Simple trial function for shallow donor D^0 states in GaAs-$Ga_{1-x}Al_xAs$ quantum-well structures

F. J. Betancur and I. D. Mikhailov
Department of Physics, Industrial University of Santander, Box Aerial 678 Bucaramanga, Colombia
(Received 4 August 1994)

A three-nonlinear-parameters trial variational function is proposed for the ground and first excited states of a hydrogenic donor at the center and off center in the GaAs quantum well in a magnetic field. Binding energies are in very good agreement with recent effective-mass calculations for the intermediate-width well and there are more accurate results in narrow wells approximating asymptotically to exact ones ($L \to 0$). Results are improved for ground and low-lying excited states, with or without an applied magnetic field in all cases, as the barrier well approaches the impurity center.

I. INTRODUCTION

Many effects such as quantum Hall effects, metal-insulator transitions, and electron localizations, are intimately related to phenomena of high magnetic fields and impurity states.[1] The theoretical study of the behavior of a hydrogenic impurity located in a quantum well has been a subject of considerable interest in recent years.[1,2]

Using the Bastard quantum-well model, it was demonstrated in both theory[3-14] and experiment[15-17] that the energy spectrum of a shallow impurity in multiple-quantum-well heterostructures depends strongly on the geometry of the structure, the position of the impurity ion, the number of wells, and the presence of a magnetic field. The model was applied to a neutral shallow donor (D^0) at the center and off center in a quantum-well semiconductor of GaAs, surrounded by layers of $Ga_{1-x}Al_xAs$, to calculate the binding energy for the ground state ($1s$-like) and low-lying excited states ($2p_{\pm}$-like) for a hydrogenic donor associated with the first subband level.

Most of the investigations have used linear combinations of Gaussian-type[5-12] or exponential[3,4,13,14] trial functions in the variational method. A study using the free-hydrogenic-atom Huzinaga[18] trial function obtained results in good agreement with simulations by the diffusion quantum Monte Carlo method[10] for intermediate and large well width (L). The Huzinaga trial function is the best in all cases, except when the barrier edge is approximated to the impurity atom sufficiently to destroy the system spheric symmetry. Otherwise the exponential trial function, perhaps, is better.

Any trial function has to take into account the symmetry aspect. The model of the hydrogenic impurity in a quantum-well structure has cylindrical symmetry, but it transforms in the central symmetry (two-dimensional hydrogenic-atom model) for narrow wells ($L \to 0$). One exact solution for this case is given by an exponential[19] function. On the other hand, for large well widths ($L \to \infty$) spherical symmetry appears, and the Huzinaga Gaussian wave function[18] becomes suitable when the impurity is located at the quantum-well center, but when it is located at the edge, the symmetry is not spherical and this function is not the best.

Taking into account the symmetry aspect, we expect improvement in the results using only three nonlinear variation parameters. Previous papers[8-11] based on Huzinaga's representation[18] have taken 13 or more linear combinations of Gaussian functions to obtain results for the binding energy that are close to experimental values. But there are cases where increasing the number of the linear variational parameters does not improve the results. For example, if the potential barrier crosses the Coulomb potential curve near the impurity center point, the wave function is strongly confined. For this case, the set Huzinaga free-hydrogenic-atom base functions become quasidependent and the minimizing processes become unstable. This situation has been observed in previous works[8-11] for narrow wells ($L \to 0$).

Some authors have used only one[5-11,13-16] or two[12] nonlinear parameters. The object of this paper is to show that results considerably improve by including only a few nonlinear variational parameters and are not improved by increasing the number of linear parameters as the impurity approaches the edge. In addition, the nonlinear parameters allow us to construct one trial function that is flexible enough to change between cylindrical and spherical symmetries. We propose a simple trial wave function with three nonlinear variational parameters to improve the stability of the calculation for narrow wells, near the edge impurity position and low-lying excited states. Our trial wave function is sufficiently flexible to change from a Gaussian-type ($L \to \infty$) to an exponential function ($L \to 0$). Results on binding energies for the ground state ($1s$-like) and low-lying excited states ($2p_{\pm}$-like) of a hydrogenic donor associated with the first subband level, as a function of quantum-well width and the impurity position, are reported. We have considered the cases as an impurity atom is located at the center and at the edge of a GaAs well with a magnetic field applied to the axis of growth of the quantum-well structure.

II. METHOD OF CALCULATION

Within the framework of an effective-mass approximation, the dimensionless Hamiltonian in cylindrical coordinates for a donor impurity located at $z = Z_i$ in a quantum

0163-1829/95/51(8)/4982(5)/$06.00

GaAs well surrounded by two semi-infinite layers of $Ga_{1-x}Al_xAs$, can be written as

$$\hat{H}=\hat{H}_1(\rho,\varphi)+\hat{H}_2(z)+\hat{H}_3(\rho,z) , \tag{1}$$

where

$$\hat{H}_1(\rho,\varphi)=-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\tfrac{1}{4}\gamma^2\rho^2-\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}-i\gamma\frac{\partial}{\partial\varphi} ,$$

$$\hat{H}_2(\rho)=-\frac{\partial^2}{\partial z^2}+V_B(z) ,$$

$$\hat{H}_3(\rho,z)=-\frac{2}{\sqrt{\rho^2+(z-Z_i)^2}} .$$

The effective Bohr radius in GaAs, $a_0^*=(\hbar^2\epsilon/m^*e^2)$, is used as the unit length and the effective Rydberg, $\mathrm{Ry}^*=(e^2/2\epsilon a_0^*)$, is the unit of energy. m^* and ϵ are the effective mass of the electron and the static dielectric constant, respectively. Z_i is the z coordinate of the impurity atom. γ is a dimensionless measure of the magnetic field, defined as $\gamma=(e\hbar B/2m^*c\mathrm{Ry}^*)$. $V_B(z)$ is the square-well potential of height V_0 and width L,

$$V_B(z)=\begin{cases}0, & |z|\le\dfrac{L}{2}\\ V_0, & |z|>\dfrac{L}{2}\end{cases} . \tag{2}$$

To calculate the eigenvalues of the Hamiltonian described by Eq. (1) following a variational approach, let us choose the trial function, with an explicit factor for the lowest-energy solution to the square well, $f_k(z)$, out of the donor variational wave function ψ:

$$\psi(\rho,z,\varphi)=G(\rho,z,\varphi)f_k(z) ,$$
$$G(\rho,z,\varphi)=e^{im\phi}\rho^{|m|}R(\rho)e^{-\beta_2(z-Z_i)^2} , \tag{3}$$

and $R(\rho)$ is defined as

$$R(\rho)=e^{-\alpha\rho^2-\beta_1\rho} . \tag{4}$$

We have taken three variational parameters, α, β_1, and β_2, for the trial function given by Eqs. (3) and (4). $G(\rho,z,\varphi)$ describes the internal states of the donor and the (unnormalized) lowest-energy solution to the square-well problem, given as

$$f_k(z)=\begin{cases}\cos kz, & |z|\le\dfrac{L}{2}\\ Ae^{-\kappa|z|}, & |z|>\dfrac{L}{2}\end{cases} . \tag{5}$$

The parameter k is determined from the energy of the first subband and the quantities A and κ are determined by the matching conditions at the interface. The form of Eq. (3) is similar to previous authors,[8-11] who have used $R(\rho)$ as an exponential or Gaussian function. For large well widths ($L\to\infty$), $R(\rho)$ as a Gaussian function gives the best results. The wave function for small well widths ($L\to 0$) becomes almost planar and the system transforms to a planar hydrogenic atom. In this case, the Schrödinger equation's exact solution is an exponential function, ($e^{-\beta_1\rho}$). It is clear that our $R(\rho)$ function has sufficient variational flexibility to be interchanged between exponential ($e^{-\beta_1\rho}$) and Gaussian ($e^{-\alpha\rho^2}$) functions.

The eigenvalues $E(\alpha,\beta_1,\beta_2)$, for $m=0$ and -1, are determined by numerically minimizing $(\langle\psi|\hat{H}|\psi\rangle/\langle\psi|\psi\rangle)$. The binding energies of the ground state (E_{1s}) and first excited (E_{2p_-}) states are determined by a variational method in the following way:

$$E=k^2+\gamma-E(\alpha,\beta_1,\beta_2) , \tag{6}$$

where k^2 is the lowest subband energy of the square well, and γ is the energy of the first Landau level. The method to calculate this energy is given in the Appendix.

III. RESULTS AND DISCUSSION

Two separate sets of calculations of the binding energies of the ground and excited states with the impurity ion located at the center and off-center of the well were performed. The results have been extrapolated to different values of the well width and barrier height, V_0, and magnetic field. For numerical computing, we assume the effective mass for GaAs as $m^*=0.067m_e$, where m_e is the free-electron mass and the static dielectric constant $\epsilon=12.5$. Values of the effective mass, m^*, and the static dielectric constant, ϵ, are constrained to be equal in GaAs and $Ga_{1-x}Al_xAs$. The barrier height, V_0, is chosen to be $0.60\,\Delta E_g$ (Ref. 8) and $0.85\Delta E_g$ (Ref. 9), where the total band-gap difference, ΔE_g, between GaAs and $Ga_{1-x}Al_xAs$ is given as a function of the Al concentration, x,[17]

$$\Delta E_g=1.155x+0.37x^2 \ \ [\mathrm{eV}] . \tag{7}$$

The value of the Al concentration, x, in the barrier layers is taken to be 0.3 throughout this work.

Apparently, it is possible to directly calculate the variational energy, $(\langle\psi|\hat{H}|\psi\rangle/\langle\psi|\psi\rangle)$, but it is necessary to take into account minimizing the process unstability, related, on one hand, with the loss of precision computing of two-dimensional integrals and, on the other hand, with the appearance of a ill-conditioned matrix. As the nonlinear variational parameters α, β_1, β_2 decrease during the minimization processes, the form of the subintegral functions becomes similar to Dirac δ-like ones and it is very difficult to compute such integrals with sufficient precision. But for our trial function, one can analytically calculate almost all integrals (see the Appendix). Besides, the minimizing process is sufficiently simple because the trial function has a few variational parameters and consists of only the single term.

In Fig. 1, we display the variation of the binding energy (units of the Rydberg effective) of the donor $1s$ state in a quantum well for $V_0=0.60\Delta E_g$ as a function of a donor position ($2Z_i/L$), without magnetic field, ($\gamma=0$), and for four different trial functions. Curve (a) presents results of calculations using the Huzinaga trial function with 13

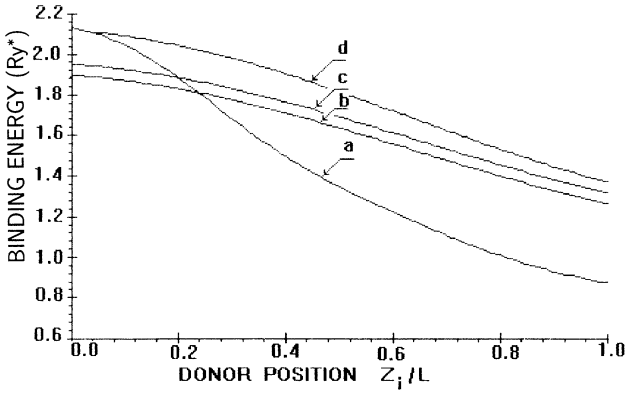

FIG. 1. Binding energies of the ground state of a shallow donor in a GaAs-$Ga_{0.7}Al_{0.3}As$ quantum well as a function of donor position ($L=1.0a_0^*$, $\gamma=0$): (a) Gaussian trial function with 13 linear variation parameters; (b) Gaussian trial function with one nonlinear variational parameter ($\beta_1=0$; $\beta_2=\alpha$); (c) Gaussian two variational parameters trial function ($\beta_1=0$), and (d) mixing three variational parameters trial function [Eqs. (3) and (4)].

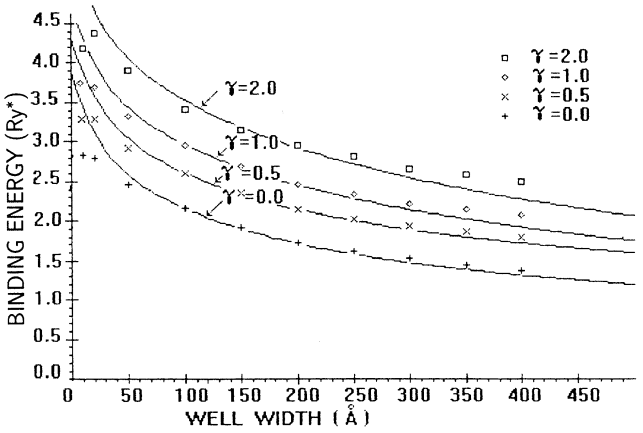

FIG. 2. Binding energies of the ground state of a shallow neutral donor in a GaAs-$Ga_{0.7}Al_{0.3}As$ quantum well as a function of the well size (L) for four different values of magnetic-field parameter: our results (solid curve) and results of Ref. 8 ($+,\times,\Diamond,\square$).

linear variational parameters from Ref. 9. Results of our calculations using the Gaussian trial function with one (b) and two (c) nonlinear variational parameters are shown. The last functions have been obtained from Eqs. (3) and (4), replacing $\beta_1=0$ and $\beta_2=\alpha$, respectively, at curve (b). Curve (d) shows results of our calculations using the three-nonlinear-variational-parameters trial function given by Eqs. (3) and (4).

From Fig. 1, three important findings seem clear: (1) the binding energy slightly increased with the number of linear parameters (a), but a drastic increase ($\sim 100\%$) is observed by using only one nonlinear variational parameter (b) when the barrier edge is near the impurity center; (2) in the last case, for each additional nonlinear parameter, the binding energy increases about 7%; and (3) our three-nonlinear-parameters trial function overcomes all results of Ref. 9 for all impurity-center positions [compare curves (d) and (a)]. In addition, the behavior of our curves (b,c,d) is much smoother than (a). This gives further support to our minimizing process.

As the impurity center approaches the edge, we see a remarkable advantage of our mixing trial function [Eq. (3)] in comparison with the Gaussian ones. A similar situation also occurs for narrow wells. Let us study the binding-energy dependence of the well size.

Figures 2 and 3 present our results (solid curves) and the previous results ($+,\times,\Diamond,\square$) of Ref. 8 for $V_0=0.85\Delta E_g$. The dependence of the binding energy of the ground state and first excited state on the impurity at the center of the quantum well is shown for different magnetic-field values as a function of the well width.

In general, our curves and previous results are similar, except in the extremes. To clarify the differences, extraction of some results for $1s$ and $2p_-$ states without magnetic field from Fig. 2 are presented in Table I. Column (c) of the table gives the exact limit energies for well width $L\rightarrow 0$ (free two-dimensional hydrogenic-atom) and $L\rightarrow\infty$ (free three-dimensional hydrogenic-atom), which have been obtained from the following formulas[19] $E_n=-(n-\frac{1}{2})^{-2}$ and $E_n=-n^{-2}$ ($n=1,2$ for $1s$ and $2p_-$, respectively).

For the $1s$ state from the table, it seems clear that our trial function provides better results for well widths smaller than 100 Å and has a true asymptotic behavior for narrow wells. In contrast, the Gaussian trial function gives erroneous asymptotic results for $L\rightarrow 0$ and differs from the exact result by more than 30%. But for $L\rightarrow\infty$, our results for the three-parameters variational trial function are slightly worse ($<4\%$) than ones from Ref. 8.

The table indicates that our results for the $2p_-$ state are in good agreement with exact ones for all limit cases. Despite the fact that the column (a) results for $2p_-$ states in the table are superior to our results, those are also in

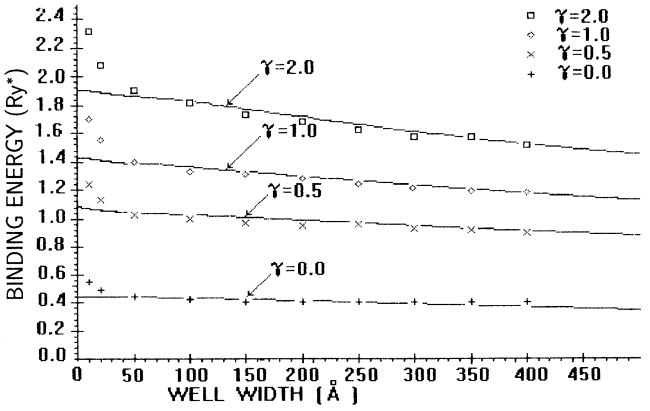

FIG. 3. Binding energies of the $2p_-$ state of a shallow neutral donor in a GaAs-$Ga_{0.7}Al_{0.3}As$ quantum well as a function of the well size (L), for four different values of magnetic-field parameters: our results (solid curve) and results of Ref. 8 ($+,\times,\Diamond,\square$).

TABLE I. Binding energies for ground and $2p_-$ states with the impurity at the center of a GaAs-$Ga_{0.7}Al_{0.3}As$ quantum well, without a magnetic field ($\gamma=0$), for different well widths: (a) results of Ref. 8, (b) results of the present work, and (c) theoretically exact limit energies. *denotes extrapolation results.

	E_B (Ry*) $1s$			E_B (Ry*) $2p_-$		
L (A)	(a)	(b)	(c)	(a)	(b)	(c)
0		3.9*	4.0	0.60*	0.444*	0.444
10	2.70	3.70		0.53	0.444	
20	2.70	3.11		0.49	0.443	
50	2.47	2.59		0.44	0.440	
100	2.17	2.17		0.42	0.432	
200	1.73	1.72		0.40	0.412	
400	1.37	1.32		0.40	0.367	
∞			1.0	0.40*	0.243*	0.25

contradiction with exact ones[19] for $L\to 0$ and ∞. Perhaps this is explained by errors of the minimizing process for Gaussian trial functions.

In addition, we have studied the dependence of the binding energy for an off-center impurity position. Our results for $L>100$ Å are in good agreement, but for $L<100$ Å, the binding energies of Ref. 8 are smaller than ours up to 11%.

IV. CONCLUSION

We have performed a theoretical calculation of the binding energies for ground ($1s$) and first excited ($2p_-$) states of shallow donors in a GaAs-$Ga_{1-x}Al_xAs$ heterostructure as a function of the size of the quantum well and the impurity position in the presence of a magnetic field, using a variational method and mixing trial wave functions. The binding energy increases dramatically with the number of nonlinear variational parameters and the best results for the binding energy were obtained by using a mixing trial function with only three nonlinear variational parameters. We show that our nonlinear-three-parameters trial mixing function gives binding-energy results overcoming previous ones when the barrier edge is near the impurity center.

ACKNOWLEDGMENTS

This research was financed by Universidad Industrial de Santander, Department of Physics. F.J.B. wishes to thank T. Szwacka for her invaluable help and generous hospitality at Universidad de los Andes (ULA) Mérida-Venezuela.

APPENDIX

The Hamiltonian [Eq. (1)] contains three variational energies,

$$E(\alpha,\beta_1,\beta_2)=E_1+E_2+E_3\ ,$$
$$E_k=\frac{\langle\psi|\hat{H}_k|\psi\rangle}{\langle\psi|\psi\rangle},\quad k=1,2,3\ , \tag{A1}$$

where $\hat{H}_k$ and ψ are given by Eqs. (1) and (3), respectively. Substituting expressions (1) and (3) in (A1) and after simplifications, one can obtain for E_1,

$$E_1=\left[\left[4\alpha^2+\frac{\gamma^2}{4}\right]J(2|m|+3)+4\alpha\beta_1 J(2|m|+2)+(\beta_1^2-4\alpha|m|)J(2|m|+1)-2|m|\beta_1 J(2|m|)+2m^2J(2|m|-1)\right]\Big/J(1)\ , \tag{A2}$$

where $J(1)$ is

$$J(1)=\frac{1}{4\alpha}-\frac{\beta_1}{2\alpha\sqrt{2\alpha}}e^{\beta_1^2/2\alpha}\int_{\beta_1/\sqrt{2\alpha}}^{\infty}e^{-u^2}du\ , \tag{A3}$$

and $J(k)$ for any k can be obtained from the recurrent relation,

$$J(k)=-\frac{1}{2}\frac{\partial}{\partial\beta_1}J(k-1)\ . \tag{A4}$$

The energies E_2 and E_3 are equal to

$$E_2=k^2+4\beta_2^2\frac{\int_{-\infty}^{\infty}f_k^2(z)(z-Z_i)^2e^{-2\beta_2(z-Z_i)^2}dz}{\int_{-\infty}^{\infty}f_k^2(z)e^{-2\beta_2(z-Z_i)^2}dz}\ , \tag{A5}$$

$$E_3=-2\int_{-\infty}^{\infty}dz\,e^{-2\beta_2(z-Z_i)^2}f_k^2(z)\times\int_0^{\infty}\frac{\rho^{2|m|+1}e^{-2\alpha\rho^2-2\beta_1\rho}}{\sqrt{\rho^2+(z-Z_i)^2}}d\rho\Big/\langle\psi|\psi\rangle\ . \tag{A6}$$

[1]For a review, see articles in *High Magnetic Field in Semiconductor Physics III*, edited by G. Landwehr, Springer Series in Solid-State Sciences Vol. 101 (Springer, Berlin, 1992).
[2]S. Huant *et al.*, Phys. Rev. Lett. **65**, 1486 (1990).
[3]G. Bastard, Phys. Rev. B **24**, 4714 (1981).
[4]S. Chaudhuri, Phys. Rev. B **28**, 4480 (1983).
[5]R. L. Greene and K. K. Bajaj, Solid State Commun. **45**, 825 (1983).
[6]R. L. Greene and P. Lane Phys. Rev. B **34**, 951 (1986).
[7]C. Priester *et al.*, Phys. Rev. B **30**, 6029 (1984).
[8]R. L. Greene and K. K. Bajaj, Phys. Rev. B **31**, 913 (1985).
[9]P. Lane and Ronald L. Greene, Phys. Rev. B **33**, 5871 (1986).
[10]T. Pang and S. G. Louie, Phys. Rev. Lett. **65**, 1635 (1990).
[11]N. Nguyen *et al.*, Phys. Rev. B **48**, 14 226 (1993).
[12]T. Szwacka and J. Blinowski, Phys. Rev. B **45**, 6043 (1992).
[13]Y. Yafet, W. Keyes, and E. N. Adams, J. Phys. Chem. Solids

1, 137 (1956).
[14]K. Tanaka, M. Nagaoka, and Y. Yamabe, Phys. Rev. B **28**, 7068 (1983).
[15]N. C. Jarosik *et al.*, Phys. Rev. Lett. **54**, 1283 (1983).
[16]C. Aldrich and R. L. Greene, Phys. Status Solidi B **93**, 343 (1979).
[17]H. J. Lee *et al.*, Phys. Rev. B **21**, 659 (1980).
[18]S. Huzinaga, J. Chem. Phys. **42**, 1293 (1965).
[19]W. Kohn and J. M. Luttinger, Phys. Rev. **98**, 915 (1955).