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ON THE LIFETIME OF QUASI-STATIONARY LEVELS DURING TUNNELING IN A RESONANT TUNNEL STRUCTURE

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Abstract. We investigate field emission in resonant tunneling heterostructures with one quantum well and two barriers, as well as the influence of the lifetime of resonant metastable levels formed in the well on it. The problem of the tunneling time of a quantum particle (electron) through a structure with a barrier and two barriers and a well is also considered. Stationary and nonstationary Schrodinger equations are used. The lifetimes of metastable levels are determined and their effect on tunnel current is investigated.

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1. INTRODUCTION

Resonant tunneling structures (RTS), which are nanoscale heterostructures with field emission, are widely used in electronics as sources of very high current densities (up to 10^{14} A/m²) [1–3]. They also form the basis for designing resonant tunneling diodes (RTD), transistors, quantum cascade lasers (QCL) of the "Stark ladder" type, THz transistors and switches [4–11], as well as other devices. For all these applications, switching times, response times, and overall transient times are crucial [11,12].

RTS is characterized by having one, two, or several quantum wells separated by barriers, where quasi-stationary resonance levels can arise [13]. We will refer to the electron-emitting left electrode as the cathode (denoted by the subscript c) and the right electrode as the anode (subscript a). For the intermediate electrode (grid), the subscript g will be used. In the case of equal electrochemical potentials of the electrodes $\mu_c = \mu_a$, the quantum potential V(x) between the two electrodes (in a diode structure) resembles an inverted parabola on a pedestal and can be strictly described by an infinite series of images that account for the electron work functions [1]. Approximating this series with an inverted parabola is rather crude [1,14]. A more accurate approximation is a fourth-order inverted parabola [1,2]. In this work, we will use an even more precise approximation for the potential in the diode $0 < x < d$ under anode voltage U_a:

$$V(x) = E_{Fc} + W_c \frac{(1-\alpha/d)(1+\delta/d)^2}{(1-\delta/d)^2\varepsilon} \times$$

$$\times\left[1 - \frac{\delta d}{\left(x+\delta(1-x/d)\right)\left(d-x+x\delta/d\right)}\right] - \frac{eU_a x}{d}. \quad (1)$$

In this formula, $\alpha = \delta\left(2\ln(2)+1\right)$ represents the cathode work function, assumed equal for both the cathode and anode $W_c = W_a$, and is related to the parameter (gap size) δ by the equation:

$$W_a = e^2/(16\pi\varepsilon_0\delta).$$

For simplicity, we will further assume equal Fermi energies $E_{Fc} = E_{Fa}$ for the electrodes. Under potential $V(x)V(x)V(x)$, the boundary conditions are $V(0) = E_{Fa}$ at the cathode and $V(d) = E_{Fa} - eU_a = \mu_a$, at the anode, meaning the quantum potential V coincides with the electrochemical potentials. In cases with different work functions (and materials of the cathode and anode), an additional term $(E_{Fa} - E_{Fc})x/d$ should be added to (1). The accuracy of equation (1) is no worse than 1%. Diode structures do not allow for extremely high current densities. Current increase

occurs through resonant tunneling (RT), where one or more quantum wells are surrounded by barriers [1–3]. Reflections from the barriers interfere, and the total reflection coefficient cancels out. For simplicity, we further consider a single-well structure with three electrodes: cathode (source), grid (gate), and anode (drain). Equation (1) applies both to a vacuum gap ($\varepsilon = 1$), and a dielectric gap between electrodes. In the absence of an anode voltage $U_a = 0$, the potential in the center of the gap is:

$$V\left(d/2\right) = E_{Fc} + \frac{W_c\left(1-\alpha/d\right)\left(1+\delta/d\right)^2}{\left(1-\delta/d\right)^2\varepsilon}.$$

For a work function of 3.6 eV, the corresponding value is $\delta = 0.1$. Thus, for typical work functions of materials (2–5 eV) and typical electrode and gap sizes, RTS structures on the order of nanometers satisfy the inequalities $\delta/d << 1$, $\alpha / d << 1$. In the absence of anode voltage, the inequality $V\left(d/2\right) \approx E_{Fc} + W_c/\varepsilon$ holds. A dielectric with dielectric permittivity ε reduces the barrier height by a factor of ε.

Suitable and convenient dielectrics for RTS include CVD (Chemical Vapor Deposition) diamond ($\varepsilon = 5.6$, bandgap 2.5 eV) [15] and beryllium oxide (BeO, $\varepsilon = 6.7$, bandgap 10.6 eV). These dielectrics significantly reduce the barrier height and have the highest thermal conductivity, which is essential for high current densities [2,3]. Although CVD diamond with 88% sp^3 hybridization has a density of 88.2% of crystalline diamond, its dielectric constant can be taken as 5.6 due to the presence of a small graphite phase. Electrodes can be made of metals or doped semiconductors. Beryllium has the highest Fermi energy (14.6 eV), relatively low work function (3.92 eV), and the highest thermal conductivity among metals. To construct a complex profile V (Fig. 1), equation (1) is applied twice – once for the cathode-grid gap (replacing $U_a \to U_g$) and once for the grid-anode gap, assuming $E_{Fc} \to E_{Fc} - eU_g$. On the grid, the quantum potential is constant and determined by its electrostatic potential U_g.

In RTDs and QCLs, highly conductive layers are usually considered electrically free, meaning the potential along them is not fixed and decreases [4–12]. Figure 1 shows typical profiles of V(x) for diode and triode structures under different anode (U_a) and grid (U_g) voltages for copper electrodes. To form a quantum well, a grid voltage $U_g = E_{Fc}/e$ was applied. The energy E is measured from the

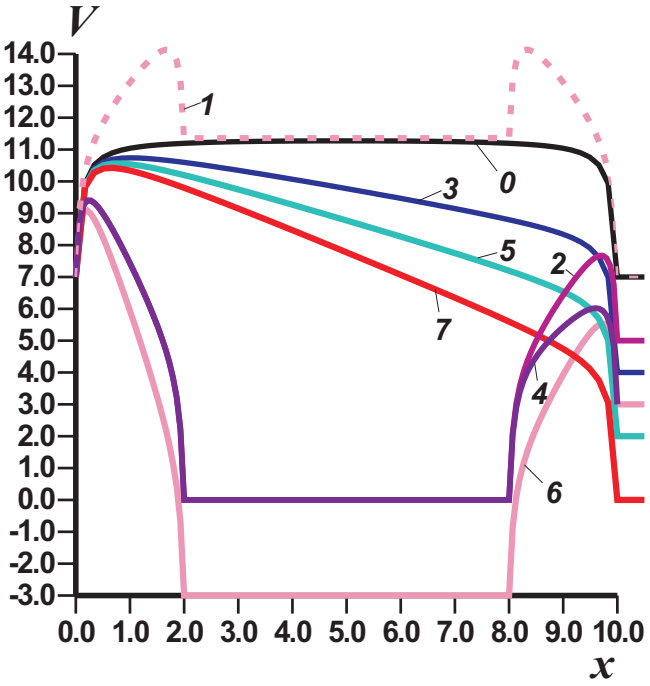

Fig. 1. Potential Barrier Profile V (eV) as a Function of Distance x (nm) in a vacuum diode (curves 0, 3, 5, 7) and a vacuum triode (curves 1, 2, 4, 6). The curve numbers for the diode correspond to the anode voltage U_a in volts. For the triode curves 2 and 4, the grid voltage $U_g = E_F$ is specified, and their numbers correspond to the anode voltage. For curve 1, $U = 0$, $U_g = W_c/e$, while for curve 6, $U_a = 4$ V and $U_g = 3$ V. The work functions are $E_{F_c} = 7$ eV and $W_c = 4.36$ eV (copper electrodes).

conduction band bottom of the cathode, which coincides with the bottom of the well.

If an energy level E_n exists in the formed quantum well, it is quasi-stationary, as there is always an identical level at both the cathode and anode, allowing the electron to tunnel between them. Tunneling can occur both leftward to the cathode and rightward to the anode. Subsequently, the electron transitions from this level to the Fermi level of the corresponding electrode, from which it can enter the power supply circuit, as only electrons near the Fermi level participate in the diffusion current.

The issue of quasi-stationary level lifetime (decay time) in a spherically symmetric quantum well has been addressed in several works, such as [16–18]. However, the lifetime of quasi-stationary levels in a one-dimensional Cartesian RTS has not been strictly studied. This time is closely related to the tunneling time of a single particle through the structure (its dwell time). There is extensive literature on the introduction of various time definitions (see, for example, the reference list in [19]). The topic

of tunneling times remains under discussion, with several paradoxes. Tunneling times are closely linked to the switching times of tunnel devices [11]. RTS devices such as RTDs, QCLs, and other structures are typically modeled using rectangular potentials modified by the term $-eU_a x/d$ [11]. This approach is a rough approximation because high voltages lead to a barrier shape close to a triangle on a pedestal [1]. Schrödinger equation (SE) calculations show that such a barrier is orders of magnitude more transparent than a rectangular barrier of the same height and base width. A semiclassical approximation is often used [16], which can be integrated exactly for a triangular barrier [20]. However, this method is accurate only up to a pre-exponential factor and is quite imprecise in the narrow upper part of the barrier, as it neglects the reflected electron wave [20]. For narrow barriers, the reflected wave contributes significantly. In the analysis of RTS with two or more rectangular barriers, resonance levels are usually defined as the penetration of a particle through identical barriers to the left or right with the same energy as in the well [13]. However, real RTS structures differ. Upon reaching the cathode or anode with a given energy, the particle transitions to the Fermi level of the electrode, emitting or absorbing an energy quantum, and exits the structure with this energy, as any current in conductors is generated by electrons near the Fermi level. Under stationary tunneling (constant anode voltage), the number of electrons tunneling from the cathode is exponentially greater than the number tunneling from the anode, resulting in a constant emission current closing through the power supply. The emergence of resonance levels E'_n leads to resonant tunneling (RT), accompanied by an increase in current, as the barrier becomes fully transparent for electrons with energy $E = E'_n$. Quasi-stationary levels arise with increasing well width. These energy levels are complex: $\tilde{E}_n = E'_n - iE''_n$. The parameter E''_n determines the level lifetime $\tau_n = 2\hbar / E''_n$. The smaller the lifetime, the broader the energy level, the wider the energy range satisfying the condition $E \approx E'_n$, and the greater the number of electrons undergoing resonant tunneling. Thus, determining the lifetimes (complex energies $\tilde{E}_n$) of quasi-stationary levels and their dependence on quantum potential configurations is crucial, which is the primary aim of this study. For field emission, the number of electrons incident per second on the barrier within a velocity interval $v_z + dv_z$ and energy range is: $d\nu(v_z) = n^+(k)v_z dv_z$,

where

$$n^+(k) = \frac{m_e^2 k_B T}{2\pi^2\hbar^3} \times \times \ln\left(1 + \exp\left(\frac{E_{Fc} - E(k)}{k_B T}\right)\right) v_z. \quad (2)$$

Equation (2) is derived by averaging over all transverse velocities of the Fermi gas electrons in the metal cathode and is presented for finite temperatures. For cold emission (T = 0), the spectrum is limited by the Fermi energy:

$$n^+(k) = m_e^2\left(E_{Fc} - E(k)\right)/\left(2\pi^2\hbar^3\right)v_z.$$

Although the actual tunneling process involves a multi-speed electron flux determining the total tunnel current density:

$$J^+(U_a) = \frac{-em_e}{2\pi^2\hbar^3}\int_0^{\mu_c} D^+(E,U_a)(\mu_c - E)dE, \quad (3)$$

this problem can be treated as single-particle tunneling with a specified energy E.

The electron charge is taken as $q_e = -e$, so the positive electron flux from the cathode results in a positive anode current $-J^+(U_a)$ through a unit cross-section. The upper limit in equation (3) is on the order of several electronvolts, which is consistent with non-relativistic quantum mechanics. For thermionic-field emission (at T~2000K), equation (2) should be used, with the upper limit in equation (3) extended by a few eV due to the logarithmic decay.

For T = 0, the total current density $J = J^+ - J^-$ is determined by tunneling in both directions with transmission coefficients $D^{\pm}(E) = 1 - \left|R^{\pm}\right|^2$, derived from reflection coefficients $R^{\pm}$. To determine $R^{\pm}$, the Schrödinger equation is solved. The expression for J^- is obtained by substituting $\mu_c \to \mu_a$, $D^+ \to D^-$.

For a symmetric potential ($U_a = 0$), the tunneling coefficient T(E)T(E)T(E) is always $D^+ = D^-$. For a weakly asymmetric potentials.

2. LIFETIME OF THE LEVEL BASED ON THE STATIONARY SCHRÖDINGER EQUATION SOLUTION

The stationary Schrödinger equation (SSE):

$$\left(-\frac{(\hbar\partial_x)^2}{2m_e} + V(x)\right)\psi(x) = 0$$

is most conveniently solved for V(x) using the wave impedance transformation method. For a constant potential V_n in the region $x_n < x < x_{n+1}$, the wave impedance is introduced as:

$$z_n(E) = -i\psi(x) / \psi'(x) = 1 / k_n,$$

where:

$$\psi(x) = A \exp(ik_n x)$$

is the wave function (WF) of an electron moving in the direction of x electron,

$$k_n = \sqrt{2me(E - V_n)}/\hbar.$$

Let $z_0(x_{n+1})$ be the impedance on the right side. It transforms into the input impedance on the left side according to the formula:

$$Z_i(x_n) = z_n \frac{z_0 - iz_n \mathrm{tg}(k_n(x_{n+1} - x_n))}{z_n - iz_0 \mathrm{tg}(k_n(x_{n+1} - x_n))}. \quad (4)$$

Setting $z_0 = Z_i(x_n)$, we apply this formula iteratively for each segment until we obtain the input impedance at the cathode $Z_{ic}(0)$ and the reflection coefficient from the cathode side:

$$R^+ = (1 - k_0 Z_{ic}(0)) / (1 + k_0 Z_{ic}(0)).$$

Here,

$$k_0 = k_c = \sqrt{2m_e E} / \hbar.$$

For the initial iteration at the anode, we assume:

$$k_a = \sqrt{2m_e(E - E_{Fc} + eU_a)}/\hbar,$$
$$z_0 = 1/k_a.$$

It is worth noting that in typical tunneling through a barrier, $k_a = k_0$ is taken, i.e., the motion is considered only up to the turning point. Such transparency is $\tilde{D}^+ = \tilde{D}^-$. However, after passing this point, the electron moves quasi-classically, gaining energy eU_a. This results in lowering the Fermi level at the anode by eU_a, necessitating the use of the adjusted value k_a.

This concept can be illustrated using an infinitely narrow step-like barrier: $V = 0$ at $x < 0$ and $V = -eU_a$ at $x > 0$. For such a barrier, the quasi-classical approximation gives full transparency, $D = 1$, $R = 0$. However, under the strict solution, the reflection from the step is:

$$R = (k_0 - k_a) / (k_0 + k_a)$$

and $D < 1$. Applying formula (4) is equivalent to matching the wave function and its derivative. Clearly, the energy levels $E_n = E_n' - iE_n''$ can be defined as the complex roots of the equation:

$$R^+(E_n) = 0.$$

The transparency from the anode to the cathode D^- is determined by reverse transformation, where at the anode we take:

$$k_a = \sqrt{2m_e E} / \hbar,$$
$$z_0 = 1 / k_a$$

and

$$R^- = (1 - k_0 Z_{ia}(d)) / (1 + k_0 Z_{ia}(d)).$$

The difference between D^+ and D^- increases with increasing U_a. When $eU_a > E_{Fc}$, tunneling from the anode becomes impossible. After tunneling, the electron always transitions to the Fermi level of the corresponding electrode, either releasing or absorbing energy $e|E - E_{F(a,c)}|$ depending on the sign of the energy difference. This process is diffusive, occurring over a distance on the order of the electron mean free path, and does not affect the wave tunneling process itself. If tunneling occurs from a level below the Fermi energy, heating of the corresponding electrode occurs (Nottingham effect): the departing electron is replaced by an electron from the Fermi level. For $U_a = 0$, we obtain a symmetric structure in the form of a quantum well between two barriers (see Fig. 1, curves 0 and 1). In this case, the condition:

$$R^+(E_n) = R^-(E_n) = 0$$

yields energy levels from which the particle can tunnel equally to the left or right. Otherwise, the condition $R^+(E_n) = 0$ gives the levels from which the particle can escape to the anode, while $R^-(E_n) = 0$ corresponds to levels leading to cathode transitions. Calculations show that the levels approximately coincide within their width. For example, if $eU_a > E_{FA}$, all energy levels at the anode become negative, making transitions to positive energy levels on the cathode impossible. It is evident that for $E < 0$, when $|R^-(E)| \equiv 1$, i.e. meaning no solutions exist for the equation $R^-(E) = 0$. In this case, the cathode impedance $1/k_c$ becomes imaginary, and the cathode acts as an infinitely long, fully reflective

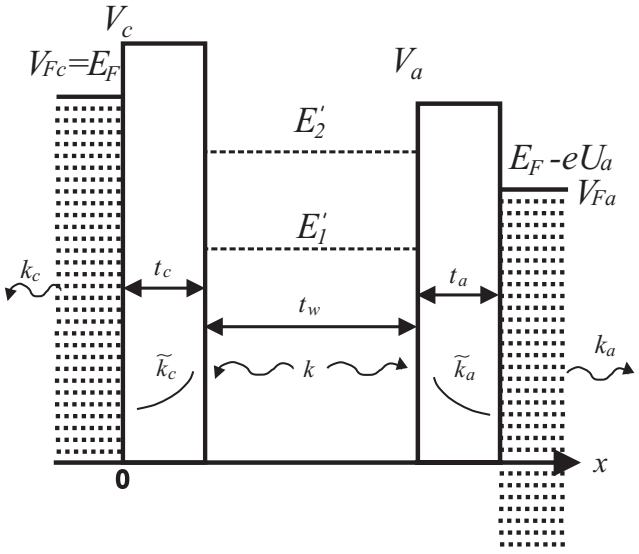

Fig. 2. Schematic potential distribution V in a single-well RTS at $U_g = E_F/e$. Dashed lines indicate the energy levels at the cathode, anode, and two metastable levels.

step for the anode. Positive energies at the anode can only exist at non-zero temperatures, i.e., under thermionic emission conditions. Solutions to the equation $R^+(E) = 0$ always exist for levels on the cathode side. Thus, for an asymmetric potential, two types of energy levels exist. Resonant tunneling is primarily considered for asymmetric potentials, as this condition ensures a continuous current.

Another possible approach to solving the stationary Schrödinger equation involves using transfer matrices [1–3] $\hat{T}(E)$. The structure matrix is defined by piecewise-constant potential V approximations and multiplying the segment matrices. The characteristic equation for determining tunneling levels at the anode takes the form [1, 3]:

$$ik_c(E) = \frac{T_{21}(E) - ik_a(E)T_{22}(E)}{T_{11}(E) - ik_a(E)T_{12}(E)}. \qquad (5)$$

Another method involves using the sweep method. In addition to finding $R^{\pm}(E)$ and $D^{\pm}(E)$ this approach allows for determining the wave function amplitudes $A_n^{\pm}\psi\left(\pm ik_n(x - x_n)\right)$ and the charge distribution in the barrier and well region under known incident particle fluxes from the cathode $n^+(k)v_z dv_z$ and the anode $n^-(k)v_z dv_z$.

This, in turn, enables the estimation of changes in the quantum potential V due to space charge effects under high currents [2]. Such estimation requires iterative solutions of the Poisson equation (PE) and the Schrödinger equation. However, these numerical methods are less convenient for our analysis of resonant level influence on electron emission.

We derive the exact solution of the Schrödinger equation (SE) for the model potential $\tilde{V}(x)$, described by two rectangular barriers of height V_c at the cathode and V_a at the anode (see Fig. 2). To better match the real potential, the barrier widths t_c and T_a are taken approximately half the size of the bases of the actual near-triangular barriers on a rectangular pedestal (Fig. 1, curves 2, 4, 6), while the well width t_u is correspondingly increased. It is possible to achieve an exact correspondence between the width of a triangular barrier and the width of a rectangular barrier with equal heights by equating their transparencies $D_{rec}(E) = D_{tre}(E)$. This correspondence depends on the energy. Averaging over the energy range, we obtain a coefficient of approximately $t_{rec} \approx 0.5t_{tre}$. In the quantum well, the SE solution takes the form:

$$\psi(x) = A_w^+ \exp\left(ik_0(x - t_c)\right) + A_w^- \exp\left(-ik_0(x - t_c)\right).$$

In the barrier region near the cathode, the wave function (WF) is:

$$\psi(x) = A_c^+ \exp\left(-\tilde{k}_A x\right) + A_c^- \exp\left(\tilde{k}_A x\right),$$

Similarly, in the barrier region near the anode, the wave function is:

$$\psi(x) = A_a^+ \exp\left(-\tilde{k}_a(x - t_c - t_w)\right) + \\ + A_a^- \exp\left(\tilde{k}_a(x - t_c - t_w)\right).$$

Here, we introduced the following notations:

$$\tilde{k}_c = \sqrt{2m_e(V_c - E)},$$
$$\tilde{k}_a = \sqrt{2m_e(V_a - E)},$$
$$k_0 = \sqrt{2m_e E}.$$

The wave function at the cathode represents an outgoing wave:

$$\psi(x) = A_c \exp(-ik_0 x).$$

Similarly, at the anode:

$$\psi(x) = A_a \exp\left(ik_0(x - d)\right).$$

Here, $A_a = k_0$, $d = t_c + t_w + t_a$ is the size of the structure. The task is to match the wave functions and their derivatives at the boundaries. There are eight unknowns, four boundaries, and thus eight conditions.

Calculating the eighth-order determinant without numerical methods is challenging, so we iteratively eliminate unknowns. The results of this elimination are provided in the Appendix. By defining the function $f(E)$ according to formula (A2) from the Appendix, the characteristic equation takes the form:

$$E = V_a \frac{\left(f\left(E\right)-1\right)^2}{\left(f\left(E\right)-1\right)^2 - \left(f\left(E\right)+1\right)^2}. \qquad (6)$$

This equation allows for the iterative search for complex roots $\tilde{E}_n$. Assuming the function f is large in magnitude (corresponding to wide barriers), we obtain $E \approx -V_c f\left(E\right)/4$. As the well expands from a very narrow width, the energy level first appears near V_a [21]. For such a level, the decay rate $\tilde{k}_a \approx 0$ is:

$$\mathrm{tg}\left(k_0 t_w\right) \approx k_0/\tilde{k}_a.$$

Assume there is such a level:

$$\tilde{E}_1 = V_a\left(1-\delta_1\right),$$

where δ_1 is small. Also, let:

$$\delta << \Delta = V_c/V_a - 1.$$

Calculating the function f, we obtain:

$$\tilde{k}_c \approx \tilde{k}\left(1+\delta/\left(2\Delta\right)\right),$$

$$\exp\left(2\tilde{k}_c t_c\right) \approx \exp\left(2\tilde{k}t_c\right)\left(1+\delta/\left(2\Delta\right)\right),$$

Where

$$\tilde{k} = \sqrt{2m_e V_a \Delta}/\hbar.$$

As well as:

$$k_0 \approx \tilde{k}\left(1-\delta/2\right)/\sqrt{\Delta},$$

$$k_0/\tilde{k}_c \approx \left(1-\delta_1\left(1+1/\Delta\right)/2+\delta_1^2/\left(4\Delta\right)\right)/\sqrt{\Delta}.$$

Let us set $\tilde{k}_a = 0$, and rewrite the introduced condition as

$$\left(t_w\tilde{k}/\sqrt{\Delta}\right) = \sqrt{\Delta}.$$

Then we have

$$f \approx \frac{\exp\left(2\tilde{k}t_c\right)}{4\Delta - \delta_1(\Delta+1)\left(1+t_w\tilde{k}\right)} \times$$

$$\times\{\delta_1(\Delta+1)(1+t_w\tilde{k}) -$$

$$-\left(\delta_1^2/2\right)\left[\Delta + 2\Delta\left(t_w\tilde{k}\right)^2 + (\Delta+1)\left(1+t_w\tilde{k}\right)\right]\}.$$

For the left side of equation (A2), we get

$$\frac{1+ik_0/\tilde{k}_a}{1-ik_0/\tilde{k}_a} \approx 1+\delta_1\frac{1+i\sqrt{\Delta}}{\left(\Delta+1\right)^2},$$

from which the correction δ_1 can be found, expanding further:

$$\delta_1 = \frac{16\exp\left(-2\tilde{k}t_c\right)}{\left(1+1/\Delta\right)\left(1+t_w\tilde{k}\right)} +$$

$$+\frac{4\delta\exp\left(-2\tilde{k}t_c\right)}{\left(1+1/\Delta\right)\left(1+t_w\tilde{k}\right)} \times$$

$$\times\left[4\frac{1+i\sqrt{\Delta}}{\left(\Delta+1\right)^2} - \left(1+1/\Delta\right)\left(1+t_w\tilde{k}\right)\right].$$

We can neglect the second-order term. To find the exact roots of equation (6), let us consider a well surrounded by infinitely wide barriers, i.e., potential steps of height V_c and V_a. In such a well, stationary energy levels $E_n < V_a$ are possible. The problem of an asymmetric well has been solved and studied in [21]. With the notation

$$k_{0n} = \sqrt{2m_e E_n}/\hbar$$

it has the solution

$$k_{0n}t_w = n\pi - \arcsin\left(\frac{k_{0n}\hbar}{\sqrt{2m_e V_c}}\right) -$$

$$-\arcsin\left(\frac{k_{0n}\hbar}{\sqrt{2m_e V_a}}\right) = g\left(E_n\right) \qquad (7)$$

which gives real energy levels. Rewrite equation (7) as

$$\mathrm{tg}\left(k_{0n}t_w\right) = k_{0n}t_n,$$

where

$$t_n = \frac{k_{0n}+\tilde{k}_c}{\tilde{k}_c\tilde{k}_a - k_{0n}^2}.$$

Choosing the well width from the condition of the existence of one level:

$$t_w > t_0 = \frac{\pi/2 - \arcsin\left(V_a/V_c\right)}{\sqrt{2m_e V_c}/\hbar},$$

we get

$$E_n = \frac{\left(\hbar g\left(E_n\right)/t_w\right)^2}{2m_e}.$$

From this equation, we find the real values of E_1 by the bisection method in the interval $\left[\left(0,V_0\right)\right.$. For the existence of multiple levels, the well must be several times wider than t_0. Then we find E_n, $n = 1,2,...,N$. The values of E_n are used as initial approximations $\tilde{E}_n^{(0)} = E_n$ for the iterations according to equation (6). As a result, we obtain all the levels from which a particle can escape to both the anode and the cathode. To increase the current, the widest possible well should be used, for which the electrode material should have the maximum electron mean free path (MFP). The MFP can be significantly increased by using cryogenic temperatures. Let us consider the derivation of equation (7), where the wave functions (WF) on the cathode and anode sides are taken as

$$\psi\left(x\right) = A_c \exp\left(\tilde{k}_a\left(1 - i\delta_c\right)x\right),$$

$$\psi\left(x\right) = A_a \exp\left(-\tilde{k}_a\left(1 - i\delta_a\right)\left(x - t_w\right)\right),$$

i.e., the barriers are partially transparent. Here

$$\tilde{k}_c = \sqrt{2m_e\left(V_c - E_n'\right)}/\hbar,$$

$$\tilde{k}_a = \sqrt{2m_e\left(V_a - E_n'\right)}/\hbar,$$

and small corrections are taken as

$$\delta_c = E_n''/\left(2V_c - 2E_n'\right),$$

$$\delta_a = E_n''/\left(2V_a - 2E_n'\right).$$

In reality, they are associated with the finite width of the barriers and the finite lifetime of the levels. In the well $0 < x < t_w$, we take

$$\psi\left(x\right) = A\sin\left(k_{0n}\left(1 + \delta_n\right)x + \delta\right),$$

where

$$\tilde{E}_n = \left(1 + \delta_n\right)^2\left(k_{0n}\hbar\right)^2/\left(2m_e\right),$$

and the small correction δ_n needs to be found. As a result, we obtain the characteristic equation for it:

$$\mathrm{tg}\left(k_{0n}\left(1 + \delta_n\right)t_w\right) = k_{0n}\left(1 + \delta_n\right)\times$$

$$\times\frac{\tilde{k}_a\left(1 - i\delta_a\right) + \tilde{k}_c\left(1 - i\delta_c\right)}{\tilde{k}_c\tilde{k}_a\left(1 - i\delta_a\right)\left(1 - i\delta_c\right) - k_{0n}^2\left(1 + \delta_n\right)^2}.$$

Introducing the notations

$$\delta'_{an} = \delta_a/\delta_n, \quad \delta'_{cn} = \delta_c/\delta_n.$$

Primed quantities are not small. Considering (8), to obtain the correction, expansion up to the second order in δ_n^2 should be used. We obtain $\delta_n = A_n/B_n$, where

$$A_n = \frac{t_w}{t_n} + k_{0n}^2 t_n t_w - 1 + \frac{i\left(\delta'_{an}\tilde{k}_a + \delta'_{cn}\tilde{k}_c\right)}{\tilde{k}_a + \tilde{k}_c} -$$

$$-\frac{2i\tilde{k}_c\tilde{k}_a\left(\delta'_{an} + \delta'_{cn}\right) + 2k_{0n}}{\tilde{k}_c\tilde{k}_a - k_{0n}^2},$$

$$B_n = \frac{\tilde{k}_c\tilde{k}_a\delta'_{an}\delta'_{cn} + k_{0n}^2}{\tilde{k}_c\tilde{k}_a - k_{0n}^2} - k_{0n}^2 t_n t_w +$$

$$+4\left[\frac{i\tilde{k}_c\tilde{k}_a\left(\delta'_{an} + \delta'_{cn}\right) + k_{0n}^2}{\tilde{k}_c\tilde{k}_a - k_{0n}^2}\right]^2 +$$

$$+\frac{2i\tilde{k}_c\tilde{k}_a\left(\delta'_{an} + \delta'_{cn}\right) + 2k_{0n}^2}{\tilde{k}_c\tilde{k}_a - k_{0n}^2}.$$

For the calculation of the correction, one can assume $\tilde{E}'_n = E_n$, and then

$$\tilde{E}_n''/E_n = -\Im\left(\delta_n\right),$$

while the real part also changes:

$$E_n' = E_n\left(1 + \mathrm{Re}\left(\delta_n\right)\right).$$

In Fig. 2, two levels are shown. From the cathode, tunneling to both levels with exit to the anode is possible. In this case, the cathode heats up because its level is above the Fermi level (Nottingham effect). When transitioning from the first level to the anode, the anode cools, while transitioning from the second level heats it up. Tunneling from the anode to the second level at T=0 is impossible. The lifetime of the level exponentially decreases with the narrowing of the barriers. The barriers narrow as the field U_g increases (Schottky effect), i.e., with an increase in well depth. At $U_g > U_a + E_{Fc}/\hbar$, stationary levels are possible in the well. Narrowing of the barriers also occurs with increasing voltage U and decreasing sizes t_c and t_a. There is a critical voltage at which the barrier relative to the Fermi level disappears, becoming nearly triangular. Indeed, using equation (1), where we denote

$$W' = W_c\frac{\left(1 - \alpha/d\right)\left(1 + \delta/d\right)^2}{\left(1 - \delta/d\right)^2\varepsilon},$$

assuming $d = t_g$ and neglecting small terms, this condition can be written as:

$$V(x_0) = E_{Fc} =$$
$$= E_{Fc} + W_c'\left(1 - \delta d/\left(x_0(d - x_0)\right)\right) - eU_g x_0/d.$$

From this, we find the point x_0 where this occurs. It is very close to the cathode, so we simplify the cubic equation by replacing $d - x_0$ with d:

$$x_0 = eU_g x_0^2/(W_c' d) + \delta.$$

Solving this quadratic equation iteratively, first assuming

$$x_0 = \delta$$

and then refining:

$$x_0 = \delta + \delta^2 eU_g/(W_c' d).$$

The refinement is very small, so we obtain the critical voltage:

$$U_g = W'(d/\delta - 1)/(2e) \approx W'd/(2e\delta).$$

For a work function of about 4 eV at d=2 nm, this corresponds to a critical electric field strength at the cathode of $2.35 \cdot 10^{10}$ V/m. Thus, in RT structures with well widths of a few t_0 and narrow barrier widths t_c and t_a, a significant increase in emission current is possible simply by increasing the size t_w. However, tunneling is ballistic transport without energy loss, so the width t_w must be significantly less than the electron mean free path (MFP) in the corresponding material. The characteristic size t_w at room temperature is a few nanometers. To reduce the lifetime of levels and increase current, the barriers should be made narrow. Their narrowing is also achieved by increasing electrode voltages. It is not difficult to obtain exact solutions to equation (6), but these equations are model-based. For real potentials (Fig. 1), one should solve the exact equations (5) or $R^{\pm}(E) = 0$. The table above presents the results of iterative calculations of complex energies. Calculations based on equation (5) and the conditions $R^{\pm}(E) = 0$ agree well.

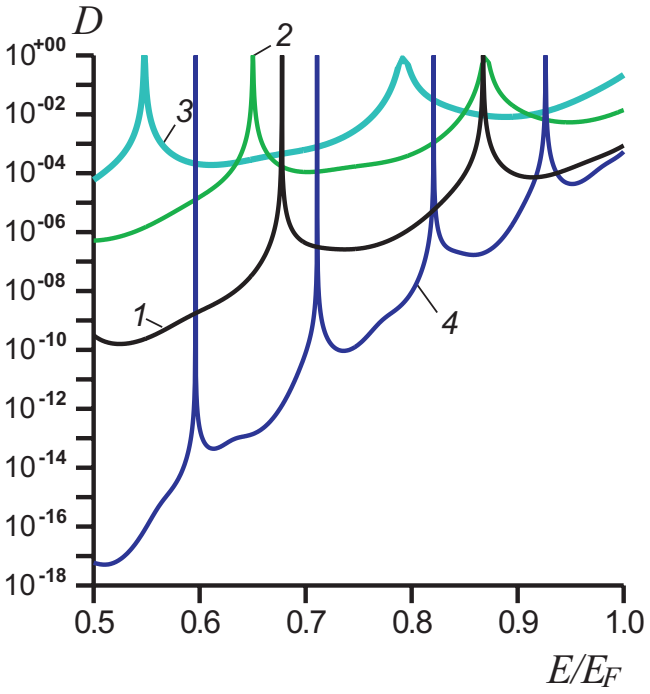

Fig. 3. Tunneling coefficient $D = D^+$ in a double-well RT structure as a function of the ratio $t = t_1 = t_2 = t_3$ depending on E/E_{F_c} at $t = t_g = 1$ nm (curves *1*, *3*) and $t = 2$ nm, $t_g = 1.5$ nm, $d = 9$ nm (curve *4*). Work function $W_c = W_g = W_a$ =4.0 eV, Fermi energy $E_{F_c} = E_{F_a}$ 5 eV, $U_a = 11$ V. $U_g = 13$ V (*1*, *4*); $U_g = 20$ V (*2*); $U_g = 25$ V (*3*)

A very simple method for determining complex levels is calculating the transparency of the structures. Figure 3 shows an example of calculating D^+ for several double-well RT structures with 2 to 4 metastable levels. Such structures are obtained with a double grid [1–3] and are more convenient for achieving resonance tunneling because two approximately equal barriers can be formed under a significant electrostatic potential U_a.

Table. Metastable levels (eV) in the range (0, E_{Fc}) for the potential in Fig. 1 at different anode voltages U_a (V):

U_a	1.0	2.0	3.0	4.0
$E_1' - iE_1''$	$0.14467 - i3.1 \cdot 10^{-4}$	$0.1445 - i2.9 \cdot 10^{-4}$	$0.1399 - i2.7 \cdot 10^{-4}$	$0.1405 - i2.7 \cdot 10^{-4}$
$E_2' - iE_2''$	$1.815 - i2.5 \cdot 10^{-3}$	$1.807 - i2.6 \cdot 10^{-3}$	$1.798 - i2.8 \cdot 10^{-3}$	$1.789 - i2.9 \cdot 10^{-3}$
$E_3' - iE_3''$	$4.4938 - i8.9 \cdot 10^{-3}$	$4.369 - i9.5 \cdot 10^{-3}$	$4.328 - i9.9 \cdot 10^{-3}$	$4.279 - i1.2 \cdot 10^{-2}$
$E_4' - iE_4''$		$6.872 - i7.2 \cdot 10^{-2}$	$6.982 - i8.3 \cdot 10^{-2}$	

Notably, the peaks for D^+ and D^- differ slightly, particularly at low energies. At $E > E_{Fc}$, $D^{\pm} \approx 1$ always holds. This case corresponds to thermionic emission if the electrode temperatures $T^{\pm} > 0$. It should be noted that for different barriers, peaks may not reach unity (incomplete resonance tunneling), associated with partial suppression of reflected electron waves. The values E'_n are determined by the peak maxima, which can be done accurately. The lifetimes E''_n are determined by the resonance widths. Typically, the levels are located near the upper regions of the well.

Let us consider how the position and width of the level affect the current contribution. Suppose there is one level $E'_1 - iE''_1$. Approximating it as an equilateral triangle with unit height, the contribution from the level is

$$\Delta J^+ = -em_e\left(E_{Fc} - E'_1\right)E''_1/\left(4\pi^2\hbar^3\right).$$

For levels near the Fermi level of the cathode, it is small. Therefore, it is important to obtain low-lying levels with a short lifetime (large width). For a single triangular potential barrier at a critical field, the semiclassical approximation gives its transparency D as

$$D \approx \exp\left(-4d\sqrt{2m_e}W^{3/2}/3\hbar eU_a\right),$$

see [20]. Here, the barrier height W is measured from the kinetic energy of the incoming electron, i.e., in our case, $W = V - E$.

For deep levels, the transparency of a single barrier is exponentially small compared to $D = 1$ in resonance tunneling. The formula works well for deep levels, but for $E = V$, its limitation becomes apparent: $D = 1$ at $W = 0$, while solving the Schrödinger equation gives $D < 1$. This limitation restricts the applicability of the Fowler–Nordheim formula to single barriers.

Nevertheless, the result can be used to estimate the lifetimes of deep levels by calculating $D_{(c,a)}$ at $W = V_{c,a} - E_n$ and determining $\delta_c = D_c$ and $\delta_a = D_a$.

3. LIFETIME OF THE LEVEL IN THE NONSTATIONARY APPROACH

The nonstationary Schrödinger equation (SE) is written as

$$\hat{S}(t,x)\psi(t,x) = V(t,x)\psi(t,x),$$

It is known to be relativistically non-covariant. Here, the operator for a free particle's Hamiltonian is denoted as

$$\hat{S}(t,x) = i\hbar\partial_t + \frac{\left(\hbar\partial_x\right)^2}{2m_e}.$$

This implies that the Green's propagator function (GPF), which describes the propagation of a particle from point x' at time t' to point x at time t, has the following form [22, 23]:

$$K_0(t-t',x-x') = \\ = \operatorname{sgn}(t-t')\sqrt{\frac{m_e}{2\pi i\hbar|t-t'|}} \times \\ \times\exp\left(\frac{i(x-x')^2 m_e}{2\hbar|t-t'|}\right), \qquad (8)$$

This expression suggests infinitely fast propagation of the perturbation. Indeed, GPF (8) defines the particle's presence at point x at time t based on its amplitude $\psi_0(x',t')$ at point x' at the initial moment t':

$$\psi_0(t,x) = \int_{-\infty}^{\infty} K_0(x-x',t-t')\psi_0(t',x')dx'.$$

If at the initial moment t_0, a probability density

$$\psi_0(t_0,x,) = \delta(x-x_0),$$

emerges at point x_0 meaning the particle is localized there, then for any later time $t > t_0$, the wavefunction exists throughout the entire infinite space:

$$\psi_0(x,t) = K_0(x-x_0,t-t_0),$$

Thus, the propagation speed of the probability density is infinite, though the density itself rapidly decreases at distant points. Here, the subscript "0" denotes a free particle (V=0).

Such a particle is generally described as a wave packet (WP) with a certain spectrum of wave numbers k and energies E. It is worth noting that the incoming particle flow described by distribution (2) also represents a WP.

The GPF (8) satisfies the initial condition

$$K_0(t-t',x-x')_{t\to t'} = \delta(x-x')$$

and the differential equation

$$\hat{S}K_0(t-t',x-x') = i\hbar\delta(t-t')\delta(x-x'),$$

(see [22]). Solving the nonstationary SE requires setting appropriate initial conditions. A convenient approach is to use the stationary case at the initial moment $t = t_0$, i.e., the wavefunction $\psi_0(x)$ and the potential $V_0(x)$.

At $t \geq t_0$, when the potential $V(x,t)$ starts changing, the wavefunction satisfies the nonstationary SE. The wavefunction for $t_0 > 0$ is governed by the Lippmann–Schwinger-type integral equation:

$$\psi(x,t) = \psi_0(x) - i\hbar^{-1}\int_0^t\int_{-\infty}^{\infty} K_0(t-t',x-x')\times$$
$$\times\left[V(t',x') - V_0(x')\right]\psi(t',x')dx'dt'. \quad (9)$$

Indeed, at t " 0,, we have $\psi(x,t) = \psi_0(x)$.. Taking the time $t > 0$ derivative of (9) and applying the operator $\hat{S}$, we obtain the SE:

$$\hat{S}\psi(x,t) = V(t,x)\psi(t',x').$$

Assume the potential

$$\Delta V(t,x) = V(t,x) - V_0(x)$$

is localized within a certain region. In this case, for small times, equation (9) can be solved rather simply. An example for a double-barrier resonant tunneling diode (RTD) is provided in [12]. This equation is particularly convenient for analyzing transient processes and tunneling times. Two cases can be considered: (a) $\Delta V(0,x) = 0$ (smooth potential change) and (b) $\Delta V(0,x) \neq 0$. We focus on the second case here. Assume a well with one metastable level between two barriers exists at $t < 0$. This level cannot be populated, as it would decay over infinite time. For simplicity, consider identical barriers of height V. The metastable level between identical barriers V is defined by the condition

$$\mathrm{th}\left(\tilde{k}_1 t_b\right)(kt_w) =$$
$$= \alpha = \frac{\sqrt{\tilde{E}_1\left(V-\tilde{E}_1\right)}}{\tilde{E}_1 - V/2},$$

see [13], where

$$\tilde{k}_1 = \tilde{k}'_1 + i\tilde{k}''_1 = \frac{\sqrt{2m_e\left(V-\tilde{E}_1\right)}}{\hbar}$$

This equation determines the level's lifetime, $t_1 = t_2 = t_b$ is the barrier width. A convenient numerical solution can be sought in the form

$$E_1 = V_0{}^2\left(\alpha(E_1)\right)/\mathrm{th}^2\left(\tilde{k}_1 t_b\right),$$

$$V_0 = \hbar^2/2m_e t_w^2,$$

expressing the arctangent via logarithmic functions. The quantities

$$\alpha = \alpha' + i\alpha'' = \sqrt{E_1(V-E_1)}/(E_1 - V/2)$$

and

$$\tilde{k}' = \tilde{k}'_1 + i\tilde{k}''_1$$

are complex. For wide barriers, we obtain

$$\tilde{k}'_1 = \sqrt{2m_e(V-E'_1)}/\hbar,$$

$$\tilde{k}''_1 = E''_1\sqrt{m_e/(2V-2E'_1)}/\hbar,$$

$$\mathrm{th}^2\left(\tilde{k}_1 t_b\right) \approx 1 - 4\exp\left(-2\tilde{k}'_1 t_b\right)\exp\left(-2i\tilde{k}''_1 t_b\right).$$

It is easiest to estimate the level by assuming it arises at the barrier boundary. In this case, α', and

$$\alpha'' \approx 3\alpha'_1 E''_1/2V$$

To simplify further calculations, introduce the dimensionless parameter

$$\delta = 4\exp\left(-2\tilde{k}'_1 t_b\right)\exp\left(-2i\tilde{k}''_1 t_b\right),$$

and obtain the energy as

$$E_1 = (V+V_0)/2 + \sqrt{V_0^2/4 + 3V_0V/2} + \delta\Delta E_1,$$

where

$$\Delta E_1 = \frac{\left(V_0{}^2/4 + 3VV_0/4\right)}{\sqrt{V_0^2 4 + 3V_0V/2}} + \frac{V_0}{2}.$$

If the well deepens by an amount ΔV, the energy at the bottom becomes negative. Assume only one stable level exists. If the center of the well is at x=0, the wavefunction inside the well takes the form of either an even or odd function:

For an even wavefunction:

$$\psi_0(x) = A_c\cos(k_1 x),$$

For an odd wavefunction:

$$\psi_0(x) = A_s \sin(k_1 x),$$

herewith

$$\psi_0(t_w/2) \neq 0, \quad \psi_0'(t_w/2) \neq 0,$$

$$k_1 = \sqrt{2m_e E_1}/\hbar.$$

Let's mark

$$\tilde{k}_0 = \sqrt{2m_e(\Delta V - E_1)}/\hbar,$$

$$\tilde{k}_1 = \sqrt{2m_e(V + \Delta V - E_1)}/\hbar,$$

$$z_0 = -i/\tilde{k}_0,\ \tilde{z}_1 = -i/\tilde{k}_1,\ z_1 = 1/k_1.$$

Then, in the case of an odd wave function, we have the characteristic equation:

$$\mathrm{tg}(k_1 t_w/2) = iZ_i/\rho_1,$$

And for the even function:

$$\mathrm{tg}(k_1 t_w/2) = -i\rho_1/Z_i.$$

The value

$$Z_i = \frac{\tilde{\rho}_1\left(\tilde{\rho}_0 - \tilde{\rho}_1 \mathrm{th}\left(\tilde{k}_1 t\right)\right)}{\tilde{\rho}_1 - \tilde{\rho}_0 \mathrm{th}\left(\tilde{k}_1 t\right)}$$

is imaginary, so the equations are real and determine the real energies. We take the normalization of the wave function (WF) from the condition of finding the particle in the well region $|x| \,''\, t_w/2$. This is an approximate condition, as there is some probability leakage through the barriers. However, with sufficiently wide barriers, it is negligible. A strict normalization can be performed, but it results in cumbersome amplitude values. In our case, the amplitudes are:

$$|A_c|^2 = \left[t_w\left(1 + \sin(t_w k_1)/(t_w k_1)\right)\right]^{-1},$$

$$|A_s|^2 = \left[t_w\left(1 - \sin(t_w k_1)/(t_w k_1)\right)\right]^{-1}.$$

It is clear that the even level should appear first, as its wave function approximately corresponds to the half-wave of de Broglie. Thus, for $t < 0$, such a populated level exists. At the moment $t = 0$, the potential $\Delta V > 0$ is suddenly switched on, and the bottom of the well rises to zero energy. In such a well, the particle cannot exist indefinitely, and the state begins to decay, described by the integral equation (IE):

$$\psi(x,t) = \psi_0(x) - i\hbar^{-1}\Delta V \times$$

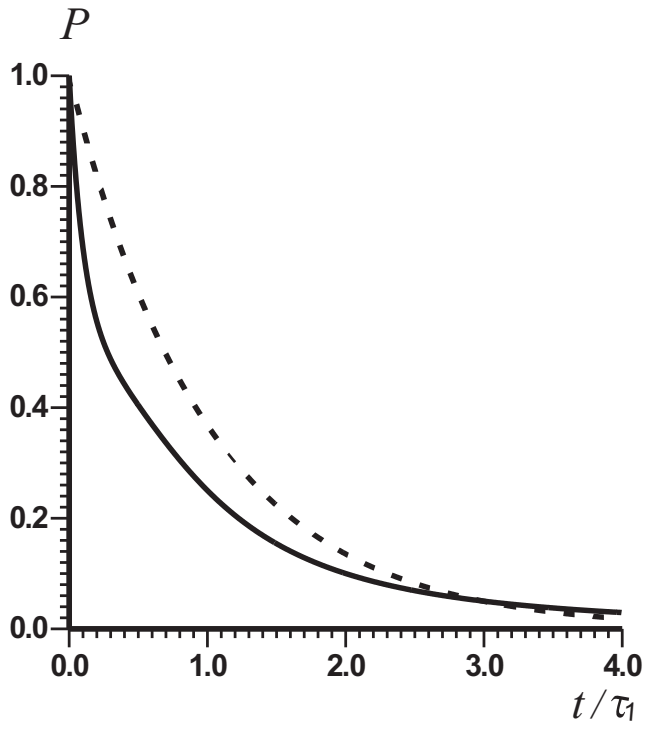

Fig. 4. Transition probability $P(t)$ according to formula (12) for the decay of a single level. The dashed curve represents exponential decay $P_0(t) = \exp(-t/\tau_1)$.

$$\times \int_0^t \int_{-t_w/2}^{t_w/2} K_0(t - t', x - x')\psi(t', x')\,dx'dt'. \qquad (10)$$

This problem can be solved numerically or by perturbation theory. In the latter case, the first approximation is:

$$\psi_{(1)}(x,t) = \psi_0(x) - i\hbar^{-1}\Delta V \times$$

$$\times \int_0^t \int_{-t_w/2}^{t_w/2} K_0(t - t', x - x')\psi_0(x')\,dx'dt'.$$

The probability of finding the particle in the well region now becomes:

$$P(t) = \int_{-t_w/2}^{t_w/2} |\psi(t,x)|^2\,dx. \qquad (11)$$

It decreases over time. Solving IE (10), we compute (11). Obviously, with the chosen normalization $P(0) = 1$. Approximating (11) with the function $P_0(t) = \exp(-t/\tau_1)$, we determine the level lifetime. The corresponding result is shown in Fig. 4, corresponding to the value $E_1''/E_1' = 0.021$,

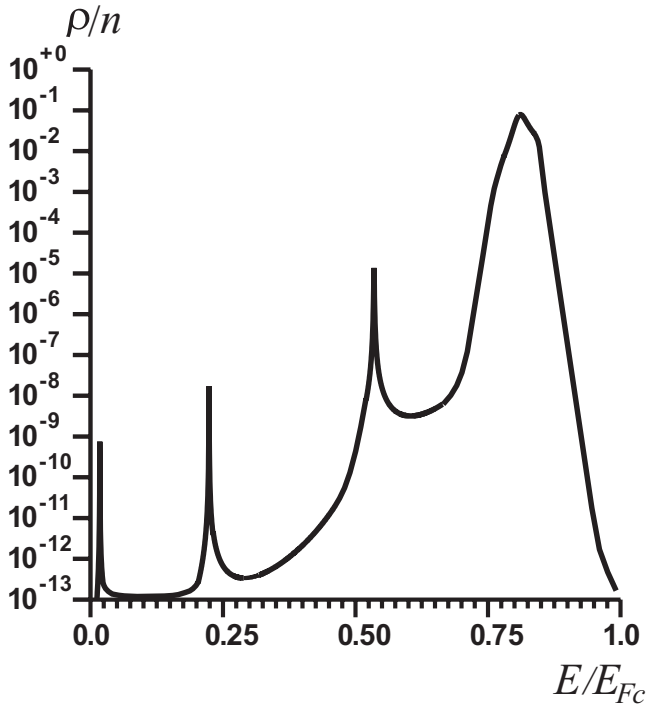

Fig. 5. Normalized particle number density ρ in the well as a function of energy E for three resonance levels (eV): 0.140552, 1.78936 eV, 4.27933 eV (see Table, $U_a = 4$ V)

$\tau_1 = 59.5$ fs. It should be noted that the decay of such a state generally does not follow an exponential law [24–35], which holds only for infinitely long-lived levels [36]. There exist continuous-spectrum states in the well that distort the exponential law. The continuous spectrum and interference lead to faster initial decay, followed by a slowdown [17, 24]. An even more complex case corresponds to multiple levels. The non-stationary approach is significantly more complicated than determining complex roots. Interestingly, for tunneling problems, calculating the probability density:

$$\rho(E) = \int \left|\psi_0(x,E)\right|^2 dx$$

both in the well region and in the barrier region shows maxima at energies corresponding to the resonance levels E′ (see Fig. 5). The result is normalized to the particle number density in both flows:

$$n(E) = n^+(E) + n^-(E) =$$
$$= \sqrt{2E} m_e^{3/2} (E_{Fc} - E)/\pi^2\hbar^3.$$

This is because all incident flows from the left and right with resonance energies E_n' pass into the well, while for other energies they are significantly reflected. Both the tunnel current density J and the probability current density j are continuous along the entire structure, including the electrodes, reflecting the conservation law of particles (probability) in non-relativistic quantum mechanics.

4. APPLICATION OF NON-STATIONARY SCHRÖDINGER EQUATION FOR DETERMINING TUNNELING TIME

Since the introduction of the concept of tunneling time in 1930, there has been no established understanding in the literature (see [19] and references therein). Paradoxes such as the Hartman effect, "superluminal" tunneling, negative tunneling time, and others are still discussed. IE (10) is quite convenient for resolving such issues and studying transient processes [12]. The level lifetime (residence time in the structure) is often associated with tunneling time. Here, instead of IE (9), we consider another approach based on series expansion for solving the non-stationary Schrödinger equation. Suppose that at $t < 0$, in the region $0 < x < d$, we have a structure with three electrodes: $U_a = 0$, and $U_g = -W_c/e$. Also, let the value ddd be sufficiently large. In this case, the potential is close to a rectangular shape with width d and height W_c relative to the Fermi level (see Figure 1, curve 0). Relative to zero, its height is $V = W_c + E_{Fc}$. If the grid voltage were zero, the potential (relative to E_{Fc}) would appear as two peaks of height W_c, separated by a gap with zero height. Curve 1 in Fig. 1 demonstrates the potential at a negative grid voltage $U_g = -W_c$, when the entire curve is elevated by W_c. Such a potential blocks the current. Suppose that at time $t = 0$, the potentials switch such that $U_a > 0$ and $U_g = E_{Fc}/e$, i.e., the problem becomes equivalent to resonant tunneling (RT). Accordingly, we need to consider the transient processes of tunneling establishment when $t > 0$ during the switch from curve 1 to curves like 2, 4. For a diode structure, this switch corresponds to curve 0 transitioning to curves 3, 5, 7, but without RT. The macroscopic change in current during such a process is quite easy to measure, unlike the tunneling time of an individual particle. It should be noted that for $t < 0$, the current was absent due to the symmetry of the structure. Also, at these times, the particle density in the structure was negligible, as the tunneling probability through a wide barrier was nearly zero. Near the edges, the density decays exponentially. By choosing a large ddd, one can assume that particles were absent in the barrier region. Switching the potentials leads to the appearance of current. It cannot

appear instantaneously, as particles need to traverse the region d, thus creating a finite transient time. We will solve the non-stationary Schrödinger equation by expanding into series in the region $0 < x < d$:

$$\Psi(t,x) = $$

$$= A\left(\sum_{n=0}^{\infty}\alpha_n(t)\cos(\chi_n x)+\sum_{n=1}^{\infty}\beta_n(t)\sin(\chi_n x)\right), \quad (12)$$

$$V(t,x) = \sum_{n=0}^{\infty}\nu_n(t)\cos(\chi_n x), \quad (13)$$

where $\chi_n = n\pi/d$. This method is applicable for multiple electrodes, but further numerical results are presented for the diode. It is not possible to use only cosines or sines in the expansion (12), as this would always result in zero probability current density. For simplicity, we will apply the method to the diode structure. The amplitude A is introduced for normalization, meaning that when it is specified, we can assume $\alpha_0 = 1$. To perform the calculations, we truncate the series (12) and (13) by an index N. Substituting (12) and (13) into the Schrödinger equation and using the orthogonality of trigonometric functions, we obtain the coupled differential equations:

$$\alpha_n'(t) = i\sum_{m=0}^{N}A_{nm}^{cc}\omega_m\alpha_m(t) +$$

$$+ i\sum_{m=1}^{\infty}A_{nm}^{cs}\omega_m\beta_m(t)\sin(\chi_m x) -$$

$$-\frac{i}{\hbar}\left(\sum_{m=0}^{N}V_{nm}^{\alpha cc}(t)\alpha_m(t) +\right.$$

$$\left.+\sum_{m=1}^{\infty}V_{nm}^{\beta cs}(t)\beta_m(t)\sin(\chi_m x)\right), \quad (14)$$

$$\beta_n'(t) = i\sum_{m=0}^{N}A_{nm}^{sc}\omega_m\alpha_m(t) +$$

$$+i\sum_{m=1}^{\infty}A_{nm}^{ss}\omega_m\beta_m(t)\sin(\chi_m x) -$$

$$-\frac{i}{\hbar}\left(\sum_{m=0}^{N}V_{nm}^{\alpha sc}(t)\alpha_m(t) +\right.$$

$$\left.+\sum_{m=1}^{\infty}V_{nm}^{\beta ss}(t)\beta_m(t)\sin(\chi_m x)\right). \quad (15)$$

Here, $\omega_n = \hbar\pi^2 n^2/\left(2m_e d^2\right)$ are the frequencies, and the matrix elements, detailed in the Appendix. These equations are quite complex if the potential depends arbitrarily on time. In the case of an abrupt potential switch, it stops depending on time, simplifying the equations. Rewriting the matrix elements, the first equation can be simplified to:

$$\alpha_n'(t) - i\omega_n\alpha_n(t) =$$

$$= f_n(t) = -\frac{i}{\hbar}V_{nn}^{\alpha cc}(t) + i\sum_{m=1}^{\infty}\tilde{A}_{nm}^{cs}(t)\beta_m(t) +$$

$$+i\sum_{m=0,m\approx n}^{N}\tilde{A}_{nm}^{cc}(t)\alpha_m(t).$$

Solving this equation using the Bernoulli method or the method of variation of arbitrary constants gives:

$$\alpha_n(t) = \alpha_n(0)\exp(i\omega_n t) +$$

$$+\exp(i\omega_n t)\int_0^t f_n(t')\exp(-i\omega_n t')dt'. \quad (16)$$

Similarly, we obtain:

$$\beta_n(t) = \beta_n(0)\exp(i\omega_n t) +$$

$$+\exp(i\omega_n t)\int_0^t g_n(t')\exp(-i\omega_n t')dt'.$$

Here, the following functions are introduced:

$$g_n(t) = -\frac{i}{\hbar}V_{nn}^{\beta ss}(t) + i\sum_{m=0}^{N}\tilde{A}_{nm}^{sc}(t)\alpha_m(t) +$$

$$+i\sum_{m=1,m\approx n}^{\infty}\tilde{A}_{nm}^{ss}(t)\beta_m(t).$$

The solution in time is sought using the discretization method: $t_m = m\Delta t$, $m = 1,2,...$, with integrals calculated using the midpoint method. If the initial values $\alpha_n(0)$, $\beta_n(0)$, are known, the equations allow us to find $\alpha_n(m\Delta t)$, $\beta_n(m\Delta t)$, using either explicit or implicit schemes.

The modified matrix elements here take a simple and clear form, for example:

$$\tilde{A}_{nm}^{\alpha cc}(t) = A_{nm}^{cc} - V_{nm}^{\alpha cc}(t)$$

If such a barrier instantaneously changes its shape at $t = 0$ to $V(x)$, these elements stop depending on time:

$$\tilde{A}_{nm}^{\alpha cc} = \omega_m A_{nm}^{cc} - V_{nm}^{\alpha cc}/\hbar$$

Their exact values can be found if the shape $V(x)$ is simple. For large U_a, it resembles a triangle placed on a rectangular base (see Fig. 1, curves 3, 5, 7). At $eU_a = E_F$, the height of the base can be taken as W, and the height of the triangle as E_F. Due to the Schottky effect, the barrier is actually somewhat lower. Calculating the integrals, we obtain:

$$V_{nm}^{\alpha cc} = \left(v_{n+m}^{c} + v_{n-m}^{c}\right)/\left(1+\delta_{n0}\right),$$

$$V_{nm}^{\beta ss} = \left(v_{n+m}^{s} - v_{n-n}^{s}\right)/\left(1+\delta_{n0}\right),$$

$$V_{nm}^{\alpha sc} = v_{n-m}^{s} + v_{n+m}^{s},$$

$$V_{nm}^{\beta ss} = v_{m-n}^{c} - v_{m+n}^{c}.$$

Here, the values of the following integrals are introduced:

$$\nu_n^c = \frac{1}{d}\int_0^d V(x)\cos\left(\chi_n x\right)dx,$$

$$\nu_n^s = \frac{1}{d}\int_0^d V(x)\sin\left(\chi_n x\right)dx.$$

For the initial symmetric wide barrier (curve 0), the height $V_0 = W + E_F$, and the coefficients $\alpha_n(t) = 0$ and $\beta_n(t) = 0$ at $t < 0$, as the probability density inside is practically absent. This approximation improves with increasing d, implying $\alpha_n(t) = 0$, $\beta_n(t) = 0$, i.e. within $\Psi(x,t) = 0$, $t < 0$. We take the initial barrier as rectangular. Then the integrals are easily computed, for example:

$$\nu_n(0) = V_0 sinc(n\pi) = V_0\delta_{n0}.$$

When this barrier under applied voltage $U_a = E_F/e$ takes the form:

$$V(x) \approx W + E_F\left(1 - x/d\right)$$

(see Fig. 1, curve 7), we obtain:

$$\nu_n^c = \left(W + E_F\right)\delta_{n0} + E_F conc(n\pi),$$

$$\nu_n^s = W conc(n\pi) + E_F sinc(n\pi).$$

In our case:

$$\nu_n^s = W conc(n\pi).$$

We assume that at the moment of voltage application, some coefficients $\alpha_n(0)$ and $\beta(0)$ instantly change from zero. This happens due to the appearance of probability current density. We find them from the continuity condition of this current density.

To the left of the barrier, the spectral wave function has the form:

$$\psi(x,k) = a^+(k)\left[\exp(ikx) + R^+(k)\exp(ikx)\right],$$

and to the right:

$$\psi\left(x,\tilde{k}\right) =$$

$$= a^-\left(\tilde{k}\right)\left[\exp\left(-i\tilde{k}\left(x-d\right)\right) - \exp\left(i\tilde{k}\left(x-d\right)\right)\right].$$

Here:

$$\psi(d,k) = 0, \quad \psi'\left(d,\tilde{k}\right) = -2i\tilde{k}a^-\left(\tilde{k}\right),$$

At high voltage:

$$\left|\psi'(d,k)/\psi'\left(0,\tilde{k}\right)\right| << 1.$$

Upon voltage application, the electrochemical potential on the cathode jumps, hence:

$$\sqrt{2m_e eU_a}/\hbar < k < \sqrt{2m_e\left(E_{Fc} + eU_a\right)}/\hbar,$$

$$0 < \tilde{k} < \sqrt{2m_e E_{Fa}}/\hbar.$$

Now the coefficients α_n, β_n in the wave function (13) at $t > 0$ become non-zero. They are dimensionless, so the amplitude A must be determined from the normalization to particle flux. The flux to the right, at large U_a, can be taken as zero:

$$j(d) = 0.$$

The flux to the left for the wave function:

$$\psi(x,k) = a^+(k)\left[\exp(ikx) + R^+(k)\exp(ikx)\right]$$

is given by:

$$j(0,k) = \frac{\hbar k\left|a^+(k)\right|^2}{m_e}\left(1 - \left|R^+(k)\right|^2\right).$$

The total flux is obtained by integration:

$$j(0) = \frac{\hbar}{m_e}\int_0^{k_F}\left|a^+(k)\right|^2\left(1 - \left|R^+(k)\right|^2\right)kdk =$$

$$= \frac{m_e}{2\pi^2\hbar^3}\int_0^{E_F}\left(1 - \left|R^+(E)\right|^2\right)\left(E_F - E\right)dE.$$

Calculating the flux into the barrier from the left at $x = 0$, we find the condition:

$$j(0) = -i\frac{\hbar}{m_e}\mathrm{Re}\,\Psi'(0,0)\Psi^*(0,0) =$$

$$= -\frac{\hbar|A|^2}{m_e}\Re\left(i\sum_{n=1}^{\infty}\chi_n\beta_n(0)\right)\left(\sum_{m=0}^{\infty}\alpha_m^*(0)\right).$$

For the flux on the right (from the anode), we find:

$$-\frac{\hbar|A|^2}{m_e}\mathrm{Re}\left(i\sum_{n=1}^{\infty}(-1)^n\chi_n\beta_n(0)\right)\times$$

$$\times\left(\sum_{m=0}^{\infty}(-1)^m\alpha_m^*(0)\right) = 0.$$

It is also necessary to equate the wave functions (WF) and their derivatives at the boundaries of the region:

$$\Psi(0,0) = A\sum_{n=0}^{\infty}\alpha_n(0),$$

$$\Psi'(0,0) = A\sum_{n=1}^{\infty}\chi_n\beta_n(0),$$

$$\Psi(0,d) = A\sum_{n=0}^{\infty}(-1)^n\alpha_n(0) = 0,$$

$$\Psi'(0,d) = A\sum_{n=1}^{\infty}(-1)^n\chi_n\beta_n(0) = 0.$$

The last equality is set to zero because we assume a high voltage and measure the energy from the conduction band edge of the cathode. We obtain six additional equations to determine the infinite number of initial conditions $\alpha_n(0)$, $\alpha_n(0)$ $\beta_n(0)$. However, using the full set of sines in (12) is redundant because the cosine system is sufficient for approximating the wave function. We introduced sines to obtain nonzero fluxes and nonzero WF derivatives at the boundaries. It is quite reasonable to assume: $\alpha_n(0) = 0$, $n > 2$, $\beta_n(0) = 0$, $n > 3$. Thus, we have six unknowns, as well as six conditions. It is sufficient to consider nonzero coefficients $\alpha_0(0)$, $\alpha_1(0)$, $\beta_1(0)$, $\beta_2(0)$. Then:

$$\alpha_1(0) = \alpha_0(0), \quad \beta_2(0) = \beta_1(0)/2,$$

and all six equations are satisfied, with:

$$j(0) = -\frac{4\pi\hbar|A|^2}{m_e d}\mathrm{Re}\left(i\beta_1(0)\alpha_0^*(0)\right).$$

It is convenient to choose:

$$\beta_1(0) = i\alpha_0(0), \quad \alpha_0(0) = 1.$$

Then:

$$j(0) = \frac{4\pi\hbar|A|^2}{m_e d},$$

and the wave function takes the form:

$$\Psi(t,x) = \sqrt{\frac{j(0)m_e d}{4\pi\hbar}}\times$$

$$\times\left(\sum_{n=0}^{\infty}\alpha_n(t)\cos(\chi_n x) + \sum_{n=1}^{\infty}\beta_n(t)\sin(\chi_n x)\right). \qquad (17)$$

From this, we find $\Psi(t,d)$ and $\Psi'(t,d)$.

Another method for solving equations (14) and (15) involves Fourier transforms:

$$\begin{pmatrix}\alpha_n(t)\\ \beta_n(t)\end{pmatrix} = \frac{1}{2\pi}\int_{-\infty}^{\infty}\begin{pmatrix}\alpha_n(\omega)\\ \beta_n(\omega)\end{pmatrix}\exp(i\omega)d\omega,$$

which requires calculating integrals. This can be done using the residue method, but this approach requires separate consideration. To solve the problem, we need to determine the initial wave function $\Psi(0,x)$ and its derivative, which will be done below. It is convenient to introduce the frequency $\omega = E/\hbar$. The incident wave packet (WP) from the left can be written as:

$$\Psi(t,0) = \int_0^{E/\hbar}\psi^+(0,\omega)\exp(-i\omega t)d\omega,$$

$$\psi^+(0,\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\Psi(0,\omega)\exp(i\omega t)d\omega.$$

Here:

$$\omega = k^2\hbar/2m_e, \quad k = \sqrt{2m_e\omega/\hbar}.$$

Neglecting back tunneling, we have on the left:

$$\Psi(t,0) = \int_0^{E/\hbar}a^+(\omega)\left(1 + R^+(\omega)\right)\exp(-i\omega t)d\omega,$$

and on the right:

$$\Psi(t,d) = \int_0^{E_F/\hbar}a^+(\omega)T^+(\omega)\exp(-i\omega t)d\omega.$$

The incident WP from the left is denoted as:

$$\Psi^+(t) = \int_0^{E/\hbar}a^+(\omega)\exp(-i\omega t)d\omega.$$

Here:

$$\psi^+(0,\omega) = a^+(\omega), \quad \psi^+(d,\omega) = a^+(\omega)T^+(\omega).$$

Defining $\Psi(x,t)$ as the solution to the nonstationary Schrödinger equation at time t, we construct the function:

$$\tilde{\Psi}(x,t) = \Psi(x,t) - \Psi(x,0).$$

It is zero outside the interval $(0,t)$, meaning it has a limited support, and:

$$\tilde{\Psi}(x,\omega) = \frac{1}{2\pi}\int_0^t \tilde{\Psi}(x,t')\exp(i\omega t')dt',$$

$$\Psi(x,\omega) = \frac{1}{2\pi}\int_{-\infty}^t \Psi(x,t')\exp(i\omega t')dt'.$$

We can construct the time-dependent reflection and transmission coefficients $R^+(t)$, $T^+(t)$. Specifically, we take:

$$R^+(t) = \Psi(0,t)/\Psi^+(t) - 1,$$

$$T^+(t) = \Psi(d,t)/\Psi^+(t).$$

Considering back tunneling, we define the incident WP from the right:

$$\Psi^-(t) = \int_0^{E/\hbar} a^-(\omega)\exp(-i\omega t)d\omega.$$

Thus, we obtain:

$$\Psi(t,0) = \Psi^+(t)\left(1 + R^+(t)\right) + T^-(t)\Psi^-(t),$$

$$\Psi(t,d) = \Psi^+(t)T^+(t) + \Psi^-(t)\left(1 + R^-(t)\right).$$

To find all coefficients, we also need to determine $\Psi'(t,x)$,Ψ'^+ and Ψ'^-. Derivatives can be found by differentiating the series. The current density at the anode is defined through the probability current density:

$$J(t_m) = -ej(t_m,d).$$

For this, when normalizing the wave function to the probability density, we use [20]:

$$j(t_m,x) =$$

$$= -\frac{i\hbar}{2m_e}[\Psi^*(t_m,x)\partial_x\Psi(t_m,x) -$$

$$-\Psi(t_m,x)\partial_x\Psi^*(t_m,x)].$$

For an arbitrary moment in time, we obtain:

$$j(t,x) = \frac{j(0)}{4}\times$$

$$\times\mathrm{Re}(-i\sum_{m=0}^{\infty}\left[\alpha_m^*(t)\cos(\chi_m x) + \beta_n^*(t)\sin(\chi_m x)\right]\times$$

$$\times\sum_{n=1}^{\infty} n\left[-\alpha_n(t)\sin(\chi_n x) + \beta_n(t)\cos(\chi_n x)\right]),$$

$$j(t,d) = \frac{j(0)}{4}\times$$

$$\times\mathrm{Re}\left(-i\sum_{m=0}^{\infty}(-1)^m\,\alpha_m^*(t)\cdot\sum_{n=1}^{\infty}(-1)^n\, n\beta_n(t)\right).$$

From this equation, it follows that:

$$j(0,d) = 0, \quad j(\Delta t,d) \sim \Delta t,$$

i.e., instantaneous tunneling and negative tunneling time are not possible. Using the spectra $\Psi(d,\omega)$ and $\Psi'(d,\omega)$, the result can be represented as:

$$j(t,d) = \frac{\hbar}{(2\pi)^2 m_e}\times$$

$$\times\,\mathrm{Re}\int_{-\infty}^{\infty}(-i)\Psi^*(d,\omega)\Psi'(d,\omega')\exp\left(i(\omega'-\omega)t\right)d\omega' d\omega.$$

For the steady-state process, the spectral wave function at the anode is:

$$\psi(x,k) = a^+(k)T^+(k)\exp\left(ik_a(x-d)\right)$$

The probability flux density for this wave function is:

$$dj(d,k) = v_a(k)\left|a^+(k)T^+(k)\right|^2 dk,$$

where the speed at the anode is:

$$v_a(k) = \sqrt{v^2(k) + 2eU_a/m_e}.$$

It should be noted that this speed is greater than $v(k)$ due to the acceleration of electrons passing through the barrier by the anode. Over the free path length, they scatter and transition to the Fermi level of the anode, with $v_a(k)$ decreasing to $v(k)$, causing the anode to heat up. The method of series used here is also convenient for solving the Schrödinger equation (SE) together with the Poisson equation (PE).

5. RESULTS AND DISCUSSION

Figs. 6 and 7 present the results of the transient process calculations, showing the establishment of the anode current in a diode with a Fermi energy of 7 eV and the probability density distribution $|\Psi(x,t)|^2$ when stepwise voltages of 3, 5, and 7 V appear at the anode. Fig. 7 shows the probability density distribution for curve 1 of Fig. 6 at different moments in time. The oscillations in probability density result from the finite sums used in the calculations. As the number of terms in the sums increases, both the oscillation amplitude and period decrease. The SE was integrated using the series method with 40 terms and an explicit calculation of the coefficients in equation (12). Expanding in other bases in (12) allows eliminating the oscillations. For example, finite elements can be used. However, the proposed series method is convenient when solving the SE and PE simultaneously, as applied in [2].

Calculations were performed using 200 time points. Curves 2 and 3 in Fig. 6 were constructed using 50 time points. For copper (Fermi energy 7 eV), we have an electron concentration of $8.5 \cdot 10^{28} \mathrm{m}^{-3}$ and a Fermi velocity $v_F = 1.57 \cdot 10^6$ m/s, meaning that a particle with this speed travels a distance $d = 10$ nm in a time $\tau = 6.35$ fs. We assumed that at the moment the voltage is applied, the probability density inside the barrier was zero. More precisely, it is symmetrically distributed relative to the center, approximately following a hyperbolic cosine distribution, increasing towards the edges, but extremely small at the edges themselves due to the near-complete reflection by the wide, nearly rectangular barrier. In this case, there is no inward probability flux into the barrier. The results shown in Fig. 6 indicate that the average transport speed of the probability density is somewhat greater than v_F, leading to the conclusion that the movement of the probability density is a collective effect caused by the interference of partial waves of the wave packet. An electron inside the barrier, or generally within a potential field, behaves as a quasiparticle defined by its interaction with many other particles. This averaged interaction determines the potential. A clear example is the potential of the image method. Such a quasiparticle is not required to behave like a free electron. Additionally, after passing the turning point for a single barrier, the electron moves quasi-classically and is accelerated by the anode. The additional velocity gained at $U_a = 5$ V is 1.33×106 m/s, approximately equal to

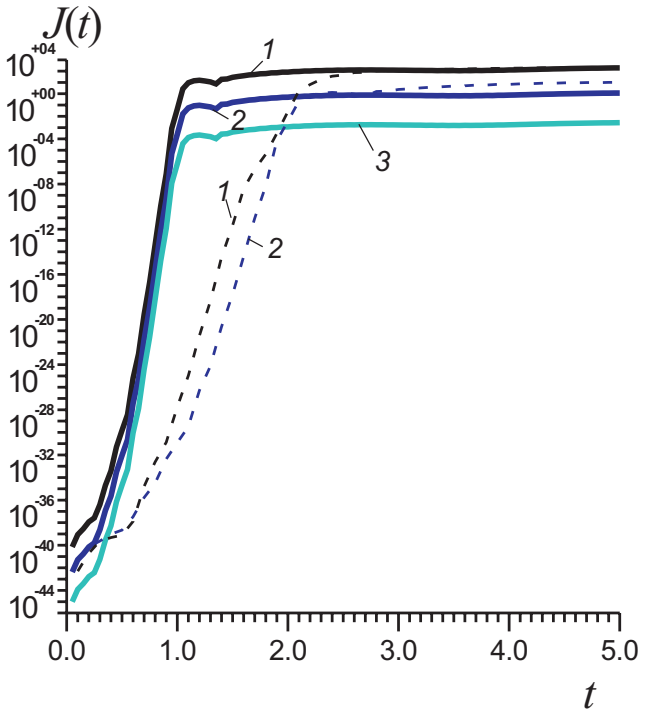

Fig. 6. Transient processes ($-J$ in A/cm², time in fs) during switching from the nearly rectangular barrier *1* to barriers *2*, *3*, and *4* in Fig. 1 (corresponding to curves *1*, *2*, and *3*).

v_F. Accordingly, the transit time is halved. A similar problem for resonant tunneling (RT) leads to a significantly longer transient process time. This can be explained by the need to form reflections from the barriers for RT to occur.

Formally, the lifetimes of the levels can be considered as an additional contribution to the transient process time. In Fig. 6, it is evident that the probability density is very small at short times. This function is asymmetric and, on average, higher near the start of the barrier but stabilizes at longer times. Similar calculations of transient processes for switching from a wide barrier to a structure with narrow, unequal barriers and a quantum well show slower current growth. This is explained by the reflections from the barriers required to form resonant levels in the well. To achieve complete RT, the barrier heights must be sufficiently close. Numerical calculations of the transparency coefficients show not only full resonances but also peaks with incomplete RT, where the maxima $D < 1$. Regarding lifetimes $\tau_n = 2\hbar/E_n''$, they are significantly shorter than the corresponding times determined at short times from transient processes as a result of wave packet evolution. This is because the wave packet contains

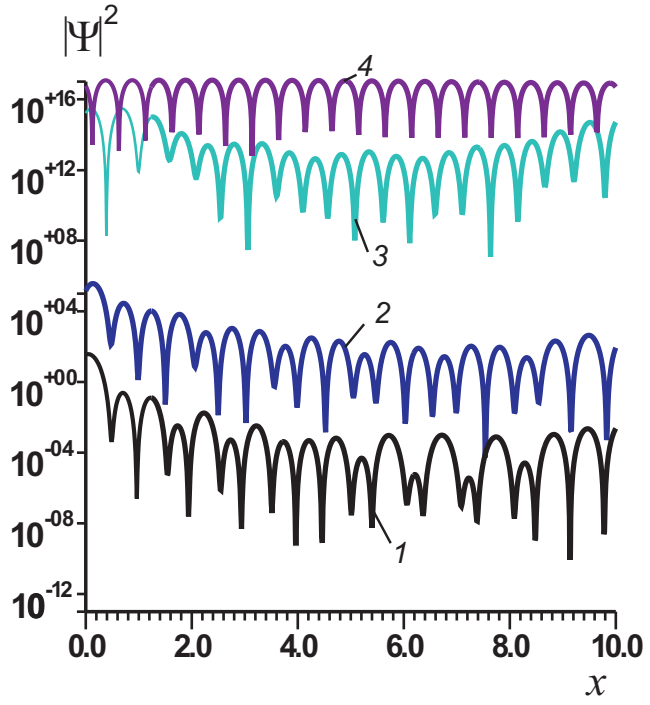

Fig. 7. Particle number density (m^3) as a function of the coordinate x (nm) in a vacuum diode structure at different moments in time (fs): 0.1 (*1*), 0.3 (*2*), 0.5 (*3*), 1.0 (*4*).

a broad energy spectrum. At longer times, the non-exponential nature of the level decay becomes evident (see, for example, [30–34]), with contributions from algebraic terms. Determining level lifetimes this way is feasible only for very narrow wave packets, which is challenging to achieve experimentally for non-relativistic quantum particles, and even more difficult to observe their passage through a barrier. This raises problems with reflecting a spectrally narrow (i.e., spatially very broad) wave packet from the barrier [18], especially when the barrier itself changes over time. However, the macroscopic current density can be measured with high accuracy.

The quantity with the dimension of velocity:

$$v(x,t) = j(x,t)/|\Psi(x,t)|^2$$

can be interpreted as the speed of the probability density movement at point x at time t. This corresponds to the concept introduced by N.A. Umov, but it cannot be interpreted as the speed of an individual particle. For a single-speed particle flow, it coincides with the particle velocity in the flow. The increase in current is accompanied by an increase in the probability density of particle presence inside the barrier. The average instantaneous speed of the wave packet (WP) passing through point x over time τ can be defined as:

$$\bar{v}(x,t,\tau) = \frac{1}{\tau}\int_{t-\tau}^{t} \frac{j(x,t')}{|\Psi(x,t')|^2}dt'. \qquad (18)$$

If the WP is finite in time, its average speed can also be determined.

Short lifetimes of quasi-stationary levels are essential for achieving high current densities in field emission. It is desirable to have as many such levels as possible, and sufficiently deep ones. Increasing the number of levels is achieved by increasing the width of the quantum well, while reducing lifetimes is achieved by using narrow-width barriers. Current growth is also facilitated by leveling the barrier heights, which can be controlled by the gate voltage and the change in the gate work function.

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APPENDIX

For the well, from the conditions at the cathode-side barrier, we have:

$$A_w^+ = \frac{A_c^+ \exp(-\tilde{k}_c t_c) + A_c^- \exp(\tilde{k}_c t_c)}{2} + \frac{\tilde{k}_c A_c^- \exp(\tilde{k}_c t_c) - \tilde{k}_c A_c^+ \exp(-\tilde{k}_c t_c)}{2ik},$$

$$A_w^- = \frac{A_c^+ \exp(-\tilde{k}_c t_c) + A_c^- \exp(\tilde{k}_c t_c)}{2} - \frac{\tilde{k}_c A_c^- \exp(\tilde{k}_c t_c) - \tilde{k}_c A_c^+ \exp(-\tilde{k}_c t_c)}{2ik}.$$

In the case of wide barriers, neglecting exponentially small terms (reflections from the left edge of the barrier with amplitude A_c^+), we find from the matching conditions at the cathode-side barrier:

$$A_w^+ \approx \frac{A_c^- \exp(\tilde{k}_c t_c)(1 - i\tilde{k}_a/k_0)}{2},$$

$$A_w^- \approx \frac{A_c^- \exp(\tilde{k}_c t_c)(1 + i\tilde{k}_a/k_0)}{2}.$$

On the other hand, the matching conditions at the anode-side barrier give:

$$A_w^+ = \frac{\exp(-ik_0t_w)\left[A_a^+ + A_a^- + i\left(A_a^+ - A_a^-\right)\tilde{k}_a/k_0\right]}{2},$$

$$A_w^- = \frac{\exp(ik_0t_w)\left[A_a^+ + A_a^- - i\left(A_a^+ - A_a^-\right)\tilde{k}_a/k_0\right]}{2}.$$

At the cathode boundary, we have the relations:

$$A_c^+ = \frac{A_c\left(1 + ik_0/\tilde{k}_c\right)}{2},$$

$$A_c^- = \frac{A_c\left(1 - ik_0/\tilde{k}_c\right)}{2}.$$

At the anode boundary, we have accordingly:

$$A_a^+ = \frac{A_a\exp\left(\tilde{k}_at_a\right)\left(1 - ik_a/\tilde{k}_a\right)}{2},$$

$$A_a^- = \frac{A_a\exp\left(-\tilde{k}_at_a\right)\left(1 - ik_a/\tilde{k}_a\right)}{2}.$$

For wide barriers, the amplitudes A_a^- and A_A^+ are small. Assuming them to be zero, we obtain:

$$A_w^+ \approx$$

$$\approx\frac{A_a\exp\left(\tilde{k}_at_a\right)\left(1-ik_0/\tilde{k}_a\right)\left(1+i\tilde{k}_a/k_0\right)\exp\left(-ik_0t_w\right)}{4},$$

$$A_w^+ \approx \frac{A_c\exp\left(\tilde{k}_ct_c\right)\left(1 - ik_0/\tilde{k}_c\right)\left(1 - i\tilde{k}_c/k_0\right)}{4},$$

$$A_w^- =$$

$$=\frac{A_a\exp\left(\tilde{k}_at_a\right)\left(1-ik_0/\tilde{k}_a\right)\left(1-i\tilde{k}_a/k_0\right)\exp\left(ik_0t_w\right)}{4},$$

$$A_w^- \approx \frac{A_c\exp\left(\tilde{k}_ct_c\right)A_c\left(1 - ik_0/\tilde{k}_c\right)\left(1 + i\tilde{k}_c/k_0\right)}{4}.$$

Equating the coefficients $A_w^{\pm}$, we get two equations:

$$A_a\exp\left(\tilde{k}_at_a\right)\left(1-ik_0/\tilde{k}_a\right)\left(1+i\tilde{k}_a/k_0\right)\exp\left(-ik_0t_w\right) =$$

$$= A_c\exp\left(\tilde{k}_ct_c\right)\left(1 - ik_0/\tilde{k}_c\right)\left(1 - i\tilde{k}_c/k_0\right),$$

$$A_a\exp\left(\tilde{k}_at_a\right)\left(1 - ik_0/\tilde{k}_a\right)\left(1 - i\tilde{k}_a/k_0\right)\exp\left(ik_0t_w\right) =$$

$$= A_c\exp\left(\tilde{k}_ct_c\right)\left(1 - ik_0/\tilde{k}_c\right)\left(1 + i\tilde{k}_c/k_0\right).$$

Dividing the first by the second, we obtain the approximate characteristic equation:

$$\frac{\left(1 - i\tilde{k}_A/k_0\right)\left(1 - i\tilde{k}_a/k_0\right)}{\left(1 + i\tilde{k}_A/k_0\right)\left(1 + i\tilde{k}_a/k_0\right)} = \exp\left(-2ik_0t_w\right). \qquad \text{(A1)}$$

To obtain the exact equation, all amplitudes must be retained. In this case, equating the coefficients gives:

$$\begin{pmatrix} A_A^+ \\ A_A^- \end{pmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}\begin{pmatrix} A_a^+ \\ A_a^- \end{pmatrix},$$

$$\begin{pmatrix} A_a^+ \\ A_a^- \end{pmatrix} = \begin{bmatrix} M_{11}^{-1} & M_{12}^{-1} \\ M_{21}^{-1} & M_{22}^{-1} \end{bmatrix}\begin{pmatrix} A_c^+ \\ A_c^- \end{pmatrix}.$$

The matrix elements $\widehat{M}$ are given by:

$$M_{11} = \exp\left(\tilde{k}_At_c\right)\tilde{M}_{11} = \exp\left(\tilde{k}_At_c\right)\times$$

$$\times\frac{\cos\left(k_0t_w\right)\left(1+\tilde{k}_a/\tilde{k}_c\right)+\left(\tilde{k}_a/k_0-k_0/\tilde{k}_A\right)\sin\left(kt_w\right)}{2},$$

$$M_{12} = \exp\left(\tilde{k}_At_c\right)\tilde{M}_{12} = \exp\left(\tilde{k}_At_c\right)\times$$

$$\times\frac{\cos\left(k_0t_w\right)\left(1-\tilde{k}_a/\tilde{k}_A\right)-\left(\tilde{k}_a/k_0+k_0/\tilde{k}_A\right)\sin\left(kt_w\right)}{2},$$

$$M_{21} = \exp\left(-\tilde{k}_At_c\right)\tilde{M}_{21} = \exp\left(-\tilde{k}_At_c\right)\times$$

$$\times\frac{\cos\left(k_0t_w\right)\left[1-\tilde{k}_a/\tilde{k}_A\right]+\left(\tilde{k}_a/k_0+k_0/\tilde{k}_c\right)\sin\left(k_0t_w\right)}{2},$$

$$M_{22} = \exp\left(-\tilde{k}_At_c\right)\tilde{M}_{22} = \exp\left(-\tilde{k}_At_c\right)\times$$

$$\times\frac{\cos\left(k_0t_w\right)\left(1+\tilde{k}_a/\tilde{k}_c\right)-\left(\tilde{k}_a/k_0-k_0/\tilde{k}_c\right)\sin\left(k_0t_w\right)}{2}.$$

Now

$$A_c^+ = A_c\left(1 + ik_0/\tilde{k}_c\right) =$$

$$= 2\left(M_{11}A_a^+ + M_{12}A_a^-\right),$$

$$A_c^- = A_c\left(1 - ik_0/\tilde{k}_c\right) =$$

$$= 2\left(M_{21}A_a^+ + M_{22}A_a^-\right).$$

Substituting $A_a^{\pm}$ in these expressions, we obtain:

$$A_c\left(1+ik_0/\tilde{k}_c\right)=M_{11}A_a\exp\left(\tilde{k}_at_a\right)\left(1-ik_0/\tilde{k}_a\right)+$$

$$+M_{12}A_a\exp\left(-\tilde{k}_at_a\right)\left(1 - ik_0/\tilde{k}_a\right),$$

$$A_c\left(1-ik_0/\tilde{k}_c\right)=M_{21}A_a\exp\left(\tilde{k}_a t_a\right)\left(1-ik_0/\tilde{k}_a\right)+$$
$$+M_{22}A_a\exp\left(-\tilde{k}_a t_a\right)\left(1-ik_0/\tilde{k}_a\right).$$

Dividing the first equation by the second, we obtain the characteristic equation:

$$\frac{1+ik_0/\tilde{k}_c}{1-ik_0/\tilde{k}_c}=f(E)= \tag{A2}$$
$$=\frac{\tilde{M}_{11}\exp\left(\tilde{k}_c t_c+\tilde{k}_a t_a\right)+\tilde{M}_{12}\exp\left(\tilde{k}_c t_c-\tilde{k}_a t_a\right)}{\tilde{M}_{21}\exp\left(\tilde{k}_a t_a-\tilde{k}_c t_c\right)+\tilde{M}_{22}\exp\left(-\tilde{k}_a t_a-\tilde{k}_c t_c\right)}.$$

For wide barriers, small terms can be neglected, resulting in the simplified form:

$$f(E)\approx\exp\left(2\tilde{k}_c t_c\right)\times$$
$$\times\frac{1+\tilde{k}_a/\tilde{k}_c+\left(\tilde{k}_a/k_0-k_0/\tilde{k}_c\right)\left(k_0 t_w\right)}{1-\tilde{k}_a/\tilde{k}_c+\left(\tilde{k}_a/k_0+k_0/\tilde{k}_c\right)\left(k_0 t_w\right)}.$$

The matrix elements appearing in equations (14) and (15) are expressed as:

$$A_{nm}^{cc}=\frac{sinc\left(\left(\chi_n-\chi_m\right)d\right)+sinc\left(\left(\chi_n+\chi_m\right)d\right)}{1+sinc\left(2\chi_n d\right)}=$$
$$=\frac{\delta_{nm}}{1+\delta_{n0}},$$
$$A_{nm}^{cs}=\frac{conc\left(\left(\chi_n-\chi_m\right)d\right)-conc\left(\left(\chi_n+\chi_m\right)d\right)}{1+sinc\left(2\chi_n d\right)}=$$
$$=\frac{(-1)^{n+m}-(-1)^{n-m}}{1+\delta_{n0}}, \tag{A3}$$
$$A_{nm}^{sc}=\frac{conc\left(\left(\chi_n-\chi_m\right)d\right)+conc\left(\left(\chi_n+\chi_m\right)d\right)}{1+sinc\left(2\chi_n d\right)}=$$
$$=\frac{2-(-1)^{n-m}-(-1)^{n+m}}{1+\delta_{n0}},$$
$$A_{nm}^{ss}=\frac{sinc\left(\left(\chi_n-\chi_m\right)d\right)-sinc\left(\left(\chi_n+\chi_m\right)d\right)}{1-sinc\left(2\chi_n d\right)}=\delta_{nm}.$$

These expressions involve the following integrals:

$$V_{nm}^{\alpha cc}(t)=\frac{2}{(1+\delta_{n0})d}\int_0^d V(t,x)\cos\left(\chi_n x\right)\cos\left(\chi_m x\right)dx,$$
$$V_{nm}^{\beta ss}(t)=\frac{2}{(1+\delta_{n0})d}\int_0^d V(t,x)\cos\left(\chi_n x\right)\sin\left(\chi_m x\right)dx,$$
$$V_{nm}^{\beta ss}(t)=2\int_0^d V(t,x)\sin\left(\chi_n x\right)\sin\left(\chi_m x\right)dx,$$
$$V_{nm}^{\alpha sc}(t)=2\int_0^d V(t,x)\sin\left(\chi_n x\right)\cos\left(\chi_m x\right)dx.$$

In equation (A3), the functions $sinc(x)=\sin(x)/x$ and $conc(x)=(1-\cos(x))/x$ are included. These functions at zero should be defined as $sinc(0)=1$, $conc(0)=0$ ensuring proper boundary conditions. Moreover, the condition $sinc(2n\pi)=\delta_{n0}$ applies at the barrier edge.

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