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Configuration interaction applied to resonant states in semiconductors and semiconductor nanostructures

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Abstract

A new method for calculating the parameters of resonant states as well as the probability of resonant scattering, capture and emission is developed. It is based on the configuration interaction method, which has been first introduced by Fano in the problem of autoionization of He. The method has been applied to resonant states induced by (i) defects in the barrier of GaAs/GaAlAs quantum well structure and (ii) acceptors in Ge under external stress. © 2001 Elsevier Science B.V. All rights reserved.

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0. Introduction

Resonant states have been studied very well in atomic physics. Semiconductors are other systems where resonant states play a significant role in physical processes. Such states appear, for example, in zero-gap semiconductors doped by shallow acceptors. The system of a special interest is uniaxially strained germanium where the generation of THz radiation has been achieved [1,2].

Here, we suggest a new method for calculating the parameters of resonant states and the probability of resonant scattering, capture and emission of carriers. The approach is based on the configuration interaction method, which was first introduced by Fano [3] in the problem of autoionization of He. The main idea is to choose two different Hamiltonians for the initial approximation: one for continuum states and the other for localized states. Then, wave functions are constructed in terms of scattering theory following to Dirac [4]. In a result, the energy shift and the width of resonant level as well as amplitude of resonant elastic scattering and capture probability by resonant states is calculated. The method is applied to resonant states induced (i) by impurities in the barrier of quantum wells and (ii) by shallow acceptors in Ge under stress.

1. Resonant states induced by localized states in barriers of QW

We will demonstrate the general idea by applying it to a system consisting of a quantum well (QW) and one impurity in the barrier. The full Hamiltonian is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(z) + V_\mathrm{d}(\mathbf{r}-\mathbf{r}_0), \tag{1.1}$$

where $V(z)$ is the QW potential and V_d is the defect potential (see Fig. 1).

As an initial approximation for the wave function of the localized state induced by the impurity we use the solution of the equation

$$\left[-\frac{\hbar^2}{2m}\Delta + V_\mathrm{d}(\mathbf{r}-\mathbf{r}_0)\right]\varphi(\mathbf{r}-\mathbf{r}_0) = E_0\varphi(\mathbf{r}-\mathbf{r}_0). \tag{1.2}$$

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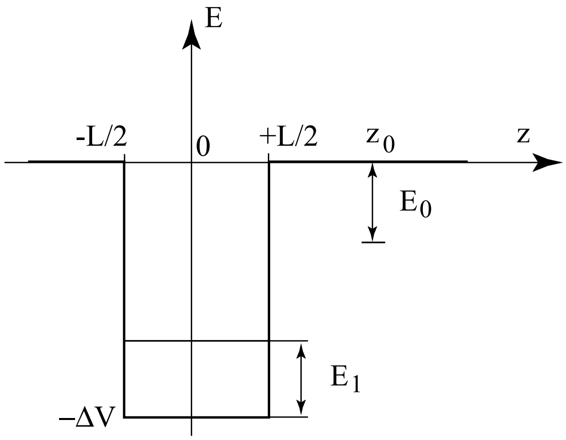

Fig. 1. A schematic of quantum well with introduced impurity level; E_0 is the binding energy of an impurity in the first approximation, E_1 is the space quantization energy.

The initial wave functions of continuum states $\psi_{\mathbf{k}}(\mathbf{r})$ satisfy the following equation:

$$\left[-\frac{\hbar^2}{2m}\Delta + V(z)\right]\psi_{\mathbf{k}}(\mathbf{r}) = E_k\psi_{\mathbf{k}}(\mathbf{r}). \tag{1.3}$$

We are considering QW with one energy level only, so that

$$E_k = -\Delta V + E_1 + \varepsilon_k, \tag{1.4}$$

where ΔV is band offset at the QW boundary (see Fig. 1), E_1 is the space quantization level and $\varepsilon_k = \hbar^2k^2/2m$ is the kinetic energy of 2D motion. So we can write for $\psi_{\mathbf{k}}(\mathbf{r})$

$$\psi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{S}}\phi(z)\exp(\mathrm{i}\mathbf{k}\rho), \tag{1.5}$$

where S is a normalizing square.

Now we consider the problem of scattering of the in-plane moving carrier by the impurity in the barrier. Following Dirac [4], we construct the wave function in terms of a scattering theory in the following form:

$$\Psi_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r}) + a_{\mathbf{k}}\varphi(\mathbf{r}-\mathbf{r}_0) + \sum_{\mathbf{k}'}\frac{t_{\mathbf{k}\mathbf{k}'}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}'} + \mathrm{i}\gamma}\psi_{\mathbf{k}'}(\mathbf{r}), \quad \gamma \to +0. \tag{1.6}$$

As long as the presence of one impurity does not perturb the continuum spectrum significantly, $\Psi_{\mathbf{k}}(\mathbf{r})$ corresponds to the energy E_k. Solving the Schrodinger equation with the full Hamiltonian (1.1) for $\Psi_{\mathbf{k}}(\mathbf{r})$, we get

$$a_{\mathbf{k}} = \frac{1}{\sqrt{S}}\frac{V_{\mathbf{k}}}{E_k - (E_0 + \Delta E) + \mathrm{i}\Gamma/2}, \tag{1.7}$$

$$t_{\mathbf{k}\mathbf{k}'} = \frac{1}{S}\frac{V_{\mathbf{k}}Z^*_{\mathbf{k}'}}{E_k - (E_0 + \Delta E) + \mathrm{i}\Gamma/2}, \tag{1.8}$$

The energy shift ΔE and the width $\Gamma/2$ of the resonant level are given by

$$\Delta E = \delta - \frac{1}{(2\pi)^2}\int \mathrm{d}^2k'\, Z^*_{\mathbf{k}'}\, W_{\mathbf{k}'} + \frac{1}{(2\pi)^2}P\int \mathrm{d}^2k'\,\frac{Z^*_{\mathbf{k}'}\,V_{\mathbf{k}'}}{E_k - E_{k'}} \tag{1.9}$$

$$\frac{\Gamma}{2} = \frac{1}{4\pi}\int \mathrm{d}^2k' Z^*_{\mathbf{k}'}V_{\mathbf{k}'}\delta(E_k - E_{k'}) \tag{1.10}$$

Here the matrix elements

$$V_{\mathbf{k}} = \sqrt{S}\langle\varphi|V_{\mathrm{d}}|\psi_{\mathbf{k}}\rangle, \quad W_{\mathbf{k}} = \sqrt{S}\langle\varphi|\psi_{\mathbf{k}}\rangle,$$

$$\delta = \langle\varphi|V(z)|\varphi\rangle \quad Z_{\mathbf{k}} = \sqrt{S}\langle\varphi|V(z)|\psi_{\mathbf{k}}\rangle,$$

$$V_{\mathbf{k}\mathbf{k}'} = S\langle\psi_{\mathbf{k}}|V_{\mathrm{d}}|\psi_{\mathbf{k}'}\rangle. \tag{1.11}$$

are introduced. In solution (1.9–1.10) we have taken into account resonant scattering only, neglecting the impurity potential scattering.

The probability of resonant elastic scattering $W_{\mathbf{k}\mathbf{k}'}$ of 2D carriers and the capture probability $W_{\mathbf{k}r}$ are given by

$$W_{\mathbf{k}\mathbf{k}'} = \frac{2\pi}{\hbar}|t_{\mathbf{k}\mathbf{k}'}|^2\,\delta(\varepsilon_k - \varepsilon_{k'}) = \frac{2\pi}{\hbar}\frac{1}{S^2}\frac{|V_{\mathbf{k}}|^2|Z_{\mathbf{k}'}|^2}{(E_k - E_0 - \Delta E)^2 + \Gamma^2/4}\delta(\varepsilon_k - \varepsilon_{k'}) \tag{1.12}$$

$$W_{\mathbf{k}r} = |a_{\mathbf{k}}|^2 = \frac{1}{S}\frac{|V_{\mathbf{k}}|^2}{(E_k - E_0 - \Delta E)^2 + \Gamma^2/4}, \tag{1.13}$$

respectively. Both probabilities contain the same resonant denominator.

The resonant scattering should be introduced into the kinetic equation when one solves the problem of the 2D carriers distribution function under an electric field applied in the plane of the quantum well. This scattering affects significantly the distribution function $f_{\mathbf{k}}$ of hot carriers [5]. The population f_r of impurities in the barrier is connected with the distribution function $f_{\mathbf{k}}$ by relation [6]

$$f_r = \sum_{\mathbf{k}} W_{\mathbf{k}r}f_{\mathbf{k}}. \tag{1.14}$$

The position of resonance E_r can be found from the condition $E_r = E_0 + \Delta E(E_k = E_r)$, where ΔE is determined by Eq. (1.9). The resonant width Γ is defined by Eq. (1.10) at $E_k = E_r$.

We will apply the above-described approach to calculate the energy level position and the width of resonant states induced by deep donor centers which appear in the barrier region of $Al_{0.3}Ga_{0.7}As$/GaAs/$Al_{0.3}Ga_{0.7}As$ heterostructure doped with Si. These centers were extensively studied experimentally [7] because they heavily affect a performance of heterostructure based electronic and optoelectronic devices.

In doped $Al_xGa_{1-x}As$ with Al content x larger than 0.27, more than a half of Si donor centers produce deep levels with binding energy $E_c \sim 155$ meV measured from the bottom of the Γ-valley [7]. The results of calculations of E_r and Γ as a function of the distance between defect and QW boundary are presented in Fig. 2 for different QW widths. We have used the band offset $\Delta V = 232$ meV, and effective masses 0.067 and 0.092 in QW and barrier regions, respectively.

2. Resonant acceptor states in uniaxially strained germanium

Germanium has a fourfold degenerate top of the valence band. When strained, it is split into two doubly degenerate states. The ground state of an acceptor shows the same behavior under uniaxial stress. At some critical value of the stress—when the splitting is larger than the acceptor binding energy—one of the split levels is shifted into the continuous spectrum of the other valence subband and becomes resonant. An effective optical transitions between resonant and localized states of the same impurities can take place. If the electric field is strong enough, an electric impurity breakdown occurs and practically all localized impurity states become depopulated. Now, the capture and emission processes lead to an effective population of resonant states. This may cause an intracenter population inversion that is the basis for THz generation [1,2].

Resonant acceptor states were considered in [6] by using the Dirac approach. It requires choosing an initial approximation Hamiltonian which should give localized states overlapping with the continuous spectrum. The approach in [6] applies for large stresses and for small quasimomenta but it fails for the region of the continuous spectrum where resonant states are present.

Using our new approach, we consider the ground resonant state induced by shallow acceptors in uniaxially strained p-Ge. As the initial approximation for localized states we choose the eigenfunctions of diagonal part of the Luttinger Hamiltonian with Coulomb

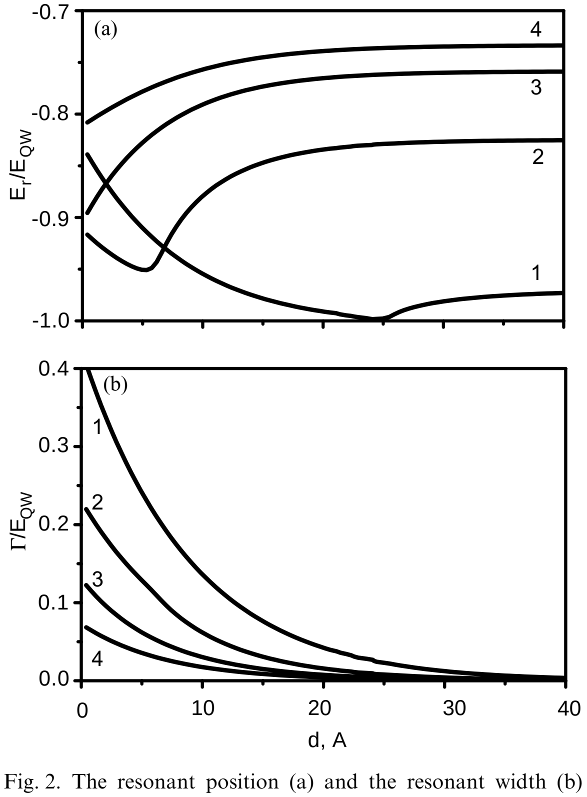

Fig. 2. The resonant position (a) and the resonant width (b) normalized by the energies of the first space quantization level as a function of the distance d between impurity and QW for the case of deep donor in $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ heterostructure. (1) $L = 5$ nm, $E_{QW} = 157.7$ meV; (2) $L = 7.5$ nm, $E_{QW} = 185.6$ meV; (3) $L = 10$ nm, $E_{QW} = 201.8$ meV; (4) $L = 12.5$ nm, $E_{QW} = 208.8$ meV.

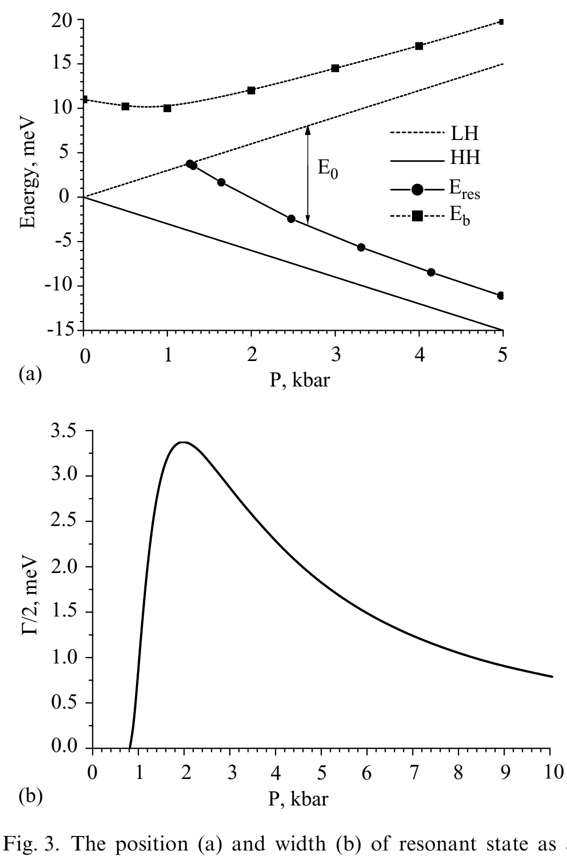

Fig. 3. The position (a) and width (b) of resonant state as a function of uniaxial stress applied to Ge in [0 0 1] direction. E_{res} is resonance position and E_b is ground localized state.

potential taken into account. For continuum states we use wave functions $\psi_{\mathbf{k}}^{\pm 1/2}(\mathbf{r})$ of free holes in cylindrical approximation for the Luttinger Hamiltonian. Following the procedure from the first section we are looking for wave functions in the form:

$$\begin{aligned}\Psi_{\mathbf{k}}^{\pm 1/2} = \psi_{\mathbf{k}}^{\pm 1/2} + a_{\mathbf{k}}^{\pm 1/2,+3/2}\varphi^{+3/2}(\mathbf{r}) \\ + a_{\mathbf{k}}^{\pm 1/2,-3/2}\varphi^{-3/2}(\mathbf{r}) + \sum_{\mathbf{k}'} \frac{t_{\mathbf{kk}'}^{\pm 1/2,+1/2}}{\varepsilon_k - \varepsilon_{k'} + i\gamma}\psi_{\mathbf{k}'}^{+1/2}(\mathbf{r}) \\ + \sum_{\mathbf{k}'} \frac{t_{\mathbf{kk}'}^{\pm 1/2,-1/2}}{\varepsilon_k - \varepsilon_{k'} + i\gamma}\psi_{\mathbf{k}'}^{-1/2}(\mathbf{r}) \qquad (1.15)\end{aligned}$$

The capture probability of holes with momentum projection $+1/2$, $W_{\mathbf{k}r}$ and the probability of elastic resonant scattering $W_{\mathbf{kk}'}$ are defined now by

$$W_{\mathbf{k}r} = \left|a_{\mathbf{k}}^{+1/2,+3/2}\right|^2 + \left|a_{\mathbf{k}}^{+1/2,-3/2}\right|^2, \qquad (1.16)$$

$$W_{\mathbf{kk}'} = \frac{2\pi}{\hbar}\left(\left|t_{\mathbf{kk}'}^{+1/2,+1/2}\right|^2 + \left|t_{\mathbf{kk}'}^{+1/2,-1/2}\right|^2\right)\delta(\varepsilon_k - \varepsilon_{k'}). \quad (1.17)$$

The expressions for the case of momentum projection $-1/2$ are similar.

The results of calculations of the resonant level shift and level width as function of stress applied along [0 0 1] direction are given in Fig. 3.

3. Conclusion

The approach for calculation of resonant state energy and lifetime as well as probabilities of resonant capture and elastic scattering are suggested and applied to resonant states induced by deep donors in the barrier of $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ QW heterostructure as well as by shallow acceptors in Ge under stress.

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