Effect of a spatially dependent effective mass on the hydrogenic impurity binding energy in a finite parabolic quantum well

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The effect of a spatially dependent effective mass in a finite GaAs/Al$_x$Ga$_{1-x}$As parabolic quantum well on hydrogenic impurity ground state ($1s$) binding energies and transition energies between a $1s$ state and low-lying excited state ($2p_{\pm}$-like) has been calculated, respectively, as a function of well width and impurity position by using the one-dimensional method. Our results are compared with Niculescu's results of constant effective mass. We find that the $1s$ state binding energies and the $1s \rightarrow 2p_{\pm}$ transition energies are greater than Niculescu results for the same well width, respectively. These results are obtained as the impurity is located at the well center. At the same time the well widths corresponding to maximum values of the $1s$ state binding energies and the $1s \rightarrow 2p_{\pm}$ transition energies are less than those of Niculescu, respectively. The physical meaning of $1/(1-\lambda)$ is discussed. [S0163-1829(98)03840-5]

I. INTRODUCTION

Since the early 1970's, many physicists have been interested in semiconductor superlattice structures. They have made numerous studies on hydrogenic impurities in square quantum wells (SQW's). But with the development of the molecular-beam epitaxy (MBE) growth method, parabolic quantum wells (PQW's) are being generated by at least two types of superlattices, namely, compositional PQW's (Ref. 1) and doping PQW's (Ref. 2). As to the former, the smooth effective PQW is obtained as a result of making an appropriate change about the width of sets of GaAs/Al$_x$Ga$_{1-x}$As layers. For this PQW, to our knowledge it is accepted by all that the alloy composition x changes continuously from the well center to the well edge. Knowledge of the influence of shallow impurities in this system leads to an understanding of the various electrical and optical properties related to the two-dimensional behavior. Up to now there have appeared some reports on impurity states in PQW's.[3–10] Luna-Acosta[3] calculated the binding energy of the hydrogenic impurity that is at the center of an infinite PQW. He adopted the variational method with a two-parameter trial wave function. Later, Learitt[4] calculated the binding energy of the hydrogenic impurity state by using another trial wave function with the extension that the impurity can be located outside the center of the PQW. Zang and Rustgi[7] examined the energy levels of hydrogenic impurities in PQW's with a magnetic field. Niculescu,[5] calculated variationally binding energies of single and double donors in finite PQW's and discussed the validity of the infinite-parabolic-well approximation. Furthermore, Niculescu[6] calculated the binding energy of the ground state of a double donor by taking into account the nonparabolicity of the conduction band. Still, there are authors who discussed the properties of the hydrogenic impurities in a parabolic quantum wire and dot.[8–10]

So far only Herling and Rustgi,[12] to our knowledge, have discussed the effect of a spatially dependent effective mass (SDEM) on the electron state in a finite PQW. No one has discussed the effect of a SDEM on hydrogenic impurities calculation in a finite PQW. In this paper, we have considered the effect of a SDEM on $1s$ hydrogenic impurity state binding energies and $1s \rightarrow 2p_{\pm}$ transition energies in a finite PQW and have obtained different results. The $1s$ state binding energies and the $1s \rightarrow 2p_{\pm}$ transition energies are greater than Niculescu's results for the same well width, respectively. These results are obtained as the impurity is located at the well center. At the same time the values of the well width corresponding to maximum values of the $1s$ state binding energies and the $1s \rightarrow 2p_{\pm}$ transition energies are less than those of Niculescu. The method used in our calculation is a one-dimensional method that is developed by Liu[13] in calculating the hydrogenic impurity binding energies in a square well. It is a kind of variational calculation. Its superiority is that the three-dimensional Schrödinger equation of the hydrogenic impurity is simplified into the one-dimensional equivalent equation by selecting a reasonable variational wave function. The one-dimensional equivalent equation has two characteristics: (a) There is no oddity and it is easily calculated; (b) it has an analytical solution that satisfies the boundary condition and has the same result as that of a bulk material when the well width L approaches 0 and ∞.

In Sec. II we show how to extend the one-dimensional method[13] to the case of infinite PQW's and finite PQW's and derive the corresponding one-dimensional equivalent equation. Our results are discussed in detail and compared with the previous theoretical results in Sec. III, and Sec. IV is our conclusion.

II. ONE-DIMENSIONAL EQUIVALENT EQUATION

For the system of a finite PQW of GaAs/Al$_x$Ga$_{1-x}$As, we take the quantum well of width $L = 2a$ (along the z direction) and height V_0. Then the potential is

$$V(z) = \begin{cases} \dfrac{1}{2}kz^2 & |z| < a \\[2mm] V_0 = \dfrac{1}{2}ka^2 & |z| \geq a, \end{cases} \tag{1}$$

where $k = 2V_0/a^2$, and a is half-well width.

Considering the effect of a SDEM, the effective mass of the electron in the well can be written[12] as

$$m_1^*(z) = g(z)m_1^*, \qquad (2)$$

where m_1^* is the value in bulk GaAs. For $0 \leqslant x \leqslant 0.4$, the band-gap expression is well approximated by $\triangle E_g = 1250x$ meV,[12] and the x is the Al concentration in GaAs/Al$_x$Ga$_{1-x}$As. The relation between the potential and band gap is[12] $V(z) = 0.6 \triangle E_g$. The effective mass of the electron in PQW is given by $m_1^*(z) = 0.0665 + 0.0835x$, so we obtained

$$g(z) = 1 + 0.4018z^2/a^2. \qquad (3)$$

If not considering the effect of a SDEM, the effective mass of the electron in the well is m_1^*, in other words, $g(z)$ equals 1.

In the effective-mass approximation, the Hamiltonian of hydrogenic impurities in a finite PQW system can be written

$$H = \begin{cases} -\nabla \dfrac{\hbar^2}{2m_1^*(z)} \cdot \nabla - \dfrac{e^2}{\varepsilon r} + \dfrac{1}{2}kz^2, & |z| < a \\[3mm] -\dfrac{\hbar^2}{2m_2^*}\nabla^2 - \dfrac{e^2}{\varepsilon r} + V_0, & |z| \geqslant a. \end{cases} \qquad (4)$$

The origin of the coordinate system is chosen at the well center and z_0 is the coordinate of the impurity along the z axis, which is perpendicular to the layer planes, where m_2^* is the effective mass of the electron in bulk Al$_x$Ga$_{1-x}$As and $r = \sqrt{x^2 + y^2 + (z-z_0)^2}$ is the distance between the electron and the hydrogenic impurity center. The Schrödinger equation and the boundary condition at $|z| = a$ are, respectively,

$$H\psi = E\psi, \qquad (5)$$

$$\psi_- = \psi_+, \qquad \frac{1}{m_1^*(z)}\frac{\partial \psi}{\partial z}\bigg|_- = \frac{1}{m_2^*}\frac{\partial \psi}{\partial z}\bigg|_+, \qquad (6)$$

where $\pm$ indicates $|z| \rightarrow a \pm 0_\pm$.

From the one-dimensional method, we chose the trial wave function,[13]

$$\psi = e^{\lambda r}f^{-1/2}W(z)\Phi. \qquad (7)$$

The expression and requirements of Φ are the same as those in Ref. 13. We can obtain an equivalent one-dimensional equation through a series of complex calculations:

$$-\frac{1}{g(z)}\frac{d^2W}{d^2z} + \frac{g'(z)}{g(z)^2}\frac{dW}{dz} + \frac{UW}{g(z)} = EW, \qquad |z| < a$$

$$-\alpha\frac{d^2W}{d^2z} + \bar{U}W = EW, \qquad |z| \geqslant a, \qquad (8)$$

where $\alpha = m_1^*/m_2^*$ and the one-dimensional equivalent potential is

$$U = U_0 + \frac{1}{2}g(z)kz^2 + 2[1 - g(z)]\frac{F_1}{F}, \qquad |z| < a \qquad (9)$$

$$\bar{U} = V_0 + \alpha U_0 + 2(\alpha - 1)\frac{F_1}{F}, \qquad |z| \geqslant a. \qquad (10)$$

In calculation, U_0, K, F, F_1, and F_2 are the same as they are in Ref. 13. The boundary condition is

$$W_- = W_+, \qquad \frac{1}{m_1^*}\frac{dW}{dz}\bigg|_- = \frac{1}{m_2^*}\frac{dW}{dz}\bigg|_+. \qquad (11)$$

In order to obtain the one-dimensional equivalent potential, we chose φ_{100} and $\varphi_{21\pm1}$ as the skeleton states, respectively, for the $1s$ state and $2p_\pm$-like state to calculate K, F, F_1, and F_2. Thus the $1s$ state and $2p_\pm$-like state energies (E) of the impurity state can be obtained by numerically solving Eq. (8). The binding energies (E_b) of the system can be obtained by $E_b = E_0 - E$, where E_0 is the $1s$ state energy of the electron in a PQW without the impurity potential. Without the effect of a SDEM, E_0 is determined by numerically solving the transcendental equation[11]

$$2\phi'(\bar{V}a^2) = \phi(\bar{V}a^2)[1 - \bar{W}\sqrt{\alpha}/(\bar{V}\alpha)], \qquad (12)$$

where $\bar{V}^2 = V_0/a^2$, $\bar{W}^2 = V_0 - E_0$, $\phi(\zeta)$ is a confluent hypergeometric function.

When we take the effect of a SDEM into account, E_0 is obtained by numerically solving the Schrödinger equation (13) subject to the boundary condition (14),

$$\left[-\frac{d}{dz}\frac{\hbar^2}{2m_1^*(z)}\frac{d}{dz} + \frac{1}{2}kz^2\right]\psi(z) = E_0\psi(z), \qquad |z| < a$$

$$\left[-\frac{\hbar^2}{2m_2^*}\frac{d^2}{dz^2} + V_0\right]\psi(z) = E_0\psi(z), \qquad |z| \geqslant a, \qquad (13)$$

$$\psi_+ = \psi_-, \qquad \psi'_+ = \psi'_-. \qquad (14)$$

In our calculation, the largest value of Al concentration x at the well edge is 0.32. So the potential well height (V_0) is 240 meV. Ignoring the difference of dielectric constants between in the well and barrier, we take the average value $\epsilon = (\epsilon_1 + \epsilon_2)/2$, where $\epsilon_1 = 12.53$ and $\epsilon_2 = 12.53 - 2.73x$,[14,15] respectively.

In the infinite PQW, the ground-state energy E is calculated with the same process as that in the finite PQW. But the calculation is made only in the well without boundary condition. E_0 is obtained by the equation $E_0 = \sqrt{\hbar^2k/4m_1^*}$. In the preceding calculation, the units of energy and distance are the electron Rydberg $R_d = m_1^*e^4/2\epsilon_0^2\hbar^2$ and Bohr radius $a_0 = \epsilon_0\hbar^2/m_1^*e^2$ in GaAs, respectively.

III. RESULTS AND DISCUSSION

It can be seen from Fig. 1 that the binding energies E_b increase with the increasing k, which is consistent with the previous results,[3,4,7] and reflects the effect of the term $\frac{1}{2}kz^2$ in the Hamiltonian (4). But we noticed that our results are greater than those in Ref. 3 and Ref. 4. This shows the one-dimensional method is suitable for calculating E_b of hydrogenic impurities in the PQW.

By adopting the one-dimensional method, the binding energies of the $1s$ hydrogenic impurity state are calculated as a function of the well width in the finite PQW for the on-center
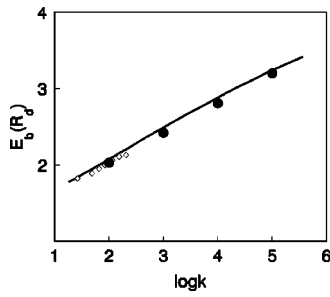
FIG. 1. Impurity binding energy E_b in an infinite PQW vs parabolic coefficient k. The solid curve indicates our result; ● indicates the results of Ref. 4, and ◇ indicates the results of Ref. 3. k is in units of R_d/a_0^2.

and the on-edge impurity. We obtained the results considering the effect of a SDEM and the results ignoring the effect of a SDEM, respectively. Figure 2 shows the following.

(i) When the effect of a SDEM is considered, the binding energies increase and the increasing values vary with the well width. The reason is that the average effective mass of the electron increases because of the effect of a SDEM and leads to a great reduction of the system energy. Moreover, the magnitude of the system energy reduction becomes less as the well becomes wider. It is the result of the gradient of the effective mass decreasing at the same degree.[12] The effective mass of the electron tends to the value of bulk material when well width L approaches 0 and ∞. Thus the effect of a SDEM becomes weak for very small or large well widths.

(ii) The qualitative dependence of E_b on L is consistent with the result of Niculescu.[5] But for the on-center impurity, our results display two aspects different from Niculescu's.[5] (a) Our E_b values are greater than Niculescu's for the same well width. The peak correction is about 22% considering the effect of a SDEM, but the peak correction is only 13% without considering the effect of a SDEM. (b) The value of the well width corresponding to the peak is about $0.25a_0$, which is less than $0.5a_0$ of Niculescu.[5] The reason for this difference might be as follows: The effect of a SDEM leads to reduction of the $1s$ state energy level,[12] and the height of barrier of our calculation is 32 meV more than that of Niculescu.

(iii) The effect of a SDEM becomes weak when the value of the well width increases to about $4a_0$ for the on-center
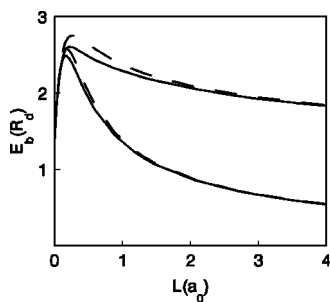

FIG. 2. Impurity binding energy E_b of the on-center (upper two curves) and the on-edge (lower two curves) impurity ground state as a function of well width. The solid curves indicate the result without the effect of a SDEM; the broken curves indicate the result with the effect of a SDEM.
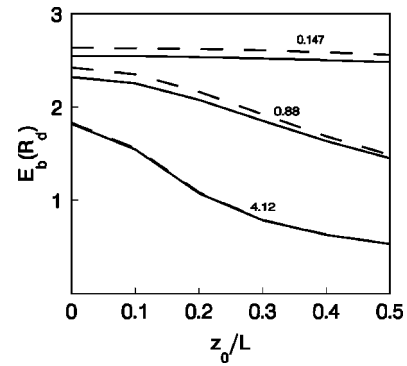

FIG. 3. Impurity binding energy E_b of the ground state for three given wells [$L=0.147a_0$ (upper two curves), $L=0.88a_0$ (middle two curves), $L=4.12a_0$ (lower two curves)], vs the position of the impurity atom in a finite PQW. The solid curves indicate the result without the effect of a SDEM; the broken curves indicate the result with the effect of a SDEM.

impurity. But for the on-edge impurity, the effect of a SDEM becomes weak when the value of the well width increases to about $2.5a_0$. We know that the system binding energies are determined by Coulomb potential, repulsion of both barriers, and the effect of a SDEM. For the on-center impurity, the whole system is symmetrical about the well center, so repulsions of the two barriers nearly offset each other. Thus the effect of a SDEM is important and its sphere of influence scope becomes wider. However, for the on-edge impurity, the symmetry of the system is destroyed. Then one barrier's strong repulsion offsets the effect of a SDEM; consequently its sphere of influence becomes narrower.

Figure 3 indicates that the binding energies reduce with the increase of the distance between the impurity and the well center in the three given wells (the values of the well width L are, respectively, $0.147a_0$, $0.88a_0$, and $4.12a_0$). This agrees qualitatively with the result of Learitt,[4] due to the weakness of the Coulomb potential with the increase of the distance between the impurity and the well center. In addition, when considering the effect of a SDEM, the increasing magnitude of the E_b varies with the impurity position in the three given wells. In a narrower well, for example, $L=0.147a_0$, the increasing values of the binding energies do not vary with the impurity position. But in a wider well such as $L=0.88a_0$, the increasing values reduce while the impurity is far away from the well center. When L is up to $4.12a_0$, the increasing values of the binding energies do not vary with the impurity position and nearly tend to zero. It is not difficult to understand the cause in a very wide well (e.g., $L=4.12a_0$) as is shown in Fig. 2. However, when the impurity is far away from the well center in a narrow well, the comprehensive effect of a SDEM and potential barrier strong repulsion leads to the results in Fig. 3. Because two barriers' strong repulsion keeps balance basically in an extremely narrow well (e.g., $L=0.147a_0$), the effect of a SDEM is not affected. But when the value of the well width increases relatively, for instance, $L=0.88a_0$, the farther the impurity is away from the well center; the more obvious the disequilibrium of two potential barriers' repulsion is, the stronger the effect of a SDEM is offset.

In addition, we calculate the $1s \rightarrow 2p_\pm$ transition energies. Figure 4 gives the $1s \rightarrow 2p_\pm$ transition energies as a function
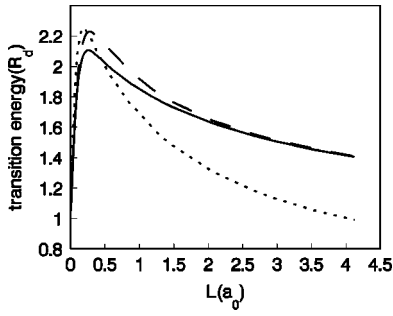
FIG. 4. The $1s \rightarrow 2p_{\pm}$ transition energy of the on-center impurity state as a function of well width. The solid curve indicates the result without the effect of a SDEM; the broken curve indicates the result with the effect of a SDEM; the dotted curve indicates the result of a square well.

of the well width for a hydrogenic impurity in the PQW. We notice that the dependence of $1s \rightarrow 2p_{\pm}$ transition energies on the well width is consistent with the conclusion of Niculescu.[5] But the values obtained for the $1s \rightarrow 2p_{\pm}$ transition energies are greater than the results of Niculescu, and the well width corresponding to the peak is less than Niculescu's. At the same time we find that there is an intersect between the curve of the PQW and that of the SQW. If we do not consider the effect of a SDEM, the well width corresponding to the intersect is $0.5a_0$. When the well width is more than $0.5a_0$, our results are in qualitative agreement with Niculescu's results.[5] The condition is reversed as the value of the well width is less than $0.5a_0$. That is to say, the values obtained for the $1s \rightarrow 2p_{\pm}$ transition energies are less than those for square wells of the same well width. The reason is that the strong confined effect of a narrow PQW makes penetration of the wave function into the potential barrier increase greatly and leads to a reduction of the transition energy in a narrow PQW. We can also see from Fig. 4 that the effect of a SDEM increases the $1s \rightarrow 2p_{\pm}$ transition energies as the value of the well width increases to about $4a_0$. The value of the well width corresponding to intersect goes to a value of $0.25a_0$. The reason is that the effect of a SDEM leads to the $2p_{\pm}$-like state energy reduction, which is less than $1s$ state energy reduction.[12] When the value of the
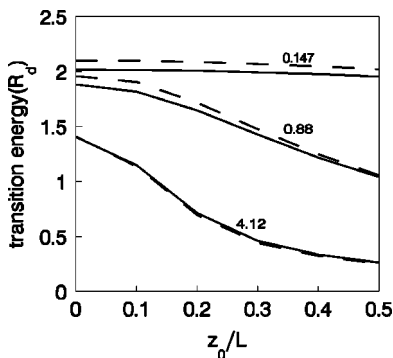

FIG. 5. The $1s \rightarrow 2p_{\pm}$ transition energy for three given wells [$L=0.147a_0$ (upper two curves), $L=0.88a_0$ (middle two curves), $L=4.12a_0$ (lower two curves)] vs the position of the impurity in a finite PQW. The solid curves indicate the result without the effect of a SDEM; the broken curves indicate the result with the effect of a SDEM.
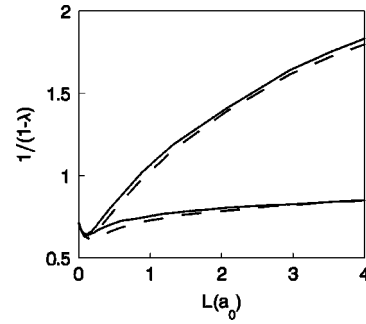

FIG. 6. The parameter $1/(1-\lambda)$ of the on-center (lower two curves) and the on-edge (upper two curves) impurity as a function of well width. The solid curves indicate the result without the effect of a SDEM; the broken curves indicate the result with the effect of a SDEM.

well width is very small or very large, the effect of a SDEM is too weak to be considered.

Figure 5 displays the $1s \rightarrow 2p_{\pm}$ transition energies as a function of impurity position for the three given wells. This shows the dependence of the $1s \rightarrow 2p_{\pm}$ transition energies on the impurity position is similar to that of the $1s$ state binding energies in the PQW.

Figure 6 shows $1/(1-\lambda)$ as the function of the well width. Its physical meaning could be interpreted as a measure of the extent of the electron density distribution.[13] Its dependence on the well width is consistent with that observed by Liu, and he gave a lengthly discussion.[13] In the case of the on-edge impurity, we can see that the electron is distributed in a relatively wider area than that of the on-center impurity. The reason is that the effect of the potential barrier's repulsion is more preponderant than the attraction of the on-edge impurity. At the same time, considering the effect of a SDEM, it can be seen that the values of $1/(1-\lambda)$ are slightly less than the values of the same well width without considering the effect of a SDEM. This shows that the radius of the impurity state becomes smaller. That is to say, the impurity attraction becomes strong, and E_b increases as is shown in the previous discussion.

IV. CONCLUSION

From the above discussion, we find that the effect of a SDEM increases the $1s$ state binding energies and the $1s \rightarrow 2p_{\pm}$ transition energies of the hydrogenic impurity. For the on-center impurity in a PQW, the effect of a SDEM is obvious for the $1s$ state binding energies and the $1s \rightarrow 2p_{\pm}$ transition energies while the well width is less than $4a_0$. But for the on-edge impurity, the effective range of a SDEM becomes narrower. The effect of a SDEM vanishes as the value of the well width exceeds $0.25a_0$. Moreover, the effect of a SDEM on the $1s$ state binding energies and the $1s \rightarrow 2p_{\pm}$ transition energies vary with the impurity position in different wells. In the extremely narrow wells, the effect of a SDEM does not vary with the impurity position. The result is that increasing values of the $1s$ state binding energies and the $1s \rightarrow 2p_{\pm}$ transition energies do not change with the variation of impurity position. In wide wells, the effect of a SDEM is obvious when the impurity is near the well center, however, the effect of a SDEM vanishes in much wider wells.

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