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# ELECTRON TRANSPORT THEORY IN SEMICONDUCTOR SYSTEMS CONTAINING PERIODICALLY ARRANGED ASYMMETRIC POTENTIAL WELLS AND BARRIERS

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**Abstract:** The transmission of electron wave functions in a material whose physical parameters vary along a specific spatial direction has been investigated from a rigorous theoretical perspective. In such systems, spatial inhomogeneity plays a crucial role in determining the quantum-mechanical behavior of charge carriers, since variations in potential energy, effective mass, or compositional profile significantly influence wave propagation. When an electron travels through a non-uniform medium, its wave function adapts to the changing environment, leading to reflection, transmission, and interference phenomena that must be described consistently within the framework of quantum mechanics.

The present analysis is based on the single-particle, time-independent Schrödinger equation, which provides a fundamental description of stationary states in quantum systems. This equation is formulated under the assumption of total energy conservation, meaning that the sum of kinetic and potential energies remains constant throughout the motion of the particle. By applying appropriate boundary conditions at interfaces where material properties change, one can determine the amplitudes of reflected and transmitted waves, as well as calculate physically measurable quantities such as transmission and reflection coefficients.

Within this formalism, elastic scattering processes of non-interacting, spinless particles are examined in detail. Elastic scattering implies that the particle’s total energy is conserved during interaction with the potential landscape, although its momentum and direction of motion may change. Particular attention is given to quantum tunneling phenomena, in which particles penetrate potential barriers even when their kinetic energy is lower than the barrier height. Such processes arise purely from the wave nature of matter and have no classical analog. Altogether, the approach provides a unified, internally consistent framework for describing wave transmission, reflection, and tunneling in spatially non-uniform quantum systems.

***Keywords:*** semiconductor structure, Schrödinger equation, elastic scattering, tunneling effect, potential barriers, quantum well, effective mass, bulk quantization.

**Аннотация:** С точки зрения строгой теории исследовано распространение волновых функций электронов в материале, физические параметры которого изменяются вдоль определенного пространственного направления. В таких системах пространственная неоднородность играет решающую роль в определении квантово-механического поведения носителей заряда, поскольку изменения потенциальной энергии, эффективной массы или профиля состава существенно влияют на распространение волн. Когда электрон движется через неоднородную среду, его волновая функция адаптируется к изменяющейся среде, что приводит к явлениям отражения, пропускания и интерференции, которые должны быть последовательно описаны в рамках квантовой механики.

Настоящий анализ основан на одночастичном, стационарном уравнении Шрёдингера, которое обеспечивает фундаментальное описание стационарных состояний в квантовых системах. Это уравнение сформулировано в предположении сохранения полной энергии, то есть сумма кинетической и потенциальной энергий остается постоянной на протяжении всего движения частицы. Применяя соответствующие граничные условия на границах раздела, где

изменяются свойства материала, можно определить амплитуды отраженных и прошедших волн, а также рассчитать физически измеримые величины, такие как коэффициенты пропускания и отражения.

В рамках данного формализма подробно исследуются процессы упругого рассеяния невзаимодействующих бесспиновых частиц. Упругое рассеяние подразумевает, что полная энергия частицы сохраняется при взаимодействии с потенциальным ландшафтом, хотя её импульс и направление движения могут изменяться. Особое внимание уделяется явлениям квантового туннелирования, при которых частицы проникают через потенциальные барьеры, даже когда их кинетическая энергия ниже высоты барьера. Такие процессы возникают исключительно из волновой природы материи и не имеют классического аналога. В целом, данный подход обеспечивает единую, внутренне непротиворечивую основу для описания передачи, отражения и туннелирования волн в пространственно неоднородных квантовых системах.

**Ключевые слова:** полупроводниковая структура, уравнение Шрёдингера, упругое рассеяние, туннельный эффект, потенциальные барьеры, квантовая яма, эффективная масса, объёмное квантование.

We examine fundamental aspects of electron wave propagation in a material whose physical parameters change exclusively along one chosen spatial direction. The analysis relies on the time-independent single-particle Schrödinger formalism to model elastic scattering and quantum tunneling phenomena of non-interacting, spinless particles under the assumption that their total energy remains conserved.

Advances in modern fabrication techniques make it possible to engineer semiconductor layers with virtually arbitrary compositional distributions (i.e., quantum well heterostructures) in order to optimize the performance of devices constructed from them [1]. Under such conditions, the description of electronic states can be reduced to analyzing the motion of a microscopic particle in a periodically modulated potential landscape. Suppose that the electron potential energy is defined piecewise as $U(x) = U_1$ for $x < x_1$ and $U(x) = U_2$ for $x > x_1$. In this situation, the corresponding electron wave function is represented in the following general form:

$$\psi_j(x) = A_j \exp(ik_j x) + B_j \exp(-ik_j x), \qquad (1)$$

where $k_j(x) = k_j = \sqrt{\frac{2m_j(E-U_j)}{\hbar^2}}$ is the wave vector, $m_j$ is the effective mass of the electrons, and $j = 1,2,3,\ldots$ denotes the layer numbers in the structure. Then, from the boundary conditions for the continuity of the wave functions [2] and electron flux, taking into account Bastard’s conditions (see, for example, [3])-which differ from standard quantum mechanical problems - it is straightforward to obtain relations connecting the amplitudes of the de Broglie waves of electrons located in adjacent regions (layers):

$$\begin{aligned} 2A_1 &= (1 + a_{21})A_2 \exp(i(k_2 - k_1)x_1) + (1 - a_{21})B_2 \exp(i(k_2 + k_1)x_1), \\ 2B_2 &= (1 - a_{21})A_2 \exp(i(k_2 + k_1)x_1) + (1 + a_{21})B_2 \exp(i(k_2 - k_1)x_1). \end{aligned} \qquad (2)$$

Here $a_{jj'} = \frac{\tilde{k}_j}{\tilde{k}_{j'}}$, where $\tilde{k}_j = \frac{k_j}{m_j}$. Equation (2) can conveniently be rewritten using the transfer matrix from region “1” to “2”:

$$\begin{bmatrix} A_1 \\ B_2 \end{bmatrix} = \hat{T}^{(21)} \begin{bmatrix} A_2 \\ B_2 \end{bmatrix} = \begin{bmatrix} T_{11}^{(21)} & T_{12}^{(21)} \\ T_{21}^{(21)} & T_{22}^{(21)} \end{bmatrix} \begin{bmatrix} A_2 \\ B_2 \end{bmatrix}, \qquad (3)$$

where

$$\begin{aligned} &T_{11}^{(21)} = T_{22}^{(21)^*} = \frac{1}{2}(1 + a_{21})e^{i(k_2-k_1)x_1}, T_{12}^{(21)} = T_{21}^{(21)^*} = \frac{1}{2}(1 - a_{21})e^{-i(k_2+k_1)x_1}, \\ &\det\left[T^{(21)}\right] = \tilde{k}_2/\tilde{k}_1 = \sqrt{\frac{m_1}{m_2}\frac{E-U_2}{E-U_1}}. \end{aligned} \qquad (4)$$

The transfer matrix $T(21)$ becomes a unimodular matrix in the case when $\tilde{k}_2 = \tilde{k}_1$, i.e., for symmetric structures [3], where the potential barrier heights and the effective electron masses are equal.

If we introduce the reflection coefficient $r$ and transmission coefficient $t$ as the ratios of the probability current densities in the reflected and transmitted waves to the probability current density of electrons in the incident wave, then by definition

$$r^{(21)} = |B_1|^2/|A_1|^2 = \left|T_{21}^{(21)}\right|^2 / \left|T_{11}^{(21)}\right|^2 \quad \text{and} \quad t^{(21)} = \frac{\tilde{k}_2}{\tilde{k}_1}\frac{|A_2|^2}{|A_1|^2} = \frac{\tilde{k}_2}{\tilde{k}_1}\frac{1}{\left|T_{11}^{(21)}\right|^2}.$$

In this context, the transmission coefficient has physical significance in classically allowed regions, where the electron wave vectors are real values. Then, for the potential chosen in our case, we have

$$r^{(21)} = \left|\tilde{k}_1 - \tilde{k}_2\right|^2 / \left|\tilde{k}_1 + \tilde{k}_2\right|^2 = \left|1 - \sqrt{\frac{m_1}{m_2}\frac{E - U_2}{E - U_1}}\right|^2 \Bigg/ \left|1 + \sqrt{\frac{m_1}{m_2}\frac{E - U_2}{E - U_1}}\right|^2.$$

In particular, for a symmetric structure, $r^{(21)} = \frac{|1-\sqrt{m_1/m_2}|^2}{|1+\sqrt{m_1/m_2}|^2}$, and it becomes zero when the effective electron masses are identical across all layers of the structure.

Currently, three-layer structures with rectangular quantum wells, featuring an additional potential dip in the center, are used to create a new generation of resonant-tunneling diodes and heterolasers with separated electronic and optical confinement [1]. Therefore, we will further analyze a structure composed of three layers, described by the potential $U(x) = U_1$ for $x < x_1$ and for $x_1 \leq x \leq x_2$; $U(x) = U_3$ for $x > x_2$ and $U(x) = U_2$ for $x > x_1$. Then, the transfer matrix $T(31) = T(32)T(21)$, with its matrix element

$$T_{11}^{(31)} = T_{11}^{(32)}T_{11}^{(21)} + T_{12}^{(32)}T_{21}^{(21)} = \frac{1}{4}\exp(ik_3x_2 - k_1x_1 - k_2(x_2 - x_1)) \times$$
$$\times \{(1 + a_{21})(1 + a_{32})\exp(2ik_2(x_2 - x_1)) + (1 - a_{21})(1 - a_{32})\}.$$

Then, for the over-barrier transmission coefficient of electrons, we have

$$t_{\text{n.b}}^{(31)} = 4\tilde{k}_1\tilde{k}_2^2\tilde{k}_3\left\{\left(\tilde{k}_2^2 + \tilde{k}_1\tilde{k}_3\right)^2 - \left(\tilde{k}_1^2 - \tilde{k}_2^2\right)\left(\tilde{k}_3^2 - \tilde{k}_2^2\right)\cos^2[k_2(x_2 - x_1)]\right\}^{-1}. \qquad (5)$$

From (5), it is evident that, firstly, $t_{n.b.}^{(31)}$ is invariant under the transformation $\tilde{k}_1 \leftrightarrow \tilde{k}_3$, which means that the electron transmission coefficient in the structure does not depend on the direction from which the electrons approach the barrier. Secondly, the over-barrier transmission exhibits an oscillatory nature. This oscillation is associated with the interference of waves reflected from the potential barrier, with its amplitude determined by the difference $(\tilde{k}_1^2 - \tilde{k}_2^2)(\tilde{k}_3^2 - \tilde{k}_2^2)$, and it vanishes when electrons have energies

$$E_j^{(0)} = \left(m_2U_j - m_jU_2\right)/\left(m_2 - m_j\right), j = 1{,}3.$$

From (5), it is evident that dimensional quantization can be observed in the electron spectrum. If such a spectrum is defined by the formula $E_-(k_y, k_z, n_-) = E(k_y, k_z) + U_2 + E_0n_-^2$, then structures with such layers, where $\tilde{k}_1 = \tilde{k}_2 = \tilde{k}_3$ with $\tilde{k}_2 = \frac{\pi n_-}{2(x_2 - x_1)}$, will be tunneling-transparent, i.e., $t_{n.b.}^{(31)} = 0$, where $n_-$ are odd integers. Interestingly, if the dimensional quantization spectrum is defined by the formula $E_+(k_y, k_z, n_+) = E(k_y, k_z) + U_2 + E_0n_+^2$, then in structures with layers where $n_+$ are even integers, the behavior of $t_{n.b.}^{(31)}$ depends on both the heights of the potential barriers and the ratio of the effective masses of electrons in adjacent layers, i.e., it is determined by the expression

$$4\tilde{k}_1\tilde{k}_2^2\tilde{k}_3\{(\tilde{k}_2^2 + \tilde{k}_1\tilde{k}_3)^2 - (\tilde{k}_1^2 - \tilde{k}_2^2)(\tilde{k}_3^2 - \tilde{k}_2^2)\}^{-1},$$

where, for $\tilde{k}_1 > \tilde{k}_2 > \tilde{k}_3$ (or $\tilde{k}_1 < \tilde{k}_2 < \tilde{k}_3$), it is possible that $t_{n.b.}^{(31)} > 1$. This indicates that, in such a structure, an enhancement of the transmission of electron de Broglie waves may occur.

Thus, depending on the nature of the dimensional quantization chosen, it is possible to either suppress or enhance the oscillatory scattering phenomena from barriers or tunneling through the barrier.

For the study of under-barrier transmission of electrons, one can use the above formula for $T_{11}^{(31)} = T_{11}^{(32)}T_{11}^{(21)} + T_{12}^{(32)}T_{21}^{(21)}$, where, for $E > U_j$ (for $j = 1{,}3$) and $E < U_2$, it is convenient to make the following transformation:

$$\tilde{k}_j \pm \tilde{k}_2 = \tilde{k}_j \pm i\kappa_2 = \sqrt{\tilde{k}_j^2 + \kappa_2^2}\exp(\pm i\phi_{j2}),$$

where $\phi_{j2} = \arctan\left(\frac{\kappa_2}{\tilde{k}_j}\right)$ and $\kappa_2 = \sqrt{\frac{2m_2}{\hbar^2}(U_2 - E)}$. Then, the under-barrier transmission coefficient has the form:

$$t_{\text{n.b}}^{(31)} = 4\tilde{k}_1\tilde{\kappa}_2^2\tilde{k}_3\left\{\left(\tilde{k}_2^2 + \tilde{\kappa}_2^2\right)\left(\tilde{k}_2^2 + \tilde{\kappa}_2^2\right)\sinh[\kappa_2(x_2 - x_1)]\right\}^{-1} \qquad (6)$$

and is symmetric with respect to the transformation $\tilde{k}_1 \leftrightarrow \tilde{k}_3$.

It is important to emphasize that in an asymmetric semiconductor configuration — and even in a symmetric one where the effective electron mass differs across individual layers — oscillatory behavior is anticipated in the energy (spectral) dependence of both the transmission probability associated with quantum tunneling and the overall transparency of the potential barrier. These oscillations arise from the interference of electron waves reflected at the interfaces of the potential barrier, while their amplitude is governed by the mismatch between the electron wave vectors inside the barrier region and those in the neighboring potential wells. Moreover, this interference effect does not vanish even in structurally symmetric systems, since variations in the effective electron mass across different regions of the heterostructure inherently sustain the phase differences responsible for the oscillatory response.

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