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Hydrogenic impurity in multilayered quantum wires

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The binding energy of the ground state of a hydrogenic impurity located at the center of a multilayered quantum wire (MLQW) is studied within the framework of the effective-mass approximation. The MLQW consists of a core wire (GaAs) coated by a cylindrical shell ($Ga_{1-x}Al_xAs$) and then embedded in the bulk ($Ga_{1-y}Al_yAs$). The calculation was performed by using a trial wave function. To make a comparison, the ground and excited states ($1s$, $2p$, and $3d$ states) binding energies of a hydrogenic impurity located at the center of a single-layered quantum wire (QW) are also calculated. It is found for small wire radius, the ground-state binding energy of the hydrogenic impurity located at the center of a MLQW behaves very differently from that of a single-layered QW. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1326467]

I. INTRODUCTION

The progress in epitaxial growth and microfabrication techniques in recent years has motivated studies of low-dimensional semiconductor structures such as two-dimensional quantum wells (QWs), one-dimensional quantum-well wires (QWWs), and zero-dimensional quantum dots (QDs).[1–8] Since Bastard's[9] pioneering works in the study of the binding energy of a hydrogenic impurity within an infinite potential-well structure, many theoretical works have been devoted to the study of the properties of impurity states in various confining systems.[9–25] The binding energy of the ground state of a hydrogenic impurity E_b in D dimension is given by[26] $E_b=[2/D-1]^2$ Ry, where Ry is the effective Rydberg. The physical properties of electrons in quantum wires are very different from those in the bulk. As a consequence of the confinement, energy levels are discrete. The existence of these atomic-like states may be utilized in future lasers where laser properties can be tailored by proper choices of well and barrier materials as well as size and shape of the wire.[27,28] The change in impurity binding energies due to the confinement effect has been observed in photoluminescence[15,29–31] and Raman-scattering[32,33] experiments on the impurities in the quantum wells.

Recently, GaAs-$Ga_{1-x}Al_xAs$ structures have been the subject of research for the following technological reasons:[34] (1) GaAs and $Ga_{1-x}Al_xAs$ both possess a direct-gap band structure, (2) single-crystal heterostructures of GaAs and $Ga_{1-x}Al_xAs$ are possible because the lattice constants of GaAs and $Ga_{1-x}Al_xAs$ are nearly identical, so that they are closely lattice matched, and, therefore, (3) abrupt spatial transitions in the energy gap are possible. However, in all of previous calculations it has been assumed that the $Ga_{1-x}Al_xAs$ layers are thick enough to confine the wave functions so that they do not leak out the wells. But superlattices were made with layer thickness ranging from a few monolayers to about 400 Å. And most attention has been focused on systems with aluminum concentration x of $Ga_{1-x}Al_xAs$ less than 0.45. In this concentration range the band gap is direct at the Γ point. The spreading of the impurity envelope wave functions depends on the potential barrier height as well as the barrier thickness. Thus, the previous calculations with single-layered approximation are not adequate for thin supperlattices, or even for moderately thick superlattices but with small aluminum concentration. The first attempt to use more than a single quantum well was done by Chaudhuri,[35] who used three quantum wells in his variational calculation of the ground-state energy of the donor electron with respect to the lowest subband level. Lane and Greene[36] calculated the binding energies and probability distributions of shallow donor states in multiple-well GaAs-$Ga_{1-x}Al_xAs$ heterostructure. Many authors[37–40] used colloidal chemistry techniques and wet chemistry to prepare the CdS/HgS/CdS multiple well in which a shell of HgS is embedded in a CdS quantum dot, forming a ''quantum-dot quantum well'' (QDQW). The homogeneous absorption and fluorescence spectra of the QDQW were investigated. Numerous studies on organic light-emitting diodes (LEDs) have used these structures as the emitting and charge-transport species.[41–43] In this work, we calculate the ground-state binding energy of the hydrogenic impurity located at the center of the multilayered quantum wire by using the effective-mass approximation. Our system is constructed as a core wire made of GaAs surrounded by a cylinder shell of $Ga_{1-x}Al_xAs$ and then embedded in the bulk of $Ga_{1-y}Al_yAs$. The barrier height V between GaAs and $Ga_{1-x}Al_xAs$ can be obtained[44] as $0.8729x$ eV from a fixed ratio $Q=0.7$ of the band-gap discontinuity $\Delta E_g=1.247x$ eV. In this article, the effective atomic units are used so that all energies are measured in the units of the effective Rydberg (Ry) and all distances are measured in the units of effective Bohr radius a_0^*. The Ry and a_0^* can be determined by $\mu e^4/2\hbar^2\varepsilon^2$ and $\varepsilon\hbar^2/\mu e^2$, where μ and ε are the electronic effective mass and the dielectric constant of GaAs material which are equal to $0.067m_e$ and 13.18, respectively. And Ry and a_0^* are equal to 5.2 meV and 104 Å, respectively. In this work, the effective-mass difference between GaAs and $Ga_{1-x}Al_xAs$

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material has been ignored. The polarization and image charge effects may be significant in the multilayered system if there is a large dielectric discontinuity between the core wire and the surrounding medium. However, this is not the case for the GaAs–$Ga_{1-x}Al_xAs$ system (the dielectric constant of $Ga_{1-x}Al_xAs$ is $13.18-3.12x$). Thus, they are safely to be ignored.

Brown and Spector[10] have calculated the single-layered quantum wire with their trial function and many authors have employed their trial function in the calculations. But the trial function of Brown is only suitable for the single-layered quantum wire and ground state. Bryant[13] has calculated $1s$, $2p$-state binding energies by the variational method in the single-layered quantum wire. However, the result of Bryant does not agree with the limiting value in some cases. In this article, we calculate the ground-state binding energy of an impurity located at the center of a multilayered quantum wire (MLQW), and the ground- and excited-state binding energies of an impurity located at the center of a single-layered quantum wire. We proposed a trial function which is modified from the result of Brown and Spector. Our calculation shows that the state energies we obtained are in better agreement with the correct limiting values in some special cases than the previous results.

II. THEORY

The Hamiltonian of a hydrogenic impurity located at the center of the MLQW is written as

$$H=-\frac{\hbar^2}{2\mu}\nabla^2-\frac{e^2}{\varepsilon(\rho^2+z^2)^{1/2}}+V(\rho), \tag{1}$$

where

$$V(\rho)=\begin{cases} 0\,, & \text{if } \rho<a \text{ (GaAs)},\\ V_2\,, & \text{if } a\leqslant\rho<b \text{ } (Ga_{1-x}Al_xAs),\\ V_3\,, & \text{if } \rho\geqslant b \text{ } (Ga_{1-y}Al_yAs),\end{cases} \tag{2}$$

assuming the trial function of the eigenstates of the Hamiltonian in the absence of impurity is in the following form:

$$\begin{aligned}&\Psi_1(\rho,\theta,z)=N_1J_l(\alpha_{nl}\rho)\rho^{n-1}e^{ikz}e^{il\theta}, \quad \text{if } \rho>a,\\ &\Psi_2(\rho,\theta,z)=[N_{21}I_l(\beta_{nl}\rho)+N_{22}K_l(\beta_{nl}\rho)]\rho^{n-1}e^{ikz}e^{il\theta},\\ &\qquad\qquad \text{if } a\leqslant\rho<b,\\ &\Psi_3(\rho,\theta,z)=N_3K_l(\gamma_{nl}\rho)\rho^{n-1}e^{ikz}e^{il\theta}, \quad \text{if } \rho\geqslant b,\end{aligned} \tag{3}$$

where

$$\alpha_{nl}=\sqrt{\frac{2\mu E_{nlk}}{\hbar^2}-k^2}, \tag{4}$$

$$\beta_{nl}=\sqrt{\frac{2\mu(V_2-E_{nlk})}{\hbar^2}-k^2}=\sqrt{V_2-\alpha_{nl}^2}, \tag{5}$$

$$\gamma_{nl}=\sqrt{\frac{2\mu(V_3-E_{nlk})}{\hbar^2}-k^2}=\sqrt{V_3-\alpha_{nl}^2}, \tag{6}$$

and J_l is an ordinary Bessel function of order l, and I_l and K_l are the modified Bessel functions of the first and second kind, respectively, of order l. Since the wave functions must be continuous at $\rho=a$ and $\rho=b$, then, the relations of N_1, N_{21}, N_{22}, and N_3 can be obtained as

$$N_1=\frac{N_{21}I_l(\sqrt{V_2-\alpha_{nl}^2}a)+N_{22}K_l(\sqrt{V_2-\alpha_{nl}^2}a)}{J_l(\alpha_{nl}a)}, \tag{7}$$

$$N_3=\frac{N_{21}I_l(\sqrt{V_2-\alpha_{nl}^2}b)+N_{22}K_l(\sqrt{V_2-\alpha_{nl}^2}b)}{K_l(\alpha_{nl}b)}. \tag{8}$$

If we set $N_{22}=N$ and $N_{21}=NN_2$, then the wave function becomes

$$\begin{aligned}\Psi_1(\rho)&=N\frac{N_2I_l(\sqrt{V_2-\alpha_{nl}^2}a)+K_l(\sqrt{V_2-\alpha_{nl}^2}a)}{J_l(\alpha_{nl}a)}\\ &\quad\times\rho^{n-1}J_l(\alpha_{nl}\rho),\\ \Psi_2(\rho)&=N[N_2I_l(\sqrt{V_2-\alpha_{nl}^2}\rho)+K_l(\sqrt{V_2-\alpha_{nl}^2}\rho)]\rho^{n-1},\\ \Psi_3(\rho)&=N\frac{N_2I_l(\sqrt{V_2-\alpha_{nl}^2}b)+K_l(\sqrt{V_2-\alpha_{nl}^2}b)}{K_l(\sqrt{V_3-\alpha_{nl}^2}b)}\\ &\quad\times K_l(\sqrt{V_3-\alpha_{nl}^2}\rho)\rho^{n-1}.\end{aligned} \tag{9}$$

Furthermore, the derivative of the wave function is continuous at $\rho=a$, thus,

$$N_2=\frac{K_l'(\sqrt{V_2-\alpha_{nl}^2}a)J_l(\alpha_{nl}a)-K_l(\sqrt{V_2-\alpha_{nl}^2}a)J_l'(\alpha_{nl}a)}{I_l(\sqrt{V_2-\alpha_{nl}^2}a)J_l'(\alpha_{nl}a)-I_l'(\sqrt{V_2-\alpha_{nl}^2}a)J_l(\alpha_{nl}a)}. \tag{10}$$

And the trial function of the eigenstates of the impurity system can then be assumed as

$$\Psi_{i1}(\rho)=N\left[\frac{K_l'(\sqrt{V_2-\alpha_{nl}^2}a)J_l(\alpha_{nl}a)-K_l(\sqrt{V_2-\alpha_{nl}^2}a)J_l'(\alpha_{nl}a)}{I_l(\sqrt{V_2-\alpha_{nl}^2}a)J_l'(\alpha_{nl}a)-I_l'(\sqrt{V_2-\alpha_{nl}^2}a)J_l(\alpha_{nl}a)}I_l(\sqrt{V_2-\alpha_{nl}^2}a)+K_l(\sqrt{V_2-\alpha_{nl}^2}a)\right]\times\frac{J_l(\alpha_{nl}\rho)}{J_l(\alpha_{nl}a)}\rho^{n-1}e^{-\lambda\sqrt{\rho^2+z^2}}, \tag{11}$$

$$\Psi_{i2}(\rho)=N\left[\frac{K_l'(\sqrt{V_2-\alpha_{nl}^2}a)J_l(\alpha_{nl}a)-K_l(\sqrt{V_2-\alpha_{nl}^2}a)J_l'(\alpha_{nl}a)}{I_l(\sqrt{V_2-\alpha_{nl}^2}a)J_l'(\alpha_{nl}a)-I_l'(\sqrt{V_2-\alpha_{nl}^2}a)J_l(\alpha_{nl}a)}I_l(\sqrt{V_2-\alpha_{nl}^2}\rho)+K_l(\sqrt{V_2-\alpha_{nl}^2}\rho)\right]\rho^{n-1}e^{-\lambda\sqrt{\rho^2+z^2}}, \tag{12}$$

$$\Psi_{i3}(\rho)=N\left[\frac{K_l'(\sqrt{V_2-\alpha_{nl}^2}a)J_l(\alpha_{nl}a)-K_l(\sqrt{V_2-\alpha_{nl}^2}a)J_l'(\alpha_{nl}a)}{I_l(\sqrt{V_2-\alpha_{nl}^2}a)J_l'(\alpha_{nl}a)-I_l'(\sqrt{V_2-\alpha_{nl}^2}a)J_l(\alpha_{nl}a)}I_l(\sqrt{V_2-\alpha_{nl}^2}b)+K_l(\sqrt{V_2-\alpha_{nl}^2}b)\right]$$
$$\times\frac{K_l(\sqrt{V_3-\alpha_{nl}^2}\rho)}{K_l(\sqrt{V_3-\alpha_{nl}^2}b)}\rho^{n-1}e^{-\lambda\sqrt{\rho^2+z^2}}, \tag{13}$$

where N is the normalization constant, and α_{nl} is the nth root satisfying the boundary condition

$$\left.\frac{\partial\Psi_2(\rho)}{\partial\rho}\right|_{\rho=b}=\left.\frac{\partial\Psi_3(r)}{\partial\rho}\right|_{\rho=b}, \tag{14}$$

and

$$N^{-2}=-\pi\frac{d(G+H+M)}{d\lambda}, \tag{15}$$

with

$$G=\int_0^a\rho\Psi_1^2(\rho)K_0(2\lambda\rho)d\rho, \tag{16}$$

$$H=\int_a^b\rho\Psi_2^2(\rho)K_0(2\lambda\rho)d\rho, \tag{17}$$

$$M=\int_b^\infty\rho\Psi_3^2(\rho)K_0(2\lambda\rho)d\rho. \tag{18}$$

The binding energy E_b of the hydrogenic impurity is defined conventionally, as the energy difference between the energy of the system without the impurity and the energy of the system with the impurity; i.e.,

$$E_b=-\lambda^2-\frac{4(G+H+M)}{\dfrac{d(G+H+M)}{d\lambda}}. \tag{19}$$

In Eq. (19) the energy and length are expressed in Rydberg and Bohr radius of the wire material, respectively. For the single-layered quantum-wire model, it is only to set $a=b$ and $V_2=V_3$.

III. RESULTS AND DISCUSSIONS

To make a comparison, we first set $V_2=V_3=V$, which is equivalent to considering the case of a single-layer quantum wire. If one plots the probability density $|\Psi(r,z)|^2$ of lower-lying states of a hydrogenic impurity located at the center of a single-layered GaAs quantum wire surrounded by $Ga_{1-x}Al_xAs$ with $x=0.1$, the results will show that only the probability density of the $1s$ state is almost concentrated in the well with radius $|a|=1a_0^*$. The leakage probability density is increased as n increases, where n is the principal quantum number. This shows that the leaking effect is prominent for the large principal quantum number for a fixed wire radius. Figure 1 shows the calculated binding energy of $1s$, $2p$, and $3d$ states with $x=0.1$. For comparison, the previous result of Bryant[13] is also presented together. One can note that for a single-layered quantum wire with very large wire radius, the impurity behaves just like a three-dimensional free-hydrogen atom, thus its level energies of a hydrogenic impurity will approach the three-dimensional value $(1/n^2)$ Ry. If the wire radius decreases, the confinement effect enhances the binding energy more prominently. Thus, the binding energy of the impurity increases monotonically with the wire radius. However, as the wire radius is further decreased, the state energy of the impurity may become higher than the confining barrier. Meanwhile, the kinetic energy of the confined electron becomes larger by the uncertainty principle, and thus increases the probability of the electron leaking outside the well. The electron behaves like a three-dimensional (3D) electron after a certain characteristic wire radius and is only weakly perturbed by the potential well. Therefore, the level energies resume $(1/n^2)$ Ry again. Our results show some discrepancies from that of Bryant.[13] However, our results are more consistent with the correct limiting value as the radius approaches zero or infinity. Thus, our results are better than that of Bryant and agree better with the corresponding value of a free atom in 3D. The binding energy of $2p$ state obtained by Bryant approaches 1 Ry as the radius approaches infinity, which disagrees with the corresponding value of a free atom in the case of 3D. In Fig. 1, we also compare the confinement of the wire and dot,[45] and our result shows the confinement in the QD is stronger. We also calculate the $1s$-, $2p$-, $3d$-state binding energies of the hydrogenic impurity in the quantum wire with infinite potential barriers. The binding energies were found to approach the corresponding limiting values $[(1/n^2)$ Ry$]$ of a free atom in 3D as the wire radius approaches infinity. As the radius decreases from infinity, the binding energies increase and approach infinity, which agrees with the previous results.[17,18]

Figure 2 shows the ground-state binding energy of a hydrogenic impurity located at the center of a multilayered quantum wire ($GaAs$-$Ga_{1-x}Al_xAs$-$Ga_{1-y}Al_yAs$) as a function of core wire radius for different shell thicknesses with the Al concentration $x=0.2$, $y=0.1$. In Fig. 2, the curve of $b-a=\infty$ is the same as the case of the single-layered quantum wire with the Al concentration $x=0.1$. Comparing the case of the single-layered QW with the multilayered QW, one can find that their binding energies are very different for small wire radius. This is due to the different leakage probability of the electron in the single-layered and multilayered QWS. For a small single-layered QW, the electron leaks to the barrier ($Ga_{1-x}Al_xAs$), and the impurity atom behaves just like a free-hydrogen atom, thus, the binding energy approaches 1 Ry. For the MLQW, the electron tunnels to the bulk region ($Ga_{1-y}Al_yAs$) and still behaves like a confined electron as the core radius approaches zero. Figure 3 shows

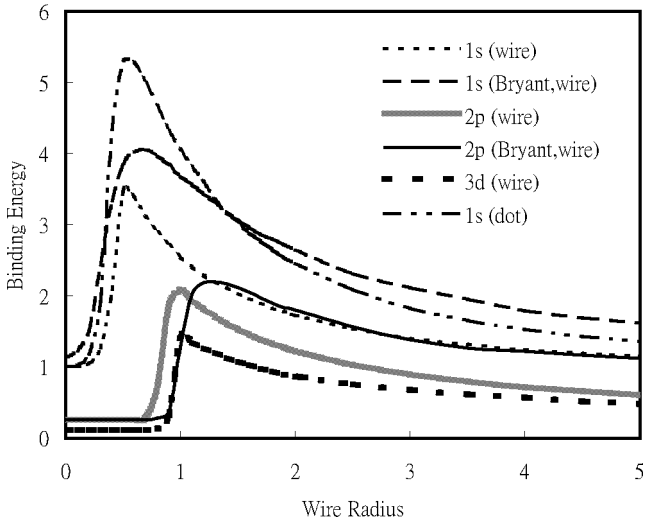

FIG. 1. 1s-, 2p-, and 3d-state binding energy of a hydrogenic impurity in a single-layered quantum wire and 1s-state binding energy of a hydrogenic impurity in quantum dot with the $Ga_{1-x}Al_xAs$ of aluminum concentration $x=0.1$, and the previous result of Bryan (Ref. 13).

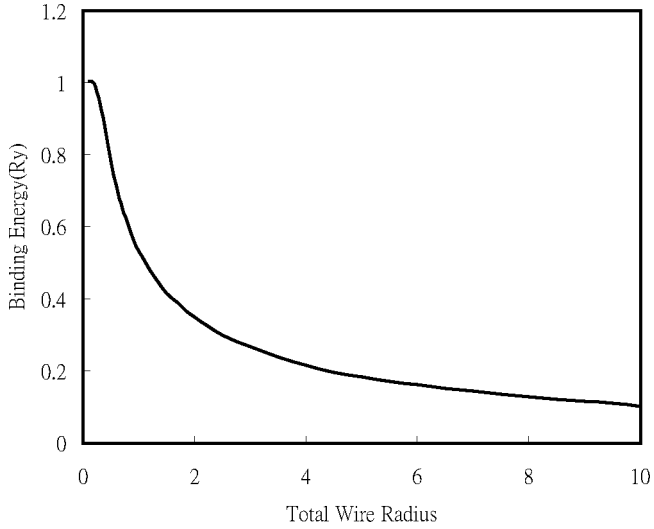

FIG. 3. Ground-state binding energy of a hydrogenic impurity located at the center of a multilayered quantum wire as a function of total wire radius with core wire radius $a=0.1a_0^*$ and the Al concentration $x=0.2$, $y=0.1$.

the binding energy decreases from 1 to 0 Ry as the total wire radius is increased. This is because the distance between the ion and the electron is increased as the total wire radius is increased, thus decreasing the binding between the electron and the impurity ion.

For small core wire radius, the electron tunnels to the bulk region for Al concentration $x=0.2$ and $y=0.1$. But, when the electron begins to leak out of the well and tunnels to the shell or bulk region, the leakage probability depends on the core wire radius and the difference of the Al concentration between the shell and bulk materials. As shown in Fig. 4, as y increases from 0.01 to 0.2, the binding energy increases from 0.671 to 1.007 Ry for $a=0.1a_0^*$ and increases from 0.625 to 2.404 Ry for $a=0.2a_0^*$. For smaller core wire radius ($a=0.1a_0^*$), the electron tunnels completely to the bulk region. For $a=0.2a_0^*$, the electron tunnels to the bulk region for $y<0.16$ and the electron tunnels to the shell region as $y>0.16$.

IV. CONCLUSION

We successfully propose a trial function for calculating the level energies of hydrogenic impurity located at the center of a single-layered quantum wire and multilayered quantum wire. Our results are satisfactory and reasonable compared with the previous result obtained by Bryant.[13]

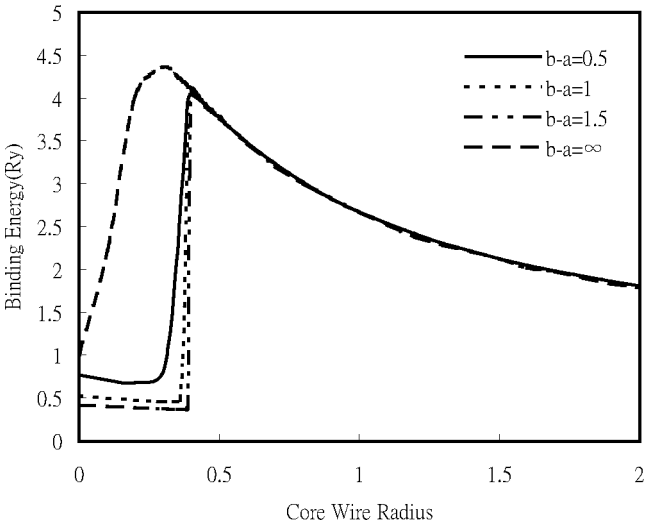

FIG. 2. Ground-state binding energy of a hydrogenic impurity located at the center of a multilayered quantum wire as a function of core wire radius for the different shell thicknesses $b-a=0.5,1,1.5,\infty a_0^*$ with the Al concentration $x=0.2$, $y=0.1$.

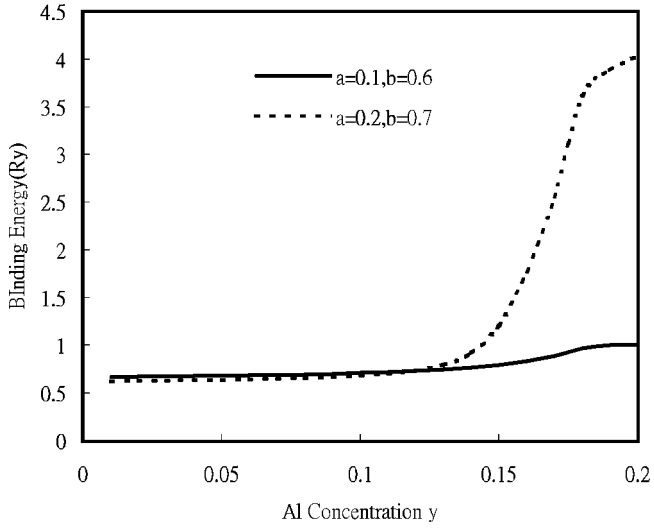

FIG. 4. Ground-state binding energy of a hydrogenic impurity located at the center of a multilayered quantum wire as a function of Al concentration of bulk material y with $x=0.2$ and $b-a=0.5a_0^*$ for $a=0.1a_0^*$ and $a=0.2a_0^*$, respectively.

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