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Variational studies of D^0 and D^- centers in magnetic fields in bulk crystals and in parabolic quantum wells

J. Blinowski* and T. Szwacka
Departamento de Física, Facultad de Ciencias, Universidad de Los Andes, Mérida, Venezuela

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A linear combination of a few Gaussian functions of variable widths and anisotropy was used as a trial function for D^0 centers in bulk crystals and in parabolic quantum wells in the presence of a magnetic field. The same types of functions with an additional correlation factor were then used for D^- ions in the bulk and in parabolic quantum wells. All integrals including the electron-electron interaction were calculated analytically. The results obtained for the bulk are very accurate for D^0 centers and quite close to the experimental data for D^- ions in GaAs. The impurities in parabolic quantum wells were not yet experimentally investigated but the present results indicate that even in the case of a uniform spatial distribution they should lead to well-defined infrared absorption maxima.

I. INTRODUCTION

The experimental evidence for the existence of ionized donor centers D^- (neutral shallow donors D^0 that bind an additional electron), first in multivalley semiconductors Si and Ge,[1-4] and afterwards in single-valley ones,[5,6] gave reason for the theoretical study of D^- centers in bulk materials. These have been done by Natori and Kamimura,[7] and Larsen.[8] Considering the D^- center as an analog of the H^- ion, they studied the bound states in the presence of a magnetic field variationally and obtained reasonable agreement with the experimental data for D^- centers in bulk GaAs.[5,6] Pang and Louie[9] calculated the ground-state binding energy of the D^- center for bulk GaAs in a magnetic field by the diffusion quantum Monte Carlo method. They obtained excellent agreement with the experimental data of Ref. 6. Recently Larsen and McCann[10] have made variational studies of two- and three-dimensional D^- centers in magnetic fields. Their results for the D^- ground-state energy in bulk materials are as good as those of Pang and Louie.[9]

The extensive magneto-optical studies of shallow donors in selectively doped GaAs-$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ multiple quantum wells[11-15] (MQW's) undertaken in the last decade have shown the importance of D^- centers in these structures. Observation of the optical spectra of two-dimensional (2D) D^- centers in GaAs-$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ MQW's was reported by Huant, Najda, and Etienne.[16] These authors interpreted a series of peaks in their magnetophotoconductivity spectra as photoionization transitions from the ground state of the 2D D^- impurity to successive Landau levels. The dominant peak, identified as the transition to the $N=1$ level, was strongly affected by the resonant polaron effect, but a weaker low-energy peak, identified as the transition to the $N=0$ level and free of any polaron effects, was also observed. Simultaneously Pang and Louie[9] calculated the binding energy for a D^- center in a quantum well identical to those studied in Ref. 16 for two values of the magnetic field perpendicular to the well. The calculated energies were lower than the lowest transition energies observed in the experiment.[16] The origin of the discrepancy became clear when Larsen and McCann[17] and Dzyubenko[18] pointed out that in strong magnetic fields the final states of dipole magneto-optical transitions from the ground state of 2D and quasi-2D D^- impurities are excited singlet p-like levels with energies above the next Landau levels. The correct identification of the final states, and detailed experimental and theoretical studies of the tilt-induced line splitting in a magnetic field, allowed for definite identification of the D^- center in a GaAs-$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ MQW by Mueller, Larsen, and Waldman.[19]

The purpose of the present paper was first to test relatively simple trial functions for D^0 and D^- donors, which would give analytical expressions for energies in bulk GaAs in a magnetic field without losing too much accuracy, and then to apply the same trial functions to donors in parabolic quantum wells. Such structures have been recently grown by molecular-beam epitaxy[20-22] by varying the Al composition x quadratically from $x=0$ at the center to some finite x_0 at the edges of the well. In this way one obtains a parabolic-shaped potential well which is still sandwiched between two barrier layers of composition $y > x_0$.

We extended the idea of Yafet, Keyes, and Adams (YKA),[23] who proposed a two-parameter variational wave function of Gaussian type for the ground state of the D^0 center, and we introduced a linear combination of a few Gaussian functions with different longitudinal and transverse radii which together with the linear coefficients play the role of variational parameters. Trial wave functions of this type give simple analytical expression for the energy for D^0 centers, and represent a very good choice for moderate and high magnetic fields. We show that by increasing the number of Gaussians it is possible to reproduce the best previous theoretical results we know of for the ground-state binding energies of the D^0 center in a magnetic field. The same type of one-electron trial function with simple correlation factor proved to be effective in the case of D^- centers in bulk GaAs in a magnetic field, although with somewhat lower accuracy than for D^0 donors.

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The advantages of the linear combination of Gaussian functions as a one-electron trial function still hold in the case of D^0 and D^- centers in parabolic $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ quantum wells. In such wells, as in square wells, the optical transitions from the ground state to the singlet p-like excited state should dominate the absorption spectra of D^- centers. Apart from the ground state, we investigated the lowest excited state of D^0 centers with the z component of the angular momentum $M_z=1$ (tending to the $2p^-$ atomic state in the low-field and to the $N=0$ Landau level in the high-field limit). For D^- we also investigated the lowest excited singlet state with $M_z=-1$ (the electrons in $1s$ and $2p^-$ orbitals in the low-field and in $N=0, M_z=0$ and $N=0, M_z=-1$ in the high-field limit). In all cases analytical expressions for the energy expectation values were obtained. We selected the excited states with $M_z=-1$, despite the fact that at high magnetic fields the dipole optical transitions in the Faraday configuration from the ground states to these states have lower oscillator strengths than the transitions to the lowest singlet states with $M_z=+1$ (with the excited electron in the $2p^+$ state in the low-field and $N=1, M_z=1$ in the high-field limit). The reason was that, in contrast to the latter, the former are practically unaffected by band nonparabolicity and polaron effects, as shown by Dzyubenko and Sivachenko[24] for square quantum wells.

In Sec. II we calculate the ground-state energy for the D^0 center in bulk GaAs and we compare our result with previous theoretical results. In Sec. III calculations of the ground and the lowest-lying p-like excited states of D^0 centers in wide parabolic quantum wells are reported. In Sec. IV we calculate the ground-state binding energy for the D^- ion in bulk GaAs and in Sec. V we investigate the two lowest singlet states of the D^- center in wide parabolic quantum wells. In all cases we consider a broad range of external magnetic fields.

II. D^0 GROUND STATE IN A BULK MATERIAL

The shallow donor center in bulk GaAs can be considered as a hydrogenlike atom. The hydrogen ground state in a magnetic field has been investigated by many authors.[8,23,25–28] YKA,[23] Larsen,[8,25] and Aldrich and Greene[26] have developed variational calculations for the ground state, Praddaude[27] has proposed an expansion of the H wave functions in Laguerre polynomials, and Cabib, Fabri, and Fiorio[28] (CFF) have investigated the Schrödinger equation numerically. So, nowadays, we have very accurate values of hydrogen ground-state energies for $\gamma \le 5$,[27,28] where the dimensionless parameter $\gamma=\hbar\omega_c/2\ \mathrm{Ry}^*$ expresses the strength of the magnetic field B; $\omega_c=eB/m^*c$, $\mathrm{Ry}^*=m^*e^4/2\hbar^2\varepsilon^2$ ($-e, m^*$ are the charge and effective mass of an electron, respectively, and ε the static dielectric constant). Unfortunately, the procedures which gave the best results for the neutral hydrogenlike atom are rather difficult to adapt to the case of the two-electron D^- center in a magnetic field.

Here, we choose the following trial wave functions for the ground state of the hydrogenlike atom in a magnetic field:

$$\psi_s^{(n)}=\sum_{i=1}^{n} A_i e^{-(\alpha_i\rho^2+\beta_i z^2)} , \tag{1}$$

where ρ, z denote cylindrical coordinates and A_i, α_i, β_i are variational parameters. As the case of $n=1$ has already been studied in Ref. 23, we focus our attention on the cases of $n>1$. The dimensionless Hamiltonian for the ground state of the hydrogenlike atom in a magnetic field, in the effective-mass approximation, is of the form

$$H=-\nabla^2-\frac{2}{r}+\tfrac{1}{4}\gamma^2\rho^2 , \tag{2}$$

where $r=[\rho^2+z^2]^{1/2}$. The energy is measured in effective Rydbergs Ry* and the effective Bohr radius $a_B^*=\hbar^2\varepsilon/m^*e^2$ is the unit of distance. The variational ground-state binding energies $E_D^{(n)}(\gamma)$ are given by

$$E_D^{(n)}(\gamma)=\gamma-\min\frac{\langle\psi_s^{(n)}|H|\psi_s^{(n)}\rangle}{\langle\psi_s^{(n)}|\psi_s^{(n)}\rangle} , \tag{3}$$

where

$$\langle\psi_s^{(n)}|H|\psi_s^{(n)}\rangle=\sum_{i,k=1}^{n} A_i A_k\Big[F(\alpha_i,\beta_i;\alpha_k,\beta_k;1) -2f(\alpha_{ik},\beta_{ik}) +\frac{\gamma^2}{4\alpha_{ik}}G(\alpha_{ik},\beta_{ik})\Big] \tag{4}$$

and

$$\langle\psi_s^{(n)}|\psi_s^{(n)}\rangle=\sum_{i,k=1}^{n} A_i A_k G(\alpha_{ik},\beta_{ik}) . \tag{5}$$

In the above expressions, the following abbreviations were used:

$$\alpha_{ik}=\alpha_i+\alpha_k,\quad \beta_{ik}=\beta_i+\beta_k , \tag{6}$$

$$G(\alpha_{ik},\beta_{ik})=(\pi/\alpha_{ik})(\pi/\beta_{ik})^{1/2} , \tag{7}$$

$$F(\alpha_i,\beta_i;\alpha_k,\beta_k;n)=\left[4n\alpha_i\left[1-\frac{\alpha_i}{\alpha_{ik}}\right]+2\beta_i\left[1-\frac{\beta_i}{\beta_{ik}}\right]\right]G(\alpha_{ik},\beta_{ik}) , \tag{8}$$

and

$$f(\alpha_{ik},\beta_{ik})=\begin{cases}\dfrac{2\pi}{[\alpha_{ik}(\beta_{ik}-\alpha_{ik})]^{1/2}}\arctan[(\beta_{ik}-\alpha_{ik})/\alpha_{ik}]^{1/2}, & \beta_{ik}>\alpha_{ik},\\ \dfrac{2\pi}{\alpha_{ik}}, & \beta_{ik}=\alpha_{ik},\\ \dfrac{2\pi}{[\alpha_{ik}(\alpha_{ik}-\beta_{ik})]^{1/2}}\operatorname{arctanh}[(\alpha_{ik}-\beta_{ik})/\alpha_{ik}]^{1/2}, & \beta_{ik}<\alpha_{ik}.\end{cases} \tag{9}$$

The minimization of (3) was performed with the use of the standard downhill simplex method in multiple dimensions described in Ref. 29. The ground-state binding energies $E_D^{(n)}(\gamma)$, for $n=2,3,7$ and $1\le\gamma\le 10$, are listed in Table I and compared with the results reported in Refs. 8, 23, 27, and 28. We can see that the improvement of $E_D^{(2)}(\gamma)$ with respect to $E_D^{(1)}(\gamma)$ is nearly the same for all values of γ considered in Table I, equal roughly to 0.1 Ry* [$E_D^{(2)}(\gamma)-E_D^{(1)}(\gamma)$ increases very slightly with γ]. Then, $E_D^{(3)}(\gamma)-E_D^{(2)}(\gamma)\cong 0.02$ Ry* is nearly one order of magnitude smaller than $E_D^{(2)}(\gamma)-E_D^{(1)}(\gamma)$ and also increases slightly with γ. This tendency continues as the number of Gaussians in the trial wave function increases. The values of $E_D^{(7)}(\gamma)$ practically coincide with the best values for the ground-state binding energies reported until now (the results of Praddaude[27] and CFF,[28] denoted in Table I as $E_D^{(P)}$).

High accuracy over a wide range of fields was obtained by Larsen[8] (binding energy $E_D^{(L)}$ in Table I) with a trial wave function of the form

$$\phi=\exp\left[-\tfrac{1}{4}\gamma'\rho^2-\frac{z^2}{b}-\chi(\rho^2+az^2)^{1/2}\right].$$

This function involves only four variational parameters (γ',b,χ,a) but does not allow for analytical calculation of the electron-electron interaction in the case of the D^- center.

It is interesting to note that the binding energies obtained by Aldrich and Greene[26] with a Gaussian basis involving 120 different Gaussians with fixed longitudinal and transverse radii can be reproduced with our trial wave function involving only five Gaussians. In conclusion, we propose rather simple (in form and easy to work with) variational wave functions for the ground state of the hydrogenlike atom in a magnetic field, which already for $n=3$ give binding energies differing by less than 0.3% from the most accurate results we know in the entire range of magnetic fields from $\gamma=1$ to 10.

TABLE I. Comparison of D^0 ground-state binding energies (in units of the effective Rydberg Ry*) calculated with different trial wave functions. The $E_D^{(n)}$ (for $n=1,2,3,7$) were obtained using variational wave functions (1), $E_D^{(L)}$ are reported in Ref. 8, and $E_D^{(P)}$ in Ref. 27 [$E_D^{(1)}$ was reported previously by YKA (Ref. 23)].

Field	Hydrogen-like-atom ground-state binding energies for various wave functions					
γ	$E_D^{(1)}$	$E_D^{(2)}$	$E_D^{(3)}$	$E_D^{(7)}$	$E_D^{(L)}$	$E_D^{(P)}$
1	1.524	1.6401	1.6579	1.662 31	1.6620	1.662 33
2	1.908	2.0228	2.0400	2.044 40	2.0438	2.044 42
3	2.191	2.3066	2.3244	2.329 04	2.3282	2.329 05
4	2.420	2.5379	2.5567	2.561 57		2.561 6[a]
5	2.616	2.7358	2.7557	2.760 77	2.7594	2.760 81[b]
10	3.331	3.4651	3.4897	3.495 55	3.4928	3.495 61[b]

[a] From Ref. 28.

[b] The results of Praddaude reported in Ref. 8.

III. D^0 STATES IN A PARABOLIC QUANTUM WELL

Let us consider a donor center placed in the central region of a relatively thick parabolic $Al_xGa_{1-x}As$ quantum well ($l_w\ge 800$ Å, where l_w denotes the thickness of the well). The Al composition x varies quadratically from $x=0$ at the center to $x=x_0$ at the edges of the well. We choose the z axis in this direction and the center of the well at $z=z_0$ (z is put equal to zero at the donor position). The dimensionless Hamiltonian for the hydrogenlike atom in a magnetic field parallel to the z axis has the form

$$H_w=H+V(z)+\gamma L_z\ , \tag{10}$$

where H is given by (2) and the potential energy of an electron in a quantum well $V(z)$ has the form

$$V(z)=\eta(z-z_0)^2\ . \tag{11}$$

L_z is the z component of the orbital angular momentum around a nucleus and its eigenvalue is zero for the D^0 ground state. We propose the following trial wave function for the ground state of the Hamiltonian (10):

$$\psi_{sw}^{(n)}=(1+\delta z)\psi_s^{(n)}\ , \tag{12}$$

where $\psi_s^{(n)}$ is given by (1). For a donor center placed in the center of the quantum well, the variational parameter δ is equal to zero. The energy of the lowest subband in the parabolic quantum well described by the potential (11) is given by $\eta^{1/2}$. The variational ground-state binding energies $E_{Dw}^{(n)}(\gamma)$ are given by

$$E_{Dw}^{(n)}(\gamma)=\gamma+\eta^{1/2}-\min\frac{\langle\psi_{sw}^{(n)}|H_w|\psi_{sw}^{(n)}\rangle}{\langle\psi_{sw}^{(n)}|\psi_{sw}^{(n)}\rangle}\ , \tag{13}$$

where

$$\langle \psi_{sw}^{(n)} | H_w | \psi_{sw}^{(n)} \rangle = \sum_{i,k=1}^{n} A_i A_k \left[F_w(\alpha_i,\beta_i;\alpha_k,\beta_k;1) - 2f(\alpha_{ik},\beta_{ik}) + 2\delta^2 \frac{\partial f(\alpha_{ik},\beta_{ik})}{\partial \beta_{ik}} + \frac{\gamma^2}{4\alpha_{ik}} G_w(\alpha_{ik},\beta_{ik}) + \eta P(\alpha_{ik},\beta_{ik}) \right] , \tag{14}$$

$$\langle \psi_{sw}^{(n)} | \psi_{sw}^{(n)} \rangle = \sum_{i,k=1}^{n} A_i A_k G_w(\alpha_{ik},\beta_{ik}) , \tag{15}$$

with

$$\begin{aligned} F_w(\alpha_i,\beta_i;\alpha_k,\beta_k;n) &= \left[1 + \frac{\delta^2}{2\beta_{ik}} \right] F(\alpha_i,\beta_i;\alpha_k,\beta_k;n) + \delta^2 \frac{2\beta_i}{\beta_{ik}} \left[1 - \frac{\beta_i}{\beta_{ik}} \right] G(\alpha_{ik},\beta_{ik}) , \\ G_w(\alpha_{ik},\beta_{ik}) &= \left[1 + \frac{\delta^2}{2\beta_{ik}} \right] G(\alpha_{ik},\beta_{ik}) , \end{aligned} \tag{16}$$

and

$$P(\alpha_{ik},\beta_{ik}) = \left[(1 - 4\delta z_0 + \delta^2 z_0^2) \frac{1}{2\beta_{ik}} + \frac{3\delta^2}{4\beta_{ik}^2} + z_0^2 \right] G(\alpha_{ik},\beta_{ik}) . \tag{17}$$

The abbreviations used here were defined already by formulas (6)–(9). It is easy to see that if the parameters η and δ are equal to zero then the expressions (14) and (15) reduce to (4) and (5), respectively, as was expected.

As the next step we consider the lowest-lying *p*-like excited state of the D^0 center with the quantum number of the L_z operator equal to -1 [the $2p(-1)$ state]. We propose the following trial wave functions for this state:

$$\psi_{pw}^{(n)} = 2^{-1/2}(x - iy)\psi_{sw}^{(n)} , \tag{18}$$

where $\psi_{sw}^{(n)}$ is given by formula (12). The transition energy from the ground $1s$ state to the $2p(-1)$ state is equal to the difference between the energy expectation values of the states:

$$\Delta E_{D^0 w}^{(n)} = \min \frac{\langle \psi_{pw}^{(n)} | H_w | \psi_{pw}^{(n)} \rangle}{\langle \psi_{pw}^{(n)} | \psi_{pw}^{(n)} \rangle} - \min \frac{\langle \psi_{sw}^{(n)} | H_w | \psi_{sw}^{(n)} \rangle}{\langle \psi_{sw}^{(n)} | \psi_{sw}^{(n)} \rangle} , \tag{19}$$

where the new quantities have the form

$$\langle \psi_{pw}^{(n)} | H_w | \psi_{pw}^{(n)} \rangle = \sum_{i,k=1}^{n} A_i A_k \left[\frac{1}{2\alpha_{ik}} F_w(\alpha_i,\beta_i;\alpha_k,\beta_k;2) + \frac{\partial f(\alpha_{ik},\beta_{ik})}{\partial \alpha_{ik}} - \delta^2 \frac{\partial^2 f(\alpha_{ik},\beta_{ik})}{\partial \alpha_{ik} \partial \beta_{ik}} + \frac{\gamma^2}{4\alpha_{ik}^2} G_w(\alpha_{ik},\beta_{ik}) + \frac{\eta}{2\alpha_{ik}} P(\alpha_{ik},\beta_{ik}) \right] - \gamma \langle \psi_{pw}^{(n)} | \psi_{pw}^{(n)} \rangle , \tag{20}$$

and

$$\langle \psi_{pw}^{(n)} | \psi_{pw}^{(n)} \rangle = \sum_{i,k=1}^{n} A_i A_k \frac{1}{2\alpha_{ik}} G_w(\alpha_{ik},\beta_{ik}) . \tag{21}$$

The final numerical results are presented in Figs. 1–3 and in Table II. We performed the calculations for two different parabolic quantum wells: one defined by $\eta = 0.25$ and the other one by $\eta = 1.0$. If we select the composition x_0 at the edges of the well equal to 0.15, the parameter $\eta = 1.0$ will correspond to a parabolic quantum well of width 800 Å, whereas $\eta = 0.25$ will correspond to a well twice as wide. [We used for the barrier height the formula $0.6(1.155x + 0.37x^2)$ eV.[30–32]]

In Fig. 1 we have plotted the ground-state binding energies for the D^0 center in an $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ parabolic quantum well defined by $\eta = 0.25$ as a function of magnetic field and for three different positions of the impurity with respect to the center of the well: (a) with the D^0 impurity placed at the center of the well, and (b) and (c) for cases when the distances between D^0 impurity and the center of the well are $0.5a_B^*$ and $1.0a_B^*$, respectively ($a_B^* = 98$ Å). The plotted binding energies were obtained with formula (13) for $n = 3$. The D^0-center ground-state binding energy as a function of magnetic field for bulk GaAs is also plotted in Fig. 1. As expected, the binding energy for the D^0 center in the well is higher than in the bulk material. This increment for a donor impurity placed in the center of the well is of the order of 30% in the absence of a magnetic field and about 15% for $\gamma = 5$. We can see also that for all donor centers placed in the central region of the well (of size 100 Å) the binding energy has very similar values (for fixed γ)— the difference is less than 3% and decreases when γ increases.

Similar curves for an $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ parabolic quantum well defined by $\eta = 1.0$ are plotted in Fig. 2. As the size of this well is twice reduced in comparison to the previous one, we have investigated donor centers placed in a central region reduced in the same proportion. In this

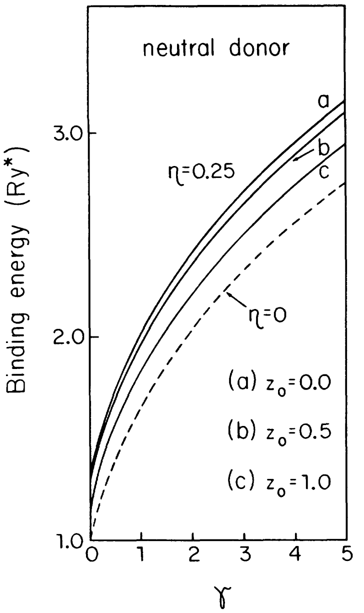

FIG. 1. Binding energy of the D^0-center ground state for an $Al_xGa_{1-x}As$ parabolic quantum well defined by $\eta=0.25$ as a function of magnetic field and for three values of the distance between the impurity and the center of the well: $z_0=0.0a_B^*$, $0.5a_B^*$, and $1.0a_B^*$. The dashed curve corresponds to results for bulk GaAs.

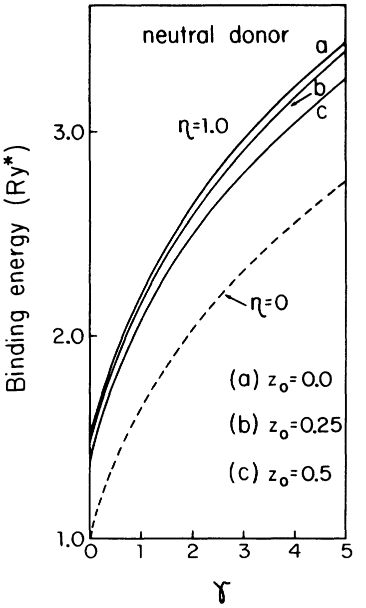

FIG. 2. Binding energy of the D^0-center ground state for an $Al_xGa_{1-x}As$ parabolic quantum well defined by $\eta=1.0$ as a function of magnetic field and for three values of the distance between the impurity and the center of the well: $z_0=0.0a_B^*$, $0.25a_B^*$, and $0.5a_B^*$. The dashed curve corresponds to results for bulk GaAs.

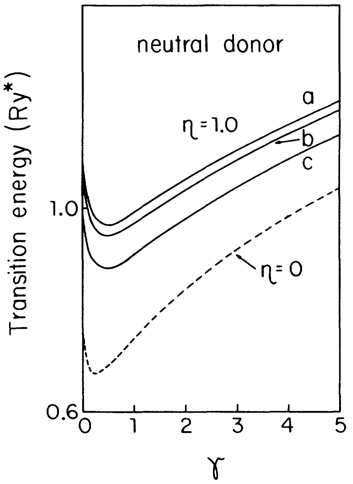

FIG. 3. Transition energy from 1s to 2p(-1) states of the D^0 center in an $Al_xGa_{1-x}As$ parabolic quantum well defined by $\eta=1.0$ as a function of magnetic field and for three values of the distance between the impurity and the center of the well: (a) $z_0=0.0a_B^*$, (b) $z_0=0.25a_B^*$, and (c) $z_0=0.5a_B^*$. The transition energy for bulk GaAs is also plotted (dashed curve).

case the increment of the ground-state binding energy for an impurity placed in the center of the well with respect to the bulk is about 50% in the absence of an external magnetic field and 20% for $\gamma=5$. When the distance between the impurity and the center of the well increases its ground-state binding energy decreases, but for impurities placed in a central region of the same size as in the previous case (equal to 100 Å) this difference is less than 7.5% for $\gamma=0$ and decreases as γ increases.

In Table II we have listed the transition energies from the ground 1s state to the lowest p-like excited state 2p(-1) for the D^0 center in the two $Al_xGa_{1-x}As$ parabolic quantum wells as a function of magnetic field and the distance between the impurity and the center of the well. These transition energies were obtained with formula (19) for $n=3$. For better illustration we have plotted some of the results reported in Table II (those corresponding to the well defined by $\eta=1.0$) in Fig. 3. In this figure the transition energy for bulk GaAs is also given. We can see that all the curves have a similar shape but the decrease of the transition energy for $\gamma<0.5$ is more pronounced in the case of the quantum well than in the case of the bulk material.[33] The increment of the 1s-2p(-1) transition energy for a D^0 impurity placed in the center of the well with respect to the bulk in the absence of a magnetic field is of the order of 50% for the

TABLE II. Transition energies (in effective Rydbergs Ry*) from 1s to 2p(-1) states of D^0 centers in $Al_xGa_{1-x}As$ parabolic quantum wells defined by $\eta=0.25$ and 1.0 as a function of magnetic field and the distance between the impurity and the center of the well (denoted by z_0 in units of a_B^*) calculated with formula (19) for $n=3$.

Field	$\Delta E^{(3)}_{D^0_w}$ ($\eta=0.25$)			$\Delta E^{(3)}_{D^0_w}$ ($\eta=1.0$)		
	z_0			z_0		
γ	0.0	0.5	1.0	0.0	0.25	0.5
0	0.951	0.921	0.830	1.098	1.072	1.003
1	0.866	0.844	0.777	0.991	0.970	0.909
2	0.939	0.921	0.865	1.057	1.037	0.979
3	1.002	0.988	0.940	1.116	1.097	1.042
4	1.057	1.045	1.003	1.167	1.149	1.097
5	1.105	1.096	1.057	1.212	1.196	1.145

well with $\eta=1.0$ and 30% for the other well, and at high magnetic fields ($\gamma=5$) drops to about 17% and 7%, respectively. As for the binding energy, the $1s$-$2p(-1)$ transition energy decreases when the impurity is shifted off the center of the well, but the decrease is rather slow. In the central region of the well, extending over 100 Å, the dispersion of the transition energies does not exceed 3% for the first and 9% for the second well, whatever the magnetic field. As a consequence, the donor centers from a relatively broad region of the well can contribute with very similar energies to the optical transitions from $1s$ to $2p(-1)$ states, making them observable in the absorption spectra. We have checked also that the oscillator strengths for dipole optical transitions from $1s$ to $2p(-1)$ states in the case of D^0 centers placed in the central region of the parabolic quantum well and for the photon polarization direction parallel to the xy plane, have for a given γ very similar values to that for the D^0 center in the bulk material.

IV. SINGLET GROUND STATE OF THE D^- ION IN A BULK MATERIAL

When the D^- ion in a magnetic field parallel to the z axis is in its singlet ground state, the dimensionless Hamiltonian in the effective-mass approximation has the form

$$\mathcal{H}=H(1)+H(2)+2/|\mathbf{r}_1-\mathbf{r}_2| , \tag{22}$$

where

$$H(i)=-\nabla_i^2-\frac{2}{r_i}+\tfrac{1}{4}\gamma^2\rho_i^2, \quad i=1,2 , \tag{23}$$

and $\mathbf{r}_1,\mathbf{r}_2$ give the positions of both electrons relative to the nucleus. The binding energy of the D^--ion singlet ground state is defined as

$$E_B(\gamma)=E_{D^0}(\gamma)+\gamma-E_{D^-}(\gamma) , \tag{24}$$

where $E_{D^0}(\gamma)$ denotes the ground-state energy of a neutral donor and $E_{D^-}(\gamma)$ is the ground-state energy of the D^- ion. In this definition of the binding energy, we assumed the same spin state for the initial and final states.

We propose the following Chandrasekhar-type[34] variational wave functions, adapted to the presence of a magnetic field, for the singlet ground state of the D^- ion:

$$\Psi_s^{(n)}(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\sqrt{2}}[\psi_s^{(n)}(\mathbf{r}_1)\psi_s'^{(n)}(\mathbf{r}_2)+\psi_s'^{(n)}(\mathbf{r}_1)\psi_s^{(n)}(\mathbf{r}_2)](1+B|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|^2+C|z_1-z_2|^2) , \tag{25}$$

where $\psi_s^{(n)}(\mathbf{r}_i)$ and $\psi_s'^{(n)}(\mathbf{r}_i)(i=1,2)$ are defined by the same equation (1) but with different sets of parameters. This means that the electrons are in the ground-state hydrogenlike atomic orbitals in the presence of a magnetic field. The repulsive interaction between the two electrons is accounted for by the correlation factor

$$(1+B|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|^2+C|z_1-z_2|^2) . \tag{26}$$

In evaluating the binding energy of the D^- ion, following Natori and Kamimura[7] we calculated both energies $E_{D^0}(\gamma)$ and $E_{D^-}(\gamma)$ within the same approximation. This means that we approximate the binding energy defined in Eq. (24) by the quantity:

$$E_B^{(n)}(\gamma)=E_{D^0}^{(n)}(\gamma)+\gamma-E_{D^-}^{(n)}(\gamma) , \tag{27}$$

where $E_{D^0}^{(n)}(\gamma)$ is the minimum expectation value of the Hamiltonian (2) obtained for the trial wave function (1) and $E_{D^-}^{(n)}(\gamma)$ is the minimum expectation value of the Hamiltonian (22) for the trial wave function (25).

In the case of the Hamiltonian (22), the expression for the variational energy $\langle\Psi_s^{(n)}|\mathcal{H}|\Psi_s^{(n)}\rangle/\langle\Psi_s^{(n)}|\Psi_s^{(n)}\rangle$ is still analytical as in the case of the Hamiltonian (2) though more complicated. Let us define first the following functions

$$K(x,y;i,j,k,l)=G(x,y)\left[1+2i\frac{B}{x}+k\frac{C}{y}+2j\left[\frac{B}{x}\right]^2+\frac{3}{4}l\left[\frac{C}{y}\right]^2+ik\frac{BC}{xy}\right] , \tag{28}$$

$$L(x,y;i,j)=G(x,y)\left[1+i\frac{B}{x}+\tfrac{1}{2}j\frac{C}{y}\right] , \tag{29}$$

$$M(x,y)=\left[1-2B\frac{\partial}{\partial x}-2C\frac{\partial}{\partial y}+2BC\frac{\partial^2}{\partial x\,\partial y}+B^2\frac{\partial^2}{\partial x^2}+C^2\frac{\partial^2}{\partial y^2}\right]f(x,y) , \tag{30}$$

$$\begin{aligned}N(x,y;v,z;i,j)={}&-f(x,y)K(v,z;i,j,1,1)\\&+G(v,z)\left\{-M(x,y)+f(x,y)+B\left[\frac{4iB}{v}+\frac{C}{z}\right]\frac{\partial f(x,y)}{\partial x}+C\left[\frac{2iB}{v}+\frac{3C}{z}\right]\frac{\partial f(x,y)}{\partial y}\right\} ,\end{aligned} \tag{31}$$

whereas $G(x,y)$ and $f(x,y)$ are defined by Eqs. (7) and (9), respectively. We introduce still further abbreviations

$$S(a_1,a_2;b_1,b_2;\mu)=\frac{1}{\tilde{a}}G(\tilde{a},\tilde{b})[\mu K(\bar{a},\bar{b};2,3,1,1)+K(\bar{a},\bar{b};1,1,1,1)] , \tag{32}$$

$$T(a_1,a_2;b_1b_2;\mu)=\frac{1}{\tilde{b}}G(\tilde{a},\tilde{b})[\mu K(\bar{a},\bar{b};1,1,3,5)+K(\bar{a},\bar{b};1,1,1,1)]\ , \tag{33}$$

where

$$\begin{aligned} \tilde{a}&=a_1+a_2, \quad \bar{a}=\frac{a_1a_2}{a_1+a_2}\ ,\\ \tilde{b}&=b_1+b_2, \quad \bar{b}=\frac{b_1b_2}{b_1+b_2}\ . \end{aligned} \tag{34}$$

Using the above abbreviations we define the following two functions,

$$\begin{aligned} I(a_1,a_2,b_1,b_2;\nu,\vartheta)=&\,2N(a_1,b_1;a_2,b_2;1,1)+\left[\frac{\gamma^2}{4}+4\nu\right]S(a_1,a_2;b_1,b_2;a_2/a_1)\\ &+2\vartheta T(a_1,a_2;b_1,b_2;b_2/b_1)+G(\tilde{a},\tilde{b})[M(\bar{a},\bar{b})-2(2B+C)L(\bar{a},\bar{b};1,1)] \end{aligned}$$

and

$$I_1(a_1,a_2,b_1,b_2)=G(\tilde{a},\tilde{b})K(\bar{a},\bar{b};1,1,1,1)\ .$$

Finally we have

$$\begin{aligned} \langle\Psi_s^{(n)}|\mathcal{H}|\Psi_s^{(n)}\rangle=\sum_{i,k=1}^{n}\ \sum_{j,l=n+1}^{2n} A_iA_jA_kA_l[&I(\alpha_{ik},\alpha_{jl},\beta_{ik},\beta_{jl};\alpha_i\alpha_k,\beta_i\beta_k)+I(\alpha_{jl},\alpha_{ik},\beta_{jl},\beta_{ik};\alpha_j\alpha_l,\beta_j\beta_l)\\ &+I(\alpha_{il},\alpha_{jk},\beta_{il},\beta_{jk};\alpha_i\alpha_l,\beta_i\beta_l)+I(\alpha_{jk},\alpha_{il},\beta_{jk},\beta_{il};\alpha_j\alpha_k,\beta_j\beta_k)] \end{aligned}$$

and

$$\langle\Psi_s^{(n)}|\Psi_s^{(n)}\rangle=\sum_{i,k=1}^{n}\ \sum_{j,l=n+1}^{2n} A_iA_jA_kA_l[I_1(\alpha_{ik},\alpha_{jl},\beta_{ik},\beta_{jl})+I_1(\alpha_{il},\alpha_{jk},\beta_{il},\beta_{jk})]\ , \tag{35}$$

where α_{ik} and β_{ik} for $i,k=1,\ldots,2n$ are defined by (6). Here α_i,β_i,A_i, for $i=1,\ldots,n$ represent the variational parameters of the one-electron wave function describing the inner orbital and for $i=n+1,\ldots,2n$ the variational parameters for the outer orbital.

The final numerical results are presented in Table III. We can see from Table III that the values of $E_B^{(n)}(\gamma)$ for $n=1,2,3$ are rather close to one another. When the number n of Gaussians in the one-electron wave function increases both $E_{D^0}^{(n)}(\gamma)$ and $E_{D^-}^{(n)}(\gamma)$ decrease by almost the same amount, so that the difference $E_{D^0}^{(n)}(\gamma)-E_{D^-}^{(n)}(\gamma)$ and as a consequence $E_B^{(n)}(\gamma)$ change very little with n. Physically, this means that the second electron, with its slowly varying wave function formed to a large extent by the magnetic field, is not affected by the fine details of the charge distribution of the first electron. Both kinetic and potential energies of the second electron are secondary factors in the energy balance of the D^- system. It is the kinetic energy of the inner, more localized electron and its potential energy which do depend on the details of the wave function of this electron and contribute decisively to the total energy of the D^- system. When the same type of trial function is used for this electron both in D^0 and D^- centers, the systematic errors resulting from the finite flexibility of the trial functions cancel to a large extent. In conclusion, the improvement on the one-electron wave function of type (1) does not change significantly the D^--ion ground-state binding energy calculated with Eq. (27). This binding energy is determined mainly by the form of the correlation factor.

TABLE III. Comparison of D^- singlet ground-state binding energies (in units of the effective Rydberg Ry*) calculated with the variational wave functions $\Psi_s^{(n)}$ given by Eq. (25) ($n=1,2,3$) with $E_B^{(L)}$ as reported in Ref. 10.

Field	D^- singlet ground-state binding energies for various wave functions in bulk GaAs			
γ	$E_B^{(1)}$	$E_B^{(2)}$	$E_B^{(3)}$	$E_B^{(L)}$
1	0.327	0.328	0.325	0.339
2	0.414	0.418	0.417	0.435
3	0.475	0.480	0.479	0.498
4	0.522	0.529	0.527	0.549
5	0.562	0.569	0.568	0.591
10	0.707	0.714	0.712	0.742

In the last column of Table III we list the best values of D^- singlet ground-state binding energies reported by Larsen and McCann.[10] We can see that their results are about 4% better than ours. These results were obtained with the help of one-electron wave functions of the form

$$f_I(\mathbf{r})=\exp(-H_I\rho^2-\kappa_Ir-\beta_Ir^2-G_Ir\rho^2)$$

and

$$f_0(\mathbf{r})=\exp[-H_0\rho^2-\kappa_0(\rho^2+\alpha_0z^2)^{1/2}]\ ,$$

and with the correlation factor given by

$$\{1+C[|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|^2+\alpha_C|z_1-z_2|^2]^{1/2}\}\ . \tag{36}$$

$H_I, H_0, \kappa_I, \ldots, \alpha_C$ are variational parameters. The investigation of different trial wave functions for the singlet ground state of the D^- ion made in Ref. 10 has shown that a correlation factor of the form (36) represents the best choice. Our results confirm that the binding energy of the D^- ion is determined mainly by the form of the correlation factor. Nevertheless, even though the correlation factor (26) gives results somewhat lower than necessary, it offers analytical expressions for the expectation values of the energy, while a correlation factor of the form (36) leads to manifold numerical integrations.

Summarizing, we propose a relatively simple class of trial wave functions suitable for the singlet ground state of negatively charged hydrogenlike ions D^- in moderate and strong magnetic fields. The essential advantage of these functions is the analytic form of all one- and two-particle integrals. The minimum value of the ground-state energy depends on the choice of the one-electron functions. The binding energy is less sensitive to this choice but depends crucially on the form of the electron-electron correlation factor. The class of trial wave functions discussed in this paper can be easily generalized for calculations of excited-state energies and optical matrix elements.

V. D^- STATES IN A PARABOLIC QUANTUM WELL

Let us consider a D^- ion placed in the central region of the parabolic $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ quantum well described already in Sec. III, and in the presence of a magnetic field parallel to the z axis. The dimensionless Hamiltonian in the effective-mass approximation has the form

$$\mathcal{H}_w=H_w(1)+H_w(2)+2/|\mathbf{r}_1-\mathbf{r}_2|+\gamma M_L\ , \tag{37}$$

where

$$H_w(i)=H(i)+\eta(z_i-z_o)^2,\quad i=1,2\ , \tag{38}$$

and $\mathbf{r}_1, \mathbf{r}_2$ give the positions of both electrons relative to the nucleus. M_L represents the component of the total orbital angular momentum along the z axis, and its eigenvalue is zero for the singlet ground state of the D^- ion. $H(i)$ for $i=1,2$ are given by the formula (23). We propose the following variational wave functions for the singlet ground state of the D^- ion:

$$\Psi_{sw}^{(n)}(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\sqrt{2}}[\psi_{sw}^{(n)}(\mathbf{r}_1)\psi_{sw}'^{(n)}(\mathbf{r}_2)+\psi_{sw}'^{(n)}(\mathbf{r}_1)\psi_{sw}^{(n)}(\mathbf{r}_2)]$$

$$\times(1+B|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|^2+C|z_1-z_2|^2)\ , \tag{39}$$

where the $\psi_{sw}^{(n)}(\mathbf{r}_i)$, for $i=1,2$, are defined by (12) and the functions $\psi_{sw}'^{(n)}(\mathbf{r}_i)$ are obtained as in the case of the D^- ion in the bulk material.

Similarly to the case of the D^- ion in the bulk material we shall define the binding energy of the D^--ion singlet ground state in a parabolic quantum well as

$$E_{Bw}^{(n)}(\gamma)=E_{D^0w}^{(n)}(\gamma)+\gamma+\eta^{1/2}-E_{D^-w}^{(n)}(\gamma)\ , \tag{40}$$

where $E_{D^0w}^{(n)}(\gamma)$ is the minimum expectation value of the Hamiltonian (10) obtained for the trial wave function (12), and $E_{D^-w}^{(n)}(\gamma)$ is the minimum expectation value of the Hamiltonian (37) for the trial wave function (39). (This means that both minimum expectation values are calculated in the same approximation.)

The expression for the variational energy $\langle\Psi_{sw}^{(n)}|\mathcal{H}_w|\Psi_{sw}^{(n)}\rangle/\langle\Psi_{sw}^{(n)}|\Psi_{sw}^{(n)}\rangle$ is analytical for any position of the D^- ion in the parabolic quantum well but it is somewhat long for ions placed at some distance from the center of the well. For D^- ions placed in the center of the well, $\langle\Psi_{sw}^{(n)}|\Psi_{sw}^{(n)}\rangle$ is still given by the formula (35) and

$$\langle\Psi_{sw}^{(n)}|\mathcal{H}_w|\Psi_{sw}^{(n)}\rangle=\langle\Psi_s^{(n)}|\mathcal{H}|\Psi_s^{(n)}\rangle+\eta\sum_{i,k=1}^{n}\ \sum_{j,l=n+1}^{2n}A_iA_jA_kA_l[T(\alpha_{ik},\alpha_{jl};\beta_{ik},\beta_{jl};\beta_{jl}^{ik})+T(\alpha_{il},\alpha_{jk};\beta_{il},\beta_{jk};\beta_{jk}^{il})]\ ,$$

where

$$\beta_{jl}^{ik}=\frac{1}{2}\left[\frac{\beta_{ik}}{\beta_{jl}}+\frac{\beta_{jl}}{\beta_{ik}}\right],\quad \beta_{jk}^{il}=\frac{1}{2}\left[\frac{\beta_{il}}{\beta_{jk}}+\frac{\beta_{jk}}{\beta_{il}}\right]\ .$$

Here, as in the case of the D^- ion in bulk material, α_{ik} and β_{ik} for $i,k=1,\ldots,2n$ are defined by (6), and A_i for $i=1,\ldots,n$ represent the variational parameters of the one-electron wave function describing the inner orbital and for $i=n+1,\ldots,2n$ the variational parameters for the outer orbital. The function $T(x,y;v,z;\mu)$ is defined by the formula (33).

Let us consider now the lowest-lying singlet p-like excited state of the D^- ion in the presence of a magnetic field, which is unbound. For this state the eigenvalue of the total orbital angular momentum along the z axis, M_L, is equal to -1. We propose the following variational wave function

$$\Psi_{pw}^{(n)}(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\sqrt{2}}[\psi_{sw}^{(n)}(\mathbf{r}_1)\psi_{pw}^{(n)}(\mathbf{r}_2)+\psi_{pw}^{(n)}(\mathbf{r}_1)\psi_{sw}^{(n)}(\mathbf{r}_2)]$$

$$\times(1+B|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|^2+C|z_1-z_2|^2)\ , \tag{41}$$

where $\psi_{sw}^{(n)}(\mathbf{r}_i)$ and $\psi_{pw}^{(n)}(\mathbf{r}_i)$ for $i=1,2$ are defined by (12) and (18), respectively. The transition energy from the singlet ground state to the singlet p-like excited state described by the variational wave function (41) is given by

$$\Delta E_{D^-w}^{(n)}=\min\frac{\langle\Psi_{pw}^{(n)}|\mathcal{H}_w|\Psi_{pw}^{(n)}\rangle}{\langle\Psi_{pw}^{(n)}|\Psi_{pw}^{(n)}\rangle}-\min\frac{\langle\Psi_{sw}^{(n)}|\mathcal{H}_w|\Psi_{sw}^{(n)}\rangle}{\langle\Psi_{sw}^{(n)}|\Psi_{sw}^{(n)}\rangle}\ , \tag{42}$$

where the expressions of the new quantities for the D^- ion placed in the center of the well are given in the Appendix.

The final numerical results are presented in Fig. 4 and

TABLE IV. Transition energies (in effective Rydbergs Ry*) from the singlet ground state to the lowest p-like singlet excited state of the D^- ion in $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ parabolic quantum wells defined by $\eta=0.25$ and 1.0 as a function of magnetic field and the distance between the ion and the center of the well (denoted by z_0 in units of a_B^*) calculated with formula (42) for $n=1$.

	$\Delta E^{(1)}_{D^-w}$ ($\eta=0.25$)			$\Delta E^{(1)}_{D^-w}$ ($\eta=1.0$)		
Field		z_0			z_0	
γ	0.0	0.5	1.0	0.0	0.25	0.5
1	0.591	0.568	0.513	0.672	0.658	0.617
2	0.712	0.687	0.645	0.823	0.806	0.760
3	0.783	0.758	0.687	0.906	0.890	0.840
4	0.837	0.813	0.734	0.966	0.949	0.898
5	0.882	0.857	0.776	1.014	0.997	0.946

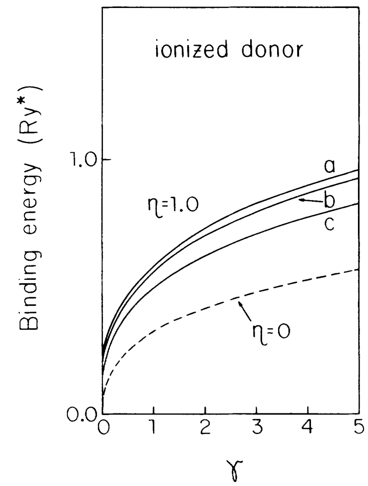

FIG. 4. Binding energy of the D^--ion singlet ground state for an $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ parabolic quantum well defined by $\eta=1.0$ as a function of magnetic field and for three values of the distance between the ion and the center of the well: (a) $z_0=0.0a_B^*$, (b) $z_0=0.25a_B^*$, and (c) $z_0=0.5a_B^*$. The dashed curve corresponds to results for bulk GaAs.

Table IV. In Fig. 4 we plotted the binding energies for the singlet ground state of the D^- ion in the parabolic $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ quantum well defined by the parameter $\eta=1.0$ as a function of magnetic field, for three different positions of the ion with respect to the center of the well: (a) for the D^- ion placed at the center of the well, and (b) and (c) for the cases when the distances between the D^- ion and the center of the well are $0.25a_B^*$ and $0.5a_B^*$, respectively. These results were obtained with formula (40) for $n=1$ (we have shown already for bulk GaAs that the binding energy is not sensitive to the number of Gaussians in the one-electron function). The singlet ground-state binding energy as a function of magnetic field for bulk GaAs is also plotted. The binding energy for the D^- ion placed in the center of this well and in the absence of a magnetic field is equal to 0.181 Ry*, while for bulk GaAs its value is 0.0555 Ry*.[35] For $\gamma=5$ the value of the binding energy for the same position of the ion in the well is 0.959 Ry* and for bulk GaAs 0.569 Ry* (we compare quantities obtained within the same approximation). We can see that for $\gamma=5$ an increment of nearly 70% for the binding energy is expected in the case of the ion in the well. When the distance between the ion and the center of the well increases, the binding energy decreases but in the central region of size 100 Å the binding energy has quite similar values for all the γ under consideration.

In Table IV we have listed the transition energies from the singlet ground state to the lowest p-like singlet excited state for the D^- ion in the two $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ parabolic quantum wells defined by $\eta=0.25$ and $\eta=1.0$. These results were obtained with formula (42) for $n=1$. As expected, the transition energy decreases when the distance between the ion and the center of the well increases but in the central region of any well the changes are small. For the well defined by $\eta=0.25$ the transition energy decreases less than 4% for ions in the central region of size 100 Å, and for the other well less than 8% in the same region, for all γ under consideration. The difference between the transition energy and the binding energy for a D^- ion placed in the center of the well defined by $\eta=0.25$ changes from 12% for $\gamma=1$ to 4% for $\gamma=5$. For the other well ($\eta=1.0$) this difference changes from 15% for $\gamma=1$ to 6% for $\gamma=5$.

In conclusion, one can expect that the intradonor absorption for D^0 as well as for D^- centers should show up in optical magnetoabsorption experiments on doped parabolic $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ wells.

APPENDIX

In the following, the explicit form of the D^--ion energy expectation value $\langle\Psi^{(n)}_{pw}|\mathcal{H}_w|\Psi^{(n)}_{pw}\rangle/\langle\Psi^{(n)}_{pw}|\Psi^{(n)}_{pw}\rangle$ for the singlet p-like state for the ion placed in the center of a parabolic quantum well is given. Let us define the following functions first

$$\tilde{S}(a_1,a_2;b_1,b_2;\mu)=\frac{\mu}{\tilde{a}}G(\tilde{a},\tilde{b})\left[\frac{a_2}{a_1}K(\bar{a},\bar{b};3,6,1,1)+K(\bar{a},\bar{b};2,3,1,1)\right]+S(a_1,a_2;b_1,b_2;a_2/a_1)\ ,$$

$$\tilde{T}(a_1,a_2;b_1,b_2;\mu)=\frac{\mu}{\tilde{b}}G(\tilde{a},\tilde{b})\left[\frac{b_2}{b_1}K(\bar{a},\bar{b};2,3,3,5)+K(\bar{a},\bar{b};2,3,1,1)\right]+T(a_1,a_2;b_1,b_2;b_2/b_1)\ ,$$

$$W(x,y;v,z)=\frac{1}{v}G(v,z)\left[-B\left[\frac{4B}{v}+\frac{C}{z}+2\right]\frac{\partial}{\partial x}+2B^2\frac{\partial^2}{\partial x^2}+2BC\frac{\partial^2}{\partial x\,\partial y}\right]f(x,y)\ ,$$

where B and C are variational parameters defined in Eq. (26), the functions $G(x,y)$, $f(x,y)$, $K(x,y;i,j,k,l)$, $S(x,y;v,z;\mu)$, and $T(x,y;v,z;\mu)$ are defined by Eqs. (7), (9), (28), (32), and (33), respectively, and $\tilde{a},\bar{a},\tilde{b},\bar{b}$, by (34). With the help of the above functions we shall define the following ones:

$$
\begin{aligned}
I_{p1}(a_1,a_2,b_1,b_2;\nu_1,\nu_2,\vartheta_1,\vartheta_2) = {} & \frac{1}{a_2}N(a_1,b_1;a_2,b_2;2,3) - \frac{\partial}{\partial a_2}N(a_2,b_2;a_1,b_1;1,1) \\
& + \frac{1}{\tilde{a}}G(\tilde{a},\tilde{b})\left(-\frac{a_1}{a_2}\bar{a}\frac{\partial}{\partial \bar{a}}+1\right)M(\bar{a},\bar{b}) \\
& + \frac{1}{\tilde{a}}\left[\left(\frac{\gamma^2}{4}+4\nu_1\right)\tilde{S}(a_1,a_2;b_1,b_2;a_1/a_2) + \left(\frac{\gamma^2}{4}+4\nu_2\right)\tilde{S}(a_2,a_1;b_1,b_2;a_1/a_2)\right. \\
& - a_2 S(a_1,a_2;b_1,b_2;a_1/a_2) + \tilde{a}S(a_1,a_2;b_1,b_2;-2\nu_1/\tilde{a}\bar{a}) \\
& + \frac{1}{\tilde{a}}\left[\left(\vartheta_1+\frac{\eta}{4}\right)\tilde{T}(a_1,a_2;b_1,b_2;a_1/a_2) + \left(\vartheta_2+\frac{\eta}{4}\right)\tilde{T}(a_1,a_2;b_2,b_1;a_1/a_2)\right] \\
& \left. - \frac{1}{\tilde{a}}G(\tilde{a},\tilde{b})\left[\frac{\gamma^2}{8\bar{a}}K(\bar{a},\bar{b};2,3,1,1) + 2(2B+C)\left(\frac{a_1}{a_2}L(\bar{a},\bar{b};2,1) + L(\bar{a},\bar{b};1,1)\right)\right]\right] ,
\end{aligned}
$$

$$
\begin{aligned}
I_{p2}(a_1,a_2,b_1,b_2;\nu_1,\nu_2,\vartheta_1,\vartheta_2;\zeta) = {} & W(a_1,b_1;a_2,b_2) + W(a_2,b_2;a_1,b_1) \\
& + \frac{1}{\tilde{a}}G(\tilde{a},\tilde{b})\left[\left(\bar{a}\frac{\partial}{\partial \bar{a}}+1\right)M(\bar{a},\bar{b}) + B(2B+C)\frac{2}{\bar{a}}G(\bar{a},\bar{b})\right] - \zeta S(a_1,a_2;b_1,b_2;-1) \\
& + \frac{1}{\tilde{a}}\left[\left(\frac{\gamma^2}{4}+4\nu_1\right)\tilde{S}(a_1,a_2;b_1,b_2;-1) + \left(\frac{\gamma^2}{4}+4\nu_2\right)\tilde{S}(a_2,a_1;b_1,b_2;-1)\right] \\
& + \frac{1}{\tilde{a}}\left[\left(\vartheta_1+\frac{\eta}{4}\right)\tilde{T}(a_1,a_2;b_1,b_2;-1) + \left(\vartheta_2+\frac{\eta}{4}\right)\tilde{T}(a_1,a_2;b_2,b_1;-1)\right] ,
\end{aligned}
$$

$$
I_{p3}(a_1,a_2,b_1,b_2) = \tfrac{1}{2}S(a_1,a_2;b_1,b_2;a_1/a_2) ,
$$

$$
I_{p4}(a_1,a_2,b_1,b_2) = \tfrac{1}{2}S(a_1,a_2;b_1,b_2;-1) .
$$

In the above expressions the functions $K(x,y;i,j,k,l),L(x,y;i,j)$, $M(x,y)$, and $N(x,y;v,z;i,j)$ are defined by Eqs. (28), (29), (30), and (31), respectively. B and C are variational parameters defined in Eq. (26). Finally we have

$$
\begin{aligned}
\langle \Psi_{pw}^{(n)}|\mathcal{H}_w|\Psi_{pw}^{(n)}\rangle = \sum_{i,k=1}^{n}\sum_{j,l=n+1}^{2n} & A_i A_j A_k A_l [I_{p1}(\alpha_{ik},\alpha_{jl},\beta_{ik},\beta_{jl};\alpha_i\alpha_k,\alpha_j\alpha_l,\beta_i\beta_k,\beta_j\beta_l) \\
& + I_{p2}(\alpha_{il},\alpha_{jk},\beta_{il},\beta_{jk};\alpha_i\alpha_l,\alpha_j\alpha_k,\beta_i\beta_l,\beta_j\beta_k;\alpha_{ik})] - \gamma\langle \Psi_{pw}^{(n)}|\Psi_{pw}^{(n)}\rangle
\end{aligned}
$$

and

$$
\langle \Psi_{pw}^{(n)}|\Psi_{pw}^{(n)}\rangle = \sum_{i,k=1}^{n}\sum_{j,l=n+1}^{2n} A_i A_j A_k A_l [I_{p3}(\alpha_{ik},\alpha_{jl},\beta_{ik},\beta_{jl}) + I_{p4}(\alpha_{il},\alpha_{jk},\beta_{il},\beta_{jk})] ,
$$

where α_{ik} and β_{ik} for $i,k=1,\ldots,2n$ are defined by (6). Here, α_i,β_i, A_i, for $i=1,\ldots,n$ represent the variational parameters of the one-electron wave function describing the inner orbital and for $i=n+1,\ldots,2n$ the variational parameters for the outer orbital.

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[*] Permanent address: Institute of Theoretical Physics, Warsaw University, ul. Hoza 69, 00-681 Warsaw, Poland.

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