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Binding of two-dimensional D^- ions in a magnetic field

Jia-Lin Zhu

Centre of Theoretical Physics, CCAST (World Laboratory), Beijing 100080, People's Republic of China and Department of Physics, Tsinghua University, Beijing 100084, People's Republic of China

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Abstract. Using the exact solutions of two-dimensional (2D) hydrogen-like donors D^0 in a magnetic field, a novel trial function is constructed for 2D D^- ions in the field. The field dependence of the binding energies and the electron correlation effect on them are studied and compared with other results.

In recent years, there have been many investigations of the electronic structure and properties of neutral shallow donors D^0 in GaAs–$Ga_{1-x}Al_xAs$ multiple-quantum-well (MQW) structures with and without doping in strong magnetic fields. Although negative-donor centres D^-, i.e. neutral shallow donors that bind an additional electron, have already been observed in bulk elemental semiconductors for more than 20 years (Gershenzon *et al* 1971, Thornton and Honig 1973, Taniguchi *et al* 1975, Norton 1976), they have been identified in quantum-well structures for only about 2 years (Huant *et al* 1990). D^- centres can be expected to form readily in intentionally doped GaAs–$Ga_{1-x}Al_xAs$ MQW structures owing to electron transfer from the $Ga_{1-x}Al_xAs$ barrier to neutral donors located in the GaAs well. Far-infrared magnetotransmission and magnetophotoconductivity measurements on the MQW structures have revealed photoionization transitions from the D^- centres to successive Landau levels (Huant *et al* 1990). It has been shown that, for D^- in quantum-well structures, the quasi-two-dimensional (Q2D) nature results in a dramatic enhancement of the binding energy with respect to the 3D case. The effective-mass model has been applied to the D^- and D^0 centres in a magnetic field in both the Q2D and the 3D cases, and the model has been solved by a diffusion quantum Monte Carlo method (Pang and Louie 1990). For the 3D case, comparison of the results with the experimental data (Huant *et al* 1990) and other calculations (Natori and Kamimura 1978, Larsen 1979a, b) shows that electron correlation effects are very important to obtain better results. For the Q2D case, there is a large increase in binding energies over those of the 3D case. It shows that the binding energies of D^- centres in a magnetic field are strongly dependent on the confined dimensionality, i.e. the dimensions and the strength of the magnetic field. Therefore, it is interesting to know the limits of the binding energies in a magnetic field in the pure 2D case and the electron correlation effect on them.

The energy levels of a 2D D^0 centre in a magnetic field can be calculated using approximation or numerical methods such as the perturbation theory, the WKB approximation (Akimoto and Hasegawa 1967), the two-point Padé approximation (MacDonald and Ritchie 1986) and numerical integral methods (Duggan 1988, Whit-

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taker and Elliott 1988, Edelstein *et al* 1989). However, analytically the series formulae of wavefunctions with exact quantum levels obtained numerically for a 2D D^0 centre in a magnetic field have been given by Zhu *et al* (1990). In this paper, based on the exact solutions, we introduce a novel trial function for 2D D^- ground states in a magnetic field. Then, the field dependence of the binding energies of a 2D D^- centre and the electron correlation effect are studied and compared with other results.

The effective Hamiltonian of a 2D D^- centre in a magnetic field perpendicular to the 2D plane can be written as follows:

$$H = H(1,W) + H(2,W) + 2/|\rho_1 - \rho_2| \tag{1}$$

with

$$H(i,W) = -[(1/\rho_i)(\partial/\partial\rho_i)(\rho_i\,\partial/\partial\rho_i) + (1/\rho_i^2)L_i^2] + (\gamma^2/4)\rho_i^2 + \gamma L_i - 2W/\rho_i \tag{2}$$

where $H(i,W)$ is the effective Hamiltonian of the 2D D^0 centre with electron i in the presence of the field, ρ_i is the displacement of electron i from the centre, $\rho_i^2 = x_i^2 + y_i^2$, $W = 1$ and γ is the magnetic field in effective atomic units. The third term on the RHS in (1) is the interaction between two electrons. We have assumed an infinitely massive ion, ignored the Zeeman spin energy, which does not affect the binding energies, and have taken all energies and lengths in units of the effective Rydberg Ryd* and the effective Bohr radius a^*, respectively. L_i in (2) is the angular momentum of electron i along the field direction. We should point out that the total angular momentum of the 2D D^- centre is equal to $L_1 + L_2$ and the total magnetic quantum number can be well defined for the D^- states.

The 2D D^- states in a magnetic field cannot be solved exactly, and approximation methods should be used. For determining the electronic structure and the binding energies of the ground states in the magnetic field, we introduce a new trial wavefunction which includes the electron correlation effect and approaches the Chandrasekhar-type trial function at $\gamma = 0$. It is as follows:

$$\Psi = A(1 + C\rho_{12})[\psi(\lambda_1,\rho_1)\psi(\lambda_2,\rho_2) + \psi(\lambda_1,\rho_2)\psi(\lambda_2,\rho_1)] \tag{3}$$

where C, λ_1 and λ_2 are variational parameters, A is the normalization constant, and $\psi(\lambda_i,\rho_i)$ is the ground-state eigenfunction of $H(i,\lambda_i)$ which is equal to $H(i,W)$ of (2) as $\lambda_i = W$. We should point out that $\psi(\lambda_i,\rho_i)$ can be obtained exactly with the use of different series forms in different regions of the radial equation (Zhu *et al* 1990). Therefore, the variational energy $E(D^-)$ is given by

$$E(D^-) = \min_{\lambda_1\lambda_2 C} \langle\Psi|H|\Psi\rangle \tag{4}$$

where

$$\langle\Psi|H|\Psi\rangle = \langle\Psi|H(1,\lambda_1)|\Psi\rangle + \langle\Psi|H(2,\lambda_2)|\Psi\rangle + \langle\Psi|2/|\rho_1 - \rho_2| - (2-2\lambda_1)/\rho_1 - (2-2\lambda_2)/\rho_2|\Psi\rangle. \tag{5}$$

The first and second terms on the RHS are calculated partly analytically and partly numerically. The third term can be calculated numerically. Then, the binding energy of the D^- ground state is as follows:

$$E_B(D^-) = E(D^0) + \gamma - E(D^-) = 2\gamma - E_B(D^0) - E(D^-) \tag{6}$$

where $E(D^0)$ is the lowest level of the Hamiltonian of (2), i.e. the D^0 ground-state energy in the magnetic field, which can be solved exactly as mentioned above, and $E_B(D^0)$ is the binding energy of the neutral donor.

We have performed a numerical calculation for the ground states of 2D D^0 and 2D D^- centres in magnetic fields and obtained the ground-state levels and the corresponding energies as shown in table 1. At zero magnetic field, the binding energies of 2D D^0 and 2D D^- centres are equal to 4 Ryd and 0.450 Ryd*, respectively. The $E_B(D^-)$ shows a dramatic increase, by a factor of 8.69, compared with the binding energy (0.0518 Ryd*) of 3D D^- centres obtained by Chandrasekhar (1944). It is reasonable that the value of the binding energy of 2D D^- centres is larger than those obtained by the experiment (Haunt *et al* 1990) and the calculation (Pang and Louie 1990) in quantum-well structures. It is interesting to point out that the value is close to the 'exact' result (0.480 Ryd*) obtained by Phelps and Bajaj (1983), and that the ratio (8.69) of 2D $E_B(D^-)$ (0.450 Ryd*) to 3D $E_B(D^-)$ (0.0518 Ryd*) obtained by using Chandrasekhar-type trial functions at $\gamma = 0$ is about the same as that (8.64) obtained by using 'exact' 2D $E_B(D^-)$ (0.480 Ryd*) and 3D $E_B(D^-)$ (0.0555 Ryd*) (Perkeris 1958, 1962). As shown in table 1, the binding energies of both 2D D^- and 2D D^0 ground states increase with increasing magnetic field γ. However, the binding energy of 2D D^- centres in lower magnetic fields increases with increasing γ much more rapidly than in higher magnetic fields, and both 2D D^- and 2D D^0 binding energies increase with increasing γ at about the same rate in higher magnetic fields, i.e. the so-called magnetic freeze-out effect. This feature has been explained by the fact that the extension of the outer orbital in a 2D D^- ion sharply decreases with increasing field even in a weak-field regime, compared with the extension of a neutral donor orbital which decreases rather slowly. In table 1, it is clearly seen that the ratio R_1 of $E_B(D^-)$ to $E_B(D^0)$ increases from 0.113 to about 0.3. The starting and limiting values of R_1 are larger than those (about 0.05 and 0.2) of 3D D^- centres obtained by Natori and Kamimura (1978). This means that the freeze-out effect of D^- centres depends on the confined dimensionality and that R_1 and its limit increase with increasing dimensionality.

Table 1. Ground-state energies $E(D^0)$ and $E(D^-)$ and binding energies $E_B(D^0)$ and $E_B(D^-)$ of 2D D^0 and D^- centres in magnetic fields γ. R_1 is the ratio of $E_B(D^-)$ to $E_B(D^0)$, and R_2 is the ratio of $\Delta E_B(D^-)$ to $E_B(D^-)$ where $\Delta E_B(D^-)$ is equal to $E_B(D^-)$ minus the binding energy obtained by using the trial function without the polarization term (see the text).

Γ	$E(D^0)$ (Ryd*)	$E(D^-)$ (Ryd*)	$E_B(D^0)$ (Ryd*)	$E_B(D^-)$ (Ryd*)	R_1	R_2
0	−4	−4.4501	4	0.450	0.113	0.330
1	−3.8961	−4.0211	4.896	1.125	0.230	0.279
3	−3.3370	−2.0916	6.332	1.760	0.278	0.252
5	−2.4521	0.3696	7.452	2.178	0.292	0.219
10	0.3694	7.4608	9.631	2.908	0.302	0.165

In order to study the electron correlation effect in D^- centres in magnetic fields, we have also calculated the ground-state levels and binding energies using the trial function without the polarization term in $\rho_{12}(C = 0)$ in (3). As shown in table 1, the ratio of R_2 of the binding energy difference due to omission of the correlation term

to the binding energy decreases monotonically from 0.330 to 0.165 when γ increases from 0 to 10. It is worthwhile pointing out that the ratio R_2 of 2D D^- centres is smaller than that of the corresponding 3D D^- centres and, particularly at $\gamma = 0$, the R_2 difference between 2D and 3D cases is larger and equal to about 0.15. The above discussion means that, as increasing confinement (increasing the strength of magnetic field or reducing the dimensionality) causes one electron with a spin to approach close to another with the opposite spin and have less room to avoid each other in a D^- centre, the electron correlation effect on the wavefunction and binding energy can become weak.

In conclusion, we have for the first time used the new trial function, which has a Chandrasekhar-type structure and consists of the exact eigenfunctions of the Hamiltonian $H(i, \lambda)$, and obtained the ground-state levels and binding energies of 2D D^- centres in magnetic fields. The calculated results have shown that the binding energies, the freeze-out effect and the electron correlation effect are strongly dependent on the confinement, i.e. the strength of magnetic field and the dimensionality. This will be useful for understanding the electronic properties in low-dimension systems and for designing some devices in the future. Finally, it is worthwhile pointing out that, using the new kind of trial function as a part of the total trial function of D^- centres in quantum-well structures, the quantum levels and binding energies can be calculated correctly and compared with other calculations and experiments. This work is in progress.

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