PHONON-ASSISTED TRAPPING BY SHALLOW IMPURITY IN QUANTUM WELL

Yuri M. Sirenko and Vladimir Mitin

Department of Electrical and Computer Engineering, Wayne State University, Detroit, Michigan 48202, USA

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We have considered the capture of electron in a quantum well by shallow donor impurity due to the interaction with an acoustical phonon. Wave functions of the nine lowest bound states have been found by variational method. We have calculated the rates of transitions between the free states and bound states as well as between different bound states. In the case of phonon wavelength much smaller than the width of the well \( L \), the transition rates are proportional to \( e^{-2}(n_e + 1/2 \pm 1/2)L^{-6} \), where \( e \) is the transferred energy, \( n_e \) is a phonon occupation number.

I. Introduction

The processes of free carrier trapping by impurity centers 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. First, proposed by Lax [2] and then improved and extended by Leningrad's group [3], treats the capture of carrier as classical descend through the quasiisotropic spectrum of highly-excited bound states due to cascade emission of low-energy acoustical phonons. The generalization of this model to the two-dimensional case was performed by Karpus [4]. Since this model is based on the assumption of the high density of impurity bound states at the negligible thermal energy, its applicability is limited to low temperatures and materials with comparatively large effective Rydberg energy [5].

In GaAs quantum wells the Rydberg energy is less than a hundred kelvins and, at room temperature, the case opposite to that of the first model is realized. Therefore we will consider only the processes with the participation of the ground and several low-excited states assuming that they give the major contribution to transport and low-frequency noise. For bulk materials the calculations of acoustical phonon assisted trapping have been performed with the help of exact coulombic wave functions of the free and several lowest bound states [6]. To our best knowledge there exist no correspondent treatment of capture by impurities in quantum wells.

In this paper we study the processes of trapping and detrapping of the electron in a quantum well by a shallow donor impurity placed either inside or outside of the well. We calculate the rates of electron transitions between the free states and several lowest bound states, as well as transitions between the different bound states assisted by the emission and absorption of longitudinal DA-phonons. Impurity bound states in quantum well are calculated within the variational method proposed by Bastard for the ground state of impurity in the infinite rectangular well [7] and generalized subsequently by a number of authors to account for different forms of confining potential, higher-excited levels, radiative transitions, etc. (for reviews see e. g. [8]).

II. Model and Calculations

Following Bastard [7] we consider the system of the infinite square quantum well at \(-L/2 < x < L/2\) and a shallow donor impurity at \((0, 0, z_0)\). In the effective-mass approximation the unperturbed Hamiltonian of the system is given by

\[
\mathcal{H} = -\frac{\hbar^2}{2m^*} \nabla^2 - e^2 \frac{\epsilon_L}{\epsilon_L R} + V_{QW}(z),
\]

where \( m^* \) is an effective mass of electron; \( \epsilon_L \) is a lattice dielectric constant; \( R = \sqrt{\rho^2 + (z - z_0)^2} \) is a distance from the impurity and \( \rho = (x, y) \) is a polar radius; term \( V_{QW}(z) \) is the quantum well potential.

For the ground and several low-excited states of Hamiltonian \( \mathcal{H} \) we use the hydrogen-like trial wave functions \( \psi_{nm} \) containing variational parameters \( \lambda_{nm} \)

\[
\psi_{nm}(r) = \frac{N_{nm}}{\lambda_{nm}^{m+1}} \rho^{|m|} P_{nm} \left( \frac{r}{\lambda_{nm}} \right) e^{-R/\lambda_{nm}} \rho^{|m|} \chi(z).
\]

(2)

Here \( m = 0, \pm 1, \pm 2, \ldots \) is a magnetic quantum number due to the cylindrical symmetry of the Hamiltonian; \( n = 1, \ldots , |m| + 1 \) is the main quantum number; \( \chi(z) \) is the transverse wave function of a lowest subband,

\[
\chi(z) = \sqrt{\frac{2}{L}} \cos \frac{\pi z}{L} \theta(L/2 - |z|),
\]

(3)

where \( \theta(z) \) is a step-function; dimensionless factors \( N_{nm} \) are chosen to normalize the wave functions to unity; functions \( P_{nm}(z) \) are polynomials of the order \( n - |m| - 1 \) with the coefficients chosen to provide orthogonality of the wave functions \( \psi_{nm} \) with the different quantum numbers. In fact, trial functions (2) are equal to the product of the transverse wave function \( \chi(z) \) of free electron in the quantum well and hydrogen-like functions corresponding
to orbital quantum number \( l = |m| \) (states with other \( l \) are not bound for a sufficiently thin well).

Minimization of the expectation value of the Hamiltonian \( \mathcal{H} \) for the trial wave functions \( \psi_{nm}(r) \) with conditions of orthonormality gives the values of the variational lengths \( \lambda_{nm} \) and ionization energies \( \epsilon_{nm} \) of the impurity bound states

\[
\epsilon_{nm} = \frac{\hbar^2 \pi^2}{2mL^2} - (\psi_{nm}|\mathcal{H}|\psi_{nm}).
\]

On Fig. 1 we plot the results of calculations for ionization energies of nine lowest bound states corresponding to \( n = 1,2,3 \) vs. the position of the impurity for the quantum well of width \( L = 150 \ \text{Å} \) (note that \( \epsilon_{nm} \) does not depend on the sign of \( m \)). For the sake of convenience the ionization energies are measured in kevins.

Electron free states are taken as unperturbed plane waves corresponding to the lowest subband,

\[
\psi_k(x) = S^{-1/2} \exp(ikx) \chi(x),
\]

where \( S \) is a layer area, and \( k = (k_x, k_y) \) is in-plane electron wave vector.

We use the Fermi golden rule to calculate the rates of transitions due to the interaction with the longitudinal DA-phonon modes:

\[
W_{i\rightarrow f}^{Q} = \frac{2\pi}{\hbar} \frac{\hbar D^2 Q^2}{2\rho \omega Q V} \left( n_Q + \frac{1}{2} \pm \frac{1}{2} \right) |\langle \psi_f | e^{iQr} | \psi_i \rangle|^2 \times \delta(\epsilon_f - \epsilon_i + \hbar \omega Q).
\]

Here \( W_{i\rightarrow f}^{Q} \) is the probability of transition between initial \((i)\) and final \((f)\) states per unit time mediated by DA-phonon with wave vector \( Q = (q_x, q_y) \); \( D \) is the deformation potential constant; \( \omega Q \) specifies phonon dispersion relationship; \( n_Q \) is the occupancy number of phonons; \( \rho L \) and \( V \) are crystal density and volume; sign "plus" corresponds to the emission and "minus" to absorption of a phonon.

We consider all possible sorts of transitions: i) trapping with \( i \equiv k \) and \( f \equiv nm \); ii) detrapping with \( i \equiv nm \) and \( f \equiv k \); iii) interlevel transitions with \( i \equiv nm \) and \( f \equiv n'm'. \) In the case of trapping one should multiply the left-hand side of Eq. (5) by the number of impurities \( N_{\text{imp}} \) in the plane \( z = z_i \) to obtain the probability for an electron to be trapped to the state \( \psi_{nm} \) of any impurity.

For the matrix element of transition with allowance for Eqs. (2) and (4) we obtain after integration over the polar angle \( \varphi \)

\[
\langle \psi_{nm} | e^{iQr} | \psi_k \rangle = \frac{2\pi N_{\text{imp}}}{\lambda_{nm+1}^{1/2}} \int_{-L/2}^{L/2} dx \chi(x)e^{iQz} \times \int_0^\infty dp \rho p e^{-2\lambda_{nm}/\lambda_{nm+1}} J_{nm}(|q - k|p),
\]

and a similar expression for the interlevel transitions (here \( J_{nm} \) is a Bessel function).

In order to find the overall transition rates \( W_{i\rightarrow f} \) we have to perform the integration over all possible phonon wave vectors \( Q \):

\[
W_{i\rightarrow f} = (2\pi)^{-3} V \int d^2Q \ W_{i\rightarrow f}^{Q}.
\]

Magnitude of \( Q \) is specified by the transition energy \( \epsilon \):

\[
\hbar \omega_Q = \epsilon,
\]

where \( \epsilon = \epsilon_{nm} + \hbar^2 k^2/(2m^*) \) or \( \epsilon = |\epsilon_{nm} - \epsilon_{n'm'}| \).

In the following we restrict ourselves by the cases of such energies of transition, \( \epsilon \), that phonon wave vector \( Q \) is (much) greater than other values of the same dimensionality, in particular

\[
Q \ L \geq 2 \pi.
\]

In GaAs this is realistic approximation for characteristic lengths of the order of hundred angstroms or larger and \( \epsilon \geq 2\pi \hbar s/L \sim 10 \div 20 \ \text{K} \). In this case due to the rapidly oscillating factors \( \exp(iz) \) and \( J_{nm}(|q - k|p) \) in Eq. (6) the trapping and detrapping rates decrease rapidly with the increase of \( Q \). Analysis of the integral in Eq. (6) shows that the main contribution to transition rates (7) is given by the "transverse" phonons with \( Q \approx q_x \gg q, k \) since the matrix element of transition decreases more rapidly with \( |q - k| \) than with \( q_x \). The same conclusion is valid for interlevel transitions.

Substituting the expression (6) for matrix element into Eqs. (5) and (7) and performing integration over phonon wave vectors \( Q \) we find the following results for the trapping rate

\[
W(k \rightarrow nm) = n_{\text{imp}} \frac{D^2}{\rho L s_e} \frac{(n_e + 1) F_{nm}}{e L^2 (Q_s L/2\pi)^3},
\]

detrapping rate

\[
\frac{dW(nm \rightarrow k)}{d(\hbar^2 k^2/(2m^*))} = \frac{m^*}{\pi \hbar^2} \frac{D^2}{\rho L s_e} \frac{n_e F_{nm}}{e L^2 (Q_s L/2\pi)^3},
\]
and the rate of interlevel transitions

\[ W(nm \rightarrow n'm') = D^3 \frac{\rho_L s_z}{\lambda_{nm} \lambda_{n'm'}} \left| \frac{Q_z L}{2 \pi} \right|^4 . \]  

(11)

Here \( n_z \) is a phonon occupation number; the value \( s_z \equiv du_{sg}/dQ \) for small \( Q \) tends to the sound velocity \( s \); factor \( n_{\text{imp}} = N_{\text{imp}}/S \) is a sheet concentration of impurities at \( z = z_i \); formfactors \( F \) are given by

\[ F_{nm} = \frac{N_{nm}^2}{2|\lambda_{nm}|^2} \left[ e^{-z_i} S_{nm}(z_i) + e^{z_i} S_{nm}(z_{-i}) \right] ; \]

\[ F_{n'm'} - n'm' = \frac{N_{n'm'}^2 N_{nm}^2}{2|\lambda_{n'm'}|^{2|\lambda_{nm}|^2}} \left[ e^{-z_i} S_{nm}(z_i) + e^{z_i} S_{nm}(z_{-i}) \right] \]

\[ \times \left[ e^{-z_i} S_{n'm'}(z_i) + e^{z_i} S_{n'm'}(z_{-i}) \right] , \]

where \( z_i = |2z_i \pm L|/\lambda_{nm} \) and \( z_{-i} = |z_i \pm L/2|/\lambda_{nm} \); functions

\[ S_{nm}(u) = e^{-u} \int_0^\infty e^{-t} P_{nm}(t/2) (t^2 - u^2)^{|\lambda_{nm}}| dt , \]

\[ S_{n'm'}(u) = e^{-u} \int_0^\infty e^{-t} (t^2 - u^2)^{|\lambda_{n'm'}}| dt \]

\[ \times P_{n'm'} \left( \frac{t}{\lambda_{n'm'}}, \frac{u}{\lambda_{nm}} + \frac{u}{\lambda_{n'm'}} \right) \]

are polynomials. Note that in equilibrium the transition probabilities (9) and (10) are related by the detailed balance equation.

The transition energies less or of the order of 100 K involved in our problem correspond to phonon wavevector \( Q \) in an almost linear part of \( \omega_Q \) dependence [9], therefore we can use the equation \( Q_z = e/\hbar s \) and the value of deformation potential constant \( D \) at \( Q = 0 \). With the help of this relation we obtain from Eqs. (9) — (11) the following dependence of the transition rates on the transferred energy and the width of the well: \( W_{e-f} \propto e^{-z_i} (n_z + 1/2 \pm 1/2) L^{-6} \) (numerical calculations show that for reasonable values of \( L \) and \( z_i \) formfactors \( F \) are of the order of unity). Thus the capture (detraping) of the carriers occurs mainly from (10) the free states near the bottom of the lowest subband. Note that the transition energy is in its turn specified by ionization energies \( \varepsilon_{nm} \), which depend strongly on \( z_i \) and \( L \) (cf. Fig. 1).

Following [3] we introduce the integral transition times \( \tau_{\text{tr}} \) and \( \tau_{\text{det}} \) which appear in the balance equations for carrier concentration. The electron capture time \( \tau_{\text{tr}} \) specifies the probability (per unit time) for "average" electron in the lowest subband to be trapped to the level \( nm \) of any impurity at \( z = z_i \) plane:

\[ 1/\tau_{\text{tr}} = \int_0^\infty f(E) W(k \rightarrow nm) dE / \int_0^\infty f(E) dE . \]  

(12)

The electron stay time \( \tau_{\text{det}} \) gives the rate of electron detrapping from the bound state \( nm \) to any free electron state in the lowest subband,

\[ 1/\tau_{\text{det}} = \int_0^\infty dE [1 - f(E)] [dW(nm \rightarrow k)/dE] . \]  

(13)

Here \( E = \hbar k^2/(2m^*), \) and \( f(E) \) is the distribution function of the electrons on the lowest subband. In the case of \( e \ll kT \) from Eqs. (9) and (10) follows that \( 1/\tau_{\text{tr}} \propto e^{-z_i} W_{e-f} \). In equilibrium the relation \( \tau_{\text{tr}}/\tau_{\text{det}} = \tau_{\text{nm}}/n_{\text{imp}} \) holds.

### III. Numerical Results

For the numerical evaluation of the transition rates we use the parameters of the GaAs: \( m^* = 0.067m_0, s = 5.24 \times 10^6 \text{cm/s}, \rho_L = 5.36 \text{ g/cm}^3, \epsilon_L = 12.5, D = 7.0 \text{ eV}. \)

The width of the well \( L \) is equal to 150 Å; both phonon and electron temperatures are equal to 300 K.

On Fig. 2 we presented inverse electron capture times \( 1/\tau_{\text{tr}} \) and capture rates \( n_{\text{cap}} = 1/\tau_{\text{tr}} \tau_{\text{nm}} \) versus the impurity position \( z_i \) for the case of the nondegenerate electrons and \( n_{\text{imp}} = 10^{10} / \text{cm}^2 \). One can see that the dependence of \( W_{e-f} \) on \( z_i \) for different states \( nm \) has the form analogous to that on Fig. 1, i.e. for the given width of the well \( L \) the behavior of trapping probabilities is specified mainly by ionization energies \( \varepsilon_{nm} \). Note that for the group of levels with \( n = 3 \) the condition (8) is hardly justified, therefore the results for \( 1/\tau_{\text{tr}} \) provide only an estimation for the actual rates.

On Fig. 3 the rates of interlevel transitions calculated with the help of Eq. (11) are plotted versus the impurity position. Two groups of transitions are presented: \( ij \) between the levels with \( n - 1 \) and \( n = 2 \); \( ij \) between the levels with \( n = 1 \) and \( n = 3 \). We plotted only the results for transitions from the upper to lower level; the rates for inverse processes differ by the factor \( \exp(-\varepsilon_{nm}/T) \) which

![Fig. 2. Inverse capture times 1/\tau_{\text{tr}} (left axis) and capture rates \( n_{\text{cap}} = 1/\tau_{\text{tr}} \tau_{\text{nm}} \) (right axis) to impurity bound state \( nm \) (indicated near the curves) vs. impurity position \( z_i \). Width of the well \( L = 150 \text{ Å}, \) electron and phonon temperatures \( T_e = T_{ph} = 300 \text{ K}; \) for calculation of 1/\tau_{\text{tr}} we used the sheet impurity concentration \( n_{\text{imp}} = 10^{10} / \text{cm}^2 \).]
Analysis of Figs 1–3 gives the following qualitative picture of the carrier trapping. For states with \( n \geq 3 \) the energy separation between levels is small being only a fraction of effective Rydberg energy and also due to the lifting of the degeneracy in quantum number \( m \). Thus, for temperature greater or of the order of 10 K the states with \( n \geq 3 \) can be treated as quasiconsecutive spectrum, therefore the transitions between the levels are fast and can be treated in the fashion of Refs. [3, 4]. The levels with \( n = 1 \) and \( n = 2 \) are separated from the other (cf. Fig. 1), this implies the existence of several distinct groups of transitions on Figs. 2 and 3. The time of capture to the ground state of the impurity is specified by the transitions from levels with \( n = 2 \), direct trapping from the free states have much lower probabilities. Note that for the capture of electron to the ground state of on-center impurity other mechanisms of trapping can dominate, namely interaction with an optical phonon or Auger-processes.

The effect of carrier trapping in quantum wells on nonequilibrium transport and noise should be examined by solving the balance equation for the electron distribution function for the free and impurity bound states with the transition rates given by Eqs. (9) – (11) and proper scattering mechanisms included (cf. [6]).

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References