UDC 621.315.592

# Analytical solution of the one-dimensional schrodinger equation with linear potential in diode

© M.V. Davidovich

Saratov National Research State University,
410012 Saratov, Russia

E-mail: davidovichmv@info.sgu.ru

Received June 27, 2024
Revised January 1, 2025
Accepted January 6, 2025

An analytical solution of the Schrodinger equation with a potential in the form of a linear function is obtained by three methods. Their results correspond to each other and to the numerical solution. The current in the vacuum diode is calculated taking into account the temperature.

**Keywords:** thermionic-field emission, Schrodinger equation, tunneling, diode.

DOI: 10.61011/SC.2024.12.60382.6826

## 1. Introduction

The potential barrier in a diode structure can be determined very accurately based on the multiple-image method [1,2]. Often in the literature problems with rectangular barriers [3] are used as exactly solvable. In some cases, the actual barrier in the diode is very close to triangular (Figure 1). The triangular shape (Figure 2) is considered in a number of papers, e. g., [4]. In fact it means a linear dependence of the potential on the coordinate, i. e., coordinate-independent force acting on the electron. The triangular shape of the barrier is closer to the reality arising in modeling real semiconductor devices, including resonant-tunnel diodes [5–8]. However, the lack of rigorous models for it leads to the use of coarser models, barriers, for example, even in the form of $\delta$-functions [7]. Although there is a formula for tunneling through a triangular barrier [9] in the quasi-classical approximation (WKB) (calculus in quantum mechanics) on which Fowler–Nordheim (FN) theory is based, it is not entirely satisfactory, as will be noted later. Although an analytical solution in the form of Airy functions is known for the triangular quantum well, it has not been used for a finite triangular quantum barrier in a diode, therefore obtaining its value is a relevant problem. The trapezoidal form of the barrier in the form of a triangle on a rectangular pedestal [4–6] (Figure 2, $b$) is often considered. The linear potential solution can also be applied to it, since the rectangular pedestal is accounted for is quite simple. Much attention has recently been paid to the study of tunneling through a triangular barrier [10–12]. The search for exactly solvable models [11,12] for the tunneling coefficient, such as using harmonic wavelets [12] and by using the Airy function method with the origin placed at the outer classical pivot point (PP) of the electron [13], is crucial. Tunneling through the triangular barrier was the basis of the FN theory, so the search for exact solutions is an urgent problem.

One-dimensional Schrödinger equation (SE)

$$[-\hbar^2\partial^2_{xx}/(2m_e) + V(x/d) - E]\psi(x/d) = 0$$

with a linear function of quantum potential

$$V(x/d) = E_{\mathrm{F}} + \tilde{W} - (\tilde{W} + eU_a)x/d.$$

at $0 \le x \le d$ in the diode has the form $\psi^*(x/d) = (ax/d-b)\psi(x/d)$. Here the dimensionless constants are denoted $a = 2m_e d^2(eU_a + \tilde{W})/\hbar^2$ and $b = 2m_e d^2(E_{\mathrm{F}} + \tilde{W} - E)/\hbar^2$, $m_e$ — mass (effective mass) of the electron, $U_a$ — anode potential, $\psi$ — wave function (WFN), $\tilde{W} = W/\varepsilon$ — effective work function (WF) considering the dielectric, $W$ — WF into vacuum, $\varepsilon$ — dielectric permittivity (DP) of the gap. In the following, we will use the following designations for dimensionless coordinates: $y = ax/d-b$, $z = y/a = x/d - b/a$, $t = x/d$, $\tau = z^3 a = \xi^3$, $\xi = a^{1/3}(t-c)$, and the ratio $c = b/a$. Therefore, the SE can be written as $\phi^*(t) = (at-b)\psi(t)$ or $\varphi^*\psi(\xi) = \xi\varphi(\xi)$. For a vacuum diode $\varepsilon = 1$, $\tilde{W} = W$. On cathode at $x < 0$ $V = 0$ is necessary, the VFN is, $\psi = \exp(ik_0x) + R\exp(-ik_0x)$ (when the incident wave amplitude is unity). Here $k_0 = \sqrt{2m_eE}/\hbar$ — wave number (WN), and at $x = d$ a linear approximation of the potential gives $V(1) = E_{\mathrm{F}} - eU_a$. Inside the WN barrier $k(x/d) = \sqrt{2m_e\left(E - V(x/d)\right)}/\hbar$ can be either imaginary or real but at the anode ($x > d$) the WN should be taken as $k_a = k_0$. This corresponds to a jump in the normalized wave impedance (WI) $\rho(x/d) = k_0/k(x/d)$ both at the cathode $\rho(0)/\rho_0 = \sqrt{1-(E_{\mathrm{F}} + \tilde{W})/E}$, and at the anode $\rho_0/\rho(1) = 1/\sqrt{1-(E_{\mathrm{F}} - \tilde{W} - eU_a)/E}$, $\rho_0 = 1$ (Figure 2). Let there is no anode voltage: $U_a = 0$. Then the barrier (for the vacuum gap) becomes rectangular with height $\tilde{W} + E_{\mathrm{F}}$. In front of it and behind it is $V = 0$, i. e. we have a potential jump $\pm(E_{\mathrm{F}} + \tilde{W})$, and also WI jumps

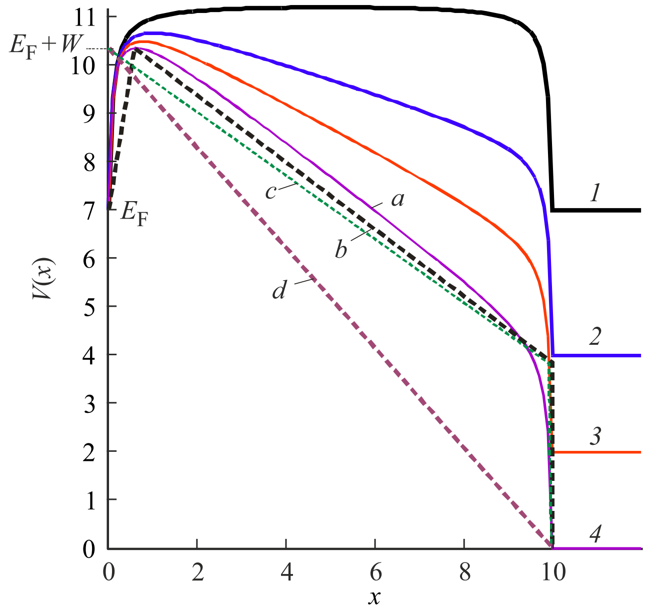


**Figure 1.** Shape of the potential barrier $V$ [eV] in a vacuum diode $d = 10$ nm as a function of coordinate $x$ (nm) at different anode voltages, V: *1* — 0, *2* — 3, *3* — 5, *4* — 7. The electrodes are made of copper $E_F = 7$, $W = 4.36$ (eV). The dashed lines $b, c$ and $d$ show linear approximations of the barrier $a$. (The colored version of the figure is available on-line).

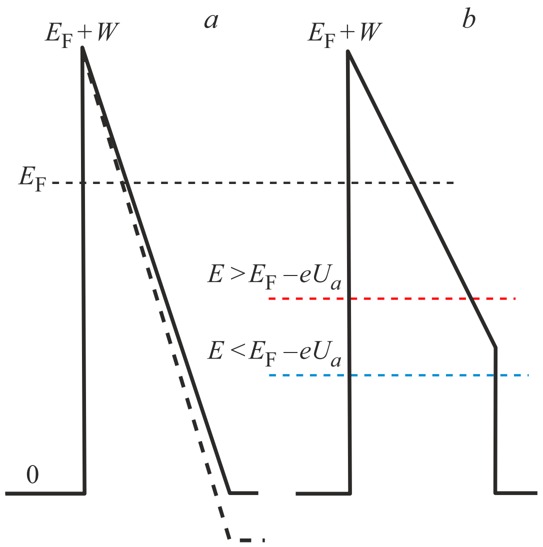


**Figure 2.** Triangular barrier ($a$) at $eU_a = E_F$ and $eU_a > E_F$ (shown by dashed line), ($b$) — triangle type barrier on pedestal at $eU_a < E_F$.

$\sqrt{1-(E_F+\tilde{W})/E}$ and $1/\sqrt{1-(E_F-\tilde{W})/E}$. Here there are two PPs $x = 0$ and $x = d$. The problem should be solved between the two PPs, i. e., the triangular barrier is reduced to a rectangular barrier in this case. Let $eU_a < E_F + \tilde{W}$. The jump in wave impedance at the anode can be both $E > E_F - \tilde{W} - eU_a$) and real (at $E < E_F - \tilde{W} - eU_a$). In the first case, we have to solve the problem from the PP $x = 0$ to PP $x = d$, and in the second case also to the $x = d$ point, but the TP is to the left: $x_{tp} < d$ (Figure 2). After the PP $x_{tp}$ the electron moves quasi-classically, accelerated by the anode, and its WFN acquires a phase incursion. It should be taken into account. Upon hitting the anode, the electron scatters at the free path length, its momentum relaxes to the Fermi momentum of the anode, the energy changes, and the wave equation for the scattering phase becomes inapplicable. Therefore, WN $k_0$, should be used, providing the law of energy conservation in the form of $|R| + |\tilde{T}| = 1$. We denote the values at the cathode by the index $c$, at the anode — by the index $a$ (we will omit them for identical electrode materials).

The above SE occurs in a vacuum tunnel diode at a large anode voltage $U_a$. It is also possible in a metal–insulator–metal (MIM) tunnel diode with metal electrodes and dielectric filling. Note that $b = 0$, if $E = E_F + \tilde{W}$ is satisfied for energy. This is the point at the apex of the triangular barrier. For it we have a general solution through the Airy functions $\psi(t) = A\,\mathrm{Ai}(a^{1/3}t) + B\,\mathrm{Bi}(a^{1/3}t)$ [14,15]. According to it,

$$1 + R = A\,\mathrm{Ai}(0) + B\,\mathrm{Bi}(0),$$

$$ik_0d(1-R) = a^{1/3}[A\,\mathrm{Ai}'(0) + B\,\mathrm{Bi}'(0)],$$

$$\tilde{T} = A\,\mathrm{Ai}(a^{1/3}) + B\,\mathrm{Bi}(a^{1/3}),$$

$$ik_0da^{-1/3}\tilde{T} = A\,\mathrm{Ai}'(a^{1/3}) + B\,\mathrm{Bi}'(a^{1/3}),$$

from where we obtain the input conductance for the narrow barrier

$$Y = (1-R)/(1+R) = 1 + ik_0d(3a)^{-1/3}\Gamma(1/3)/\Gamma(2/3),$$

i. e. the reflectance coefficient $R$ tends to zero when the barrier width $d$ tends to zero. For a finite width, we obtain a reflectance coefficient unequal to zero (contrary to the FN formula). At $d \to 0$ and therefore, $a \to 0$ we have $\psi(1) = \psi(0)$, $\psi'(1) = \psi'(0)$, $1 + R = \tilde{T}$, $1 - R = \tilde{T}$, i. e. $R = 0$, $\tilde{T} = 1$. At low $d$ we easily get $R \approx -ik_0d/4$. At $d \to \infty$ we have $B = 0$, $(1-R)/(1+R) = a^{1/3}\mathrm{Ai}'(0)/\big(ik_0d\mathrm{Ai}(0)\big) \to 0$, i. e. $R = 1$, which means a completely opaque infinite step at its level.

If the SE corresponds to a vacuum diode of length $d$, then on the surface of the cathode $V(0) = E_{Fc} + \tilde{W}$, where $E_{Fc}$ — the Fermi (FE) energy of the cathode, $\tilde{W}$ — the effective WF from the cathode relative to the FE, taking into account the Schottky effect, conductor and dielectric effects (the real WF of the cathode material $W_c$ may be much higher). Inside the cathode $V = 0$. The potential and energy are counted from the bottom of the conduction band of the cathode, so at the cathode the Fermi level (FL) $\mu_c$ (electrochemical potential) corresponds to FL:

$$\mu_c = E_{Fc}\big(1 - (\pi^2/12)(k_BT/E_{Fc})^2 + \ldots\big) \approx E_{Fc}.$$

At the anode, the FL is lower at $eU_a$, so $V(d) = E_F - eU_a$. This is a linear approximation of the real barrier [1,2] of Figure 1. Its maximum is slightly shifted from the cathode, and the shift is easily determined [1] of Figure 1, curve $a$. Therefore, it is more accurate to approximate $V(x)$ by two linear functions: from cathode to maximum and from maximum to anode (curve $b$). We will consider large voltages (strong fields) and small sizes $d$, when the barrier apex is very close to the cathode, the WF $\tilde{W}$ is small, and the function $V$ is nearly linear (Figure 1, curves $c, d$), i.e. we will take the approximation of Figure 2. In the limit case of high voltage $\tilde{W} \approx 0$, and the slope of the potential to the anode starts directly from the FE of the cathode. Inside the cathode for $x < 0$ electrons are free, $V(x) = 0$, so at the cathode the WN $k_0$, and at the cathode (at infinitesimal distance) $\kappa(0) = \sqrt{2m_e(E_F + \tilde{W} - E)}/\hbar$. In the region of the barrier, WN is imaginary $k(x) = i\kappa$, $\kappa(x) = \sqrt{2m_e\big(V(x) - E\big)}/\hbar$. In the vicinity of the anode the WN $k_a = \sqrt{2m_e(E + eU_a - E_F)}/\hbar$. For the numerical solution, the normalized WI of electron waves [3] $\rho(x) = k_0/k(x)$ are used. Inside the barrier, they are imaginary, on cathode and on anode $\rho_0 = 1$.

Next, we consider a barrier that appears abruptly from zero at $x < 0$ to $E_F + W$ at $x = 0$, and then declines linearly to $V(d)$ at anode (Figure 1, curve $d$, Figure 2). In this case, the WI jump occurs at both electrodes. Note that at $eU_a = E_F$ will be $k_a = k_c$, and there is no WI jump at the anode (Figure 2, $a$). For simplicity, we assume the cathode and anode materials are the same. If this is not the case, and also if there is dielectric filling of the cathode–anode space by a material with dielectric permittivity (DP) $\varepsilon$, then the potential should be taken as

$$V(x) = E_{Fc} + W_c/\varepsilon - [(W_c - W_a)/\varepsilon + eU_a]x/d.$$

WF is understood taking into account the Schottky effect and the mutual influence of the electrodes, i.e. considering the size $d$. Taking into account the dielectric leads to a $\varepsilon$ fold reduction in the barrier, i.e. to the replacement of $W \to W/\varepsilon$. It is convenient to assume $W = 0$, which takes place for high voltages (strong fields), when the maximum potential moves to the cathode (the barrier relative to FE disappears). In a vacuum diode, this occurs at the critical voltage $U_a = 8W_c(1 - \alpha/d)/(e\varepsilon)$ (the approximation of the potential $V$ by a 4th order parabola [2] without field application is taken). The small parameter $\alpha \ll d$ will be given later and determines the reduction of the WF $W_c$ from the cathode due to the proximity of the electrodes.

For $W_c = 4\,\text{eV}$ and $d = 2\,\text{nm}$ $\varepsilon = 1$ we have the critical anode potential $U_a \sim 34\,\text{V}$, i.e. the voltage of the critical field for the vacuum diode $\sim 1.7 \cdot 10^{10}\,\text{V/m}$. For a diode made on a diamond film using CVD (chemical vapor deposition) technology with DP $\varepsilon = 5.6$ it is $\sim 6$ times lower. If we consider a remote anode and a barrier

$$V(x) = E_F + W_c/\varepsilon - e^2/[16\pi\varepsilon_0\varepsilon(x + \delta)] - E_x x,$$

created by the electric field $E_x$, from the condition $V'(0) = 0$ of finding the maximum at the cathode we obtain the critical field $E_{xc} = e^2/(16\pi\varepsilon_0\varepsilon\delta^2) = W_e/(\varepsilon\delta)$. Here $\delta \ll d$ — a small parameter with length dimension: $W_e = e^2/(16\pi\varepsilon_0\delta)$, i.e. of the cathode $V(0) = E_F$. For WF $W_c = 4\,\text{eV}$ we have $\delta = 0.09\,\text{nm}$, and the critical field is significantly higher: $2.2 \cdot 10^{10}\,\text{V/m}$, since the barrier is significantly reduced in nanoscale structures. It is at such fields that the real potential becomes almost linear, and a triangular barrier appears for the electron with energy $E < E_F$. An approximate solution for it is known for the transparency in the quasi-classical (WKB) approximation [9]: $D \approx A\exp\big(-4d\kappa(0)/(3eU_a)\big)$, where WF $\kappa(x) = \sqrt{2m_e\big(V(x) - E\big)}/\hbar$ and $\kappa(0) = \kappa_0 = \sqrt{2m_e(E_F - E)}/\hbar$. are denotedIn it we have replaced the electric field — $E_x$ with $U_a/d$. In case of non-zero WF $W$ we will have $\kappa_0 = \sqrt{2m_e(E_F + W - E)}/\hbar$. In [9] the pre-exponential multiplier $A$ is found by neglecting the value of $\alpha = -\beta\exp(-2\gamma)$ — the backward (reflected from the trailing edge of the triangular barrier) rising wave

$$\alpha\exp\left(\int_0^x \kappa(y)dy\right) \Big/ \sqrt{\kappa(x)}$$

in region $0 < x < l$ (in [9] $\alpha = 0$) is assumed where the integral

$$\gamma = \frac{1}{\hbar}\int_0^l \sqrt{2m_e\big(V(x) - E\big)}dx$$

is calculated before the PP $l$ (of formula (24.4), (24.7) from [9]). It is determined from the condition $E = V(l)$. In our case, $l = d(E_F - E + W)/(W + eU_a)$. This is justified when the barrier length $l$ is substantial. However at $W = 0$ and near the FE $E \approx E_F$ (where there is maximum transparency) it will be $l = 0$ and $\alpha = -\beta$, so the formula for transparency is not correct. Moreover, the multiplier $A$ (formula (24.7)) derived in such a way is inversely proportional to the infinitesimal value of $\kappa(l) = 0$. This formula is given for the case of zero potential to the left and right of the barrier. Taking into account both coefficients at arbitrary potentials leads to a refinement of the formula given later in the monograph [9]:

$$A = \frac{16k_a}{k_0\big(\kappa(l) + k_a^2/\kappa(l)\big)\left[\big(1 - \exp(-2\gamma)\big)^2/\kappa(0) + \kappa(0)\big(1 + \exp(-2\gamma)\big)^2 k_a^2/k_0^2\right]},$$

which has the same drawbacks. The reason for this is the quasi-classical WFN of the forbidden region, before the exponents in which the multiplier $1/\sqrt{\kappa(x)}$ takes place. When computing the derivative of the $\partial\psi/\partial x$ WFN, only the exponents are differentiated, since the $1/\sqrt{\kappa(x)}$ multiplier is assumed to be a smooth function. However, in TP this function is not. The problem of correct definition of the multiplier $A$ is simply reduced to the fact that it is replaced by one. The same takes place in the FN formula. In this case for $E = E_F$ we get $D = 1$, which is incorrect. Of course, one can correctly take into account the derivative of $1/\sqrt{\kappa(x)}$, which leads to very complex formulas, but even this approach is approximate. Therefore, obtaining an analytical solution of the SE is a relevant issue.

The purpose of this paper is — to obtain an analytical solution of the SE with a linear potential. Since complex potential barriers have large nearly linear regions [1,2], such a solution will improve the accuracy of numerical solution of such problems using piecewise linear approximation, since they are usually solved on the basis of piecewise constant approximations of the potential [1,2]. It will also allow evaluating the accuracy of the FN formula.

## 2. Solving by means of cylindrical functions

The original SE $\psi''(t) = a(t-c)\psi(t)$ is reduced to the Airy equation $\varphi''(\xi) = \xi\varphi(\xi)$ for function $\varphi(\xi) = \psi(\xi/a^{1/3} + c)$ by replacing $\xi = a^{1/3}(t-c)$. It has a solution in the Bessel functions (see [14], 2.162(11)): $\varphi(\xi) = \sqrt{\xi}Z_{1/3}(2i\xi^{3/2}/2)$ at $\xi > 0$ and $\varphi(\xi) = \sqrt{\xi}Z_{1/3}(2\xi^{3/2}/3)$ at $\xi < 0$. Here $Z_\nu(z) = C_1 J_\nu(z) + C_2 Y_\nu(z)$ — the general solution of the Bessel equation of index $\nu = \pm 1/3$, $C_1, C_2$ — arbitrary coefficients (integration constants). However, these solutions for the diode are inconvenient because $\xi$ may go to zero in the region, and it is necessary to take a finite solution at $\xi = 0$, i.e. discard the Neumann function. Therefore, we take the general solution in the form [15] $\varphi(\xi) = C_1\,\mathrm{Ai}(a^{1/3}\xi) + C_2\,\mathrm{Bi}(a^{1/3}\xi)$. Here, the Airy functions of the 1st and 2nd kind are used: $\mathrm{Ai}(x) = \pi^{-1}\sqrt{x/3}K_{1/3}(2x^{3/2}/3)$, $\mathrm{Bi}(x) = -\sqrt{x/3}\big(I_{1/3}(2x^{3/2}/3) + I_{-1/3}(2x^{3/2}/3)\big)$, $K_\nu$ — Macdonald function

$$K_\nu(x) = (\pi/2)[I_{-\nu}(x) - I_\nu(x)]/\sin(\nu\pi),$$

$I_{\pm\nu}$ — Bessel functions of the 2nd kind. In the neighborhood of zero we have

$$\mathrm{Ai}(x) = \frac{1}{3^{2/3}\Gamma(2/3)} - \frac{x}{3^{1/3}\Gamma(1/3)} + \frac{x^3}{3^{2/3}6\Gamma(2/3)} - \frac{x^4}{3^{1/3}12\Gamma(1/3)} + \ldots,$$

$$\mathrm{Bi}(x) = \frac{1}{3^{1/6}\Gamma(2/3)} + \frac{3^{1/6}}{\Gamma(1/3)}\left(x + \frac{x^4}{12}\right) + \frac{1}{3^{1/6}\Gamma(2/3)}\frac{x^3}{6} + \ldots.$$

These functions are related at zero:

$$\mathrm{Ai}(0) = 3^{-2/3}/\Gamma(2/3) = \mathrm{Bi}(0)/\sqrt{3} = 0.355028053$$

and so are their derivatives:

$$\mathrm{Ai}'(0) = 3^{-1/3}/\Gamma(1/3) = -\mathrm{Bi}'(0)/\sqrt{3} = -0.258819403.$$

Consider the solution of the SE. To the left of the barrier we have WFN $\psi(x, E) = \exp(ik_0x) + R(E)\exp(-ik_0x)$, and to the right — $\psi(x, E) = \tilde{T}\exp\big(ik_0(x-d)\big)$. From boundary conditions we get:

$$1 + R = \mathrm{Ai}(-c)C_1 + \mathrm{Bi}(-c)C_2,$$

$$ik_0d(1-R) = a^{1/3}[\mathrm{Ai}'(-c)C_1 + \mathrm{Bi}'(-c)C_2]$$

on the left boundary, and also

$$\tilde{T} = \mathrm{Ai}\big(a^{1/3}(1-c)\big)C_1 + \mathrm{Bi}\big(a^{1/3}(1-c)\big)C_2,$$

$$ik_0d\tilde{T} = a^{1/3}\big[\mathrm{Ai}'\big(a^{1/3}(1-c)\big)C_1 + \mathrm{Bi}'\big(a^{1/3}(1-c)\big)C_2\big]$$

on the right boundary. Excluding the unknown constants, we have $C_2 = GC_1$ and

$$G = \frac{\mathrm{Ai}'\big(a^{1/3}(1-c)\big) - ik_0da^{-1/3}\mathrm{Ai}\big(a^{1/3}(1-c)\big)}{ik_0da^{-1/3}\mathrm{Bi}\big(a^{1/3}(1-c)\big) - \mathrm{Bi}'\big(a^{1/3}(1-c)\big)}, \quad (1)$$

$$C_1 = \\ = \frac{2ik_0d}{ik_0d\mathrm{Ai}(-c) + a^{1/3}\mathrm{Ai}'(-c) + [ik_0d\mathrm{Bi}(-c) + a^{1/3}\mathrm{Bi}'(-c)]G}. \quad (2)$$

The solution of the problem takes the form

$$Y = \frac{a^{1/3}[\mathrm{Ai}'(-c) + \mathrm{Bi}'(-c)G]}{ik_0d[\mathrm{Ai}(-c) + \mathrm{Bi}(-c)G]}, \quad (3)$$

$$\tilde{T} = [\mathrm{Ai}\big(a^{1/3}(1-c)\big) + \mathrm{Bi}\big(a^{1/3}(1-c)\big)G]C_1. \quad (4)$$

The reflectance coefficient is expressed as $R = (1-Y)/(1+Y)$ or as

$$R = C_1\big[\mathrm{Ai}(-c) + \mathrm{Bi}(-c)G - (a^{1/3}/ik_0d) \times [\mathrm{Ai}'(-c) + \mathrm{Bi}'(-c)G]\big]/2,$$

and for a transparent barrier we have $D = 1-|R|^2 = |\tilde{T}|^2$. For a narrow barrier at $c = 0$ it is not difficult to obtain

$$G \approx 1/\sqrt{3} - 2ik_0da^{-1/3}\mathrm{Ai}(0)/\big(\mathrm{Ai}'(0)\sqrt{3}\big).$$

## 3. Integration by the method of series

Calculating the Airy functions and their derivatives can be inconvenient, so we obtain another form of solution by integrating the original SE $\psi''(t) = a(t-b/a)\psi(t)$ by the method of series, i.e by decomposing into a power series over $t^n$: $\psi(t) = \alpha_0 + \alpha_1 t + \ldots$ with equating the coefficients at the same powers. Here, $\psi(t) = \alpha_0 + \alpha_1 t + \ldots$ $0 \le t \le 1$. We have the formula

$$\partial_{tt}^2\psi(t) = \sum_{n=2}^{\infty} n(n-1)\alpha_n t^{n-2} = a\sum_{n=0}^{\infty}\alpha_n t^{n+1} - b\sum_{n=0}^{\infty}\alpha_n t^n, \quad (5)$$

from which we obtain the recurrence formula

$$\alpha_n = (n-2)!(a\alpha_{n-3} - b\alpha_{n-2})/n!$$

Coefficients $\beta_n$ and $\gamma_n$

| $n$ | $\beta_n$ | $\gamma_n$ |
|---|---|---|
| 3 | $a/3!$ | $-b/3!$ |
| 4 | $b^2/4!$ | $2a/4!$ |
| 5 | $-4ab/5!$ | $b^2/5!$ |
| 6 | $(4a^2-b^3)/6!$ | $-6ab/6!$ |
| 7 | $\beta_1 = 9b^2a/7!$ | $\gamma_7 = (10a^2-b^3)/7!$ |
| 8 | $\beta_8 = (b^4-28a^2b)/8!$ | $\gamma_8 = 12ab^2/8!$ |
| 9 | $\beta_9 = (28a^3-16ab^3)/9!$ | $\gamma_9 = (b^4-52a^2b)/9!$ |
| 10 | $\beta_{10} = \big(100(ab)^2-b^5\big)/10!$ | $\gamma_{10} = (80a^3-20ab^3)/10!$ |

and the coefficients of $\alpha_2 = -b\alpha_0/21$, $\alpha_3 = a(\alpha_0-c\alpha_1)/3!$, $\alpha_4 = (b^2\alpha_0 + 2!a\alpha_1)/4!$, ... We find the general solution

$$\psi(t) = \alpha_0\big(1-bt^2/2 + \varphi_0(t)\big) + \alpha_1\big(t + \varphi_1(t)\big)$$

with functions

$$\varphi_0(t) = \beta_3 t^3 + \beta_4 t^4 + \ldots$$

and

$$\varphi_1(t) = \gamma_3 t^3 + \gamma_4 t^4 + \ldots,$$

$$\varphi_0(0) = \varphi_1(0) = 0.$$

The first few coefficients $\beta_n$ and $\gamma_n$ constructed from the recurrence formula are given in the table.

All coefficients can also be calculated through complex functions

$$f_n(\alpha_0, \alpha_1) = \big(a f_{n-3}(\alpha_0, \alpha_1) - b f_{n-2}(\alpha_0, \alpha_1)\big)/[n(n-1)],$$

$n = 1, 2, 3, 4, 5, 6, \ldots,$ where the first three functions are of the form: $f_0(\alpha_0, \alpha_1) = \alpha_0$, $f_1(\alpha_0, \alpha_1) = \alpha_1$, $f_2(\alpha_0, \alpha_1) = -b\alpha_0/2!$. Using these, we calculate the coefficients using the formulas

$$\alpha_n = (n-2)!\big(a f_{n-3}(\alpha_0, \alpha_1) - b f_{n-2}(\alpha_0, \alpha_1)\big)/n!,$$

$$n = 4, 5, \ldots$$

Then we calculate $\beta_n = f_n(1, 0)$, $\gamma_n = f_n(0, 1)$. The imaginary parts of $f_n(1, 0)$ and $f_n(0, 1)$ equal zero. To solve the problem, it is sufficient to know $\psi(0) = \alpha_0$, $\psi'(0) = \alpha_1$, $\psi(1)$ and $\psi'(1)$. Knowing the first two constants, the values of $\psi(1)$ and $\psi'(1)$ can be easily calculated using the recurrence formula $\alpha_n = (a\alpha_{n-3}-b\alpha_{n-2})/[n(n-1)]$.

To solve the problem, we have the equations $1 + R = \alpha_0$, $1 - R = \alpha_1/(ik_0 d)$, $\varphi(1) = \tilde{T}$, $\varphi'(1) = ik_a d\tilde{T}$. From the latter two relations we find the incoherence $\Delta = \varphi'(1)/\varphi(1) - ik_a d = 0$. From the first two we get $2 = \alpha_0 + \alpha_1/(ik_0 d)$ and $Y = (1-R)/(1+R) = \alpha_1/(ik_0 d\alpha_0)$. The solution using the functions $\varphi_0$, $\varphi_1$ and their derivatives is as follows: $\alpha_1 = \tilde{G}\alpha_0$, $\alpha_0 = 2/\big(1 + \tilde{G}/(ik_0 d)\big)$, where

$$\tilde{G} = \frac{b - \varphi_0'(1) + ik_0 d\big(1 - b/2 + \varphi_0(1)\big)}{1 + \varphi_1'(1) - ik_0 d\,\varphi_1(1)}. \qquad (6)$$

The function values included in (6) can be calculated using formulas with a finite number of terms. Since $t^n \le 1$, for a characteristic size of $d = 2\,\mathrm{nm}$ and the usual values of $eU_a \sim 5\,\mathrm{eV}$ we have $a \sim 500$, at the same time if $E_{\mathrm{F}} = 7\,\mathrm{eV}$, then value $b$ changes from zero to 740 during tunneling. In all coefficients $\beta_n$ and $\gamma_n$ the maximum degrees are less than $n/2$. Discarding the irrelevant coefficients in the Stirling formula, from the condition $n! \approx (500)^{n/2}$ we have an estimate of the maximum number of terms of the series $n \sim 60$ when its coefficients begin to decrease. This is a very tight estimate because the value (6) is computed as a function ratio. For MIM (metal−isolator−metal) type diodes, the need for a large number of series members is not entirely convenient. For SIS-(semiconductor−isolator−semiconductor)-type diodes the number of terms is much smaller. Thus, in a GaAs semiconductor diode with effective mass $m^* = 0.067m_e$ DP $\varepsilon = 14$ in layer $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ $d = 0.5\,\mathrm{nm}$ thick and at WF 4.5 eV, $U_a = 0.5\,\mathrm{V}$ we have $a = 2m^* d^2(eU_a + W/\varepsilon)/\hbar^2 = 0.36$ and $b = 0.14$ at level $E = E_{\mathrm{F}}$. In this case, 2−3 members are sufficient, i.e. we obtain a nearly analytical solution. In tunneling, $(E < E_{\mathrm{F}})b$ decreases with increasing energy, and becomes negative, but small in modulus (when the barrier is slightly exceeded). In general, using a finite number of terms in the series, we calculate (6) and determine $\alpha_0$ and $\alpha_1$. Then, using the recurrence formula, we calculate all other coefficients $\alpha_n$ to those numbers when they begin to greatly decrease. This determines the number of terms of the series needed. When calculated exactly, the $\Delta = \varphi'(1)/\varphi(1)-ik_a d$ discrepancy should be zero (low). We calculate this non-convexity and refine the coefficient iteratively: $\alpha_0^{(n+1)} = \alpha_0^{(n)}-\tau_n\Delta_n$. Here $\tau_n$ is the iteration parameter (with $\tau_n = 1$ — this is the simple iteration method). After each calculation of $\alpha_0^{(n+1)}$ $\alpha_1^{(n+1)}$ should be calculated $\alpha_1^{(n+1)} = (ik_0 d)(2-\alpha_0^{(n+1)})$ and use them to determine the new residual $\Delta$. The iteration parameter can be selected using the minimum residual method $\Delta_{n+1}$ [16]. The iterative algorithm requires the determination of several coefficients, but can be inconvenient. However, all coefficients up to the required large orders of magnitude can be computed numerically without iteration based on the above algorithm. The convergence of the method is very fast if $d < 1\,\mathrm{nm}$, barrier height of order and $< 0.5\,\mathrm{eV}$, voltage $< 1\,\mathrm{V}$, and effective mass of order and less than $0.1m_e$. Such parameters are characteristic of semiconductor tunnel diodes, when in a thin carrier-depleted layer the DP has values of 12−17, i.e the barrier is reduced by more than an order of magnitude due to the DP and small width. Exactly such barriers occur in resonant-tunnel structures made by $\mathrm{GaAs}-\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ and similar technologies.

Here is another simpler algorithm based on the row method for the variable $z = x/d - c$. For this substitution, the SE for the WFN $\varphi(z) = \psi(z + c)$ is simplified and takes the form $\varphi''(z) = az\,\varphi(z)$, $-c \le z \le 1-c$. This is also the equation for the Airy functions $\mathrm{Ai}(a^{1/3}z)$, $\mathrm{Bi}(a^{1/3}z)$. But we will use integration by the series method $\varphi(z) = \alpha_0 + \alpha_1 z + \alpha_2 z^2 + \ldots$, which leads to the recurrence formula $\alpha_n = a\alpha_{n-1}/[n(n-1)]$, $n = 3, 4, \ldots$ and to the ratios $\alpha_{3m+2}$, $m = 0, 1, 2, 3, \ldots$. According to the recurrence formula, all the coefficients of $\alpha_{3m}$ are expressed in terms of $\alpha_0$, and the coefficients of $\alpha_{3m+1}$ — in terms of $\alpha + 1$, $m = 1, 2, 3, \ldots$ as $\alpha_{3m} = \alpha_0 a^m (3m-2)!!!/(3m)!$, $\alpha_{3m+1} = \alpha_1 a^m (3m-1)!!!/(3m+1)!$. Here we denote the triple factorial: $n!!! = n(n-3)!!!$, where $1!!! = 1$, $2!!! = 2$, $3!!! = 3$ (similarly the double factorial is determined: $n!! = n(n-2)!!$, $1!! = 1$, $2!! = 2$). We have formulas $(3n)!!! = 3^n n!$, $n! = n!!!(n-1)!!!(n-2)!!!$. We make substitutions $3m = k$, $\tau = z^3 a$ and get the general solution $\Psi(\tau) = \alpha_0\big(1 + \psi_0(\tau)\big) + \alpha_1(\tau/a)^{1/3}\big(1 + a\psi_1(\tau)\big)$, where the functions

$$\psi_0(\tau) = \sum_{k=1}^{\infty} \tau^k \frac{(3k-2)!!!}{(3k)!} = \sum_{k=1}^{\infty} \tau^k \frac{1}{(3k)!!!(3k-1)!!!}, \quad (7)$$

$$\psi_1(\tau) = \sum_{k=1}^{\infty} \tau^k \frac{(3k-1)!!!}{(3k+1)!} = \sum_{k=1}^{\infty} \tau^k \frac{1}{(3k+1)!!!(3k)!!!}. \quad (8)$$

The variable in them changes within $\tau_0 \le \tau \le \tau_1$, $\tau_0 = -b^3/a^2$, $\tau_1 = (1-c)^3 a$. Next, it will be necessary to calculate their derivatives. Obviously, $\partial_x \psi_{(0,1)}(\tau) = 3az^2\psi'_{(0,1)}(\tau)/d$. The derivatives of $\tau$ of these functions are of the following form.

$$\psi_0'(\tau) = \sum_{k=1}^{\infty} \tau^{k-1} k \frac{(3k-2)!!!}{(3k)!} = \sum_{k=1}^{\infty} \tau^{k-1} \frac{k}{(3k)!!!(3k-1)!!!}, \quad (9)$$

$$\psi_1'(\tau) = \sum_{k=1}^{\infty} \tau^{k-1} k \frac{(3k-1)!!!}{(3k+1)!} = \sum_{k=1}^{\infty} \tau^{k-1} \frac{k}{(3k+1)!!!(3k)!!!}. \quad (10)$$

The diagrams of these functions and their derivatives are shown in Figure 3. The maximum modulo value of $|\tau| \sim \max(a, b^3/a^2)$, at the same time $\tau_0$ — negative, and $\tau_1$ — negative at $b < a$ in this case the series — sign-variable and rapidly converging), and at $b \sim a$ and $b < a$ value $\tau_1$ is small. Therefore, condition $(\max|\tau|)^k (3k-2)!!! = (3k)!$ leads to an estimate of $k \sim 25$. At $\tau < 1$ the convergence of the series in (7), (8) is extremely high and is sufficient to hold for several terms in the series. At $\tau = 10$ we have in (7) fifteen exact decimal places when 15 terms of the series are taken into account. At $\tau = 100$ we have nine decimal places for 15 terms of the row, and all 15 precimal places for 18 terms of the row. At $\tau = 1000$ the required number of terms of the series to obtain 15 exact signs is 34. From boundary conditions is follows that

$$1 + R(E) = \alpha_0\big(1 + \psi_0(\tau_0)\big) - \alpha_1 c\big(1 + a\psi_1(\tau_0)\big), \quad (11)$$

$$1 - R(E) = \\ = \frac{\alpha_0(3b^2/a)\psi_0'(\tau_0) + \alpha_1[1 + a\psi_1(\tau_0) - (3b^3/a)\psi_1'(\tau_0)]}{ik_0 d}, \quad (12)$$

$$\alpha_0\big(1 + \psi_0(\tau_1)\big) + \alpha_1(1-c)\big(1 + a\psi_1(\tau_1)\big) = \tilde{T}, \quad (13)$$

$$\frac{\alpha_0 3a(1-c)^2\psi_0'(\tau_1) + \alpha_1[1 + a\psi_1(\tau_1) + 3a^2(1-c)^3\psi_1'(\tau_1)]}{ik_a d} = \tilde{T}. \quad (14)$$

The solution of the problem takes the form

$$Y(E) = \frac{1-R}{1+R} \\ = \frac{(3b^2/a)\psi_0'(\tau_0) + \dddot{G}[1 + a\psi_1(\tau_0) - (3b^3/a)\psi_1'(\tau_0)]}{ik_0 d[1 + \psi_0(\tau_0) - \dddot{G}(c + b\psi_1(\tau_0))]}, \quad (15)$$

$$\dddot{G} = \frac{ik_0 d(1 + \psi_0(\tau_1)) - 3a(1-c)^2\psi_0'(\tau_1)}{1 + a\psi_1(\tau_1) + 3a^2(1-c)^3\psi_1'(\tau_1) - ik_0 d(1-c)(1 + a\psi_1(\tau_1))}. \quad (16)$$

The coefficients are calculated by the formulas $\alpha_1 = \dddot{G}\alpha_0$,

$$\alpha_0 = 2\Bigg[1 + \psi_0(\tau_0) + \frac{3b^2\psi_0'(\tau_0)}{ik_0 da} \\ - \dddot{G}\bigg(c + ca\psi_1(\tau_0) - \frac{1 + a\psi_1(\tau_0) - 3b^3\psi_1'(\tau_0)/a}{ik_0 d}\bigg)\Bigg]^{-1}. \quad (17)$$

At high anode voltage, the right TP is almost equal to $d$ (Figure 2), and then the triangular barrier stands on the pedestal $\Delta V$, i.e. $V(x) \approx E_F + W - (W + eU_a - \Delta V)x/d$. To approximate the curve $a$ (or 4) (Figure 1) we have $\Delta V \approx 4$ eV. In this case $a = 2m_e d^2(eU_a - \Delta V + W)/\hbar^2$, and for $d = 1$ nm in the vacuum diode we have $a = 163$. The functions (7), (8) and their derivatives (9), (10) are easily calculated at low or negative $\tau$ (with sign-variable coefficients), but also at sufficiently high $\tau$. They are independent of the structure parameters, can be computed once (Figure 3), tabulated or approximated, and expressed through Airy functions (we do not address this issue here). 100 terms of the series were used. The results do not change when 200 terms are taken into account. The $a$ coefficient decreases greatly at $d < 1$ and in the case of low $U_a$. At the same time, the effective WF $W$ also decreases due to the proximity of the electrodes. At $U_a = 0$ and $d > 1$ the barrier is approximated by the rectangular (constant) potential $V = W$ (Figure 1, curve *1*), for which instead of (7) and (8), the fundamental solutions of the SE are as follows

$$\cos\Big(x\sqrt{2m_e(E_F + W_c - E)}/\hbar\Big)$$

and

$$\sin\Big(x\sqrt{2m_e(E_F + W_c - E)}/\hbar\Big).$$

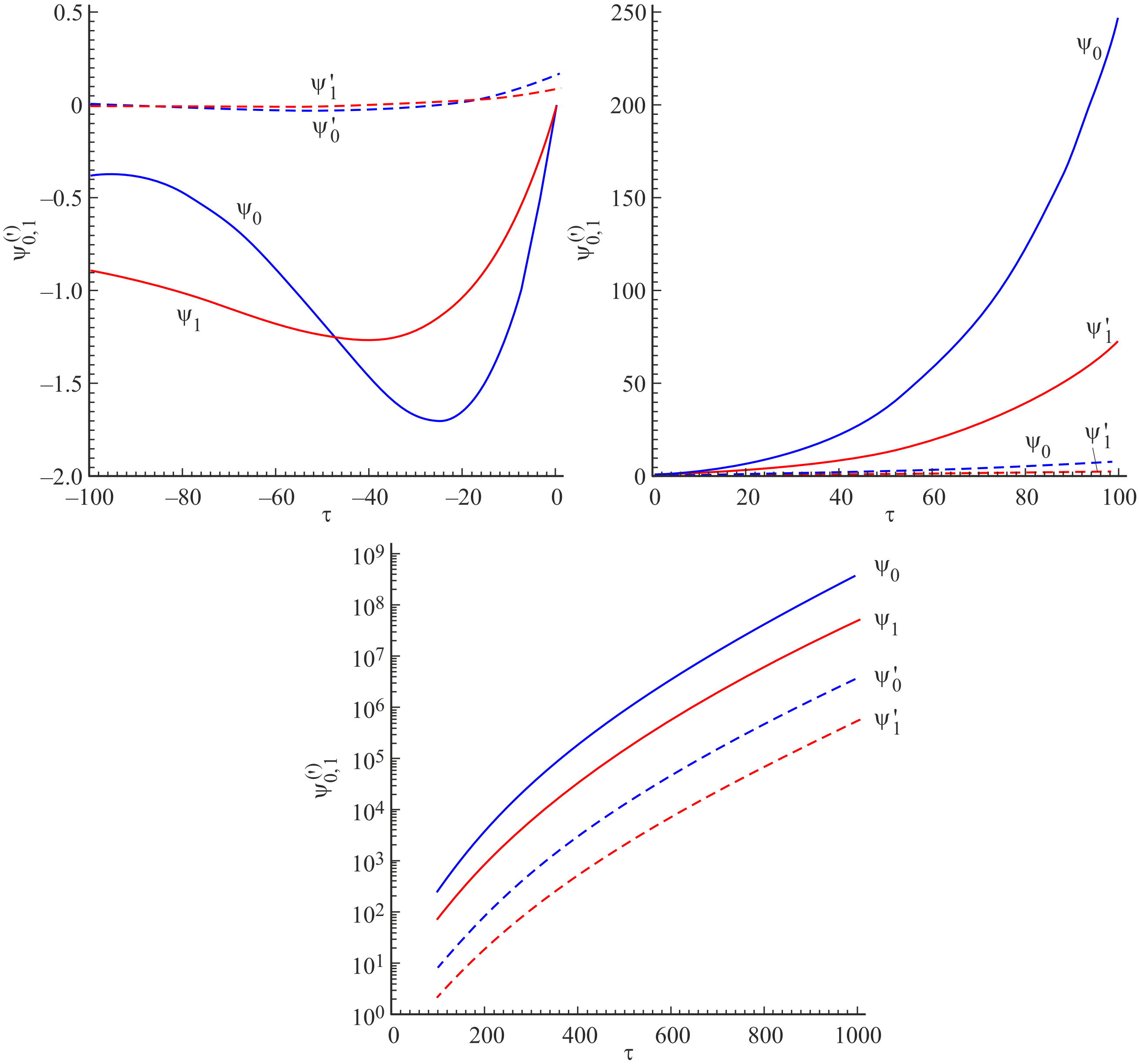


**Figure 3.** Diagrams of functions (7)–(10).

## 4. Analysis of solutions, results and conclusions

Let us consider the obtained solutions. At $d = 0$ we have $a = b = 0$, $\tau_0 = \tau_1 = 0$, $\psi'_0(0) = 1/6$, $\psi'_1(0) = 1/12$, $\psi_0(0) = \psi_1(0) = 0$. In 1st order by $d$ we take $\dddot{G} = ik_0 d$. In the same order $Y(E) = \dddot{G}/ik_0 d = 1_0$, i.e. $R = 0$, $D = 1$, $T = 1 + R = 1$. This is an infinitely narrow barrier. If $d > 0$, we have the PP of $l = d(E_\mathrm{F} + W - E)/(eU_a + W)$ and the transparency of $\tilde{D} = |\tilde{T}|^2 = 1 - |\tilde{R}|^2$. In the case of $l = d$ there must be $E = E_\mathrm{F} - eU_a$, and the small neighborhood of this level must be excluded from the solution, since the WN for it is zero. If $E_\mathrm{F} - eU_a > 0$, the barrier takes the form of a triangle $W + eU_a$ high on a pedestal $E_\mathrm{F} - eU_a$ high (Figure 2, $b$). Tunneling to the level below the pedestal $(0 < E \le E_\mathrm{F} - eU_a)$ is possible if the electron preliminarily from it passes to the FL of the anode $E_\mathrm{F} - eU_a$ absorbing the energy quantum $E_\mathrm{F} - eU_a - E$. At the same time on the cathode due to the Nottingham effect the energy quantum $E_\mathrm{F} - E$ is released. Thus, the total heat release for one act of electron transition is equal to $eU_a$ and occurs due to the work of the power source. This same energy is also released during tunneling from higher levels when the electron at the anode gives up energy $E - E_\mathrm{F} + eU_a$ by transitioning to the FL of the anode. The release or absorption of energy occurs at the free path length due to the interaction of electrons with electrode phonons. The tunneling at $E \le E_\mathrm{F} - eU_a$ is small. At very high voltage $eU_a \gg E_F$ we have the narrow triangular barrier of Figure 2, $a$ (dashed line).

For small $a$ and $b$ it is quite convenient to use the decomposition (5) with coefficients from the table. Thus at $d = 1$ nm, $W = 2$ eV, $E_F = 0.5$ eV, effective mass $0.067m_e$, DP $\varepsilon = 14$ we have $a = 2.02$, and for the electron at the barrier apex ($E = E_F + W/\varepsilon = 0.64$ eV) we have $b = 0$ and $\varphi_0(t) \approx 2t^3/3! + 16t^6/6! + 224t^9/9! + \ldots$, $\varphi_1(t) \approx 4t/4! + 40t^7/7! + 640t^{10}/10! + \ldots$. Since $t \le 1$, the terms of the series are greatly decreasing, and at $t = 1$ the third terms give maximum corrections $< 0.2$ i.e., they can be omitted and the solution can be taken in the form of $\psi(t) = \alpha_0(1 + 2t^3/3! + 16t^6/6!) + \alpha_1(t + 4t^4/4! + 40t^7/7!)$. This case corresponds to a GaAs doped diode with a carrier-depleted layer $Ga_{1-x}Al_xAs$ $d = 1$ nm thick. We reduced the WFs according to the mutual influence of the electrodes. At $d = 2$ nm, the WF will increase slightly, but the contribution of $W/\varepsilon$ is small, and all the coefficients will increase by about 4 times, and the result can be applied to such a diode as well. For the barrier apex $b = 0$, and we will get $R \approx -ik_0d/4 - (k_0d)^2/12 \approx -ik_0d/4$.

Let us consider the case of a particle at the apex of the triangular barrier ($eU_a = E_F$, $E = E_F + \tilde{W}$) for other solutions. For (13) at $b = 0$ we have $\tau_0 = 0$, $\tau_1 = a = k_0^2d^2$, $\tau = at^3$ and $Y = \dddot{G}/(ik_0d) \neq 1$, i.e. there is no complete passage of the barrier (as dictated by the FN formula). Let the barrier be narrow, i.e. $a = k_0^2d^2 \ll 1$ and $\psi_0(a) \approx 1/6$, $\psi_1(a) \approx a/12$, $\psi_0'(a) \approx 1/6$, $\psi_1'(a) \approx 1/12$. Then $\dddot{G} \approx ik_0d - (k_0d)^2/2$, $Y(E) \approx 1 + ik_0d/2$ and have the reflectance coefficient $R \approx -ik_0d/4$ as stated above. It is small, but non zero. If $\tau_1 = a \gg 1$, then this corresponds to a wide barrier (rectangular step) and should result in total reflection. In this case $1 < \psi_1'(\tau_1) \ll \psi_0'(\tau_1) \ll \psi_1(\tau_1) \ll \psi_0(\tau_1)$ (see also Figure 3), so we have

$$\dddot{G} = \frac{ik_0d\psi_0(\tau_1) - 3a\psi_0'(\tau_1)}{a\psi_1(\tau_1)[1 - ik_0d] + 3a^2\psi_1'(\tau_1)} \approx -\frac{\psi_0(\tau_1)}{a\psi_1(\tau_1)}. \quad (18)$$

At $\tau_1 = a = 100$ $\dddot{G} \approx -0.0029268$, and at $\tau_1 = a = 5000$ will be $\dddot{G} \approx -0.000016043$. In both cases the input conductance is small, imaginary: $Y(E) = -i\dddot{G}/(k_0d) = i0.00029288$ in the first case and $Y(E) = i2.269 \cdot 10^7$ in the second case. These correspond to practically unitary reflectance coefficients. Only when the barrier is substantially exceeded does the reflectance coefficient tend to zero. In particular, let $E \gg E_F + W$. In this case of motion high above the barrier the value of $b \approx -(k_0d)^2$ is negative and large modulo, $-b \gg a$, $\tau_0 \approx \tau_1 \approx -b^3/a^2$, all functions and their derivatives from negative values are small and $\psi_{(0,1)}(\tau_0) \approx \psi_{(0,1)}(\tau_1)$, $\psi_{(0,1)}'(\tau_0) \approx \psi_{(0,1)}'(\tau_1)$. We thus obtain

$$\dddot{G} = \frac{ik_0da\left(1 + \psi_0(\tau_0)\right) + 3b^2\psi_0'(\tau_0)}{a + aa\psi_1(\tau_1) - 3b^3\psi_1'(\tau_1) + ik_0db\left(1 + a\psi_1(\tau_1)\right)}.$$

At high $-b$ we have $\dddot{G} \approx -\psi_0'(\tau_0)/\left(b\psi_1'(\tau_0)\right) \approx 0$, i.e. $Y \approx 1$ and $R \approx 0$, which corresponds to over-barrier passage.

In the cylindrical function-based model for the particle at the barrier apex at $b = 0$ and $c = 0$ we have the reflectance coefficient

$$R = C_1\left[ik_0d\left(\mathrm{Ai}(0) + \mathrm{Bi}(0)G\right) - a^{1/3}\left(\mathrm{Ai}'(0) + \mathrm{Bi}'(0)G\right)\right]/2$$

$$= C_1\left[ik_0d\mathrm{Ai}(0)(1 + \sqrt{3}G) - a^{1/3}\mathrm{Ai}'(0)(1 - \sqrt{3}G)\right]/2,$$

$$C_1 = \frac{2}{\mathrm{Ai}(0) + \mathrm{Bi}(0)G} = \frac{2}{\mathrm{Ai}(0)(1 + \sqrt{3})G},$$

$$G = \frac{a^{1/3}\mathrm{Ai}'(a^{1/3}) - ik_0d\mathrm{Ai}(a^{1/3})}{ik_0d\mathrm{Bi}(a^{1/3}) - a^{1/3}\mathrm{Bi}'(a^{1/3})}.$$

For short lengths of $d$ we have

$$G \approx -\mathrm{Ai}'(a^{1/3})/\mathrm{Bi}'(a^{1/3}) \approx -1/\sqrt{3}$$

and therefore

$$R = -2\sqrt{3}(3a)^{1/3}\Gamma(2/3)/[\Gamma(1/3)(1 + \sqrt{3})] \approx 0.$$

For long lengths of $G \approx 0$, $C_1 = 2/\mathrm{Ai}(0)$, conductance $Y = i0.729a^{1/3}/(k_0d)$ — a value small modulo and $R \approx 1 - 1.458ia^{1/3}/(k_0d) \approx 1$.

The barrier profiles shown in Figure 1 are obtained by formula [1,2]

$$Y(x) = E_F + \tilde{W}\left[1 - \frac{\delta d}{\left(x + \delta(1 - x/d)\right)(d - x + x\delta/d)}\right] - eU_a\frac{x}{d}. \quad (19)$$

It naturally differs from the linear approximation used above and gives the real image-based barrier profile in the diode, taking into account the WF of the cathode material $W_d = e^2/(16\pi\varepsilon_0\delta)$. In it the value $\tilde{W} = W_c(1 - \alpha/d)/\varepsilon$ determines the barrier height taking into account the influence of the anode and dielectric, $\alpha = \delta\left(1 + 2\ln(2)\right)$. The real barrier height $W = V(x_{\max}) - E_F$ above the Fermi level (Figure 1) is somewhat smaller. It is determined by the right-hand term and can be calculated from equation $V'(x_{\max}) = 0$. The curves in Figure 1 correspond to relatively low voltages in a vacuum diode with copper electrodes and are shown for clarity. Closer to the triangular profile is the curve *4* (or $a$) for the anode voltage $U_a = 7$ V. The linear approximation corresponds to the line $c$. A more accurate approximation is given by the broken line $b$. To plot it, we need to determine the energy $E_{tp}$, where the maximum of the second derivative of $-V''(x_{tp})$ occurs. This is PP. In our case, $E_{tp} \approx 4$ eV, $x_{tp} \approx d$. One can approximate the barrier using three broken lines, but two is enough. As $U_a$ increases, the point $x_{tp}$ approaches $d$, the maximum shifts to the cathode, and the c-type profile describes the barrier more and more accurately. In Figure 4, the $D(E, U_a)$ transparencies for the curves in Figure 1 are

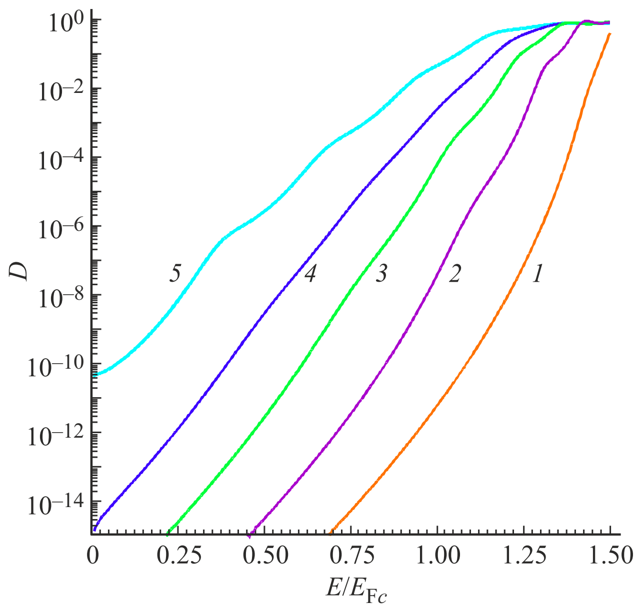


**Figure 4.** The barrier transparency of the vacuum diode is $d = 2$ nm at $U_a$, V: *1* — 1, *2* — 4, *3* — 7, *4* — 10, *5* — 15.

shown. They are then used to calculate the current density (Figure 5), determined for the thermal field emission from the cathode by the integral [1,2]

$$J(U_a, T) = \frac{em_e k_B T}{2\pi^2 \hbar^3} \times \int_0^{3E_F} D(E, U_a) \ln\left(1 + \exp\left(\frac{E_F - E}{k_B T}\right)\right) dE. \quad (20)$$

In Figure 6, transparency (in the formulas *) based on formulas (6) and (15) for the triangular barrier heights $E_F + W = 8$ eV and $E_F = 7$ eV at $d = 2$ nm, $d = 1$ nm and $d = 0.5$ nm are shown. They are compared with the numerical solution of the SE by the wave impedance transformation method using 300 steps. The results are seen to be almost the same. Results based on formula (6) are obtained using 20 members in series and two iterations. From computational point of view, the results based on formula (15) are preferable to those based on formulas (3) and (6). They require substantially less computational cost than the numerical solution of SE.

The results in Figure 5 are given for different cathode and anode temperatures. The formula (20) corresponds to a degenerate electron gas in the metal, with the electrons distributed according to the Fermi–Dirac (at $T = 0$ the upper limit is $E_F$). In (20), instead of the infinite limit, the upper limit $3E_F$ is taken. This is more than sufficient to account for thermionic emission at the cathode temperature $T < 2000$ K. The upper limit of $2E_F$ is quite sufficient, since at $k_B T \sim 0.2$ eV the logarithm can be replaced by a small exponent, and at $D(E, U_a) \approx 1$ for the remainder of the integral at $E_F = 7$ eV we obtain a value of $1.26 \cdot 10^{-16}$. The density (20) is positive and determines the anodic current, although negatively charged electrons from the cathode tunnel ($e > 0$). At $T > 0$ electrons with positive energy at the anode can also tunnel to the cathode, and the tunneling

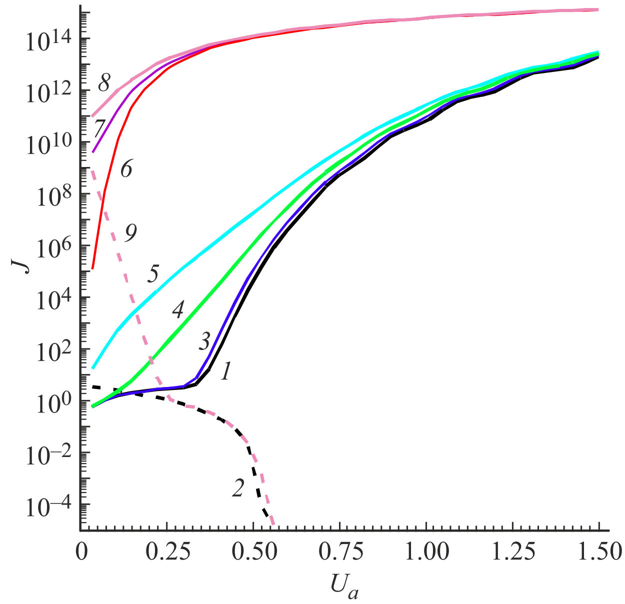


**Figure 5.** VAC of a vacuum diode (Am$^{-2}$/V) $d = 2$ nm long (curves *1–5*) and the same CVD diamond-filled diode (*7–9*) at different temperatures, K: $T_c = T_a = 300$ (*1, 2, 6*), 800 (*3, 7*), $T_c = 1500$, $T_a = 300$ (*4*), $T_c = T_a = 1200$ (*5, 8, 9*). The dashed curves *2* and *9* show the inverse current densities for curves *1* and *8*, respectively. $E_{Fc} = E_{Fa} = 7$, $W_c = W_a = 4.36$ eV.

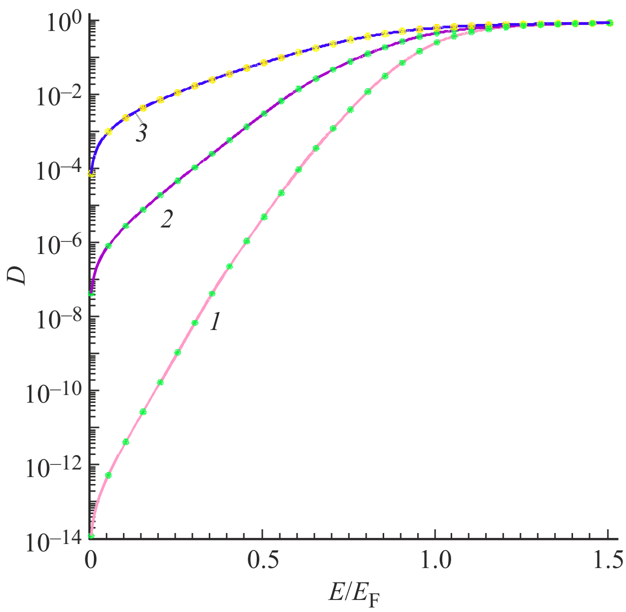


**Figure 6.** Transparency $D$ based on the numerical solution of the SE for $d = 2$ nm (curve *1*), 1 nm (*2*), and 0.5 nm (*3*), and also results based on formula (15) (***) for the first two cases and formula (6) (***) for the third case. (A color version of the figure is provided in the online version of the paper).

coefficient $D(E, U_a)$ is the same (consider $T_e = T_a = T$). However, the number of such electrons is proportional to $k_B T \ln\left(1 + \exp\left((E_F - eU_a - E)/(k_B T)\right)\right)$, i.e. substantially less than at the cathode in formula (20). At low temperature this number is proportional to $E_F - eU_a - E$, whereas at the cathode it is proportional to $E_F - E$. The electron density near the bottom of the conduction band is maximum, and the value of $E_F - eU_a - E$ determines higher energy levels relative to the conduction band bottom of the anode than $E_F - E$ relative to the analogous bottom of the cathode. At $eU_a = E_F$ and $T_a = 0$ there are no electrons with positive energies at the anode to tunnel to the cathode (all filled levels are negative), and there is no reverse current. At low anode voltages or with highly heated electrodes in the diode, the total current should be considered as the difference of the two electron fluxes from the cathode and from the anode.

## 5. Conclusion

The following results were obtained over the course of this study: In diode structure with sharpened apex quantum potential (for a narrow barrier), the modulus of the reflectance coefficient for energy at the apex level is small, of the order of $k_0 d$, and as $d$ decreases, it tends to zero. At very high anode voltages, the barrier virtually disappears, becoming a linear bevel into the quantum well. For a very wide barrier and low anodic voltage, the modulus $|R|$ is close to unity and only at some excess of the barrier does it begin to tend to zero. In diode structures at small anode voltages, tunneling in both directions must be taken into account. High-current diode nanostructures should be made using good dielectrics with high thermal conductivity such as diamond and BeO. This leads to a great decrease in barrier, operating voltages, and an increase in current.

In conclusion, let us note the following. In the paper, exactly solvable models for the triangular barrier have been obtained. They are applicable to diode and to triode (transistor) structures if the barriers are close to triangular in shape, which is often the case with narrow barriers and substantial voltages. Exactly solved models have an advantage over approximate models in the validity of the results. In particular, the triangular barrier model is more preferable than the rectangular one and even more so than the $\delta$-shaped. The advantage of the derived model over numerical solutions of the SE is that it is faster, which is essential in unsteady device models when subjected to alternating stress with a large number of changes in barrier heights [8]. For complex multi-pit and multi-barrier structures, the resulting models allow us to plot a dimensionless transfer (transfer) matrix of the entire structure and thus increase the simulation speed. The matrix relates the WFN and its derivative on both sides of the structure. If there are several such areas, the full matrix is defined as a product of the matrices. Compared to a piecewise constant potential approximation, where it is necessary to use on the order of several hundred products of such matrices [1], this leads to a substantial gain and a reduction in numerical error. The applied method of integrating the SE can be used for parabolic approximation of the potential, including parabolas of order 4, which describe the form (19) more exactly. It should be noted that the functions (7)–(10) appear to be more convenient than the Airy functions.

### Funding

This study was supported by the Ministry of Education and Science of the Russian Federation under a state order (No. FSRR-2023-0008).

### Conflict of interest

The author declares that he has no conflict of interest.

## References

[1] M.V. Davidovich, I.S. Nefedov, O.E. Glukhova, M.M. Slepchenkov. J. Appl. Phys., **130**, 204301 (2021). DOI: 10.1063/5.0067763
[2] M.V. Davidovich. ZhTF, **94** (1), 32 (2024). (in Russian). DOI: 10.61011/JTF.2024.01.56899.170-23
[3] E.A. Nelin. UFN, **177**, 307 (2007). (in Russian). DOI: 10.3367/UFNr.0177.200703d.0307
[4] Yu.A. Chaplygin, V.K. Nevolin, V.A. Petukhov. DAN **436** 2 (179). (in Russian). DOI: 10.1134/S1028335811010058
[5] K.S. Grishakov, V.F. Elesin, Semiconductors, **50**, 1092 (2016). DOI: 10.1134/S1063782616080121
[6] I.I. Abramov, I.A. Goncharenko, N.V. Kolomeitseva. Semiconductors, **41**, 1375 (2007). DOI: 10.1134/S106378260711019X
[7] V.F. Elesin, I.Yu. Kateev, M.A. Remnev. Semiconductors, **43**, 257 (2009). DOI: 10.1134/S1063782609020250
[8] M.V. Davidovich. JETP Letters, **110** (7), 472 (2019). DOI: 10.1134/S0370274X19190068
[9] A.S. Davydov. *Kvantovaya mekhanika* (Nauka, M., 1973). (in Russian).
[10] Z. Ahmed, D. Ghosh, S. Kumar, N. Turumella. Eur. J. Phys., **39** (2), 025404 (2018). DOI: 10.1088/1361-6404/aa8c0c
[11] R. Elpelt, O. Wolst, H. Willenberg, S. Malzer, G.H. Döhler. Phys. Rev. B, **69**, 205305 (2004). DOI: 10.1103/PhysRevB.69.205305
[12] E.-S. Malureanu. U.P.B. Sci. Bull., Ser. A, **76** (2), 251 (2014).
[13] R.G. Forbes, J. Deane. Proc. Royal Soc. A, **467** (2134), 2927 (2011). DOI: 10.1098/rspa.2011.0025
[14] E. Kamke. *Spravochnik po obyknovennym differentsial'nym uravneniyam* (M., Izdatelstvo inostr.lit., 1950). (in Russian).
[15] L.D. Landau, E.M. Lifshitz. *Kvantovaya mechanika. Nerelyativistskaya teoriya* (GIFML, M., 1963). (in Russian).
[16] M.V. Davidovich, A.K. Kobets, K.A. Sayapin. Fizika volnovykh protsessov i radiotekhnicheskiye sistemy, **24** (3), 18 (2021). (in Russian). DOI: 10.18469/1810-3189.2021.24.3.18-27

*Translated by J.Savelyeva*