Change of symmetry of the barrier D^- ground state in finite magnetic fields

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The states of the barrier D^- center which consists of a positive ion located on the z axis at a distance from the x-y plane and two electrons in the same plane bound by the ion are investigated based on a direct diagonalization method in finite and relatively high magnetic fields. The energies of the barrier D^- states, the binding energies for the barrier D^- states, and the expectation values of both the distance of the electron from the origin and distance between two electrons are obtained as functions of the applied magnetic field strength γ perpendicular to the x-y plane and the distance ζ between the positive ion and the x-y plane. The effects of the higher Landau levels become small as γ and ζ increase. The change of symmetry of the barrier D^- ground state is possible in finite magnetic fields. Both the distance of the electron from the origin and distance between two electrons vary discontinuously with the changes of symmetry of the barrier D^- ground states. Our calculations indicate that the phase transitions of the barrier D^- ground states can be observed in real systems. [S0163-1829(97)11407-2]

I. INTRODUCTION

A negative hydrogenic donor center (D^-) in semiconductors consists of a single positive ion and two electrons which are bound to the positive ion. It is analogous to a negative hydrogen ion (H^-). Recently there has been much experimental and theoretical interest in the problem of D^- centers in quasi-two-dimensional systems. Since the existence of D^- centers in center-doped GaAs/Al_xGa_{1-x}As multiple quantum wells was first reported by Huant, Najda, and Etienne[1] many experimental[2–5] and theoretical[6–10] investigations for D^- centers in quantum wells have been carried out.

A system in which two electrons confined to the x-y plane are bound by a positive ion in the same plane is called a strictly two-dimensional D^- center. This model gives us important informations on the behavior of D^- centers at the middle of a narrow quantum well. It is well known that in the strong-magnetic-field limit if one takes account of only the lowest Landau level, exact solutions for this model exist.[11–13] Recently Fox and Larsen[14] proposed a model called a barrier D^- center. It is a model obtained by generalizing the strictly two-dimensional model by retaining electron confinement in the x-y plane, but moving the positive ion to a distance ζ from the plane on the z axis. They have shown that exact solutions for the problem of barrier D^- centers exist in the strong-magnetic-field limit and, in such a limit, the symmetry of the barrier D^- ground state changes as ζ increases from zero.

The work by Fox and Larsen motivated us to perform the present work. We are interested in the behavior of the barrier D^- center in finite magnetic fields. When a frame of the strong-magnetic-field limit is removed and the effects of the higher Landau levels are taken into account, we investigate how the symmetry of the barrier D^- ground state changes as functions of the applied magnetic field strength γ and the distance ζ. We calculate the energies of barrier D^- states applying the direct diagonalization method[15] which Dzyubenko and Sivachenko used, because a number of excited states can be treated under this framework. The results obtained by using this method will be valid in finite and relatively high magnetic fields and can be compared with those calculated by Fox and Larsen[14] in the strong-magnetic-field limit. As a consequence of our calculations, it is found that the effects of the higher Landau levels become small as γ and ζ increase. The change of symmetry of the barrier D^- ground state is possible in finite magnetic fields. Both the distance of the electron from the origin (in this paper, the origin is taken as the projection of the positive ion on the x-y plane) and distance between two electrons vary discontinuously with the changes of symmetry of the barrier D^- ground state. The phase diagram indicates that the phase transitions of the barrier D^- ground states can be observed in real systems with vary narrow quantum wells.

In Sec. II we present the model of barrier D^- center and describe the direct diagonalization method to calculate the various quantities associated with the barrier D^- states. In Sec. III we calculate the energies of the barrier D^- states, the binding energies for the barrier D^- states and the expectation values of both the distance of the electron from the origin and distance between two electrons. Finally we show the phase diagram for the barrier D^- ground states and comment on the application of our results to real systems.

II. FORMULATION

The Hamiltonian for the barrier D^- center in the effective-mass approximation when the magnetic field is applied perpendicular to the x-y plane is given by

$$H = h_D(1) + h_D(2) + \frac{2}{|\vec{\rho}_1 - \vec{\rho}_2|}, \tag{1}$$

where $h_D(j)$ is the barrier donor Hamiltonian for the jth electron given by

$$h_D(j)=h_0(j)-\frac{2}{(\rho_j^2+\zeta^2)^{1/2}}, \tag{2}$$

$$h_0(j)=2\gamma(a_j^\dagger a_j+\tfrac{1}{2}), \tag{3}$$

where $h_0(j)$ is the free-particle Hamiltonian for the jth electron, $\vec{\rho}_j$ is the position of the jth electron in the x-y plane, and ζ is the distance between the fixed positive ion on the z axis and the x-y plane. We have used an effective Bohr radius a_B^* as the unit of length and an effective Rydberg R^* as the unit of energy. $\gamma=\hbar\omega_c/2R^*$ is the dimensionless magnetic field strength, where $\omega_c=eB/m^*c$, B is the strength of the applied magnetic field perpendicular to the interface, and m^* is the conduction-band mass. The eigenstates and eigenvalues for $h_0(j)$ are given by

$$|N_j,M_j\rangle_j=\frac{(a_j^\dagger)^{N_j}(b_j^\dagger)^{M_j}}{\sqrt{N_j!M_j!}}|0,0\rangle_j, \tag{4}$$

$$\epsilon_{N_j}=2\gamma(N_j+\tfrac{1}{2}), \tag{5}$$

where a_j and b_j are inter-Landau-level and intra-Landau-level ladder operators for the jth electron defined by[16]

$$a_j=\left(\frac{\gamma}{2}\right)^{1/2}\left(\frac{z_j^*}{2}+\frac{2}{\gamma}\frac{\partial}{\partial z_j}\right), \tag{6}$$

$$b_j=\left(\frac{\gamma}{2}\right)^{1/2}\left(\frac{z_j}{2}+\frac{2}{\gamma}\frac{\partial}{\partial z_j^*}\right), \tag{7}$$

where we used complex numbers to represent two-dimensional vectors, i.e., $z=x+iy$. N_j is the Landau-level quantum number, and M_j is the oscillator quantum number. $|N_j,M_j\rangle_j$ are also the eigenstates of an angular momentum operator along the z axis with the eigenvalue $L_j=N_j-M_j$. Throughout this paper we neglect Zeeman energies associated with the electron spins.

The total Hamiltonian H is invariant under rotation about the z axis and under interchange of indices 1 and 2. Therefore its eigenstates are classified according to the z component of the total angular momentum L and their symmetry under interchange of the indices 1 and 2.[11,14] We take symmetrized (singlet) or antisymmetrized (triplet) products of the eigenstates for the jth free Hamiltonian as basis states for the total Hamiltonian. They are written as

$$|N_1,M_1;N_2,M_2\rangle^\pm=\{|N_1,M_1\rangle_1|N_2,M_2\rangle_2 \pm|N_2,M_2\rangle_1|N_1,M_1\rangle_2\}, \tag{8}$$

where the $+$ sign is for singlet states and the $-$ sign for triplet states, and permutation between two electrons is represented by exchanging the indices of the free-particle eigenstates, retaining their quantum numbers. Then the eigenstates for the total Hamiltonian are given by linear combinations of the basis states

$$|L\rangle^\pm=\sum_{N_1,M_1,N_2,M_2} C^\pm_{N_1,M_1,N_2,M_2}|N_1,M_1;N_2,M_2\rangle^\pm, \tag{9}$$

where summation should be done under the conditions that $L=L_1+L_2=N_1-M_1+N_2-M_2$. The eigenvalues $E^\pm_{D^-}(L)$, and the expansion coefficients $C^\pm_{N_1,M_1,N_2,M_2}$, are determined by solving the Schrödinger equations

$$H|L\rangle^\pm=E^\pm_{D^-}(L)|L\rangle^\pm. \tag{10}$$

One-electron binding energies $\varepsilon_B^\pm(L)$ associated with these eigenvalues are defined as

$$\varepsilon_B^\pm(L)=E^\pm_{D^-}(L)-(E_{D^0}+\gamma), \tag{11}$$

where E_{D^0} is the ground-state energy for the barrier donor Hamiltonian. E_{D^0} is determined by solving the appropriate Schrödinger equations in which the ground state for the barrier donor Hamiltonian is given by linear combinations of the eigenstates with zero angular momentum for the free-particle Hamiltonian. $\varepsilon_B^\pm(L)$ is negative for bound states, and positive for unbound states. We evaluate the interaction terms between the fixed positive ion and the electron numerically. Using the simple relationship between the representation of symmetrized or antisymmetrized products of free-particle eigenstates and the representation of products of the center-of-mass and relative motion eigenstates, the interaction terms between two electrons can be evaluated analytically.[12,16]

What we have to do is to solve the Schrödinger equations (10). As has been pointed out, Fox and Larsen[14] showed that exact solutions for the problem of barrier D^- centers exist in the strong-magnetic-field limit. The energy differences between the different Landau levels are proportional to γ, whereas the energies due to the Coulomb interaction terms are proportional to $\gamma^{1/2}$. Therefore mixing between different Landau levels is ignored in the strong-magnetic-field limit. The exact solutions in the strong-magnetic-field limit are obtained by diagonalizing the total Hamiltonian within the lowest Landau level ($N_1=N_2=0$). In this paper, we remove the restriction that the magnetic-field strength is infinite, and take account of the mixing between the different Landau levels. Since it is almost impossible to take account of all the Landau levels, we are content to solve the appropriate secular determinant by taking account of basis states in the low-lying $N_{\rm mix}$ Landau levels, where N_1 and N_2 should satisfy the condition $N_{\rm mix}\geqslant N_1+N_2+1$. The results obtained under this framework will be valid in finite and relatively high magnetic fields. We consider only the state which gives the minimum energy among the states classified according to L and the symmetry under interchange of indices 1 and 2, since we are interested in the change of symmetry of the barrier D^- ground state as functions of ζ and γ.

III. RESULT AND DISCUSSION

We are now in a position to represent our numerical calculations. Figure 1 shows the γ dependence of the ground-state energies of the barrier donor center for $\zeta=0.1$ and 0.5. We have taken account of the low-lying $N_{\rm mix}$ Landau levels. Results obtained by taking $N_{\rm mix}=1$, 4, and 7 are shown by the dotted, broken, and solid lines, respectively. Here we note that the barrier donor center consists of only one electron so that in this case N, the Landau-level quantum number of the electron, satisfies the condition $N_{\rm mix}\geqslant N+1$. It is

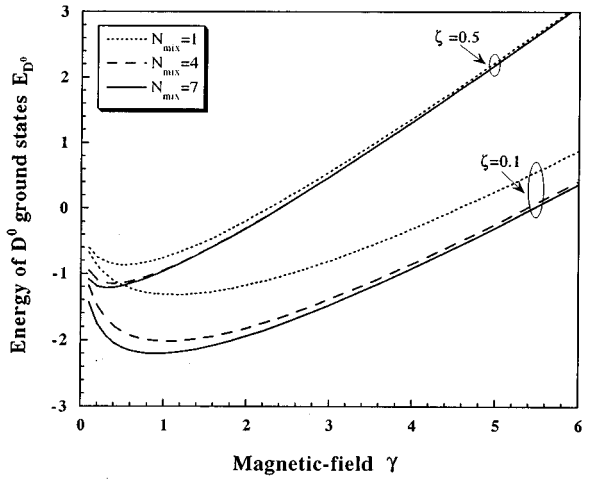

FIG. 1. The ground-state energies E_{D^0} (in units of R^*) of the barrier donor center for $\zeta=0.1$ and 0.5 as a function of γ. The solid and broken lines show the results obtained by taking account of the seven and four low-lying Landau levels, respectively. The dotted lines show the results within the lowest Landau level.

found that the energies of the barrier donor states become low and approach to the true ones with increasing N_{mix}, as is expected from the procedure of diagonalization.[17]

Figure 2 shows the γ dependence of the energies of the singlet barrier D^- states with $L=0$ (a) and the triplet states with $L=-3$ (b) for $\zeta=0.1$ and 0.5. Similar to the case of the barrier donor center, the results obtained by taking account of the low-lying $N_{\mathrm{mix}}=1$, 4, and 7 Landau levels are shown by the dotted, broken, and solid lines, respectively. The dotted lines correspond to the results which are extrapolated from those obtained by Fox and Larsen in the strong-magnetic-field limit to a finite regime of magnetic field. When we take $N_{\mathrm{mix}}=7$, we take account of 72 basis states for the singlet barrier D^- states with $L=0$ and 112 basis states for the triplet states with $L=-3$. It is found that the energies of the barrier D^- states become low, and approach to the true ones with increasing N_{mix}. For large γ and ζ our method of calculation is a good approximation because the effects of the higher Landau levels become small, as explained below. But it is not so good an approximation for small γ and ζ even if we take $N_{\mathrm{mix}}=7$. For example, for the strictly two-dimensional model ($\zeta=0$), calculations based on the variational method of Larsen and McCann[18] give more accurate energies of D^- states with lower angular momentum than ours. The differences between the dotted lines and the other lines represent the effects of the higher Landau levels. These effects become small as γ and ζ increase. This is reasonable because if γ increases the lowest eigenvalues of the total Hamiltonian agree asymptotically with the ground state energies obtained in the strong-magnetic-field limit. On the other hand, when ζ increases, the interaction terms between the electrons do not change while the interaction terms between the positive ion and the electron become small. In consequence of this it is found that the contributions from the off-diagonal elements between different Landau levels to the ground state energies with definite angular momentum and the symmetry become small as ζ increases.

The binding energies for the barrier D^- states obtained by

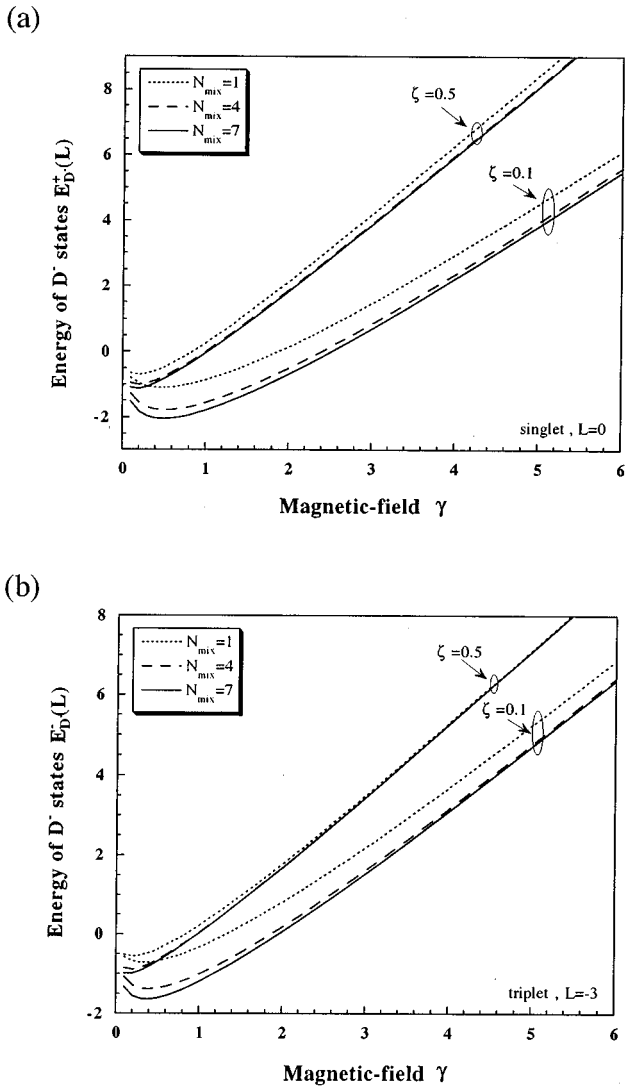

FIG. 2. The energies $E^-_{D^-}(0)$ and $E^+_{D^-}(-3)$ (in units of R^*), respectively, of the singlet barrier D^- states with $L=0$ (a) and the triplet barrier D^- states with $L=-3$ (b) for $\zeta=0.1$ and 0.5 as a function of γ. The solid and broken lines show the results obtained by taking account of the seven and four low-lying Landau levels, respectively. The dotted lines show the results within the lowest Landau level.

taking account of the seven low-lying Landau levels at $\zeta=1.0$ as a function of γ are plotted in Fig. 3. The solid and dotted lines indicate the singlet and triplet states, respectively. An examination of Fig. 3 indicates that the sequence of the barrier D^- ground states is $L=0$, singlet $\rightarrow$ $L=-1$, triplet $\rightarrow$ $L=-2$, singlet $\rightarrow$ $L=-3$, triplet $\rightarrow$ $L=-4$, singlet $\rightarrow$ $L=-5$, triplet whereby γ passes at 0.16, 1.18, 2.46, 3.83, and 5.24. The ground states with $|L|>5$ are not bound. This shows that the change of symmetry of the barrier D^- ground state, which has been predicted in the strong-magnetic-field limit,[14] is also possible in finite magnetic fields. This change of symmetry is caused by the competition between the Coulomb attractive force and the Coulomb repulsive force.

To show that the change of symmetry of the barrier D^- ground state is caused by the competition between the Cou-

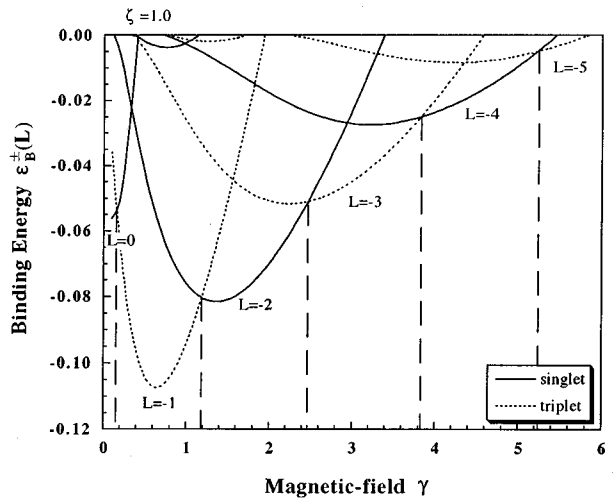

FIG. 3. The binding energies (in units of R^*) of the barrier D^- center for $\zeta=1.0$ as a function of γ. All the bound states obtained within the seven low-lying Landau levels are shown. The solid and dotted lines show the symmetric (singlet) and antisymmetric (triplet) states, respectively.

lomb attractive force and the Coulomb repulsive force, in the case of $\zeta=1.0$ we plot the expectation values $\sqrt{\langle\rho_j^2\rangle}$ of the distance of the electron from the origin (a) and the expectation values $\sqrt{\langle|\vec{\rho}_1-\vec{\rho}_2|^2\rangle}$ of the distance between two electrons (b) for various barrier D^- states obtained by taking account of the seven low-lying Landau levels as a function of γ in Figs. 4. The solid and the dotted lines indicate the singlet and triplet states, respectively. In Fig. 4(b) the angular momentum quantum numbers L take, from left, $0,-1,-2,-3,-4$, and -5 for singlet states and $-2,-1,-4,-3$, and -5 for triplet states. The solid lines for $L=0$ and -1, and the dotted lines for $L=-2$ and -1, are almost degenerated, respectively. The phase transitions for $L\rightarrow L-1$ occur at the broken lines parallel to the vertical line. It is found that both the expectation values $\sqrt{\langle\rho_j^2\rangle}$ and $\sqrt{\langle|\vec{\rho}_1-\vec{\rho}_2|^2\rangle}$ become large as $|L|$ increases. Then both the Coulomb attractive and Coulomb repulsive energies become small. Since the energies due to the Coulomb attractive force terms are functions of γ and ζ, the optimum number L also depends on γ and ζ. The expectation values of the distance of the electron from the origin are almost independent on the symmetry of the barrier D^- states. For even (odd) L the expectation values of the distance between two electrons for the singlet (triplet) states are larger than those for the triplet (singlet) states, as is expected from the fact that the singlet states have only even relative angular momentum and the triplet states have only odd relative angular momentum.[12] Then for even (odd) L the energies for the singlet (triplet) barrier D^- states are lower than those for the triplet (singlet) barrier D^- states. Therefore the symmetry of the barrier D^- ground state changes when L becomes $L-1$. These properties are analogous to those for the two-electron system in a harmonic quantum dot.[19,20] Figure 4 indicates that both the distance of the electron from the origin and distance between two electrons vary discontinuously when the symmetry of the barrier D^- ground states changes.

In Fig. 5 we show the phase diagram for the barrier D^-

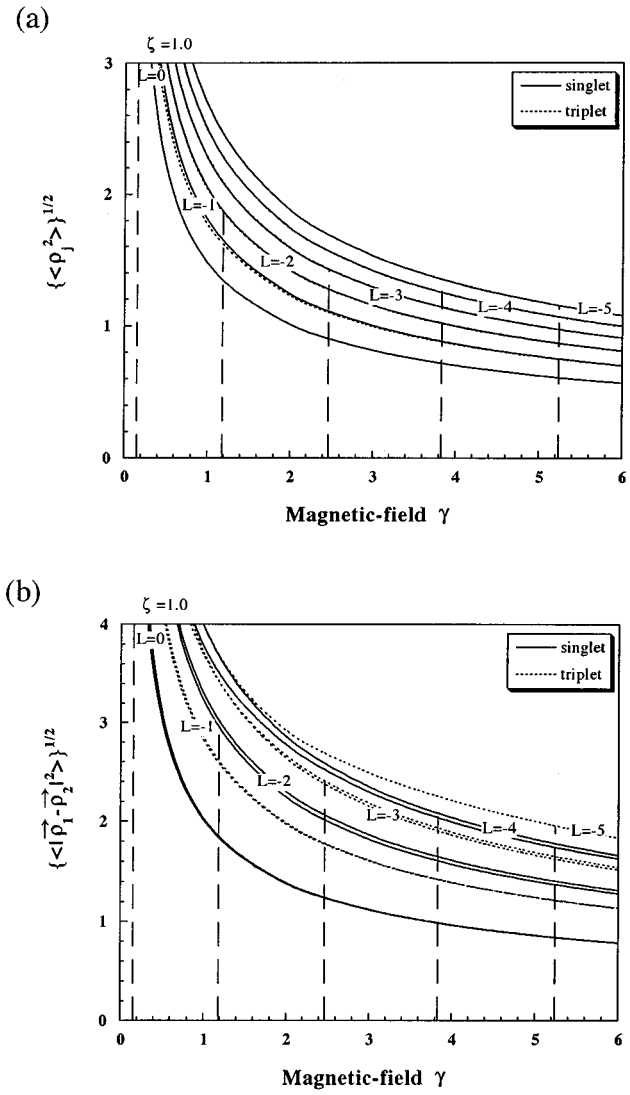

FIG. 4. The expectation values (in units of a_B^*) of the distance of the electron from the origin (a) and the distance between two electrons (b) for $\zeta=1.0$ as a function of γ. All the expectation values are obtained by taking account of the seven low-lying Landau levels. The solid and dotted lines show the symmetric (singlet) and antisymmetric (triplet) states, respectively. In (b) the angular momentum quantum numbers L take, from left, $0,-1,-2,-3,-4$, and -5 for the singlet states and $-2,-1,-4,-3$, and -5 for the triplet states.

ground states. The dotted and solid lines are calculated by taking account of the low-lying one and seven Landau levels, respectively. The dotted lines indicate the results obtained by applying the results in the strong-magnetic-field limit[14] to a finite regime of magnetic field. The boundaries representing the phase transitions for $L\rightarrow L-1$ do not depend on the energies of the barrier donor ground states, as is shown directly from Eq. (11). Therefore the differences between the dotted lines and the solid lines associated with the phase transitions represent the effects of the higher Landau levels for the energies of the barrier D^- states. It is found that for a certain values of ζ the phase transitions for $L\rightarrow L-1$ occur at larger γ as $N_{\rm mix}$ increases. This phase diagram is compared with that for two-electron states in a harmonic quantum dot.[19,20]

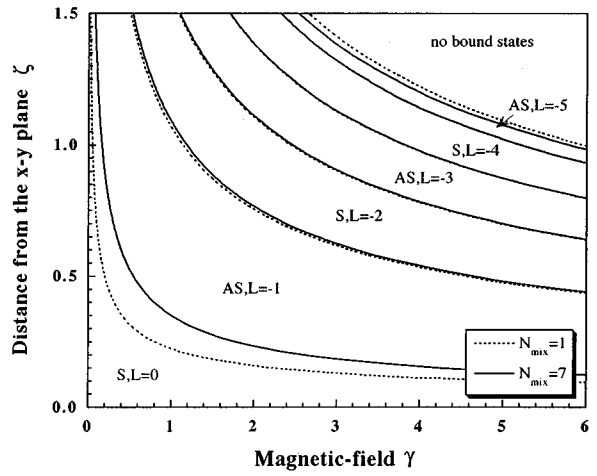

FIG. 5. The phase diagram for the barrier D^- ground states. The solid lines show the results within the seven low-lying Landau levels, and the dotted lines show the results within the lowest Landau level.

In contrast with the quantum dot model in which all states are bound, there are no bound states for the barrier D^- center in a certain region of γ and ζ. This is the magnetic vaporization of the barrier D^- center discussed by Fox and Larsen in the strong-magnetic-field limit.[14] The boundaries representing the magnetic vaporization which are determined from Eq. (11) depend on the barrier donor ground-state energies. Because the effects of the higher Landau levels for the energies of the barrier D^- states become small as γ and ζ increase, the difference between the dotted and solid lines associated with the magnetic vaporization is almost determined by the difference of the barrier donor ground-state energies calculated for $N_{\mathrm{mix}}=1$ and 7. The phase transition and magnetic vaporization of the D^- center in a more realistic quantum-well model were also discussed by Zhu and Xu[21] based on a variational method in the case of low angular momentum. This indicates that these are not special phenomena for the model of a strictly two-dimensional electron system. Although our calculations are based on the strictly two-dimensional electron system, our phase diagram would be applied to real systems in which the quantum-well width is much smaller than the distance between the positive ion and the center of the well. In such a case the effect of smearing the electronic wave functions in the z direction which would occur in a well of nonzero width can be neglected. For example, for the case of very narrow GaAs quantum wells, if we take the effective mass of GaAs, $m^*=0.067m_e$, and the static dielectric constant of GaAs, $\epsilon_0=12.5$, we obtain $a_0^*=98.7$ Å, $R^*=5.83$ meV, and $\gamma=0.148\ B(\mathrm{T})$. Then it is expected that the phase transition for $L=0(\mathrm{singlet})\rightarrow L=-1$ (triplet) occurs at $B=17.4$ (T) for the case of the positive ion located at 20 Å from the center of the well, the phase transition for $L=-1$ triplet $\rightarrow L=-2$ (singlet) occurs at $B=7.8$ (T) for the case of the positive ion located at 100 Å from the center of the well; and the magnetic vaporization of the D^- center occurs at $B=16.7$ (T) for the case of the positive ion located at 150 Å from the center of the well.

To conclude, we calculated the energies of the various barrier D^- states, the binding energies for the barrier D^- states, and the expectation values of both the distance of the electron from the origin and distance between two electrons based on the direct diagonalization method as functions of γ and ζ. The effects of the higher Landau levels become small as γ and ζ increase. The change of symmetry of the barrier D^- ground state, which has been predicted in the strong-magnetic-field limit, is also possible in finite magnetic fields. Both the distance of the electron from the origin and distance between two electrons vary discontinuously when the symmetry of the barrier D^- ground states changes. It is also found that the magnetic vaporizations occur at sufficiently large values of γ and ζ. Based on the phase diagram obtained by our calculation, the phase transitions of the barrier D^- ground states are expected to be observed in experiments concerning barrier D^- states in a very narrow quantum well.

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[1] S. Huant, S. P. Najda, and B. Etienne, Phys. Rev. Lett. **65**, 1486 (1990).
[2] E. R. Mueller, D. M. Larsen, J. Waldman, and W. D. Goodhue, Phys. Rev. Lett. **68**, 2204 (1992).
[3] S. Holmes, J. P. Cheng, B. D. McCombe, and W. Schaff, Phys. Rev. Lett. **69**, 2571 (1992).
[4] S. Huant, A. Mandray, J. Zhu, S. G. Louie, T. Pang, and B. Etienne, Phys. Rev. B **48**, 2370 (1993).
[5] J. G. S. Lok, A. K. Geim, J. C. Maan, I. Marmorkos, F. M. Peeters, N. Mori, L. Eaves, T. J. Foster, P. C. Main, J. W. Sakai, and M. Henini, Phys. Rev. B **53**, 9554 (1996).
[6] T. Pang and S. G. Louie, Phys. Rev. Lett. **65**, 1635 (1990).
[7] J. L. Dunn, E. P. Pearl, and C. A. Bates, J. Phys. Condens. Matter **5**, 7815 (1993).
[8] E. R. Mueller, D. M. Larsen, W. D. Goodhue, and J. Waldman, Phys. Rev. B **51**, 2326 (1995).
[9] J. M. Shi, F. M. Peeters, and J. T. Devreese, Phys. Rev. B **51**, 7714 (1995).
[10] M. Fujito, A. Natori, and H. Yasunaga, Phys. Rev. B **51**, 4637 (1995).
[11] D. M. Larsen and S. Y. McCann, Phys. Rev. B **45**, 3485 (1992).
[12] A. H. MacDonald, Solid State Commun. **84**, 109 (1992).
[13] A. B. Dzyubenko, Phys. Lett. A **165**, 357 (1992).
[14] H. L. Fox and D. M. Larsen, Phys. Rev. B **51**, 10 709 (1995); **52**, 16 937 (1995).
[15] A. B. Dzyubenko and A. Y. Sivachenko, Phys. Rev. B **48**, 14 690 (1993).

[16] A. H. MacDonald and D. S. Ritchie, Phys. Rev. B **33**, 8336 (1986).
[17] D. M. Larsen, Phys. Rev. B **44**, 5629 (1991).
[18] D. M. Larsen and S. Y. McCann, Phys. Rev. B **46**, 3966 (1992).
[19] U. Merkt, J. Huser, and M. Wagner, Phys. Rev. B **43**, 7320 (1991).
[20] M. Wagner, U. Merkt, and A. V. Chaplik, Phys. Rev. B **45**, 1951 (1992).
[21] J.-L. Zhu and S. Xu, Phys. Rev. B **50**, 12 175 (1994).