Nanotechnology 12 (2001) 457–461 PII: S0957-4484(01)28320-2

Configuration interaction applied to resonant states in semiconductors and semiconductor nanostructures

A A Prokofiev[1], **I N Yassievich**[1], **A Blom**[2], **M A Odnoblyudov**[2] **and K-A Chao**[2]

[1]Ioffe Physico-Technical Institute, RAS, 194021 St Petersburg, Russia
[2] Fasta Tillståndets Teori, Sölvegatan 14 A, S-223 62 Lund, Sweden

Received 11 July 2001
Published 27 November 2001
Online at stacks.iop.org/Nano/12/457

Abstract
A new approach for calculation of resonant state parameters is developed. The method proposed allows us to solve different scattering problems, such as scattering and capture probability as well as calculations of shifts and widths of energy levels. It has been applied to the problem of resonant states induced by impurities in the barrier of quantum wells and by strain in uniaxially stressed germanium.

Introduction

Quasistationary (or resonant) states have been extensively studied in atomic physics. Semiconductors are other systems where resonant states play a significant role in physical processes. Such states appear, for example, in gapless semiconductors when doped by shallow acceptors. A system of 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 the wavefunctions are constructed in terms of scattering theory following Dirac [4]. As a result, the energy shift and the width of resonant level as well as the amplitude of resonant elastic scattering and the capture probability by resonant states can be 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

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

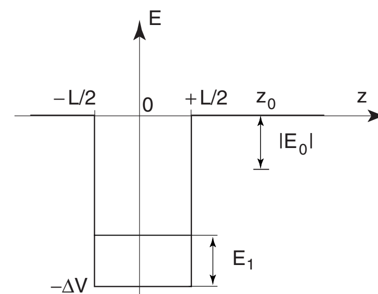

Figure 1. The parameters of the well and impurity.

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(z) + V_{\rm d}(\boldsymbol{r} - \boldsymbol{r}_0), \qquad (1)$$

where the potential of the QW $V(z)$ is shown in figure 1; $V_{\rm d}$ is the defect potential and $\boldsymbol{r}_0 = (0, 0, z_0)$ is the position of the defect.

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

$$\left[-\frac{\hbar^2}{2m}\Delta + V_{\rm d}(\boldsymbol{r} - \boldsymbol{r}_0)\right]\varphi(\boldsymbol{r} - \boldsymbol{r}_0) = E_0\varphi(\boldsymbol{r} - \boldsymbol{r}_0). \qquad (2)$$

The initial wavefunctions of continuum states $\psi_{\boldsymbol{k}}(\boldsymbol{r})$ satisfy the following equation:

$$\left[-\frac{\hbar^2}{2m}\Delta + V(z)\right]\psi_{\boldsymbol{k}}(\boldsymbol{r}) = E_k\psi_{\boldsymbol{k}}(\boldsymbol{r}). \qquad (3)$$

0957-4484/01/040457+05$30.00 © 2001 IOP Publishing Ltd Printed in the UK

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

$$E_k = -\Delta V + E_1 + \varepsilon_k, \tag{4}$$

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

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{S}}\phi(z)\mathrm{e}^{\mathrm{i}k\rho}, \tag{5}$$

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 wavefunction in terms of scattering theory in the following form:

$$\Psi_{\boldsymbol{k}}(\boldsymbol{r}) = \psi_{\boldsymbol{k}}(\boldsymbol{r}) + a_{\boldsymbol{k}}\varphi(\boldsymbol{r}-\boldsymbol{r}_0) + \sum_{k'}\frac{t_{\boldsymbol{k}\boldsymbol{k}'}}{\varepsilon_k - \varepsilon_{k'} + \mathrm{i}\gamma}\psi_{\boldsymbol{k}'}(\boldsymbol{r}),$$
$$\gamma \to 0. \tag{6}$$

As the presence of one impurity does not perturb the continuum spectrum significantly, $\Psi_{\boldsymbol{k}}(\boldsymbol{r})$ corresponds to the energy E_k. Solving the Schrödinger equation with the full Hamiltonian (1) for $\Psi_{\boldsymbol{k}}(\boldsymbol{r})$ one obtains the following expressions for $a_{\boldsymbol{k}}$ and $t_{\boldsymbol{k}\boldsymbol{k}'}$:

$$\begin{aligned} a_{\boldsymbol{k}} &= \frac{1}{\sqrt{S}}\frac{V_{\boldsymbol{k}}}{E_k - (E_0 + \Delta E) + \mathrm{i}\Gamma/2}, \\ t_{\boldsymbol{k}\boldsymbol{k}'} &= \frac{1}{S}\frac{V_{\boldsymbol{k}} Z^*_{\boldsymbol{k}'}}{E_k - (E_0 + \Delta E) + \mathrm{i}\Gamma/2}. \end{aligned} \tag{7}$$

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

$$\Delta E = \delta - \frac{1}{(2\pi)^2}\int \mathrm{d}^2k'\, Z^*_{\boldsymbol{k}'} W_{\boldsymbol{k}'} + \frac{1}{(2\pi)^2} P\int \mathrm{d}^2k' \frac{Z^*_{\boldsymbol{k}'}V_{\boldsymbol{k}'}}{E_k - E_{k'}}, \tag{8}$$

$$\frac{\Gamma}{2} = \frac{1}{4\pi}\int \mathrm{d}^2k'\, Z^*_{\boldsymbol{k}'}V_{\boldsymbol{k}'}\delta(E_k - E_{k'}). \tag{9}$$

Here the matrix elements

$$\begin{aligned} V_{\boldsymbol{k}} &= \sqrt{S}\langle\varphi|V_{\mathrm{d}}|\psi_{\boldsymbol{k}}\rangle, \qquad & W_{\boldsymbol{k}} &= \sqrt{S}\langle\varphi|\psi_{\boldsymbol{k}}\rangle, \\ \delta &= \langle\varphi|V(z)|\varphi\rangle, \qquad & Z_{\boldsymbol{k}} &= \sqrt{S}\langle\varphi|V(z)|\psi_{\boldsymbol{k}}\rangle, \end{aligned} \tag{10}$$

are introduced. In solution (7) we have taken into account resonant scattering only neglecting the impurity potential scattering.

The probability of resonant elastic scattering $W_{\boldsymbol{k}\boldsymbol{k}'}$ of two-dimensional carriers and the capture probability $W_{\boldsymbol{k}r}$ are given by

$$W_{\boldsymbol{k}\boldsymbol{k}'} = \frac{2\pi}{\hbar}|t_{\boldsymbol{k}\boldsymbol{k}'}|^2\delta(\varepsilon_k - \varepsilon_{k'}), \qquad W_{\boldsymbol{k}r} = |a_{\boldsymbol{k}}|^2, \tag{11}$$

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 two-dimensional carrier distribution function under an electric field applied in the plane of the QW. This scattering significantly affects the distribution function $f_{\boldsymbol{k}}$ of hot carriers [5]. The population f_{r} of impurities in the barrier is connected with the distribution function $f_{\boldsymbol{k}}$ by the relation [6]

$$f_{\mathrm{r}} = \sum_{\boldsymbol{k}} W_{\boldsymbol{k}r} f_{\boldsymbol{k}}. \tag{12}$$

We shall apply the above-described approach to calculate the energy level position and width of resonant states induced by deep donor centres which appear in the barrier region of $Al_{0.3}Ga_{0.7}As$/GaAs/$Al_{0.3}Ga_{0.7}As$ heterostructures which are doped by Si. These centres have been extensively studied experimentally [7–9] because they heavily affect the performance of heterostructure-based electronic and optoelectronic devices.

It has been shown [7] that in doped $Al_xGa_{1-x}As$ with Al content x larger than 0.27 more than half of the Si donor centres produce deep levels with binding energy $E_{\mathrm{c}} \approx 155$ meV measured from the bottom of the Γ valley.

We shall describe these localized deep states in the framework of a zero-range potential model [10]. According to this model, we take the normalized wavefunction of the isolated localized impurity state of the form

$$\phi(\boldsymbol{r}) = \sqrt{\frac{\kappa}{2\pi}}\frac{\mathrm{e}^{-\kappa r}}{r}. \tag{13}$$

The parameter κ is related to the energy of the localized state

$$E_0 = -\frac{\hbar^2\kappa^2}{2m_b}. \tag{14}$$

To calculate the matrix element $V_{\boldsymbol{k}}$ (see equation (10)) with a generally unknown impurity potential $V_{\mathrm{d}}(\boldsymbol{r})$ we express it in the form

$$V_{\boldsymbol{k}} = \langle\phi|\frac{\hbar^2}{2m_b}\nabla^2 + E_0|\psi_{\boldsymbol{k}}\rangle. \tag{15}$$

The position of resonance E_{r} can be found from the condition

$$E_{\mathrm{r}} = E_0 + \Delta E(E_k = E_{\mathrm{r}}), \tag{16}$$

where $\Delta E(E_k)$ is determined by equation (8). The resonant width Γ is defined by equation (9) at $E_k = E_{\mathrm{r}}$. The results of calculation of E_{r} and Γ as a function of the distance between the defect and the QW boundary are presented in figure 2 for different QW widths. We have used the value of 232 meV for the band offset ΔV between the Γ points in the conduction bands of GaAs and $Al_{0.3}Ga_{0.7}As$, and the values 0.067 and 0.092, respectively, for the effective masses in the QW and the barrier region.

2. Resonant acceptor states in uniaxially strained germanium

Tetrahedrally coordinated semiconductors (e.g. GaAs, Ge, Si) have a fourfold degenerate top of the valence band. When strained, the top of the valence band is split into two doubly degenerate states. The ground state of an acceptor shows the same behaviour 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

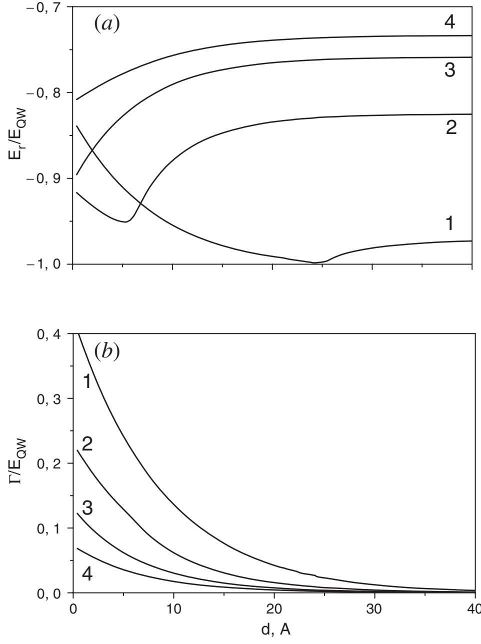

Figure 2. The resonant position (a) and the resonant width (b) normalized by the energies of the first space quantization level as a function of the distance d between the impurity and the QW for the case of a deep donor in the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ heterostructure. (1) $L = 50$ Å, $E_0 = 157.7$ meV; (2) $L = 75$ Å, $E_0 = 185.6$ meV; (3) $L = 100$ Å, $E_0 = 201.8$ meV; (4) $L = 125$ Å, $E_0 = 208.8$ meV.

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 capture and emission processes lead to an effective population of resonant states. This may cause an intracentre population inversion that is the basis for THz generation [1, 2].

Resonant acceptor states were considered in [6] by using the Dirac approach, which requires choosing an initial approximation Hamiltonian giving 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 shall consider the ground resonant state induced by shallow acceptors in uniaxially strained p-Ge along [001] and [111] directions.

As the initial approximation for localized states we choose the diagonal part of the Luttinger Hamiltonian and the Coulomb potential of an acceptor in the same way as in [6]:

$$\varphi^{+3/2}(\boldsymbol{r}) = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \varphi(\boldsymbol{r}) \qquad \varphi^{-3/2}(\boldsymbol{r}) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} \varphi(\boldsymbol{r}) \tag{17}$$

where

$$\varphi(\boldsymbol{r}) = \frac{1}{\sqrt{\pi a^2 b}} \exp\left(-\sqrt{\frac{\rho^2}{a^2} + \frac{z^2}{b^2}}\right). \tag{18}$$

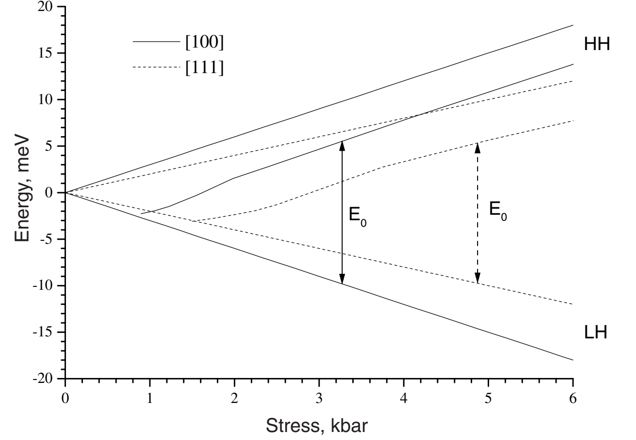

Figure 3. The position of the resonant state as a function of stress. Solid curves correspond to splitting of the top of the valence band and the position of the resonant level for the [001] stress direction and dashed ones to the [111] stress direction. We set the zero reference energy at the valence-band edge, and adopt the convention that the valence-band energy is positive.

Variational calculation gives $a = 114$ Å, $b = 61.2$ Å and binding energy $E_A = 4.69$ meV for stress applied along [001] and $a = 108$ Å, $b = 55.7$ Å, $E_A = 5.01$ meV for stress along [111].

For continuum states we use the eigenfunctions $\psi_{\boldsymbol{k}}^{\pm 1/2}(\boldsymbol{r})$ of the full Luttinger Hamiltonian for free holes in the cylindrical approximation taking strain into account. Following the procedure from the first section we are looking for wavefunctions in the form

$$\Psi_{\boldsymbol{k}}^{\pm 1/2} = \psi_{\boldsymbol{k}}^{\pm 1/2} + a_{\boldsymbol{k}}^{\pm 1/2,+3/2} \varphi^{+3/2}(\boldsymbol{r}) + a_{\boldsymbol{k}}^{\pm 1/2,-3/2} \varphi^{-3/2}(\boldsymbol{r}) + \sum_{\boldsymbol{k}'} \frac{t_{\boldsymbol{k}\boldsymbol{k}'}^{\pm 1/2,+1/2}}{\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}'} + \mathrm{i}\gamma} \psi_{\boldsymbol{k}'}^{+1/2} + \sum_{\boldsymbol{k}'} \frac{t_{\boldsymbol{k}\boldsymbol{k}'}^{\pm 1/2,-1/2}}{\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}'} + \mathrm{i}\gamma} \psi_{\boldsymbol{k}'}^{-1/2}. \tag{19}$$

The probabilities of capture $W_{\boldsymbol{k}r}^{+1/2}$ and elastic resonant scattering $W_{\boldsymbol{k}\boldsymbol{k}'}^{+1/2}$ of holes with momentum projection $+1/2$ are now defined by

$$W_{\boldsymbol{k}r}^{+1/2} = \left|a_{\boldsymbol{k}}^{+1/2,+3/2}\right|^2 + \left|a_{\boldsymbol{k}}^{+1/2,-3/2}\right|^2. \tag{20}$$

$$W_{\boldsymbol{k}\boldsymbol{k}'}^{+1/2} = \frac{2\pi}{\hbar}\left(\left|t_{\boldsymbol{k}\boldsymbol{k}'}^{+1/2,+1/2}\right|^2 + \left|t_{\boldsymbol{k}\boldsymbol{k}'}^{+1/2,-1/2}\right|^2\right)\delta(\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}'}). \tag{21}$$

The expressions for holes with momentum projection $-1/2$ are similar. We have carried out calculations taking into account non-resonant scattering by the Coulomb potential in the first order only; the details will be presented in a separate paper.

Coefficients $a_{\boldsymbol{k}}^{\pm 1/2}$, $t_{\boldsymbol{k}\boldsymbol{k}'}^{\pm 1/2,\pm 3/2}$ as well as resonant capture and elastic scattering probabilities $W_{\boldsymbol{k}r}^{\pm 1/2}$ and $W_{\boldsymbol{k}\boldsymbol{k}'}^{\pm 1/2}$ contain the resonant denominator $E_k - E_0 + \mathrm{i}\Gamma/2$.

Here E_0 is the calculated resonance position counted from the top of the valence band (see figure 3). The result of calculations of the resonant level width as a function of stress applied along [001] and [111] directions is given in figure 4.

It is convenient to present the capture probability (20) in a form similar to the Breite–Wigner model [5, 10]; $\varepsilon_{\boldsymbol{k}} = E_0$:

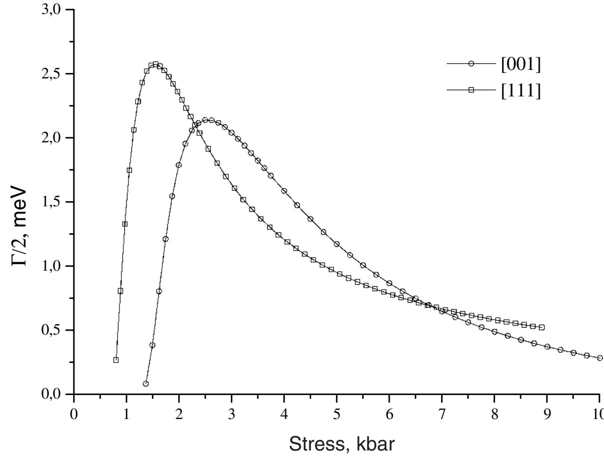

Figure 4. The width of the resonant state as a function of stress applied along the [001] and [111] directions.

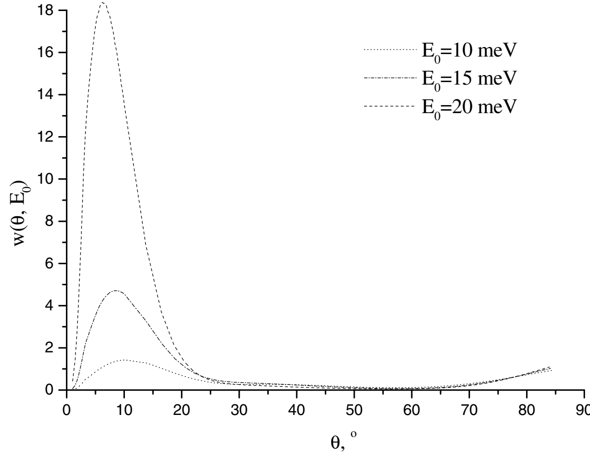

Figure 5. Angular dependence of $w(\theta, E_0)$ (see (22)). $\theta = \arctan(k_\perp/k_z)$, $E_0 = 10, 15, 20$ meV. Stress along [001]. Cylindrical approximation.

$$W_{kr}^{+1/2} = \frac{1}{V}\frac{\Gamma}{(\varepsilon_k - E_0)^2 + \Gamma^2/4}\frac{\pi}{4\sqrt{E_0}} \times \left\{\left[\frac{1}{k_\perp}\frac{\partial\varepsilon_k}{\partial k_\perp} + \frac{1}{k_z}\frac{\partial\varepsilon_k}{\partial k_z}\right]^{3/2}\right\}\Bigg|_{\varepsilon_k = E_0} w(\theta, E_0), \tag{22}$$

$$w(\theta, E_0) = \frac{4\sqrt{E_0}}{\pi\Gamma}\left\{\left(\left|A_k^{+1/2,+3/2}\right|^2 + \left|A_k^{+1/2,+3/2}\right|^2\right) \times \left(\frac{1}{k_\perp}\frac{\partial\varepsilon_k}{\partial k_\perp} + \frac{1}{k_z}\frac{\partial\varepsilon_k}{\partial k_z}\right)^{-3/2}\right\}\Bigg|_{\varepsilon_k = E_0}. \tag{23}$$

The results of calculations of $w(\theta, E_0)$ for Ge under stress along the [001] axis as a function of angle θ between wavevector $\boldsymbol{k}$ and stress axis are presented in figure 5 for $0 < \theta < \pi/2$. Note that $w(\theta, E_0) = w(\pi - \theta, E_0)$.

The expression obtained for elastic scattering probability contains two terms: (i) Coulomb potential scattering in the Born approximation and (ii) resonant elastic scattering, which can be presented in the following form:

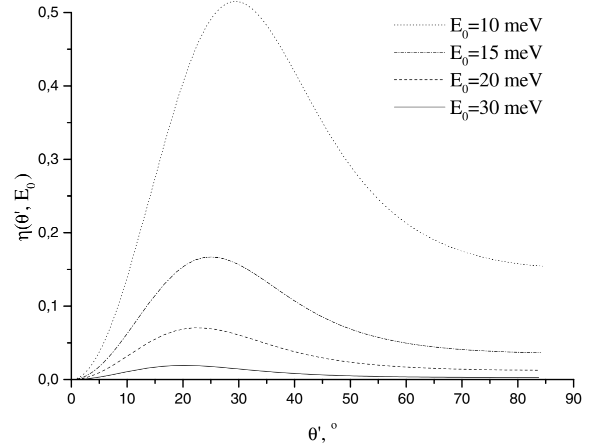

Figure 6. Angular dependence of $\eta(\theta', E_0)$ (see (25)). $\theta' = \arctan(k'_\perp/k'_z)$, $E_0 = 10, 15, 20, 30$ meV. Stress along [001]. Cylindrical approximation.

$$\tilde{W}_{kk'}^{+1/2} = \frac{2\pi}{\hbar}\sigma_{kk'}^{r}\frac{1}{V^2}\frac{\pi}{4}\left(\frac{1}{k_\perp}\frac{\partial\varepsilon_k}{\partial k_\perp} + \frac{1}{k_z}\frac{\partial\varepsilon_k}{\partial k_z}\right)^2 \delta(\varepsilon_k - \varepsilon_{k'}). \tag{24}$$

It is convenient to present the cross-section $\sigma_{kk'}^{+1/2}$ in the form

$$\sigma_{kk'}^{+1/2} = \pi a^2 b \frac{\Gamma}{(\varepsilon_k - E_0)^2 + \Gamma^2/4}E_0^{3/2} \times \left\{\left(\frac{1}{k_\perp}\frac{\partial\varepsilon_k}{\partial k_\perp} + \frac{1}{k_z}\frac{\partial\varepsilon_k}{\partial k_z}\right)^{-1/2}\right\}\Bigg|_{\varepsilon_k = E_0} w(\theta, E_0)\eta(\theta', E_0), \tag{25}$$

where a and b are parameters of the initial approximation for the resonant state obtained by the variational procedure (18), and the nondimensional factor $\eta(\theta', E_0)$ is defined by

$$\eta(\boldsymbol{k}') = \left\{\frac{64}{\left[1 + b^2k_z'^2 + a^2k_\perp'^2\right]^4}\frac{\left|b(\boldsymbol{k}')\right|^2 + \left|c(\boldsymbol{k}')\right|^2}{N_l(\boldsymbol{k}')^2} \times \left[\frac{\hbar^2}{2mE_0}a_+(\boldsymbol{k}') + 1\right]^2\right\}\Bigg|_{\varepsilon_{k'} = E_0}. \tag{26}$$

The results of numerical calculations of $\eta(\theta', E_0)$ for Ge strained along [001] are presented in figure 6.

One can see that resonant scattering and capture are absent for holes moving along [001]. The probabilities of capture and elastic scattering increase with θ and achieve a maximum at $\theta = 10^\circ$ and 20°, respectively.

Note that elastic resonant scattering takes place and formulae (22), (24) are valid only if the lifetime $\hbar/\Gamma$ in the resonant state is so small that no perturbation of the wavefunction could take place during this time.

It can be easily shown that $W_{kk'}^{+1/2} = W_{kk'}^{-1/2}$ and $W_{kr}^{+1/2} = W_{kr}^{-1/2}$. In the presence of an external electric field, distribution functions of holes with different projection of inner momenta are equal: $f_k^{+1/2} = f_k^{-1/2}$.

The resonant state population f_r should be found from the equation

$$f_r = \sum_k W_{kr}^{+1/2} f_k^{+1/2} + \sum_k W_{kr}^{-1/2} f_k^{-1/2}. \tag{27}$$

3. Conclusion

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

Acknowledgments

This work has been partially supported by the RFBR (grants 01-02-16265, 00-15-96768, 00-02-17429, 01-02-02011), The Swedish Foundation for International Cooperation in Research and Higher Education (contract 99/527 (00)) and a NorFA Grant. AAP also thanks the Swedish Institute for a Visby Programme Grant.

References

[1] Altukhov I V, Chirkova E G, Kagan M S, Korolev K A, Sinis V P, Odnoblyudov M A and Yassievich I N 1999 *Zh. Eksp. Teor. Fiz.* **88** 51
[2] Gousev Yu P, Altukhov I V, Korolev K A, Sinis V P, Kagan M S, Haller E E, Odnoblyudov M A, Yassievich I N and Chao K-A 1999 *Appl. Phys. Lett.* **75** 757
[3] Fano U 1961 *Phys. Rev.* **124** 1866
[4] Dirac P A M 1981 *Principles of Quantum Mechanics* 4th edn (Oxford: Clarendon)
[5] Prokofiev A A, Odnoblyudov M A and Yassievich I N 2001 *Semiconductors* **35** 586
[6] Odnoblyudov M A, Yassievich I N, Chistyakov V M and Chao K A 2000 *Phys. Rev.* B **62** 2486
[7] Schubert E F and Ploog K 1984 *Phys. Rev.* B **30** 7021
[8] Nelson R J 1977 *Appl. Phys. Lett.* **31** 351
[9] Lang D V and Logan R A 1977 *Phys. Rev. Lett.* **39** 635
[10] Landau L D and Lifshiz E M 1977 *Quantum Mechanics. Non-Relativistic Theory* 3rd edn (New York: Pergamon) p 673