E_n(l,W=1)\ , \tag{8}$$

and

$$E_{nB}(m,D^0)=E_n(m,W=0)-E_n(m,W=1)\ , \tag{9}$$

for 3D and 2D QD's, respectively. It is worthwhile to point out that for the parabolic potentials,

$$\begin{aligned}&E_n(l,W=0)=(l+2n+\tfrac{3}{2})\gamma\ ,\\ &E_n(m,W=0)=(|m|+2n+1)\gamma\ ,\quad n=0,1,2,3\ldots,\end{aligned} \tag{10}$$

and for the rectangular potentials with $V_0=\infty$ Ry*,

$$\begin{aligned}&E_n(l,W=0)=(X_{nl}/R_0)^2\ ,\\ &E_n(m,W=0)=(Y_{nm}/R_0)^2\ ,\end{aligned} \tag{11}$$

where X_{nl} and Y_{nm} are the nth roots of the lth-order spherical and mth-order cylindrical Bessel functions, respectively. Therefore, the binding energies $E_B(D^0)$ of the ground states are given by

$$\begin{aligned}&E_B(D^0)=\tfrac{3}{2}\gamma-E_0(l=0,W=1)\ ,\\ &E_B(D^0)=\gamma-E_0(m=0,W=1)\ ,\end{aligned} \tag{12}$$

for the 3D and 2D parabolic potentials, and

$$\begin{aligned}&E_B(D^0)=\frac{9.870}{R_0^2}-E_0(l=0,W=1)\ ,\\ &E_B(D^0)=\frac{5.783}{R_0^2}-E_0(m=0,W=1)\ ,\end{aligned} \tag{13}$$

for the 3D and 2D rectangular potentials.

The Hamiltonian for a D^- in a QD is given by

$$H=\begin{cases}H(1,W)+H(2,W)+\dfrac{2}{r_{12}} & \text{for 3D QD's}\\ H(1,W)+H(2,W)+\dfrac{2}{\rho_{12}} & \text{for 2D QD's}\end{cases}, \tag{14}$$

where $H(i,W)$ is the Hamiltonian of the ith electron and the positive donor ion in the QD as shown in Eq. (6), $2/r_{12}$ and $2/\rho_{12}$ are interaction terms of the two 3D and two 2D electrons, respectively.

Compared with the binding energy of a D^0 center in QD's as mentioned above, the binding energy of the D^- ground state in the QD's is defined as follows:

$$\begin{aligned}E_B(D^-)&=E(D^0)+E_0-E(D^-)\\ &=2E_0-E_B(D^0)-E(D^-)\ ,\end{aligned} \tag{15}$$

where $E(D^-)$ is the lowest level of the Hamiltonian of Eq. (14), i.e., the D^- ground-states energy in QD's, E_0 and $E(D^0)$ are, respectively, the lowest levels of an electron in the QD's without and with the Coulomb potential, and $E_B(D^0)$ is the binding energy of the neutral donor, which is equal to $E_0-E(D^0)$.

In order to study the γ, R_0, and V_0 dependence of the binding energies of D^0 and D^- centers in QD's and the dimensionality and potential-shape effects of QD's on them, numerical calculations have been performed for 2D and 3D rectangular-potential QD's (2D and 3D RQD's) of R_0 between 0 and $15a^*$ with different V_0 and 2D and 3D parabolic-potential QD's (2D and 3D PQD's) of γ between 0 and 10. In Fig. 1, we have plotted the binding energies $E_B(D^0)$ and $E_B(D^-)$ of D^0 and D^- centers as a function of R_0 for 2D and 3D RQD's with $V_0=\infty$, 80 Ry* and 40 Ry*, respectively. It is readily seen that as R_0 decreases both the $E_B(D^0)$ and $E_B(D^-)$ in 2D and 3D RQD's with $V_0=\infty$ Ry* increase monotonically from their 2D and 3D values to quasi-zero-dimensional ones.

However, for finite $V_0=80$ and 40 Ry*, as R_0 decreases the binding energies increase continuously until their maxima and, then, decrease fast. The positions of the maxima of D^0 centers are much the same as those of D^- centers. It is interesting to point out that as R_0 approaches zero from the positions of the maximum binding energies the values of 3D RQD's decrease to the 3D limits (1 and 0.0518 Ry*) much faster than those of 2D RQD's to the 2D limits (4 and 0.454 Ry*), as shown in Fig. 1. It is easy to understand if we note that there are different decreasing rates of confinement regions between 3D and 2D RQD's as R_0 decreases.

Two QD's are defined to have the same "confinement" if the ground-state energy of a free electron in one of the QD's is equal to that in the other. In Figs. 2(a) and 2(b) binding energies of D^0 and D^- centers, respectively, are plotted as functions of γ for PQD's (solid lines) and also for RDQ's (dashed lines) for which $V_0=\infty$ and which have the same confinement at given γ as the PQD's at

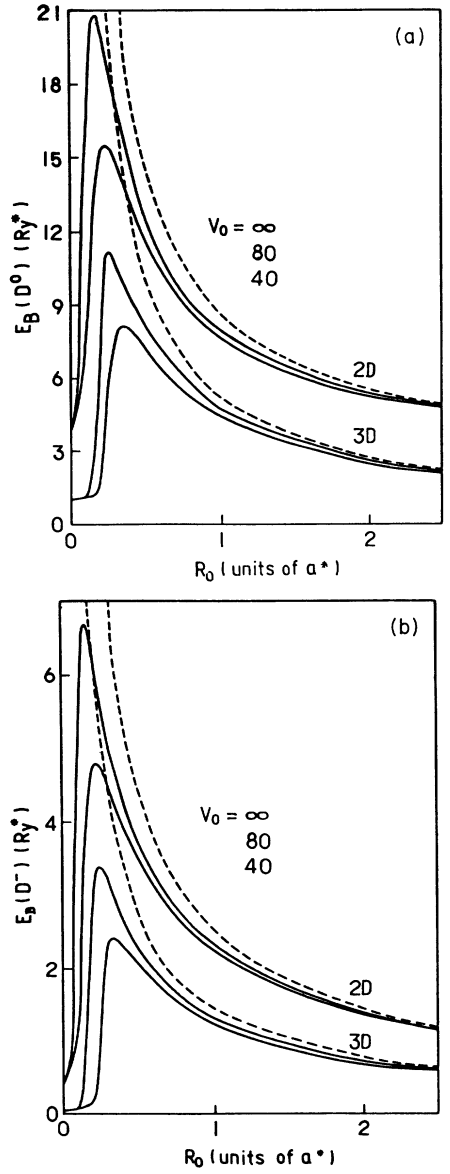

FIG. 1. Quantum-dot radius dependence of binding energies $E_B(D^0)$ and $E_B(D^-)$ of (a) D^0 and (b) D^- ground states in 2D and 3D RQD's with $V_0=\infty$ (dashed lines), 80 (upper solid lines), and 40 (lower solid lines) Ry*, respectively. $E_B(D^0)$ and $E_B(D^-)$ of $R_0=0$ a^* with $V_0=40$ and 80 Ry* are 4 and 0.454 Ry* for 2D RQD's and 1 and 0.0518 Ry* for 3D RQD's.

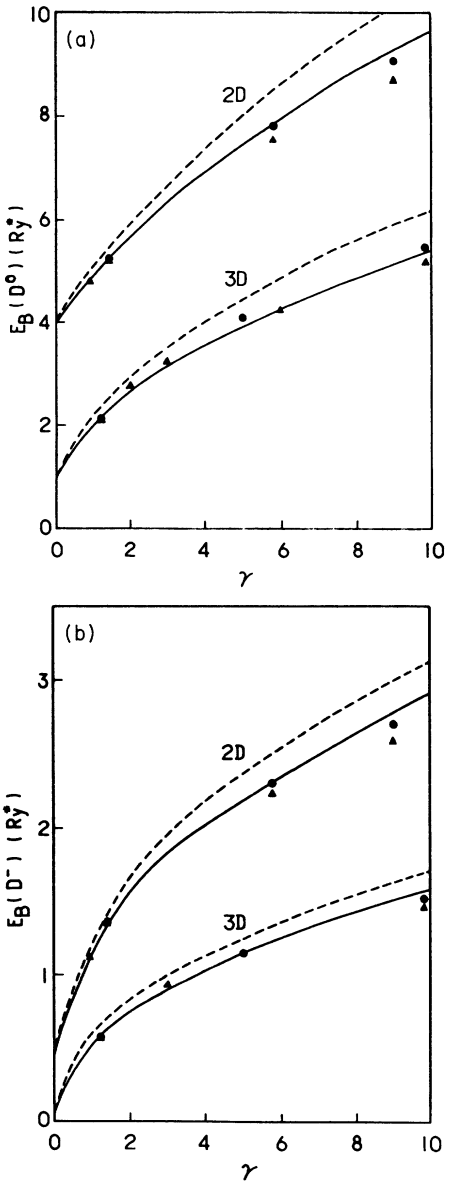

FIG. 2. Binding energies $E_B(D^0)$ and $E_B(D^-)$ of (a) D^0 and (b) D^- ground states in 2D and 3D RQD's with $V_0=\infty$ Ry* (dashed lines) and 2D and 3D PQD's (solid lines) vs γ. For each dimensionality (2D or 3D) data plotted at a given value of γ correspond to systems with the same confinement as a PQD at that value of γ and that dimensionality. At $V_0=\infty$ the connection between γ and R_0 for PQD's and RQD's with the same confinement (see the text) is $\gamma=6.580/R_0^2$ in 3D and $\gamma=5.783/R_0^2$ in 2D. The same connection is used in all of the following figures. The solid circle and triangles represent those of 2D and 3D RQD's with $V_0=80$ and 40 Ry*, respectively. $E_B(D^0)$ and $E_B(D^-)$ of $\gamma=0$ are 4 and 0.454 Ry* for 2D and 1 and 0.0518 Ry* for 3D.

that γ. At $V_0=\infty$, the connection between γ and R_0 for PQD's and RQD's with the same confinement is $\gamma=6.580/R_0^2$ in 3D and $\gamma=5.783/R_0^2$ in 2D. The closeness of corresponding dashed and solid lines in Fig. 2 suggests that the shape of the confining potential is less important than the confinement in determining the binding energy of D^0 and D^- centers. It is easily seen that the differences of the binding energies between PQD's and infinite barrier RQD's are about the same as the ones between the RQD's with $V_0=\infty$ and 80 Ry* and smaller than ones between the RQD's with $V_0=\infty$ and 40 Ry* in the γ regions between 0 and 10.

As shown in Eq. (5), the correlation term of two electrons is included in the Chandrasekhar-type trial function. Using the trial function with and without the polarization term in the equation and making a comparison between the two cases, the electron-correlation effect can be roughly studied. The ratio R, defined by the binding-energy difference due to omission of the Cr_{12} or $C\rho_{12}$ over the binding energy, is plotted for PQD's and RQD's in Fig. 3. It is readily seen that in the regime, in which γ is slightly larger than zero, the R is larger for 2D QD's than for 3D QD's even though the R (0.342) is smaller for the unconfined 2D case than that (0.479) for the unconfined 3D case. This is an interesting dimensionality effect of QD's. Clearly, the R is weakly dependent on the potential shape as shown in the figure.

In Table I, the binding energies obtained by different variational and diffusion Monte Carlo calculations are given for 3D and 2D D^- ions[24–26] in the absence of magnetic field and a 3D D^- ion in the magnetic field ($\gamma=100$),[9] which has the same behavior as one in QWW's. It is clearly shown that for the 3D case, the error of the Chandrasekhar binding energy appears to be

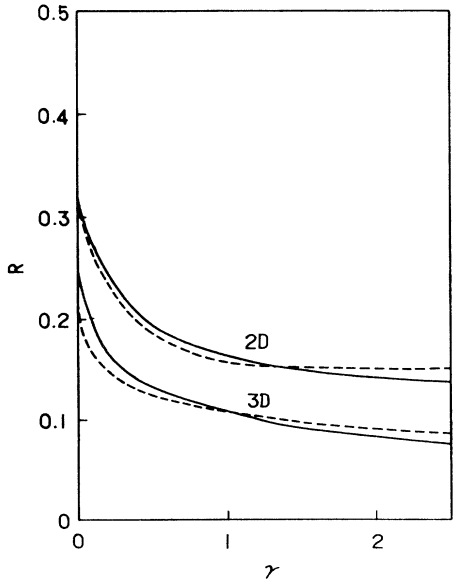

FIG. 3. Ratio R of the binding-energy difference due to omission of the Cr_{12} or $C\rho_{12}$ to the binding energy vs γ for 2D and 3D PQD's (upper and lower solid lines) and 2D and 3D RQD's with $V_0=\infty$ Ry* (upper and lower dashed lines).

TABLE I. Binding energies of 3D and 2D D^- ions without magnetic field and a 3D D^- ion in magnetic field $\gamma=100$, i.e., a quasi-one-dimensional D^- ion. The superscripts *a*, *b*, *c*, *d*, and *e* refer, respectively, to Refs. 19, 24, 25, 9, and 26 where the values are found.

Binding Energy $E_B(D^-)$ (Ry*)			
	3D	2D	Q1D
No correlation	0.0270	0.307	1.14[a]
Chandrasekhar	0.0518	0.454	1.44[a]
Best variational	0.0555[b]	0.480[c]	1.533[d]
Diffusion Monte Carlo	0.056[e]	0.511[e]	

comparable to the statistical fluctuations (0.002 Ry*) of the Monte Carlo calculation,[26] and for the 2D case, however, the error seems considerably greater.[8,9] We believe that the electron-correlation effect is dependent not only on the dimensionality but also on the multiple expansion of the electron-electron interaction and it is the reason why the error of the Chandrasekhar binding energy is different for 3D and 2D cases. Then, it is interesting to know the binding energy of a 3D D^- ion in a strong magnetic field, for example, $\gamma=100$ obtained by the Monte Carlo method and to compare the result with the variational one.[9]

III. RATIO OF D^- TO D^0 BINDING ENERGY

In order to achieve a better understanding of the dimensional characteristics of D^0 and D^- centers and the dimensionality and potential-shape effects of QD's on binding energies, we have calculated the ratio σ of D^- to D^0 binding energy in different QD's. For the unconfined 3D and 2D cases, the σ is respectively equal to 0.0518 and 0.114 in the present work and 0.056 and 0.128 in the work of Louie and Pang.[26] In Fig. 4, the ratio σ has been shown as a function of γ between 0 and 10 for 3D and 2D QD's. As γ increases σ increases from their 2D and 3D values until about certain constants, respectively. The limit value of σ is about 0.3 for 3D and 2D PQD's and 0.28 for 3D and 2D RQD's while it is about 0.2 for the corresponding QWW's.[20] It means that the difference of the limiting σ between different QD's is much smaller than that between QD's and QWW's and that σ is weakly dependent on the potential-shape.

It is worthwhile to note that in the γ regime between 0 and 3, the σ of 3D QD's can be larger than that of 2D QD's even though it is much smaller in the unconfined 3D case than in the unconfined 2D case and both of $E_B(D^0)$ and $E_B(D^-)$ of 3D QD's are smaller than the corresponding ones of 2D QD's. The results are qualitatively consistent with those of Ref. 8 in which Pang and Louie reported both of $E_B(D^0)$ and $E_B(D^-)$ for a 10 nm $GaAs/Ga_{0.7}Al_{0.3}As$ well in a magnetic field. The $E_B(D^0)$ is equal to 2.92 and 3.89 (Ry*) and the $E_B(D^-)$ 0.77 and 1.13 (Ry*) for a dimensionless magnetic field of $\gamma=1$ and 3, respectively. Then, the ratio σ 0.264(0.77/2.92) and 0.290(1.13/3.89) is larger than that (0.230 and 0.278) of the 2D PQD's with the same value of γ and about the same as that (0.268 and 0.288) of the corresponding 3D

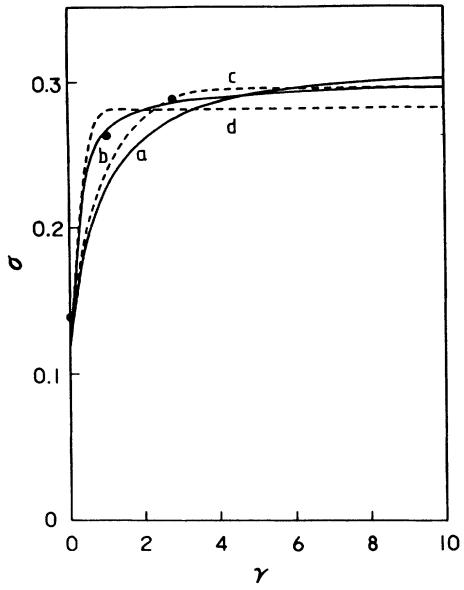

FIG. 4. Ratio σ of $E_B(D^-)$ to $E_B(D^0)$ vs γ for 2D (solid line a) and 3D (solid line b) PQD's and 2D (dashed line c) and 3D (dashed line d) RQD's, respectively. σ of $\gamma=0$ is 0.0518 and 0.114 for 3D and 2D cases, respectively. The solid circles represent those of 2D QW's in Ref. 8 (see the text).

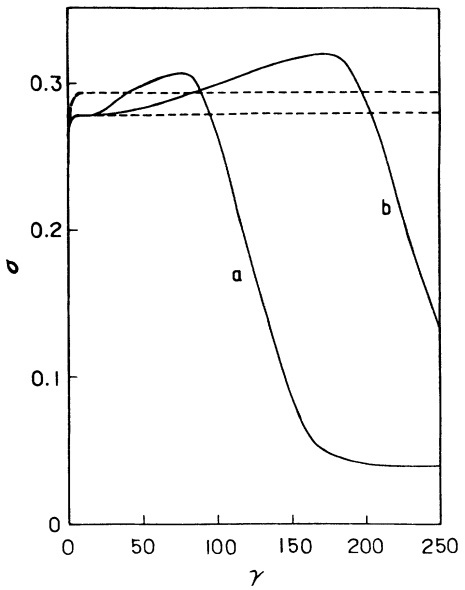

FIG. 5. Ratio σ of $E_B(D^-)$ to $E_B(D^0)$ vs γ for 3D PQD's (upper dashed line), 3D RQD's with $V_0=40$ (solid line a), 80 (solid line b), and ∞ Ry* (lower dashed line).

PQD's, as shown in the figure.

The ratios σ of 3D RQD's with $V_0=\infty$, 80, 40 Ry*, and 3D PWD's have been plotted as a function of γ between 0 and 250 in Fig. 5. The limit values of the ratios are, respectively, equal to 0.280 and 0.294 for 3D RQD's with $V_0=\infty$ Ry* and 3D PQD's. The ratios of 3D RQD's with $V=40$ and 80 Ry* increase and approach their maxima (0.306 and 0.320) and, then, decrease and approach 3D limit as γ increase from zero.

IV. SUMMARY AND CONCLUSION

In order to study the well-radius and barrier-height dependence of the binding energy $E_B(D^-)$ of a D^- ion in 2D and 3D RQD's, a numerical calculation has been performed by using a Chandrasekhar-type trial function. Comparing $E_B(D^0)$ and $E_B(D^-)$ of 2D and 3D RQD's with those of 2D and 3D PQD's, we have found that the former is larger than the latter on the same confinement condition and that the effect of a parabolic potential on $E_B(D^0)$ and $E_B(D^-)$ can be equivalent to that of a rectangular potential with reasonable R_0 and V_0. We have calculated the ground-state energies with the trial function with and without the polarization term. It has been found that the correlation effect on $E_B(D^-)$ is important in a small γ regime and that the finite value of C of Eq. (5) not only brings in the important correlation effect, but also modifies the behavior of the single-electron orbitals. The variation of the ratio R with γ is quite different for 2D and 3D QD's while the variation is slightly different for different potential shapes of QD's. In addition, our calculations are also qualitatively consistent with the results of Ref. 8 on the basis of the analysis of σ.

In conclusion, the study of the binding energy, electron correlation, and ratio σ in different QD's is important not only for understanding the electronic structures in low dimensions but also for explaining the experiments about D^- centers in narrow quantum wells in a magnetic field[8] and in other kinds of quantum-well structures. Since quantum wells in a magnetic field form a kind of QD's between 3D and 2D PQD's and D^- centers could be located anywhere in QD's, it should be interesting to study the positional dependence of D^- states in RQD's, PQD's, and other kinds of quantum dots. Finally, it is worthwhile to point out that the D^- excited states can be quite different between different QD's. This is an interesting subject to study.

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[1]J.-L. Zhu, J.-J. Xiong, and B.-L. Gu, Phys. Rev. B **41**, 6001 (1990), and references quoted therein for neutral donors in 2DQW's, QWW's, and QD's.

[2]J.-L. Zhu, J.-H. Zhao, W.-H. Duan, and B.-L. Gu, Phys. Rev. B **46**, 7546 (1992).

[3]S. Huant, S. P. Najda, and B. Etienne, Phys. Rev. Lett. **65**, 1486 (1990).

[4]E. R. Mueller, D. M. Larsen, J. Waldman, and W. D. Goodhue, Phys. Rev. Lett. **68**, 2204 (1992).

[5]S. Holmes, J.-P. Cheng, B. D. McCombe, and W. Schaff, Phys. Rev. Lett. **69**, 2571 (1992).

[6]A. Mandray, S. Huant, and B. Etienne, Europhys. Lett. **20**, 181 (1992).

[7]J.-P. Cheng, Y. J. Wang, B. D McCombe, and W. Schaff, Phys. Rev. Lett. **70**, 489 (1993).

[8]T. Pang and S. G. Louie, Phys. Rev. Lett. **65**, 1635 (1990); S. G. Louie and T. Pang, in *New Horizons in Low-Dimensional Electron Systems,* edited by H. Aoki (Kluwer Academic, Dordrecht, 1992), p. 445.
[9]D. M. Larsen and S. Y. McCann, Phys. Rev. B **45**, 3485 (1992); **46**, 3966 (1992).
[10]S. Huant, A. Mandray, G. Martinez, M. Grynberg, and B. Etienne, Surf. Sci. **263**, 565 (1992).
[11]J.-L. Zhu, J. Phys. Condens. Matter **4**, 6119 (1992).
[12]N. P. Sandler and C. R. Proetto, Phys. Rev. B **46**, 7707 (1992).
[13]A. H. MacDonald, Solid State Commun. **84**, 109 (1992).
[14]E. Glaser, B. V. Shanabrook, R. L. Hawkins, W. Beard, J. M. Mercy, B. D. McCombe, and D. Musser, Phys. Rev. B **36**, 8185 (1987).
[15]N. C. Jarosik, B. D. McCombe, B. V. Shanabrook, J. Comas, J. Ralston, and G. Wicks, Phys. Rev. Lett. **54**, 1283 (1985).
[16]S. Huant, R. Stepniewski, G. Martinez, V. Thierry-Mieg, and B. Etienne, Superlatt. Microstruct. **5**, 331 (1989).
[17]J. M. Shi, F. M. Peeters, G. Q. Hai, and J. T. Devereese, Phys. Rev. B **44**, 5692 (1991).
[18]S. P. Najda, C. J. Armistead, C. Trager, and R. A. Stradling, Semicond. Sci. Technol. **4**, 439 (1989).
[19]D. M. Larsen, Phys. Rev. Lett. **42**, 742 (1979); Phys. Rev B **20**, 5217 (1979).
[20]A. Natori and H. Kamimura, J. Phys. Soc. Jpn. **44**, 1216 (1978).
[21]H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer-Verlag, Berlin, 1957); S. Chandrasekhar, J. Astrophys. **100**, 176 (1944).
[22]See, e.g., D. ter. Haar, *Problems in Quantum Mechanics* (Pion Limited, London, 1975), p. 34.
[23]J.-L. Zhu, Phys. Rev. B **39**, 8780 (1989); J.-L. Zhu, Y. Cheng, and J.-J. Xiong, *ibid.* **41**, 10 792 (1990).
[24]C. L. Perkeris, Phys. Rev. **112**, 1649 (1958); **126**, 1470 (1962).
[25]D. E. Phelps and K. K. Bajaj, Phys. Rev. B **27**, 4883 (1983).
[26]S. G. Louie and T. Pang, in *New Horizons in Low-Dimensional Electron Systems* (Ref. 8), p. 455.