acta phys. slov. 33 (1983), No. 2

TUNNELLING THROUGH COMBINED POTENTIAL STRUCTURES II. SOME EXAMPLES

S. TAKÁCS[1]), Bratislava

The general results for the tunnelling of particles through the system barrier-well-barrier (BWB), evaluated in a recent work of the author, are used for calculating some problems which can be important in the theory of electric and thermal conductivity of crystalline solids with impurities or in disordered structures.

The temperature and electric-field dependence of the total transmission coefficient and the total amount of energy conducted by electrons with the Maxwell—Boltzmann distribution are calculated. They determine the electric conductivity and the electron component of the thermal conductivity of solids, respectively.

The transmission time τ of electrons through the system BWB is shown to have analogous maxima as the transmission coefficient D. By comparing this time with the transition time $\bar{\tau}$ between free states of the incoming electrons and the bound states of the well not occupied at this time (e. g. near ionized impurities)-which is also calculated in this paper- the trapping probability of electrons by ionized impurities $\approx \tau/\bar{\tau}$ is given. It is shown further that the resonance tunnelling leads to negative-resistance regions in the current-voltage characteristics.

The eigen-energies of the system BWB, which were needed for determining the time $\bar{\tau}$, are shown to be always larger than the eigen-energies of the corresponding single well.

ТУННЕЛИРОВАНИЕ ЧЕРЕЗ КОМБИНИРОВАННЫЕ ПОТЕНЦИАЛЬНЫЕ СТРУКТУРЫ

II. НЕКОТОРЫЕ ПРИМЕРЫ

Общие результаты автора по проблеме туннелирования частиц через систему барьер-яма-барьер (БЯБ), полученные в предыдущей работе, применены для вычисления некоторых проблем, которые могут иметь важное значение в теории электропроводимости и удельной теплопроводности твердых кристаллических тел с примесями, или неупорядоченных структур.

Вычислена зависимость от температуры и от электрического поля полного коэффициента прохождения и полной энергии, перенесенной электронами, которые подчиняются распределению Максвелла–Больцмана. Эти величины определяют

[1]) Elektrotechnický ústav CEFV SAV, Dúbravská cesta, 842 39 BRATISLAVA, Czechoslovakia.

соответственно электропроводимость и электронную составляющую удельной теплопроводности твердых тел.

В работе показано, что время τ перехода электронов через системы БЯБ имеет аналогичные максимумы так же, как и коэффициент прохождения D. На основе сравнения этого времени с временем $\bar{\tau}$ перехода между свободными состояниями поступающих электронов и связанными состояниями ямы, которые в это время не заняты (например, вблизи ионизированных примесей) также вычисленное в работе, определена вероятность захвата электронов ионизированными примесями $\approx \tau/\bar{\tau}$. Кроме того, показано, что резонансный туннельный эффект приводит к областям с отрицательным дифференциальным сопротивлением в вольт-амперной характеристике. Показано также, что собственные энергии системы БЯБ, которые необходимы для вычисления $\bar{\tau}$, всегда больше собственных энергий соответствующей ямы.

I. INTRODUCTION

In our recent paper [1], cited in the following as I, we have shown how the quantum-mechanical transmission coefficient of the system barrier-well-barrier (BWB, denoted also as double barrier in the following) depends on the characteristic parameters of the potential barriers and the potential well between the barriers. We emphasized mainly the deviations of the results from such where the barriers can be treated as acting independently on the particle tunnelling.

In this contribution, we use the general results of I for calculating some other parameters which can be useful mainly in the theory of electrical and thermal conductivity of crystalline solids with impurities, or in disordered structures.

In Section II, we calculate the total transmission coefficient and the total energy transferred by the electrons through the system barrier-well-barrier assuming the distribution of electrons by the Maxwell—Boltzmann distribution function. In Sect. III, the time is calculated during which the electrons stay "in" the double barrier. This time is very important for the determination of the transition probability of the transmitted electrons into a bound state, not occupied at this time (e. g. near ionized impurities in solids). This transition probability is calculated in section V. For these calculations we have to know the eigenstates of the system BWB, which are therefore determined in Section IV.

II. THE TOTAL PERMITTIVITY OF THE DOUBLE BARRIER WITH THE DISTRIBUTION FUNCTION FOR THE PARTICLES

If the electrons in solids have to transmit through the system of the type BWB (Fig. 1), two parameters are very important in calculating the electronic transport properties:

a) the total number of electrons passing the double barrier system (i. e. the total transmission coefficient D_t of the electrons with the given distribution function f;

b) the total amount of energy, transferred by the electrons through the double barrier system.

The first quantity will determine the electrical, the second the electron contribution to the thermal conductivity.

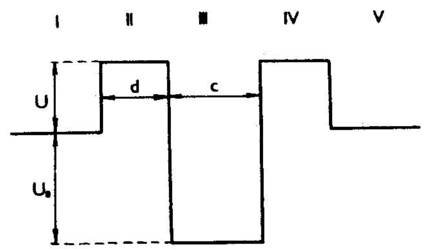

Fig. 1. The definition of the parameters of the double barrier and the division into different regions.

For the Maxwell—Boltzmann distribution function we have

$$f(v) = \sqrt{\frac{k^3}{\pi}}\, v^2 e^{-kv^2}$$

with the mean velocity

$$\bar{v} = \frac{2}{\sqrt{k\pi}}, \quad k = \frac{4m}{3\pi k_B T},$$

or

$$f(E) = 2\sqrt{\frac{E}{\pi}}\,(k_B T)^{-3/2} e^{-E/k_B T}$$

with the mean energy $\bar{E} = 3k_B T/2$ (k_B — Boltzmann constant).

We obtain then for the total transmission coefficient D_t and the totally transmitted energy E_t

$$D_t = \int_0^\infty D(E) f(E)\, dE = \frac{2}{\sqrt{\pi}} n^{3/2} \int_0^\infty z^{1/2} e^{-zn} D(z)\, dz,$$

$$E_t = \int_0^\infty E D(E) f(E)\, dE = \frac{2}{\sqrt{\pi}} n^{5/2} \int_0^\infty z^{3/2} e^{-zn} D(z)\, dz,$$

where

$$z = \frac{E}{U}, \quad n = \frac{U}{k_B T} = \frac{T_0}{T}$$

(U is the barrier height).

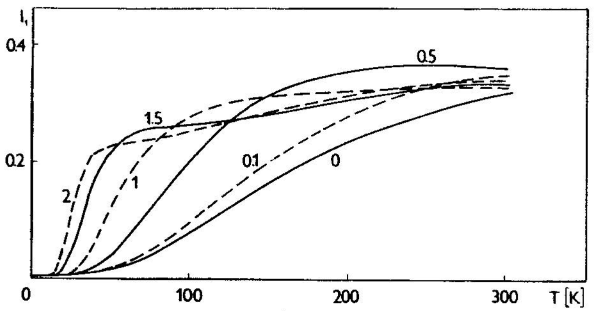

Fig. 2a

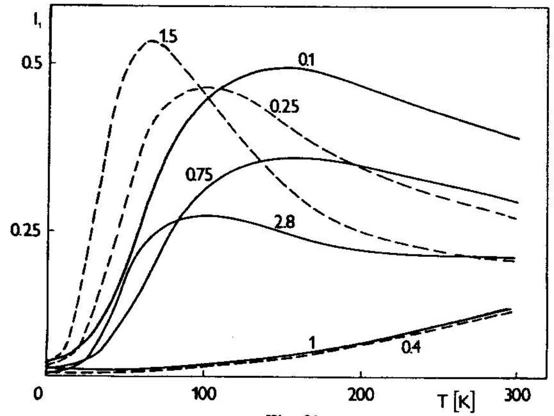

Fig. 2b

For $D(E) = 1$ we have

$$D_t = 1, \quad E_t = \frac{3}{2} k_B T.$$

We would like to mention that the influence of the electric field F on the electron distribution function can be included in the first approximation by changing the effective temperature of the electron gas T_{eff}, e. g. $T_{eff} = T(1 + \beta F^2)$.

Without restriction of generality, we can assume that the mean energy of the electrons at 300 K is equal to the barrier height U. For other values of U it is sufficient to provide the corresponding transformation on the temperature axis.

Then we have $T_0 = 450$ K and

$$D_t = I_1 = \frac{2}{\sqrt{\pi}} \left(\frac{450}{T}\right)^{3/2} \int_0^{\infty} z^{1/2} e^{-zn} D(z)\, dz,$$

$$E_t = \frac{2}{\sqrt{\pi}} \left(\frac{450}{T}\right)^{5/2} k_B T \int_0^{\infty} z^{3/2} e^{-zn} D(z)\, dz = k_B T . I_2.$$

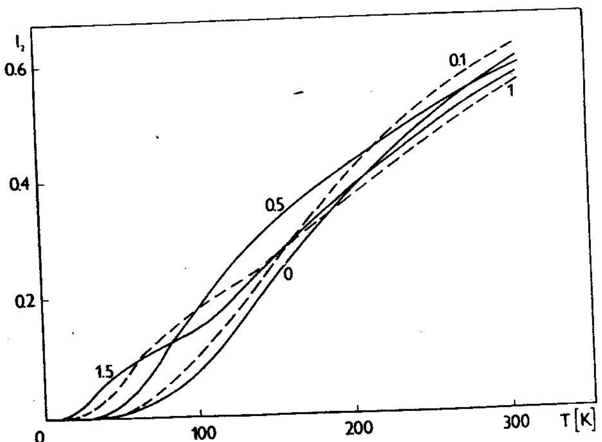

Fig. 2c

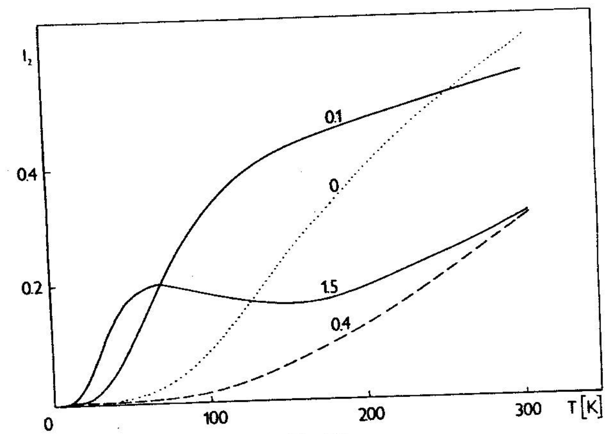

Fig. 2d

Fig. 2. The temperature dependence of the functions $I_1 = D_t$ and $I_2 = E_t/(3k_BT/2)$ for the double barrier with $y = |U_0|/U = 0$ — curves a) and c) and $y = 5$ — curbes b) and d). The curves represent shallow ($y = 0$) and deep ($y = 5$) double barriers. The numbers at the curves mean the ratios $b = c/d$ (well/barrier width). The barrier height is assumed to be $U = 3k_BT/2$ with $T = 300$ K. For other values of U it is sufficient to provide the corresponding transformation on the temperature axis.

In Figs. 2 one can see that the temperature dependence of both quantities can greatly differ. One obtains some typical curves in cases where the maxima of the transmission coefficient are at smaller or higher values of the electron energies, or the maximum of $D(E)$ even does not exist, respectively.

It is evident from these figures in which cases the transmission coefficient can be approximated with some average value (mainly I_1 does not depend very much on the temperature at higher T), or with the temperature dependence of the mean transmission coefficient (i. e. without the resonant tunnelling). The last approximation is very crude, as we can see from these figures. This can be very important in the theory of disordered materials [2].

III. THE TRANSMISSION TIME OF THE PARTICLE THROUGH THE SYSTEM BARRIER-WELL-BARRIER

The time of the particle in the system during the tunnelling process is somewhat dubious [3]. By solving the time-dependent Schrödinger equation we obtain that the particle described by the plane wave

$$\Psi = A e^{ikx - i(E/\hbar)t},$$

will be transmitted through the barrier instantaneously [3]. This result -a bit surprising- is not in contradiction with the theory of relativity, as in the non-relativistic Schrödinger equation the propagation velocity of particles is not limited.

We have therefore to use another procedures for calculating the transmission time τ of real particles.

One of the possibilities is the determination of the transmission time of the particle (being at the time $t=0$ in one of the wells) through the barrier into the other well (Fig. 3).

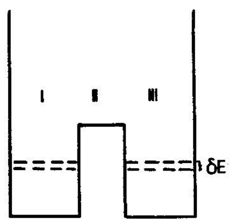

Fig. 3. The calculation of the transformation time between two wells separated by a potential barrier.

The time τ is then [3]

$$\tau = \frac{1}{2}\frac{\pi\hbar}{\delta E}$$

where

$$\delta E = \hbar^2 \frac{k\delta k}{m}$$

and δk is the splitting of the wave function in the well I due to the presence of the well III (Fig. 3).

Since

$$\delta E \sim e^{-\frac{\sqrt{2mU}}{\hbar}d},$$

one finds that the tunnelling is a very slow process. We see already from the

principles of this method that it is convenient in such case where the particles are sufficiently localized.

For quantitative calculations of the transmission time τ, one can use another procedure [4, 5], which is analogous to the calculation of the life-time of metastable states of the potential well in [6]. This method is suitable for our calculations with combined potentials, too.

The "particle" is characterized by the wave packet

$$\Psi(x, t) = \frac{1}{2\Delta E}\int_{E_0-\Delta E}^{E_0+\Delta E} \Psi_E(x, t)\, dE$$

with the mean energy E_0. The characteristic dimension of the wave packet is considered to be very small ($\Delta E/E \ll 1$); finally we shall apply the limiting procedure ($\Delta E \to 0$).

The wave packet, coming to the system BWB from the left, is divided after tunnelling into the transmitted part,

$$\Psi_t(x, t) = A_5(k) e^{(ikx - i(E/\hbar)t)},$$

(because there is no particle coming from the right, we have $B_5 = 0$), and into the reflected part (a "mixture" of the original packet with the reflected wave function)

$$\Psi_r(x, t) = [A_1 e^{ikx} + B_1 e^{-ikx}] e^{-i(E/\hbar)t}.$$

We have adopted the notations from paper I.

Since at the time $t=0$ there exists only the wave packet coming from the left to the double barrier, there should be $A_1 = 1$. Besides, from the narrow wave packet (i. e. $\Delta E/E \ll 1$) we can assume

$$|A_5(k)| \approx |A_5(k_0)|, \quad |B_1(k)| \approx |B_1(k_0)|$$

and therefore

$$A_5(k) = |A_5(k_0)| e^{i\alpha_1(k)}, \quad B_1(k) = |B_1(k_0)| e^{i\alpha_2(k)}.$$

If the original wave packet contained the component $\sim e^{-i\omega t}$, the transmitted part will contain the component

$$A_5 \sim e^{i(\alpha_2 - \omega t)} = e^{i\alpha_0 - i\omega(t-\tau)}$$

where the expansion

$$\alpha_2(k) = \alpha_0 + \left(\frac{d\alpha_2}{d\omega}\right)_{\omega=\omega(k_0)}, \quad \left(\frac{d\alpha_2}{d\omega}\right)_{\omega=\omega(k_0)} = \tau$$

had been used, which is allowed for the sufficiently narrow wave packet, too.

It is then obvious that

$$\tau = \frac{d(\arg A_5)}{d\omega} \tag{1}$$

will mean the time by which the particle motion is delayed in the double barrier system (with respect to such a particle which has no obstacle in its way, i. e. a free particle).

From paper I, we have for our combined potential

$$\arg(A_5) = \operatorname{arctg} \frac{\left[\frac{1}{2} F_1 - F_2 \operatorname{tgh}^2(Kd)\right] \operatorname{tg}(k_3 c) - F_4 \operatorname{tgh}(Kd)}{1 + \operatorname{tgh}^2(Kd) + F_3 \operatorname{tgh}(Kd) \operatorname{tg}(k_3 c)} = \operatorname{arctg} \frac{L}{M}$$

and

$$\tau = \hbar \frac{d(\arg A_5)}{dE} = \frac{\hbar}{U} \frac{d(\arg A_5)}{dz}, \qquad (2)$$

with $z = E/U$.

We can see in Fig. 4 that the function $\tau(z)$ has maxima analogous to the maxima of the transmission coefficient $D(z)$.

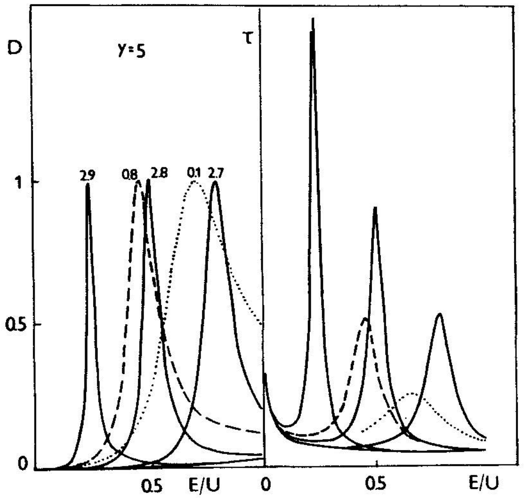

Fig. 4. The characteristic maxima of the transmission coefficient D and the transmission time τ for $y = 5$. The curves correspond to different values of $b = c/d$.

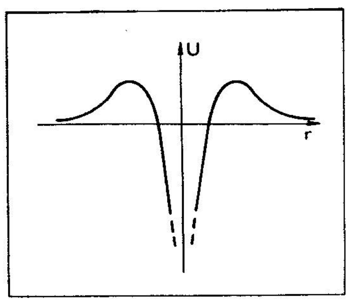

Fig. 5. Scheme of the potential near ionized impurities.

The existence of sharp maxima of τ can be important for some physical problems (α-decay in atomic physics, solids with ionized impurities, etc.). Namely, analogous potential structures form around such impurities (Fig. 5). Near the narrow "well" (which corresponds to the Coulomb potential of the ionized impurity) a "cloud" of negative charge is built up (the valence electrons are attracted by the positive ions), which acts as a barrier for the conduction electrons.

The probability for "trapping" the conduction electrons by such an impurity is then proportional both to the time which the electron spends near the well and to the transition probability of the electron with energy E to the bound state of the well (energy E_0).

IV. EIGENENERGIES OF THE SYSTEM BARRIER-WELL-BARRIER

For the trapping of electrons by ionized impurities, the eigenstates of the system are to be determined. These eigenstates can exist only for $E_0 < 0$, as for $E > 0$ there is a finite probability for the particle to escape from the well.

The existence of the eigenstates of the system BWB is naturally always important (e. g. also for the α-decay).

The corresponding wave functions for $E_0 < 0$ are in the individual regions (see Fig. 1 for determining these regions)

$$\varphi_{I} = A_1 e^{K_1 x} \qquad (3)$$

$$\varphi_{II} = A_2 e^{K_2 x} + B_2 e^{-K_2 x}$$

$$\varphi_{III} = A_+ \cos(\varkappa x), \quad \text{or} \quad A_- \sin(\varkappa x)$$

$$\varphi_{IV} = A_4 e^{K_2 x} + B_4 e^{-K_2 x}$$

$$\varphi_{V} = B_5 e^{-K_1 x}$$

where A_+ and A_- correspond to the even and odd symmetry of the wave function in the well, respectively,

$$K_1 = \frac{\sqrt{-2mE_0}}{\hbar}, \quad K_2 = \frac{\sqrt{2m(U - E_0)}}{\hbar}, \quad \varkappa = \frac{\sqrt{2m(|U_0| + E_0)}}{\hbar}.$$

Due to the boundary conditions for $x \to \pm\infty$, $B_1 = A_5 = 0$.

The calculation method is the same as in paper I. From the continuity conditions of the wave functions and its derivatives on the boundaries between the regions we have

$$B_5 = A_1, \quad B_2 = A_4, \quad B_4 = A_2,$$

as well as the condition for the *existence* of the bound state for even and odd symmetry, respectively:

$$\text{(even)} \qquad \operatorname{tg} \frac{\varkappa c}{2} = \frac{K_2}{\varkappa} \frac{\operatorname{tgh}(K_2 d) + \frac{K_1}{K_2}}{1 + \frac{K_1}{K_2} \operatorname{tgh}(K_2 d)} = \frac{K_1}{\varkappa} H,$$

(odd) $$\operatorname{ctg}\frac{\varkappa c}{2}=-\frac{K_1}{\varkappa}H,$$

where
$$H=\frac{1+\frac{K_2}{K_1}\operatorname{tgh}(K_2 d)}{1+\frac{K_1}{K_2}\operatorname{tgh}(K_2 d)}.$$

It is evident that with respect to the single well, the additional term $H>1$ appears in these conditions.

Therefore, the eigenenergies of the system BWB are always larger than for the corresponding well only.

This is apparent also from the following considerations (we consider now the even symmetry in details). The "new" bound state is formed in both systems (single barrier and barrier-well-barrier, respectively) for $E\to 0$. This leads to the condition

(well) $$\operatorname{tg}\frac{ab'\sqrt{y}}{2}=0,\quad \text{or}\quad \frac{ab'\sqrt{y}}{2}=\pi n,\qquad n=0,1,2,\ldots$$

(BWB) $$\operatorname{tg}\frac{ab\sqrt{y}}{2}=\frac{\operatorname{tgh}(\alpha)}{\sqrt{y}},\quad \text{or}\quad \frac{ab\sqrt{y}}{2}=\operatorname{arctg}\frac{\operatorname{tgh}(\alpha)}{\sqrt{y}}+\pi n.$$

The "new" bound state is formed (e. g. by increasing the value of b, leaving α, z constant) always "sooner" for the single well and it has always a smaller energy than the energy of the corresponding bound state of the structure BWB (Fig. 6).

Relatively, the difference of the eigenenergies are larger for the "shallow" well, but absolutely they are larger for the "deep" well (the depth always with respect to the barrier height).

Thus, e. g. for $\alpha=2$, $y=5$ there is
$$b'_n=\frac{\pi}{\sqrt{5}}n\approx 1.4n,$$
$$b_n\approx 0.18+1.4n,$$
for $\alpha=2$, $y=1$
$$b'_n=\pi n$$
$$b_n=0.767+n.$$

Even for
$$\frac{ab\sqrt{y}}{2}<\operatorname{arctg}\frac{\operatorname{tgh}(\alpha)}{\sqrt{y}}$$
there does not exist any bound state in the double barrier system (as well known, for the single potential well there is always at least one bound state in the one-dimensional case!).

A further undoubtedly interesting result is that the "new" bound state is formed in the system BWB at such parameters for which the transmission coefficient is

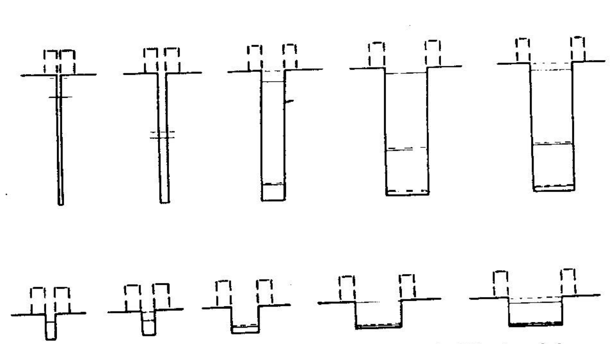

Fig. 6. The positions of the eigenstates of the double barrier (dashed line) and the corresponding single well (full lines) for $y=5$ and $y=2$, for different well widths.

approaching maximum at $E\to 0$. The "resonant" state of the system BWB is therefore ***transformed continously*** into the bound state.

The same conclusions are true for the odd symmetry of the wave function in the potential well. Knowing the eigenenergies of the system BWB we can determine the trapping probability of electrons by such system.

V. TRAPPING THE PARTICLES BY THE POTENTIALL WELL BETWEEN THE BARRIERS

As already mentioned, the trapping probability of the particle will be proportional to the transition probability P between the free states (with energy E) and the "bound" state (eigenstate) of the system BWB, as well as to the time which the particle stays "in" the system BWB. Since the transition probability in the time unit is the reciprocal value of the time $\bar{\tau}$ needed for the transition between the two states, the product $P\tau$ is essentially the ratio transmission/transition time $\tau/\bar{\tau}$.

The probability amplitude for finding the particle with energy E_0 at the time t, previously in the state with energy E at the time $t=0$, by stimulated emission (the transition of the particle with energy E into the eigenstate with energy E_0 by emitting the photon with frequency $\omega_{12}=(E-E_0)/\hbar$) is [4, 7]
$$a^{em}(t)=-\frac{e}{im}\int_0^{\infty}\mathrm{d}\omega A^*(\omega)\frac{e^{i(\omega_{12}+\omega)t}-1}{i(\omega_{12}+\omega)}h^{em},$$
where the photon spectrum is described by the vector potential of the electromagnetic field
$$\mathbf{A}(r,t)=-ie\int_0^{\infty}[A(\omega)e^{i(kr-\omega t)}-A^*(\omega)e^{-i(kr-\omega t)}]\,\mathrm{d}\omega$$
and
$$h^{em}=\int_{-\infty}^{\infty}\varphi e^{-ikx}(\partial\Psi/\partial x)\,\mathrm{d}x.$$

Here, Ψ is the wave function (2) from paper I (see Appendix) with $|A_1|^2 = 1$ (the particle is coming from the left).

For the transition probability in the time unit

$$P = \frac{\mathrm{d}}{\mathrm{d}t}\left(|a^{em}(t)h^{em}|^2\right) = (a\dot{a}^* + \dot{a}a^*)|h^{em}|^2$$

we have after integration

$$P = \frac{16\pi^2 e^2 \hbar^2 c^2}{m^2 d^2 (E+E_0)}|h|^2 \approx \frac{7.4\times 10^{10}}{\alpha^2(z+z_0)}|h|^2,$$

where $|h|^2$ is normalized to be dimensionless:

$$h = \int_{-\infty}^{\infty} \bar{\varphi} e^{-ikx}\frac{\partial \Psi}{\partial x}\,\mathrm{d}x. \tag{4}$$

For the even symmetry with

$$\xi = \frac{x - d - \frac{c}{2}}{d} = \frac{x}{d} - 1 - \frac{b}{2}, \quad V_2 = \alpha\sqrt{1+z_0}, \quad V_3 b = \alpha b\sqrt{y - z_0},$$

$$z_0 = E_0/U, \quad |W_1|^2 = 1/Q, \quad Q = \frac{1}{\alpha\sqrt{z_0}} + \frac{\sinh(V_2)}{V_2}\left[\frac{\cosh(V_2)}{1+z_0} + \right.$$

$$\left. + 2\sqrt{\frac{z_0}{1+z_0}}\sinh(V_2)\right] + \frac{1}{z+z_0} + \frac{\left[\cosh(V_2) + \sqrt{\frac{z_0}{1+z_0}}\sinh(V_2)\right]^2}{2V_3\cos\frac{V_2 b}{2}} \times$$

$$\times [V_3 b + \sin(V_3 b)],$$

we obtain

$$\bar{\varphi} = \bar{W}\begin{cases} e^{\alpha\sqrt{z_0}\xi}, \quad \xi \leqslant -1 - \frac{b}{2} \\ e^{-\alpha\sqrt{z_0}(1+b/2)}\left\{\cosh\left[\alpha\sqrt{1+z_0}\left(1+\frac{b}{2}+\xi\right)\right] + \sqrt{\frac{z_0}{1+z_0}} \times \right. \\ \left. \quad \times \sinh\left[\alpha\sqrt{1+z_0}\left(1+\frac{b}{2}+\xi\right)\right]\right\}, \quad -\frac{b}{2} - 1 \leqslant \xi \leqslant 1 + \frac{b}{2}, \\ e^{-\alpha\sqrt{z_0}(1+b/2)}\frac{\cos(\alpha\sqrt{y - z_0}\xi)}{\cos\frac{V_3 b}{2}}\left[\cosh(\alpha\sqrt{1+z}) + \right. \\ \quad \left. + \sqrt{\frac{z_0}{1+z_0}}\sinh(\alpha\sqrt{1+z})\right], \quad |\xi| \leqslant \frac{b}{2}, \\ e^{-\alpha\sqrt{z_0}(1+b/2)}\left\{\cosh\left[\alpha\sqrt{1+z_0}\left(1+\frac{b}{2}-\xi\right)\right] + \right. \\ \quad \left. + \sqrt{\frac{z_0}{1+z_0}}\sinh\left[\alpha\sqrt{1+z_0}\left(1+\frac{b}{2}-\xi\right)\right]\right\}, \quad \frac{b}{2} \leqslant \xi \leqslant 1 + \frac{b}{2}, \\ e^{-\alpha\sqrt{z_0}\xi}, \quad \xi \geqslant 1 + \frac{b}{2}. \end{cases} \tag{5}$$

Analogously for the odd symmetry

$$\bar{\varphi} = \bar{W}_1\begin{cases} e^{\alpha\sqrt{z_0}\xi}, \quad \xi \leqslant -1 - \frac{b}{2} \\ e^{-\alpha\sqrt{z_0}(1+b/2)}\left\{\cosh\left[\alpha\sqrt{1+z_0}\left(1+\frac{b}{2}+\xi\right)\right] + \sqrt{\frac{z_0}{1+z_0}} \times \right. \\ \left. \quad \times \sinh\left[\alpha\sqrt{1+z_0}\left(1+\frac{b}{2}+\xi\right)\right]\right\}, \quad -\frac{b}{2} - 1 \leqslant \xi \leqslant -\frac{b}{2}, \\ e^{-\alpha\sqrt{z_0}(1+b/2)}\frac{\sin(\alpha\sqrt{y - z_0}\xi}{\sin\frac{V_3 b}{2}}\left[\cosh(\alpha\sqrt{1+z}) + \right. \\ \quad \left. + \sqrt{\frac{z_0}{1+z_0}}\sinh(\alpha\sqrt{1+z})\right], \quad |\xi| \leqslant \frac{b}{2}, \\ e^{-\alpha\sqrt{z_0}(1+b/2)}\left\{\cosh\left[\alpha\sqrt{1+z_0}\left(1+\frac{b}{2}-\xi\right)\right] + \right. \\ \quad \left. \sqrt{\frac{z_0}{1+z_0}}\sinh\left[\alpha\sqrt{1+z_0}\left(1+\frac{b}{2}-\xi\right)\right]\right\}, \quad \frac{b}{2} \leqslant \xi \leqslant 1 + \frac{b}{2}, \\ e^{-\alpha\sqrt{z_0}\xi} \quad \xi \geqslant 1 + \frac{b}{2}, \end{cases}$$

$$|\bar{W}_1|^2 = \frac{1}{Q'}, \quad Q' = \frac{1}{\alpha\sqrt{z_0}} +$$

$$+ \frac{\sinh(V_2)}{V_2}\left[\frac{\cosh(V_2)}{1+z_0} + 2\sqrt{\frac{z_0}{1+z_0}}\sinh(V_2)\right] +$$

$$+ \frac{1}{z+z_0} + \frac{\left[\cosh(V_2) + \sqrt{\frac{z_0}{1+z_0}}\sinh(V_2\right]^2}{2V_3\sin^2\frac{V_4 b}{2}}[V_3 b - \sin(V_3 b)].$$

Since the calculation of the complete overlapping integral (4) is very tedious, we give only the basic formulae in the Appendix.

In Figs. 7, the dependence of $\tau/\bar{\tau}$ on the energy of the incoming particles is shown for even and odd symmetry. We show only the transitions into the highest bound states, as the transition probabilities into the lower states are always much smaller; besides, for not very large electrical fields and not very high temperatures only the highest states will be ionized.

From these figures the following statements can be made for the characteristic

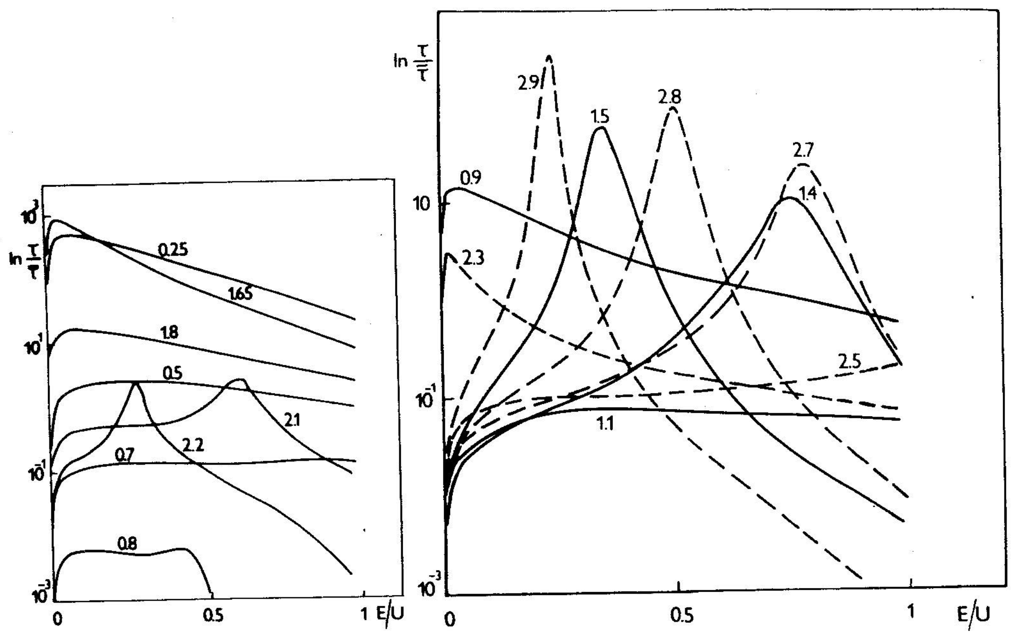

Fig. 7. The ratio transmission/transition time $\tau/\bar{\tau}$ for the even (a) and odd (b) symmetry of the wave function of the double barrier with $y=5$ as the function of the energy of the incoming particles E. The numbers at the curves mean again the ratio $b=c/d$. For $\tau/\bar{\tau}\gtrsim 1$ the particle will be trapped with a very large probability by the impurity.

behaviour of the trapping probability $\approx\tau/\bar{\tau}$ (for $\tau\gtrsim\tau$, the particle will very probably be trapped).

For the eigenstates near the top of the well ($z_0 \ll y$) the trapping probability decreases with the increasing energy of the incoming particles (or it remains nearly unchanged), whereas for lower eigenenergies ($z_0 \approx y$) the quantity $\tau/\bar{\tau}$ has clearly visible maxima. This holds both for the even and for the odd symmetry.

As already mentioned above, this type of $\tau/\bar{\tau}(E)$ dependence can be very important in solids with ionized impurities. Let the electron system in the solid be represented by the Maxwell—Boltzmann distribution function f for the given temperature T. If the electric field F is not very large, its influence on the electrons can be included by introducing the effective temperature (depending of F) in f. The maximum in F is then shifted to higher energies with the increasing electric field. Until this maximum is below the maximum of $\tau/\bar{\tau}$, the trapping probability of the electrons will increase. At the overlapping of the two maxima (for $\tau/\bar{\tau}$ and for f), the total trapping of the electrons will be approximately maximum, too.

Next, the total trapping will decrease, which results in the increased concentration of the conduction electrons and therefore in the increased electrical conductivity.

The electrical resistivity has therefore a component which at first increases with temperature (the trapping probability of the conduction electrons increases) and after reaching its maximum, it begins to decrease. Some analogous results were obtained experimentally [8]. The mechanism is very similar to the Gunn effect.

VI. DISCUSSION AND COMMENTS

The examples given in this paper show the importance of the resonance tunnelling in solids. The same is true for tunnelling between two superconductors as shown in the following paper [9].

We compare now our results with the calculations of the lifetime of quasi-stationary states in analogous systems [10, 11]. This was treated for the attractive short-range potentials δ-function combined with the attractive [10] and repulsive [11] Coulomb interaction. The last system resembles the problem of ionized impurities, calculated in the previous section. However, the Coulomb part leads to a very large width for $E\to 0$ and to very large barriers for the particles (some eV), which cannot be built up in semiconductors (mainly due to the shielding by conduction electrons). In addition, the potential well is not of a very short range as it is caused also by the Coulomb interaction.

We obtain the life-time in our theory by reversing the time variable: the tunnelling time gives then also the life-time of the corresponding eigenstates. It is from eq. (11) of [1],

$$\mathrm{tg}\left(\frac{\alpha b}{2}\sqrt{y+z}\right)\to 0 \quad \text{for} \quad z=E/U\to 0$$

and

$$\tau\approx\frac{\hbar}{U}\,\frac{(\sqrt{y}-1)\cosh^2(\alpha)(y-1)}{2\sqrt{z}(y+1)} \quad \text{for} \quad y\gg 1.$$

This gives a much slower increase for $E\to 0$ than that of the δ-like will. It cannot be explained only by the "brightening" of the barrier with decreasing energy due to the very long-ranged Coulomb potential.

We would like to mention that this is not the first known case in which the δ-like potential leads to different results [12].

With respect to the time τ_0 (tunnelling time through the barrier without the well in between),

$$\tau_0 \approx \frac{\hbar}{U}\frac{\operatorname{tgh}(\alpha)}{2\sqrt{z}}$$

we have

$$\frac{\tau}{\tau_0} \approx \frac{\sqrt{y-1}}{2}\sinh(2\alpha),$$

which depends mainly on the parameters of the barrier, in qualitative agreement with our calculations.

The time τ_0 is in a very good agreement with the qualitative considerations of [13]. Due to these the tunnelling time should depend in practical examples ($\operatorname{tgh}(\alpha) \approx 1$) mainly on the height of the barrier U and not on its width. This is in accordance with Heisenberg's uncertainty relation. Namely, the uncertainty in the electron energy during the crossing of the potential well is $\approx U$. The time due to this uncertainty is

$$\tau \approx \hbar / U.$$

I would like to acknowledge useful discussions with Doc. Dr. Ľ. Hrivnák.

APPENDIX

Here, we give only the principles for calculating the overlaping integral (4) for the "ďeven" symmetry. The wave function Ψ for the incoming wave is given by [1]

$$\Psi_j = A_j e^{ik_j x} + B_j e^{-ik_j x}.$$

With the notations

$$T_1 = \alpha\sqrt{z}, \quad T_2 = \alpha\sqrt{1-z}, \quad T_3 = \alpha\sqrt{z+y},$$

we have

$$\frac{\partial\Psi}{\partial x} = \frac{1}{d}\begin{cases} iT_1[A_1 e^{iT_1(\xi+1+\frac{b}{2})} - B_1 e^{-iT_1(\xi+1+\frac{b}{2})}] \\ T_2[-A_2 e^{iT_2(\xi+1+\frac{b}{2})} + B_2 e^{-iT_2(\xi+1+\frac{b}{2})}] \\ iT_3[A_3 e^{iT_3(\xi+1+\frac{b}{2})} - B_3 e^{-iT_3(\xi+1+\frac{b}{2})}] \\ T_2[-A_4 e^{iT_2(\xi+1+\frac{b}{2})} + B_4 e^{-iT_2(\xi+1+\frac{b}{2})}] \\ iT_1 A_5 e^{iT_1(\xi+1+\frac{b}{2})}. \end{cases}$$

The integral (4) consists of 5 parts; in front of the barrier, (1), in the first barrier (2), in the well between the barriers (3), in the second barrier (4) and beyond the system BWB (5):

$$I_1 = iW_1T_1\int_{-\infty}^{-1-b/2} e^{V_1\xi}[A_1 e^{iT_1(\xi+1+\frac{b}{2})} - B_1 e^{-iT_1(\xi+1+\frac{b}{2})}]e^{-ikx}\,d\xi,$$

$$I_2 = W_2T_2\int_{-1-b/2}^{-b/2}\left\{\cosh\left[V_2\left(\xi+1+\frac{b}{2}\right)\right] + \sqrt{\frac{z_0}{1+z_0}}\sinh\left[V_2\left(\xi+1+\frac{b}{2}\right)\right]\right\}\times$$
$$\times[-A_2 e^{-T_2(\xi+1+\frac{b}{2})} + B_2 e^{T_2(\xi+1+\frac{b}{2})}]e^{-ikx}\,d\xi,$$

$$I_3 = iW_3T_3\int_{-b/2}^{b/2}\cos(V_3\xi)[A_3 e^{iT_3(\xi+1+\frac{b}{2})} - B_3 e^{-iT_3(\xi+1+\frac{b}{2})}]e^{-ikx}\,d\xi,$$

$$I_4 = W_4T_2\int_{b/2}^{1+b/2}\left\{\cosh\left[V_2\left(1+\frac{b}{2}-\xi\right)\right] + \sqrt{\frac{z_0}{1+z_0}}\sinh\left[V_2\left(1+\frac{b}{2}-\xi\right)\right]\right\}\times$$
$$\times[-A_4 e^{-T_2(1+\frac{b}{2}+\xi)} + B_4 e^{T_2(1+\frac{b}{2}+\xi)}]e^{-ikx}\,d\xi,$$

$$I_5 = iW_5T_1A_5\int_{1+b/2}^{\infty} e^{-V_1\xi}e^{iT_1(1+\frac{b}{2}+\xi)-ikx}\,d\xi,$$

where

$V_1 = \alpha\sqrt{z_0}$, $V_2 = \alpha\sqrt{1+z_0}$, $V_3 = \alpha\sqrt{y-z_0}$, $V_4 = \alpha\sqrt{y+z_0}$, $V_0 = \alpha\sqrt{1-z_0}$, $kx = \frac{E-E_0}{\hbar c}x \approx d^2(z+z_0)\frac{2\times 10^{-3}}{\delta}\left(1+\frac{b}{2}+\xi\right) = (V_0^2+T_1^2)\frac{2\times 10^{-3}}{\delta}\left(1+\frac{b}{2}+\xi\right)$, $d = \delta\times 10^{-8}$ cm, $W_1 = W_5 = W$, $W_2 = W_4 = We^{-V_1(1+b/2)}$, $W_3 = We^{-V_1(1+b/2)}$

$$\frac{\cosh(V_2) + \sqrt{z_0/(1+z_0)}\sinh(V_2)}{\cos\frac{V_3 b}{2}}.$$

These results are due to $2\times 10^{-3}/\delta \ll 1$ approximately

$$I_1 = iW_1T_1e^{-V_1(1+\frac{b}{2})}\left[\frac{A_1}{V_1+iT_1} - \frac{B_1}{V_1-iT_1}\right],$$

$$I_2 = \frac{W_2T_2}{2}\left\{\left(1+\sqrt{\frac{z_0}{1+z_0}}\right)\left[-\frac{A_2(e^{V_2-T_2}-1)}{V_2-T_2} + \frac{B_2(e^{V_2+T_2}-1)}{V_2+T_2}\right]+\right.$$
$$\left.+\left(1-\sqrt{\frac{z_0}{1+z_0}}\right)\left[\frac{A_2(e^{-V_2-T_2}-1)}{V_2+T_2} + \frac{B_2(e^{-V_2+T_2}-1)}{T_2-V_2}\right]\right\},$$

$$I_3 = -\frac{2W_3T_3}{V_3^2-T_3^2}\left(V_3\cos\frac{V_3b}{2}\sin\frac{T_3b}{2} + T_3\sin\frac{V_3b}{2}\cos\frac{T_3b}{2}\right)\times$$
$$\times(A_3e^{iT_3(1+\frac{b}{2})} + B_3e^{-iT_3(1+\frac{b}{2})}),$$

Table 1

The eigenenergies of the single potential well and the double barrier (BWB) for different b-values ($b = c/d$ is the ratio between the barrier and the well width).

$a=2,\ y=1$

b	0.5	0.768	0.8	1	1.5	2	2.4	3	3.15	3.5	3.9	4	4.7	5	6.25	7	7.1
well	0.19	0.34	0.35	0.45	0.63	0.73	0.79	0.85	0.858	0.878	0.898	0.902	0.924	0.932	0.953	0.961	0.962
									10^{-14}	0.06	0.166	0.192	0.357	0.411	0.587	0.659	0.667
																0.107	0.124
BWB	—	3×10^{-4}	0.03	0.01	0.51	0.67	0.74	0.82	0.835	0.861	0.884	0.889	0.916	0.924	0.949	0.959	0.96
									—	—	—	0.034	0.256	0.33	0.545	0.629	0.638
																—	0.011

$a=2,\ y=5$

b	0.1	0.18	0.185	0.5	0.7	1	1.4	1.5	1.55	1.6	2	2.2	2.3	2.5	2.99	3	3.2
well	0.23	0.67	0.7	2.51	3.22	3.85	4.29	4.36	4.387	4.42	4.59	4.67	4.72	4.717	4.792	4.793	4.815
								0.14	0.267	0.404	1.53	2.18	2.52	2.526	3.156	3.167	3.357
															0.257	0.276	0.671
BWB	—	—	0.01	2.25	3.08	3.78	4.25	4.33	4.362	4.39	4.58	4.64	4.66	4.71	4.787	4.788	4.811
								—	—	0.414	1.35	1.86	2.07	2.44	3.105	3.116	3.315
															—	0.016	0.482

$$I_4=\frac{W_4T_2}{2}\left\{\left(1+\sqrt{\frac{z_0}{1+z_0}}\right)\left[-\frac{A_4(e^{V_2+T_2}-1)}{V_2+T_2}+\frac{B_4(e^{V_2-T_2}-1)}{V_2-T_2}\right]+\right.$$

$$\left.+\left(1-\sqrt{\frac{z_0}{1+z_0}}\right)\left[\frac{A_4(e^{-V_2+T_2}-1)}{T_2-V_2}-\frac{B_4(e^{-V_2-T_2}-1)}{V_2+T_2}\right]\right\},$$

$$I_5=\mathrm{i}\,W_5A_5T_1\,\frac{e^{2i(T_1-V_1)(1+\frac{b}{2})}}{V_1-\mathrm{i}T_1},$$

where the coefficients A_j, B_j are to be determined from the formulae given in paper [1].

The most important contribution to the overlapping integral (4) comes from region III (the wave function decreases exponentially in barriers). Neglecting the other contributions

$$|h|^2=|I_3|^2=\frac{4W_3^2T_3^2}{(V_3^2-T_3^2)^2}\left(V_3\cos\frac{V_3b}{2}\sin\frac{T_3b}{2}+T_3\sin\frac{V_3b}{2}\cos\frac{T_3b}{2}\right)^2\times$$

$$\times\left\{|A_3|^2+|B_3|^2+2\,\mathrm{Re}\,(A_3B_3^*)\cos\left[2T_3\left(1+\frac{b}{2}\right)\right]-\right.$$

$$\left.-2\,\mathrm{Im}\,(A_3B_3^*)\sin\left[2T_3\left(1+\frac{b}{2}\right)\right]\right\}.$$

REFERENCES

[1] Takács, S.: Acta Phys. Slov. *30* (1980), 193.
[2] Krempaský, J., Dieška, P.: Phys. Stat. Sol. (b) *56* (1973), 365.
[3] Kane, E. O.: *Tunnelling phenomena in solids* (Eds. Burstein, E., Lundqist, S.). Plenum Press, New York 1969.
[4] Jánossy, L., Király, P., Werner, A.: Acta Phys. Hung. *43* (1977), 31.
[5] Pišút, J., Gomolčák, L.: *Kvantová mechanika*, ALFA Bratislava 1975.
[6] Bohm, D.: *Quantum Theory*, Prentice-Hall, New York 1952.
[7] Heitler, W.: *The Quantum Theory of Radiation*, Clarendon Press, Oxford 1952.
[8] Ridley, B. K., Watkins, T. B.: J. Phys. Chem. Solids *22* (1961), 155.
[9] Janetka, I.: Acta Phys. Slov., *following paper*

[10] Grinberg, A. A.: Fiz. techn. poluprov. *11* (1977), 1909.
[11] Beljavskij, V. I., Sviridov, V. V.: Fiz. techn. poluprov. *15* (1979), 979.
[12] Olejníková, B., Hrivnák, Ľ., Kedro, M.: Phys. Stat. Sol. (b) *107* (1981), 451.
[13] Roy, D. K.: *Tunnelling and negative resistance phenomena in semiconductors*. Pergmamon Press, Oxford—New York—Toronto—Sidney—Paris—Frankfurt 1977.