Free carrier absorption in quantum well in consideration of the interaction with impurities

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Abstract. Intrasubband transitions caused by light absorption in a parabolic quantum well is considered taking into account the scattering by ionized impurity centers. To calculate the scattering matrix element Born approximation is used, and the interaction with the impurity is described via screened Coulomb potential. An analytical expression for the absorption coefficient is obtained based on the initial absorption of a photon and a further scattering on ionized impurity center. Absorption coefficient frequency characteristics and dependence on the width of the quantum well is examined.

1. Introduction
It is known that the direct light absorption by free carriers is impossible, since it contradicts conservation laws of energy and momentum. Availability of phonons, impurities and other lattice defects enable light absorption, since scattering on a third particle provides a necessary change in a momentum. Free carriers absorption (FCA) is an effective tool to identify and assess the mechanisms of scattering. FCA was reviewed in massive semiconductors in the second-order of perturbation theory, taking into account various mechanisms of scattering [1], including ionized impurities [2].

The most interesting case of FCA is in the low-dimensional structures. Owing to dimensional quantization (for example in one direction in quantum wells), energy subbands arise which make possible transitions not only in one subband (intrasubband transitions), but also transition between two subbands (intersubband transitions) [3].

Intrasubband transition in the quantum wells (QW) cause a great interest due to its unique characteristics: large dipole momentum, ultra-fast relaxation, great opportunity to control the transitions wave length [4-6]. It is important not only for the fundamental physics, but also for development of new technological applications. Many devices are developed based on intrasubband and intersubband transitions in heterostructures from QW. For example, infrared photodetectors [7, 8], superfast optical modulators [9], optical switches [10] and quantum cascade lasers [11].

One of the first theoretical works devoted to light absorption by free carriers in size quantized structures are the works of Kazaryan et al [12, 13], where within the second order of perturbation theory frequency dependency of absorption coefficient is obtained for nondegenerate electronic gas in QW and in quantum well wires. Scattering mechanisms on acoustic phonons [12] and the ionized impurity centers [13] are considered. Later FCA in QW had been studied by many authors, taking into account scattering on acoustic phonons [14], polar and non polar optical phonons [15,16,17], and also on the ionized screened impurities [18, 19]. In the studied works confinement potentials had been approximated by single rectangular, and also doubled [20] (applied to quantum cascade lasers) finite or infinite rectangular potentials.
On the other hand, there is a need to create more realistic model of the confinement potential which takes into account both physicochemical properties of structure and its geometry. The first form height and shape of the potential barrier on the interface, and the geometry defines symmetry of a Hamiltonian (in lack of external fields). For these purposes various models of the confinement potential for low-dimensional systems were applied [21-25]. As a first approximation the confinement potential can be approximated by parabolic one. With regard to the problem considered in the presented work it allows to obtain analytical expression for absorption coefficient. Let us notice, that ideal parabolic approximation of the confinement potential works fine for low energy levels. Further, it is assumed that confinement potential of QW looks like

\[ V_{\text{conf}}(z) = \frac{m^* \omega_0^2 z^2}{2}, \]  

where \( m^* \) – effective mass of electron, \( \omega_0 \) – frequency defined by virial theorem according to a relation \( \omega_0 = \frac{\hbar}{m^* a} \), where \( a \) – is QW width. For the exact equality we will present \( \omega_0 \) in a form

\[ \omega_0 = \frac{\gamma \hbar}{m^* a^2}, \]

where \( \gamma \) – some adjustable parameter providing exact equality in (2).

2. Theory
Calculations are carried out on the basis of the standard theory of quantum transitions, according to the general formula:

\[ \alpha = \sqrt{\frac{\varepsilon}{cN}} \sum_i P_i f_i, \]

where \( \varepsilon \) – dielectric constant, \( N \) – quantity of the photons falling on the QW in a unit of time per unit area, \( c \) – light speed, \( f_i \) – charge distribution function, \( P_i \) – transition probability (count of transition per unit time).

Expression for \( P_i \) in the second order of the perturbation theory has an appearance [26-28]:

\[ P_i = \frac{2\pi}{\hbar} \sum_f \sum_{m} \left| \frac{M^r_{im}}{E_i - E_m + \hbar \omega} \right|^2 \delta(E_f - E_i - \hbar \omega), \]

where \( E_i \) – initial state energy, \( E_f \) – finit state energy, \( E_m \) – middle state energy, \( M^r_{im} \) – matrix element, caused by absorption of a photon, \( M^l_{im} \) – matrix element, caused by scattering on ionized impurity centers. In \( z \) direction electron located in parabolic QW, and in the plane \((x, y)\) there is a two-dimensional translational symmetry (see Figure 1).

It is supposed that incident light is linearly polarized, and incident angle is not specified. It should be mentioned, that for the intrasubband transitions one should demand that light incidence is not parallel to QW plane (vector of polarization is not perpendicular to QW plane), and vice versa for intersubband transitions [3]. This requirement is equivalent to that if polarization vector \( x, y \) components are non-zero: \( E_{x,y} \neq 0 \) (figure 1).

In case of initial absorption of a photon (figure 2, transition \( imf \)), transition \( i \rightarrow m \) is followed by absorption of a photon (Figure. 2), and the transition of \( m \rightarrow f \) corresponds to the scattering on
ionized impurity centers. At initial scattering (figure 2, transition \( im'f \)) we have: \( i \rightarrow m' \) – scattering on the impurity center and \( m' \rightarrow f \) – photon absorption. \( m \) and \( m' \) states are virtual.

We use Born approximation for calculation of a scattering matrix element. We will consider the elastic mechanism of scattering on ionized impurity. In Figure 3 the change of a two-dimensional wave vector of an electron in case of elastic scattering mechanism is represented: \( \vec{k} \) is a wave vector of an electron before interaction with impurity, and \( \vec{k}' \) – after interaction. As it can be seen from figure the angle of a scattered wave vector lies in an interval \((-\pi, \pi)\). As it can be obtained from figure 3 the absolute value if of wave vectors difference can be presented as

\[
|\vec{k}' - \vec{k}| = 2k \sin \frac{\theta}{2}, \quad \text{(5)}
\]

\( \theta \) – is scattering angle.

Wave function is

\[
|\phi\rangle = \frac{1}{\sqrt{S}} \frac{1}{\sqrt{2^n n!}} \left( \frac{\gamma}{\pi a^2} \right)^{1/4} e^{\frac{k_0}{\gamma}} e^{-\frac{\gamma z^2}{2a^2}} H_n \left( \frac{\sqrt{\gamma} z}{a} \right), \quad \text{(6)}
\]

where \( a \) – QW width, \( S \) – surface area, \( H_n \) – Hermite polynomials.

In further calculations we will consider that at first there is an absorption of a photon, and then scattering on the impurity center (pic. 2, transition of \( imf \)). The energy spectrum:

\[
E_i = \frac{\hbar^2 k_i^2}{2m} + \frac{\hbar \omega_{osc}}{2} ; \quad E_m = \frac{\hbar^2 k_m^2}{2m} + \frac{\hbar \omega_{osc}}{2} + \hbar \omega;
\]

\[
E_f = \frac{\hbar^2 k_f^2}{2m} + \frac{\hbar \omega_{osc}}{2} \quad \hbar \omega_{osc} = \frac{2\hbar^2}{m a^2}
\]

where \( \hbar \omega \) – photon energy. Note that processes like \( i \rightarrow m \rightarrow f \) and \( i \rightarrow m' \rightarrow f \) have equal probabilities.
Taking into account an expression (6) the matrix element caused by absorption of a photon has a form:

\[
M_{nm} = \langle \phi_n | H' | \phi_m \rangle = \frac{1}{aS} \left[ \frac{1}{1} \int e^{i\vec{k}_\omega \cdot \vec{r}} e^{-\frac{i\vec{r}^2}{2a^2}} H_{nm}(z/a) \right] \left( \frac{\epsilon}{mc} \right) e^{i\vec{p}_\omega \cdot \vec{r}} e^{-\frac{i\vec{r}^2}{2a^2}} H_z(z/a) d\vec{r} =
\]

\[
= \frac{2\pi^2}{S} \frac{\sqrt{2\pi}}{\epsilon} \left( \frac{\hbar e}{mc} \right) \left( \frac{\hbar^2}{\sqrt{n}} \right)
\]

(8)

And the matrix element of scattering is:

\[
M'_{nf} = \langle \phi_f | V_{\text{Yukawa}} | \phi_n \rangle = \int_0^{\infty} \int_0^{\infty} \phi_f V_{\text{Yukawa}} \phi_m \rho d\rho dz =
\]

\[
= \frac{2\pi \varepsilon^2}{S} \left( \frac{1}{\varepsilon} \right) \exp \left( -\frac{1}{4\gamma} \left( k^2 + \frac{1}{L_D^2} \right) \right),
\]

(9)

where \( k = |\vec{k}_f - \vec{k}_n| \), \( L_D \) - is Debye screening length, and scattering potential is takne in the form (Debye-Hucke, Yukava)

\[
V_{\text{Yukawa}} = \frac{Ze^2}{\varepsilon \sqrt{\rho^2 + z^2}} \exp \left( -\frac{\sqrt{\rho^2 + z^2}}{L_D} \right); \quad \text{where} \quad L_D = \sqrt{\frac{\varepsilon k_T a}{4\varepsilon^2 n_e}}.
\]

(10)

For absorption coefficient calculation (see eq. (4)) in case of initial absorption of a photon and further scattering on ionized impurity we use expression [29]

\[
\alpha(\omega) = \frac{1}{N \cdot \sqrt{c / n}} \left( \frac{2S}{(2\pi)^2} \right) \int d^2k d^2k' \left\{ \frac{2\pi}{\hbar} \frac{|M_{nf}|^2}{|M_{nf}|^2} \delta(E_f - E_n - \hbar\omega) \right\} f(k)[1 - f(k')],
\]

(11)

where \( f(k) \) and \( f(k') \) are the probabilities of filling of initial and final states (Fermi-Dirac distribution), \( N \) – quantity of the incident photons per square (considered one-photon absorption), \( n \) – refraction index.

We consider a nondegenerate electronic gas with a temperature \( T \), neglecting \( f(k') = 0 \); \( f(k) \) is the Boltzmann distribution function

\[
f(k) = \frac{n_e}{N_e} e^{-\frac{E}{k_B T}} = \frac{n_e}{2L m k_B T} \left( \frac{2\pi\hbar^2}{m k_B T} \right)^{3/2} e^{-\frac{E}{k_B T}},
\]

(12)

where \( n_e \) – concentration of 2D free electrons.

Substituting the expressions of the matrix elements (8), (10) in (11), and taking into account a distribution function (12), we will receive the following expression for absorption coefficient:

\[
\alpha(\omega) = C \left( 3 + \frac{\hbar\omega}{2E_T} + \frac{1}{16} \left( \frac{\hbar\omega}{E_T} \right)^2 \right) \left( \frac{1}{\hbar\omega} \right)^4 \frac{1}{8E_T} \exp \left( \frac{m a^2}{2\gamma} \right) \left( \frac{1}{mL_D^2} \right) - \frac{1}{\hbar^2} \left( \frac{1}{1 + \frac{h^2}{mL_D^2}} \right)
\]

(13)

where we have used the following notations:

\[
E_T = k_B T;
\]

\[
C = 1504n_N \frac{\hbar^2 e^6 E_T}{e^{3/2} a m^{3/2} c} \exp \left( \frac{\hbar\omega_{\text{osc}}}{2E_T} + \frac{a^2}{2\gamma E_T^2} \right)
\]

(14)

\( N_i \) – concentration of the 2D ionized impurities, \( \varepsilon \) – the dielectric constant.
The difference between absorption coefficients between screened and pure Coulomb potentials can be presented as

$$\alpha_{\text{Yukawa}}(\omega) = \alpha_{\text{Coulomb}}(\omega) \exp \left( \frac{a^2}{2 \gamma L_D^2} \right) \left( 1 + \frac{\hbar^2}{mL_D^2 \hbar \omega} \right) .$$

(15)

### 3. Results

All numerical calculations are made for QW of GaAs with the following parameters: $m^* = 0.067 m_e$, $\varepsilon = 13.8$, $E_p = 5.275$ meV, $a_p = 104$ Å. Are received the results for one type of processes – with initial absorption of a photon and further scattering on the ionized impurity. Since other possible sequence of transitions (with initial scattering on the ionized impurity) is equiprobable, it is natural to expect that the result should be the same. The analysis of frequency dependence of absorption coefficient shows dependence of $\alpha(\omega) \sim \frac{1}{\omega^{3/2}}$. Therefore, for parabolic QW the absorption coefficient with the increase of photon energy decreases faster in comparison with result for a massive sample $- \frac{1}{\omega^{3/2}}$ [1].

Absorption coefficient dependence on light frequency for various QW widths is presented on figure 4. It is visible, that the absorption shifts to the bigger values of photon energy with the reduction of QW width. Calculations are made for temperature $T=77$K, as at higher temperatures phonon scattering mechanism dominates.

![Figure 4. Dependence of absorption coefficient on incident photon energy at various values of QW widths.](image)

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