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On Transmissions through a Symmetrical Triple Delta-Barrier

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Abstract: The solution of the Schödinger equation is examined for the energy-potential function that equals the sum of the three delta-functions of the equal strength. The transfer matrix method is employed to derive an analytical formula of the transmission coefficient for the symmetrical triple delta-barrier. The transmission coefficient is shown to exhibit absolute maxima and two kinds of relative minima. The maximum and minimum conditions are obtained. Some attributes of the transmission coefficient are established.
Keywords: Schödinger wave equation, Dirac delta-function, rectangular barrier, transmission coefficient.
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1. Introduction

This paper presents a simple model of conduction electrons in a sandwich structure A-B-A-B-A-B-A, where B is a very narrow single crystalline layer embedded in (being lattice-matched on both its sides with) a bulk crystal A. Neglecting space charge effects and adopting the Wannier one band approximation [1], one can diagrammatically represent the sandwich structure A-B-A-B-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 three narrow layers B embedded in the bulk crystal A are modelled by the one-dimensional rectangular barriers. In the case of the very narrow layer B, one can formally let the width of the rectangular barrier tend to the zero and, simultaneously, its height tends to the infinity whilst keeping their product to be constant. Then, the potential-energy function representing the rectangular barrier in Fig. 1 becomes the delta-function whose strength g is equal to the product of the width and the height of the original rectangular barrier. Though the delta-function is a very simplified form of the original potential-energy function, it still enables one to get a proper insight into the transmissions through the narrow and high barrier structures [2 6]. Therefore, it must be also interesting for one to find the analytical solution of the transmission problem through the symmetrical triple delta-barrier. The transmissions through the triple rectangular barrier were studied in [7 11]. However, the transmission coefficient for the triple rectangular barrier appears to be very intricate. A very simple expression for the transmission coefficient is presented in this paper.

The organisation of this paper is as follows. In the next section, the Schrödinger wave equation is employed to obtain the wave function for the potential-energy function, which corresponds to the limiting case of the rectangular triple barrier structure shown in Fig. 1.

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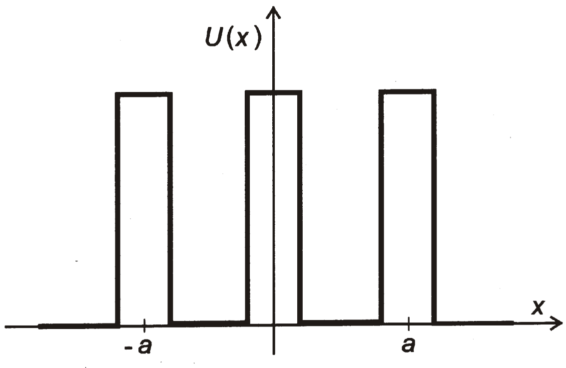

Fig. 1. Schematic diagram of the electron potential energy in the triple barrier structure.

In the third section, the wave function is used to derive an analytical formula of the transmission coefficient for the symmetrical triple delta-barrier. Some attributes of the transmission coefficient are also presented in the third section. The fourth section is devoted to discussion.

2. Solution of the Schrödinger equation

The one-dimensional stationary Schrödinger wave equation,

$$\frac{\hbar^2 \quad ^2}{m \quad x} \quad U(x) \quad E \qquad (x) \quad 0,$$

is solved for the potential-energy function

$$U(x) \quad g \ (x \quad a) \quad g \ (x) \quad g \ (x \quad a).$$

Here x represents the spatial variable, E is the energy of a particle (a conduction electron), m is its effective mass, $\hbar$ is the reduced Planck constant, (x) is the Dirac delta-function, g is its strength (a positive value of the strength corresponds to the barrier, while a negative value would correspond to the well), $2a$ is the width ofthe triple delta-barrier.

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.

$$(x) \quad \{1 \qquad (x \quad a)\} \ _I(x) \quad \{ \ (x \quad a) \qquad (x)\} \ _{II}(x)$$

$$\{ \ (x) \qquad (x \quad a)\} \ _{III}(x) \qquad (x \quad a) \ _{IV}(x)$$

$$\{1 \qquad (x \quad a)\} \ A_I \mathrm{e}^{\ ikx} \quad B_I \mathrm{e}^{\ ikx} \qquad \{ \ (x \quad a) \qquad (x)\} \ A_{II} \mathrm{e}^{\ ikx} \quad B_{II} \mathrm{e}^{\ ikx}$$

$$\{ \ (x) \qquad (x \quad a)\} \ A_{III} \mathrm{e}^{\ ikx} \quad B_{III} \mathrm{e}^{\ ikx} \qquad \{ \ (x \quad a)\} \ A_{IV} \mathrm{e}^{\ ikx} \quad B_{IV} \mathrm{e}^{\ ikx} \quad .$$

Here (x) is the Heaviside step function ($(x) \quad 0$ if $x \quad 0$ and $(x) \quad 1$ if $x \quad 0$). The subscript I refers to the spatial region ($\quad , \ a)$ that is on the left-hand side of the triple delta-barrier, the subscript II to the spatial region (a,0), the subscript III to the spatial region $(0, a)$ and the subscript IV to the spatial region $(a, \quad)$ that is on the righthand side of the triple delta-barrier. The symbols $A_{\rm I}, B_{\rm I}; A_{\rm II}, B_{\rm II}; A_{\rm III}, B_{\rm III}$ and A_{IV}, B_{IV} represent the amplitudes of those two plane waves in these four spatial regions. The positive wave number k is introduced by the relation $E \quad \hbar^2 k^2 / 2m$.

Subjecting the wave function $\quad (x)$ to the connection formulas at the points $x_1 \quad a$, $x_2 \quad 0$ and $x_3 \quad a$ (Appendix), one finally obtains that the wave function on the lefthand side of the triple delta-barrier can be written in the form

$$_I(x) \quad A_I \mathrm{e}^{\quad ikx} \quad \{r(k)A_I \quad t(k)B_{IV}\}\mathrm{e}^{\quad ikx}$$

and on the right-hand side in the form

$$_{IV}(x) \quad t(k)A_I \quad \frac{r^*(k)t(k)}{t^*(k)} B_{IV} \quad \mathrm{e}^{\quad ikx} \quad B_{IV}\mathrm{e}^{\quad ikx} \; .$$

Here the quantities $t(k)$ and $r(k)$ are, respectively, given by the relations

$$t(k) \quad \frac{8k^3 \mathrm{e}^{\quad 2ika}}{(2k \quad i \quad)^3 \mathrm{e}^{\quad 2ika} \quad 4k \quad ^2 \quad 2i \quad ^3 \quad (2k \quad i \quad) \quad ^2 \mathrm{e}^{\quad 2ika}} \, ,$$

$$\frac{r(k)}{t(k)} \quad \frac{i}{8k^3} \quad (2k \quad i \quad)^2 \mathrm{e}^{\quad 2ika} \quad 2 \quad ^2 \quad 4k^2 \quad (2k \quad i \quad)^2 \mathrm{e}^{\quad 2ika}$$

and $\quad 2mg / \hbar^2$.

Evidently, $A_{\rm I}$ is the amplitude of the plane wave impinging upon the triple delta-barrier from the left-hand side, $r(k)A_{\rm I}$ is the amplitude of its reflected wave and $t(k)A_{\rm I}$ is the amplitude of its transmitted wave; $B_{\rm IV}$ is the amplitude of the plane wave impinging upon the triple delta-barrier from the right-hand side, $\quad r^*(k)t(k)B_{\rm IV} \; / \, t^*(k)$ is the amplitude of its reflected wave and $t(k)B_{\rm IV}$ is the amplitude of its transmitted wave. The quantities $t(k)$ and $r(k)$, respectively, represent the transmission and reflection amplitude (actually, $r(k)$ is the reflection amplitude from the left and $\quad r^*(k)t(k) / t^*(k)$ is the reflection amplitude from the right, they differ only in a phase). The transmission coefficient is defined by the relation $T(k) \quad t^*(k)t(k)$. The reflection coefficient can be obtained from the well-known relation, namely $R(k) \quad r^*(k)r(k) \quad 1 \quad T(k)$.

3. Transmission coefficient

After straightforward algebra one can derive a formula of the transmission coefficient for the symmetrical triple delta-barrier,

$$T(k) \quad \frac{4k^6}{4k^6 \quad ^2 \quad (2k\cos(ka) \quad \sin(ka))^2 \quad k^2 \quad ^2} \, .$$

In the limit $a \quad 0$, the three delta-barriers join into a single delta-barrier,

$$\lim_{a \quad 0} T(k) \quad \frac{4k^2}{4k^2 \quad (3 \quad)^2} \quad T_0(k) \, ,$$

where $T_0(k)$ is the transmission coefficient for the single delta-barrier of the strength $3g$.

In the limit $k \quad 0$, one gets

$$\lim_{k \quad 0} T(k) \quad \lim_{k \quad 0} \frac{4k^2}{4k^2 \quad {}^2\{(2 \quad a)^2 \quad 1\}^2} .$$

Thus, $\lim_{k \quad 0} T(k) \quad 0$, if $(2 \quad a)^2 \quad 1$, and $\lim_{k \quad 0} T(k) \quad 1$, if $a \quad 1$ or if $a \quad 3$. Consequently, the transmission coefficient for the symmetrical triple delta-barrier has its absolute minimum at the value $k \quad 0$. Only the transmission coefficient for the symmetrical triple delta-well of the strength $g \quad \hbar^2 / 2ma$ or the strength $g \quad 3\hbar^2 / 2ma$ would have its absolute maximum at the value $k \quad 0$.

Evidently, the transmission coefficient $T(k)$ has an infinite number of absolute maxima, $T_{\max}(k) \quad 1$. They take place at all the positive values of the wave number k that are determined by the maximum (resonance) condition,

$$(2k\cos(ka) \quad \sin(ka))^2 \quad k^2 \quad 0 .$$

This equation immediately yields the asymptotic value of the abscissa of the nth maximum of the function $T(k)$. It tends either to the value $ka \quad / 3 \quad (n \quad 1) \quad / 2$, where $n \quad 1, 3, 5, \ldots$, or to the value $ka \quad 2 \quad / 3 \quad (n \quad 2) \quad / 2$, where $n \quad 2, 4, 6, \ldots$. To find minima of the transmission coefficient $T(k)$, one has to differentiate the function $T(k)$ and to equate its first derivative to the zero. Thus,

$$\frac{dT(k)}{dk} \quad \frac{a \quad {}^2 T^2(k)}{k^6} \{(2k\cos(ka) \quad \sin(ka))^2 \quad k^2\}$$

$$(2k\cos(ka) \quad \sin(ka)(2k\sin(ka) \quad \cos(ka)) .$$

To obtain this very simple expression for the first derivative, one has to keep only the term that is proportional to the width of the triple delta-barrier. Evidently, this approximation is justifiable only in the case of the transmissions through the wide triple delta-barrier, i.e. when $1 \quad ka$.

So, the relative minima of the transmission coefficient $T(k)$ should approximately occur at the positive values of the wave number k that obey one of the minimum conditions,

$$2k\cos(ka) \quad \sin(ka) \quad 0 , \qquad 2k\sin(ka) \quad \cos(ka) \quad 0 .$$

When the first minimum condition is satisfied the transmission coefficient $T(k)$ can be arranged into the form

$$\frac{4k^2}{4k^2 \quad {}^2} \quad T_{s\min}(k) .$$

It is easy to show that $T_0(k) \quad T_{s\min}(k)$, i.e. the transmission coefficient for the symmetrical triple delta-barrier in its shallow minima (Figs. 2a and 2b) is greater than the transmission coefficient for the single delta-barrier of the threefold strength. One also obtain from the minimum condition that the abscissa of the nth shallow minimum of the function $T(k)$ tends to the value $ka \quad / 2 \quad (n \quad 1)$, where $n \quad 1, 2, 3, \ldots$.

When the second minimum condition is satisfied the transmission coefficient $T(k)$ can be arranged into the form

$$\frac{4k^6}{4k^6 \quad {}^2(3k^2 \quad {}^2)^2} \quad T_{d\min}(k) .$$

It is easy to show that $T_{d\min}(k) \quad T_0(k)$, i.e. the transmission coefficient for the symmetrical triple delta-barrier in its deep minima (Figs. 2a and 2b) is smaller than the trans-

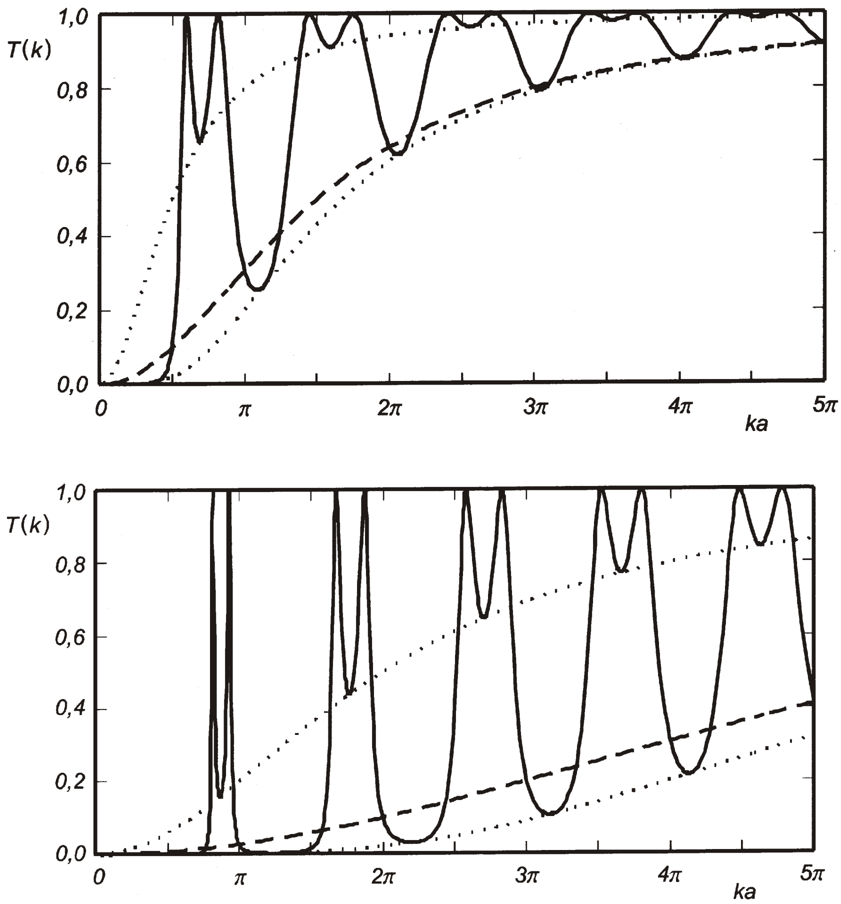

Fig. 2. Plot of the transmission coefficients. a) *a* , b) *a* 4 .

mission coefficient for the single delta-barrier of the threefold strength. The abscissa of the *n*th deep minimum of the function $T(k)$ approaches the value $ka \quad n$, where $n \quad 1, 2, 3, \ldots$.

It should be recalled that the resonant tunnelling, i.e. an ideal transmission (without a reflection) through a multibarrier structure is a result of the constructive interference between the waves just transmitting through the single barrier and those being reflected off the next barriers ([12] and references cited therein). The stronger the barriers are, the smaller the intensity of the transmitted waves is and the more pronounced the interference becomes. It has been also shown that the transmission coefficient for the symmetrical triple delta-barrier in its deep minima is smaller than the transmission coefficient for the single delta-barrier arisen by joining the three delta-barriers of the triple delta-barrier. It follows; there also exists some destructive interference between the waves just transmitting through the single barrier and those being reflected off the next barriers.

In Figs. 2a and 2b, the transmission coefficients $T(k)$, $T_{s\min}(k)$, $T_0(k)$, and $T_{d\min}(k)$ are drawn for the two values of the dimensionless parameter $\quad a$, namely in Fig. 2a for $\quad a$ and in Fig. 2b for $\quad a \quad 4$. In both the figures, the full curves depict the transmission coefficient $T(k)$. These two full curves demonstrate the existence of absolute maxima and two kinds of relative minima in the transmissions through the symmetrical triple delta-barrier. As expected, the depth of minima becomes larger as the strength of the delta-barriers increases. The dashed curves show the transmission coefficient $T_0(k)$ and the dotted curves the transmission coefficients $T_{s\min}(k)$ and $T_{d\min}(k)$. These curves demonstrate the validity of the inequality $T_{d\min}(k) \quad T_0(k) \quad T_{s\min}(k)$. It is also seen from Figs. 2a and 2b that the transmission coefficients $T_{s\min}(k)$ and $T_{d\min}(k)$ excellently trace the shallow and deep minima of the transmission coefficient $T(k)$, respectively. This confirms the appropriateness of the approximation made in the derivation of the minimum conditions. Further, it is seen that the abscissas of maxima and minima approach their calculated asymptotic values. Furthermore, one easily derives that both the transmission coefficients $T(k)$ and $T_0(k)$ have the same value when one of the following three conditions is satisfied: $\sin(ka) \quad 0$, $2k\sin(ka/2) \quad \cos(ka/2) \quad 0$, $2k\cos(ka/2) \quad \sin(ka/2) \quad 0$. Thus, the dashed curve intersects the full curve at the points with the abscissas $ka \quad n$, where $n \quad 1, 2, 3, \ldots$, as well as at the points, whose abscissas also tend to the values $ka \quad n$. Therefore, in the region of high wave numbers, the dashed curve finally touches the full curve in its deep minima. Evidently, all the transmission coefficients gradually approach the unity when the wave number tends to the infinity. This asymptotic behaviour of the transmission coefficients can easily be verified analytically as well, $\lim_{k} T(k) \quad \lim_{k} T_{d\min}(k) \quad \lim_{k} T_0(k) \quad \lim_{k} T_{s\min}(k) \quad 1$.

These are the characteristics proper to the transmissions through the symmetrical triple delta-barrier.

4. Discussion

There has been a rising interest in the study of the transmissions through multibarrier structures. Despite of a great deal of theoretical and experimental work on them ([12, 13] and references cited therein), many of their properties have not been understood yet and the need for the models of the multibarrier structures has not decreased. Such an archetype of the triple barrier structure has been presented in this paper. As far as the author knows, calculations on the triple delta-barrier has not been carried, out yet, though the transmission coefficient for the double delta-barrier is available e.g. in [3 6]. The treatment of the triple delta-barrier shows that there exist two kinds of relative minima of the transmission coefficient. They should manifest themselves in the largeness of the peak-to-valley ratios of the current-voltage characteristics.

Appendix

Three connection formulas are to be obtained from the continuity condition for the wave function $\quad (x)$ at the points $x_1 \quad a$, $x_2 \quad 0$ and $x_3 \quad a$, namely $(\ a \quad 0) \quad (\ a \quad 0)$, $(0) \quad (\ 0)$ and $(a \quad 0) \quad (a \quad 0)$. Thus,

$$A_{II}\mathrm{e}^{\ \ ika} \quad B_{II}\mathrm{e}^{\ ika} \quad A_I\mathrm{e}^{\ \ ika} \quad B_I\mathrm{e}^{\ \ ika},$$

$$A_{III} \quad B_{III} \quad A_{II} \quad B_{II},$$

$$A_{IV}\mathrm{e}^{\ \ ika} \quad B_{IV}\mathrm{e}^{\ ika} \quad A_{III}\mathrm{e}^{\ \ ika} \quad B_{III}\mathrm{e}^{\ \ ika}.$$

A formal integration of the Schrödinger equation around the points $x_1 \quad a, x_2 \quad 0$ and $x_2 \quad a$ leads to the relations expressing the discontinuity of the first derivative of the wave function at these points [2 6], i.e. $(\ a \quad 0) \quad (\ a \quad 0) \quad 2mg\ (\ a)/\hbar^2$, $(\ 0) \quad (\ 0) \quad 2mg\ (0)/\hbar^2$ and $(a \quad 0) \quad (a \quad 0) \quad 2mg\ (a)/\hbar^2$, where $(x) \quad \mathrm{d}\ (x)/\mathrm{d}x$. These three discontinuity relations also yield three other connection formulas,

$$ik(A_{II}\mathrm{e}^{\ \ ika} \quad B_{II}\mathrm{e}^{\ ika}) \ \ ik(A_I\mathrm{e}^{\ \ ika} \quad B_I\mathrm{e}^{\ ika}) \quad (A_I\mathrm{e}^{\ \ ika} \quad B_I\mathrm{e}^{\ ika}),$$

$$ik(A_{III} \quad B_{III}) \ \ ik(A_{II} \quad B_{II}) \quad (A_{II} \quad B_{II}),$$

$$ik(A_{IV}\mathrm{e}^{\ \ ika} \quad B_{IV}\mathrm{e}^{\ ika}) \ \ ik(A_{III}\mathrm{e}^{\ \ ika} \quad B_{III}\mathrm{e}^{\ ika}) \quad (A_{III}\mathrm{e}^{\ \ ika} \quad B_{III}\mathrm{e}^{\ ika}),$$

where $\quad 2mg/\hbar^2$. The connection formulas can be written in the form of matrices,

$$\begin{matrix} A_{II} \\ B_{II} \end{matrix} \quad M(\mathrm{II,I}) \begin{matrix} A_I \\ B_I \end{matrix}, \quad \begin{matrix} A_{III} \\ B_{III} \end{matrix} \quad M(\mathrm{III,II}) \begin{matrix} A_{II} \\ B_{II} \end{matrix}, \quad \begin{matrix} A_{IV} \\ B_{IV} \end{matrix} \quad M(\mathrm{IV,III}) \begin{matrix} A_{III} \\ B_{III} \end{matrix}.$$

The elements of the transfer matrices M(II, I), M(III, II) and M(IV, III) are given by

$$M_{11}(\mathrm{II,I}) \quad M_{22}^*(\mathrm{II,I}) \quad M_{11}(\mathrm{III,II}) \quad M_{22}^*(\mathrm{III,II}) \quad M_{11}(IV,\mathrm{III}) \quad M_{22}^*(\mathrm{IV,III}) \quad \frac{2k \quad i}{2k},$$

$$M_{12}(\mathrm{II,I}) \quad M_{21}^*(\mathrm{II,I}) \quad \frac{i}{2k}\mathrm{e}^{\ 2ika}, \quad M_{12}(\mathrm{III,II}) \quad M_{21}^*(\mathrm{III,II}) \quad \frac{i}{2k},$$

$$M_{12}(\mathrm{IV,III}) \quad M_{21}^*(\mathrm{IV,III}) \quad \frac{i}{2k}\mathrm{e}^{\ 2ika}.$$

It is easy to show that det M(II, I) = det M(III, II) = det M(IV, III) = 1.

The three consecutive transfers are to be joined into one,

$$\begin{matrix} A_{IV} \\ B_{IV} \end{matrix} \quad M(\mathrm{IV,III})M(\mathrm{III,II})M(\mathrm{II,I}) \begin{matrix} A_I \\ B_I \end{matrix} \quad M(\mathrm{IV,I}) \begin{matrix} A_I \\ B_I \end{matrix}, \ \text{ where}$$

$$M_{11}(\mathrm{IV,I}) \quad M_{22}^*(\mathrm{IV,I}) \quad \frac{1}{t^*(k)}$$

$$\frac{\mathrm{e}^{\ 2ika}}{8k^3}\{(2k \quad i\ )^3\mathrm{e}^{\ 2ika} \quad 4k^{\ 2} \quad 2i^{\ 3} \quad (2k \quad i\ )^{\ 2}\mathrm{e}^{\ 2ika}\},$$

$$M_{12}(\mathrm{IV,I}) \quad M_{21}^*(\mathrm{IV,I}) \quad \frac{r^*(k)}{t^*(k)}$$

$$\frac{i}{8k^3}\{(2k \quad i\ )^2\mathrm{e}^{\ 2ika} \quad 2^{\ 2} \quad 4k^2 \quad (2k \quad i\ )\mathrm{e}^{\ 2ika}\}.$$

It is easy to obtain that

$$\det M(\mathrm{IV},\mathrm{I}) \quad \frac{1 \quad r(k)r^{*}(k)}{t(k)t^{*}(k)} \quad \det M(\mathrm{IV},\mathrm{III})\det M(\mathrm{III},\mathrm{II})\det M(\mathrm{II},\mathrm{I}) \quad 1.$$

The two new-introduced quantities $t(k)$ and $r(k)$ enable one to express the relation between the amplitudes of the first and fourth spatial region in the simple form,

$$B_{\mathrm{I}} \quad r(k)A_{\mathrm{I}} \quad t(k)B_{\mathrm{IV}}\,, \quad A_{\mathrm{IV}} \quad t(k)A_{\mathrm{I}} \quad \frac{r^{*}(k)t(k)}{t^{*}(k)}B_{\mathrm{IV}}\,.$$

These expressions for the amplitudes B_{I} and A_{IV} are used to establish the form of the wave function (x) on the left-hand and on the right-hand side of the triple delta-barrier.

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