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ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

Liviu Gr. Ixaru

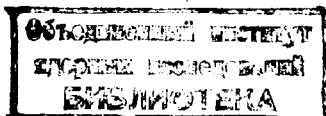
ON THE PENETRABILITIES IN QUANTUM  
MECHANICS

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The tunnel effect has been firstly notified forty years ago when G. Gamow<sup>1/</sup>, trying a theoretical description for alpha decay of heavy nuclei, has pointed out that in the frame of quantum mechanics, contrary to the classical mechanics case, a particle can pass through a potential barrier even if the maximum height of the barrier is larger than the particle energy.

During the following years important efforts have been made in order to study this effect in greater detail<sup>2-4/</sup> and, with that end in view, a new ad hoc parameter, named as penetrability or transparency, has been introduced.

As a matter of fact, there are several distinct definitions for this parameter or, in other words, the tunnel effect is quantitatively marked by an ensemble of parameters and although each of the elements belonging to this ensemble has the same name—penetrability, they are carrying different physical meanings.

Of course, approximate calculation formulae can be derived for each penetrability depending on the approximations involved in the estimations of the wave functions.

Unfortunately, the existence of distinct definitions of the penetrability, on the one hand, and of various approximate formulae corresponding to each definition, on the other hand, is often unobserved. More exactly one compares usually different approximate formulae as if they would come from one and the same definition and this often leads to some confusions.

The aim of this paper is to review briefly some distinct definitions for penetrabilities and to obtain exact calculation formulae as well as JWKB-approximate formulae for each penetrability.

The potential used here has a simplest form but is in the author's views to continue this work by extending these estimations for potentials having more complicated forms.

### 1. The Statement of the Problem

The tunnel effect is mainly involved during the study of two kinds of physical processes: scattering and decay.

Both processes have a common characteristic feature: the positions<sup>x)</sup> of the particles taking part in such processes are strongly time-dependent. So, in a collision, for example, at  $t \rightarrow -\infty$  when the experiment starts, the particles, which are very far apart, are ejected towards one another. While time passing they bring together nearer and nearer, interact and finally ( $t \rightarrow +\infty$ ) move off again.

Obviously, a rigorous treatment of such a problem can be performed by solving a time-dependent Schroedinger equation and using wave packets in order to localize involved particles.

As Goldberger and Watson have shown in their brilliant book on collisions<sup>/5/</sup>, this rigorous treatment leads to results which are identical<sup>xx)</sup> to those given by the formal treatment (or, as one often says, the formal theory).

According to this theory both scattering and decay processes can be described by a time-independent Schroedinger equation and specific character of each of them is incorporated in the boundary conditions which are to be imposed in order to solve this equation.

<sup>x)</sup> Obviously, within the quantum mechanics language, this word is an improper one. It indicates usually the space region where the wave function is significantly different from zero.

<sup>xx)</sup> We tacitly suppose anywhere in this paper that the Hamilton operator is a time-independent one.

One of the most important consequences of different boundary conditions is, as is well known, that for a scattering process the energy spectrum is real and continuous while it is complex and discrete for a decay one.

The present paper will use the formal theory only.

It is perhaps worthwhile to illustrate the formal theory on a simplest case. This insertion is made only due to didactic reasons and certain readers could reading this papers simply by skipping over these considerations.

Our example is the one-dimensional collision of two particles having the masses  $m_1$  and  $m_2$ , respectively.

Let us denote by  $x_1$  and  $x_2$  their positions and suppose that their mutual interaction is described by the potential function  $V(x_1 - x_2)$  where, as one sees on fig. 1,  $\lim_{x_1 - x_2 \rightarrow -\infty} V = 0$  and  $\lim_{x_1 - x_2 \rightarrow +\infty} V = V \neq 0$ .

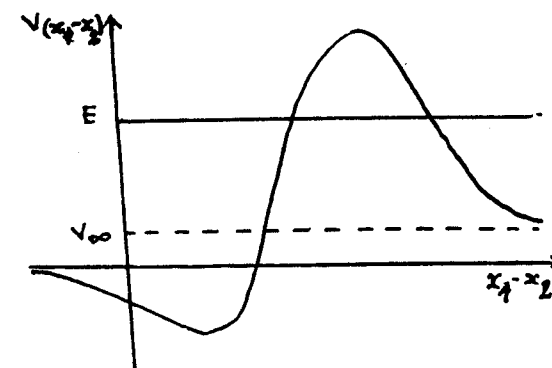


Fig. 1.

As we previously said, this process can be described by solving a time-independent Schroedinger equation, i.e.,

$$-\frac{\hbar^2}{2m_1} \frac{d^2 \Psi(x_1, x_2)}{dx_1^2} - \frac{\hbar^2}{2m_2} \frac{d^2 \Psi(x_1, x_2)}{dx_2^2} + V(x_1 - x_2) \Psi(x_1, x_2) = E \Psi(x_1, x_2) \quad (1)$$

subject to certain boundary conditions.

In the following we will establish these conditions. In order to settle our ideas, let us suppose that at the beginning of the experiment ( $t \rightarrow -\infty$ ) the particle  $m_1$  is coming from the left while  $m_2$  from the right side of fig.2, and  $\hbar k_1, \hbar k_2$  are their momenta. Obviously, in this case  $k_1$  is a positive and  $k_2$  a negative quantities. The wave function corresponding to this moment is

$$e^{i k_1 x_1} \cdot e^{i k_2 x_2} \quad (x_2 \gg x_1). \quad (2)$$

The particles are going on their nearness and interact with each other. After that they move off again, in such a manner that at  $t \rightarrow +\infty$  two situations can take place:



Fig.2

a). Each particle is returning towards its initial region ( $m_1$  on the left side and  $m_2$  on the right one, on fig.2). b) The particles have interchanged their positions and  $m_1$  is now on the right, while  $m_2$  on the left. If we denote by  $\hbar k'_1, \hbar k'_2, \hbar \lambda_1, \hbar \lambda_2$  the momenta of the particles in each of two possibilities just mentioned above, the wave functions of our system are

$$e^{i k'_1 x_1} \cdot e^{i k'_2 x_2} \quad (x_2 \gg x_1) \quad (3)$$

corresponding to a) case (in any rate  $k' > 0$ ) and

$$e^{i \lambda_1 x_1} \cdot e^{i \lambda_2 x_2} \quad (x_2 \ll x_1) \quad (4)$$

for b) case. Here  $\lambda_1 > 0$ .

So far we have used the intuition only.

The second stage in finding the boundary conditions consists in the application word for word of the formal theory prescription:

1. We ignore the physical evidence that the wave functions (2), on the one hand, and (3), (4) on the other hand, are taking place at distinct times.

2. We remark that both (2) and (3) are valid within the same spatial domain ( $x_2 \gg x_1$ ) and urge for  $\Psi$  to be a linear combination of them, i.e.:

$$\Psi(x_1, x_2) = C_1 e^{i(k_1 x_1 + k_2 x_2)} + C_2 e^{i(k'_1 x_1 + k'_2 x_2)} \quad (x_2 - x_1 \gg 0) \quad (5)$$

In addition

$$\Psi(x_1, x_2) = C_3 e^{i(\lambda_1 x_1 + \lambda_2 x_2)} \quad (x_2 - x_1 \ll 0) \quad (6)$$

yielding as a linear combination of (4) itself.

3. The wave numbers  $k_1, k_2, k'_1, k'_2, \lambda_1, \lambda_2$  satisfy the equations

$$\frac{\hbar^2 k_1^2}{2m_1} + \frac{\hbar^2 k_2^2}{2m_2} = \frac{\hbar^2 k'_1{}^2}{2m_1} + \frac{\hbar^2 k'_2{}^2}{2m_2} = E, \quad (7)$$

$$\frac{\hbar^2 \lambda_1^2}{2m_1} + \frac{\hbar^2 \lambda_2^2}{2m_2} = E - V_\infty, \quad (8)$$

due to the energy conservation law, and

$$k_1 + k_2 = k'_1 + k'_2 = \lambda_1 + \lambda_2 \quad (9)$$

by the force of the momentum conservation law.

As a conclusion, the equations (5), (6) satisfying (7), (8), (9) are the boundary conditions of (1) for the problem under consideration.

This problem can be reduced to a simpler one by performing, as usually, the coordinate transformation:

$$r = x_1 - x_2 \quad (10)$$

$$x = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} \quad (11)$$

Using them the equation (1) becomes:

$$-\frac{\hbar^2}{2(m_1+m_2)} \frac{d^2\Psi(r,x)}{dx^2} - \frac{\hbar^2}{2m} \frac{d^2\Psi(r,x)}{dr^2} + V(r)\Psi(r,x) = E\Psi(r,x) \quad (12)$$

while the boundary conditions (5), (6) get the following aspect

$$\Psi(r,x) = e^{i(k_1+k_2)x} (C_1 e^{ipr} + C_2 e^{-ipr}) \quad (r \ll 0) \quad (13)$$

$$\Psi(r,x) = C_3 e^{i(k_1+k_2)x} e^{-iqr} \quad (14)$$

Here:

$$m = \frac{m_1 m_2}{m_1 + m_2} \quad (15)$$

$$p = \frac{1}{m_1 + m_2} (m_2 k_1 - m_1 k_2) = -\frac{1}{m_1 + m_2} (m_2 k'_1 - m_1 k'_2) \quad (16)$$

$$q = \frac{1}{m_1 + m_2} (m_2 \lambda_1 - m_1 \lambda_2). \quad (17)$$

By taking as a guide the separation of the functions which we see in the equations (13), (14) of the boundary conditions we will introduce the new function  $\Psi(r)$  defined as<sup>x)</sup>:

$$\Psi(r,x) = e^{i(k_1+k_2)x} \Psi(r). \quad (18)$$

Now, by straightforward calculation, it is easy to verify that  $\Psi(r)$  is the solution of the equation

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi(r)}{dr^2} + V(r)\Psi(r) = \epsilon\Psi(r) \quad (19)$$

for  $r \in (-\infty, +\infty)$ , subject to the boundary conditions

$$\Psi(r) = C_1 e^{ipr} + C_2 e^{-ipr} \quad (r \ll 0) \quad (20)$$

$$\Psi(r) = C_3 e^{-iqr} \quad (r \gg 0), \quad (21)$$

<sup>x)</sup> The fact that the same  $\Psi$  is appearing in both sides of the equation (18) is not to induce confusions: the left hand  $\Psi$  is obeying (1) while the right hand  $\Psi$  is obeying (19).

where

$$\epsilon = E - \frac{\hbar^2}{2(m_1+m_2)} (k_1+k_2)^2 \quad (22)$$

represents the energy in c.m.s.

One remark is to be made: the usual quantities involved in all the definitions for the penetrabilities are  $|\Psi(x_1, x_2)|^2$  and the current density  $J$  which is defined as

$$J_\phi = \frac{1}{2} (\phi^*(x_1, x_2) v \phi(x_1, x_2) - \phi(x_1, x_2) v \phi^*(x_1, x_2)) \quad (23)$$

where

$$v = -i\hbar \left( \frac{1}{m_1} \frac{d}{dx_1} - \frac{1}{m_2} \frac{d}{dx_2} \right) \quad (24)$$

is the velocity operator. By using (10) and (11) it is easy to see that

$$|\Psi(x_1, x_2)|^2 = |\Psi(r)|^2 \quad (25)$$

and

$$J_{\Psi(x_1, x_2)} = J_{\Psi(r)} = \frac{1}{2} (\Psi^*(r) v \Psi(r) - \Psi(r) v \Psi^*(r)), \quad (26)$$

where  $v$  expressed in  $r, x$  variables is

$$v = -\frac{i\hbar}{m} \frac{d}{dr}, \quad (27)$$

i.e. it does not depend on  $x$ . As a conclusion, all the subsequent considerations can be performed in c.m.s.

## 2. Penetrabilities for the One-Dimensional Scattering Problems

As we can see from the equation (16),  $p$  is a positive quantity. Consequently, as the formal theory says, the first term of the right part of (19) represents a wave propagating from the left to the right, or, in the language of the old variables  $x_1$  and  $x_2$  the both

particles  $m_1$  and  $m_2$  approach each other nearer and nearer (fig.3a). The second term is a wave propagating in the opposite sense or, in other words, the distant  $m_1$  and  $m_2$  particles move off again and again. (See fig.3b). As it concerns  $\Psi(r)$  given by (20), it represents a wave propagating from the left to the right but corresponding to the case when  $m_1$  and  $m_2$  have interchanged their positions (fig.3c).

Intuitively, the penetrability must characterize the transition from the situation envisaged on fig.3a to that represented of fig.3c. We now denote by  $P$  the projection operator on the outgoing functions (i.e. corresponding to fig.3a, 3b):

$$P \Psi(r) \Big|_{r \rightarrow -\infty} = C_1 e^{ip_1 r} ; P \Psi(r) \Big|_{r \rightarrow +\infty} = C_2 e^{iq_1 r} \quad (28)$$

The first definition for the penetrabilities is <sup>[6-8]</sup> :

$$P_{+\infty, -\infty} = \frac{J_{O \Psi(r) | r \rightarrow +\infty}}{J_{O \Psi(r) | r \rightarrow -\infty}} = \frac{q}{p} \left| \frac{C_2}{C_1} \right|^2 \quad (29)$$

As we can see this definition connects the value of currents in the extreme regions of the real axis and for this reason we will call it asymptotic current penetrability (ACOP). It provides only a gross information about the potential  $V(r)$ .

A more subtle information would be obtained by defining the penetrabilities for limited regions of the real axis. For example, it would be necessary to study only the penetrability of the first barrier belonging to the potential  $V(r)$ , shown on fig.4. In order to do it we approximate  $V(r)$  by a sequence of step functions and consider the intervals  $i = [r_1, r_{i+1}]$  and  $j = [r_j, r_{j+1}]$  bordering this barrier.

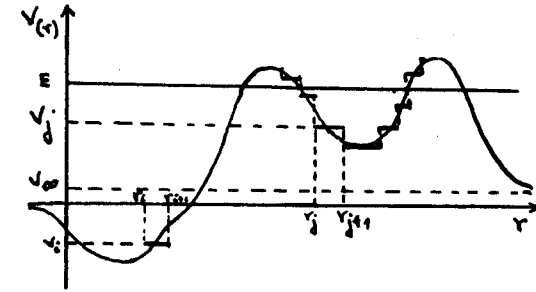
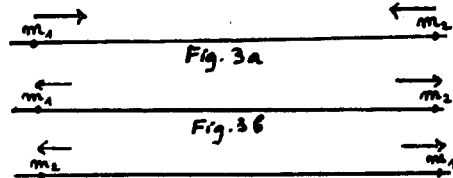


Fig.4

The Schrodinger equation is :

$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi(r)}{dr^2} + V_i \Psi(r) = \epsilon \Psi(r) \quad (30)$$

within  $i$  interval, and

$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi(r)}{dr^2} + V_j \Psi(r) = \epsilon \Psi(r) \quad (31)$$

within  $j$  interval.

Now, by denoting:

$$p_i = \frac{1}{\hbar} \sqrt{2m(\epsilon - V_i)}, \quad q_j = \frac{1}{\hbar} \sqrt{2m(\epsilon - V_j)} \quad (32)$$

we must solve the Schrodinger equation (19) for the interval  $[r_1, r_{i+1}]$ , subject to the boundary conditions

$$\Psi(r) = C_{11} e^{ip_1 r} + C_{21} e^{-ip_1 r} \quad (r \rightarrow r_1) \quad (33)$$

$$\Psi(r) = C_{1j} e^{iq_j r} \quad (r \rightarrow r_{j+1}) \quad (34)$$

We can now define a local one-dimensional penetrability (LCOP) for this barrier:

$$P_{j,i} = \frac{J_{O \Psi(r) | r=r_{j+1}}}{J_{O \Psi(r) | r=r_1}} = \frac{q_j}{p_i} \left| \frac{C_{1j}}{C_{11}} \right|^2 \quad (35)$$

As we remark, the LCOP definition is inadequate when  $p_1$  or  $q_1$  are very small. This is, perhaps, the reason for which Gamow have avoided to define penetrabilities using the currents.

The asymptotic Gamow one-dimensional penetrability (AGOP) is simply<sup>1,9/</sup>:

$$P_{+\infty, -\infty} \equiv \frac{|\Psi(r)|_{r \rightarrow +\infty}^2}{|\Psi(r)|_{r \rightarrow -\infty}^2} = \left| \frac{C_2}{C_1} \right|^2 \quad (36)$$

while for the local Gamow-type penetrability (LGOP) the definition is:

$$P_{j,1} \equiv \frac{|\Psi(r)|_{r=r_1+1}^2}{|\Psi(r)|_{r=r_1}^2} = \left| \frac{C_{1j}}{C_{11}} \right|^2 \quad (37)$$

### 3. Penetrabilities for the Three-Dimensional Scattering Problems

According to the formal theory, the scattering of the two particles  $m_1$  and  $m_2$  is described, in c.m.s., by the time-independent equation<sup>x)</sup>:

$$-\frac{\hbar^2}{2m} \Delta \Psi(\vec{r}) + v(r) \Psi(\vec{r}) = \epsilon \Psi(\vec{r}). \quad (38)$$

Here  $m$  is, as usually, the reduced mass of two particles, (15). The boundary conditions which are to be imposed are generally rather complicated but they get a simplest form if we additionally impose as the two particle system to have a given total angular momentum  $\ell$ . In this case, by using spherical coordinates  $(r, \theta, \phi)$ , the wave function can be separated<sup>xx)</sup>:

$$\Psi(\vec{r}) = \frac{\Psi(r)}{r} Y_{\ell m}(\theta, \phi). \quad (39)$$

Here  $Y_{\ell m}(\theta, \phi)$  is the familiar spherical function, the eigenfunction of the operator

x) We suppose that the mutual interaction potential  $v(r)$  is a central one.

xx) Again we are not to fall into confusion as  $\Psi$  is appearing within both sides of (39).

$$\nabla_{\theta, \phi}^2 = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} (\sin \theta \frac{\partial}{\partial \theta}) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \quad (40)$$

subject to the condition to be continuous, single-valued and finite throughout the ranges  $0 \leq \theta \leq \pi$ ,  $0 \leq \phi \leq 2\pi$  and normalized as:

$$\int d\Omega Y_{\ell m}^*(\theta, \phi) Y_{\ell' m'}(\theta, \phi) = \delta_{\ell \ell'} \delta_{m m'} \quad (41)$$

By inserting (39) into (38) we find that  $\Psi(r)$  satisfies the equation

$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi(r)}{dr^2} + v(r) \Psi(r) = \epsilon \Psi(r) \quad (42)$$

for  $r \in [0, +\infty)$  and

$$v(r) = U(r) + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} \quad (43)$$

In order to fix our ideas, let us suppose that  $v(r)$  have for  $r > 0$  the form given on fig.1. The boundary conditions for (42) are, according to the formal scattering theory requests:

$$\Psi(0) = 0 \quad (44)$$

coming from the fact that  $\Psi(\vec{r})$  of (39) must be a finite one at the origin and

$$\Psi(r) = C_1' e^{iqr} + C_2' e^{-iqr} \quad (r \gg 0). \quad (45)$$

Now, the current for the three-dimensional problem has a similar definition as for the one-dimensional case, i.e.

$$\vec{j}_{\phi}(\vec{r}) = \frac{1}{2} (\phi^*(\vec{r}) \vec{C} \phi(\vec{r}) - \phi(\vec{r}) \vec{C} \phi^*(\vec{r})), \quad (46)$$

where

$$\vec{C} = -\frac{i\hbar}{m} \nabla_{\vec{r}} = -\frac{i\hbar}{m} \left( \vec{i}_r \frac{\partial}{\partial r} + \vec{i}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \vec{i}_\phi \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right). \quad (47)$$



Due to the fact that in this three-dimensional case we are dealing with surface we must take into account the flux of particles through-out a surface  $S$  :

$$\Phi = \int_S \vec{j} \cdot \vec{n} dS \quad (48)$$

In this definition  $d\vec{S} = \vec{n} dS$  and  $\vec{n}$  is the unit vector normal to the surface element  $dS$  and if  $S$  is the surface of a  $r$  radius sphere we have  $d\vec{S} = \vec{e}_r r^2 d\Omega = \vec{e}_r r^2 d(\cos\theta) d\phi$ . If we calculate the flux by using (39) and the relations

$$\vec{e}_r \cdot \vec{e}_\theta = 0, \quad \vec{e}_r \cdot \vec{e}_\phi = 0 \quad (49)$$

we easily obtain:

$$\Phi(r) = \int_S \vec{j} \cdot \vec{n} dS = -\frac{i\hbar}{2m} \left( \Psi^*(r) \frac{d\Psi(r)}{dr} - \Psi(r) \frac{d\Psi^*(r)}{dr} \right) = J_{\Psi(r)} \quad (50)$$

As a conclusion the flux value is given by calculating the current for the function  $\Psi(r)$ .

At the first sight it would seem that the definition for the penetrabilities given in the one-dimensional case could be extrapolated word by word for the three-dimensional one. This is not the case at least for the following reasons:

1. In the one-dimensional case the domain of  $r$  was  $(-\infty, +\infty)$  while now it is  $[0, +\infty)$  and at least asymptotic penetrabilities can not be introduced.

2. Let us look what physical meaning would have a LCOP for the three-dimensional case. Supposing that  $j$  is at very large distance we would have, according to (35) and (45):

$$P_{+\infty, j} = \frac{q}{p_j} \left| \frac{C_{j1}'}{C_{j1}} \right|^2 \quad (51)$$

but, if for the one-dimensional problem the function  $C_{j0} e^{iqr}$  really represents the particles which have already passed through the barrier, the term  $C_{j1}' e^{iqr}$  of the last problem represents both the escaped particles and the incident particles after their reflection on the bar-

rier. Consequently such a "penetrability" really describes a mixture between tunnel and reflection effect.

In order to define the penetrabilities for the three-dimensional problem generally one renounces the scattering-type boundary conditions (44), (45), by replacing them by a new one:

$$\Psi(r) = C_{j0} e^{iqr} \quad (52)$$

and no condition at the origin <sup>x)</sup>.

This new problem (42), (52) is alike <sup>xx)</sup> the one-dimensional one and consequently LCOP and LGOP applied to it really represent the tunnel effect. We will call them LCTP and LGTP.

Besides them there are in the literature other definitions. For example we can adopt for local penetrability the definition:

$$P_{j, l} = \frac{m}{\hbar} \frac{J_0 \Psi(r) |_{r=r_{j+1}}}{|\Psi(r)|^2_{r=r_j}} = \frac{q_j |C_{j1}|^2}{|C_{j1}|^2 + |C_{j2}|^2 + C_{j1}^* C_{j2} e^{-2ip_j r_j} + C_{j1} C_{j2}^* e^{2ip_j r_j}} \quad (53)$$

which, in the partial asymptotic case becomes

$$P_{+\infty, j} = \frac{m}{\hbar} \frac{J_0 \Psi(r) |_{r \rightarrow +\infty}}{|\Psi(r)|^2_{r=r_j}} = \frac{q |C_{j0}|^2}{|C_{j1}|^2 + |C_{j2}|^2 + C_{j1}^* C_{j2} e^{-2ip_j r_j} + C_{j1} C_{j2}^* e^{2ip_j r_j}} \quad (54)$$

<sup>x/</sup> The solution of (42), (52) is different from zero at the origin and consequently it seems to be meaningless from physical point of view. This is only one of the short comings of the formal theory in the framework of which we are working. In reality (42), (52) are the formal theory equations for the particle spreading problem that is, if we would rigorously study the problem of the spreading of particles continuously ejected by a particle generator situated at the origin of the reference system we would obtain the same results as solving (42), (52).

<sup>xx/</sup> In fact they are identical except the  $r$  domain, because (20) does not impose any restrictive conditions on  $\Psi(r)$ .

Those definitions are currently used by Wigner's group<sup>/10-16/</sup> and for this reason they will be called LWTP and AWTP, respectively.

Both definitions have a peculiar surprising feature: according to them the penetrability has the dimension (length)<sup>-1</sup>, contrary to the other reviewed definitions which are dimensionless.

In order to avoid this, Lane and Thomas<sup>/17/</sup> have used the definition:

$$P_{j,l} = \frac{m r_l}{\hbar} \frac{\int_0^j \Psi(r) |_{r=r_{j+1}}}{|\Psi(r)|^2_{r=r_l}} \quad (55)$$

for local penetrability (LLTP) and

$$P_{+\infty,l} = \frac{m r_l}{\hbar} \frac{\int_0^j \Psi(r) |_{r \rightarrow +\infty}}{|\Psi(r)|^2_{r=r_l}} \quad (56)$$

for the asymptotic one<sup>x)</sup>. Both (55), (56) are dimensionless.

Finally, it is worthwhile to point out again that for the three-dimensional scattering problem all the penetrability definitions are coming not from the scattering equation (42), (44), (45), but from the ad hoc equation (42), (52).

#### 4. Comparison between Various Definitions of the Penetrabilities

As we have already shown the Schroedinger equation yielding formulae for penetrabilities are the same for one-dimensional and three-dimensional problems except the domain of  $r$ .

We put down again this equation:

$$-\frac{\hbar^2}{2m} \frac{d^2 \Psi(r)}{dr^2} + V(r) \Psi(r) = \epsilon \Psi(r) \quad (57)$$

with the condition

$$\Psi(r) = C_3 e^{-iqr} \quad (r \gg 0) \quad (58)$$

<sup>x)</sup> The same definition is used by Vogt<sup>/18/</sup>.

and choose as a potential the function

$$V(r) = \begin{cases} 0 & r \leq r_1 \\ V_0 & r_1 < r \leq r_2 \\ V_\infty & r_2 < r \end{cases} \quad (59)$$

(See the fig.5).

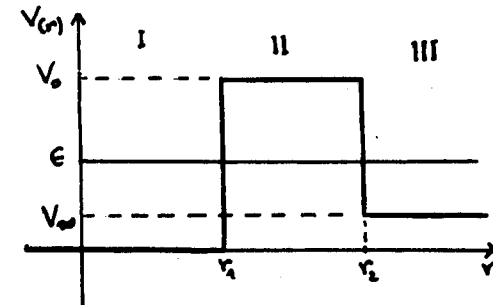


Fig.5

#### a) Exact Calculation Formulae

According to this form of the potential we solve the Schroedinger equation within each of the domains I, II, III, as on the fig.5, and after that we connect the solutions at the joining points  $r_1$  and  $r_2$ . If we denote:

$$p = \frac{1}{\hbar} \sqrt{2m\epsilon}, \quad \omega = \frac{1}{\hbar} \sqrt{2m(V_0 - \epsilon)}, \quad q = \frac{1}{\hbar} \sqrt{2m(\epsilon - V_\infty)} \quad (60)$$

we find:

$$\Psi(r) = C_1^I e^{ipr} + C_2^I e^{-ipr} \quad r \in I \quad (61)$$

$$\Psi(r) = C_1^{II} e^{i\omega r} + C_2^{II} e^{-i\omega r} \quad r \in II \quad (62)$$

$$\Psi(r) = C_1^{III} e^{iqr} + C_2^{III} e^{-iqr} \quad r \in III \quad (63)$$

Using the boundary condition (58) we obtain

$$C_1^{III} = C_2^I, \quad C_2^{III} = 0. \quad (64)$$

We now connect (61), (62), (63) by requiring that at the joining points  $r_1$  and  $r_2$  the functions and their first derivative be equal. So, we have at the  $r_1$  joining point:

$$C_1^I e^{ipr_1} + C_2^I e^{-ipr_1} = C_1^{II} e^{\omega r_1} + C_2^{II} e^{-\omega r_1} \quad (65)$$

$$ip C_1^I e^{ipr_1} - ip C_2^I e^{-ipr_1} = \omega C_1^{II} e^{\omega r_1} - \omega C_2^{II} e^{-\omega r_1} \quad (66)$$

and at the  $r_2$  joining point

$$C_1^{II} e^{\omega r_2} + C_2^{II} e^{-\omega r_2} = C_3 e^{iqr_2} \quad (67)$$

$$\omega C_1^{II} e^{\omega r_2} - \omega C_2^{II} e^{-\omega r_2} = iq C_3 e^{iqr_2} \quad (68)$$

By introducing the notations

$$B_1 = \frac{C_2^I}{C_1^I}, \quad A_2 = \frac{C_1^{II}}{C_1^I}, \quad B_2 = \frac{C_2^{II}}{C_1^I}, \quad A_3 = \frac{C_3}{C_1^I} \quad (69)$$

the equations (65), (66), (67) and (68) constitute the system:

$$\begin{aligned} B_1 e^{-ipr_1} - A_2 e^{\omega r_1} - B_2 e^{-\omega r_1} &= -e^{ipr_1} \\ -ip B_1 e^{-ipr_1} - \omega A_2 e^{\omega r_1} + \omega B_2 e^{-\omega r_1} &= -ipe^{ipr_1} \end{aligned} \quad (70)$$

$$A_2 e^{\omega r_2} + B_2 e^{-\omega r_2} - A_3 e^{iqr_2} = 0$$

$$\omega A_2 e^{\omega r_2} - \omega B_2 e^{-\omega r_2} - iq A_3 e^{iqr_2} = 0.$$

As we can see, in order to estimate the penetrabilities, only  $A_3$  and  $B_1$  must be calculated. After easy but rather long calculation by means of the determinantal method we obtain from (70):

$$A_3 = \frac{-4ip\omega e^{ipr_1} e^{-iqr_2}}{\omega^2 (e^{\omega(r_2-r_1)} - e^{-\omega(r_2-r_1)}) - i(p+q)\omega (e^{\omega(r_2-r_1)} + e^{-\omega(r_2-r_1)}) - qp (e^{\omega(r_2-r_1)} - e^{-\omega(r_2-r_1)})} \quad (71)$$

$$B_1 = -e^{2ipr_1} \frac{\omega^2 (e^{\omega(r_2-r_1)} - e^{-\omega(r_2-r_1)}) + i(p-q)\omega (e^{\omega(r_2-r_1)} + e^{-\omega(r_2-r_1)}) + qp (e^{\omega(r_2-r_1)} - e^{-\omega(r_2-r_1)})}{\omega^2 (e^{\omega(r_2-r_1)} - e^{-\omega(r_2-r_1)}) - i(p+q)\omega (e^{\omega(r_2-r_1)} + e^{-\omega(r_2-r_1)}) - qp (e^{\omega(r_2-r_1)} - e^{-\omega(r_2-r_1)})} \quad (72)$$

If the involved barrier is thick enough (i.e., for example  $\omega(r_2-r_1) > 10$ ) the term  $e^{-\omega(r_2-r_1)}$  is very small as compared with  $e^{\omega(r_2-r_1)}$ . By supposing that this happens for our barrier, we will neglect  $e^{-\omega(r_2-r_1)}$ , and with this fine approximation,

$$A_3 = -\frac{4ip\omega}{(\omega-ip)(\omega-iq)} e^{ipr_1} e^{-iqr_2} e^{-\omega(r_2-r_1)} \quad (73)$$

$$B_1 = -\frac{\omega+ip}{\omega-ip} e^{2ipr_1} \quad (74)$$

Now, because for the chosen potential the regions bordering the barrier are just asymptotical, the asymptotic penetrabilities will be equal to the local penetrabilities.

Using (73), (74) we obtain the following formulae:

$$\begin{aligned} \text{ACOP, LCOP} & \\ \text{LCTP} & \quad P_{+\infty, -\infty} = \frac{q}{p} |A_3|^2 = \frac{16p\omega^2 q}{(\omega^2+p^2)(\omega^2+q^2)} e^{-2\omega(r_2-r_1)} \quad (75) \end{aligned}$$

$$\begin{aligned} \text{AGOP, LGOP} & \\ \text{LGTP} & \quad P_{+\infty, -\infty} = |A_3|^2 = \frac{16p^2\omega^2}{(\omega^2+p^2)(\omega^2+q^2)} e^{-2\omega(r_2-r_1)} \quad (76) \end{aligned}$$

$$\begin{aligned} \text{AWTP, LWTP} & \quad P_{+\infty, 1} = \frac{q |A_3|^2}{1 + |B_1|^2 + B_1 e^{-2ipr_1} + B_1^* e^{2ipr_1}} = \\ & = \frac{8q\omega^2 p^2}{(\omega^2+p^2)(\omega^2+q^2)(1 - \cos 2[p(r_1-r_1) + \arctg \frac{p}{\omega}])} e^{-2\omega(r_2-r_1)} (\text{length})^{-1} \quad (77) \end{aligned}$$

$$\text{ALTP, LLTP} \quad P_{+\infty,1} = \frac{8q\omega^2 p^2 r_1}{(\omega^2 + p^2)(\omega^2 + q^2)(1 - \cos 2[p(r_1 - r_1) + \arctg \frac{q}{\omega}])} e^{-2\omega(r_2 - r_1)} \quad (78)$$

b) JWKB Formulae

As is well known the solution of the equation (57) with the boundary condition (58), is, in the JWKB approximation<sup>/19/</sup>

$$\Psi(r) = \begin{cases} \phi(r) e^{i \int_{r_2}^r \phi(\xi) d\xi} e^{i \frac{\pi}{4}} & r > r_2 \\ \phi(r) e^{i \int_r^{r_2} \phi(\xi) d\xi} & r_1 < r < r_2 \\ 2\phi(r) e^{i \int_r^{r_1} \phi(\xi) d\xi} \cos \left[ \int_r^{r_1} \phi(\xi) d\xi - \frac{\pi}{4} \right] & r < r_1 \end{cases} \quad (79)$$

where

$$\phi(r) = \frac{1}{h} \sqrt{2m|V(r) - \epsilon|} \quad (80)$$

and  $r_1, r_2$  are the inner and outer turning points, i.e. the roots of the equation  $V(r) - \epsilon = 0$ . For our potential we immediately obtain

$$\Psi(r) = \begin{cases} \frac{1}{q} e^{i \frac{\pi}{4}} e^{-iqr_2} e^{iqr} & r > r_2 \\ \frac{1}{\omega} e^{-\omega r_2} e^{-\omega r} & r_1 < r < r_2 \\ \frac{1}{p} e^{i \frac{\pi}{4}} e^{\omega(r_2 - r_1)} e^{-ipr_1} e^{ipr} + \frac{1}{p} e^{-i \frac{\pi}{4}} e^{-\omega(r_2 - r_1)} e^{ipr_1} e^{-ipr} & r < r_1 \end{cases} \quad (81)$$

By inspecting this formula we get  $A_8$  and  $B_1$ :

$$A_8 = \left(\frac{p}{q}\right)^{1/2} e^{ipr_1} e^{-iqr_2} e^{-\omega(r_2 - r_1)} \quad (82)$$

$$B_1 = e^{-i \frac{\pi}{2}} e^{2ipr_1} \quad (83)$$

The penetrabilities:

$$\text{ACOP, LCOP} \quad P_{+\infty, -\infty} = \frac{q}{p} |A_8|^2 = e^{-2\omega(r_2 - r_1)} \quad (84)$$

$$\text{AGOP, LGOP} \quad P_{+\infty, -\infty} = |A_8|^2 = \frac{p}{q} e^{-2\omega(r_2 - r_1)} \quad (85)$$

$$\text{AWTP, LWTP} \quad P_{+\infty, 1} = \frac{p}{2(1 - \cos 2[p(r_1 - r_1) + \frac{\pi}{4}])} e^{-2\omega(r_2 - r_1)} \frac{1}{(\text{length})} \quad (86)$$

$$\text{ALTP, LLTP} \quad P_{+\infty, 1} = \frac{pr_1}{2(1 - \cos 2[p(r_1 - r_1) + \frac{\pi}{4}])} e^{-2\omega(r_2 - r_1)} \quad (87)$$

Some final remarks:

1. The formula (84), having unity as preexponential factor corresponds only to ACOP, LCOP, LCTP, in the frame of the JWKB approach and can not be used for estimating other penetrabilities as Poggenburg did<sup>/20/</sup>.

2. Gamow and Crichfield<sup>/9/</sup>, using the JWKB approach, have obtained for AGOP the formula

$$P_{+\infty, -\infty} = 4 \frac{p}{q} e^{-2\omega(r_2 - r_1)} \quad (88)$$

The appearance of the factor 4 is due to the fact that they connect the JWKB functions at the turning points, that is to say exactly where they do not hold. The rigorous treatment by Fröman<sup>/19/</sup> leads to the formula (85).

3. The discrepancies between exact and JWKB penetrabilities are embodied within the function

$$f(p, \omega, q) = \frac{|A_8|_{\text{JWKB}}^2}{|A_8|_{\text{EXACT}}^2} = \frac{p}{q} \frac{(\omega^2 + p^2)(\omega^2 + q^2)}{16p^2 \omega^2} = \frac{(a^2 + 1)(\beta^2 + 1)}{16a\beta} = f(a, \beta), \quad (89)$$

where

$$\alpha = \frac{p}{\omega}, \quad \beta = \frac{q}{\omega} \quad (90)$$

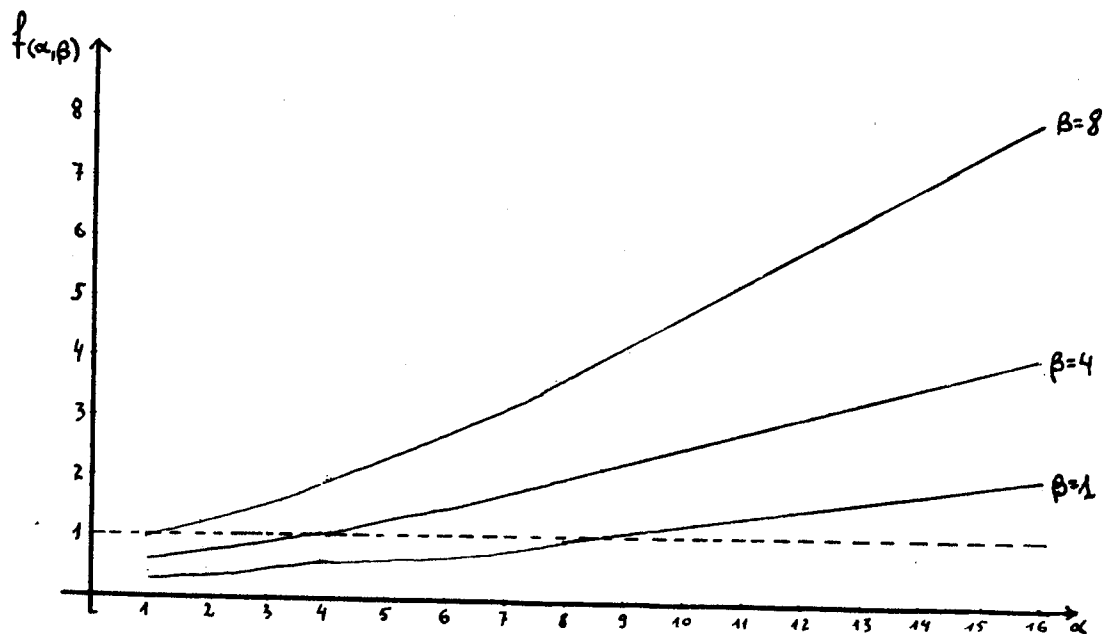


Fig.6

The fig .6 presents  $f(\alpha, \beta)$  for  $\alpha > 1$  and several  $\beta \geq 1$ . The other values are easily derived from this figure if we note that

$$f(\alpha, \beta) = f\left(\alpha, \frac{1}{\beta}\right) = f\left(\frac{1}{\alpha}, \beta\right) = f\left(\frac{1}{\alpha}, \frac{1}{\beta}\right).$$

The conclusion is the JWKB approximation underestimates the penetrabilities if  $\alpha$  and  $\beta$  are about unity and overestimates them for  $\alpha$  and  $\beta$  strongly different of 1.

5. It is perhaps a shocking fact that the denominator of Wigner and Lane-Thomas penetrabilities becomes vanishing for certain values of  $r_1$ . Generally, in the concrete problems, these penetrabilities are to be calculated at  $r_1$ 's where  $|\Psi(r_1)|^2$  is maximum.

6. The penetrabilities can not be experimentally measured because the problems (19), (20), (21) and (42), (52) yielding penetrabilities are corresponding to the one-dimensional scattering and three-dimensional particle spreading processes which are, obviously, non-experimental ones.

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