

## Theory of resonant states of hydrogenic impurities in quantum wells

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The binding energy and the density-of-states spectrum of resonant impurity states in quantum well structure have been theoretically studied with variation of the impurity position taken into account, using the multisubband model and the resolvent operator technique. Calculations for the  $2p_0$  resonant state in a GaAs-Al<sub>0.2</sub>Ga<sub>0.8</sub>As quantum well have been performed. It has been found that there can be a considerable resonant coupling in the  $2p_0$  state, causing a  $\sim 0.1$  ps capture or escape time of electrons between the  $2p_0$  localized state and the first subband states. The maximum shift of the impurity energy is in general of the order of 0.1 meV, much smaller than the maximum binding energy of the  $2p_0$  state.

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### I. INTRODUCTION

The study of the electronic states of a hydrogenic impurity in a semiconductor quantum-well (QW) structure has been a subject of considerable interest for the last two decades.<sup>1-15</sup> There have been numerous reports on calculations of the impurity states in such a system.<sup>1-14</sup> However, most of the studies are restricted to the calculation of the binding energies of the ground state or some low-lying excited states attached to the first subband.<sup>1-10</sup> In general, the calculation relies on the variational technique accompanied with a proper trial function. For the ground state, a good trial function should keep the calculation not too complicated and give the expectation energy of the state as low as possible. Typical forms for the trial function are bound and expressed as a linear combination of Gaussian orbitals<sup>2,11</sup> or as products of the envelope function of the first subband edge and a single or a linear combination of Gaussian (or exponential) orbitals.<sup>1,3-9</sup> Making use of the cylindrical symmetry of the systems, it is not difficult to obtain proper trial functions for the excited states below the first subband, such as the  $2p_{\pm}$  states.<sup>2,3,6-9,11</sup> However, the trial function for the  $2p_0$  state, which is cylindrically symmetric and has a node along the growth direction, has to be chosen with caution. When the  $2p_0$  donor level lies below the lowest subband for a wide QW, it is a localized state and a bound trial function is reasonable. Such a state is orthogonal to other localized impurity states below the first subband and can therefore be obtained simultaneously with the ground state in a matrix diagonalization.<sup>2,11</sup> It has been confirmed that as the QW width reduces, the on-center  $2p_0$  donor level moves with the second subband and then overlaps with the continuum of the first-subband states.<sup>3,6,8</sup> This indicates that the  $2p_0$  state should be attached to the second subband rather than the first one. Consequently, a trial function has been proposed in the form of the envelope function of the second-subband edge multiplying a linear combination of Gaussian or exponential orbitals.<sup>8,12</sup> However, such a trial function of the  $2p_0$  state, which when below the first subband has to stay orthogonal to the ground state, becomes inconvenient for an asymmetric system (with an impurity in an asymmetric QW or an off-center impurity in a symmetric QW).

When the  $2p_0$  state lies above the first subband, it may be

resonant with the first subband and no longer localized. The bound trial function becomes questionable for such a state which is composed of a bound part and an extending part. Priester *et al.*, first pointed out the resonance behavior of impurity states attached to higher-order subbands.<sup>12</sup> They proposed a type of trial function for the bound part and treated the resonant coupling with the technique of resolvent operators. Since then, the  $2p_0$  state has been treated with various trial functions.<sup>11-14</sup> The investigations were, nevertheless, restricted to symmetric systems where the  $2p_0$  state has an odd parity, leading to no coupling with the first subband. In this case the  $2p_0$  state is localized. This allows us to write down easily a proper trial function for the  $2p_0$  state. When the impurity is away from the QW center, the parity breaks down and the  $2p_0$  state is in resonance with the first subband. It is not trivial to determine a proper trial function for the bound part of the state since it is not a stationary state of the whole system and need not be orthogonal to other localized impurity states below the first subband.

The resonance of the  $2p_0$  state has been observed in resonant Raman scattering experiments.<sup>15</sup> The resonant states can serve as hot-carrier traps for the mechanism leading to a negative differential conductance.<sup>16</sup> They are also expected to play an important role in achievement of intrainpurity population inversion for terahertz stimulated emission.<sup>17</sup> It is therefore of scientific and technical importance to have a theoretical method for the investigation of the resonant impurity states. However, until now there has not existed any report on a treatment of the resonant impurity states in an asymmetric system.<sup>18</sup>

In this paper, we will theoretically study resonant states of a shallow donor arbitrarily lying in a two-dimensional QW structure based on the multisubband model. The density-of-states (DOS) spectra of the resonant states are obtained using the resolvent operator technique. For illustration, we calculate the binding energy, the DOS spectrum width, and the resonance energy shift of the  $2p_0$  state in a QW as a function of the impurity position. Considerable coupling is found. It causes a capture or escape time as short as  $\sim 0.1$  ps. The paper is organized as follows. In the following section, we present a theory of resonant impurity states in a QW. The calculated results of the  $2p_0$  state in GaAs-Al<sub>0.2</sub>Ga<sub>0.8</sub>As QW

are given in Sec. III. Finally, the conclusion is drawn in Sec. IV.

## II. THEORY

The effective-mass Hamiltonian for an electron bound to a donor in a QW structure can be written as

$$H = H_0 + V_c(\mathbf{r}), \quad (1)$$

where  $H_0$  is the impurity-free Hamiltonian and can be written as

$$H_0 = -\frac{\partial}{\partial z} \frac{1}{m_r(z)} \frac{\partial}{\partial z} - \nabla_{\parallel}^2 + V_0(z). \quad (2)$$

$V_c$  is the Coulomb potential energy of the impurity, having the following expression:

$$V_c(r) = -\frac{2}{\kappa(z) \sqrt{\rho^2 + (z - z_i)^2}}. \quad (3)$$

The Hamiltonian is written in the dimensionless form in which the energy and the length are in units of the effective Rydberg  $R^*$  ( $R^* = m_0^* e^4 / 2\epsilon_0^2 \hbar^2$ ) and effective Bohr radius  $a^*$  ( $a^* = \hbar^2 \epsilon_0 / m_0^* e^2$ ) of the well material, respectively. ( $m_0^*$  and  $\epsilon_0$  are the effective mass and the static dielectric constant, respectively, of the material making up the well.) The  $z$  axis is chosen to be along the growth direction of the layers.  $m_r(z)$  is the relative effective mass, defined as the ratio of the effective mass at  $z$  to that of the well material,  $m_0^*$ . Here  $V_0(z)$  is the potential energy of the two-dimensional QW in the absence of the impurity.  $\kappa(z)$  is the relative dielectric constant at  $z$  with respect to that of the well material. The impurity is assumed to be at  $\rho = 0$  and  $z = z_i$ .

The impurity-free Schrödinger equation

$$H_0 \psi_{n\mathbf{k}} = E_{n\mathbf{k}} \psi_{n\mathbf{k}} \quad (4)$$

can be readily solved with the eigenfunctions expressed as

$$\psi_{n\mathbf{k}} = \frac{1}{\sqrt{A}} e^{i\mathbf{k} \cdot \boldsymbol{\rho}} f_n(z), \quad (5)$$

where  $n$  is the subband index,  $\mathbf{k}$  is the in-plane wave vector, and  $A$  is the area of the QW for normalization of the eigenfunctions.

The wave functions of resonant states can be divided into two parts: a bound part and an extending part. Consider the energy  $E_I$  of an impurity state of interest to lie between the bottoms of the  $(\nu - 1)$ th and the  $\nu$ th subbands: that is,  $E_{\nu-1, \mathbf{k}=0} < E_I < E_{\nu, \mathbf{k}=0}$ . This impurity state is conventionally called as being attached to the  $\nu$ th subband. It may be in resonance with the mutually overlapped  $(\nu - 1)$  lowest subbands (subbands 1, 2, ...,  $\nu - 1$ ). The wave function of the resonant state as  $\rho \rightarrow \infty$  can be written in a linear combination of solutions of the Schrödinger equation, which now can be regarded to be impurity free—that is,

$$\psi^{(\nu m)} = \psi_B^{(\nu m)} + \psi_X^{(\nu m)}, \quad (6)$$

where

$$\psi_B^{(\nu m)}(\rho \rightarrow \infty, \phi, z) = e^{im\phi} \sum_{n \geq \nu} C_n^{(\nu m)} K_n[\text{Im}(k_n \rho)] f_n(z), \quad (7a)$$

$$\psi_X^{(\nu m)}(\rho \rightarrow \infty, \phi, z) = e^{im\phi} \sum_{n < \nu} C_n^{(\nu m)} H_n^{(1)}(k_n \rho) f_n(z), \quad (7b)$$

with  $k_n = \sqrt{E_I - E_{n\mathbf{k}=0}}$ . Here  $K_n$  is the modified Bessel function of the second kind of order  $n$  and  $H_n^{(1)}$  is the Hankel function of the first kind of order  $n$ . The  $\phi$ -dependent function  $e^{im\phi}$ , where  $m$  is an integer, arises from the cylindrical symmetry of the system.  $C_n^{(\nu m)}$ 's are coefficients of the linear combination. It is clear that  $k_n$  is imaginary for  $n \geq \nu$  ( $E_I < E_{n\mathbf{k}=0}$ ) and real for  $n < \nu$  ( $E_I > E_{n\mathbf{k}=0}$ ). With the help of the fact that, as  $\rho \rightarrow \infty$ ,

$$K_n[\text{Im}(k_n \rho)] \rightarrow \frac{e^{-\text{Im}(k_n \rho)}}{\sqrt{2\pi \text{Im}(k_n \rho)}} \quad (8a)$$

and

$$H_n^{(1)}(k_n \rho) \rightarrow \sqrt{\frac{2}{\pi k_n \rho}} e^{-i(n/2 + 1/4)\pi} e^{ik_n \rho}, \quad (8b)$$

we know that  $\psi_B^{(\nu m)}$  in Eq. (7a) decays with  $\rho$  and should correspond to the bound part of the resonant state attached to the  $\nu$ th subband, while  $\psi_X^{(\nu m)}$  in Eq. (7b) behaves divergently as outgoing waves and should be responsible for the extending part. Since the plane waves  $e^{i\mathbf{k} \cdot \boldsymbol{\rho}}$  can serve as a complete set of basis functions for expressions of the  $\rho$ -dependent envelope functions multiplying by  $e^{im\phi}$ , the bound part  $\psi_B^{(\nu m)}(\rho \rightarrow \infty)$  in Eq. (7a) can be thought of as a linear combination of higher-subband states  $\psi_{n\mathbf{k}}$  with  $n \geq \nu$  while the extending part  $\psi_X^{(\nu m)}(\rho \rightarrow \infty)$  in Eq. (7b) is in a linear combination of lower-subband states  $\psi_{n\mathbf{k}}$  with  $n < \nu$ . It is therefore easy to divide the impurity resonant state into the bound and extending parts if the wave function over the whole range is assumed to be in the form

$$\psi^{(\nu m)} = e^{im\phi} \sum_{n=1}^{\infty} Y_n^{(\nu m)}(\rho) f_n(z) = \psi_B^{(\nu m)} + \psi_X^{(\nu m)}, \quad (9)$$

where

$$\psi_B^{(\nu m)} = e^{im\phi} \sum_{n=\nu}^{\infty} Y_n^{(\nu m)}(\rho) f_n(z) \quad (10a)$$

and

$$\psi_X^{(\nu m)} = e^{im\phi} \sum_{n=1}^{\nu-1} Y_n^{(\nu m)}(\rho) f_n(z). \quad (10b)$$

Comparing Eq. (10) with Eq. (7), we find that the  $\rho$ -dependent functions  $Y_n^{(\nu m)}$  should have the asymptotic behavior that, as  $\rho \rightarrow \infty$ ,

$$Y_n^{(\nu m)} \rightarrow C_n^{(\nu m)} K_n[\text{Im}(k_n)\rho] \quad (11a)$$

for  $n \geq \nu$  and

$$Y_n^{(\nu m)} \rightarrow C_n^{(\nu m)} H_n^{(1)}(k_n \rho) \quad (11b)$$

for  $n < \nu$ . Since the set of plane waves  $e^{i\mathbf{k}\cdot\boldsymbol{\rho}}$  is complete for expressions of all  $e^{im\phi} Y_n^{(\nu m)}(\rho)$ , it is concluded that the bound part of the resonant state is attributed entirely to the subband states with  $n \geq \nu$ , while the extending part is composed only of the subband states with  $n < \nu$ . Due to the orthogonality of the subband states, we have

$$\langle \psi_{n\mathbf{k}} | \psi_B^{(\nu m)} \rangle = 0 \quad (12a)$$

for  $n < \nu$  and thus

$$\langle \psi_X^{(\nu m)} | \psi_B^{(\nu m)} \rangle = 0. \quad (12b)$$

That is, the bound part is orthogonal to all lower-subband states and also to the extending part. Similarly, the extending part is orthogonal to all higher-subband states. Note that in the expansion (10a), the continuous unconfined subbands above the barriers as well as the confined subbands with  $n \geq \nu$  must be included to give a complete set of basis functions for the localized function  $\psi_B^{(\nu m)}$ .

It is convenient in derivation of formulas to decompose the Hilbert space into two subspaces  $\mathcal{S}_B^{(\nu)}$  and  $\mathcal{S}_X^{(\nu)}$ , where  $\mathcal{S}_B^{(\nu)}$  is the space with all higher-subband states  $\psi_{n\mathbf{k}}$  ( $n \geq \nu$ ) as basis vectors and  $\mathcal{S}_X^{(\nu)}$  is the one with all lower-subband states  $\psi_{n\mathbf{k}}$  ( $n < \nu$ ) as basis vectors. A projection operator  $P_\nu$  is defined to project a state onto the subspace  $\mathcal{S}_B^{(\nu)}$ . Accordingly, the total Hamiltonian in Eq. (1) can be written as

$$H = H_U^{(\nu)} + H_C^{(\nu)} + (1 - P_\nu) V_c (1 - P_\nu), \quad (13)$$

where

$$H_U^{(\nu)} = P_\nu (H_0 + V_c) P_\nu + H_0 (1 - P_\nu) \quad (14a)$$

and

$$H_C^{(\nu)} = (1 - P_\nu) V_c P_\nu + P_\nu V_c (1 - P_\nu). \quad (14b)$$

$H_U^{(\nu)}$  is the Hamiltonian of the uncoupled system in which there is no intersubspace coupling—i.e.,

$$\langle \psi_B | H_U^{(\nu)} | \psi_X \rangle = 0, \quad (15)$$

if  $\psi_B \in \mathcal{S}_B^{(\nu)}$  and  $\psi_X \in \mathcal{S}_X^{(\nu)}$ . In writing Eq. (14a), we have made use of the fact that  $P_\nu$  commutes with  $H_0$  such that  $(1 - P_\nu) H_0 (1 - P_\nu) = H_0 (1 - P_\nu)$ . Here  $H_C^{(\nu)}$  is the term for intersubspace coupling. The third term in Eq. (13) is for scattering within subspace  $\mathcal{S}_X^{(\nu)}$  and gives a second-order smaller effect if the impurity states and the resonant coupling are of main interest. This term will thus be neglected. From the physical viewpoint, the bound part of the resonant state  $\psi_B^{(\nu m)}$  should be stationary if the coupling  $H_C^{(\nu)}$  were switched off. That is,  $\psi_B^{(\nu m)}$  is an eigenstate of  $H_U^{(\nu)}$ . Since the lower-subband states  $\psi_{n\mathbf{k}} \in \mathcal{S}_X^{(\nu)}$  are also eigenstates of  $H_U^{(\nu)}$ , as can be easily seen from Eq. (14a), the uncoupled Hamiltonian, which will be regarded to be zeroth order, is

diagonal in the representation for which  $\psi_B^{(\nu m)}$  and all the lower-subband states  $\psi_{n\mathbf{k}} \in \mathcal{S}_X^{(\nu)}$  serve as basis functions. Note that the localized states  $\psi_B^{(\nu m)}$  attached to different subbands  $\nu$  are eigenstates of different Hamiltonians  $H_U^{(\nu)}$ . The orthogonality between those localized states is not guaranteed. In some cases, there is more than one localized state which is attached to a common subband and has the same symmetry of axial rotation. An additional index—say,  $j$ —is required as well as the indices  $(\nu m)$  to characterize these states. These states  $\psi_B^{(\nu m j)}$  must be mutually orthogonal because they are distinct eigenstates of the same Hamiltonian  $H_U^{(\nu)}$ .

To find the bound part of a resonant state, we imagine that the resonant coupling is at present switched off. Define a space  $\mathcal{S}_B^{(\nu m)}$  in which each element can be expressed in the form of the right of Eq. (10a) with the specific indices  $(\nu m)$ . All the localized states  $\psi_B^{(\nu m j)}$ ,  $j = 1, 2, \dots$ , characterized by the same  $(\nu m)$  are therefore in  $\mathcal{S}_B^{(\nu m)}$ . We first restrict our attention to  $\psi_B^{(\nu m 1)}$  which is the lowest of all the states  $\psi_B^{(\nu m j)}$ . The state  $\psi_B^{(\nu m 1)}$  is the *ground* state in the space  $\mathcal{S}_B^{(\nu m)}$  of the uncoupled Hamiltonian  $H_U^{(\nu)}$  even if it may not be the ground state in the space  $\mathcal{S}_B^{(\nu)}$  and in the whole Hilbert space. What the problem becomes now is to find a set of  $Y_n^{(\nu m)}(\rho)$  ( $n \geq \nu$ ) in Eq. (10a) such that the expectation energy  $E_I^{(\nu m)} = \langle \psi_B^{(\nu m)} | H_U^{(\nu)} | \psi_B^{(\nu m)} \rangle$ , which is also equal to  $\langle \psi_B^{(\nu m)} | H | \psi_B^{(\nu m)} \rangle$ , has the lowest energy. To this end, we use the variation method with trial functions for  $Y_n^{(\nu m)}(\rho)$  in the following form:

$$Y_n^{(\nu m)}(\rho) = \rho^{|m|} \sum_l C_{nl}^{(\nu m)} e^{-\alpha_l^{(\nu m)} \rho^2} \quad (16)$$

for  $n \geq \nu$ . Such an expression has the asymptotic behavior that  $Y_n^{(\nu m)} \rightarrow \rho^{|m|}$  as  $\rho \rightarrow 0$  and  $Y_n^{(\nu m)} \rightarrow 0$  as  $\rho \rightarrow \infty$ , in consistency with the asymptotic behavior of the solution of the uncoupled Schrödinger equation. The coefficients  $C_{nl}^{(\nu m)}$  are linear variational parameters, and  $\alpha_l^{(\nu m)}$  can serve as nonlinear variational parameters. For a given set of  $\alpha_l^{(\nu m)}$ , a matrix eigenvalue problem for the coefficients  $C_{nl}^{(\nu m)}$  can be obtained by means of variations applied to the expectation energy  $E_I^{(\nu m)}$  with respect to  $C_{nl}^{(\nu m)}$ . The coefficients are then obtained simply by matrix diagonalization. By varying the nonlinear parameters  $\alpha_l^{(\nu m)}$ , we have more degrees of freedom to obtain a lower  $E_I^{(\nu m)}$  which corresponds to a more accurate solution. The set of  $\alpha_l^{(\nu m)}$  leading to the minimum energy gives the best solution in the framework of the trial function in the form of Eqs. (10a) and (16). The other states  $\psi_B^{(\nu m j)}$ ,  $j \neq 1$ , can be obtained simultaneously with the lowest state  $\psi_B^{(\nu m 1)}$  by the matrix diagonalization. The binding energy of the localized state  $\psi_B^{(\nu m j)}$  is defined to be  $E_B^{(\nu m j)} = E_{\nu 0} - E_I^{(\nu m j)}$ , where  $E_I^{(\nu m j)}$  is the energy of the states  $\psi_B^{(\nu m j)}$ . Since the total Hamiltonian  $H$  depends on the QW structure and the impurity position  $z_i$ , the resulting energy  $E_I^{(\nu m j)}$  and parameters  $C_{nl}^{(\nu m j)}$  and  $\alpha_l^{(\nu m j)}$  (and thus  $\psi_B^{(\nu m j)}$ ) are also functions of the QW structure and  $z_i$ . The Gaussian orbitals chosen for composition of the trial function make

tractable the integrals encountered in calculations of the matrix elements of the eigenvalue problem. However, the multisubband trial function in the form of Eq. (10a) has the shortcoming that an accurate solution requires a large amount of higher subbands to be included in the variational method for an impurity state in a wide well, regardless of the impurity position. Since we are mainly interested in the resonant impurity states which appear only in a sufficiently narrow well, we will not encounter the difficulty in the present paper.

In the expression (10a), we have included all the higher subbands ( $n \geq \nu$ ) for the trial function of the localized states  $\psi_B^{(\nu m j)}$ . The more subbands the trial function contains, the more accurate the solution is. However, for a QW surrounded by finite barriers, the subbands with bottoms above the barriers merge into a continuum, causing difficulty in the treatment of the variational technique. In fact, the inclusion of all higher  $f_n(z)$  with  $n \geq \nu$  in Eq. (10a) serves to form a complete basis set to accurately construct the  $z$ -dependent component of the localized states  $\psi_B^{(\nu m j)}(\rho, \phi, z)$  for an arbitrary  $\rho$ . To solve this problem, we discretize the continuum of subbands by putting two infinite potential walls enclosing the QW structure in the  $z$  direction as long as the walls are far away from each other such that the impurity states of interest will not be affected by the enclosure. The resulting discrete subbands can thus mathematically serve as a basis set to accurately construct the  $z$ -dependent component of the localized states but do not influence the physical results of interest. The distance between the infinite walls should be chosen with caution to avoid compression of the impurity wave functions by the walls. On the other hand, it will require inclusion of more subbands in the calculation to obtain an accurate binding energy of an impurity state in a larger space enclosed by the walls.

Now we switch on the resonant coupling  $H_C^{(\nu)}$  between the localized state  $\psi_B^{(\nu m j)}$  and the subspace  $\mathcal{S}_X^{(\nu)}$ . The resonant states can be treated with the technique of resolvent operators. Let  $G^{(0)}$  and  $G$  be the resolvent operators for the uncoupled system  $H_C^{(\nu)}$  and the total system  $H$ , respectively. We have

$$G^{(0)} = (E - H_U^{(\nu)} + i0^+)^{-1} \quad (17a)$$

and

$$G = (E - H + i0^+)^{-1}. \quad (17b)$$

The DOS spectrum of the single impurity state  $\psi_B^{(\nu m j)}$  can be expressed as

$$n_B^{(\nu m j)}(E) = -\frac{1}{\pi} \text{Im}[G_{BB}], \quad (18)$$

where  $G_{BB} = \langle \psi_B^{(\nu m j)} | G | \psi_B^{(\nu m j)} \rangle$ . To find the matrix element  $G_{BB}$ , the two resolvent operators are related to each other through the Dyson equation

$$G = G^{(0)} + G^{(0)} H_C^{(\nu)} G. \quad (19)$$

Since  $H_U^{(\nu)}$  is diagonal in the representation for which  $\psi_B^{(\nu m j)}$  and all  $\psi_{n\mathbf{k}} \in \mathcal{S}_X^{(\nu)}$  are basis functions,  $G^{(0)}$  is also diagonal

in the representation. Making use of this property and vanishing intrasubspace coupling of  $H_C^{(\nu)}$ , we obtain the following equalities from Eq. (19):

$$G_{BB} = G_{BB}^{(0)} + G_{BB}^{(0)} \sum_{n < \nu, \mathbf{k}} V_{B, n\mathbf{k}} G_{n\mathbf{k}, B} \quad (20a)$$

and

$$G_{n\mathbf{k}, B} = G_{n\mathbf{k}, n\mathbf{k}}^{(0)} V_{n\mathbf{k}, B} G_{BB}, \quad (20b)$$

where

$$G_{BB}^{(0)} = \langle \psi_B^{(\nu m j)} | G^{(0)} | \psi_B^{(\nu m j)} \rangle = (E - E_I^{(\nu m j)} + i0^+)^{-1}, \quad (21a)$$

$$G_{n\mathbf{k}, n\mathbf{k}}^{(0)} = \langle \psi_{n\mathbf{k}} | G^{(0)} | \psi_{n\mathbf{k}} \rangle = (E - E_{n\mathbf{k}} + i0^+)^{-1}, \quad (21b)$$

$$G_{n\mathbf{k}, B} = \langle \psi_{n\mathbf{k}} | G | \psi_B^{(\nu m j)} \rangle, \quad (21c)$$

$$V_{B, n\mathbf{k}} = V_{n\mathbf{k}, B}^* = \langle \psi_B^{(\nu m j)} | V_c | \psi_{n\mathbf{k}} \rangle. \quad (21d)$$

Substituting  $G_{n\mathbf{k}, B}$  in Eq. (20b) into Eq. (20a), we can have

$$G_{BB} = [F(E) + i\Gamma(E)]^{-1}, \quad (22)$$

with

$$\begin{aligned} F(E) &= E - E_I^{(\nu m j)} - \sum_{n < \nu, \mathbf{k}} P \frac{|V_{B, n\mathbf{k}}|^2}{E - E_{n\mathbf{k}}} \\ &= E - E_I^{(\nu m j)} - \frac{1}{\pi} \sum_{n < \nu} P \int_{E_{n0}}^{\infty} \frac{\Gamma_n(E')}{E - E'} dE', \end{aligned} \quad (23)$$

$$\Gamma(E) = \pi \sum_{n < \nu, \mathbf{k}} |V_{B, n\mathbf{k}}|^2 \delta(E - E_{n\mathbf{k}}) = \sum_{n < \nu} \Gamma_n(E), \quad (24)$$

and

$$\Gamma_n(E) = \frac{A}{4} |V_{B, n\mathbf{k}}|^2 \quad \text{with } k = \sqrt{E - E_{n0}}. \quad (25)$$

The area  $A$  in Eq. (25) will be canceled out with that in  $|V_{B, n\mathbf{k}}|^2$ . Here  $Px^{-1}$  means to take the Cauchy principal value of  $x^{-1}$ . The resonance energy  $E_R^{(\nu m j)}$  of the impurity state is obtained by finding the peak position of the DOS spectrum  $n_B^{(\nu m j)}(E)$ , and the spectrum width is approximated by  $\Gamma(E_R^{(\nu m j)})$ , which reflects the capture time of an electron into the localized state  $\psi_B^{(\nu m j)}$  from the subband states  $\psi_{n\mathbf{k}} \in \mathcal{S}_X^{(\nu)}$  and also the escape time of an electron from the localized to the subband states. The time is estimated using the relation  $\tau = \hbar/2\Gamma(E_R^{(\nu m j)})$ . The resonant coupling causes an energy shift of  $\Delta E^{(\nu m j)} = E_R^{(\nu m j)} - E_I^{(\nu m j)}$ . It is noted that the DOS spectrum  $n_B^{(\nu m j)}(E)$  is due to a single resonant state and has dimension of inverse energy. For a low doping concentration, impurities are far from each other so that the interaction between the impurities is negligible. Consequently, the total DOS spectrum due to all the impurities is the sum of all the single-impurity spectra, which is simply the single-impurity spectrum multiplying the number of impurities.



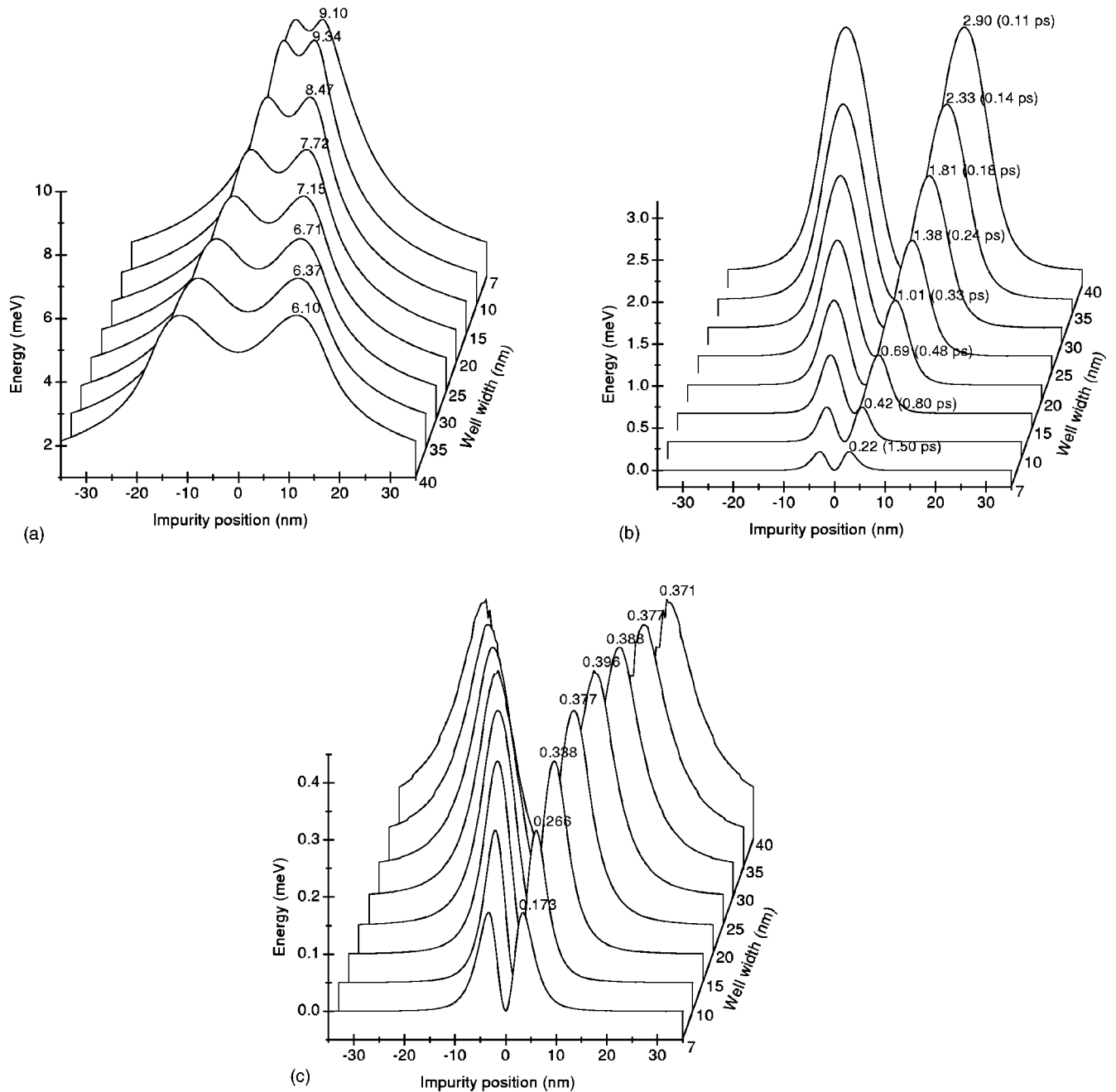


FIG. 1. Waterfall plots of (a) the binding energy, (b) the DOS spectrum width, and (c) the shift of resonance energy of the  $2p_0$  state in GaAs- $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$  QW structures as a function of the impurity position for various well widths. Each of the numbers shown in the figures represents the peak value for each well width. In (b), the corresponding capture or escape times at the peaks are also shown.

### III. NUMERICAL RESULTS AND DISCUSSION

We present numerical results to give an illustration of the resonant states. Calculations are performed for the  $2p_0$  or  $\psi^{(201)}$  resonant impurity state ( $\nu=2$ ,  $m=0$ ,  $j=1$ ) in a QW structure consisting of a GaAs well sandwiched by  $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$  barriers. The  $2p_0$  state lies above the first-subband edge and attached to the second subband for an on-center impurity in the QW well with a width less than some critical value ( $\sim 60$  nm).<sup>3</sup> In the calculation of the bound part of the  $2p_0$  state, we use the trial functions (10a) and (16) consisting of nine lowest subbands in subspace  $\mathcal{S}_B^{(2)}$

( $n=2-10$ ) and five Gaussian orbitals ( $l=0-4$ ). Two infinite potential walls 60 nm apart are artificially imposed to surround the QW structures to discretize the continuum of the subbands above the  $\text{Al}_{0.2}\text{Ga}_{0.8}\text{As}$  barriers. It has been made sure that the walls do not significantly compress the  $2p_0$  state and the first subband states. The problem becomes a  $45 \times 45$  matrix eigenvalue equation for each set of the parameters  $\alpha_l^{(20)}$ . The accuracy of the numerical results has been confirmed by observation of the convergence of the data with increasing the number of terms used in the expression of the trial function. The five nonlinear variational pa-

parameters  $\alpha_l^{(20)}$  are under the restriction of  $\alpha_l^{(20)} = \alpha + \beta_l$  where  $\alpha$  is treated as a nonlinear variational parameter but  $\beta_l$  are fixed to be  $\beta_l = 0.25l^3$  for  $l=0-4$ . In the calculations, the effective mass and the low-temperature band gap for the  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  material system are assumed to be  $(0.067 + 0.083x)m_e$  and  $1.519 + 1.447x - 0.15x^2$  eV, respectively, according to Casey and Panish,<sup>19</sup> where  $m_e$  is the free electron mass. The barrier height is assumed to be 0.65 of the band gap difference. The static dielectric constant of  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  is adopted by a linear interpolation between those of GaAs (12.58) and AlAs (10.06).

Figures 1(a), 1(b), and 1(c) are the waterfall plots of the binding energy  $E_B^{(201)}$ , the spectrum width  $\Gamma(E_R^{(201)})$ , and the shift of resonance energy  $\Delta E^{(201)}$ , respectively, of the  $2p_0$  state as a function of the impurity position  $z_i$  for various well widths. The origin is chosen at the center of the QW. The binding energy of the  $2p_0$  depends on the electronic distribution probability around the impurity position. As a consequence, the binding energy exhibits two peaks associated with the two maxima of the electronic distribution probability of the  $2p_0$  state. Furthermore, the maximum electronic distribution probability can be enhanced by a reduction of the well width. This causes an increase of the binding energy with the well width decreasing, as can be seen from Fig. 1(a). Further reduction of the well width can nevertheless push up the energy level to be close to the barrier height, leading to a widespread electronic distribution and thus a reduction of the binding energy. This explains the lower binding energy for the 7-nm well than for the 10-nm well.

The spectrum width  $\Gamma(E_R^{(201)})$  reflects the resonant coupling strength, which depends on the impurity position and the resonance energy relative to the lowest subband bottom, i.e.,  $E_R^{(201)} - E_{10}$ , through the coupling matrix elements in Eq. (24). When the impurity is at the well center, the parity difference of the bound  $\psi_B^{(201)}$  and the first subband states  $\psi_{1k}$  causes no coupling ( $\Gamma=0$ ), shown in Fig. 1(b). The spectrum width goes through a maximum and then reduces toward zero as the impurity moves away from the well center. The maximum spectrum width of a wider well is larger than that of a narrower well. This is because the energy difference  $E_R^{(201)} - E_{10}$  is smaller for a wider well. For a large value of  $k_R = \sqrt{E_R^{(201)} - E_{10}}$ ,  $\psi_{1k_R}$  exhibits a rapid oscillation along  $\rho$ , resulting in a small overlap integral for the spectrum width. In Fig. 1(b) we show the value of the maximum spectrum width for each of the wells. It can be as large as

$\sim 3$  meV. We also show the value of the capture or escape time associated with the maximum resonant coupling for each well width. It ranges approximately from 0.1 to 1 ps.

The resonance energy shift  $\Delta E^{(201)}$  shown in Fig. 1(c) exhibits more complicated variations with the impurity position. As can be seen from Eq. (23), it depends on the resonance energy level  $E_R^{(201)}$  and the coupling strength  $\Gamma(E)$  over a range of energy. Therefore, a wider well can virtually have a more significant energy shift than a narrower one. Since  $\Gamma(E)$  in principle decays with  $E$ , the coupling is expected to cause a blueshift of the impurity level, i.e.,  $\Delta E^{(201)} > 0$ . As can be seen, the maximum shift is of the order of 0.1 meV. For wide wells, such as those of width  $> 30$  nm, the resonance energy  $E_R^{(201)}$  is close to the first-subband bottom  $E_{10}$ . This may cause reduction of the blueshift or even a redshift of the impurity level ( $\Delta E^{(201)} < 0$ ), which does not show in the waterfall plot of Fig. 1(c). According to the calculated results, the redshift can be as large as tenths of meV for a wide well. The energy shift is in general much smaller than the binding energy.

#### IV. CONCLUSION

We have presented the formulas for calculations of the characteristics of resonant impurity states in QW structures by dividing the total system into an uncoupled system and the resonant coupling. The division depends on which subband the impurity state of interest is attached to. The bound part of the resonant state is a stationary state in the uncoupled system and has been obtained by the variational method with a multisubband trial function. After having found out the representation in which the uncoupled Hamiltonian is diagonal, we treat the resonant coupling with the technique of the resolvent operators and obtain the spectrum of the resonant impurity state. The numerical results of the binding energy, the DOS spectrum width, and the energy shift of the  $2p_0$  state have been presented. The spectrum width can be as large as several meV, causing a capture or escape time of  $\sim 0.1$  ps. The energy shift is in general less than 0.4 meV, much smaller than the binding energy.

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