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Transitions of the ground state and electron–electron correlations in barrier D^- centres in magnetic fields

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Abstract. The relation between the electron–electron correlations and magnetic-field-induced angular momentum transitions in the barrier D^- centre is investigated based on a variational method. The Chandrasekhar-type variational wavefunctions for the barrier D^- states are constructed based on the exact solutions in the strong-magnetic-field limit. The energies of the barrier D^- states, the binding energies, the electron densities, the angular correlations, and the average distances between the two electrons are obtained as functions of the applied magnetic field strength γ and the distance ζ between the positive ion and the plane where the two electrons reside. When the transitions of the barrier D^- ground state occur for finite ζ with increasing γ, the strong correlations appear in the electron densities, the angular correlations, and the average distances between the two electrons. As a consequence of detailed considerations of the relation between the angular correlations and the strength of binding, we find that the magnetic-field-induced angular-momentum transitions occur as a result of the strong correlations in the barrier D^- states.

1. Introduction

It is well known that the effects of interparticle correlations are enhanced by a reduction of dimensionality and strong external magnetic fields. One of the simplest systems in which electronic 'many-body' effects can be studied is a system of negative donor centres (D^-) in semiconductors. D^- centres are formed by neutral donors (D^0) trapping an extra electron. Today it is possible to create more stable D^- centres in selectively doped multiple quantum wells [1–6] compared with bulk semiconductors [7]. Quasi-two-dimensional (Q2D) D^- centres in strong magnetic fields are suitable for studying the effects of electron–electron correlations, and a number of experimental [1–6, 8–10] and theoretical [11–18] investigations for the Q2D D^- centres have been reported in recent years.

So far most of the theoretical investigations have been concerned with systems of D^- centres in which donor impurities are δ doped at the centre of the quantum wells [2, 6, 11–17]. Recently Zhu and Xu [19] investigated the Q2D D^- states which are formed away from the centre of the quantum wells, using a variational method. They showed that the ground state for such a system changes from the s-like singlet state to the p-like triplet state with increasing magnetic field. Fox and Larsen [20] have proposed a model called a barrier D^- centre in which two electrons confined to the x–y plane are bound by a positive ion at a distance ζ from the plane. This is one of the simplest models for the Q2D D^- centres which are formed near the barrier edge or inside the barrier. They showed that the transitions of the ground state occur between the states with $L = 0 \sim 5$

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as a function of the distance ζ using the exact solutions for the barrier D^- centre in the strong-magnetic-field limit (where $-L$ is the z component of the total angular momentum). In our previous work [21] we investigated the problem of the barrier D^- centre based on a direct diagonalization method in which mixing between the different Landau levels is taken into account. We showed that the transitions of the barrier D^- ground state also occur in finite magnetic fields. Marmorkos *et al* [22] investigated the remote D^- states with $L = 0 \sim 2$ in double quantum wells using a numerical technique which solves the two-electron Schrödinger equation. They indicated that the electron–electron correlations are related closely to the magnetic-field-induced angular-momentum transitions. Recently an experimental study for such problems was reported [10].

Although the barrier D^- centre is an idealized model, it includes essential physics concerning the magnetic-field-induced angular-momentum transitions which occur as off-centre effects of the D^- centre in the quantum wells. Understanding the barrier D^- centre is useful for clarifying phenomena concerning the Q2D D^- state away from the centre of the quantum well. In the model of the barrier D^- centre, the electron–ion Coulomb attraction is always dominant compared with the electron–electron Coulomb repulsion when $\zeta = 0$ (strictly two-dimensional models [23–25]). In this case the transitions of the D^- ground state do not occur. On the other hand, the effects of the Coulomb attraction decrease as ζ increases from zero. As the magnetic field strength γ increases the Coulomb repulsion eventually comes to dominate over the Coulomb attraction. In this case the transitions of the D^- ground state occur. When the role of Coulomb repulsion which tends to keep electrons as far apart as possible is important, the electrons can lower their energy most effectively by forming highly correlated states. Therefore the effects of the electron–electron correlations on the magnetic-field-induced angular-momentum transitions are very important. In fact, Fox and Larsen showed that at larger values of ζ the strong angular correlations exist in the barrier D^- states in the strong-magnetic-field limit [20]. Marmorkos *et al* showed that the angular correlation of the remote D^- state with zero angular momentum strengthens until a certain value of the magnetic field, whereas it weakens at larger fields [22]. They concluded that such a correlation gives rise to the magnetic-field-induced angular-momentum transitions. The states with relatively large angular momentum offer the possibility of achieving a relatively high degree of correlation.

The purpose of the present paper is to investigate systematically the relation between the electron–electron correlations and the magnetic-field-induced angular-momentum transitions in the problem of the barrier D^- centre including the states with large angular momentum. Here we use a variational method instead of the direct diagonalization method because the number of parameters included is much smaller and the physical picture of the electrons in the barrier D^- state is clearer in the variational method than in the direct diagonalization method. So far, many investigations for Q2D D^- states with small angular momentum ($L = 0, 1$ for the singlet state and $L = 1, 2$ for the triplet state) have been reported, but there are no variational calculations for the Q2D D^- states with large angular momentum. We extend conventional variational methods [2, 6, 16, 17, 26] which use Chandrasekhar-type variational functions [27] for D^- states with small angular momentum to apply to barrier D^- states with large angular momentum. We construct Chandrasekhar-type variational wavefunctions of the barrier D^- states based on the exact solutions [20] in the strong-magnetic-field limit. It is expected that our variational calculations are accurate in relatively high magnetic fields. The validity of our variational functions will be discussed by comparing the energies of the barrier D^- states with those obtained based on the direct diagonalization method [21]. To clarify the mechanism of the transitions of the barrier D^- ground state and to have a clear understanding of the electron states of the barrier D^-

centre, we calculate the binding energies, the electron densities, the angular correlations, and the average distances between the two electrons. For finite ζ the transitions of the barrier D^- ground state occur as a function of the magnetic field strength γ. In this case the strong correlations appear in the electron densities, the angular correlations, and the average distances between the two electrons. As a consequence of detailed considerations of the relation between the angular correlations and the strength of binding, we find that the magnetic-field-induced angular-momentum transitions occur as a result of the strong correlations in the barrier D^- states.

In section 2 we present the model of the barrier D^- centre, the variational calculation procedure for the energies of the barrier D^- states, and the method of calculation for the various physical quantities. In section 3 we show the results of variational calculations for the energies of the barrier D^- states and discuss the validity of the variational wavefunctions employed. Using the variational functions obtained we calculate the binding energies for the barrier D^- states, the electron densities, the angular correlations, and the average distances between the two electrons. We argue the relation between the electron–electron correlations and the magnetic-field-induced angular-momentum transitions. Finally we summarize the results in section 4.

2. Formulation

In the effective-mass approximation, the Hamiltonian for the barrier D^- centre in a magnetic field along the z axis is written as

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

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

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

$$h_0(j) = -\nabla_j^2 + \frac{\gamma}{i}\frac{\partial}{\partial \varphi_j} + \frac{1}{4}\gamma^2\rho_j^2. \tag{3}$$

Here $\vec{\rho}_j$ is the position vector of the jth electron in the x–y plane, φ_j is the angle between $\vec{\rho}_j$ and the x axis, ζ is the distance between the fixed positive ion and the x–y plane, and we took the origin as the projection of the positive ion on the x–y plane. $h_0(j)$ is the free electron Hamiltonian in the magnetic field applied perpendicular to the x–y plane. The unit of length is an effective Bohr radius a_B^* and the unit of energy is an effective Rydberg R^*. $\gamma = \hbar\omega_c/2R^*$ is the dimensionless magnetic field strength and is equal to the lowest Landau level energy of the free electron in units of R^*, where the cyclotron frequency ω_c is given by $\omega_c = eB/m^*c$, B is the strength of the applied magnetic field and m^* is the conduction-band mass. Throughout the 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 the two electrons. Therefore its eigenstates are classified according to the z component of the total angular momentum and their symmetry under interchange of the two electrons. In the strong-magnetic-field limit the exact solutions for the total Hamiltonian H exist [20]. Based on the exact solutions [20, 23–25] in this limit we take the following Chandrasekhar-type variational functions for the low-lying barrier D^- states

$$\Psi_{L,\Lambda}(\vec{\rho}_1, \vec{\rho}_2) = F_{L,\Lambda}(\vec{\rho}_1, \vec{\rho}_2)\left(1 + \Xi\ |\vec{\rho}_1 - \vec{\rho}_2|^2\right) \tag{4}$$

where

$$F_{L,\Lambda}(\vec{\rho}_1, \vec{\rho}_2) = \sum_{L_1} C_{L_1,L_2,\Lambda}\, G_{L_1,L_2,\Lambda}(\vec{\rho}_1, \vec{\rho}_2) \tag{5}$$

$$G_{L_1,L_2,\Lambda}(\vec{\rho}_1, \vec{\rho}_2) = \psi_{L_1}(\vec{\rho}_1)\, \psi'_{L_2}(\vec{\rho}_2) + \Lambda\, \psi'_{L_2}(\vec{\rho}_1)\, \psi_{L_1}(\vec{\rho}_2) \tag{6}$$

$$\psi_{L_j}(\vec{\rho}) = \rho^{L_j} \exp(-\mathrm{i}L_j\varphi - \xi_{L_j}\rho^2). \tag{7}$$

$-L$ represents the z component of the total angular momentum ($L = 0, 1, 2, \ldots$) and Λ is the index representing the symmetry of the wavefunctions under interchange of the two electrons: $\Lambda = +1$ corresponds to the (symmetric) singlet states and $\Lambda = -1$ corresponds to the (antisymmetric) triplet states. The one-particle variational functions ψ_{L_j} are the eigenfunctions of an angular momentum along the z axis with the eigenvalue $-L_j$, and the functions $\psi'_{L_j}(\vec{\rho})$ are defined by the same equation (7) with different parameters ξ'_{L_j}. Here ξ_{L_1}, ξ'_{L_2}, $C_{L_1,L_2,\Lambda}$ and Ξ are variational parameters. The summation over L_1 is taken from zero to $[L/2]$ for the singlet states ($L \geqslant 0$) and to $[(L-1)/2]$ for the triplet states ($L > 0$), respectively, where $[a]$ means the maximum integer not exceeding a (Gauss's notation). $L_2 = L - L_1 \geqslant L_1$. In the variational functions employed the electron–electron correlations of the system are taken into account by taking linear combinations of the functions $G_{L_1,L_2,\Lambda}(\vec{\rho}_1, \vec{\rho}_2)$ and the correlation factor $(1 + \Xi\ |\vec{\rho}_1 - \vec{\rho}_2|^2)$.

We determine numerically the variational parameters ξ_{L_1}, ξ'_{L_2}, $C_{L_1,L_2,\Lambda}$ and Ξ so that the energies of the barrier D^- states

$$E_{D^-}(L, \Lambda) = \frac{\langle \Psi_{L,\Lambda} |\ H\ | \Psi_{L,\Lambda} \rangle}{\langle \Psi_{L,\Lambda}\ |\ \Psi_{L,\Lambda} \rangle} \tag{8}$$

are minimized. Because of the normalization condition of the wavefunction all of $C_{L_1,L_2,\Lambda}$ are not independent variational parameters. We can assume $C_{0,L,\Lambda} = 1$. For example, for the singlet barrier D^- state with $L = 2$ there are six variational parameters (ξ_0, ξ_1, ξ'_1, ξ'_2, $C_{1,1,S}$, Ξ). Owing to the simple form of the variational wavefunctions the four-dimensional integrals over the coordinates of the two electrons can be done analytically.

One-electron binding energies, $\varepsilon_B(L, \Lambda)$, are defined as

$$\varepsilon_B(L, \Lambda) = E_{D^-}(L, \Lambda) - (E_{D^0} + \gamma) \tag{9}$$

where E_{D^0} is the ground state energy for the barrier donor Hamiltonian and γ is the lowest Landau level energy of the free electron. E_{D^0} is calculated variationally with the wavefunction having the same form for $L_j = 0$ in (7). $\varepsilon_B(L, \Lambda)$ are negative for bound states and positive for unbound states.

We can easily calculate various physical quantities with the simple variational functions employed. In order to have a clear understanding of the electron states of the barrier D^- centre we calculate the following physical quantities. The electron densities defined by

$$n_{L,\Lambda}(\vec{\rho}) = \sum_{j=1}^{2} \frac{\langle \Psi_{L,\Lambda} |\ \delta(\vec{\rho} - \vec{\rho}_j)\ | \Psi_{L,\Lambda} \rangle}{\langle \Psi_{L,\Lambda}\ |\ \Psi_{L,\Lambda} \rangle} \tag{10}$$

represent the probability of finding an electron at a position $\vec{\rho}$ in the x–y plane. The probabilities of finding two electrons at a certain relative angle φ between $\vec{\rho}_1$ and $\vec{\rho}_2$ are defined as

$$g_{L,\Lambda}(\varphi) = \frac{\langle \Psi_{L,\Lambda} |\ \delta(\varphi - \varphi_{12})\ | \Psi_{L,\Lambda} \rangle}{\langle \Psi_{L,\Lambda}\ |\ \Psi_{L,\Lambda} \rangle}. \tag{11}$$

In the present paper we call $g_{L,\Lambda}$ the angular correlation functions. They represent the angular correlations between the two electrons. The average distances between the two electrons are given as

$$\overline{\rho_{12}}(L,\Lambda) = \left[\frac{\left\langle \Psi_{L,\Lambda}\right| \left|\vec{\rho}_1 - \vec{\rho}_2\right|^2 \left|\Psi_{L,\Lambda}\right\rangle}{\left\langle \Psi_{L,\Lambda} \mid \Psi_{L,\Lambda}\right\rangle}\right]^{\frac{1}{2}}. \tag{12}$$

By considering the binding energies $\varepsilon_B(L,\Lambda)$ together with the above mentioned quantities $n_{L,\Lambda}(\vec{\rho})$, $g_{L,\Lambda}(\varphi)$ and $\overline{\rho_{12}}(L,\Lambda)$, we can clarify the relation between the electron–electron correlations and the magnetic-field-induced angular-momentum transitions in the barrier D^- centre.

3. Result and discussion

We now show the results of the variational calculations for the energies of the barrier D^- states. Using the variational wavefunctions in (4) the variational parameters are determined so that the energies $E_{D^-}(L,\Lambda)$ in (8) are minimized. Figure 1 typically shows the γ dependence of the energies of the singlet barrier D^- states with $L = 2$ at $\zeta = 0.1$ and 0.5. The solid lines show the results based on the present variational calculation. To show the accuracy of the present calculation the corresponding results based on the direct diagonalization method in which mixing among the low-lying $N_{\text{mix}} = 7$ Landau levels is taken into account [21] are included in this figure (dotted lines). These results with $N_{\text{mix}} = 7$ are the best results obtained before [21]. Except for the weak magnetic field for which the results based on the direct diagonalization method are not expected to be accurate, the energies obtained with the present calculation are always higher than those obtained previously. But the differences between these energies are very small, and they become smaller as ζ increases. For the other states we obtained results similar to those for the singlet states with $L = 2$. These results indicate that the simple variational functions employed are a relatively good approximation for the barrier D^- states.

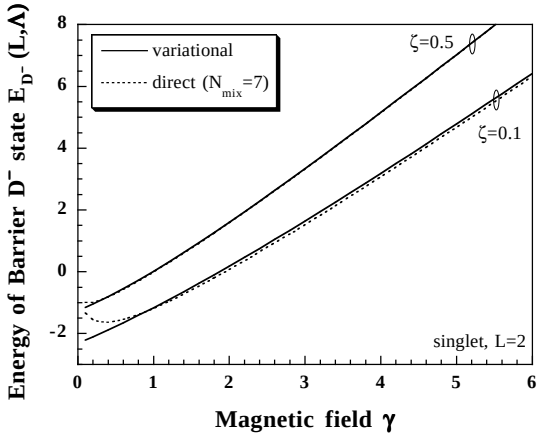

Figure 1. The energies $E_{D^-}(2,S)$ (in units of R^*) of the singlet barrier D^- states with $L = 2$ at $\zeta = 0.1$ and 0.5 as a function of γ. The solid lines show the results based on the present variational calculation. The dotted lines show the corresponding results based on the direct diagonalization method of [21].

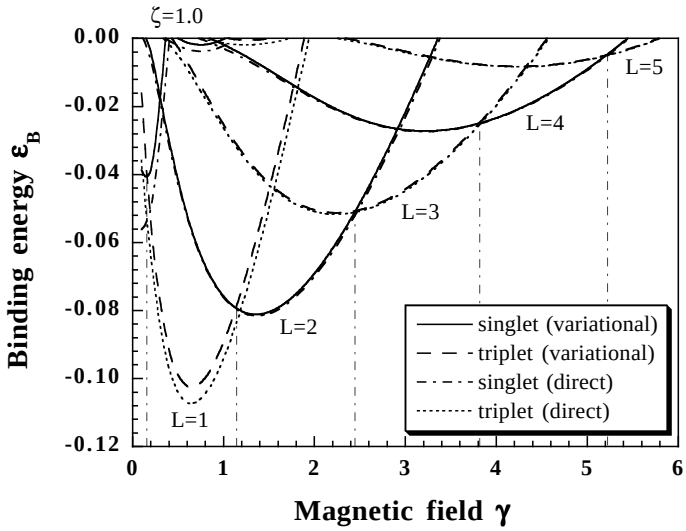

Figure 2. The binding energies ε_B (in units of R^*) for the barrier D^- states at $\zeta = 1.0$ as a function of γ. The solid and dashed lines represent, respectively, the present results for the singlet and triplet states. As a comparison, the previous results [21] for the singlet and triplet states are shown by the dashed–dotted and dotted lines, respectively.

We plot the binding energies $\varepsilon_B(L, \Lambda)$ in (9) at $\zeta = 1.0$ as a function of γ in figure 2. As a comparison, the previous results are also shown in figure 2. The solid and broken lines represent the present results for the singlet and triplet states, respectively, while the dashed–dotted and dotted lines represent the previous results for the singlet and triplet states, respectively. Here we show only the bound states ($\varepsilon_B < 0$). We should note that a consistent way to test the accuracy of a calculation is the direct comparison of the energies E_{D^-} and not the binding energies ε_B which result from the difference between the energies E_{D^-} and E_{D^0}. As shown in figure 2, however, it is found that the present results are in good agreement with the previous ones. This indicates that we can investigate the physics concerning the magnetic-field-induced angular-momentum transitions using the present variational functions. From the present results the transitions ($L \to L + 1$) of the barrier D^- ground state occur at $\gamma = 0.16$, 1.14, 2.45, 3.82 and 5.23.

To clarify the mechanism of the transitions of the barrier D^- ground state and to have a clear understanding of the electron states of the barrier D^- centre, we investigate the electron densities $n_{L,\Lambda}(\vec{\rho})$ in (10), the angular correlation functions $g_{L,\Lambda}(\varphi)$ in (11), and the average distances between the two electrons $\overline{\rho_{12}}(L, \Lambda)$ in (12) using the variational wavefunctions in (4). Figure 3(a) shows the electron densities as a function of the position vector $\vec{\rho}$ and figure 3(b) shows the angular correlation functions as polar plots of φ for the singlet barrier D^- states with $L = 2$ at $\zeta = 0.5$. Figure 4 shows the same quantities as figure 3 for the triplet states with $L = 5$ at $\zeta = 1.0$. In all the plots the solid, broken, and dotted lines represent the results at $\gamma = 0.4$, 2.0, and 6.0, respectively. $n(\vec{\rho})$ do not depend on the angle of $\vec{\rho}$ because of the rotational invariance about the z axis of the system. From the definitions of $n(\vec{\rho})$ and $g(\varphi)$ they satisfy the relations $\int \mathrm{d}\vec{\rho}\, n(\vec{\rho}) = 2$ and $\int \mathrm{d}\varphi\, g(\varphi) = 1$. The average distances between the two electrons for the singlet states with $L = 2$ at $\zeta = 0.5$ and the triplet states with $L = 5$ at $\zeta = 1.0$ are given in table 1, for $\gamma = 0.4$, 2.0, and 6.0. In figures 3(a) and 4(a) when γ is small ($\gamma = 0.4$), the electron densities $n(\vec{\rho})$ have

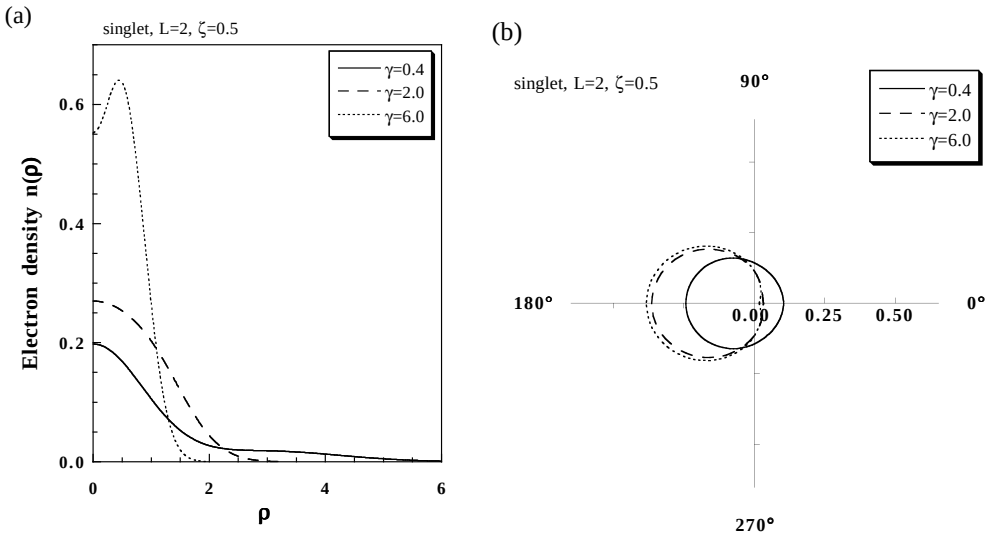

Figure 3. The radial electron densities $n(\rho)$ as a function of $\rho = |\vec{\rho}|$ (a) and the polar plots of the angular correlation functions $g(\varphi)$ (b) for the singlet barrier D^- states with $L = 2$ at $\zeta = 0.5$. The solid, broken, and dotted lines show the results for $\gamma = 0.4$, 2.0, and 6.0, respectively. $n(\rho)$ are in units of $(a_B^*)^{-2}$.

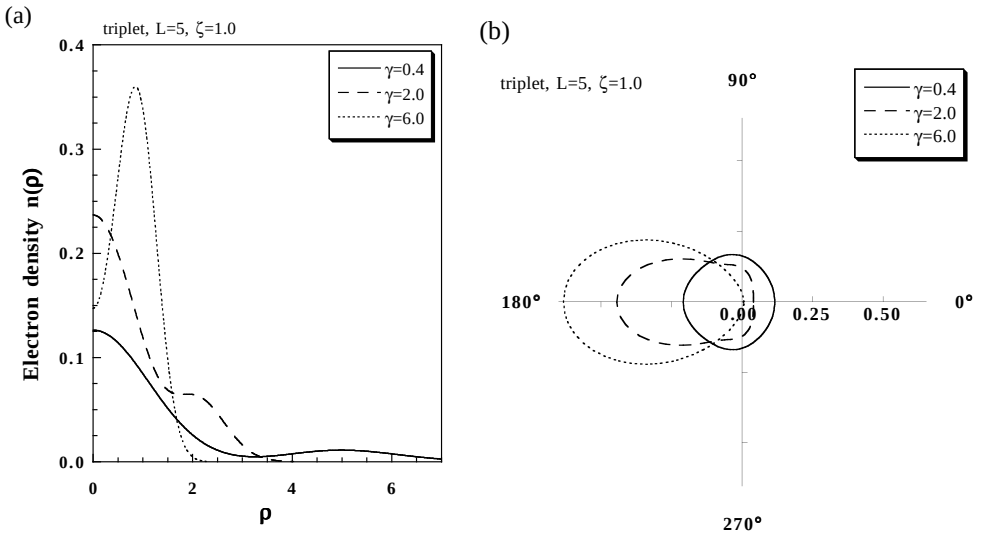

Figure 4. As figure 3, but for the triplet barrier D^- states with $L = 5$ at $\zeta = 1.0$.

large peaks at the origin and successive peaks are a significant distance apart. In the case of small γ, the angular correlations are relatively weak as shown in figures 3(b) and 4(b). These results indicate that the electron–ion Coulomb attraction is strong and the barrier D^- states consist of the inner electron strongly bound by the positive ion and the outer electron weakly bound. For the triplet state with $L = 5$ at $\gamma = 0.4$ the average distance of 5.98 between the two electrons is roughly equal to the distance 5.0 between the two peaks

in $n(\vec{\rho})$. On the other hand, with increasing γ the role of the electron–electron Coulomb repulsion, which tends to keep electrons as far apart as possible, increases as a result of the confinement due to magnetic fields. In fact, when γ is large ($\gamma = 6.0$) $n(\vec{\rho})$ have peaks at $\rho(> 0)$ and the angular correlations are strong. It is also found that the average distances between the two electrons are roughly equal to twice the distances between the origin and the position of the peak in $n(\vec{\rho})$. For example, $\overline{\rho_{12}} = 1.40$ is roughly equal to $2 \times 0.5 = 1.0$ for the singlet state with $L = 2$ at $\gamma = 6.0$.

Table 1. The average distances $\overline{\rho_{12}}$ (in units of a_B^*) between the two electrons for the singlet barrier D^- states with $L = 2$ at $\zeta = 0.5$ and for the triplet states with $L = 5$ at $\zeta = 1.0$ for several points of γ.

	$\overline{\rho_{12}}$	
γ	singlet, $L = 2$ ($\zeta = 0.5$)	triplet, $L = 5$ ($\zeta = 1.0$)
0.4	4.33	5.98
2.0	2.31	3.09
6.0	1.40	1.99

Here we would like to comment briefly on the effects of the correlation factor $(1 + \Xi\ |\vec{\rho}_1 - \vec{\rho}_2|^2)$ and the linear combination of the functions $G_{L_1,L_2,\Lambda}$. The correlation effects are taken into account only through the correlation factor for the states with small angular momentum ($L = 0, 1$ for the singlet state and $L = 1, 2$ for the triplet state), while not only the correlation factor but also the linear combination of the functions $G_{L_1,L_2,\Lambda}$ contribute to the electron–electron correlations for the states with large angular momentum. As a result of our calculations it is found that the contributions to the energies of the barrier D^- states through the correlation factor are about a few per cent for the states with small angular momentum but negligibly small for the states with large angular momentum. In order to calculate the energies of the barrier D^- states more accurately we must consider different forms of the correlation factor [26]. The role of the correlation factor will then be more important. The contributions to the other physical quantities through the correlation factor are as small as those to the energies of the barrier D^- states. Therefore changes of the angular correlations for the states with small angular momentum are caused only through the correlation factor but most changes of the angular correlations for the states with large angular momentum arise through the linear combination of the functions $G_{L_1,L_2,\Lambda}$.

It is known that the magnetic-field-induced angular-momentum transitions also occur in quantum dots in which a few interacting electrons exist [28–30]. It is understood that these phenomena in the two different systems are caused by competition between the confining potential energy and the interaction energy [20, 21, 28–30]. The confining potential is a harmonic potential for the quantum dot system. The corresponding confining potential is a Coulomb attractive potential by the positive ion for the barrier D^- centre. Here again we would like to show that the transitions for the barrier D^- ground state are caused by competition between the attractive potential and the repulsive potential. We divide the energies $E_{D^-}(L, \Lambda)$ of the barrier D^- states into two parts, $E_1(L, \Lambda)$ and $E_2(L, \Lambda)$. $E_1(L, \Lambda)$ are given as the expectation values of the Coulomb repulsive potential which is the last term in (1) and $E_2(L, \Lambda)$ are given as $E_{D^-}(L, \Lambda)$ minus $E_1(L, \Lambda)$. We define the differences of E_1 and E_2 between the states with (L, Λ) and (L', Λ') as follows,

$$\Delta E_1^{(L,\Lambda)\to(L',\Lambda')} = E_1(L, \Lambda) - E_1(L', \Lambda') \tag{13}$$

and

$$\Delta E_2^{(L,\Lambda)\to(L',\Lambda')} = E_2(L,\Lambda) - E_2(L',\Lambda'). \tag{14}$$

ΔE_1 represent the differences of the Coulomb repulsive energy between the two electrons and ΔE_2 represent the differences of the Coulomb attractive energy between the electron and the positive ion when the state of the system changes from (L, Λ) to (L', Λ'). We plot ΔE_1 and $-\Delta E_2$ for the transitions $(1, A) \to (2, S)$ and $(3, A) \to (4, S)$ at $\zeta = 1.0$ as a function of γ in figure 5. The solid and dotted lines represent ΔE_1 and $-\Delta E_2$, respectively. It is found that for the transitions $(L \to L+1)$ ΔE_1 are always positive and ΔE_2 are always negative. The vertical lines represent the points of γ (denoted γ_L) at which the transitions of the ground state for $L \to L+1$ occur. The differences of the binding energies ε_B between the different states are

$$\varepsilon_B(L,\Lambda) - \varepsilon_B(L',\Lambda') = \Delta E_1^{(L,\Lambda)\to(L',\Lambda')} + \Delta E_2^{(L,\Lambda)\to(L',\Lambda')}. \tag{15}$$

At $\gamma = \gamma_L$ the differences of the binding energies are equal to zero and ΔE_1 are exactly equal to $|\Delta E_2|$. For $\gamma < \gamma_L$, ΔE_1 are smaller than $|\Delta E_2|$, while for $\gamma > \gamma_L$ the reverse applies. That is, it is found that the transitions of the barrier D^- ground state occur when the gain of the Coulomb repulsive energy ΔE_1 becomes larger than the loss of the Coulomb attractive energy $|\Delta E_2|$. On the other hand, no such transition occurs in the case $\zeta = 0$ in which the electron–ion Coulomb attraction is always dominant. For such transitions to occur it is essential that the electron–electron Coulomb repulsion comes to dominate over the electron–ion Coulomb attraction.

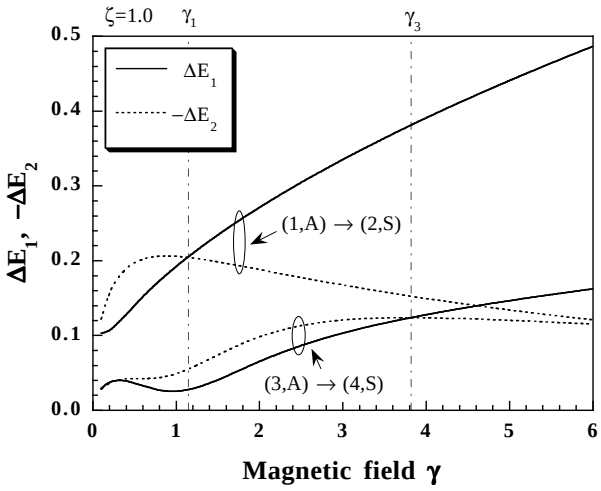

Figure 5. ΔE_1 and $-\Delta E_2$ (in units of R^*) for the transitions of the barrier D^- ground state $(1, A) \to (2, S)$ and $(3, A) \to (4, S)$ at $\zeta = 1.0$ as a function of γ. The solid and dotted lines represent ΔE_1 and $-\Delta E_2$, respectively.

When the Coulomb repulsion comes to dominate over the Coulomb attraction, the electron–electron correlations play important roles [20, 22]. Here we investigate a relation between the electron–electron correlations and the magnetic-field-induced angular-momentum transitions in detail. Figures 6(a) and (b) show the angular correlation functions $g_{L,\Lambda}(\varphi)$ for the triplet states with $L = 3$ and the singlet states with $L = 4$, respectively, at $\zeta = 1.0$ for several points of γ. These figures show that the angular correlation for each state almost reaches the maximum around the point at which the strength of binding for the

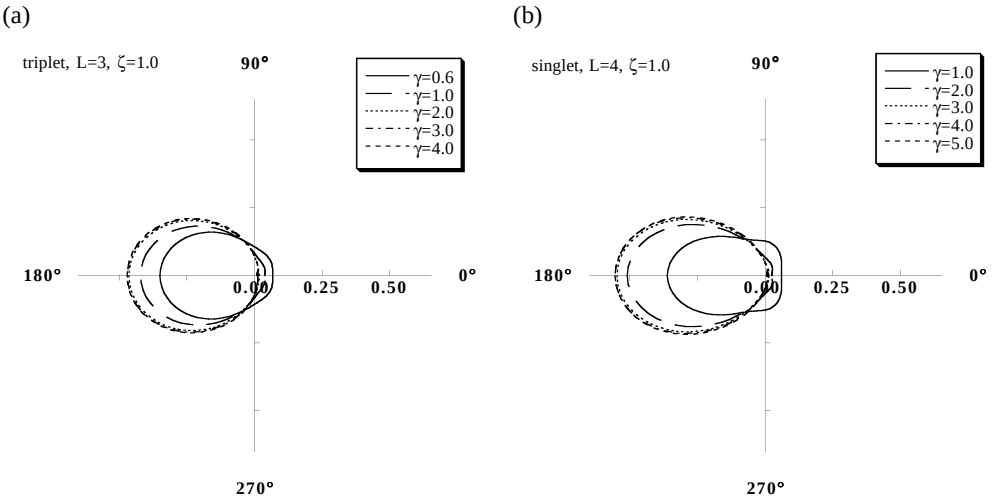

Figure 6. The angular correlation functions $g(\varphi)$ for the triplet barrier D^- states with $L = 3$ (a) and for the singlet states with $L = 4$ (b) at $\zeta = 1.0$ for several points of γ.

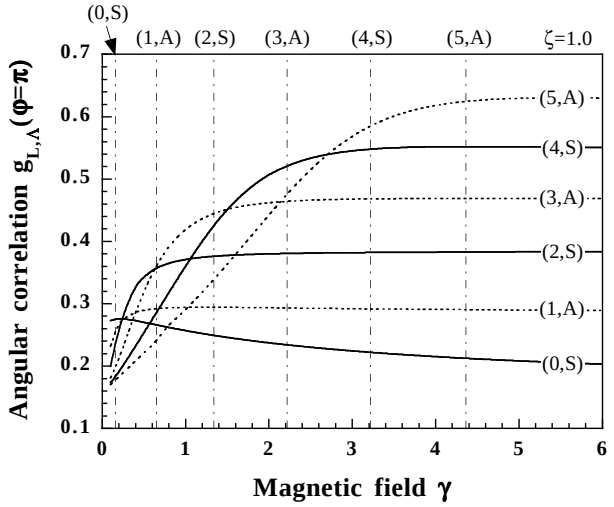

Figure 7. The angular correlation functions $g(\varphi)$ at $\varphi = \pi$ and $\zeta = 1.0$ as a function of γ. The solid and broken lines represent the results for the singlet and triplet states, respectively.

state becomes maximum ($\gamma \sim 2.0$ for the triplet state with $L = 3$ and $\gamma \sim 3.0$ for the singlet state with $L = 4$) as γ increases and it remains almost unchanged for larger γ. In order to show this more clearly we plot in figure 7 the γ dependence of the angular correlation functions $g_{L,\Lambda}(\varphi)$ at $\varphi = \pi$. The results for the singlet and triplet states are represented by the solid and broken lines, respectively. Here we show only the states concerning the transitions of the ground state. The vertical lines in figure 7 represent the points at which the strength of binding for each state reaches a maximum. Here we consider that the strength of the angular correlations is well expressed by the angular correlation functions $g_{L,\Lambda}(\varphi)$ at $\varphi = \pi$. In figure 7 it is clearly shown that except for the singlet state with $L = 0$ the

angular correlation function at $\varphi = \pi$ for each state reaches almost the maximum around the point at which the strength of binding for the state becomes maximum and it remains almost unchanged for larger γ. The different behaviour for the singlet state with $L = 0$ is related to the fact that the state has no angular correlation in the strong-magnetic-field limit. Marmorkos *et al* studied the effects of the electron–electron correlations for the remote D^- states with $L = 0$ and 1 in double quantum wells [22]. They showed that the angular correlation at $\varphi = \pi$ for the state with zero angular momentum reaches the maximum at a certain value of the magnetic field, whereas it decreases at larger fields. Although there are some differences between the more realistic quantum well model and the present model for the barrier D^- centre, our results for the singlet state with $L = 0$ are qualitatively consistent with the results of Marmorkos *et al*. However, for the states with $L \geqslant 2$ we cannot see any decrease of the angular correlations at $\varphi = \pi$ after they reach the maximum. States with large L can reach a larger maximum angular correlation compared with states with smaller L. In figure 7 it is also shown that the value of the magnetic field at which the angular correlation becomes maximum is larger for the state with large L than for the state with small L. Based on the relation between the angular correlations and the strength of binding for each barrier D^- state we can understand that the change of the angular correlations as shown in figure 7 gives rise to the magnetic-field-induced angular-momentum transitions. That is, the strength of binding for the barrier D^- ground state for a given L increases by making the correlations between the electrons strong until the angular correlation of the state becomes a maximum as γ increases. The strength of binding decreases as γ increases further and the state reaches the unbound but localized state [20, 22] because the angular correlation is almost unchanged and the energy of the state increases as a result of the confinement due to magnetic fields. The transition of the ground state for $L \rightarrow L + 1$ occurs at a certain value of γ as the state with larger L can reduce its energy by making the correlations stronger.

4. Summary

We investigated the relation between the electron–electron correlations and the magnetic-field-induced angular-momentum transitions for the problem of the barrier D^- centre based on the variational method. The Chandrasekhar-type variational wavefunctions of the barrier D^- states are constructed based on the exact solutions in the strong-magnetic-field limit. Using these variational functions we calculated the energies of the barrier D^- states, the binding energies, the electron densities, the angular correlations, and the average distances between the two electrons. By comparing the energies of the barrier D^- states based on the present variational method with those based on the direct diagonalization method, it is found that our variational calculations give a relatively good approximation for the barrier D^- states. The number of parameters included in the present variational method is much smaller than that used in the direct diagonalization method, so that we can easily calculate various physical quantities within the variational method. For finite ζ the transitions of the barrier D^- ground state occur as a function of γ. In this case the strong correlations appear in the electron densities, the angular correlations, and the average distances between the two electrons. As a consequence of the detailed investigations on the relation between the angular correlations and the strength of binding for each barrier D^- state, we found the following. Except for the singlet state with $L = 0$ the angular correlation for each barrier D^- state becomes strong until a certain value of γ and then it remains almost unchanged for larger γ. The state with large L can reach a larger maximum angular correlation compared with the state with small L and the value of the magnetic field at

which the angular correlation becomes maximum is larger for the state with large L than for the state with small L. The strength of binding for each barrier D^- state increases until the angular correlation of the state becomes maximum as γ increases. For larger γ the angular correlation remains almost unchanged and the strength of binding decreases. All the barrier D^- states eventually become unbound. It is understood that the change of the angular correlation for each barrier D^- state gives rise to the magnetic-field-induced angular-momentum transitions.

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