

On the tunneling of electrons out of the potential well in an electric field

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Abstract The exact solution of the non-stationary problem of the tunneling of electrons out of the one-dimensional potential well by the steady electric field when it is suddenly switched on is obtained. The formula for the tunnel current density is found. The results obtained are compared with those of stationary tunneling theory that corresponds to the adiabatic switching on of the electric field. It is noted that the especially strong dependence of the tunnel current on the way the electric field is switched on arises in the case of the well a few bound states. This dependence should be taken into account while analysing experimental data on tunneling (atom ionisation, for example) in an electric field.

1. Introduction

In this paper the exact solution of the non-stationary problem of the electron tunneling out of the one-dimensional well in a steady electric field is given. The main result is that the electron tunneling out of the well is a quantum transition of the electron from the bound state in the well to the state which represents a super position of both quasi-stationary states and continuous spectra states and the subsequent simultaneous penetration of the electron wave 'through' the barrier via the channels corresponding to the bound electron states in the well.

We consider the electron tunneling out of the well under the influence of an electric field as a non stationary quantum mechanical problem. The electric field causing the tunnel transition is assumed to be switched on at some moment of time. The initial condition imposed on the solution of the Schrödinger time equation corresponds to the localised electron state in the well. Such an approach was used by Drukarjev (1951) while investigating the particle transfer through the potential barrier in the case of the long-range potential. The present paper generalises Drukarjev's results to the case of the long-range potential describing the electric field. This case turns out to be technically more complicated than that of the short-range potential as the energy distribution function for the initial state is not a meromorphic function which is in agreement with the results of Krylov and Fock (1947)

To formulae for the wavefunction of the bound state disintegrating under the influence of the electric field and for the electron tunnel current density out of the well are derived in the following sections. The case of the well with the single bound state is considered. The results obtained are compared with those of the stationary theory of tunneling. The difference between them is considerable especially in the case of the well with a few bound states and also remains in the case of the well with the single bound state. This is accounted for by the fact that in the non-stationary theory under the influence of the field impact due to the switching on of the electric field, the electron is largely knocked out of the initial level and goes over to the wavepacket state that does not make any appreciable contribution to the tunnel current. In the appendix we present formulae for the wavefunctions of stationary states and derive some relations required for the tunnel current calculation

2. The wavefunction

Let us consider the problem of electron tunneling out of the one-dimensional potential well $V_0(z) = V_0[\theta(-z-L) + \theta(z)]$ under the influence of the electric field \mathcal{E} , which is switched on at the moment of time $t = 0$ in the half-plane $z > 0$. The Hamiltonian of the model is written as follows

$$H(z, t) = H_0(z) + \theta(t)H_{\text{int}}(z) \quad (1)$$

$$H_0(z) = -\frac{1}{2m} \frac{d^2}{dz^2} + V_0(z); \quad H_{\text{int}}(z) = -e\mathcal{E}z\theta(z)$$

The potential energy of an electron $V_1(z)$ at $t > 0$ is represented in figure 1. We shall search for the solution $\psi_E(z, t)$ of the Schrödinger time equation with the Hamiltonian $H(z, t)$, satisfying the initial condition

$$\psi_E(z, 0) = \varphi_E(z) \quad (2)$$

where $\varphi_E(z)$ is the eigenfunction of the Hamiltonian $H_0(z)$ with the eigenvalue E ($E < V_0$).

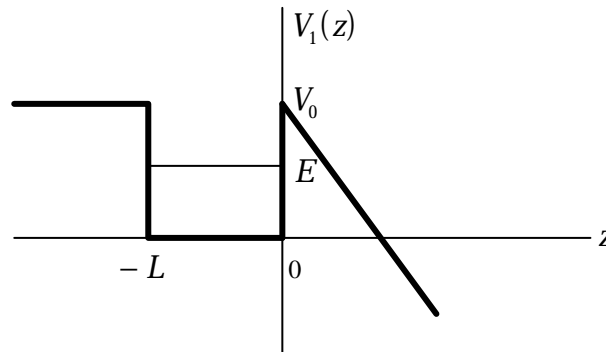


Figure 1. Potential energy of the electron in an electric field

(V_0 and L - are the depth and width of potential well)

We expand the wavefunction $\mathbf{y}_E(z, t)$ in terms of the eigenfunction $\phi_E(z)(E < V_0)$ and $\phi_{E\sigma}(z)(E > V_0)$ of the Hamiltonian $H_0(z) + H_{\text{int}}(z)$:

$$\Psi_E(z, t) = \int_{-\infty}^{V_0} dE' e^{-iE't} F_1(E') + \int_{V_0}^{\infty} dE' e^{-iE't} F_2(E') \quad (3)$$

$$F_1(E') = a_{E'}(E) \phi_{E'}(z); \quad F_2(E') = \sum_{\sigma=\pm 1} a_{E'\sigma}(E) \phi_{E'\sigma}(z) \quad (4)$$

Here the index σ takes into account the double degeneration of energy levels at $E > V_0$, the constant coefficient $a_{E'}(E)$ and $a_{E'\sigma}(E)$ are determined by the initial condition (2):

$$a_{E'}(E) = \int dz \phi_{E'}^*(z) \phi_E(z) \quad (5)$$

$$a_{E'\sigma}(E) = \int dz \phi_{E'\sigma}^*(z) \phi_E(z); \quad \sigma = \pm 1$$

Using the formulae given in the appendix functions $F_1(E')$ and $F_2(E')$ may be transformed into the form

$$F_n(E') = \frac{\delta m'}{\pi k_2'} \frac{\left[\kappa_1 \Lambda_1(E') P_n(E') - i k_2' \Lambda_2(E') \right] (y')^{1/2} H_{1/3}^{(1)}(\zeta')}{\left(y_0' \right)^{1/2} H_{1/3}^{(1)}(\zeta_0') - \frac{i}{k_2'} \frac{d}{dz} \left[\left(y_0' \right)^{1/2} H_{1/3}^{(1)}(\zeta_0') \right] P_n(E')} + c.c. \quad (6)$$

where the prime (') means that in the corresponding quantity one ought to put $E = E'$,

$$P_1(E') = i \frac{\cos k_2' L + \frac{\kappa_1'}{k_2'} \sin k_2' L}{\sin k_2' L - \frac{\kappa_1'}{k_2'} \cos k_2' L} \quad (7)$$

the function $P_2(E')$ is determined by the right-hand side of formula (7) if κ_1' is replaced by $-i k_1'$. The rest of the notation is given in appendix 1. It should be noted that formula (3) and (6) are precise. The errors arising in the subsequent relations are connected only with the approximate calculations of the integrals involved in (3) and (A2.6).

First of all, we fix the argument phase of Hankel's functions $H_{\frac{1}{3}}^{(n)}(\zeta)$ ($n=1,2$), namely, we assume that $y = |y|e^{-i\pi}$ at $y < 0$. Besides, for simplicity we shall later calculate the wavefunction $\psi_E(z, t)$ at $z > b$ (see figure 1).

To calculate the integrals involved in (3), let us consider the contour integrals $I_n = \int_{C_n} dE' e^{-iE't} F_1(E')$, ($n=1,2$), $I_3 = \int_{C_3} dE' e^{-iE't} F_2(E')$, where the contours C_n ($n=1,2,3$) in the plane of complex variable E' are shown in figure 2. Note that for the functions $F_1(E')$ and $F_2(E')$ the point $E' = V_0 = E_1$ is the branch point and the points $E' = 0 = E_2$ and $E' = V_0(1 - z/b) \equiv E_3$ are not singular. Nevertheless, for convenience the contours C_n pass around all these points along the infinitely small circle arcs shown in figure 2.

Firstly, we consider the integral I_1 . It can be shown that the function $F_1(E')$ behaves like

$$\exp\left[-\frac{2}{3}(2m)^{\frac{1}{2}}(b/V_0)|V_0 - E'|^{\frac{3}{2}}\left(\cos\frac{3}{2}\psi + i\sin\frac{3}{2}\psi\right)\right]$$

$$\text{at } -(E' - V_0) = |E' - V_0|e^{i\psi}, \quad \text{Re } E' \rightarrow -\infty$$

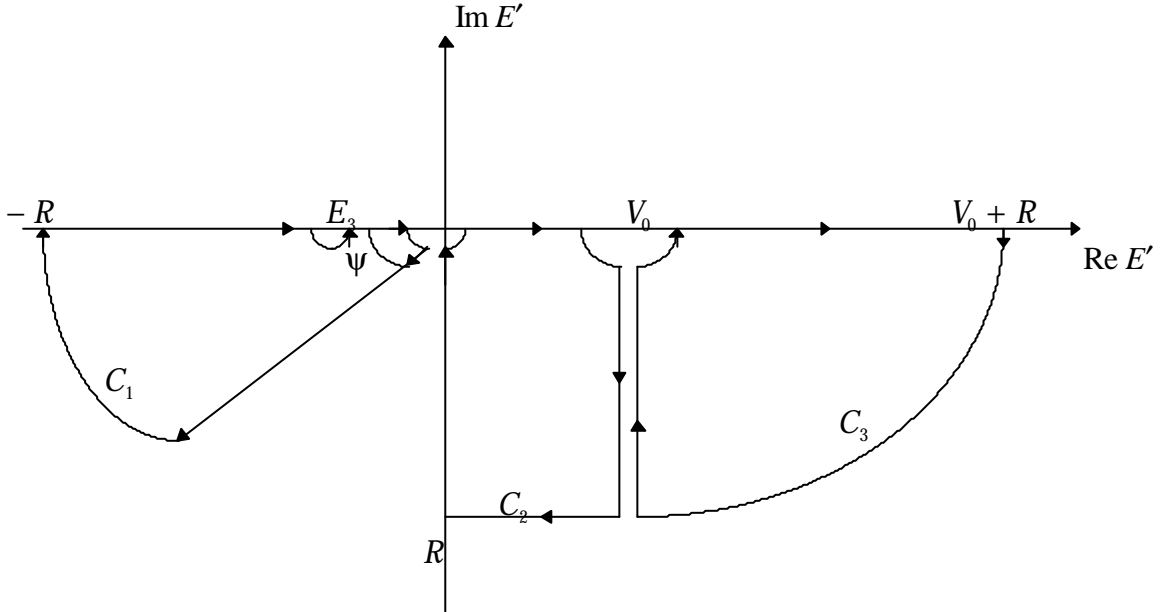


Figure 2. The integration contours in the plane of a complex variable E'

Therefore, the angle ψ (see contour C_1) must be in the interval $(0, \frac{1}{3}\pi - 0)$; in this case the integral along the contour C_1 are of the radius $R \rightarrow \infty$ vanishes. The integrals along the arcs of the radius $r \rightarrow 0$ vanish as well. Applying Cauchy's theorem on residues to the integral I_1 , we obtain the formula

$$\begin{aligned} & \int_{-\infty}^0 dE' e^{-iE't} F_1(E') = \\ & = e^{i\psi} \int_0^{\infty} dx \exp(ixte^{i\psi}) F_1(xe^{-i\pi+i\psi}) - 2\pi i \sum_{\text{Re } s C_1} e^{-iE't} F_1(E') \end{aligned}$$

where $\sum_{\text{Re } s C_1}$ is the sum of residues in the poles located inside the contour C_1 .

The integrals I_2 and I_3 are investigated analogously. By means of the formulae obtained in this way we arrive at the following expression for the wavefunction

$$\begin{aligned} \Psi_E(z, t) = & \int_0^{\infty} dx \left\{ \exp[i\psi + ixte^{i\psi}] F_1(xe^{-i\pi+i\psi}) - ie^{-xt} F_1(xe^{-i\pi/2}) \right\} + \\ & + ie^{-iV_0 t} \int_0^{\infty} dx e^{-xt} \left[F_1(V_0 + xe^{-i\pi/2}) - F_2(V_0 + xe^{-i\pi/2}) \right] - \\ & - 2\pi i \left[\sum_{\text{Re } s C_1, C_2} e^{-iE't} F_1(E') + \sum_{\text{Re } s C_3} e^{-iE't} F_2(E') \right] \end{aligned} \quad (8)$$

Formula (8) is correct if the condition

$$t - \xi^{\frac{2}{3}} V_0^{-1} (z/b - 1)^{\frac{2}{3}} > 0, \quad \xi \equiv (2mV_0 b^2)^{\frac{2}{3}} \quad (9)$$

is satisfied. It can be shown that with increasing z the wavefunction sharply decreases if the opposite inequality is fulfilled.

We investigate the asymptotic behaviour of integrals involved in the right-hand side of the expression (8) at $t \rightarrow \infty$.

We shall now proceed with the evaluation of the first of the integrals. As the integrand rapidly decreases with increasing x , the main contribution is made by a small vicinity of the point $x = 0$. Taking into consideration that the point $x = 0$ is not singular and that

$$\left. \frac{d^n F_1(E)}{dE^n} \right|_{E=xe^{-i\pi+i\psi}} = \left. \frac{d^n F_1(E)}{dE^n} \right|_{E=xe^{-i\pi/2}}$$

at $x \rightarrow +0$; $n = 0, 1, \dots$, and integrating by parts, we arrive at the conclusion that this integral vanishes at $t \rightarrow \infty$.

In the second integral the point $x = 0$ is the branch point of the integral. Owing to this fact, the integral does not vanish. The following representation takes place:

$$F_1(V_0 + xe^{-i\pi/2}) - F_2(V_0 + xe^{-i\pi/2}) = \sqrt{x} \mathcal{F}(x, z) \quad (10)$$

where the function $\mathcal{F}(x, z)$ has no singularity at $x = 0$. In view of the rapid decrease of the integrand with increasing x , we may replace the function $\mathcal{F}(x, z)$ by its expansion in a power series in x , retaining only the first two expansion terms

$$\mathcal{F}(x, z) = \mathcal{F}_0(z) + x \mathcal{F}_1(z) \quad (11)$$

The formula for $\mathcal{F}_0(z)$, which can be easily deduced with the aid of the equalities (6), (10) and (11) is given by

$$\begin{aligned} \mathcal{F}_0(z) = & (\delta m / \pi) 2ib \sqrt{2m} e^{i\pi/4} y^{1/2} H_{3/3}^{(1)}(\zeta) [b \kappa_1 \Lambda_1(V_0) + \Lambda_2(V_0) B] \times \\ & \left[Ab \sqrt{2mV_0} \sin(L\sqrt{2mV_0}) + B \cos(L\sqrt{2mV_0}) \right]^{-2} \end{aligned} \quad (12)$$

Here the following notation is used ($\Gamma(x)$ is Euler's gamma function)

$$\begin{aligned} y = (z/b)\xi, & \quad A = -2i3^{-1/6} \Gamma^{-1}\left(\frac{2}{3}\right), \\ B = \pi^{-1} 3^{2/3} \xi e^{i\pi/6} \Gamma\left(\frac{2}{3}\right), & \quad \xi = (2mV_0 b^2)^{1/3} \end{aligned}$$

Making use of the above formulae, we obtain

$$\begin{aligned} i e^{-iV_0 t} \int_0^\infty dx e^{-xt} \left[F_1(V_0 + xe^{-i\pi/2}) - F_2(V_0 + xe^{-i\pi/2}) \right] = \\ = i \frac{\sqrt{\pi}}{2t^{3/2}} e^{-iV_0 t} \left\{ \mathcal{F}_0(z) + \frac{2}{3t} \mathcal{F}_1(z) + \dots \right\} \end{aligned} \quad (13)$$

Now we turn to computing the last term in (8). One can easily show that in the regions $\text{Re } E' < 0$ and $\text{Re } E' > V_0$ the poles of the functions $F_1(E')$ and $F_2(E')$ are such (denote them by $E_0 - i\Gamma_0$) that $\Gamma_0 \neq 0$ at $\varepsilon \rightarrow 0$. In the region $0 < \text{Re } E' < V_0$ the picture is quite different: here $\Gamma_0 \rightarrow 0$ at $\varepsilon \rightarrow 0$. Denote the maximum value of the imaginary part of poles in the region $0 < \text{Re } E' < V_0$ by Γ_{\max} . Consider such times t , at which $\Gamma_{\max} t \leq 1$, but $\Gamma_0 t \gg 1$, where Γ_0 is the imaginary part of poles lying outside the region $0 < \text{Re } E' < V_0$. It is obvious that at such times in the formula for the wavefunction one can retain only the residues in poles for which $0 < \text{Re } E' < V_0$. Therefore, we shall further take into account only the residues in these poles. It will henceforth be supposed that the inequality

$$\tilde{y} \equiv \xi \frac{V_0 - E}{V_0} \gg 1 \quad (14)$$

is fulfilled. The above mentioned poles of the function $F_1(E)$, making the greatest contribution to the wavefunction are determined by the dispersion equation:

$$\begin{aligned} & (k_2^2 - \kappa_1^2) \sin k_2 L - 2\kappa_1 k_2 \cos k_2 L + \\ & + (72\tilde{\zeta})^{-1} \left[(5k_2^2 + 7\kappa_1^2) \sin k_2 L + 2\kappa_1 k_2 \cos k_2 L \right] + \\ & + (i/2)(k_2^2 + \kappa_1^2) \sin k_2 L e^{-2\tilde{\zeta}} = 0, \quad \tilde{\zeta} = \frac{2}{3} \tilde{y}^{3/2} \end{aligned} \quad (15)$$

To derive the latter equation we used the asymptotic formulae for Hankel's functions at large argument value.

In the absence of an electric field, equation (15) reduces to equation (A1.4) defining the energy levels $E_n^{(0)}$ of bound electron states in the potential well. The roots E_n of equation (15) are of the form:

$$\begin{aligned} E_n &= E_n^{(0)} + \Delta E_n - i\Gamma_n \\ \Gamma_n &= V_0^{-1} E_n^{(0)} (V_0 - E_n^{(0)}) \left[1 + \frac{1}{2} L \kappa_1(E_n^{(0)}) \right]^{-1} \exp(-2\tilde{\zeta}_n) \\ \Delta E_n &= -\frac{1}{4} E_n^{(0)} \xi^{-3/2} \left[(V_0 - E_n^{(0)}) / V_0 \right]^{-1/2} \left[1 + \frac{1}{2} L \kappa_1(E_n^{(0)}) \right]^{-1}, \quad \tilde{\zeta}_n = \tilde{\zeta} \Big|_{E=E_n^{(0)}} \end{aligned} \quad (16)$$

The following remark is appropriate here. The general decay theory of the unstable system prepared at some moment of time is formulated in the book (Goldberger and Watson 1964) This theory can be applied only to those cases when the poles $E_0 - i\Gamma_0$ of the functions of type $F_1(E')$ and $F_2(E')$ have a limited imaginary part. In the electron tunnelling problem in an electric field the functions $F_n(E')$, as

one may show, have poles with $|\Gamma_0| \rightarrow 0$, which makes Goldberger and Watson's theory inapplicable to the tunnelling investigation.

Neglecting, in accordance with what has been said above, the exponentially small terms, we arrive at the formula

$$-2\pi i \sum_{\text{Re } s < C_2} e^{-iE't} F_1(E') = \sum_n g_n(E) e^{-iE_n t} y_n^{1/2} H_{1/3}^{(1)}(\zeta_n) \quad (17)$$

where the following notation is used:

$$y_n = \xi \left(\frac{z}{b} - 1 + \frac{E_n^{(0)}}{V_0} \right), \quad \zeta_n = \frac{2}{3} y_n^{3/2}$$

$$g_n(E) = \frac{1}{2} e^{i\frac{2\pi}{3}} \left(\frac{\pi}{3} \right)^{\frac{1}{2}} \delta \xi^{\frac{1}{4}} (2mV_0)^{\frac{1}{2}} \left(\frac{V_0 - E_n^{(0)}}{V_0} \right)^{\frac{3}{4}} \frac{E_n^{(0)}}{V_0} \times \quad (18)$$

$$\times \left[1 + \frac{1}{2} L \kappa_1(E_n^{(0)}) \right]^{-1} [\kappa_1 \Lambda_1(E_n) - \kappa_1(E_n) \Lambda_2(E_n)] e^{-\tilde{\zeta}_n}, \quad \kappa_1 \equiv \kappa_1(E)$$

Taking into account formulae (8), (13) and (17), we finally obtain the following expression for the wavefunction

$$\Psi_E(z, t) = i \frac{\sqrt{\pi}}{2t^{3/2}} e^{-iV_0 t} \mathcal{F}_0(z) + \sum_n g_n(E) e^{-iE_n t} y_n^{1/2} H_{1/3}^{(1)}(\zeta_n) \quad (19)$$

3. The tunnel function and discussion

The wavefunction (19) has the same structure as in the short-range potential case (Drukarjev 1951). The first term in the right-hand side of (19) describes a damping transient due to the switching on of an electric field and spreading out of the wavepacket in time. As is known (Baz *et al* 1971) this term predominates over the second one only during a small time interval after switching on the field and also at very large times when the second term becomes exponentially small. Of most interest is the intermediate time region in which the first term can be neglected. In this region the electron tunnel current density is of the form:

$$j_E(z, t) = j_E^{(1)}(t) + j_E^{(2)}(z, t)$$

$$j_E^{(1)}(t) = (3e/\pi m) \xi b^{-1} \sum_n |g_n(E)|^2 e^{-2\Gamma_n t}; \quad (20)$$

$$j_E^{(2)}(z, t) = \sum_{\substack{n, n' \\ (n \neq n')}} g_n g_{n'}^* e^{-it(E_n - E_{n'}^*)} \frac{ie}{2m} y_n^{1/2} H_{1/3}^{(1)}(\zeta_n) \vec{\partial}_z [y_{n'}^{1/2} H_{1/3}^{(1)}(\zeta_{n'})]^*$$

The quantity $j_E^{(1)}(t)$ is the independent of time (at $\Gamma_n t \ll 1$) component of the tunnel current. The oscillating in the time and the space part of current $j_E^{(2)}(z, t)$ is a result of interference between the transition amplitudes corresponding to the electron jumping from the level E in the well to the neighbouring levels. Note that in the formula for $j_E^{(1)}(t)$ we have neglected the smooth dependence on z , arising from $\Gamma_n \neq 0$.

According to formulae (3), (19) and (20) the physical picture of the electron tunnelling phenomenon out of the potential well is as follows. Under the influence of the field impact due to the switching on of an electric field the electron goes over from the stationary state in the well to the state which is superposition of the quasistationary states (i.e. of the states with the finite lifetime $\tau_n = \Gamma_n^{-1}$) and of the continuous spectra states. The tunnelling is a leaking of the electron wave simultaneously through the barrier via those channels which correspond to the energy levels $E_n^{(0)}$ in the well.

Consider the case $L(2mV_0)^{1/2} < \pi$, when there is a single bound state in the well. In this case the total tunnel current $j_E(z, t)$ (20) reduces to the quantity $j_E^{(1)}(t)$, only the term n in (20) corresponding to $E_n^{(0)} = E$ being retained. Calculate the quantity $g_n(E) \equiv g(E)$. Making use of the formula (A2.9), we can easily show that the following equality takes place when condition (A2.8) is satisfied:

$$\kappa_1 \Lambda_1(E') - \kappa_1(E') \Lambda_2(E') \approx \frac{\pi^{1/2}}{4\kappa_1(E)} \frac{E' - E}{V_0} \left(\frac{V_0}{V_0 - E} \right)^{1/4} \xi^{3/4} \quad (21)$$

Putting $E' - E = E_n - E_n^{(0)} \approx \Delta E_n$ in (21) and using (16) and (18), we receive

$$g(E) = -e^{i\frac{2}{3}\pi} \frac{\delta\pi}{16\sqrt{3}} \left(\frac{V_0 - E}{V_0} \right)^{-1/2} \left(\frac{E}{V_0} \right)^2 \xi^{-1/2} [1 + \frac{1}{2} L\kappa_1(E)]^{-2} e^{-\xi} \quad (22)$$

While investigating the electron tunnelling out of the well, the stationary problem is usually studied i.e. the electric field \mathcal{E} is supposed to act constantly in time, without switching on and off. The solution to the stationary Schrödinger equation $H\phi_E(z) = E\phi_E(z)$ with the Hamiltonian $H = H_0(z) + H_{\text{int}}(z)$, obeying the outgoing-wave boundary condition (Baz *et al* 1971, Blokhintsev 1961), is looked for. The outgoing wave condition consists in the requirement that outside the barrier there be only the waves that correspond to the knocking out of the well electrons. Compare the results of the stationary theory of tunnelling with those obtained in this paper. To this end we derive the stationary theory formulae which are analogous to

(18) and (19). As is seen from formula (A1.1) for $\phi_E(z)$, the outgoing-wave condition in the tunnelling problem being considered is expressed by the equality

$$\tilde{R}^{(2)}(E) = 0 \quad (23)$$

which is equivalent to the dispersive equation (15). According to (A1.1), in the region $z > 0$ the electron wavefunction supplemented with the factor e^{-iEt} may be represented in the form (compare with relation (19))

$$\phi_E(z, t) = \tilde{g}(E)^{1/2} H_{\nu}^{(1)}(\zeta) e^{-iEt} \quad (24)$$

$$\tilde{g}_E(E) = \frac{1}{2} \tilde{d} \tilde{R}^{(1)}(E)$$

The constant \tilde{d} is defined by the condition

$$\phi_E(z) = \varphi_E(z) \quad \text{at} \quad z < 0 \quad \text{and} \quad \Gamma_n \rightarrow 0$$

the wavefunctions $\phi_E(z)$ and $\varphi_E(z)$ being expressed by relations (A1.1) and (A1.3). This condition gives: $\tilde{d} = \delta \exp(L\kappa_1)$. Taking into account the relationships (A1.1), (23) and (24), we have

$$\tilde{g}(E) = \delta e^{i\frac{2}{3}\pi} \left(\frac{\pi}{3}\right)^{\frac{1}{2}} \left(\frac{V_0 - E}{V_0}\right)^{\frac{1}{4}} \xi^{\frac{1}{4}} e^{-\zeta} \quad (25)$$

The tunnel current density in the state (24) is given by

$$j_{E_n}(z, t) \equiv (ie/2m) \phi_{E_n}(z, t) \tilde{d} \partial_z \phi_{E_n}^*(z, t) = 2\Gamma_n e^{-2\Gamma_n t}$$

The ratio of the quantities $g(E)$ (22) and $\tilde{g}(E)$ (25) is

$$\frac{g(E)}{\tilde{g}(E)} = -\frac{\pi^{1/2}}{32} \left(\frac{V_0 - E}{V_0}\right)^{-\frac{3}{4}} \left(\frac{E}{V_0}\right)^2 \xi^{-3/4} \left(1 + \frac{1}{2} L\kappa_1\right)^{-2} \approx (e\mathcal{E})^{1/2} \quad (26)$$

According to (26), the electron tunnel current calculated within the consistent non-stationary theory turns out much smaller than in the stationary theory. This is due to the fact that under the influence of the field impact the electron is largely knocked out of the initial bound state, passing to the continuous spectra states. Then the wavepacket formed by these continuous spectra states is spread out in time but in the intermediate time range mentioned above the wavepacket described by the first term in the right-hand side of (19) does not make any appreciable contribution to the tunnel current.

The present theory describes the case of the sudden switching on of an electric field when under the action of the field impact an intense ‘shaking’ of the system takes place. The stationary theory seems to describe the tunnelling in a different limiting case - when the electric field is switched on adiabatically. The appreciable dependence of the tunnel current value upon the way the electric field is switched on should be taken into account while analysing the experimental data on tunnelling (atom ionisation, for instance) in an electric field.

It is of interest that the electric field has a marked effect on the character of the spreading out of the wavepacket in time. Indeed, in the case being considered the wavepacket is spread out in time according to the law $t^{-3/2}$, while in the short-range potential case it is spread out according to the law $t^{-1/2}$ (Drukarjev 1951).

Note that in the stationary tunneling theory, in which the outgoing-wave boundary condition is used, the wavefunction $\phi_E(z, t)$ (24) is exponentially divergent at $z \rightarrow +\infty$. Indeed, making use of the asymptotic formula for the Hankel function and of the formula $E = E' - i\Gamma$ ($E' \equiv \text{Re } E, \Gamma > 0$), we obtain

$$\phi_E(z, t) \approx \exp\left[(\Gamma/V_0)(z/b - 1 + E'/V_0)^{1/2} \xi^{3/2}\right] \text{ at } z \rightarrow +\infty$$

This difficulty is absent, in accordance with the known conclusion (see, for instance, Drukarjev 1951, Blokhintsev 1961, Nussenzveig 1972), in the non-stationary theory of tunnelling.

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Appendix 1. The stationary state wavefunctions

The solutions of the stationary Schrödinger equation with the Hamiltonian $H_0(z) + H_{\text{int}}(z)$ (see equation (1)) are the form

$$\begin{aligned} \phi_{E1}(z) &= d \cdot \left\{ \theta(-z-L)(e^{ik_1z} + \gamma^* e^{-ik_1z}) + \theta(-z)\theta(z+L) \left[(\alpha_1 + \gamma^* \alpha_{-1}^*) e^{ik_2z} + (\alpha_{-1} + \gamma^* \alpha_1^*) e^{-ik_2z} \right] \right. \\ &\quad \left. + \frac{1}{2} \theta(z) \left[y^{1/2} H_{\gamma/3}^{(1)}(\zeta) R^{(1)}(E) + y^{1/2} H_{\gamma/3}^{(2)}(\zeta) R^{(2)}(E) \right] \right\}, \\ \phi_{E,-1}(z) &= \phi_{E1}^*(z), \quad (E > V_0); \\ \phi_E(z) &= \tilde{d} \left\{ \theta(-z-L) e^{\kappa_1 z} + \theta(-z)\theta(z+L) \left(\tilde{\delta}_{-1} e^{ik_2z} + \tilde{\delta}_1 e^{-ik_2z} \right) \right. \\ &\quad \left. + \frac{1}{2} \theta(z) \left[y^{1/2} H_{\gamma/3}^{(1)}(\zeta) \tilde{R}^{(1)}(E) + y^{1/2} H_{\gamma/3}^{(2)}(\zeta) \tilde{R}^{(2)}(E) \right] \right\}, \quad (E < V_0). \end{aligned} \tag{A1.1}$$

Here the following notation is introduced: $H_{\frac{2}{3}}^{(n)}(\zeta)$ - is the Hankel function,

$$\begin{aligned} k_1 &= [2m(E - V_0)]^{\frac{1}{2}}, \\ \kappa_1 &= [2m(V_0 - E)]^{\frac{1}{2}}, \quad k_2 = \begin{cases} (2mE)^{\frac{1}{2}}, & E > 0 \\ -i\kappa_2 = -i(2m|E|)^{\frac{1}{2}} & E < 0, \end{cases} \\ \alpha_\sigma &= \frac{1}{2}(1 + \sigma k_1/k_2) \exp[iL(\sigma k_2 - k_1)], \quad \sigma = \pm 1, \\ R^{(1)}(E) &= \pm \frac{1}{3} \pi \cdot k_2 b \xi^{-1} \left[\beta_1^{(-)}(E) - \gamma^* \beta_1^{(+)}(E) \right], \end{aligned} \quad (\text{A1.2})$$

$$\beta_n^{(+)}(E) = \alpha_1^* L_n^{(-)}(\zeta_0) - \alpha_{-1}^* L_n^{(+)}(\zeta_0), \quad \beta_n^{(-)}(E) = \alpha_1 L_n^{(+)}(\zeta_0) - \alpha_{-1} L_n^{(-)}(\zeta_0),$$

$$L_n^{(\pm)}(\zeta) = y^{\frac{1}{2}} H_{\frac{2}{3}}^{(n)}(\zeta) \pm (i/k_2)(d/dz) [y^{\frac{1}{2}} H_{\frac{2}{3}}^{(n)}(\zeta)], \quad (n = 1, 2)$$

$$\gamma^* = \left(\left| \beta_2^{(-)} \right| / \left| \beta_2^{(+)} \beta_1^{(+)} \right| \right) \left[\left| \beta_2^{(-)} \right| - (2/k_2) \xi^{\frac{1}{2}} b^{-\frac{1}{2}} (3k_1/\pi)^{\frac{1}{2}} \right],$$

$$|d|^2 = \left\{ 4\pi \cdot k_1/m \left(\left| \beta_1^{(+)} \right| / \left| \beta_2^{(+)} \right|^2 \right) \left[\left| \beta_1^{(+)} \right| - (2/k_2) \xi^{\frac{1}{2}} b^{-\frac{1}{2}} (3k_1/\pi)^{\frac{1}{2}} \right] \right\}^{-1},$$

$$\tilde{\delta}_\sigma = \frac{1}{2}(1 + i\sigma \kappa_1/k_2) \exp(-i\sigma \cdot k_2 L - \kappa_1 L), \quad \sigma = \pm 1,$$

$$\tilde{R}^{(1)}(E) = \pm \frac{1}{3} \pi \cdot k_2 \xi^{-1} b \left[\tilde{\delta}_{-1} L_2^{(+)}(\zeta_0) - \tilde{\delta}_1 L_2^{(-)}(\zeta_0) \right],$$

$$b = V_0/eE, \quad \zeta = \frac{2}{3} y^{\frac{2}{3}}, \quad y = \xi \cdot b^{-1} (z - b + Eb/V_0),$$

$$\zeta_0 = \zeta|_{z=0}, \quad y_0 = y|_{z=0}, \quad |\tilde{d}|^2 = \frac{2}{3} m \xi^{-1} b |\tilde{R}^{(1)}(E)|^{-2}, \quad \xi = (2mV_0 b^2)^{\frac{1}{3}}.$$

The following orthogonality and normalisation conditions take place

$$\begin{aligned} \int dz \phi_{E'\sigma'}^*(z) \phi_{E\sigma}(z) &= \delta_{\sigma'\sigma} \delta(E' - E), \\ \int dz \phi_{E'\sigma'}^*(z) \phi_E(z) &= \delta(E' - E) \end{aligned}$$

The formula for the wavefunction of the electron stationary state with the energy E in the well

$V_0(z)$ is written

$$\begin{aligned} \phi_E(z) &= \delta \left\{ \theta(-z-L) e^{\kappa_1 L} (\cos k_2 L + (\kappa_1/k_2) \sin k_2 L) e^{\kappa_1 z} \right. \\ &\quad \left. + \theta(-z) \theta(z+L) \frac{1}{2} \left[(1 + i\kappa_1/k_2) e^{ik_2 z} + (1 - i\kappa_1/k_2) e^{-ik_2 z} \right] + \theta(z) e^{-\kappa_1 z} \right\} \end{aligned} \quad (\text{A1.3})$$

$$\delta = (\kappa_1 E/V_0)^{\frac{1}{2}} \left(1 + \frac{1}{2} L \kappa_1 \right)^{-\frac{1}{2}}.$$

The normalisation constant δ is defined by the condition $\int dz |\phi_E(z)|^2 = 1$. The electron energy levels E in the well are the roots of the dispersion equation;

$$(k_2^2 - \kappa_1^2) \sin k_2 L - 2\kappa_1 k_2 \cos k_2 L = 0. \quad (\text{A1.4})$$

Appendix 2. Calculation of the coefficients $a_{E'\sigma}(E)$ and $a_{E\sigma}(E)$.

The quantity $a_{E'\sigma}(E)$, defined by (5) may be readily reduced to the form

$$a_{E'\sigma}(E) = \frac{\delta}{E' - E} \int_0^\infty dz \phi_{E'\sigma}^*(z) H_{\text{int}}(z) e^{-\kappa_1 z}, \quad \kappa_1 \equiv \kappa_1(E), \quad (\text{A2.1})$$

$\delta = \delta(E)$. In the derivation of this formula we have made use of the relation (A1.3).

Let us introduce the notation

$$Y_{E'\sigma}(\kappa) = \int_0^\infty dz \phi_{E'\sigma}^*(z) e^{-\kappa z}, \quad (\text{A2.2})$$

The coefficient $a_{E'\sigma}(E)$ is expressed in terms $Y_{E'\sigma}(\kappa)$ by the relation:

$$a_{E'\sigma}(E) = [\delta/(E' - E)] \cdot e^{\mathcal{E}} (d/d\kappa) Y_{E'\sigma}(\kappa) \Big|_{\kappa=\kappa_1(E)}, \quad (\text{A2.3})$$

The function $Y_{E'\sigma}(\kappa)$ satisfies the equation:

$$e^{\mathcal{E}} (d/d\kappa) Y_{E'\sigma} - (E' - V_0 + \kappa^2/2m) Y_{E'\sigma} = (2m)^{-1} \left(\phi_{E'\sigma}^*(z) \vec{\partial}_z e^{-\kappa z} \right) \Big|_{z=0}.$$

The solution of this equation obeying the condition $Y_{E'\sigma}(\infty) = 0$ is of the form:

$$Y_{E'\sigma}(\kappa) = \frac{\kappa}{2me^{\mathcal{E}}} \int_0^\infty d\eta \cdot \exp \left\{ -\frac{(E' - V_0)\kappa}{e^{\mathcal{E}}} \eta - \kappa^3 \frac{(1+\eta)^3 - 1}{6me^{\mathcal{E}}} \right\} \left[\kappa(1+\eta) \phi_{E'\sigma}^*(z) + \frac{d}{dz} \phi_{E'\sigma}^*(z) \right] \Big|_{z=0} \quad (\text{A2.4})$$

With the aid of (A2.3) and (A2.4), we obtain the sought after relationship

$$a_{E'\sigma}(E) = \delta \left\{ \Lambda_1(E') \kappa_1 \phi_{E'\sigma}^*(z) + \Lambda_2(E') \frac{d}{dz} \phi_{E'\sigma}^*(z) \right\} \Big|_{z=0}, \quad (\text{A2.5})$$

where the functions $\Lambda_n(E')$ ($n = 1, 2$), are defined by the equalities

$$\Lambda_n(E') = \frac{\kappa_1}{2me^{\mathcal{E}}} \int_0^\infty d\eta \cdot a_n(\eta) \cdot \exp \left\{ -\frac{(E' - V_0)\kappa_1}{e^{\mathcal{E}}} \eta - \kappa_1^3 \frac{(1+\eta)^3 - 1}{6me^{\mathcal{E}}} \right\} - \frac{1}{2m(E' - E)};$$

$$a_1(\eta) = 1 + \eta, \quad a_2(\eta) = 1. \quad (\text{A2.6})$$

One can easily show that the quantity $a_{E\sigma}(E)$ is defined by the right-hand side of the equality (A2.5) after replacing $\phi_{E'\sigma}^*(z)$ by $\phi_{E\sigma}^*(z)$ in it.

Write out approximate expression for the functions $\Lambda_n(E')$, derived under the assumption that

$$\kappa_1^3/6me\mathcal{E} \equiv \beta \gg 1, \quad (\text{A2.7})$$

in two limiting cases.

Case 1. $|E' - E| \ll V_0$ or, to be more precise,

$$|\gamma|(3\beta)^{-1/2} \ll 1, \quad \gamma \equiv (E' - E)\kappa_1/e\mathcal{E}. \quad (\text{A2.8})$$

In this case

$$\Lambda_n(E') = (2me\mathcal{E} \cdot \kappa_1)^{-1/2} \left(\frac{1}{2}\pi^{1/2} + \varepsilon_n / 3(3\beta)^{1/2} - \gamma / (12\beta)^{1/2} \right) - 1/2m(E' - E), \quad (\text{A2.9})$$

$$\varepsilon_1 = 1, \quad \varepsilon_2 = -\frac{1}{2};$$

Case 2. $V_0 - E' \ll V_0 - E \sim V_0$, (A2.10)

In this case

$$\Lambda_n(E') = -\frac{1}{2m} \frac{(V_0 - E')^2}{(E' - E)(V_0 - E)^2} - \tilde{\varepsilon}_n \frac{2me\mathcal{E}}{\kappa_1^5}, \quad (\text{A2.11})$$

$$\tilde{\varepsilon}_1 = 1, \quad \tilde{\varepsilon}_2 = 2.$$

References

- Baz A I, Zel'dovich Ja B and Perelomov A M 1971 *Scattering, reactions and decay in the nonrelativistic quantum mechanics* (Moscow: Nauka) (in Russian)
- Blokhintsev D I 1961 *Foundations of quantum mechanics* (Moscow: Vysshaja shola) (in Russian)
- Drukarjev D F 1951 *Zh. Eksp. Teor. Fiz.* **21** 59-68
- Goldberger M and Watson K 1964 *Collision theory* (New York: Wiley)
- Krylov N S and Fock V A 1947 *Zh. Eksp. Teor. Fiz.* **17** 93-107
- Landau L D and Lifshitz E M 1958 *Quantum mechanics* (Reading, Mass.: Addison-Wesley)
- Nussenzveig H M 1972 *Causality and dispersion relations* (New York: Academic)