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THE SIMILARITY BETWEEN THE CHARGED PARTICLE MOTION IN AN ELECTRIC FIELD AND THE LIGHT BEAM PROPAGATION IN A TRANSPARENT MEDIUM

The similarity between the charged particle motion in an electrostatic field, and the light beam propagation in refracting transparent medium is considered. The existing similarity makes it possible to apply the concepts and methods of the ordinary geometrical optics in an absolutely new branch of science – "electronic optics". It also makes it possible to construct electronic devices (electronic microscope, modern oscillograph tubes) similar to the corresponding optical instruments.

Keywords: similarity, electronic optics, electronic microscope.

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TRANSMISSION AND REFLECTION OF HOLES FROM SINGLE BARRIER IN A SEMICONDUCTOR HETEROSTRUCTURES

The quantum mechanical problem of tunneling and reflection of holes from a barrier in a semiconductor heterojunction has been analyzed. By using the Luttinger Hamiltonian to describe the dynamics of holes, the inherent anisotropy, non-parabolicity and heavy and light hole mixing at the top of the valence band has been taken into account. The general relations among the reflectivities and transmissivities are obtained. These analytical results are complemented by numerical calculations for volt-ampere characteristics.

Keywords: Light and heavy holes, quantum barrier, transmission and reflection coefficients.

Introduction. Tunneling and reflection from one dimensional square barrier are traditional problems of quantum mechanics With the arrival of the manufactured semiconductor heterostructures, these problems became also of practical interest, as the epitaxial growth heterointerface between two different semiconductors is almost an ideal realization of a step potential.

Many theoretical methods have been applied to study the semiconductor band structure, electronic and optical properties [1]. These methods can be divided into two general classes: the super cell approach in which the heterostructure is viewed as a material with a large unit cell [2], and the boundary condition approach in which bulk wave functions for each of the constituent semiconductors are matched at the heterostructure interfaces [3,4]. Within the latter category, the envelope function approach, based on the effective mass approximation [5] is easy to apply.

As a consequence of the degeneracy at the top of the valence band, one is forced to use a multiband effective mass theory, that in the case of GaAs-$Al_xGa_{1-x}As$ implies the use of the 4 × 4 Luttinger Hamiltonian [6], at least for energies smaller than the bottom of the Γ_7 spin split off doublet (~ 340 *meV*).

The aim of the present paper is to generalize the well-known textbook results for the transmission and reflection of electrons by one dimensional potential to the case of holes described by the 4 × 4 Luttinger Hamiltonian. The understanding of the dynamics of holes against simple obstacles such as barriers is quite important, as they can considered as the building blocks of more complicated devices, such as double barrier resonant tunneling systems and superlatticies.

The calculation scheme differs, however, in an important point: while the bulk solutions of [7] are linear combinations of four component vectors, our use of a canonical transformation of the Luttinger Hamiltonian decouples it into two 2 × 2 blocks [8], and greatly simplifies the numerical calculations. A similar approach is used in [9].

The volt-ampere dependence shows the influence of holes mixing on the volt-ampere characteristics.

The single-tunnel barrier. Consider the elementary quantum mechanics of the problem posed in Fig.1 of light and heavy holes (LH and HH) with kinetic energy E, incident on a barrier of height U (>E) and thickness a. This simple tunneling problem can be realized in practice with a thin AlGaAs barrier, say about 3*nm* thick with about 40 per cent Al, between layers of GaAs. For the moment, we consider the GaAs layers to be doped so as to produce a Fermi energy E_F (a few tens meV for $10^{18} cm^{-3}$ concentration and that the AlGaAs layer is undoped. The traditional approach is to consider the solutions to the Schrodinger equation with Luttinger 4×4 matrix Hamiltonian on each side of (and within) the barrier, and to analyze the progress of a normalized plane-wave incident from the left.

We start with the standard Luttinger Hamiltonian and differential operator $\left(1/i\right)\left(\partial/\partial z\right)$ involved explicitly [6]:

$$H^2_{4\times4}\left(k_x, k_y, k_z = \frac{1}{i}\frac{d}{dx}\right) = \begin{bmatrix} P+Q & L & M & 0 \\ L^* & P-Q & 0 & M \\ M^* & 0 & P-Q & -L \\ 0 & M^* & -L^* & P+Q \end{bmatrix} + V(z), \qquad (1)$$

where

$$P=\frac{\hbar^2}{2m}\left[\gamma_1(k_x^2+k_y^2)-\frac{d}{dz}\gamma_1\frac{d}{dz}\right], Q=\frac{\hbar^2}{2m}\left[\gamma_2(k_x^2+k_y^2)+2\frac{d}{dz}\gamma_2\frac{d}{dz}\right],$$

$$L=\frac{\sqrt{3}\hbar^2}{im}\gamma_3(k_x-ik_y)\frac{d}{dz}, M=\frac{\sqrt{3}\hbar^2}{2m}\left[\gamma_2(k_x^2-k_y^2)-2i\gamma_3k_xk_y\right],$$

$V(z)=\Delta E\Theta\left(z+{z_0}/{2}\right)\Theta\left(z-{z_0}/{2}\right)$ is the barrier potential (ΔE being the valence band offset) and the hole energy has been counted as positive. In equation (1), m is the free electron mass, and $\gamma_1,\gamma_2,\gamma_3$ are the Luttinger parameters corresponding to the barrier and semi-infinite layer material.

The basis set in the above Hamiltonian can be expressed as

$$u_{h1}=\left|{3}/{2},{3}/{2}\right\rangle=\frac{1}{\sqrt{2}}(X+iY)\vec{\alpha}, \tag{2}$$

$$u_{l1}=\left|{3}/{2},{1}/{2}\right\rangle=\frac{i}{\sqrt{6}}(X+iY)\vec{\beta}-2Z\vec{\alpha}, \tag{3}$$

$$u_{l2}=\left|{3}/{2},-{1}/{2}\right\rangle=\frac{1}{\sqrt{6}}(X-iY)\vec{\alpha}-2Z\vec{\beta}, \tag{4}$$

$$u_{h2}=\left|{3}/{2},-{3}/{2}\right\rangle=\frac{i}{\sqrt{2}}(X-iY)\vec{\beta}, \tag{5}$$

where $\vec{\alpha}$ is the spin up and $\vec{\beta}$ is the spin down wave functions.

Exact solution of the effective-mass equation. The potential $U(z)$ is the square potential which vanishes inside the barrier and equals U in the barrier. The Hamiltonian (1) acts on a four-component envelope function $F=(F_1,F_2,F_3,F_4)$ and the hole wave functions are approximately given by

$$\Psi(\vec{r})=F_1(\vec{r})u_{h1}+F_2(\vec{r})u_{l1}+F_3(\vec{r})u_{l2}+F_4(\vec{r})u_{h2}. \tag{6}$$

In approximation that the Bloch functions (2)-(5) are equal in the two materials, boundary conditions can be expressed in terms of the envelope functions alone.

The potential $U(z)$ breaks the translation symmetry along z; however, k_x and k_y remain good quantum numbers and we can set $F_i(x,y,z)=e^{i(xk_x+yk_y)}f_i(z)$.

The boundary conditions require the continuity of each component $f_i(z)$ of the envelope function and the following vector [10]

$$\begin{bmatrix} (\gamma_1-2\gamma_2)\frac{d}{dz} & \sqrt{3}\gamma_3(k_x-ik_y) & 0 & 0 \\ -\sqrt{3}\gamma_3(k_x+ik_y) & (\gamma_1+2\gamma_2)\frac{d}{dz} & 0 & 0 \\ 0 & 0 & (\gamma_1+2\gamma_2)\frac{d}{dz} & -\sqrt{3}\gamma_3(k_x-ik_y) \\ 0 & 0 & \sqrt{3}\gamma_3(k_x+ik_y) & (\gamma_1-2\gamma_2)\frac{d}{dz} \end{bmatrix} \begin{bmatrix} f_1(z) \\ f_2(z) \\ f_3(z) \\ f_4(z) \end{bmatrix}. \quad (7)$$

The continuity of vector (7) generalizes the usual derivative boundary condition, and is equivalent to the Hermiticity of the effective-mass Hamiltonian; it implies the conservation of the current through the boundary, provided the Bloch functions at both sides are taken to be equal.

For each E, we find the eigenfunctions of the Luttinger Hamiltonian with a given $\vec{k}_{||} = \vec{i}k_x + \vec{j}k_y$, and with the corresponding values k_z. They are denoted by $\pm k_l$, $\pm k_h$ out of the barrier and by $\pm q_l$, $\pm q_h$ in the barrier, where E is replaced by $U - E$. Then, we take the most general linear combination of bulk solutions, and we impose boundary conditions at the two interfaces.

The hole wave function in the cylindrical coordinate $(k_{||}, k_z, \varphi)$ out of the barrier region is:

$$\Psi_{out} = \begin{Bmatrix} c_1 e^{ik_h z} + c_2 e^{-ik_h z} + c_3 e^{ik_l z} + c_4 e^{-ik_l z} \\ c_1 F_h e^{ik_h z} + c_2 F_h^* e^{-ik_h z} + c_3 F_l e^{ik_l z} + c_4 F_l^* e^{-ik_l z} \end{Bmatrix}, \quad (8)$$

where $F_{l;h} = U_{l;h} + iW_{l;h}$, $U_{l;h} = \frac{M_a}{a_{20} + k_{l;h}^2 a_4}$, $W_{l;h} = \frac{k_{l;h} L_a}{a_{20} + k_{l;h}^2 a_4}$, $M_a = \frac{\sqrt{3}k_{||}^2}{2m}\bar{\gamma}$, $\bar{\gamma} = \sqrt{\gamma_2^2 \cos^2 2\varphi + \gamma_3^2 \sin^2 2\varphi}$, $L_a = \frac{\sqrt{3}\gamma_3 k_{||}}{m}$, $a_{20} = a_3 k_{||}^2 - E$, $a_3 = \frac{\gamma_1 - \gamma_2}{2m}$, $a_4 = \frac{\gamma_1 + 2\gamma_2}{2m}$. $F_{l;h}^*$ is complex conjugate of $F_{l;h}$.

$$k_{l;h}^2 = (6c - n)k_{||}^2 - \gamma_1 E \pm \pm\sqrt{4\gamma_2^2 E^2 + 4\gamma_1(n - 3c)k_{||}^2 E + 12n(3n - z)k_{||}^4 + 3cnk_{||}^4 \sin^2 2\varphi}, \quad (9)$$

$$n = \gamma_1^2 - 4\gamma_2^2, \; c = \gamma_3^2 - \gamma_2^2.$$

Transmission coefficient. The conservation of wave number $\vec{k}_{||}$ in each region corresponds to an assumption of secular reflection and transmission by the boundary.

The transmission T_n and reflection R_n coefficients through channel n are, for example, in the case of an incoming HH state $(c_1 = 1, c_2 = c_3 = c_4 = 0)$:

$$T_{HH} = \frac{\left\langle \psi^{t}_{HH} \left| \hat{j}_z \right| \psi^{t}_{HH} \right\rangle_n}{\left\langle \psi^{in}_{HH} \left| \hat{j}_z \right| \psi^{in}_{HH} \right\rangle_0}, \; R_{HH} = \frac{\left\langle \psi^{r}_{HH} \left| \hat{j}_z \right| \psi^{r}_{HH} \right\rangle_n}{\left\langle \psi^{in}_{HH} \left| \hat{j}_z \right| \psi^{in}_{HH} \right\rangle_0}, \tag{10}$$

where indexes n and 0 correspond to transmitting or reflecting and incoming amplitudes in the wave function (8), and the probability current-density operator may be related to the boundary condition matrix (7) using the definition of the current density conveniently written in a matrix form and in terms of the Luttinger parameters [5]

$$j_z = \mathrm{Re}\left(\psi^{+} \hat{j}_z \psi\right). \tag{11}$$

This definition of the current density is appropriate to guarantee the conservation of law of current to the envelope-function space in multi-band effective mass theory [11].

Then we will always have

$$T_{HH} + T_{LH} + R_{HH} + R_{LH} = 1 \tag{12}$$

without exceptions.

The tunneling currents due to the light hole and heavy hole incident states are calculated as:

$$\begin{aligned} J_{HH} &= \frac{e}{4\pi^3} \int d^3k \left[f(E) - f(E+eV) \right] T_{HH}(\vec{k}) v_{zHH}(\vec{k}), \\ J_{LH} &= \frac{e}{4\pi^3} \int d^3k \left[f(E) - f(E+eV) \right] T_{LH}(\vec{k}) v_{zLH}(\vec{k}), \end{aligned} \tag{13}$$

where $f(E)$ is the Fermi –Dirac distribution function. Since the population ratio of the heavy hole to the light hole is proportional to the 3/2 power of the effective mass ratio, the heavy holes make up 89% of the total hole population the injection electrode. Nevertheless, the light hole current is dominant, because the tunneling probability increases exponentially as the effective mass decreases. However, this may also depend on the thickness of the barrier.

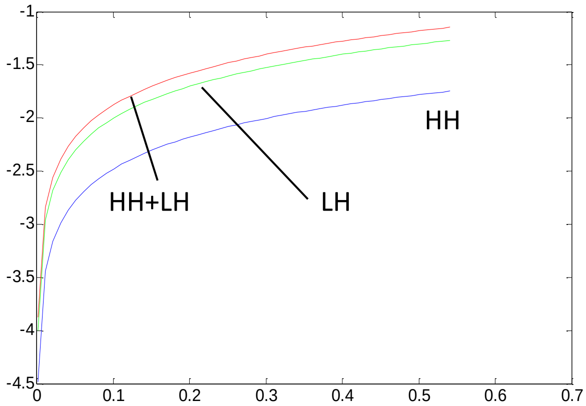

Fig.

In Figure above, the thickness of the barrier is a=75 nm, the current of the light hole is higher relative to the heavy holes. When the thickness of the barrier a=25nm, the location of volt-ampere relationships vary inversely. This explains the dynamics of changes of light and heavy holes through each other.

Conclusions. This work has been devoted to the theoretical study of the quantum mechanical problem of tunneling and reflection of holes from the barrier in semiconductor heterostructures. The calculation has been carried out within the framework of the envelope function approach which is based on the effective mass approximation. By using the Luttinger Hamiltonian to describe the dynamics of holes close at the top of the valence band, we have taken into account exactly the band non-parabolicity, anisotropy, and heavy and light holes mixing away from Brillouin zone centre.

We also provide a complete set of numerical results concerning the reflection and tunneling of holes impinging on barriers.

The Current-Voltage dependence essentially depends not only on quantum number $k_{||}$ ($\vec{k}_{||} = \vec{i}k_x + \vec{j}k_y$), but also on the barrier thickness.

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ԽՈՌՈՉՆԵՐԻ ԱՆՑՈՒՄԸ ԵՎ ԱՆԴՐԱԴԱՐՁՈՒՄԸ ԱՌԱՆՁԻՆ ԲԱՐԻԵՐԻՑ ԿԻՍԱՀԱՂՈՐԴՉԱՅԻՆ ՀԵՏԵՐՈԿԱՌՈՒՑՎԱԾՔՆԵՐՈՒՄ

Առանձնացված քվանտային ուղղանկյուն բարիերի համար լուծված է անցման և անդրադարձման քվանտամեխանիկական խնդիրը խոռոչների համար: Առաջարկված է Լատտինջերի հավասարման լուծման համար հարմար եղանակ, որով 4 × 4 չափի Լատտինջերի համիլտոնյանը բերվում է 2 × 2 չափի համիլտոնյանի, որի լուծումները համեմատաբար ավելի հեշտ է գտնել: Ստացված ալիքային ֆունկցիաներով հաշվվել են անցման և անդրադարձման գործակիցները, ինչպես նաև վոլտ-ամպերային բնութագրերը: Ուսումնասիրռած է վոլտ-ամպերային բնութագրերի կախումը բարիերի լայնությունից:

Առանցքային բառեր. ծանր և թեթև խոռոչներ, քվանտային բարիեր, անցման և անդրադարձման գործակիցներ:

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ПРОХОЖДЕНИЕ И ОТРАЖЕНИЕ ДЫРОК ОТ ОДИНОЧНОГО БАРЬЕРА ПОЛУПРОВОДНИКОВЫХ СТРУКТУР

Решена квантово-механическая задача прохождения и отражения дырок от одиночного прямоугольного квантового барьера. Предложен удобный способ решения уравнения Латтинжера, с помощью которого латтинжеровский гамильтониан размерностью 4 × 4 приведен к виду 2 × 2. С помощью волновых функций рассчитаны коэффициенты прохождения и отражения от барьера, а также вольт-амперные характеристики такой структуры. Исследованы зависимости вольт-амперных характеристик от толщины барьера.

Ключевые слова: тяжелые и легкие дырки, квантовый барьер, коэффициенты прохождения и отражения.