Nonradiative Capture of Electrons in Quantum Wells and Wires by Shallow Donor Impurities

By

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The capture of electrons in a quantum well or wire by shallow donor impurities due to the interaction with an acoustic phonon is considered. Wave functions of several lowest bound states are found by the variational method. The rates of transitions between the free and bound states as well as between different bound states are calculated. In the case of well or wire width \( L \) less than or of the order of the effective Bohr radius and greater than the phonon wavelength, the transition rates are proportional to \( \varepsilon^{-2}(n_e + 1/2 \pm 1/2) L^{-4} \), where \( \varepsilon \) is the transferred energy, and \( n_e \) a phonon occupation number.

1. Introduction

The processes of carrier capture by impurities are known to have a strong influence on noise and transport in semiconductor structures. In this paper we study the processes of trapping and detrapping of the electron in a quantum well (QWL) or quantum wire (QWR) by a shallow donor impurity placed either inside or outside of the well or wire.

From a large number of results pertinent to the defects in the bulk [1 to 3] we mention two models for capture of an electron by a shallow Coulombic impurity: (i) the cascade model based on the assumption of a quasicontinuous highly-excited bound states spectrum and (ii) the direct calculation of transition probabilities between free states and several low-excited bound states.

In the cascade-capture model, originally introduced by Lax [4] and further elaborated by the Leningrad group [5], the capture of carriers is treated as classical descent through the quasicontinuous spectrum of highly-excited bound states due to cascade emission of low-energy acoustic phonons. A solution of the obtained balance equations for the electron distribution function can be found analytically in several limiting cases or with the help of the Monte Carlo simulation [2, 5]. The generalization of this model to the two-dimensional case was performed by Karplus [6]. Since the cascade-capture model is based on the assumption of a high density of impurity bound states at negative thermal energy, its applicability is limited [7] to low temperatures and materials with comparatively large effective Rydberg energy \( R \).

In GaAs quantum wells the impurity ground state ionization energy is of the order of 100 K (in bulk material \( R \approx 65 \) K) 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. The first quantum-mechanical formulation of the

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problem in bulk materials is due to Ascarelli and Rodriguez [8] who proposed a model, where the capture takes place through the hydrogen-like states 1s, 2s, 3s, and 4s of the impurity center. The capture and various transitions are accompanied by emission and absorption of one deformational acoustic phonon. Subsequent generalizations of the calculations [9] included higher values of the main quantum number \( n \leq 7 \), nonzero angular momentum, different polarization of the emitted phonons, etc.

Since the pioneering work of Bastard [10] a considerable amount of work dealt with the theoretical calculation of the binding energies of shallow impurities in quantum wells, wires, and dots, as well as an experimental observation of the infrared radiative transitions between the ground and excited levels of an impurity [11].

In this paper we consider different mechanisms of the relaxation, namely, nonradiative capture of electrons in quantum wells or wires to the ground and low-excited states. We have calculated the rates of electron capture, ionization, and transitions between different bound states of a shallow donor impurity assisted by emission or absorption of a deformational acoustic phonon (for our preliminary results see [12, 13]).

The results are presented as follows: Section 2 introduces the model and describes the variational procedures for the calculation of the impurity bound states, in Section 3 the expressions for the transition rates are obtained, Section 4 contains numerical results and a discussion.

2. Hamiltonian and Variational Procedure

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

\[
\mathcal{H} = -\frac{\hbar^2}{2m^*} \nabla^2 - \frac{e^2}{\varepsilon_L R} + V_{\text{conf}},
\]

(1)

where \(m^*\) is the effective mass of the electron, \(\varepsilon_L\) the lattice dielectric constant, \(R = \sqrt{x^2 + (z - z_0)^2}\) the distance from the impurity, \(q^2 = x^2 + y^2\), \(V_{\text{conf}}\) is the quantum well potential.

The Hamiltonian (1) describes also the system of a rectangular quantum wire of infinite depth and shallow Coulombic impurity located at \((x_0, y_0, 0)\). In this case the distance from the impurity is given by \(R = [(x - x_0)^2 + (y - y_0)^2 + z^2]^{1/2}\) and the 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 the Hamiltonian \(\mathcal{H}\) in QWL we use the hydrogen-like trial wave functions \(\psi_{nm}\) containing the variational parameters \(\lambda_{nm}\),

\[
\psi_{nm}(r) = \frac{N_{nm}}{\lambda_{nm}}^m q^{|m|} \mathcal{A}_{nm} \left( \frac{R}{\lambda_{nm}} \right) e^{-R/\lambda_{nm}} e^{i\lambda_{nm} r} Z(z),
\]

(2)

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

\[
Z(z) = \sqrt{\frac{2}{L_z}} \cos \frac{nz}{L_z} \Theta \left( \frac{L_z}{2} - |z| \right),
\]

(3)
where $\Theta(x)$ is the step function, the dimensionless factors $N_{nm}$ normalize the wave functions to unity. The functions $\beta_{nm}(u)$ are polynomials of the order $n - |m| - 1$ with coefficients chosen so as to provide orthogonality of the wave functions $\psi_{nm}$ with the different numbers; for $n = |m| + 1$ we take $\beta_{nm}(u) = 1$, for $n = |m| + 2$ we have $\beta_{nm}(u) = 1 + a_{nm} u$, and for $n = |m| + 3$ take $\beta_{nm}(u) = 1 + a_{nm} u + b_{nm} u^2$. Note that the functions (2) do not depend on the sign of $m$. Below we consider bound states with the main quantum number $n = 1, 2, 3$.

The trial functions (2) represent the generalization of Bastard's trial function [10] and are equal to the product of the transverse wave function $Z(z)$ of the 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).

For the bound states of the impurity in a quantum wire we choose the following odd and even trial functions containing variational lengths $\lambda_{np}$:

$$
\psi_{np}(r) = N_{np} \left( \frac{x}{\lambda_{np}} \right)^{\lambda_{np}} e^{-R x} c^{-R \lambda_{np}} X(x) Y(y).
$$

(4)

Fig. 1.

Fig. 1. Ionization energies of impurity bound states $\varepsilon_{nm}$ vs. the width of the well $L_x$. Solid, long-dashed, and short-dashed lines correspond to states with $m = 0, 1, $ and $2$, respectively. Thick lines correspond to $z_i = 0$, thin lines to $z_i = L_x/2$.

Fig. 2. Ionization energies of impurity bound states vs. impurity position in quantum well and wire. Thin lines $\varepsilon_{np}$ vs. $z_i$ in the quantum well of width $L_x = 10$ nm. The main quantum number $n$ is indicated near the lines; solid, dashed, and dotted lines correspond to $m = 0, 1, $ and $2$, respectively. Thick lines $\varepsilon_{np}$ vs. $z_i$ in the quantum wire, $y_i = 0, L_x = L_y = 10$ nm. Solid line corresponds to ground 1s (1s) state; dashed line to 21 (2p) first excited state.
Here \( p \) is the parity of the wave function with respect to coordinate \( z \) (\( p = 0 \) for even and \( p = 1 \) for odd states); \( n = p + 1, p + 2, \ldots \); the factors \( N_{np} \) and the coefficients of the polynomial \( \bar{c}_{np}(w) \) of order \( n - p - 1 \) are chosen to provide orthonormality of the set (4). The functions \( X(x) \) and \( Y(y) \) can be obtained from (3) by changing \( L_z \) to \( L_x \) or \( L_y \). The wave functions (4) are equal to the product of the transverse wave function \( X(x) \) \( Y(y) \) of the free electron in QWR and hydrogen-like functions corresponding to \( m = 0 \) and \( l = p \).

A standard variational procedure gives the bound states \( \psi_{mnp} \) \( \psi_{np} \) and the ionization energies \( \varepsilon_{nmp} \) \( \varepsilon_{np} \) measured from the bottom of the lowest subband.

Fig. 1 presents the dependence of the ionization energies of impurity bound states in the GaAs QWL on the width of the well \( L_x \). As seen from the figure, the trial set of wave functions (2) reproduces correctly the results of the 3D and 2D [14] Coulomb problems \( \varepsilon^{(3D)}_{nm} = \mu/(n + 1) \) \( \lambda^{(2D)}_{nm} = \mu/(n + 1/2) \) \( \varepsilon^{(3D)}_{nm} = \mu/(n + 1) \) \( \lambda^{(2D)}_{nm} = \mu/(n + 1/2) \) \( \mu \), where \( \mu \equiv m^*e^2/2\hbar^2 \) and \( \varepsilon_{nm} = \mu/(n + 1) \) \( \lambda_{nm} = (n + 1) \) \( \mu \) for on-center defects, as well as the result \( \varepsilon_{nm} = \mu/(n + 1) \) \( \lambda_{nm} = (n + 1) \) \( \mu \) for on-edge impurities [15]. In a quantum well of finite width the degeneracy in the magnetic quantum number \( m \) is removed and higher values of \( m \) correspond to deeper states.

In Fig. 2 we plot the ionization energies of several lowest states in a 10 nm wide QWL and the two lowest states in a 10 nm \( \times \) 10 nm QWR versus the impurity position for the parameters of GaAs.

3. Transition Rates

We use the Fermi Golden Rule to calculate the transition rates due to the interaction with the longitudinal DA-phonon modes,

\[
W_{ij}^{Q} = \frac{2\pi}{2} \frac{hD^{2Q}z}{2\hbar \omega_{Q}V} \left( n_{Q} + \frac{1}{2} \right) \left( \frac{1}{2} + \delta \left( \varepsilon_{i} - \varepsilon_{j} \right) \right) \delta \left( \varepsilon_{i} - \varepsilon_{j} \right) \delta \left( \varepsilon_{i} - \varepsilon_{j} \right)
\]

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

Electron free states are taken as unperturbed plane waves with wave vector \( k \) corresponding to the lowest subband, where \( k \equiv (k_{x}, k_{z}) \) in the case of QWL, and \( k \equiv k_{z} \) for the case of QWR. The approximation of the undistorted electron wave function in the vicinity of the Coulomb center is good for all energies in the case of a quantum well. In fact, for \( L < a_{B} \) even in the worst case of on-center impurity and extremely low electron energies, the inaccuracy of the final results will not exceed the 2D Sommerfeld factor [14] \( Z = 2 \). However, in the case of extremely thin quantum wire and \( \hbar^{2}k^{2}/2m^{*} < \mu \) the use of the unperturbed electron wave function will lead to an overestimation of (de)trapping rates since the 1D Sommerfeld factor [16] \( Z \rightarrow 0 \) for \( k \rightarrow 0 \).

We consider all possible sorts of transitions: (i) trapping with \( i \equiv k \) and \( f \equiv nm \) for QWL (or \( f \equiv np \) for QWR); (ii) detrapping with \( i \equiv nm \) (or \( i \equiv np \)) and \( f \equiv k \); (iii) interlevel transitions with \( i \equiv nm \) and \( f \equiv n'm' \) (or \( i \equiv np \) and \( f \equiv n'p' \)). In the case of trapping one should multiply the left-hand side of (5) by the number of impurities \( N_{imp} \) in the plane \( z = z_{j} \) or the line \( (x = x_{i}, y = y_{j}) \) to obtain the probability for an electron to be trapped by any impurity.
In order to find the overall transition rates \( W_{i\rightarrow f} \) we have to perform the integration over all possible phonon wave vectors \( \mathbf{Q} \).

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

(6)

The magnitude of \( Q \) is specified by the transition energy \( \varepsilon \),

\[
h\omega_Q = \varepsilon,
\]  

(7)

where in the case of QWL \( \varepsilon = \varepsilon_{nm} + \hbar^2k^2/2m^* \) or \( \varepsilon = |\varepsilon_{nm} - \varepsilon_{n'm'}| \) for the QWR case the subscript \( m \) should be replaced by \( p \). Note that for small transition energies corresponding to the linear part of the \( \omega_Q \) dependence we have \( Q \varepsilon = \varepsilon/\hbar s \) with \( s \) being the sound velocity.

In the following we will assume the following conditions satisfied: (i) the width of the well (or diameter of the wire) is smaller than or of the order of the Bohr radius (in GaAs \( a_B \approx 10 \text{ nm} \),

\[
L < a_B \quad \text{(for QWL),} \quad \max (L_x, L_y) < a_B \quad \text{(for QWR)},
\]  

(8)

(ii) large transferred energies \( \varepsilon \): the phonon wave vector \( Q \varepsilon \) defined by (7) is greater than other values of the same dimensionality, in particular,

\[
Q L_z > 2\pi \quad \text{(for QWL),} \quad Q \min (L_x, L_y) > 2\pi \quad \text{(for QWR)}.
\]  

(9)

In GaAs this is a realistic approximation for characteristic lengths of the order of ten nm and \( \varepsilon \geq \hbar ks/L \approx 10 \text{ to } 20 \text{ K} \).

Under these assumptions due to the rapidly oscillating factors \( \exp(i\mathbf{Qr}) \) in transition matrix elements the trapping and detrapping rates decrease rapidly with the increase of \( Q \). Analysis of the integral in (6) shows that in case of QWL the main contribution to transition rates is given by the “transverse” phonons with \( Q \approx Q_x \gg Q_y, Q_z, k \). In the case of QWR, since the matrix elements decrease more rapidly for the wider limits of integration, the dominant contribution to the integral in (6) is given by the phonons with \( Q \approx Q_y \gg Q_x, Q_z, k \), or \( Q \approx Q_z \gg Q_x, Q_y, k \) for the cases \( L_x < L_y \) and \( L_y < L_x \), respectively.

Substituting (5) to (6) and performing the integration over the phonon wave vector \( \mathbf{Q} \) we find the following transition probabilities of the electron in the quantum well:

- trapping rate,

\[
W(k \rightarrow nm) = n_{imp}^{(2)} D^2 \frac{n_{\varepsilon} + 1}{\pi k_s \varepsilon^2 L_z^2 (Q L_z/2\pi)^2},
\]  

(10)

- detrapping rate,

\[
\frac{dW(nm \rightarrow k)}{d(\hbar^2 k^2/2m^*)} = \frac{m^* D^2}{\pi \hbar^2 k_s \varepsilon^2 L_z^2 (Q L_z/2\pi)^2},
\]  

(11)

and the rate of interlevel transitions,

\[
W(nm \rightarrow n'm') = \frac{D^2}{\varepsilon^2 n_{\varepsilon} + 1/2 \pm 1/2} \frac{\mathcal{F}_{nm,n'm'}}{\varepsilon_{nm}^2 \varepsilon_{n'm'}^2 L_z^2 (Q L_z/2\pi)^2}.
\]  

(12)

Here \( n_{\varepsilon} \) is the phonon occupation number, the value \( s \varepsilon \equiv d\omega_Q/dQ \) for small \( Q \) tends to the sound velocity \( s \) the factor \( n_{imp}^{(2)} \) is the sheet concentration of impurities in the plane \( z = z_f \).
For the quantum wire we obtain:

\[ W(k \to np) = (2\pi)^4 \frac{n_{np}^{(1)}}{\lambda_{np} \, \hat{q}, \hat{S}, \hat{S}_e} \frac{D^2}{\hat{\rho}^2} \frac{n_e + 1}{L_x^6 + L_y^6} \left[ \mathcal{F}_{np}^{(x)} \mathcal{F}_{np}^{(y)} \right], \]  

(13)

detrapping rate,

\[ \frac{dW(np \to k)}{d(h^2k^2/2m^*)} = (2\pi)^4 \frac{m^*}{\pi\hbar^2k^2} \frac{D^2}{\hat{\rho}^2} \frac{n_e}{\hat{q}, \hat{S}, \hat{S}_e} cL^2 \frac{Q_e^{(x)}}{L_x^6} + \frac{Q_e^{(y)}}{L_y^6}, \]  

(14)

and the rate of interlevel transitions,

\[ W(np \to n'p') = (2\pi)^4 \frac{D^2}{\hat{\rho}^2} \frac{n_e + 1/2 \pm 1/2}{L_x^6 + L_y^6} \left[ \mathcal{F}_{np}^{(x) \pm} \mathcal{F}_{np}^{(y) \pm} \right], \]  

(15)

Here \( n_{np}^{(1)} \) is the one-dimensional impurity concentration at \((x = x, y = y)\), the form factors \( \mathcal{F} \) for (10) to (15) are given in the Appendix. Note that in equilibrium the transition probabilities (10), (11) and (13), (14) are related by the detailed balance equation.

The transition energies less than or of the order of 100 K involved in our problem correspond to the phonon wave vector \( \mathbf{Q} \) in the almost linear part of the \( \omega_\mathbf{Q} \) dependence, therefore we can use the equation \( \mathbf{Q} = \epsilon/\hbar s \) and the value of the deformation potential constant \( D \) at \( \mathbf{Q} = 0 \). With the help of this relation we obtain from (10) to (15) the following dependence of the transition rates on the transferred energy and the width of the well or wire:

\[ W_{i \to f} \propto \epsilon^{-2} (n_e + 1/2 \pm 1/2) L^{-6}, \]  

(16)

where \( L = L_x \) for QWL and \( L = \min(L_x, L_y) \) for QWR. Thus, the capture (ionization) of carriers occurs mainly from (to) the free states near the bottom of the lowest subband. Note that the transition energy in its turn is specified by the ionization energies \( \epsilon_{nm} \) and \( \epsilon_{np} \) which depend strongly on the impurity position and the transverse dimensions of QWL or QWR (cf. Fig. 1 and 2).

Following [1] we introduce the integral transition times \( \tau^{tr} \) and \( \tau^{detr} \) which appear in the balance equations for the carrier concentration. The electron capture time \( \tau^{tr}_{nm} \) specifies the probability (per unit time) for the “average” electron in the lowest subband of the QWL to be trapped to the level \((nm) \) of any impurity in the plane \( z = z_p \).

\[ \frac{1}{\tau^{tr}_{nm}} = \int_0^\infty f(E) \, W(k \to nm) \, dE \left/ \int_0^\infty f(E) \, dE \right., \]  

(17)

The electron stay time \( \tau^{detr}_{nm} \) gives the rate of electron detrapping from the bound state \((nm) \) to any free electron state in the lowest subband,

\[ \frac{1}{\tau^{detr}_{nm}} = \int_0^\infty dE \left[ 1 - f(E) \right] \left[ \frac{dW(nm \to k)}{dE} \right]. \]  

(18)
Here \( E = \frac{h^2 k^2}{2m^*} \), and \( f(E) \) is the distribution function of the electrons on the lowest subband. In the case of \( \varepsilon \ll T \) from (10) and (11) follows that \( 1/\tau^{\text{tr}} \propto 1/\tau^{\text{det}} \propto e^{-5L^{-6}} \). In equilibrium the relation \( \tau^{\text{tr}} / n_{\text{sp}} \rho = \tau^{\text{det}} / n_{\text{car}} \rho \) holds.

After replacement of \( nm \) by \( np \), the same relations will be applicable to (de)trapping of the electron in QWR to (from) an impurity at given \( x = x_p, y = y_p \).

4. Numerical Results and Discussion

For the numerical evaluation of the transition rates we use the parameters of GaAs: effective mass \( m^* = 0.067m_0 \), sound velocity \( s = 5.24 \times 10^5 \text{ cm/s} \), dielectric constant \( \varepsilon_1 = 12.5 \), crystal density \( \rho_0 = 5.36 \text{ g/cm}^3 \), deformation potential constant \( D = 7.0 \text{ eV} \); both phonon and electron temperatures are equal to 300 K.

The results of numerical calculations of \( 1/\tau^{\text{tr}} \) versus the impurity position are presented in Fig. 3. Thin and thick lines show the capture rates to the bound states of an impurity in a 10 nm wide QWL and a 10 nm \( \times 10 \text{ nm} \) QWR, respectively. One can see that the dependence of \( 1/\tau^{\text{tr}} \) on the impurity position for different states has the form analogous to

![Fig. 3. Inverse capture times \( 1/\tau^{\text{tr}} \) and \( 1/\tau^{\text{det}} \) to impurity bound states vs. impurity position in QWL and QWR. Impurity concentrations \( n_{\text{imp}}^{(2)} = 10^{15} \text{ cm}^{-2} \) in QWL and \( n_{\text{imp}}^{(3)} = 10^7 \text{ cm}^{-1} \) in QWR. Other parameters and notations are as in Fig. 2.](image)

![Fig. 4. Rates of transitions \( W(nm \rightarrow nm') \) in a quantum well between impurity bound states \( nm \) and \( nm' \) with the emission of acoustic phonons vs. the impurity position \( z_p \). Width of the well \( L = 10 \text{ nm} \). The quantum number \( m \) of the initial state is equal to 1, 2, and 3 for solid, dashed, and dotted lines; thick and thin lines correspond to on-center and interface impurities, respectively. Lattice temperature \( T_{\text{lat}} = 300 \text{ K} \).](image)
that in Fig. 2, i.e., for the given cross-section of QWL or QWR the behavior of trapping probabilities is specified mainly by the ionization energies $\varepsilon_{nm}$ or $\varepsilon_{m'}$

Note that for comparable ionization energies the capture probability in QWR is essentially higher than that in QWL. 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. On the other hand, proper inclusion of the quasi-one-dimensional Sommerfeld factor to the calculation of (de)trapping in QWR would lead to some decrease in transition rates, especially for free electron energies, $\hbar k^2/2m^*$, less than or of the order of the Rydberg energy $\mathcal{R} \approx 70\, \text{K}$.

In Fig. 4 the rates of interlevel transitions in QWL calculated with the help of (12) are plotted versus the impurity position $z_i$. We present only the results for transitions from the upper to the lower level; the rates for inverse processes differ by the factor $\exp(-\varepsilon_{nm}/T)$ which is close to unity at room temperature. For transitions with rates greater than approximately $10^9\, \text{s}^{-1}$ (9) is not fulfilled and corresponding results are only qualitative.

The analysis of Fig. 1 to 4 gives the following qualitative picture of the carrier trapping in QWL. 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 a temperature higher than or of the order of $10\, \text{K}$ the states with $n \geq 3$ can be treated as quasicontinuous spectrum, therefore the transitions between the levels are fast and can be treated in the fashion of [1, 6].

The levels with $n = 1$ and $n = 2$ are separated from the others; this implies the existence of several distinct groups of transitions in Fig. 1 to 4. 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 has much lower probability.

Since the distance between the energy levels $\varepsilon_{20}$ and $\varepsilon_{21}$ is much smaller than to other levels, the transitions between states 20 and 21 are much faster than to any other states. Therefore it is possible to introduce a combined “level 2” and to calculate the effective transition rates as the individual ones weighted with the degeneracy of the level. Say, for transitions between “level 2” and the ground state we have

$$W(10 \to 2) = W(10 \to 20) + 2W(10 \to 21)$$

and

$$W(2 \to 10) = \frac{1}{2} W(10 \to 20) + \frac{3}{2} W(10 \to 21).$$

Note that for the direct capture of electrons to the ground state of an 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 (10) to (15) and proper scattering mechanisms included [17].

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Appendix

The form factors of electron transitions in a quantum well (cf. (10) to (12)) are given by

$$\mathcal{F}_{nm} = \frac{N_{nm}^2}{2^{2(|m|+1)}} \left[ e^{-z^+ S_{nm}(z^+)} + e^{-z^- S_{nm}(z^-)} \right],$$

$$\mathcal{F}_{nm \rightarrow n'm'} = \frac{N_{nm}^2 N_{n'm'}^2}{2^{2(|m|+|m'|)+1}} \frac{\lambda_{nm}^{2(|m|+|m'|)+1}}{\lambda_{nm}^{2(|m|+|m'|)+1}} \left[ e^{-z^+ S_{nm \rightarrow n'm'}(z^+)} + e^{-z^- S_{nm \rightarrow n'm'}(z^-)} \right],$$

where $z_{\pm} = (2z_1 \pm L)/\lambda_{nm}$ and $Z_{\pm} = (z_1 \pm L/2)/\lambda$; we introduced $\lambda = \lambda_{nm}/\lambda_{n'm'}$.

The functions

$$S_{nm}(u) = e^u \int_{\tfrac{\lambda}{u}}^{\frac{\lambda}{2}} \varphi_{nm}^2 \left( \frac{t}{2} \right) e^{-t (t^2 - u^2)^{|m|}} t \, dt,$$

$$S_{nm \rightarrow n'm'}(u) = e^u \int_{\tfrac{\lambda}{u}}^{\frac{\lambda}{2}} \varphi_{nm}^2 \left( \frac{\lambda t}{\lambda_{nm}} \right) \varphi_{n'm'}^2 \left( \frac{\lambda t}{\lambda_{n'm'}} \right) e^{-t (t^2 - u^2)^{|m|+|m'|}} t \, dt$$

can be reduced to polynomials.

For a quantum wire the form factors in (13) to (15) have the form

$$\mathcal{F}^{(x)}_{np} = \frac{4\lambda_{np} N_{np}^2}{L^2} \int_{-L/2}^{L/2} dy \cos^4 \frac{\pi y}{L} \left[ S_{np}(x^+) + S_{np}(x^-) \right],$$

$$\mathcal{F}^{(y)}_{np \rightarrow n'p'} = \frac{8\lambda_{np} N_{np}^2 N_{n'p'}^2}{L^2} \int_{-L/2}^{L/2} dy \cos^4 \frac{\pi y}{L} \left[ S_{np \rightarrow n'p'}(X^+) + S_{np \rightarrow n'p'}(X^-) \right],$$

where $\lambda = \lambda_{np}/\lambda_{n'p'}$. Functions

$$S_{np \rightarrow n'p'}(u) = \int_0^{\pi} d\theta \left( \frac{\lambda t}{\lambda_{np}} \right)^{2p} \left( \frac{\lambda t}{\lambda_{n'p'}} \right)^{2p'} \exp \left( -\sqrt{t^2 + u^2} \right) \varphi_{np}^2 \left( \frac{\lambda t}{\lambda_{np}} \right) \varphi_{n'p'}^2 \left( \frac{\lambda t}{\lambda_{n'p'}} \right)$$

can be expressed in terms of the Bessel functions of second kind. Expressions for $\mathcal{F}^{(y)}$ are obtained from $\mathcal{F}^{(x)}$ by interchanging $x$ and $y$.

References


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