TUNNELLING THROUGH COMBINED POTENTIAL STRUCTURES I. GENERAL CALCULATIONS

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The procedure for calculating the relations between two arbitrary amplitudes of wave functions in different regions of the system potential barrier-well-barrier is evaluated. The knowledge of these relations enables to calculate the probabilities of finding the particle in these regions, and thus the transmission probability, too. The procedure is carried out for step-like potentials with arbitrary heights and widths. These general results are then applied to symmetric systems (equal barriers on both sides of the potential well). Especially "shallow" and "deep" wells are considered. In both cases interesting results concerning the resonance tunnelling effects (ideal transmission of particles with special energies) are obtained.

The intervals are determined, in which the transmission coefficient D has a maximum ($D = 1$) for particle energies smaller than the height of the potential barrier.

For well depth equal to the barrier height conditions are studied under which the system is ideally permeable for particles with infinitesimally small energies.

ТУННЕЛИРОВАНИЕ ЧЕРЕЗ КОМБИНИРОВАННЫХ ПОТЕНЦИАЛНЫЕ СТРУКТУРЫ I. ОБЩИЕ ВЫЧИСЛЕНИЯ

В работе рассматривается метод вычисления соотношения между двумя произвольными амплитудами волновой функции в разных областях системы барьер–яма–барьер. Знание этих соотношений позволяет вычислить вероятности нахождения частицы в этих областях и в то же самое время вероятность прохождения частиц. Этот метод применен к скачкообразным потенциалам произвольной высоты и ширины. Полученные общие результаты затем применены к симметричной системе (одинаковые барьеры с обеих сторон ямы). В частности, рассмотрены случаи «мелких» и «глубоких» ям. В обоих частных случаях получаются интересные результаты, связанные с резонансным туннельным эффектом (идеальное прохождение частиц с определенной энергией).

Определены также области, в которых для частиц с энергией меньше высоты потенциального барьера в коэффициенте прохождения D появляется максимум ($D = 1$).

В случае, когда глубина ямы равняется высоте барьера, определены условия, при которых для частиц с бесконечно малыми энергиями система идеально прозрачна.

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I. INTRODUCTION

The possibility of particle transmission through regions in which the potential is higher than the kinetic energy of the particles (tunnelling) is one of the most interesting quantum phenomena and its experimental verification belongs to the most efficient proofs of the quantum mechanics — as no classic analogy with this phenomenon is known. Meanwhile, the non-zero amplitude of the bound state wave function of a potential hole beyond the hole expresses the same phenomenon (unless the height of the potential walls is infinite — the particle in the hole can be localized only in this case).

In addition to some already "classical" systems (e.g. the α-decay of atomic nuclei), the existence of the tunnel effect was shown in solids by measuring the tunnelling current (mainly in systems metal–insulator–metal, further in systems with semiconductors, later also with superconductors), as well as in the field emission of electrons from solid surfaces.

For M–I–M systems, the linear voltage-current dependence was clearly proved, as calculated from the theory with constant electronic density of states near the Fermi energy. The situation is much more complicated for systems with semiconductors (e.g. $p-n$ junctions), due to more complicated forms of the density of states and due to basic changes of the potentials with the electric field (the well-known differences in the forward and reverse direction, etc.).

In the last two decades, the experimental possibilities for the tunnelling research in solids have enormously increased. Together with the theoretical progress in this field, the results of this research have helped us considerably to extend our knowledge of the electron states in solids.

The method of tunnelling hamiltonian [1, 2] represents the basic microscopic approach in the theory of tunnelling in solids. However, this method is too complicated for application in special systems, as the microscopic calculations are very complicated for real forms of the barrier potential (or, if one wants, e.g., to obtain the dependence of the tunnelling characteristics on the form of the potential). Hence, the use of different approximations is necessary in practical calculations. One of these approximations, the one-dimensionality of the system considered, is the most frequently used. It has been very well substantiated in many different cases, so, e.g., in the tunnelling of normal and superconducting electrons through thin films, the field emission of electrons from surfaces, etc.

The most applicable theory with some corresponding experimental results was worked out for the study of normal and superconducting electron tunnelling through thin dielectric layers [1, 2], as well as for the spectroscopy of gas atoms on solid surfaces [3]. In the latter example, a procedure for calculating the amplitude of the electron vawe functions was elaborated by combining the method of wave function overlapping (in cases when the relative tunnelling probabilities are

needed) and the WKB method (for calculating the absolute values of the tunnelling characteristics). The form of the corresponding potential was no more a simple example of the potential barrier.

The calculations of tunnelling characteristics with complicated potentials have been carried out only in the last two decades [4], although the existence of the resonance tunnelling (i.e. maxima in the tunnelling probabilities) has been known for a long time [5]. The maxima in the tunnelling characteristics — as the result of these resonances — have experimentally been well established [4].

In addition to the "classic" example of the Kronig-Penney model, where the resonance tunnelling causes the appearance of filled (in some cases ideally conducting) and forbidden bands of the electron states, tunnelling through complicated potentials can be important in different cases, e.g. semiconductors [6] and even in biological systems (transmission of ions and molecules through the bilipides of membranes) [7]. It is therefore somewhat surprising to see that the existence of the resonance tunnelling (the enhanced tunnelling probability of the barriers with a potential well in between, compared with the barrier alone) has been neglected in those cases where the form of the potential is unambiguously of the form barrier–well–barrier (BWB) [6, 8].

So far mainly [9, 10] double potential barriers with different mutual distances have been studied.

However, a potential well between the barriers (well relatively to the potential far from the system BWB) can substantially change the transmission probability and other tunnelling parameters [11], mainly with regard to the fact that stable eigenstates (bound states) of the well exists (there does not exist any bound state for the double barrier system without the well!).

The study of those combined potential structures can be important in solid state physics (ionized impurities in solids), but also in biological systems, in the theory of α-decay, etc.

There are only a few papers dealing with the influence of the form of the potential barrier on the tunnelling characteristics [9, 12—15]. However, all these papers confirm the result that the "finenesses" in the potential form are not so important as one would expect at first sight.

The same statement is true for the combined potentials, as we shall show in another paper: the results remain nearly the same not only qualitatively, but even quantitatively.

Since in in some cases the motion of electrons in such complicated potential structures is assumed to be the fundamental mechanism of the electric transport (e.g. in fine-grained and disordered materials [8, 16]) and because the experimental facilities and the interest in tunnelling phenomena have enormously increased in the last years [8, 17], we study some phenomena connected with the tunnelling of electrons through double barriers with a well between them.

In the present paper we evaluate the procedure for calculating the relations between the wave function amplitudes in different regions (outside the barrier, in the barriers, in the well) and thus the probabilities of finding the particle in these regions. In the next paper [18], these results will be applied to some special problems in solid state physics.

II. ASYMMETRIC DOUBLE BARRIER

The system barrier–well–barrier (Fig. 1) can arise by various mechanisms, e.g. as the result of space charge near the contacts of different materials [6]. In many cases

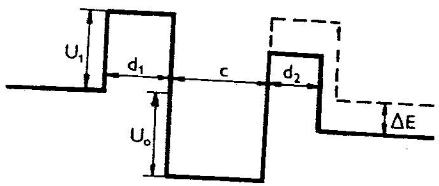

Fig. 1. The parameters of the system barrier–well–barrier.

the system with $U_0<0$ will be more frequently realistic, as e.g. for the double Schottky barrier [6]. Generally, the potential behind the well can be different from that in front of it (for example due to applied electric fields).

Throughout the paper we confine ourselves to one-dimensional calculations. Some remarks about three-dimensional effects will be given later [18]. The volume is then divided into five regions and we calculate the transmission probability for arbitrary values of the barrier and well heights and widths.

We therefore take the potential of the following form:

$$\begin{array}{llll} \text{(I)} & U=0 & \text{for} & x<0, \\ \text{(II)} & U=U_1 & \text{for} & 0<x<d_1, \\ \text{(III)} & U=U_0 & \text{for} & d_1<x<c+d_1, \\ \text{(IV)} & U=U_2 & \text{for} & c+d_1<x<c+d_1+d_2, \\ \text{(V)} & U=\Delta E & \text{for} & x<c+d_1+d_2. \end{array} \tag{1}$$

The solutions of the Schrödinger equation in these regions are

$$\begin{aligned} \Psi_I &= A_1 e^{ik_1x} + B_1 e^{-ik_1x} \\ \Psi_{II} &= A_2 e^{ik_2x} + B_2 e^{-ik_2x} \\ \Psi_{III} &= A_3 e^{ik_3x} + B_3 e^{-ik_3x} \\ \Psi_{IV} &= A_4 e^{ik_4x} + B_4 e^{-ik_4x} \\ \Psi_V &= A_5 e^{ik_5x} + B_5 e^{-ik_5x} \end{aligned} \tag{2}$$

where

$$k_1=\frac{\sqrt{2mE}}{\hbar}, \quad k_2=\frac{\sqrt{2m(E-U_1)}}{\hbar}, \quad k_3=\frac{\sqrt{2m(E-U_0)}}{\hbar},$$
$$k_4=\frac{\sqrt{2m(E-U_2)}}{\hbar}, \quad k_5=\frac{\sqrt{2m(E+\Delta E)}}{\hbar}. \tag{3}$$

For calculating the transmission probability

$$D=\left|\frac{A_5}{A_1}\right|^2$$

or the reflection probability, $R=1-D$, a formal method was developed by Kane [19]. However, the results of this method are too complicated when one is trying to use them for general potential forms.

Our method is somewhat similar, but the evaluation is simpler and the results are more lucid.

The amplitudes of the wave functions (2) are to be determined from the continuity conditions of these functions and of their derivatives on the connections of neighbouring regions.

In the following considerations we assume that the particle is coming from the left to the system BWB (i.e. amplitude $B_5=0$). We obtain then the following system of equations from the continuity conditions

$$A_1+B_1=A_2+B_2$$

$$\begin{aligned} &A_2e^{ik_2d_1}+B_2e^{-ik_2d_1}=A_3e^{ik_3d_1}+B_3e^{-ik_3d_1}, \\ &A_3e^{ik_3(d_1+c)}+B_3e^{-ik_3(d_1+c)}=A_4e^{ik_4(d_1+c)}+B_4e^{-ik_4(d_1+c)}, \\ &A_4e^{ik_4(c+d_1+d_2)}+B_4e^{-ik_4(c+d_1+d_2)}=A_5e^{ik_5(c+d_1+d_2)}, \end{aligned}$$

$$k_1(A_1-B_1)=k_2(A_2-B_2),$$

$$\begin{aligned} &k_2(A_2e^{ik_2d_1}-B_2e^{-ik_2d_1})=k_3(A_3e^{-ik_3d_1}-B_3e^{-ik_3d_1}), \\ &k_3(A_3e^{ik_3(d_1+c)}-B_3e^{-ik_3(d_1+c)})=k_4(A_4e^{ik_4(d_1+c)}-B_4e^{-ik_4(d_1+c)}), \\ &k_4(A_4e^{ik_4(c+d_1+d_2)}-B_4e^{-ik_4(c+d_1+d_2)})=k_5A_5e^{ik_5(c+d_1+d_2)}. \end{aligned}$$

After a simple rearrangement we have then

$$\begin{aligned} &A_1g_1+B_1h_1=A_2 \\ &A_1h_1+B_1g_1=B_2 \end{aligned}$$

$$\begin{aligned} &A_2g_2e^{i(k_2-k_3)d_1}+B_2h_2e^{i(-k_2-k_3)d_1}=A_3 \\ &A_2h_2e^{i(k_2+k_3)d_1}+B_2g_2e^{i(-k_2+k_3)d_1}=B_3 \end{aligned}$$

$$A_3 g_3 e^{i(k_3-k_4)(c+d_1)} + B_3 h_3 e^{i(-k_3-k_4)(c+d_1)} = A_4$$
$$A_3 h_3 e^{i(k_3+k_4)(c+d_1)} + B_3 g_3 e^{i(-k_3+k_4)(c+d_1)} = B_4$$

$$A_4 g_4 e^{i(k_4-k_5)(c+d_1+d_2)} + B_4 h_4 e^{i(-k_4-k_5)(c+d_1+d_2)} = A_5$$
$$A_4 h_4 e^{i(k_4+k_5)(c+d_1+d_2)} + B_4 g_4 e^{i(-k_4+k_5)(c+d_1+d_2)} = B_5$$

where $h_i = \frac{1}{2}\left(1 - \frac{k_i}{k_{i+1}}\right)$, $g_i = \frac{1}{2}\left(1 + \frac{k_i}{k_{i+1}}\right)$, $i = 1, \ldots, 4$.

This can be simplified by the matrix notation

$$a_i = p^{(i)} a_{i-1}, \tag{5}$$

where $a_i = \begin{pmatrix} A_i \\ B_i \end{pmatrix}$ and $p^{(i)}$ are 2×2 matrices with the components of the left side of the equation pairs (4):

$$p^{(1)} = \begin{pmatrix} p_{11}^{(1)} & p_{12}^{(1)} \\ p_{21}^{(1)} & p_{22}^{(1)} \end{pmatrix} = \begin{pmatrix} g_1 & h_1 \\ h_1 & g_1 \end{pmatrix},$$
$$p^{(2)} = \begin{pmatrix} p_{11}^{(2)} & p_{12}^{(2)} \\ p_{21}^{(2)} & p_{22}^{(2)} \end{pmatrix} = \begin{pmatrix} g_2 e^{i(k_2-k_3)d_1} & h_2 e^{i(-k_2-k_3)d_1} \\ h_2 e^{i(k_2+k_3)d_1} & g_2 e^{i(-k_2+k_3)d_1} \end{pmatrix}, \tag{6}$$

etc.

By assuming that the particles are coming from the left ($B_5 = 0$), one obtains immediatly

$$B_4 = -A_4 \frac{p_{21}^{(4)}}{p_{22}^{(4)}}$$

as well as

$$A_5 = A_4\left(p_{11}^{(4)} - \frac{p_{21}^{(4)} p_{12}^{(4)}}{p_{22}^{(4)}}\right).$$

The further procedure is then very easy, but rather cumbersome: the equations (4) are to be rearranged in the way to obtain $A_{i+1}(A_i)$ and $B_i(A_i)$, respectively.

For convenience we introduce the notations

$$L_i = \frac{p_{11}^{(i)}}{p_{22}^{(i)}} = e^{2i(k_i-k_{i+1})f_i}, \quad K_i = \frac{h_i}{g_i} e^{-2ik_{i+1}f_i}, \quad H_i = \frac{p_{21}^{(i)}}{p_{22}^{(i)}} = \frac{h_i}{g_i} e^{2ik_if_i},$$

$$G_i = p_{22}^{(i)}(L_i - K_i H_i) = p_{22}^{(i)}\left(1 - \frac{h_i^2}{g_i^2} e^{2i(k_{i-1}-k_i)f_i}\right),$$

where $f_1 = 0$, $f_2 = d_1$, $f_3 = d_1 + c$, $f_4 = d_1 + c + d_2$, and then consecutively

$$M_4 = H_4, \qquad M_5 = 0,$$

$$M_j = \frac{H_j + M_{j+1} L_j}{1 + M_{j+1} K_j}, \qquad j = 1, 2, 3.$$

We obtain then

$$B_i = -M_i A_i, \quad A_{i+1} = A_i \frac{G_i}{1 + M_{i+1} K_i}, \qquad i = 1, 2, 3, 4.$$

In this way one can obtain the dependence of two arbitrary amplitudes of the wave functions (2).[1])

Hence, we have also the $A_5(A_1)$ dependence which was our main task in the calculation of the transmission probability:

$$A_5 = A_1 \frac{G_1 G_2 G_3 G_4}{(1 + M_4 K_3)(1 + M_3 K_2)(1 + M_2 K_1)}.$$

After elementary modifications and substituting the components of the matrices (6), this expression has the form

$$\frac{A_5}{A_1} = (g_4^2 - h_4^2)(g_3^2 - h_3^2)(g_2^2 - h_2^2)(g_1^2 - h_1^2) e^{ik_2d_1 + ik_3c + ik_4d_2 - ik_5(c+d_1+d_2)} \times$$
$$[(g_1 g_2 + h_1 h_2 e^{2ik_2d_1})(g_3 g_4 + h_3 h_4 e^{2ik_4d_2}) + e^{2ik_3c}(g_1 h_2 + h_1 g_2 e^{2ik_2d_1})$$
$$\times (h_3 g_4 + h_4 g_3 e^{2ik_4d_2})]^{-1}.$$

Since there holds

$$g_1^2 - h_1^2 = \frac{1}{4}\left(1 + 2\frac{k_1}{k_2} + \frac{k_1^2}{k_2^2} - 1 + 2\frac{k_1}{k_2} - \frac{k_1^2}{k_2^2}\right) = \frac{k_1}{k_2},$$

$$g_2^2 - h_2^2 = \frac{k_2}{k_3},$$

etc.,

the result is

$$\frac{A_5}{A_1} = \frac{k_1}{k_5} e^{-ik_5(c+d_1+d_2)}[(g_1 g_2 e^{-ik_2d_1} + h_1 h_2 e^{ik_2d_1})(g_3 g_4 e^{-ik_4d_2} +$$
$$+ h_3 h_4 e^{ik_4d_2}) e^{-ik_3c} + (g_1 h_2 e^{-ik_2d_1} + h_1 g_2 e^{ik_2d_1})(h_3 g_4 e^{-ik_4d_2} +$$
$$+ h_4 g_3 e^{ik_4d_2}) e^{ik_3c}]^{-1}. \tag{7}$$

This general result is used for the calculation of the transmission probability D in the next section, as well as for calculating the transmission time of the particle through the system barrier–well–barrier in a following paper [18].

[1]) From these amplitudes not only the transition probabilities, but also other quantities (e.g. the transmission time) can be calculated [18].

III. SYMMETRIC DOUBLE BARRIER

In this section we pay attention to the case of two identical potential barriers with a potential well (relatively to the barrier height) between them (Fig. 1, dotted lines).

This means

$$U_2 = U_1 = U$$
$$d_2 = d_1 = d,$$
$$\Delta E = 0.$$

Then we have

$$k_2 = k_4 = \mathrm{i}K, \qquad K = \frac{\sqrt{2m(U-E)}}{\hbar},$$
$$k_1 = k_5,$$
$$g_1 = \frac{1}{2}\left(1 + \frac{k_1}{\mathrm{i}K}\right), \quad h_1 = g_1^*,$$
$$g_2 = \frac{1}{2}\left(1 + \frac{\mathrm{i}K}{k_3}\right), \quad h_2 = g_2^*,$$
$$g_3 = \frac{1}{2}\left(1 + \frac{k_3}{\mathrm{i}K}\right), \quad h_3 = g_3^*,$$
$$g_4 = \frac{1}{2}\left(1 + \frac{\mathrm{i}K}{k_1}\right), \quad h_4 = g_4^*.$$

The result is then

$$\left|\frac{A_5}{A_1}\right|^{-1} = \Big|\cos(k_3c)[\cosh^2(Kd) + \sinh^2(Kd)] + F_3 \sin(k_3c)\sinh(Kd)\cosh(Kd) + \mathrm{i}\Big\{\frac{1}{2}\sin(k_3c)[F_1\cosh^2(Kd) - F_2\sinh^2(Kd)] - F_4\cos(k_3c)\sinh(Kd)\cosh(Kd)\Big\}\Big|, \tag{8}$$

$$\arg\left(\frac{A_5}{A_1}\right) = \mathrm{arctg}\,\frac{\frac{1}{2}[F_1 - F_2\tanh^2(Kd)]\,\mathrm{tg}(k_3c) - F_4\tanh(Kd)\,\mathrm{tg}(k_3c)}{1 + \tanh^2(Kd) + F_3\tanh(Kd)\,\mathrm{tg}(k_3c)},$$

where

$$F_1 = \frac{k_1}{k_3} + \frac{k_3}{k_1}, \qquad F_2 = \frac{K^2}{k_1k_3} + \frac{k_1k_3}{K^2},$$
$$F_3 = \frac{K}{k_3} - \frac{k_3}{K}, \qquad F_4 = \frac{K}{k_1} - \frac{k_1}{K}. \tag{9}$$

The transmission probability $D = |A_5/A_1|^2$ of the symmetric double barrier is then given by

$$\frac{8}{D} = (4 + F_1^2)\cosh^4(Kd) + (4 + F_2^2)\sinh^4(Kd) + 2(F_1F_2 + 4)\sinh^2(Kd) \times \cosh^2(Kd)] + \cos(2ck_3)[(4 - F_1^2)\cosh^4(Kd) + (4 - F_2^2)\sinh^4(Kd) + 2(3F_4^2 - F_3^2 + 8)\sinh^2(Kd)\cosh^2(Kd)] + 4\sin 2ck_3) \times \sinh(Kd)\cosh(Kd)[(2F_3 - F_1F_4)\cosh^2(Kd) + (2F_3 + F_2F_4)\sinh^2(Kd). \tag{10}$$

IV. DISCUSSION

IV.1. Shallow wells between the barriers

The dependence of the transmission coefficient D for the symmetric double barrier with not too deep wells is given in Fig. 2 for different values of the parameter $\alpha = \frac{\sqrt{2mU}}{\hbar}d$, different ratios of the well and barrier width $b = c/d$, and different ratios of the well depth to the barrier height $y = |U_0/U|$. These curves are very interesting and demonstrate the existence of minima and maxima of the transmission coefficient D.

From the relation (10) one obtains the conditions for the extremes (minima and maxima) of the function $D(E)$:

$$\mathrm{tg}(2ck_3) = 4\sinh(Kd)\cosh(Kd) \times \frac{(2F_3 - F_1F_4)\cosh^2(Kd) + (2F_3 + F_2F_4)\sinh^2(Kd)}{(4 - F_1^2)\cosh^4(Kd) + (4 - F_2^2)\sinh^4(Kd) + 2(3F_4^2 - F_3^2 + 8)\sinh^2(Kd)\cosh^2(Kd)}. \tag{11}$$

One has then two types of the solutions of (11), as there are two independent combinations for the sin $(2ck_3)$ and cos $(2ck_3)$ which fulfil the condition (11). Therefore we have maxima

$$D_{\max} = 1, \tag{12}$$

corresponding to

$$\cos(2ck_3) = \frac{1}{-\sqrt{1 + \mathrm{tg}^2(2ck_3)}}, \tag{13}$$
$$\sin(2ck_3) = \frac{\mathrm{tg}(2ck_3)}{-\sqrt{1 + \mathrm{tg}^2(2ck_3)}},$$

and minima

$$D_{\min} = \frac{4}{[F_1\cosh^2(Kd) + F_2\sinh^2(Kd)]^2}, \tag{14}$$

corresponding to the functions sin $(2ck_3)$ and cos $(2ck_3)$ with positive signs of the roots in equation (13).

The value of D_{min} is always smaller or at most equal to the transmission coefficient of the double thickness barrier (without well) for the given energy, as $F_1 \geq 2$, $F_2 \geq 2$.

The existence of "loss-free" transmission for energies smaller than the height of the barrier is at first somewhat surprising and it assumes the existence of some kind of resonance waves of the given energy in the barriers.

This case is like the quantum-mechanical "transmission" of the simple potential well [2], where only waves with special frequencies are ideally transmitted, because one has interferences on the walls only for these frequencies.

Bohm [2] compares the effect with the classical optics, where sharp interferences occur due to sudden changes of the optical coefficients (e.g. in the neighbourhood of boundaries).

The total transmission of the double barriers with a well (i.e. the total transmission of the system in the case when the particles come with equal probability independently of the energy) is much larger than for the single barrier with double thickness (this means the limiting case $c \to 0$).[2]

The number of maxima increases very markedly with the increasing value of α (for not very deep wells) and the width of the maxima is narrowed (mainly for the maxima in the small energy regions). On the other hand, it is somewhat surprising that the maxima are shifted to higher energies with the deepening of the potential well. With the deepening of the well we have a smaller number of the maxima of $D(E)$ (and therefore also the number of resonances), which is surprising if we consider that the number of eigen-states of the given potential well is increasing with the increasing well depth.

It is also very interesting that for $U_0 < 0$ (i.e. if we have a "true" well between the barriers) there is a finite distance c' between the barriers, for which $D = 1$ for infinitesimally small energies of the particles ($k_1 \to 0$).

Hence, e. g. for $U_0 = -U_1$ this occurs for

$$\operatorname{tg}(2c'k_3) = \frac{2 \sinh(K'd)}{1 - \sinh^2(2K'd)}, \tag{15}$$

where $K' = \sqrt{2mU/\hbar}$.

If $K'd \gg 1$, the condition (15) means

$$\cos(2c'k_3) = -1 \tag{15'}$$

[2]) This is valid in the case where D has a maximum. As we shall see later this is no more true for deep wells.

and the distance c' is then

$$c' = \sqrt{\frac{2}{m|U_0|}}\,\pi\hbar\left(n - \frac{1}{2}\right) = \frac{h}{\sqrt{2m|U_0|}}\left(n - \frac{1}{2}\right), \tag{16}$$

where n is an integer.

For the barrier height of about 1 eV (we assume further the equal depth of the

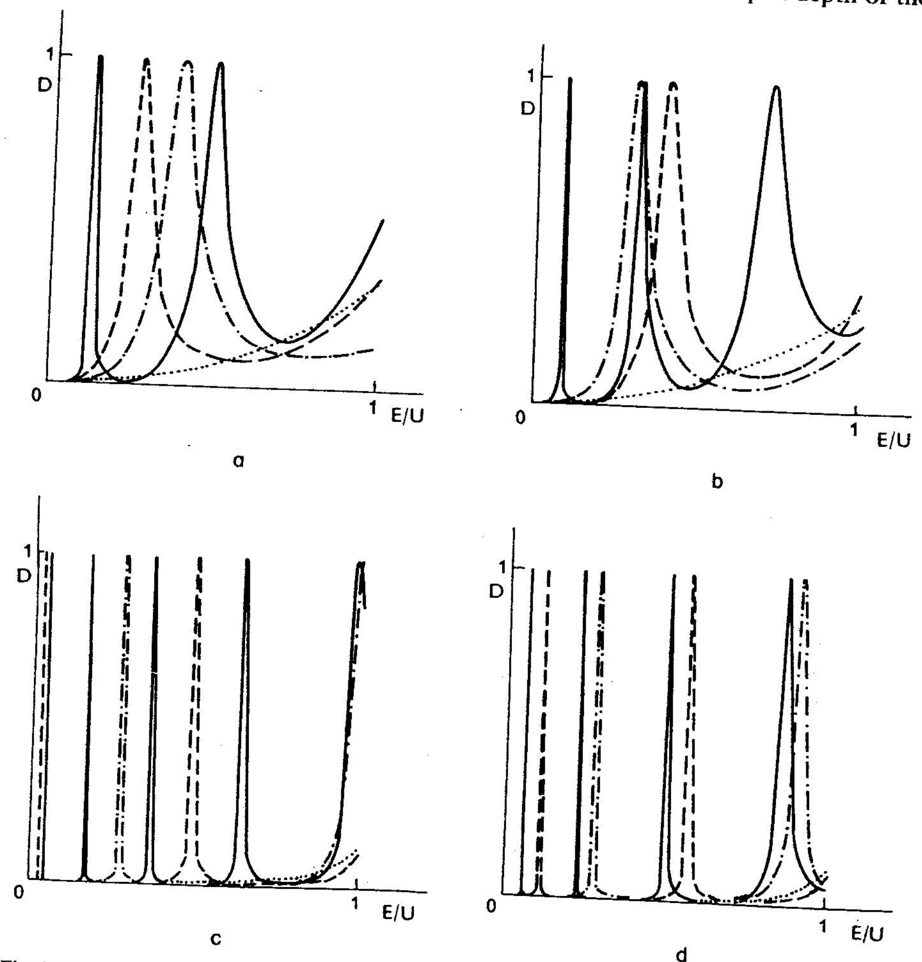

Fig. 2. The transmission coefficient D of two identical potential barriers with height U and width d, separated by a well with depth U_0 and width c, for energies smaller than the potential barrier height $(E < U)$. —— $y = |U_0/U| = 0$, - - - $y = 1$, –·–·– $y = 2$, ····· $c = 0$ (double barrier without well).
a) $\alpha = \sqrt{2m\,U}d/\hbar = 1$, $b = c/d = 3\pi/2$, b) $\alpha = 1$, $b = 2\pi$, c) $\alpha = 2$, $b = 5\pi/4$, d) $\alpha = 2$, $b = 3\pi/2$.

well) the smallest distance is then c_{min}, for which the system BWB will be ideally permitive for the infinitesimal energies, about

$$c_{min} \approx 10^{-7}\ \text{cm}. \tag{17}$$

The relation (15′) is relatively well fulfilled for $d > 10^{-7}$ cm. For the barrier height of about 1 eV and the width $d > 10^{-7}$ cm the relation (16) is therefore independent of the barrier width d and the minimum distance between the barriers (with identical well depths) for which $D(E \to 0) = 1$ is given by (17).

In some cases (e.g. in electron motions in fine-grained or disordered structures), the knowledge of the transmission coefficient above the barrier height can be useful, too. Our results for D and $A_j(A_k)$ are also valid for this case, but one has to consider that some functions are then complex for $E > U_1$. The resulting value for the transmission probability is naturally real.

In Figs. 3, the results for particle energies higher than the barrier height are shown, too.

IV.2. "Deep" wells between the barriers

We concentrate now our attention upon the case of a deep well (i.e. large values of $y = |U_0/U|$, which can be very important in solid state physics (see [18]). Figs. 4a, b show the transmission coefficients for $\alpha = 2$ and $y = 5, 20$ and different distances between the barriers $b = c/d$.

It can be seen from these figures that for not very large values of b there is at most one maximum for $E < U$. The intervals with maxima and without them

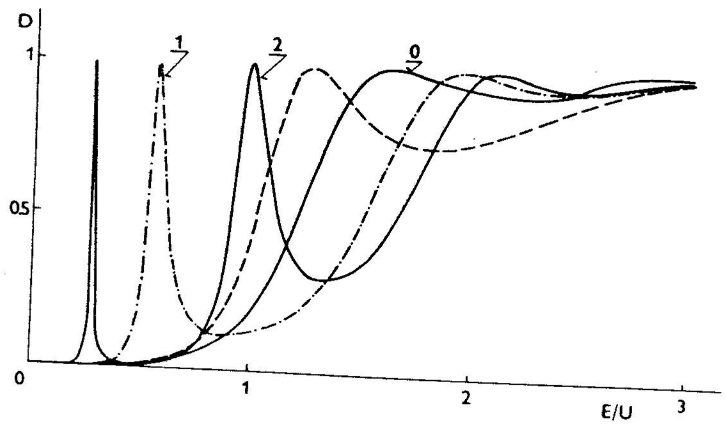

Fig. 3. The transmission coefficient for $\alpha = 2$ and $y = 0$ (which represents all features of "shallow" wells between the barriers). The ratio b is given at the corresponding curves.

"alternate" almost periodically. The value of the lower (b_1) and upper (b_2) limits of these intervals with the maximum of D,

$$b_1 < b < b_2,$$

can be obtained from the conditions

$$\lim_{E \to 0} D(E) = 1 \quad \text{and} \quad \lim_{E \to 1} D(E) = 1,$$

respectively.

These conditions result in transcendental equations

$$\operatorname{tg}(2\alpha b_1 \sqrt{y}) = \frac{4 \sinh(\alpha) \cosh(\alpha) \left[\sqrt{y} \cosh^2 \alpha) - \frac{1}{\sqrt{y}} \sinh^2(\alpha) \right]}{y \cosh^4(\alpha) + \frac{1}{y} \sinh^4(\alpha) - 6 \sinh^2(\alpha) \cosh^2(\alpha)},$$

$$\operatorname{tg}(2\alpha b_2 \sqrt{1+y}) = \frac{4\alpha\sqrt{1+y}[y(\alpha^2+1)+\alpha^2]}{y(\alpha^2+1)^2 + 2y\alpha^2(\alpha^2-1) + \alpha^2(\alpha^2-4)}.$$

These equations seem to be very complicated at first sight, but after some rearrangement and using the relations

$$\operatorname{tg}(2x) = \frac{2 \operatorname{tg}(x)}{1 - \operatorname{tg}^2(x)}, \quad \operatorname{tg}(4x) = \frac{4 \operatorname{tg}(x)}{1 - 6 \operatorname{tg}^2(x) + \operatorname{tg}^4(x)}$$

we have

$$\operatorname{tg}\left(\frac{\alpha}{2} b_1 \sqrt{y}\right) = \frac{\operatorname{tgh}(\alpha)}{\sqrt{2}},$$

$$\operatorname{tg}\left(\frac{\alpha}{2} b_2 \sqrt{1+y}\right) = \frac{\alpha^2(1+y)+y}{2\alpha\sqrt{1+y}} \left[-1 \pm \sqrt{1 + \frac{4\alpha^2(1+y)}{[\alpha^2(1+y)+y]^2}} \right].$$

One has therefore radical changes in the transmission coefficient of the system BWB (i.e. with or without a maximum) with relatively small changes of the parameters. The differences are really very large, as one can see from Figs. 4 (mainly for larger values of y). One can see from the obtained results (mainly in this section) that the most important parameter of the system BWB is the combination $\alpha b \sqrt{y}$. This will be confirmed by our further calculations, too [18].

The drastic changes of the transmission coefficient are transferred also into the total transmission of the system BWB (e.g. with the Maxwell—Boltzmann distribution function [18]).

V. SOME COMMENTS

One could think that some results of this paper (e.g. the sharpness of the maxima, the exact value of $D_{max} = 1$) are the consequence of the model (sudden changes of the potential between the barriers and the well). One can show, however, that this is not the case: also for smooth changes of the potential and even for potentials with "tails" there are similar results. Therefore the step-like structures of the potential describe the tunnelling phenomena very well also for combined potential structures.

The results for the transmission coefficient of the system barrier-well (or well-barrier) are very interesting, too. However, as we do not know such systems in reality, we do not give the reults here.

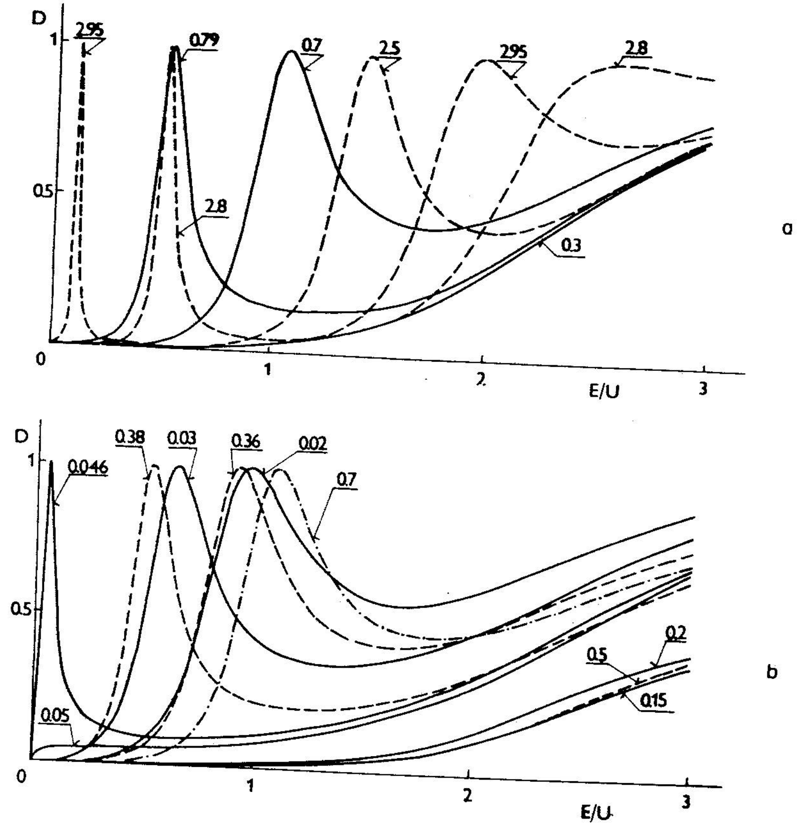

Fig. 4. The transmission coefficient for $\alpha = 2$ and $\dot{y} = 5$ (a), $y = 20$ (b), which are the case for "deep" and "very deep" wells, respectively. The numbers are the b values.

Concluding we wish to remark upon the biological aspects of tunneling in biological structures (e.g. through bilipides of membranes). As far as the transfer of ions is considered, it seems to be all right: the electrically charged particles tunnel through the potentials created by the electrostatic fields (but it is very important that one single ion can change appreciably the potential structure in the neighbourhood after tunneling). For other materials (saccharides, macromolecules), the potential can be influenced if the concentration of the given substance is changed on one side of the membrane (it can mean, e.g., the enhancement of the ground state energy of other molecules) and the potential can be built up by electrostatic, electromagnetic, but mainly by osmotic fields.

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Received September 20th, 1979