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On Transmissions through a Biased Delta-Barrier Embedded in a Crystalline Lattice

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Abstract: The solution of the one-dimensional Schrödinger-Wannier wave equation is examined for the potential-energy function that describes a delta-barrier under the application of a constant perpendicular electrical field. General expressions for the transmission and reflection coefficient are derived. The perpendicular components of the group velocities of the particles transmitted through the biased delta-barrier are involved in them. The transmission coefficients for two different dispersion functions are juxtaposed: for the quadratic function and for the Kane function. The particles with the Kane energy spectrum are shown to exhibit an exceptional behaviour in the transmissions through the biased delta-barrier.

Keywords: Schrödinger-Wannier wave equation, Dispersion function, Dirac delta-function, Rectangular barrier, Transmission coefficient.

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1. Introduction

This paper presents a theory of conduction electrons in a sandwich structure A-B-A that finds itself in a constant electrical field perpendicular to its interfaces. B is a very narrow single crystalline layer embedded in (being lattice-matched on both its sides with) a bulk crystal A. Attention is focused mainly on the non-quadracity of the dispersion function of the conduction band and its influence on the transmission properties of electrons tunnelling through the biased sandwich structure. Neglecting space charge effects and adopting the Wannier one band approximation [1], one can diagrammatically represent the biased sandwich structure A-B-A by the flat-band scheme shown in Fig. 1. (The horizontal full lines in Fig. 1 correspond to the lower boundary of the conduction band in the regions A and B.) Thus, the narrow layer B embedded in the bulk crystal A is modelled by a one-dimensional rectangular barrier of a width w_0 and a height U_0. The applied constant electrical field perpendicular to the interfaces of the sandwich structure is simulated by lowering the boundary of the conduction band, i.e. by establishing a one-dimensional rectangular well of an infinite extent and a finite depth eV in that region A in which the electrical potential is higher (e is the elementary charge and V is the applied bias voltage). So, in each region the potential energy of an electron is replaced by its average value. The transmission through the potential sketched in Fig. 1 was studied for the first time by Nordheim [2]. (Cf. also [3], where early history of quantum tunnelling is presented.)

In the case of a very narrow layer B, one can formally let the width of the rectangular barrier tend to the zero and simultaneously the height of the barrier tend to the infinity whilst keeping the product w_0U_0 to be constant. Then, the potential-energy function that represents the rectangular barrier in Fig. 1 becomes a delta-function of the strength $g = w_0U_0$. Although the delta-function is a very simplified potential-energy function, it enables us to get a proper insight into the transmissions through the narrow and high barrier structures [4, 5]. This is also why the delta-function potentials were often employed throughout many parts of the solid-state physics as a very convenient approximation to more structured and therefore more difficult, shortranged potentials (cf. e.g. references cited in [6]). Therefore, it is also interesting to examine the transmission through the biased delta-barrier that is embedded in a crystalline lattice.

As a rule, the effective-mass Schrödinger wave equation used to be employed in solving transmission problems. Thus, the energy spectrum of transmitting particles was supposed to be quadratic. Notwithstanding, even if the energy spectrum is approximated by a quadratic function, a question is, how to choose the appropriate effective-mass value. The energy spectrum is quadratic only in the alkali metals and in the $A^{III}B^{V}$ semiconductors near the bottom of their conduction band. In the majority of other substances, the non-quadraticity of the energy spectrum plays an important role. Therefore, the use of the effective-mass approximation is insufficient and the real energy spectrum should be taken into consideration. (E.g. the Kane energy spectrum is convenient to go beyond the quadratic energy spectrum in a narrow-gap semiconductor [7].) In an approach to the transmission through the unbiased delta-barrier, Bezák [6] took into account the possible non-quadraticity of the energy spectrum. Instead of the Schrödinger equation, he solved the Schrödinger-Wannier equation for the corresponding potential-energy function. In this way, he respected that the energy spectrum of the transmitting particles did not have to be quadratic and discussed some consequences of this non-quadraticity for the transmission through the unbiased delta-barrier. In our paper, his treatment is extended on the biased delta-barrier.

The organisation of this paper is as follows. In the next section, the Schrödinger-Wannier wave equation is employed to obtain the wave function for the potential-energy function, which corresponds to the limiting case of the rectangular barrier structure shown in Fig. 1. The wave function is then used to derive the general expressions for the transmission and reflection coefficient for the biased delta-barrier embedded in a crystalline lattice. The third section is devoted to the exemplification of the transmission coefficient for the two different dispersion functions. Finally, some concluding remarks are presented in the fourth section.

2. Solution of the Schrödinger-Wannier Equation

The one-dimensional stationary Schrödinger-Wannier wave equation [1],

$$\left[\mathcal{E}\left(-i\frac{\partial}{\partial x}\right) + U(x) - E\right]\psi(x) = 0, \quad (1)$$

is solved for the potential-energy function

$$U(x) = g\,\delta(x) - eV\,\theta(x). \quad (2)$$

Here x represents the spatial variable, E is the energy of a particle (a conduction electron), (x) is the Dirac delta-function and g is its strength. (A positive value of the strength corresponds to a barrier, while a negative value would correspond to a well.) (x) is the Heaviside step function ($(x)\quad 0$ if $x\quad 0$ and $(x)\quad 1$ if $x\quad 0$), e is the elementary charge, V is the bias voltage applied to the delta-barrier. The dispersion function of the conduction band $\mathcal{E}(k)$ is supposed to be even and growing for the positive wave number k and to tend to the infinity in the limit k . The definition region of the function $\mathcal{E}(k)$ is not confined to the first Brillouin zone only from the mathematical reasons. This deliberate simplification is tolerable for such values of the wave number k that are much smaller than the inverse value of the lattice constant.

Evidently, the wave function (x) is to be sought in the form of plane waves running from the left to the right and vice versa, i.e.

$$\begin{aligned} (x)\quad & \{1\quad (x)\}\ {}_{I}(x)\quad (x)\ {}_{II}(x) \\ & \{1\quad (x)\}\{A_I e^{\,i\,k_1\quad i0\ x}\quad B_I e^{\,i\,k_1\quad i0\ x}\}\quad (x)\{A_{II} e^{\,i\,k_2\quad i0\ x}\quad B_{II} e^{\,i\,k_2\quad i0\ x}\}. \end{aligned} \tag{3}$$

A_I, B_I and A_{II}, B_{II} are, respectively, the amplitudes of these two plane waves in the regions that are separated one from another by the point $x\quad 0$. The subscript I refers to the spatial region ($,\ 0)$ that is on the left-hand side of the biased delta-barrier; the subscript II refers to the spatial region ($,\ 0)$ that is on the right-hand side of the biased delta-barrier. The positive wave numbers k_1 and k_2 are introduced by the relation $E\quad \mathcal{E}(k_1)\quad \mathcal{E}(k_2)\quad eV$.

The continuity condition for the wave function (x) at the points $x\quad 0$ yields a connection formula, namely $A_I\quad B_I\quad A_{II}\quad B_{II}$. Another connection formula is derived in Appendix A. It states $\{A_I\quad B_I\}\mathcal{K}(k_1)\quad \{A_{II}\quad B_{II}\}\mathcal{K}(k_2)\quad i\quad \{A_I\quad B_I\}$, where, $\quad 2mg/\hbar^2$, $\mathcal{K}(k)\quad m\ \mathcal{E}(k)/\hbar^2\ k$. m is the effective mass of the particle at the bottom of the conduction band, i.e. $m\quad \hbar^2/(\ ^2\mathcal{E}(k)/\ ^2k)_{k\ 0}$. In the present treatment, the value of $^2\hbar^2/2m\quad 2mg^2/\hbar^2$ will be taken as an empirical parameter characterising the delta-barrier.

The two connection formulae can be rewritten as follows:

$$B_I\quad r(k_1,k_2)A_I\quad \sqrt{\frac{\mathcal{K}(k_2)}{\mathcal{K}(k_1)}}\,t(k_1,k_2)B_{II} \tag{4a}$$

$$A_{II}\quad \sqrt{\frac{\mathcal{K}(k_1)}{\mathcal{K}(k_2)}}\,t(k_1,k_2)A_I\quad \frac{r^*(k_1,k_2)t(k_1,k_2)}{t^*(k_1,k_2)}B_{II}\,, \tag{4b}$$

where

$$t(k_1,k_2)\quad \frac{2\sqrt{\mathcal{K}(k_1)\mathcal{K}(k_2)}}{\mathcal{K}(k_1)\quad \mathcal{K}(k_2)\quad i}\,,\quad r(k_1,k_2)\quad \frac{\mathcal{K}(k_1)\quad \mathcal{K}(k_2)\quad i}{\mathcal{K}(k_1)\quad \mathcal{K}(k_2)\quad i}\,. \tag{4c}$$

It is easy to show that $t^*(k_1,k_2)\,t(k_1,k_2)\quad 1\quad r^*(k_1,k_2)\,r(k_1,k_2)$.

Thus, the wave function on the left-hand side and the wave function on the right-hand side of the biased delta-barrier are, respectively, of the form

$${}_I(x)\quad A_I e^{\,i\,k_1\quad i0\ x}\quad r(k_1,k_2)A_I\quad \sqrt{\frac{\mathcal{K}(k_2)}{\mathcal{K}(k_1)}}\quad t(k_1,k_2)B_{II}\ e^{\,i\,k_1\quad i0\ x}\,, \tag{5a}$$

$${}_{II}(x)\quad \sqrt{\frac{\mathcal{K}(k_1)}{\mathcal{K}(k_2)}}t(k_1,k_2)A_I\quad \frac{r^*(k_1,k_2)t(k_1,k_2)}{t^*(k_1,k_2)}B_{II}\ e^{\,i\,k_2\quad i0\ x}\quad B_{II}e^{\,i\,k_2\quad i0\ x}\,. \tag{5b}$$

A_I is the amplitude of the plane wave impinging upon the biased delta-barrier from the left-hand side, $r(k_1,k_2)A_I$ is the amplitude of the reflected wave and $\sqrt{\mathcal{K}(k_1)/\mathcal{K}(k_2)}\,t(k_1,k_2)A_I$ is the amplitude of the transmitted wave; B_{II} is the amplitude of the plane wave impinging upon the biased delta-barrier from the right-hand side, $r^*(k_1,k_2)t(k_1,k_2)B_{II}/t^*(k_1,k_2)$ is the amplitude of the reflected wave and $\sqrt{\mathcal{K}(k_2)/\mathcal{K}(k_1)}\,t(k_1,k_2)B_{II}$ is the amplitude of the transmitted wave.

Obviously (Appendix B), the quantities $t(k_1,k_2)$ and $r(k_1,k_2)$, respectively, represent the transmission and reflection amplitude. (Actually, $r(k_1,k_2)$ is the reflection amplitude from the left and $r^*(k_1,k_2)t(k_1,k_2)/t^*(k_1,k_2)$ is the reflection amplitude from the right. They differ only in a phase.) The transmission coefficient is defined by the relation $T(k_1,k_2) \quad t^*(k_1,k_2)t(k_1,k_2)$. The reflection coefficient can be obtained from the well-known relation, namely $R(k_1,k_2) \quad r^*(k_1,k_2)r(k_1,k_2) \quad 1 \quad T(k_1,k_2)$.

Thus, the transmission and reflection coefficient for the biased delta-barrier are, respectively, given by the relations

$$T(k_1,k_2) \quad \frac{4\mathcal{K}(k_2)\mathcal{K}(k_1)}{\{\mathcal{K}(k_2) \quad \mathcal{K}(k_1)\}^2 \quad {}^2}\ , \tag{6a}$$

$$R(k_1,k_2) \quad \frac{\{\mathcal{K}(k_2) \quad \mathcal{K}(k_1)\}^2 \quad {}^2}{\{\mathcal{K}(k_2) \quad \mathcal{K}(k_1)\}^2 \quad {}^2}\ . \tag{6b}$$

Evidently, the positive wave numbers k_1 and k_2 represent those components of the wave vectors that are perpendicular to the biased delta-barrier. The dispersion function $\mathcal{E}(k)$ also involves components of the wave vectors that are parallel to and continuous across the biased delta-barrier. Two functions, a quadratic function and a non-quadratic function, are introduced as the dispersion functions of the conduction band in the next section, where the corresponding analytical expressions for the quantity $\mathcal{K}(k) \quad m \quad \mathcal{E}(k)/\hbar^2 \quad k$ is obtained, too.

Of course, if there is no external bias voltage applied to the delta-barrier, i.e. If $V \quad 0$, then $\mathcal{K}(k_2) = \mathcal{K}(k_1)$ and Eqs. (6a) and (6b) are reduced to those derived by Bezák [6]. If $\quad 0$, then Eqs. (6a) and (6b) represent respectively the transmission and reflection coefficient for a rectangular well of an infinite extent and a finite depth eV (cf. e.g. [4, 5, 8, 9], where a rectangular barrier of an infinite extent and a finite height is examined).

It is worth mentioning that the transmission coefficient, as well as the reflection coefficient, does not change if one exchanges the delta-barrier for the delta-well, i.e. if one exchanges $\quad 2mg/\hbar^2$ for $\quad 2m(\quad g)/\hbar^2$. The invariance of the transmission and reflection coefficient with respect to the replacement of g by $g \quad g$ is a specific consequence due to the use of the delta-function potential. It will be broken if one uses a barrier with a finite height U_0 and a finite width w_0 or a well with a finite depth $\quad U_0$ and a finite width w_0 (cf. [6] for more details). Further, the transmission over a finite well is ideal in certain cases; i.e. the transmission coefficient equals the unity for certain values of the energy of the transmitting particle [4, 8, 9]. Such a phenomenon is not present in the transmissions through a delta-well.

3. Exemplification of the Transmission Coefficient

In this section, the transmission coefficient is exemplified for the two different dispersion functions of the conduction band: for the quadratic function and for the Kane function.

The quadratic energy spectrum is defined by these relations

$$\mathcal{E}_Q(k) \quad \frac{(k^2 \quad k_{||}^2)\hbar^2}{2m}, \quad \mathcal{K}_Q(k) \quad m\frac{\mathcal{E}_Q(k)}{\hbar^2 \quad k} \quad k, \tag{7}$$

where $k_{||}$ is the component of the wave vector parallel to and continuous across the biased delta-barrier.

Using the relation $k_{||} \quad k_1 \tan$, where is the impact angle (0 / 2), and the relation

$$E \quad \frac{(k^2 \quad k_{||}^2)\hbar^2}{2m} \quad \frac{(k^2 \quad k_{||}^2)\hbar^2}{2m} \quad eV, \tag{8}$$

one obtains

$$\mathcal{K}_Q(k_1) \quad k_1 \quad \frac{\sqrt{2Em}}{\hbar}\cos \quad \mathcal{K}_Q(E,0,\ ) \tag{9a}$$

$$\mathcal{K}_Q(k_2) \quad k_2 \quad \frac{\sqrt{2(eV \quad E\cos^2\ )m}}{\hbar} \quad \mathcal{K}_Q(E,0,\ ). \tag{9b}$$

Then, the transmission coefficient of the particle with the quadratic energy spectrum acquires the form (formula (6a))

$$T_Q(k_1,k_2) \quad T_Q(E,V,\ ) \quad \frac{4\mathcal{K}_Q(k_2)\mathcal{K}_Q(k_1)}{\{\mathcal{K}_Q(k_2) \quad \mathcal{K}_Q(k_1)\}^2 \quad ^2} \tag{10}$$

$$\frac{4\sqrt{(eV \quad E\cos^2\ )E}\cos}{\{\sqrt{(eV \quad E\cos^2\ )} \quad \sqrt{E}\cos\ \}^2 \quad \frac{^2\hbar^2}{2m}}.$$

If the energy of the transmitting particle and the bias voltage applied to the delta-barrier is sufficiently small, i.e. if $E \quad ^2\hbar^2/2m$ and $eV \quad ^2\hbar^2/2m$, then the transmission coefficient grows with the energy and the applied bias voltage as

$$T_Q(E,V,\ ) \quad \frac{8\sqrt{(eV \quad E\cos^2\ )E}\,m\cos}{^2\hbar^2}. \tag{11}$$

Evidently, the transmission coefficient $T_Q(E,V,\ )$ does not exhibit any exceptional dependence on its variables in the region of small energies and small applied bias voltages.

In the limit E , one gets $\lim_{E} T_Q(E,V,\ ) \quad 1$; i.e. the transmission coefficient $T_Q \ E,V,$ behaves normally in the high-energy region, too.

The most popular non-quadratic, still isotropic, energy spectrum with the same effective mass m is one defined by the Kane dispersion function [7]. It is of the form

$$\mathcal{E}_K(k) \quad \frac{E_g}{2} \quad 1 \quad \frac{2(k^2 \quad k_{||}^2)\hbar^2}{mE_g} \quad 1 \tag{12a}$$

and

$$\mathcal{K}_K(k) \quad m\frac{\mathcal{E}_K(k)}{\hbar^2 \quad k} \quad \frac{k}{1 \quad \frac{2(k^2 \quad k_{||}^2)\hbar^2}{mE_g}^{1/2}} \quad \frac{k}{1 \quad \frac{2\mathcal{E}_K(k)}{E_g}}, \tag{12b}$$

where E_g is the width of the forbidden gap and the meaning of the other symbols is evident.

Near the band edge, i.e. when $(k^2 \quad k_{||}^2)\hbar^2 / 2m \quad E_g$, the Kane dispersion function is reduced to the quadratic dispersion function. Therefore, in the region of small energies and small applied bias voltages, all the results for the Kane dispersion function will be transformed into those obtained with the use of the quadratic dispersion function. Thus, essential differences between the transmission coefficients $T_Q(E,V, \quad)$ and $T_K(E,V, \quad)$ are to be expected only at high energies or with high applied bias voltages, i.e. when $E_g \quad E$ or $E_g \quad eV$.

Employing the relations $k_{||} \quad k_1 \tan$ and

$$E \quad \frac{E_g}{2} \quad 1 \quad \frac{2(k_1^2 \quad k_{||}^2)\hbar^2}{mE_g}^{1/2} \quad 1 \quad \frac{E_g}{2} \quad 1 \quad \frac{2(k_2^2 \quad k_{||}^2)\hbar^2}{mE_g}^{1/2} \quad 1 \quad eV, \tag{13}$$

one gets

$$\mathcal{K}_K(k_1) \quad \frac{\sqrt{2(E_g \quad E)E_g E m}}{(E_g \quad 2E)\hbar}\cos \quad \mathcal{K}_K(E,0, \quad), \tag{14a}$$

$$\mathcal{K}_K(k_2) \quad \frac{\sqrt{2\{(E_g \quad E)E\cos^2 \quad (E_g \quad 2E \quad eV)eV\}E_g m}}{(E_g \quad 2E \quad 2eV)\hbar} \quad \mathcal{K}_K(E,V, \quad). \tag{14b}$$

Thus, the transmission coefficient of the particle with the Kane energy spectrum can be written in this form (formula (6a))

$$T_K(k_1,k_2) \quad T_K(E,V, \quad) \quad \frac{4\mathcal{K}_K(k_2)\mathcal{K}_K(k_1)}{\{\mathcal{K}_K(k_2)+\mathcal{K}_K(k_1)\}^2 \quad ^2}$$

$$\frac{4\frac{\sqrt{\{(E_g \quad E)E\cos^2 \quad (E_g \quad 2E \quad 2eV)eV\}(E_g \quad E)E}}{(E_g \quad 2E \quad 2eV)(E_g \quad 2E)}\cos}{\frac{\sqrt{(E_g \quad E)E\cos^2 \quad (E_g \quad 2E \quad 2eV)eV}}{E_g \quad 2E \quad 2eV} \quad \frac{\sqrt{(E_g \quad E)E}}{E_g \quad 2E}\cos \quad \frac{^2\hbar^2}{2mE_g}}. \tag{15}$$

If the energy, as well as the applied bias voltage, is sufficiently small, i.e. if $E \quad E_g$ and $eV \quad E_g$, the transmission coefficient $T_K(E,V, \quad)$ can be approximated by the expression

$$T_K(E,V, \quad) \quad T_Q(E,V, \quad) \quad \frac{4\sqrt{(eV \quad E\cos^2 \quad)E}\cos}{\{\sqrt{eV \quad E\cos^2} \quad \sqrt{E}\cos \quad\}^2 \quad \frac{^2\hbar^2}{2m}}. \tag{16}$$

Thus, in the region of small energies and small applied bias voltages, the transmission coefficients $T_K(E,V, \quad)$ and $T_Q(E,V, \quad)$, Eqs. (15) and (10), exhibit the similar dependence on their variables.

However, in the limit $E \quad$, one gets

$$\lim_{E} T_K(E,V,\ ) \quad \frac{\cos^2}{\cos^2 \quad \frac{^2\hbar^2}{2mE_g}} . \tag{17}$$

So, the transmission coefficient $T_K(E,V,\ )$, Eq. (15), behaves anomalously in the high-energy region. Unlike the transmission coefficient $T_Q(E,V,\ )$, Eq. (10), it does not approach the unity in this energy region. In the case of the Kane energy spectrum, the perpendicular components of the group velocities of the transmitting particle, i.e. the quantities $\mathcal{K}_K(E,0,\ )\hbar/m$ and $\mathcal{K}_K(E,V,\ )\hbar/m$, Eqs. (14a) and (14b), are limited by the value $\sqrt{E_g/2m}\cos$ as $\lim_{E} \mathcal{K}_K(E,0,\ )\hbar/m \quad \lim_{E} \mathcal{K}_K(E,V,\ )\hbar/m \quad \sqrt{E_g/2m}\cos$. This is why the transmission coefficient $T_K \ E,V,$ tends to its own anomalous asymptotic value (not equalling the unity) that corresponds to the transmission of the particle with the asymptotic value of the perpendicular component of the group velocity. It is worth mentioning that this asymptotic value of the transmission coefficient is not influenced by the bias voltage applied to the delta-barrier.

To examine the behaviour of the transmission coefficient in the high-energy region from a little more general point of view one can consider a class of the dispersion functions that behave as

$$\mathcal{E}(k) \quad (k^2 \quad k_{||}^2)\ ,\quad 0 \qquad . \tag{18}$$

Then, one easily derives

$$\mathcal{K}(k) \quad m\frac{\mathcal{E}(k)}{\hbar^2\ k} \quad 2\ k(k^2 \quad k_{||}^2)\ ^{1} \tag{19a}$$

and

$$\mathcal{K}(E,0,\ ) \quad 2\ E^{2\ \ 1/2} \cos\ , \tag{19b}$$

$$\mathcal{K}(E,V,\ ) \quad 2\ (E \quad eV)\ ^{1/} \sqrt{(E \quad eV)^{1/} \quad E^{1/}\ \sin^2}\ . \tag{19c}$$

It is seen from the two previous relations that if $1/2$, both the perpendicular components of the group velocities of the transmitting particle, i.e. the quantities $\mathcal{K}\ (E,0,\ )\hbar/m$ and $\mathcal{K}\ (E,V,\ )\hbar/m$, diverge in the limit E . Employing Eq. (6a), one concludes that in this case the transmission coefficient goes to the unity in the high-energy region. On the other hand, if $0 \quad 1/2$, both the perpendicular components of the group velocities of the transmitting particle approach a zero value in the limit E and therefore the transmission coefficient tends to the zero in the high-energy region. If $1/2$, both the perpendicular components of the group velocities of the transmitting particle approach the same non-zero finite value in the limit E . Because of this the transmission coefficient tends to an asymptotic value that is greater than the zero and less than the unity. (The Kane dispersion function just corresponds to the case $1/2$.)

The dependence of the transmission coefficient on the dimensionless variables E/E_g and eV/E_g is, respectively, shown graphically in Figs. 2 and 3 for the four different values of the impact angle . In both the figures, the value of the parameter $^2\hbar^2/2m$, which characterises the strength of the delta-barrier, is chosen to be equal to E_g as well as the energy of the transmitting particle equals E_g in Fig. 3. In both the figures, the full curves correspond to the transmission coefficient of the particle with the quadratic energy spectrum $T_Q(E,V,\ )$, Eq. (10); the dashed curves to the transmission coefficient of the particle with the Kane energy spectrum $T_K(E,V,\ )$, Eq. (15). The first uppermost full and dashed curves are drawn for the impact angle 0, the second full and dashed curves for $/6$, the third full and dashed curves for $/4$ and the fourth full and dashed curves for $/3$. In Fig. 2, all the four full curves gradually tend to the unity and all the four dashed curves steeply approach their asymptotic values; the first uppermost dashed curve steeply approaches 1/2, the second dashed curve 3/7, the third dashed curve 1/3 and the fourth dashed curve 1/5 (formula (17) with $^2\hbar^2/2mE_g\ \ 1$ and sequentially 0, $/6$, $/4$, $/3$). Both the transmission coefficients $T_Q(E,V,\ )$ and $T_K(E,V,\ )$ vary very slowly in the region of small applied bias voltages which is depicted in Fig. 3.

In the region of high applied bias voltages, i.e. If $E\ \ eV$, one, however, obtains

$$T_Q(E,V,\ )\ \ \frac{4\sqrt{eVE}\,\cos}{eV\ \ \frac{^2\hbar^2}{2m}} \tag{20}$$

and $\lim_{V} T_Q(E,V,\ )\ \ 0$. Hence, the particle with the quadratic energy spectrum totally reflects from the well of an infinite extent and an infinite depth. In this infinite well, this particle should move with an infinite group velocity as $\lim_{V} \mathcal{K}_Q(E,V,\ )\hbar/m$ (formula (9b).

On the other hand,

$$\lim_{V} T_Q(E,V,\ )\ \ \frac{2\dfrac{\sqrt{(E_g\ \ E)E}}{E_g\ \ 2E}\cos}{\left(\dfrac{1}{2}\ \ \dfrac{\sqrt{(E_g\ \ E)E}}{E_g\ \ 2E}\cos\right)^2\ \ \dfrac{^2\hbar^2}{2mE_g}}. \tag{21}$$

Thus, in the region of high applied bias voltages, the transmission coefficient $T_K(E,V,\ )$, Eq. (15), exhibits quite a different behaviour than the transmission coefficient $T_Q(E,V,\ )$, Eq. (10), does. Unlike the particle with the quadratic energy spectrum, the particle with the Kane energy spectrum has a finite group velocity in the infinite rectangular well, as $\lim_{V} \mathcal{K}_K(E,V,\ )\hbar/m\ \ \sqrt{E_g/2m}$ (formula (14b)).

To examine the differences between the transmission coefficients $T_Q(E,V,\ )$ and $T_K(E,V,\ )$, Eqs. (10) and (15), in the region of high applied bias voltages, it is appropriate to look into the value of the perpendicular component of the group velocity of the particle in the infinite rectangular well which is to be obtained from Eq. (19c). That relation states

$$\mathcal{K}\ (E,V,\ )\ \ 2\ (E\ \ eV)^{\ 1/\ }\sqrt{(E\ \ eV)^{1/}\ \ E^{1/}\sin^2}\ . \tag{22}$$

It is seen from the previous relation that if $1/2$, the perpendicular component of the group velocity of the particle $\mathcal{K}\ (E,V,\ )\hbar/m$ approaches an infinite value in the limit V . Employing Eq. (6a), one concludes that, in this case, the transmission coefficient tends to zero in the region of high applied bias voltages. On the other hand, if $0\ \ 1/2$, the perpendicular component of the group velocity of the particle approaches a zero value in the limit V and therefore the transmission coefficient tends to the zero in the region of high applied voltages. If $1/2$ (the Kane dispersion function just corresponds to this case), the perpendicular component of the group velocity of the particle approaches a non-zero finite value. Only in this case, therefore, the transmission coefficient tends to a non-zero asymptotic value in the region of high applied bias voltages.

4. Concluding Remarks

The transmission as well as reflection coefficient for the biased delta-barrier embedded in a crystalline lattice is given by a very simple formula, which involves the perpendicular components of the group velocities of the transmitting particles. The Bloch theory of the crystalline lattice is involved in the present treatment of the transmission problem by means of the dispersion function defining the conduction band of electrons. The wave function, which is the solution of the Schrödinger-Wannier wave equation, represents an envelope of the Bloch wave functions. Interband transitions due to the biased delta-barrier were supposed not to take place. Therefore, the Schrödinger-Wannier wave equation without interband matrix elements was employed in our transmission problem. The two dispersion functions used in the exemplification of the transmission coefficient are isotropic. It is evident that the formulae for the transmission and reflection coefficient can directly be used also in the case of anisotropic dispersion functions.

In the region of small energies and small applied bias voltages, there are no essential differences among the transmission coefficients of particles with the different energy spectra. However, there are crucial differences among them in the region of high energies. These differences seem to be very important since transmissions through a barrier usually take place at energies that are well above the bottom of the conduction band. Further, there are also differences among the transmission coefficients in the region of high bias voltages applied to the barrier. Evidently, in the case of high bias voltages applied to the barrier as well as in the case of the large strength of the barrier it is necessary to incorporate interband matrix elements into the theory.

Similar results are believed to be valid with more realistic potentials modelling the biased barrier embedded in a crystalline lattice. Thus, the main conclusion of the present treatment is that the effective mass approximation is not suitable for determining the transmission coefficient of particles with the non-quadratic energy spectrum. The real energy spectrum must be considered.

Appendix A

In the case of the quadratic energy spectrum, $\mathcal{E}_Q(k) \quad (k^2 \quad k_{||}^2)\hbar^2/2m$, the formal integration of the Schrödinger equation around the point $x \quad 0$ leads to the relation expressing the discontinuity of the first derivative of the wave function at this point [4, 5], i.e. $\quad 0 \qquad 0 \quad 2mg \quad 0/\hbar^2$, where $\quad a \quad (d \quad x/dx)_{x \quad a}$. This discontinuity relation yields another connection formula for the wave function $\quad x$, Eq. (3), namely $(A_I \quad B_I)k_1 \quad (A_{II} \quad B_{II})k_2 \quad 2i(A_I \quad B_I)mg/\hbar^2$.

In the case of the non-quadratic energy spectrum, the second connection formula could be determined in a similar way. To avoid either finding the relations among the higher-order derivatives of the wave function or differentiating the Heaviside step function to an infinite order (the Maclaurin series for the function $\mathcal{E}(k)$ generally involves an infinite number of terms), it is appropriate to insert the wave function $\quad x$, Eq. (3), into the Schrödinger-Wannier wave equation, Eq. (1), in the form of the Fourier integral, $x \qquad f(\ )e^{i \ x} d$, where f is the Fourier original to the wave function, i.e.

$$f(\ ) \quad \int^{0} \{A_I e^{\ ik_1 x} \quad B_I e^{\ ik_1 x}\} e^{\ i \quad i0 \ x} dx \quad \int_{0} \{A_{II} e^{\ ik_2 x} \quad B_{II} e^{\ ik_2 x}\} e^{\ i \quad i0 \ x} dx$$

$$\frac{iA_I}{k_1 \quad i0} \quad \frac{iB_I}{k_1 \quad i0} \quad \frac{iA_{II}}{k_2 \quad i0} \quad \frac{iB_{II}}{k_2 \quad i0}. \tag{A.1}$$

Then, one gets the equation

$$\frac{\mathcal{E}(\ ) \quad \mathcal{E}(k_1)}{k_1 \quad i0} A_I \quad \frac{\mathcal{E}(\ ) \quad \mathcal{E}(k_1)}{k_1 \quad i0} B_I \quad \frac{\mathcal{E}(\ ) \quad \mathcal{E}(k_2)}{k_2 \quad i0} A_{II}$$

$$\frac{\mathcal{E}(\ ) \quad \mathcal{E}(k_2)}{k_2 \quad i0} B_{II} \quad i(A_I \quad B_I) g \frac{e^{i \ x} d}{2} \quad 0. \tag{A.2}$$

It is satisfied, when

$$\text{v.p.} \quad \frac{A_I}{\quad k_1} \quad \frac{B_I}{\quad k_1} \quad \frac{1}{\mathcal{E}(\ ) \quad \mathcal{E}(k_2)} \quad \frac{A_{II}}{\quad k_2} \quad \frac{B_{II}}{\quad k_2} \quad \frac{1}{\mathcal{E}(\ ) \quad \mathcal{E}(k_1)}$$

$$\frac{i(A_I \quad B_I) g}{(\mathcal{E}(\ ) \quad \mathcal{E}(k_1))(\mathcal{E}(\ ) \quad \mathcal{E}(k_2))} \quad 0, \tag{A.3}$$

where the symbol v.p. means the Cauchy principal value.

As the function $\mathcal{E}(\ )$ is even and growing for the positive variable , the equation $\mathcal{E}(\ ) \quad E \quad 0$ has two roots, $_{1,2} \qquad k$. Because of it, it is valid that

$$\text{v.p.} \frac{1}{\mathcal{E}(\ ) \quad \mathcal{E}(k)} \quad \frac{1}{\frac{\mathcal{E}(k)}{k}} \text{v.p.} \frac{1}{\quad k} \quad \frac{1}{\quad k}. \tag{A.4}$$

Thus, Eq. (A.3) can be rewritten into the form

$$\text{v.p.} \frac{1}{(\quad k_1)(\quad k_2)} \quad \frac{\mathcal{E}(k_1)}{k_1} A_I \quad \frac{\mathcal{E}(k_2)}{k_2} A_{II} \quad i(A_I \quad B_I) g$$

$$\text{v.p.} \frac{1}{(\quad k_1)(\quad k_2)} \quad \frac{\mathcal{E}(k_1)}{k_1} B_I \quad \frac{\mathcal{E}(k_2)}{k_2} B_{II} \quad i(A_I \quad B_I)g$$

$$\text{v.p.} \frac{1}{(\quad k_1)(\quad k_2)} \quad \frac{\mathcal{E}(k_1)}{k_1} A_I \quad \frac{\mathcal{E}(k_2)}{k_2} B_{II} \quad i(A_I \quad B_I)g$$

$$\text{v.p.} \frac{1}{(\quad k_1)(\quad k_2)} \quad \frac{\mathcal{E}(k_1)}{k_1} B_I \quad \frac{\mathcal{E}(k_2)}{k_2} A_{II} \quad i(A_I \quad B_I)g \quad 0. \tag{A.5}$$

Hence,

$$(A_I \quad B_I)\frac{\mathcal{E}(k_1)}{k_1} \quad (A_{II} \quad B_{II})\frac{\mathcal{E}(k_2)}{k_2} \quad 2i(A_I \quad B_I)g. \tag{A.6}$$

This is the second connection formula. It is, in fact, exactly of the same form as that obtained in the case of the quadratic energy spectrum since then $\mathcal{E}(k)/\quad k \quad k\hbar^2/m$.

Appendix B

The presentation of the physical significance of the quantities $t(k_1, k_2)$ and $r(k_1, k_2)$ can be started with the derivation of the continuity equation for the wave function obeying the Schrödinger-Wannier wave equation and with the identification of the incident, transmitted and reflected flux in the probability current density.

If the function $\quad (x;t)$ satisfies the non-stationary Schrödinger-Wannier wave equation,

$$\mathcal{E} \quad i\frac{}{x} \quad U(x) \quad i\hbar\frac{}{t} \quad (x;t) \quad 0, \tag{B.1}$$

then the probability-density function, $\quad x;t \quad {}^* \; x;t \quad x;t$, will evolve according to the equation

$$\frac{x;t}{t} \quad {}^* \, x;t \; \mathcal{E} \quad i\frac{}{x} \quad x;t \qquad x;t \; \mathcal{E} \quad i\frac{}{x} \quad x;t \;. \tag{B.2}$$

To arrange the right-hand side of this equation it is appropriate to represent the wave function by its Fourier integral, $\quad x;t \qquad f \quad ;t \; e^{i \; x} d \quad / \, 2$. Then, previous equation acquires the usual form of the continuity equation

$$\frac{(x;t)}{t} \quad \frac{j(x;t)}{t}, \tag{B.3}$$

where the probability-current-density function is given by

$$j(x;t) \qquad \frac{d}{} \quad \frac{d}{} \quad \frac{\mathcal{E}(\;) \quad \mathcal{E}(\;)}{(\qquad)\hbar} \; f(\;;t) f^*(\;;t) e^{i} \qquad x. \tag{B.4}$$

For stationary states of the energy E, assuming that the potential-energy function $U(x)$ is independent of time t, one has $\quad x;t \qquad e^{\;iEt/\hbar}$ and $f(\;;t) \quad f(\;)e^{\;iEt/\hbar}$, so that the explicit time dependence of the functions $\quad x;t$ and $j(x;t)$ disappears and thus the Eq. (B. 3) reduces to $j(x)/\quad x \quad 0$ with

$$j(x) \quad \frac{d}{} \quad \frac{d}{} \quad \frac{\mathcal{E}(\ )\quad \mathcal{E}(\ )}{(\qquad)\hbar} \; f(\ ) f^{*}(\ ) e^{i \qquad x} . \qquad \text{(B.5)}$$

For the wave function in the form of plane waves (formula (A1)), the integration is straightforward, though tedious. Performing the integration one obtains

$$j(x) \quad \{1 \qquad (x)\}\{A_I^* A_I \quad B_I^* B_I\}\frac{\mathcal{E}(k_1)}{\hbar \ k_1} \qquad (x)\{A_{II}^* A_{II} \quad B_{II}^* B_{II}\}\frac{\mathcal{E}(k_2)}{\hbar \ k_2}$$

$$\{1 \qquad (x)\}\, j_I(k_1,k_2) \qquad (x)\, j_{II}(k_1,k_2) . \qquad \text{(B.6)}$$

Using Eqs. (4a) and (4b), one can easily show that the probability-current-density function is continuous at the point $x \quad 0$, because

$$j_I(k_1,k_2) \quad \{A_I^* A_I \quad B_I^* B_I\}\frac{\mathcal{E}(k_1)}{\hbar \ k_1}$$

$$\{1 \quad r^*(k_1,k_2) r(k_1,k_2)\} A_I^* A_I \frac{\hbar \mathcal{K}(k_1)}{m} \quad t^*(k_1,k_2) t(k_1,k_2) B_{II}^* B_{II} \frac{\hbar \mathcal{K}(k_2)}{m}$$

$$\{r^*(k_1,k_2) t(k_1,k_2) A_I^* B_{II} \quad r(k_1,k_2) t^*(k_1,k_2) B_{II}^* A_I\}\frac{\hbar\sqrt{\mathcal{K}(k_1)\mathcal{K}(k_2)}}{m} \qquad \text{(B.7a)}$$

and

$$j_{II}(k_1,k_2) \quad \{A_{II}^* A_{II} \quad B_{II}^* B_{II}\}\frac{\mathcal{E}(k_2)}{\hbar \ k_2}$$

$$t^*(k_1,k_2) t(k_1,k_2) A_I^* A_I \frac{\hbar \mathcal{K}(k_1)}{m} \quad \{1 \quad r^*(k_1,k_2) r(k_1,k_2)\} B_{II}^* B_{II} \frac{\hbar \mathcal{K}(k_2)}{m}$$

$$\{r^*(k_1,k_2) t(k_1,k_2) A_I^* B_{II} \quad r(k_1,k_2) t^*(k_1,k_2) B_{II}^* A_I\}\frac{\hbar\sqrt{\mathcal{K}(k_1)\mathcal{K}(k_2)}}{m} . \qquad \text{(B.7b)}$$

Thus, the probability-current-density function is indeed constant for the wave function in the form of plane waves.

If $B_{II} \quad 0$, the wave function $\quad x \ $, Eq. (5), represents a particle that is incident on the biased delta-barrier from $\quad$ with the wave function $A_I e^{\ i\ k_1 \ \ i0\ x}$. The interaction with the biased delta-barrier produces a reflected wave $r(k_1,k_2)A_I e^{\ i\ k_1 \ \ i0\ x}$, which escapes to $\quad$, and a transmitted wave $\sqrt{\mathcal{K}(k_1)/\,\mathcal{K}(k_2)}\, t(k_1,k_2)A_I e^{\ i\ k_2 \ \ i0\ x}$, which moves off to $\quad$. It is seen from Eq. (B.7) that the incident flux, the reflected flux and the transmitted flux are, respectively, $A_I^* A_I \hbar\mathcal{K}(k_1)/m$, $r^*(k_1,k_2)r(k_1,k_2)A_I^* A_I \hbar\mathcal{K}(k_1)/m$ and $t^*(k_1,k_2)t(k_1,k_2)A_I^* A_I \hbar\mathcal{K}(k_1)/m$. Thus, the quantities $t(k_1,k_2)$ and $r(k_1,k_2)$ are, respectively, the transmission and reflection amplitude. The transmission and reflection coefficient are given by the relations $T(k_1,k_2) \quad t^*(k_1,k_2)t(k_1,k_2)$ and $R(k_1,k_2) \quad r^*(k_1,k_2)r(k_1,k_2)$, respectively.

If $A_I \quad 0$, the wave function $\quad (x)$ can be interpreted in a similar fashion. It represents a particle that is incident on the biased delta-barrier from $\quad$.

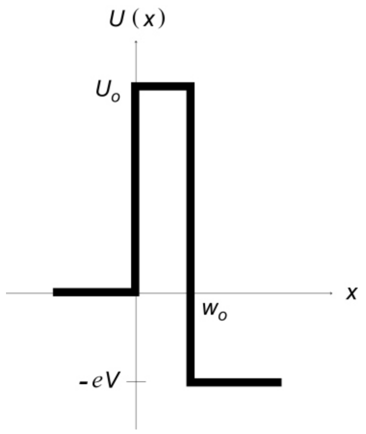

Fig. 1. Schematic diagram of the corresponding electron potential energy in a biased rectangular barrier.

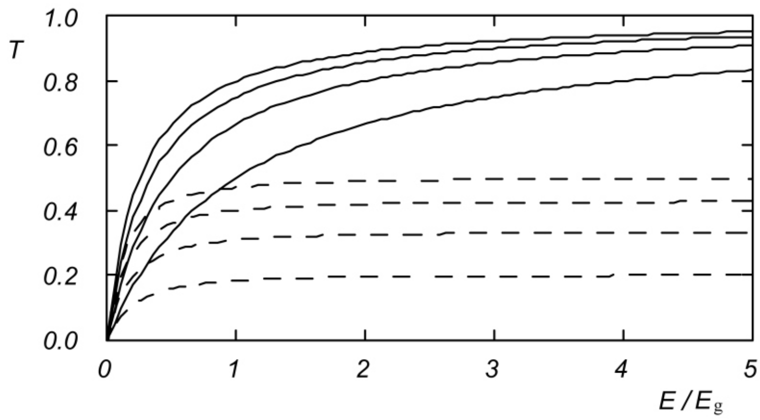

Fig. 2. Plot of the transmission coefficient for the biased delta-barrier versus the energy variable.

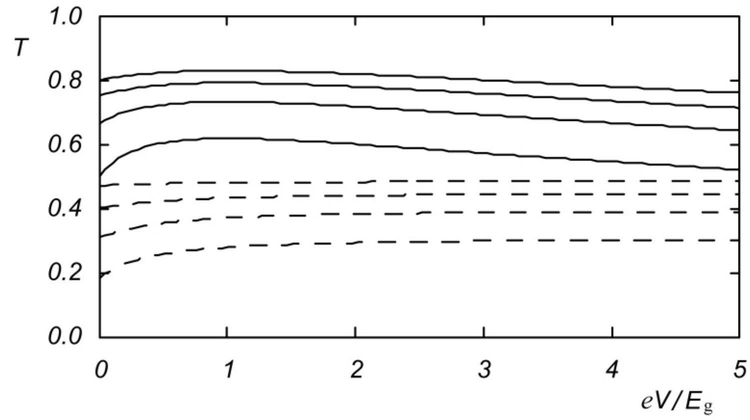

Fig. 3. Plot of the transmission coefficient for the biased delta-barrier versus the voltage variable.

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