# Effect of a finite-width barrier on binding energy in modulation-doped quantum-well structures

Hao Chen and Shixun Zhou
*Department of Physics, Fudan University, Shanghai, People's Republic of China*
(Received 21 April 1987)

The ground bound state of hydrogenic impurity in a double quantum well consisting of alternate layers of $Ga_{1-x}Al_xAs$ and GaAs is investigated. The dependence of the binding energy on the impurity position in the barrier, on the barrier heights of the quantum well, and on the thickness of the wells and the barrier is calculated. The results of the present calculation in the single well limit agree with previous results and have much simpler formula expressions. The condition under which the impurity and the electron are separated from each other in the ground state is given.

## I. INTRODUCTION

Due to the progress in the epitaxial crystal-growth techniques such as metalorganic chemical vapor deposition and molecular-beam epitaxy, studies of the hydrogenic shallow impurity state in a quantum well consisting of alternate layers of GaAs and $Ga_{1-x}Al_xAs$ have recently attracted considerable attention.

Some authors[1-3] calculated the impurity binding energy in a single quantum well with the infinite or finite potential barrier height in the $Ga_{1-x}Al_xAs$ regions as functions of the GaAs well thickness and the position of the impurity which is located in the GaAs well. But the more important and realistic case of doping is the modulation doping, the case of the impurity location inside the $Ga_{1-x}Al_xAs$ barrier region, in order to achieve a high electron mobility parallel to the GaAs well layers.[4] Tanaka *et al.*[5] and Greene and Bajaj[6] dealt with the case of the modulation doping in the single-quantum-well structure. The only study to date of the effects of finite-width barriers was done by Chaudhuri,[7] who calculated the binding energy in $GaAs/Ga_{1-x}Al_xAs$ three-quantum-well structure, which is valid for the thin- or small-barrier-height superlattice, but the impurity was located at the center in the middle GaAs well.

In this paper we propose a model of double quantum well with the hydrogenic impurity inside the $Ga_{1-x}Al_xAs$ barrier region in order to investigate the tunneling effect in the modulation-doped quantum-well structure.

In Sec. II we derive the formula expressions of the binding energy in the $Ga_{1-x}Al_xAs/GaAs$ double-quantum-well structures, and give the formulas in the single-quantum-well limit which agree with previous results but have much simpler expressions. In Sec. III the results of the variational calculations are presented. In Sec. IV a brief summary is presented.

## II. BINDING-ENERGY FORMULAS IN A DOUBLE QUANTUM WELL

In the framework of the effective-mass approximation, the Hamiltonian for an electron is given by

$$H=-\nabla^2-2/r+V(z)\ , \tag{1}$$

where

$$V(z)=\begin{cases}V_0, & |z|<b,\ a+b<|z|<+\infty\\ 0, & b<|z|<a+b\ .\end{cases} \tag{2}$$

The Hamiltonian is written in a dimensionless form so that all energies are expressed in units of the effective Rydberg $R^*=m^*e^4/2\hbar^2\epsilon^2\sim 5.83$ meV and all distances are expressed in units of the effective Bohr radius $a^*=\hbar^2\epsilon/m^*e^2$ ($\sim$ 98.7 Å), where $m^*$ and $\epsilon$ are the electronic effective mass and the dielectric constant, respectively, of GaAs. The small differences in the effective masses and dielectric constants of GaAs and $Ga_{1-x}Al_xAs$ have been neglected. The position of donor impurity is represented by $(0,0,z_i)$, and $r=[x^2+y^2+(z-z_i)^2]^{1/2}$. The origin of the coordinate system is chosen to be at the center of the central barrier (Fig. 1). The barrier height $V_0$ is obtained from the 85% rule[8] of the band-gap discontinuity $\Delta E_g$ for donor impurity

$$V_0=0.85\Delta E_g\ , \tag{3}$$

and

$$\Delta E_g=1.155X+0.35X^2\ , \tag{4}$$

(Ref. 9) in eV.

We use the simple trial wave function for the ground state of $H$ in Eq. (1) as

$$\psi=Nf(z)g(x,y,z,z_i,\lambda)\ , \tag{5}$$

where $N$ is the normalization constant. $f(z)$ is the ground-state eigenfunction of $H$ without the Coulomb impurity potential

$$f(z)=\begin{cases}De^{-k'z}, & a+b<z<+\infty\\ A\sin(kz)+B\cos(kz), & b<z<a+b\\ \cosh(k'z), & |z|<b\\ -A\sin(kz)+B\cos(kz), & -a-b<z<-b\\ De^{k'z}, & -\infty<z<-a-b\ ,\end{cases} \tag{6}$$

 

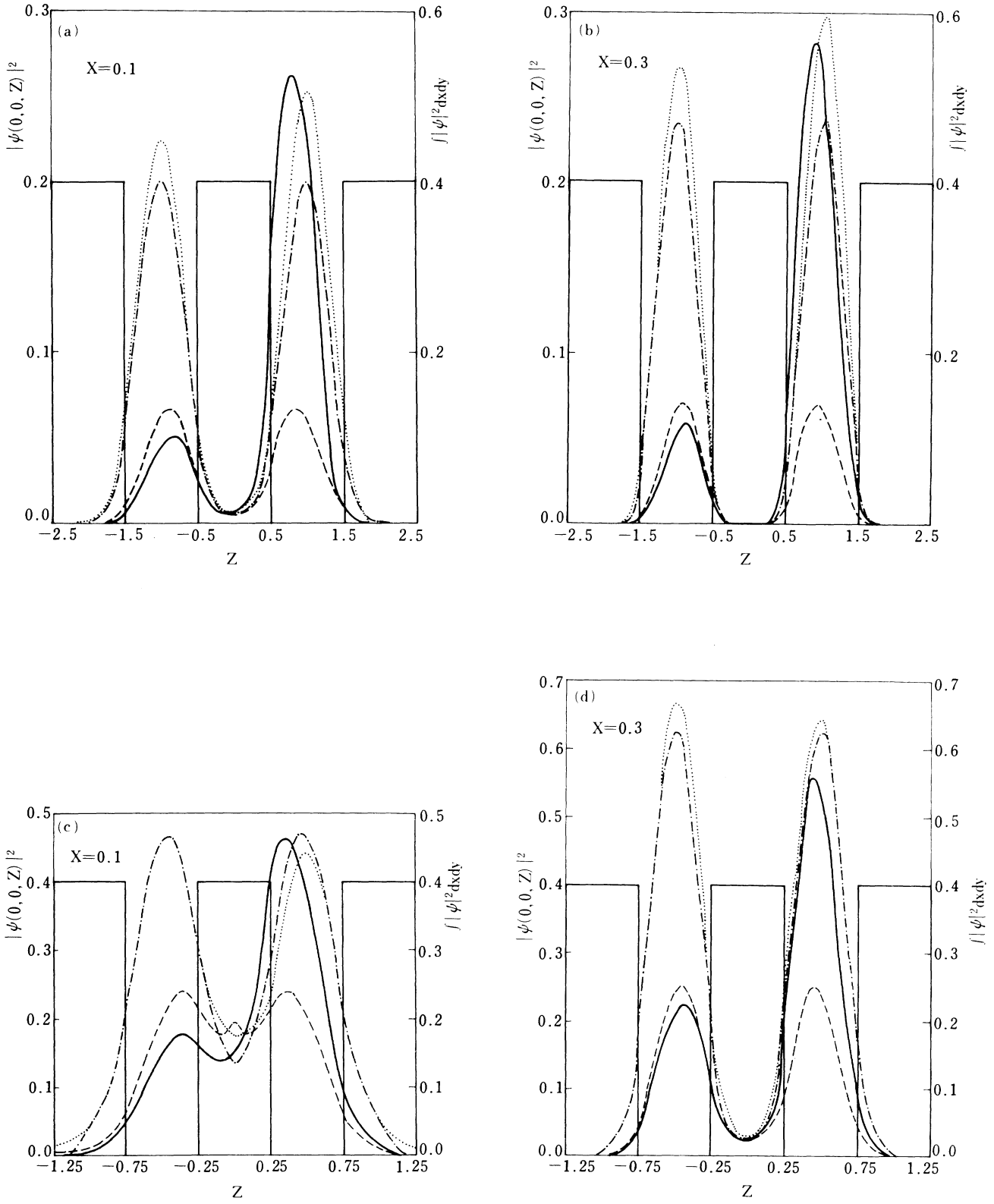


FIG. 1. Electron density distribution $|\psi(0,0,z)|^2$ and $\int\int|\psi|^2dx\,dy$ vs position along the axis normal to the interfaces. The solid and dashed curves are for impurity ratio position, $\alpha=0.0$ and 1.0, respectively, for $|\psi(0,0,z)|^2$. The dotted and dot-dashed curves are for $\alpha=0.0$ and 1.0, respectively, for $\int\int|\psi|^2dx\,dy$. (a) and (b) are for equal well and barrier thicknesses $a=L=1.0$, and (c) and (d) for $a=L=0.5$.

where

$$k=(E_0)^{1/2} \text{ and } k'=(V_0-E_0)^{1/2} . \tag{7}$$

$E_0$ is the eigenenergy of an electron in the potential given by Eq. (2). By matching $\psi$ and $d\psi/dz$ at the interfaces $z=b$, $a+b$, the eigenenergy $E_0$ can be given by the solution of the following equation:

$$[k^2-k'^2\tanh(k'b)]\tan(ka)-kk'[1+\tanh(k'b)]=0 . \tag{8}$$

The variational function $g(x,y,z,z_i,\lambda)$ is the hydrogenic eigenfunction containing the variational parameter $\lambda$,

$$g(x,y,z,z_i,\lambda)=e^{-r/\lambda} . \tag{9}$$

The variational binding energy $E_b$ felt by an electron injected from the impurity is given by

$$E_b=E_0-\min\langle\psi\mid H\mid\psi\rangle . \tag{10}$$

The normalization constant $N$ and the expectation values of $H$ are as follows:

$$\begin{aligned}N=(\tfrac{1}{2}\pi)^{1/2}\{&D^2[K_1(\lambda,k')+K_6(-\lambda,-k')]+0.5(A^2+B^2)[K_2(\lambda,0)+K_5(-\lambda,0)]\\&+0.5(A^2-B^2)[I_2(\lambda,k)+I_5(-\lambda,-k)]+AB[J_2(\lambda,k)+J_5(-\lambda,-k)]+0.5[K_3(\lambda,0)+K_4(-\lambda,0)]\\&+0.25[K_3(\lambda,k')+K_3(\lambda,-k')+K_4(-\lambda,k')+K_4(-\lambda,-k')]\}^{-1/2} ,\end{aligned} \tag{11}$$

$$\begin{aligned}\langle\psi\mid-\nabla^2+V(z)\mid\psi\rangle=k^2+1/\lambda^2+2\pi N^2\{&2D^2[P_1(\lambda,k')+P_6(-\lambda,-k')]+(A^2+B^2)[P_2(\lambda,0)+P_5(-\lambda,0)]\\&-(A^2-B^2)[S_2(\lambda,k)+S_5(-\lambda,k)]-2AB[R_2(\lambda,k)-R_5(-\lambda,k)]\\&+P_3(\lambda,0)+P_4(-\lambda,0)\\&+0.5[P_3(\lambda,k')+P_3(\lambda,-k')+P_4(-\lambda,k')+P_4(-\lambda,-k')]\} ,\end{aligned} \tag{12}$$

$$\begin{aligned}\langle\psi\mid-2/r\mid\psi\rangle=2\pi N^2\{&-D^2[Q_1(\lambda,k')-Q_6(-\lambda,-k')]-0.5(A^2+B^2)[Q_2(\lambda,0)-Q_5(-\lambda,0)]\\&+0.5(A^2-B^2)[T_2(\lambda,k)-T_5(-\lambda,k)]+AB[M_2(\lambda,k)+M_5(-\lambda,k)]\\&-0.25[2Q_3(\lambda,0)-2Q_4(-\lambda,0)+Q_3(\lambda,k')+Q_3(\lambda,-k')-Q_4(-\lambda,k')-Q_4(-\lambda,-k')]\} .\end{aligned} \tag{13}$$

The integrals $K_n$, $I_n$, $J_n$, $P_n$, $S_n$, $R_n$, $Q_n$, $T_n$, and $M_n$ are defined in the Appendix. The subscript $n$ denotes the region of integration.

In Eq. (12) we put the expectations of the operators $-\nabla^2$ and $V(z)$ together and pick up the kinetic term of a free electron, $k^2$, in order to obtain a simple expression. In the single-quantum-well limit ($b\to 0$), the right-hand side of Eq. (12) reduces to the following result:

$$\langle\psi\mid-\nabla^2+V(z)\mid\psi\rangle=k^2+1/\lambda^2 . \tag{14}$$

Equation (14) is consistent with the results of previous authors[7,10] and has much simpler expression. [In fact, the third and fourth terms in Eq. (10b) can be canceled by Eq. (10d) in Ref. 7.] Meanwhile, Eqs. (11) and (13) reduce to the following results, respectively:

$$\begin{aligned}N=(2/\pi\lambda^3)^{1/2}(1+1/\Delta^2-e^{-2a/\lambda}\{&1+a/\lambda+(1/\Delta)(a/\lambda+1/\Delta)\cos(2ka)-(\lambda k/2\Delta)(1+2a/\lambda+2/\Delta)\sin(2ka)\\&-[\cos^2(ka)/(1+\lambda k')][1+2a/\lambda+1/(1+\lambda k')]\})^{1/2} ,\end{aligned} \tag{15}$$

$$\langle\psi\mid-2/r\mid\psi\rangle=-\pi N^2\lambda^2\{1+1/\Delta-e^{-2a/\lambda}[1+(1/\Delta)\cos(2ka)-(\lambda k/\Delta)\sin(2ka)-2\cos^2(ka)/(1+\lambda k')]\} , \tag{16}$$

where

$$\Delta=1+\lambda^2k^2 . \tag{17}$$

Here the results in Eqs. (15)–(17) are just the same as the corresponding expressions obtained by previous authors.[7,10]

It is easy to get electron density distribution at $(0,0,z)$

$$|\psi(0,0,z)|^2=N^2|f(z)|^2\exp(-2|z-z_i|/\lambda) , \tag{18}$$

and total electron density distribution in the superlattice layers

$$\int\int|\psi|^2dx\,dy=N^2|f(z)|^2[0.5\lambda^2+\lambda|z-z_i|\exp(-2|z-z_i/\lambda)] . \tag{19}$$

## III. RESULTS

The ground states of the above Hamiltonian are found by using the general variational method. Then the binding energy $E_b$ is calculated through Eqs. (11)–(13).

The results are displayed in the figures. The barrier thickness is $L=2b$. The parameter $\alpha=z_i/b$ is the ratio position of the modulated impurity which is doped inside the positive barrier region, $0\leq z_i\leq b$.

In the case of the modulation doping, electrons and impurities are separated from each other, so a high electron mobility in the superlattice layers can be achieved.[4] In Figs. 1(a)–1(d), the dependence of the separation of electron and impurity on the well-barrier size and the composition of alloy in the ground state are shown. Figures 1(a)–1(d) show the electron density distribution for $L=a=1.0$ and 0.5, $x=0.1$ and 0.3, and $\alpha=0$ and 1. The solid and dashed curves are for the electron density distribution $|\psi(0,0,z)|^2$. The dotted and dot-dashed curves are for the total electron density distribution $\int\int|\psi|^2dx\,dy$ in superlattice layers. The electron density distribution is mainly localized to the well region for $L=a=1.0$ [Figs. 1(a) and 1(b)], especially for the high alloy composition, $x=0.3$, so that the impurity and the electron are separated from each other in the ground state. But if the well-barrier size goes to a smaller value, for example, $L=a=0.5$ [Figs. 1(c) and 1(d)], the impurity and the electron are not separated. Figures 1(a) and 1(b) show that the electron are not spread to the next-nearest-neighbor wells, so that our double-well model with parameters of $L=a=1.0$ is valid. From these figures one can judge at which condition the electron is separated from the impurity in the ground state.

Figure 2 shows the binding energy $E_b$ as a function of the well thickness $a$, with the barrier thickness $L$, and the ratio doping position $\alpha$ as parameters for two barrier heights corresponding to aluminum composition $x=0.1$ and 0.3. The curves with $L=0$ corresponding to the case of a single well limit coincide with those obtained by Chaudhuri.[7] In the figure one can find that the binding energy, $E_b=E_0-\min\langle\psi|H|\psi\rangle$ has a maximum. The on-edge donor increases the binding energy and causes the maximum of the binding energy to shift to the large well thickness $a$. With the increase in the donor composition $x$, the maximum of the binding energy goes to the small well size. When $x=0.3$, $L=2.0$, and $\alpha\leq 0.5$, the maximum of $E_b$ almost does not appear. The situation looks like the one of the infinite-barrier-height model,[1] and gives the condition in which the infinite-barrier-height model is valid.

Figure 3 shows the binding energy $E_b$ as a function of the barrier thickness $L$, with the well size $a$ and the ratio doping position $\alpha$ as parameters, and the donor composition is $x=0.3$. The on-edge donor causes the minimum of the binding energy.

Figure 4 shows the binding energy $E_b$ as a function of the ratio position $\alpha$ of the modulated impurity. Figure 5 presents the binding energy $E_b$ as a function of the well thickness when the GaAs and $Ga_{1-x}Al_xAs$ layer thicknesses are equal for alloy compositions $x=0.1$ and 0.4 of $Ga_{1-x}Al_xAs$ and ratio positions $\alpha=0$ and 1 of the impurity.

## IV. SUMMARY

We derive the formula expressions of binding energy in a double-quantum-well structure, and obtain a simpler formula for the single-quantum-well limit. The variational calculations for the ground binding energy have been done. The more distant from the edge of the barrier the modulation-doping impurity is, the lower the binding energy is.

The electron density distribution $|\psi(0,0,z)|^2$ and the quantity $\int\int|\psi|^2dx\,dy$ are shown for different well-barrier parameters and impurity positions. The situation

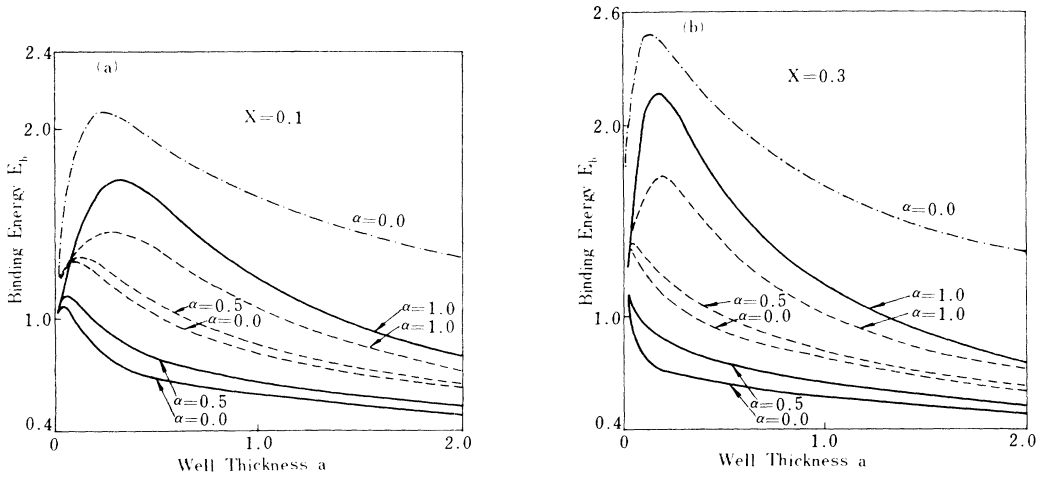


FIG. 2. Binding energy for the hydrogenic-donor ground state as a function of the GaAs layer thickness $a$ for different $Ga_{1-x}Al_xAs$ layer thicknesses $L$ and different impurity ratio positions, $\alpha=2z_i/L$. The solid, dashed, and dot-dashed curves are for barrier thicknesses $L=2.0$, 1.0, and 0.0, respectively. (a) and (b) are for the alloy composition $x=0.1$ and 0.3 of $Ga_{1-x}Al_xAs$, respectively.

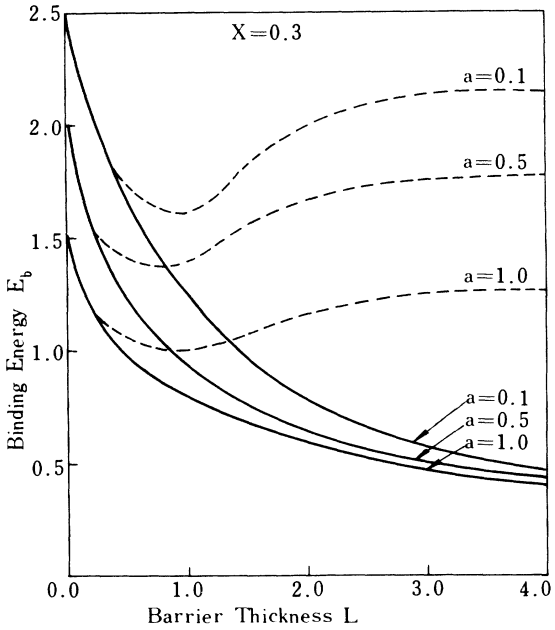


FIG. 3. Binding ground energy as functions of the $Ga_{1-x}Al_xAs$ layer thickness $L$ for different well widths $a$ and different impurity ratio positions $\alpha$. The solid and dashed curves are for the impurity on-center and on-edge, respectively.

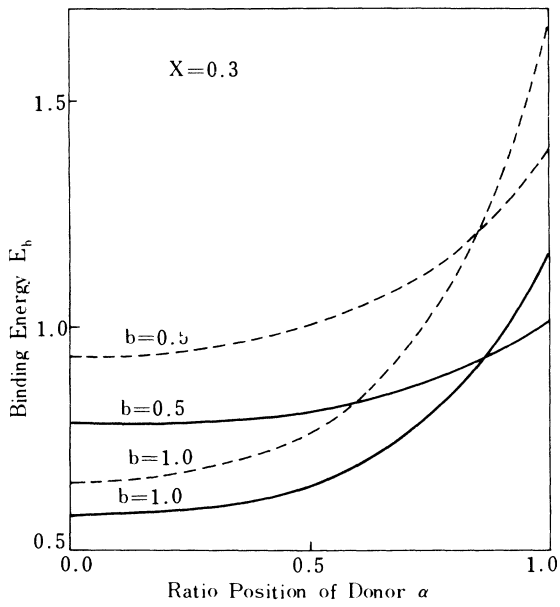


FIG. 4. Binding ground energy as functions of impurity ratio position for different well-barrier sizes. The solid and dashed curves are for the well thicknesses $a = 1.0$ and 0.5, respectively.

which is dealt with in this paper is valid for the thin- or small-barrier-height superlattices, and the impurity is located in the $Ga_{1-x}Al_xAs$ barrier region.

## ACKNOWLEDGMENTS

The authors are grateful to Mr. X. M. Xiong and Y. Zhu for helpful discussions. This work was supported by the Foundation for Higher Education under Grant No. 2(1985) of People's Republic of China. One of the authors (H.C.) would like to thank Professor Abdus Salam, the International Atomic Energy Agency (IAEA), and United Nations Educational, Scientific, and Cultural Organization (UNESCO) for hospitality at the International Center for Theoretical Physics, Trieste, where part of the work was done.

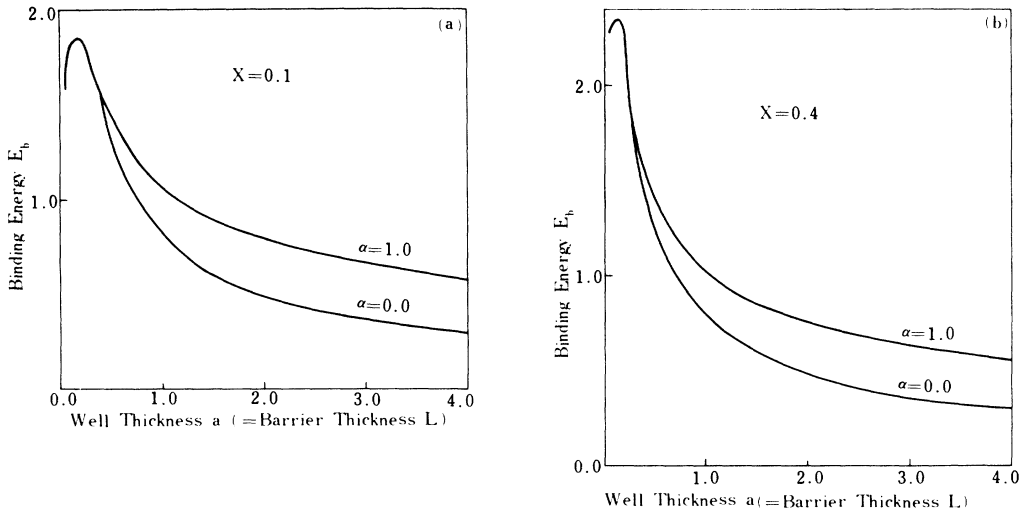


FIG. 5. Binding ground energy as functions of the well thickness when the well and barrier thickness are equal for different alloy compositions of $Ga_{1-x}Al_xAs$. (a) and (b) are for the alloy composition $x = 0.1$ and 0.4, respectively, of $Ga_{1-x}Al_xAs$.

## APPENDIX

The coefficients $A$, $B$, and $D$ in the eigenfunction $f(z)$ are obtained from the matching conditions at the interfaces as

$$A=\sin(kb)\cosh(k'b)+(k'/k)\cos(kb)\sinh(k'b)\ ,$$

$$B=-(k'/k)\sin(kb)\sinh(k'b)+\cos(kb)\cosh(k'b)\ ,$$

$$D=\{A\sin[k(a+b)]+B\cos[k(a+b)]\}\exp[k'(a+b)]\ .$$

The integrals involved in the normalization constant and the expectation value of the Hamiltonian are defined as the following:

| $n$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| $z_n$ | $-\infty$ | $-a-b$ | $-b$ | $z_i$ | $b$ | $a+b$ | $+\infty$ |

$$K_n(\lambda,k')=[0.25\lambda^2/(1+\lambda k')][-z+z_i+0.5\lambda+0.5\lambda/(1+\lambda k')]\exp[2(z-z_i)/\lambda+2k'z]\,|_{z_n}^{z_{n+1}}\ ,$$

$$I_n(\lambda,k)=(0.25\lambda^2/\Delta)[(z-z_i-\lambda/\Delta)\cos(2kz)+\lambda k\,(z-z_i-0.5\lambda-\lambda/\Delta)\sin(2kz)]\exp[2(z-z_i)/\lambda]\,|_{z_n}^{z_{n+1}}\ ,$$

$$\Delta=1+\lambda^2k^2\ ,$$

$$J_n(\lambda,k)=I_n(\cos\rightarrow\sin,\ \sin\rightarrow-\cos)\ ,$$

$$P_n(\lambda,k')=0.25(z-z_i)\exp[2(z-z_i)/\lambda+2k'z]\,|_{z_n}^{z_{n+1}}\ ,$$

$$Q_n(\lambda,k')=[0.5\lambda^2/(1+\lambda k')]\exp[2(z-z_i)/\lambda+2k'z]\,|_{z_n}^{z_{n+1}}\ ,$$

$$S_n(\lambda,k)=0.25(z-z_i)\cos(2kz)\exp[2(z-z_i)/\lambda]\,|_{z_n}^{z_{n+1}}\ ,$$

$$R_n(\lambda,k)=S_n(\cos\rightarrow\sin)\ ,$$

$$T_n(\lambda,k)=(0.5\lambda^2/\Delta)[\cos(2kz)+\lambda k\sin(2kz)]\exp[2(z-z_i)/\lambda]\,|_{z_n}^{z_{n+1}}\ ,$$

$$M_n(\lambda,k)=T_n(\cos\rightarrow\sin,\ \sin\rightarrow-\cos)\ .$$


[1]G. Bastard, Phys. Rev. B **24**, 4714 (1981).

[2]C. Mailhiot, Y. C. Chang, and T. C. McGill, Phys. Rev. B **26**, 4449 (1982).

[3]R. L. Greene and K. K. Bajaj, Solid State Commun. **45**, 825 (1983).

[4]R. Dingle, H. Stormer, A. C. Gossard, and W. Wiegmann, Appl. Phys. Lett. **23**, 665 (1978).

[5]K. Tanaka, M. Nagaoka, and T. Yambe, Phys. Rev. B **28**, 7068 (1983).

[6]R. L. Greene and K. K. Bajaj, Solid State Commun. **53**, 1103 (1985).

[7]S. Chaudhuri, Phys. Rev. B **28**, 4480 (1983).

[8]R. Dingle, in *Festkorper-Probleme*, Vol. XV of *Advances in Solid State Physics*, edited by H. J. Queisser (Pergamon Vieweg, Braunschweig, 1975).

[9]H. J. Lee, L. Y. Jurarel, J. C. Wooley, and A. J. Springthorpe, Phys. Rev. B **21**, 659 (1980).

[10]K. Jayakumar and S. Balasubramanian, Phys. Rev. B **32**, 6904 (1985).