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Phonon-assisted trapping and detrapping of an electron in quantum wells and wires by ionized impurity

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Abstract

We consider the capture and ionization of an electron in quantum wells and wires by a shallow donor impurity due to the interaction with acoustical phonons. In the case of phonon wavelengths much smaller than the width of wells or wires, L, the transition rates are proportional to $\varepsilon^{-5}(n_\varepsilon + 1/2 \pm 1/2)\,L^{-6}$, where ε is the transferred energy and n_ε is the phonon occupation number.

The processes of carrier trapping by impurities are known to play an important role in transport and noise properties of semiconductor structures [1]. Two approaches exist for the description of capture by a shallow attractive center in bulk semiconductors. The first [2] treats the capture of a carrier as a classical descent through the quasicontinuous spectrum of *highly excited* bound states due to cascade emission of low-energy acoustical phonons and is applicable to low temperatures and materials with large effective Rydberg energies (see also [3] for the two-dimensional case).

At room temperature in GaAs the case opposite to that of the first model is realized (i.e. only a few states participate). Therefore, we will consider only the processes with the participation of the ground and several *low-excited* states (cf. [4] for bulk and [5] for quantum wells). In this paper we study the processes of trapping and detrapping of the electron in quantum wells and wires by a shallow donor impurity placed either inside or outside the well or wire due to the interaction with longitudinal DA phonons.

We consider the system of the infinite square *quantum well* (QW) at $-L_z/2 < z < L_z/2$ and a shallow donor impurity at $(0, 0, z_i)$. In the effective-mass approximation the unperturbed Hamiltonian of the system is given by

$$\mathscr{H} = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\varepsilon_L R} + V_{\text{conf}}, \tag{1}$$

where m^* is the effective mass of the electron, ε_L is a lattice dielectric constant, $R = [x^2 + y^2 + (z - z_i)^2]^{1/2}$ is the distance from the impurity and term V_{conf} is the quantum well potential.

Hamiltonian (1) also describes the system of a rectangular *quantum wire* (QWR) of infinite depth and shallow Coulombic impurity located at $(x_i, y_i, 0)$. In this case the distance from the impurity is given by $R = [(x - x_i)^2 + (y - y_i)^2 + z^2]^{1/2}$, and confining potential $V_{\text{conf}} = 0$ for $|x| < L_x/2$ and $|y| < L_y/2$; otherwise $V_{\text{conf}} = \infty$.

For the ground and several low-excited states of Hamiltonian $\mathscr{H}$ of the QW we use the hydrogen-

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like trial wave functions ψ_{nm} containing variational parameters λ_{nm}:

$$\psi_{nm}(\boldsymbol{r}) = \frac{N_{nm}}{\lambda_{nm}^{|m|+1}} \rho^{|m|} \mathscr{P}_{nm}\left(\frac{R}{\lambda_{nm}}\right) \mathrm{e}^{-R/\lambda_{nm}} \mathrm{e}^{\mathrm{i}m\varphi} \chi(z). \tag{2}$$

Here $m = 0, \pm 1, \pm 2, \ldots$ is a magnetic quantum number due to the cylindrical symmetry of the Hamiltonian; $n = |m| + 1, |m| + 2, \ldots$ is the main quantum number; $\chi(z)$ is the transverse wave function of the lowest subband; dimensionless factors N_{nm} are chosen to normalize the wave functions to unity; functions $\mathscr{P}_{nm}(u)$ are polynomials of the order $n - |m| - 1$ with the coefficients chosen to provide orthogonality of the wave functions ψ_{nm} with the different quantum numbers. In fact, the trial functions (2), being a modification of Bastard's variational function [6], are equal to the product of the transverse wave function $\chi(z)$ of a free electron in the QW and hydrogen-like functions corresponding to orbital quantum number $l = |m|$ (states with other l are not bound for a sufficiently thin well).

For the bound states of an impurity in the QWR we choose the following odd and even trial functions containing variational lengths λ_{np}:

$$\psi_{np}(\boldsymbol{r}) = \frac{N_{np}}{\lambda_{np}^{1/2}} \left(\frac{z}{\lambda_{np}}\right)^{p} \mathscr{P}_{n-1}^{(p)}\left(\frac{R}{\lambda_{np}}\right) \mathrm{e}^{-R/\lambda_{np}} X(x)\, Y(y). \tag{3}$$

Here p is a parity of the wave function with respect to coordinate z ($p = 0$ for even states and $p = 1$ for odd states), $n = p + 1, p + 2, \ldots$, factors N_{np} and the coefficients of the polynomial $\mathscr{P}_{np}(u)$ of order $n - p - 1$ are chosen to provide orthonormality of the set (3). Wave functions (3) are equal to the product of the transverse wave function $X(x)\,Y(y)$ of a free electron in the QWR and hydrogen-like functions corresponding to $m = 0$ and $l = p$.

A standard variational procedure gives the bound states ψ_{nm}, Ψ_{np} and ionization energies ε_{nm}, ε_{np} measured from the bottom of the lowest subband. Fig. 1 plots the ionization energies of several lowest states in 100 Å wide QW and two lowest states in 100 × 100 Å QWR versus the impurity position.

The wave functions and ionization energies obtained are used to calculate the rates of transitions

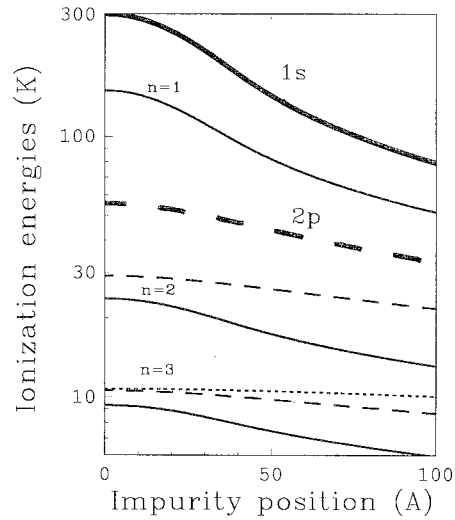

Fig. 1. Ionization energies of impurity bound states (K) versus impurity position (Å) in QW and QWR. *Thin lines*: ε_{nm} versus z_i in the *quantum well* of width $L_z = 100$ Å. Main quantum number n is indicated near the lines; solid, dashed, and dotted lines correspond to $m = 0, 1$, and 2. *Thick lines*: ε_{np} versus x_i in the *quantum wire*, $y_i = 0$, $L_x = L_y = 100$ Å. Solid line corresponds to ground 10 (1s) state, dashed line to 21 (2p) first excited state.

involving bound and free states of an electron. We start with a consideration of the processes in a *quantum well*. The transitions are assisted by emission and absorption of the longitudinal DA phonons with dispersion ω_q. The transferred energy ε is equal to $|\varepsilon_{nm} - \varepsilon_{n'm'}|$ for interlevel transitions and $\varepsilon = \varepsilon_{nm} + E$ for trapping/detrapping, where $E = \hbar^2 k^2/2m^*$ is the energy of a free electron state. The required phonon wave vector Q_ε is specified by the energy conservation law, $\hbar\omega_{Q_\varepsilon} = \varepsilon$. For calculation of the transition rates we use the Fermi golden rule and perform the summation over phonon wave vector $\boldsymbol{Q}$.

In the following we restrict ourselves to the cases of such energies of transition, ε, that the phonon wave vector Q_ε is (much) greater than other values of the same dimensionality, in particular $Q_\varepsilon L_z \geqslant 2\pi$. In GaAs this is a realistic approximation for characteristic lengths of the order of 100 Å or larger and $\varepsilon \geqslant 2\pi\hbar s/L \sim 10$–$20$ K (here s is the sound velocity). In this case, due to the rapidly oscillating factor $\exp(\mathrm{i}\boldsymbol{Q}\boldsymbol{r})$ in the matrix elements of transition,

the trapping and detrapping rates decrease rapidly with an increase of Q. Analysis shows that the main contribution to the transition rates is given by the "transverse" phonons with $Q \approx Q_z \gg Q_x, Q_y, k$.

In the limit of a phonon wavelength much smaller than the width of the well we find the following results for the transition rates (probabilities of processes per unit time): trapping rate

$$W(\boldsymbol{k} \to nm) = (2\pi)^4 n_{\mathrm{imp}}^{(2)} \frac{D^2}{\rho_{\mathrm{L}} s_\varepsilon} \frac{(n_\varepsilon + 1)\mathscr{F}_{nm}}{\varepsilon Q_\varepsilon^4 L_z^6}, \tag{4}$$

detrapping rate

$$\frac{\mathrm{d}W(nm \to \boldsymbol{k})}{\mathrm{d}(\hbar^2 k^2/2m^*)} = (2\pi)^4 \frac{m^*}{\pi\hbar^2} \frac{D^2}{\rho_{\mathrm{L}} s_\varepsilon} \frac{n_\varepsilon \mathscr{F}_{nm}}{\varepsilon Q_\varepsilon^4 L_z^6}, \tag{5}$$

and the rate of interlevel transitions

$$W(nm \to n'm') = (2\pi)^4 \frac{D^2}{\rho_{\mathrm{L}} s_\varepsilon} \times \frac{(n_\varepsilon + 1/2 \pm 1/2)\mathscr{F}_{nm \to n'm'}}{\lambda_{nm}\lambda_{n'm'} \varepsilon Q_\varepsilon^4 L_z^6}. \tag{6}$$

Here n_ε is the phonon occupation number; the value $s_\varepsilon \equiv \mathrm{d}\omega_Q/\mathrm{d}Q$ for small Q tends to the sound velocity s; D is a deformation potential constant; ρ_{L} is the crystal density; $n_{\mathrm{imp}}^{(2)}$ is the sheet concentration of impurities at $z = z_i$; $\mathscr{F}_{nm \to n'm'}$ are form factors given by

$$\mathscr{F}_{nm \to n'm'} = N_{nm}^2 N_{n'm'}^2 \times (\lambda^{2(|m|+|m'|+1)} / \lambda_{nm}^{2|m|+1} \lambda_{n'm'}^{2|m'|+1}) \times [\mathrm{e}^{-z_+} S(z_+) + \mathrm{e}^{-z_-} S(z_-)],$$

where $\lambda \equiv \lambda_{nm}\lambda_{n'm'}/2(\lambda_{nm} + \lambda_{n'm'})$ and $z_\pm = |z_i \pm L_z/2|/\lambda$; functions

$$S(u) = \mathrm{e}^u \int_u^\infty \mathrm{e}^{-t}(t^2 - u^2)^{|m|+|m'|} t\,\mathrm{d}t \times \mathscr{P}_{nm}^2(\lambda t/\lambda_{nm})\,\mathscr{P}_{n'm'}^2(\lambda t/\lambda_{n'm'})$$

are polynomials. Expressions for form factors $\mathscr{F}_{nm}$ can be obtained from that for $\mathscr{F}_{nm \to n'm'}$ by taking the limit $\lambda_{n'm'} \gg \lambda_{nm}$ and setting $N_{n'm'}^2 = \lambda_{n'm'}/\lambda_{nm}$ and $m' = 0$.

We have also calculated the transition rates for electrons in rectangular *quantum wires* in the presence of an impurity. In the case of comparatively large transition energies, $Q_\varepsilon \max(L_x, L_y) \geqslant 2\pi$, the rates of trapping, detrapping, and interlevel transitions can be obtained from Eqs. (4)–(6) after the following modifications: quantum numbers $nm, \boldsymbol{k}$, sheet impurity concentration $n_{\mathrm{imp}}^{(2)}$, and density of states $m^*/\pi\hbar^2$ must be changed to np, k_z, $n_{\mathrm{imp}}^{(1)}/\lambda_{np}$, and $m^*/\pi\hbar^2 k_z \lambda_{np}$ correspondingly; $\mathscr{F}/L_z^6$ must be replaced by $\mathscr{F}^{(x)}/L_x^6 + \mathscr{F}^{(y)}/L_y^6$. Form factors are given by

$$\mathscr{F}_{np \to n'p'}^{(x)} = 2\lambda N_{np}^2 N_{n'p'}^2 \int_{-L_y/2}^{L_y/2} \mathrm{d}y \cos^4(\pi y/L_y) \times [S(x_+) + S(x_-)],$$

where $\lambda \equiv \lambda_{np}\lambda_{n'p'}/2(\lambda_{np} + \lambda_{n'p'})$ and $x_\pm = [(x_i \pm L_x/2)^2 + (y - y_i)^2]^{1/2}/\lambda$, and functions

$$S(u) = \int_0^\infty \mathrm{d}t \left(\frac{\lambda t}{\lambda_{np}}\right)^{2p} \left(\frac{\lambda t}{\lambda_{n'p'}}\right)^{2p'} \exp(-\sqrt{t^2 + u^2}) \times \mathscr{P}_{np}^2\left(\frac{\lambda t}{\lambda_{np}}\right) \mathscr{P}_{n'p'}^2\left(\frac{\lambda t}{\lambda_{n'p'}}\right)$$

can be expressed in terms of the Bessel functions of the second kind. Form factors $\mathscr{F}_{np}$ can be derived from that for $\mathscr{F}_{np \to n'p'}$ by taking the limit $\lambda_{n'p'} \gg \lambda_{np}$ and setting $N_{n'p'} = 1$ and $p' = 0$. Expressions for $\mathscr{F}^{(y)}$ are obtained from $\mathscr{F}^{(x)}$ by interchanging x and y.

From Eqs. (4)–(6) one can obtain the following dependence of the transition rates on the transferred energy and the width of the well: $W_{\mathrm{i}\to\mathrm{f}} \propto \varepsilon^{-5}(n_\varepsilon + 1/2 \pm 1/2) L_z^{-6}$, for the rectangular quantum wire L_z^{-6} should be changed to $L_x^{-6} + L_y^{-6}$. Thus, the capture (ionization) of the carriers occurs mainly from (to) the free states near the bottom of the lowest subband.

Following [2] we introduce the inverse electron capture time $1/\tau_{nm}^{\mathrm{tr}}$ (or $1/\tau_{np}^{\mathrm{tr}}$) which gives the probability (per unit time) for an "average" electron in the lowest subband to be trapped to the level np (or np) of *any* impurity at the $z = z_i$ plane (or at line $x = x_i$, $y = y_i$), $1/\tau_{nm}^{\mathrm{tr}} = \int_0^\infty f(E)\, W(\boldsymbol{k} \to nm)\,\mathrm{d}E / \int_0^\infty f(E)\,\mathrm{d}E$. In the case of $\varepsilon \ll T$ it follows that $1/\tau^{\mathrm{tr}} \propto \varepsilon^{-5} W^{-6}$ from Eq. (4).

The results of numerical calculations of $1/\tau^{\mathrm{tr}}$ versus the impurity position are presented in Fig. 2. Parameters corresponding to GaAs are chosen, electron and phonon temperatures $T_{\mathrm{e}} = T_{\mathrm{ph}} = 300$ K, and the electrons are assumed to be nondegenerate. Thin and thick lines show the capture

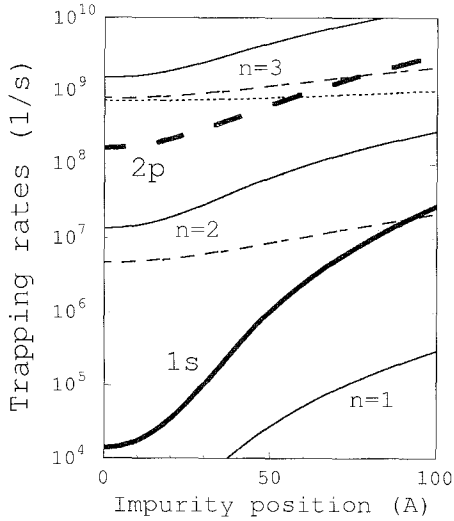

Fig. 2. Inverse capture times $1/\tau_{nm}^{tr}$ and $1/\tau_{np}^{tr}$ to impurity bound states versus impurity position in QW and QWR. Impurity concentrations $n_{imp}^{(2)} = 10^{10}/cm^2$ in QW and $n_{imp}^{(1)} = 10^5/cm$ in QWR. Other parameters and notations are as in Fig. 1.

rates to the bound states of impurity in 100 Å wide QW and 100×100 Å QWR, correspondingly. One can see that the dependence of $1/\tau_{tr}$ on the impurity position for different states has a form analogous to that in Fig. 1, i.e. for a given cross-section of QW or QWR the behavior of trapping probabilities is specified mainly by ionization energies ε_{nm} or ε_{np}. Note that for comparable ionization energies the capture probability in QWR is essentially higher than that in QW. This is partially due to the difference in the density of states – in QWR there are relatively more electrons near the bottom of the subband, where the capture rate is higher.

Analysis of Figs. 1 and 2 and results for the interlevel transition rates (cf. [5]) give the following qualitative picture of the carrier trapping. For highly excited states ($n \geqslant 3$ in QW) the energy separation between levels is small, being only a fraction of the effective Rydberg energy. Thus, for temperatures greater than or of the order of 20 K, these states can be treated as constituting a quasicontinuous spectrum; therefore, the transitions between the levels are fast and can be treated in the fashion of Refs. [2,3]. Since the levels with $n = 1$ and $n = 2$ are separated from the others (cf. Fig. 1), capture to the ground state occurs via levels with $n = 2$, and direct trapping from the free states has much lower probabilities.

Acknowledgements

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