Single Potential Barrier in High-Frequency Electromagnetic Field

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Abstract: The electron transport across a single potential barrier under the influence of a high-frequency scalar electric potential and strong electromagnetic vector potential is investigated. The scalar potential modulates the barrier height and generates the higher order harmonics. The strong vector potential modifies the barrier profile and its transmittance.

Key-Words: Single potential barrier, high-frequency signal, scalar potential, vector electromagnetic potential.

1 Introduction
Recent rapid progress in nanoelectronics and high frequency technologies necessitates that heterojunctions, superlattices, low-dimensional semiconductor structures, quantum wells and barriers are standard building blocks of recently developed nanoscale semiconductor devices that find their application in the field of microwave and submillimeter technology or in photonics. The existence of the quantum wells and barriers results in quantum-based mechanism of electron transport, the thermionic emission across the barrier, the thermionic-field-emission or and the tunnelling through the barrier. These effects should be treated by means of appropriate methods of quantum physics.

Typical situation in electronics is that a dc-bias together with a small ac-signal is applied to the structure. The calculation of potential barrier transmittance with dc-bias only is a classical and well-known problem of quantum mechanics. The application of a high-frequency signal to the barrier was studied only in the last decade. The terahertz frequency band that is usually considered as the range between 300 GHz – 3 THz, sometimes up to 30 THz (this corresponds to the submillimeter up to the far infrared wavelength band 1 mm – 10 µm) becomes recently very attractive for investigation.

However, the study of transport in intensely driven nanoscale systems is a growing field due to the recent development of a broad class of devices, such as terahertz high frequency detectors, quantum resonant tunnelling diodes or triodes for use in quantum communication, terahertz quantum cascade lasers based on quantum dots etc. The investigation of the response to the intense time-dependent excitation is important as devices are only useful if they can process a time varying information.

2 Potential barrier without ac signal
The single potential barrier is the simplest nanostructure and it will be investigated throughout this paper. Consider that electrons incident the barrier from the left. In this case, the electron wave function left from the barrier (region A), right from the barrier (region C), and inside the barrier region B is

\[ \varphi_A(x) = e^{ik_0 x} + r_0 e^{-ik_0 x} \]
\[ \varphi_C(x) = t_0 e^{iq_0 x} \]
\[ \varphi_B(x) = a_0 f(x) + b_0 g(x) \]

(1)

The function \( \varphi_B(x) \) carries the information on the potential barrier; it is the solution of the stationary Schrödinger equation

\[ H_{dc} \varphi_B = E \varphi_B, \quad H_{dc} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \]

(2)

For the rectangular barrier \( f, g \) are plane waves

\[ f(x) = e^{ip_0 x}, \quad g(x) = e^{-ip_0 x} \]

(3)

where \( p_0 \) is real for \( E > V_{max} \) (this corresponds to the electron emission over the barrier) and \( p_0 \) is imaginary, \( p_0 = ik_0 \) for \( E < V_{max} \) (electron tunneling through the barrier). If the dc bias is applied to the barrier, its profile is changed from rectangular to trapezoidal and the plane waves in (3) should be replaced by the Airy functions. For a general barrier profile the numerical solution of (2) is necessary. The transmission amplitude of a rectangular barrier of thickness \( x_B \) is

\[ t_0 = \frac{4k_0 e^{-ik_0 x_B}}{(k_0 + p_0)(1 + \frac{q_0}{p_0})e^{-ip_0 x_B} + (k_0 - p_0)(1 - \frac{q_0}{p_0})e^{ip_0 x_B}} \]

(4)
3 Barrier with scalar electric modulation

Consider the potential barrier, which height is modulated by the high-frequency scalar electrostatic potential. The wave function inside the barrier region is the solution of the time-dependent Schrödinger equation

\[
i\hbar \frac{\partial \Psi_B}{\partial t} = (H_{dc} + H_{ac}) \Psi_B , \quad H_{ac} = eV_{ac} \cos(\omega t)
\]  

(5)

It is a direct consequence of the Floquet theorem [1], [2] that the solution of (5) is

\[
\Psi_B(x, t) = \exp\left(-i \frac{E}{\hbar} t\right) \exp\left(-i \frac{eV_{ac}}{\hbar \omega} \sin(\omega t)\right) \varphi_B(x)
\]

(6)

If the Bessel function expansion is applied

\[
\exp\left(-i \frac{eV_{ac}}{\hbar \omega} \sin(\omega t)\right) = \sum_{p = -\infty}^{\infty} J_p\left(\frac{eV_{ac}}{\hbar \omega}\right) \exp(-ip\omega t)
\]

(7)

the wave function (6) can be considered as a wave modulated by the first order and higher order harmonics \( \exp(-ip\omega t) \), \( p = \pm 1, \pm 2, \ldots \). The quantum point of view offers another interpretation: electron inside the barrier region can absorb or emit one or more energy quanta \( \hbar \omega \).

Of course, if electrons with energy \( E + p\hbar \omega \) are generated inside the barrier region, they propagate also in region C right from the barrier, and their wave function is

\[
\Psi_C(x, t) = \exp\left(-i \frac{E}{\hbar} t\right) \sum_{n = -\infty}^{\infty} t_n \exp(-in\omega t) \exp(\pm iq_n x)
\]

(8)

If we restrict the consideration only to a small signal and to a rectangular potential barrier, it is possible to find the following analytical formula for the first order harmonics

\[
t_{\pm 1} = \pm \frac{eV_{ac}}{2\hbar \omega} t_0 \times \frac{\cos(p_0 x_B) + i (p_0 + k_0 q_0/p_0) \sin(p_0 x_B) - 1}{\left( k_0 + p_0 \cos(p_0 x_B) + i (p_0 + k_0 q_0/p_0) \sin(p_0 x_B) \right)}
\]

(9)

The single electron current density for the function (8) can be now calculated using the standard rules of quantum physics; the results in general is

\[
j^{(dc)}_{\text{trans}} = \sum_{n=0}^{N} j^{(n0)}_{\text{trans}}
\]

\[
j^{(n0)}_{\text{trans}} = e \frac{-\hbar q_0}{m} \left[ T_n \exp(-in\omega t) + T_n^* \exp(in\omega t) \right]
\]

(10)

where the complex amplitudes \( T_n \) are related to the transmission amplitudes \( t_n \) in (8); as an example we give the explicit formulae for the \( dc \) part and the first order harmonics:

\[
j^{(dc)}_{\text{trans}} = e \frac{-\hbar q_0}{m} \left[ t_0 t_0^* \right]
\]

\[
j^{(n0)}_{\text{trans}} = e \frac{-\hbar q_0}{m} \left[ t_0 t_{n-1} + t_0^* t_{n} \right] e^{-in\omega t} + \left[ t_0^* t_{n-1} + t_0 t_{n} \right] e^{in\omega t}
\]

(11)

Equations (5) and (8) imply the following conclusion. If the potential barrier is modulated by a harmonics high frequency signal (5), higher order harmonics are present in the electric current, which flows through the structure. The origin of the harmonics is related to the quantum character of the electron transport in the barrier region (to the absorption or emission of energy quanta) rather then to the nonlinearity of the I-V or C-V characteristics, thus their existence is an intrinsic property of the single-barrier structure. The effect of quantum absorption or emission and transmission amplitudes are drawn in Figs. 2 and 3.
The effect of emission or absorption of energy quantum on the wave function. The real part of the electron wave functions if no absorption or emission occurs, one energy quantum is absorbed or emitted, i.e. the first order harmonics is generated. It can be clearly seen along the time axis from the time variation of the wave function how the electron energy is changed (the coordinate and time are in some relative units).

4 Electromagnetic modulation

The investigation in the part 3 was focused on the high-frequency response of a quantum structure (potential barrier) for time-varying scalar electrostatic potential. As a next step we generalize the investigation to the coupling of quantum structure to infrared electromagnetic field described by the vector potential.

Instead of (2), (5) we consider now the following time-dependent Schrödinger equation

\[ i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t) = \left[ \frac{1}{2m} (\vec{p} - e\vec{A})^2 + V(\vec{r}) \right] \psi(\vec{r}, t) \]  

(12)

where \( \vec{A}(\vec{r}) \) is the vector potential of the electromagnetic field and \( V(\vec{r}) \) is the scalar electrostatic potential energy, the potential barriers at heterojunction interfaces or the external applied bias can be described by this function. It is known [3], [4] that the so called Kramers-Henneberger unitary transformation can be applied to Eq. (12). We introduce the new wave function

\[ \tilde{\psi}(\vec{r}, t) = \Omega \psi(\vec{r}, t) \]

(13)

where the unitary operator \( \Omega \) is related to the vector field potential by the following relations

\[ \Omega = \Omega_1 \Omega_2 \]

(14)

\[ \tilde{\Omega}_1 = \exp \left[ -i \int_{-\infty}^{t} \vec{A}(\tau) \cdot \vec{V} d\tau \right] \]

\[ \tilde{\Omega}_2 = \exp \left[ \frac{i e^2}{\hbar 2m} \int_{-\infty}^{t} \vec{A}^2(\tau) d\tau \right] \]

As \( \tilde{\Omega}_1 \) is a translation operator, its action on an arbitrary function of coordinates \( f(\vec{r}) \) reads

\[ \tilde{\Omega}_1 f(\vec{r}) = f(\vec{r} + \vec{a}(t)) \]

(15)

\[ \vec{a}(t) = -\frac{e}{m} \int_{-\infty}^{t} \vec{A}(\tau) d\tau \]
Thus, the transformed wave function defined by Eq. (12) satisfies the differential equation
\[ i\hbar \frac{\partial}{\partial t} \varphi(\vec{r}, t) = \left[ \frac{1}{2m} \hat{p}^2 + V(\vec{r} + \vec{a}(t)) \right] \varphi(\vec{r}, t) \] (16)

According to Eq. (16), the electron motion in the presence of a strong electromagnetic field may be described by Schrödinger equation for an electron subjected to a time-dependent potential that oscillates with the frequency of the electromagnetic wave. The last statement follows from the relation
\[ \frac{d^2}{dt^2} \vec{a}(t) = -\frac{e}{m} \frac{d}{dt} A(t) = \frac{e}{m} \vec{E}(t) \] (17)

The parameter \( \vec{a}(t) \) represents the classical displacement of a free electron from its center of oscillation in a radiation field with electric field intensity \( \vec{E}(t) \); it is usually called the laser-dressing parameter.

Some simplification of Eq. (16) is possible if the angular frequency \( \omega \) of the electromagnetic wave is as high that the time of flight \( \tau_F \) of the electron through the quantum structure obeys \( \tau_F \gg 1 \). Consider the Fourier expansion of the dressed potential \( V(\vec{r} + \vec{a}(t)) \)

\[ V(\vec{r} + \vec{a}(t)) = \int V(\vec{q}) \exp[i\vec{q}(\vec{r} + \vec{a}(t))] d\vec{q} \] (18)

If the dressing parameter is \( \vec{a}(t) = \alpha \cos(\omega t) \vec{n} \), the Fourier expansion Eq. (27) reads

\[ V(\vec{r} + \vec{a}(t)) = \int d\vec{q} V(\vec{q}) \sum_{m=\infty}^{+\infty} J_m(\alpha \vec{n}) \exp(-im\omega t) \] (19)

In the high-frequency limit the electron is subjected to the time-averaged potential \( \langle V(\vec{r} + \vec{a}(t)) \rangle \), thus only the term with \( m = 0 \) in Eq. (19) determines the electron state. Eq. (19) with \( m = 0 \) only can be easily integrated according to formulae given in [5] and the time-independent averaged potential \( \langle V(\vec{r} + \vec{a}(t)) \rangle \) can be used in Eq. (16). The result is that the profile of the potential barrier is changed, as it is demonstrated in Fig. 4 for the rectangular potential barrier. Schrödinger equation (16) is in this way converted into the equation with time independent and spatially varying potential that can be solved by means of the Floquet theory with non-uniform potential [6] or by some numerical method. The transmittances of the original rectangular barrier and of the modified barrier are compared in Fig. 4.

5 Conclusions
The high-frequency scalar electric potential (5) modulates the barrier height and generates the higher order harmonics as energy quanta of the signal can be absorbed or emitted, see Figs. 2, 3. The strong vector electromagnetic potential (12) modifies the barrier profile and its transmittance, see Fig. 4.

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