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Matrix Method for Simulating the Tunneling Transfer

V. A. Fedirko[a], S. V. Polyakov[b], and D. A. Zenyuk[a]

[a] *Moscow State Technological University, Vadkovskii per. 3a, Moscow, 127994 Russia*
[b] *Institute for Mathematical Modeling, Russian Academy of Sciences, Miusskaya pl. 4a, Moscow, 125047 Russia*
e-mail: vfed@mail.ru, polyakov@imamod.ru

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Abstract—We develop an efficient approach for computer simulation of stationary scattering and tunneling transfer across an arbitrary one-dimensional potential barrier. New algorithms and programs were worked out and tested and the convergence of the method in question was examined.

Keywords: tunneling transfer, vacuum microstructures, potential barrier, transfer matrix method.
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1. INTRODUCTION AND STATEMENT OF THE PROBLEM

Physical models may subsume a great variety of phenomena pertaining to the tunnel effect, namely, the α-decay, the Josephson effect, the cold field-emission of electrons, impurity conduction of semiconductors, low-temperature chemical reactions, and many more. A significant role is played by quantum tunneling effects in advanced nanoelectronic devices (see, e.g., [1]).

Exact numerical solutions for the tunneling transfer problem can be obtained only for a very limited number of potential barriers. The universally employed WKB approximation requires certain restrictions and is incapable of providing acceptable accuracy. In addition, this approach by itself is unable to adequately take into account resonance effects. This proves the relevance of the further development of efficient methods of computer simulations of the tunneling transfer across arbitrary potential barriers. With this aim in mind, in this paper we analyze and develop the transfer matrix method [2–5].

The tunneling transfer coefficient in one-dimensional geometry is governed by a solution of the boundary-value problem for the stationary Schrödinger equation

$$\frac{d}{dx^2}\psi^2 + \frac{2m}{\hbar^2}[E - V(x)]\psi = 0; \quad x \in [0, a], \tag{1}$$

where $V(x)$ is a potential barrier concentrated in the region $0 < x < a$. For the sake of specificity, we assume that we are dealing with transport along the positive direction from left to right. We also assume that the wave function assumes the form of a plane wave

$$\begin{aligned} \psi_L(x) &= \exp[ik_L x] + R\exp[-ik_L x], \quad k_L = \sqrt{\frac{2m(E - V_L)}{\hbar^2}}, \\ \psi_R(x) &= T\exp[ik_R(x - a)], \quad k_R = \sqrt{\frac{2m(E - V_R)}{\hbar^2}} \end{aligned} \tag{2}$$

to the left and right of the barrier. For convenience in our subsequent calculations, the amplitude of a wave incident to the barrier is taken to be unity; this does not impair the generality. Mixed boundary conditions are determined from the continuity of the wave function and its first derivative on the boundaries of the barrier:

$$\psi(0) = \psi_L(0), \quad \psi'(0) = \psi'_L(0); \quad \psi(a) = \psi_R(a), \quad \psi'(a) = \psi'_R(a).$$

The tunneling coefficient D is defined to be [6] the ratio of the current density in the transmitted wave to the current density in the incident wave. In the general problem statement, when a barrier cannot be regarded as concentrated in some finite interval, the wave amplitudes are governed by the solutions of Eq. (1) with asymptotics (2).

2. TRANSFER MATRIX METHOD

The fundamental principle underlying this method is the segmentation of the barrier into N parts, usually of the same size in the spatial coordinate, followed by subsequent approximation of the potential function so that the wave functions would have a fairly simple analytical expression on each of the segments [2, 3]. The most suitable in this respect are the constant and linear functions.

In the case of piecewise-constant interpolation, a fundamental solution of the Schrödinger equation is represented on each segment as the superposition of two plane waves,

$$\psi_j(x) = C_j \exp[ik_j x] + D_j \exp[-ik_j x], \quad k_j = \sqrt{\frac{2m(E-V_j)}{\hbar^2}}, \quad j = 1, \ldots, N.$$

The continuity requirement about the wave function and its first derivative in the matrix form are then as follows:

$$M_j = \frac{1}{2}\begin{pmatrix} (1+S_j)\exp[-i(k_{j+1}-k_j)x_j] & (1-S_j)\exp[-i(k_{j+1}+k_j)x_j] \\ (1-S_j)\exp[i(k_{j+1}+k_j)x_j] & (1+S_j)\exp[i(k_{j+1}-k_j)x_j] \end{pmatrix},$$
$$S_j = \frac{k_j}{k_{j+1}}, \quad C_0 = 1, \quad C_{N+1} = T, \quad D_0 = R, \quad D_{N+1} = 0. \tag{3}$$

Applying this procedure to all junction points of the segments, with due account for the boundary conditions, reduces the initial problem to solving the following system of linear equations

$$\begin{pmatrix} 0 \\ T \end{pmatrix} = M \begin{pmatrix} R \\ 1 \end{pmatrix}, \quad M = \prod_{k=0}^{N} M_k, \tag{4}$$

where T are R are amplitudes of the incident and transmitted waves, respectively, $D = |T|^2$, M is the transfer matrix for the region with the barrier, which is obtained by multiplication of the transfer matrices M_k at all junction points of segments. This approach is also capable of incorporating changes in the effective mass (for example, while modeling the transfer in heterostructures) by introducing a similar piecewise-constant approximation for the dependence of the effective mass on the coordinate:

$$m_j = m\left(\frac{x_{j-1}+x_j}{2}\right), \quad j = 1-N, \quad m_0 = m_L, \quad m_{N+1} = m_R.$$

A similar analysis also applies to piecewise linear approximation. In this case, the analytical solution of the Schrödinger equation on a segment will be linear combinations of Airy functions (see [6–8]):

$$\psi_j(x) = C_j Ai(z_j) + D_j Bi(z_j), \quad j = 1, \ldots, N,$$
$$z_j = -\sqrt[3]{\frac{2mF_j}{\hbar^2}}\left(x_j + \frac{E-V_j}{F_j} - x\right), \quad F_j = \frac{V_{j+1}-V_j}{x_{j+1}-x_j}.$$

Applying the above continuity conditions reduces the initial problem to solving the system

$$\begin{pmatrix} 1 \\ R \end{pmatrix} = M \begin{pmatrix} T \\ 0 \end{pmatrix}, \quad M = M_L^{-1}\tilde{M}M_R, \quad M_L = \begin{pmatrix} 1 & 1 \\ ik_L & -ik_L \end{pmatrix}, \quad M_R = \begin{pmatrix} 1 & 1 \\ ik_R & -ik_R \end{pmatrix},$$
$$\tilde{M} = M_{00}M_{01}^{-1}M_{11}M_{12}^{-1}\ldots M_{ii}M_{i,i+1}^{-1}\ldots M_{N-1,N-1}M_{N-1,N}^{-1},$$
$$M_{j,i} = \begin{pmatrix} Ai(z) & Bi(z) \\ -\sqrt[3]{\frac{2mF_j}{\hbar^2}}Ai'(z) & -\sqrt[3]{\frac{2mF_j}{\hbar^2}}Bi'(z) \end{pmatrix}, \quad z = -\sqrt[3]{\frac{2mF_j}{\hbar^2}}\left(x_j + \frac{E-V_j}{F_j} - x_i\right), \tag{5}$$

where the matrices M_L and M_R are introduced to incorporate the boundary conditions, and the matrix $\tilde{M}$ is the transfer matrix.

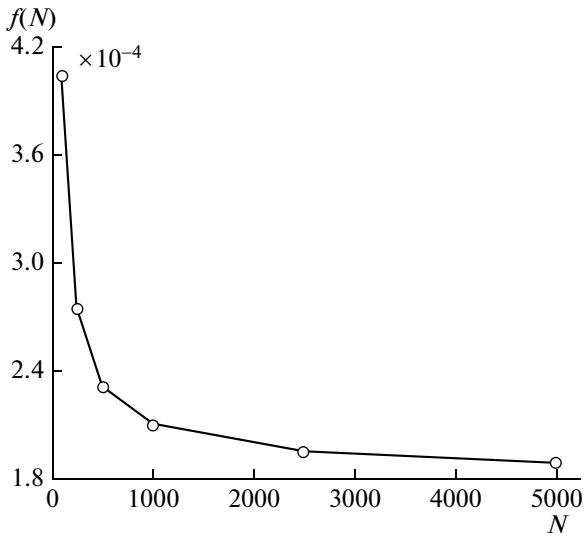

Fig. 1. Absolute error of the method using a piecewise linear approximation for the Péschl–Teller barrier.

The methods in questions take adequate account of various quantum–mechanical effects, for example [2, 4, 5], the permeability resonance when the particle energy agrees with the energy of quasi-bound states in a potential well [9].

In [4, 5], the convergence of the above approach has been numerically investigated for piecewise linear interpolation. A significant disadvantage of this method is the failure of convergence in the case when the energy level of the particle agrees with one of the values of V_j which approximate the potential. As is seen from (3), in this case k_j vanishes. A model problem for the transfer across a triangular barrier was used to obtain the analytical expression for permeability [5]

$$D = \frac{4r}{k}\frac{1}{\left[Ai(z) - \frac{r}{k}Bi'(z)\right]^2 + \left[\frac{r}{k}Ai'(z) + Bi(z)\right]^2},$$

$$r = \sqrt[3]{\frac{2mF}{\hbar^2}}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad z = -r\frac{E - V_0}{F},$$

with a deterioration in convergence being manifested in the case $E \approx V_j$.

The method involving piecewise linear approximation has been tested using the more advanced Péschl–Teller modified barrier

$$V(x) = \frac{V_0}{\cosh^2 \beta x}, \tag{6}$$

for which an exact analytical solution obtainable by means of the Gauss hypergeometric functions is known [6, 8]. The scattering problem on such a barrier includes, for example, the problem of ballistic transport of electrons across convergent channels with dimensional quantization in nanoelectronic structures [10], the dimensionless parameter

$$s = \frac{1}{2}\left[\sqrt{\left|\frac{8mV_0}{\beta^2\hbar^2} - 1\right|} - 1\right]$$

being the fundamental parameter that governs the transfer of electrons across a barrier of such a type.

The norm of the difference between the exact $D(E)$ and approximate $D^N(E)$ values of the tunneling coefficient

$$f(N) = \left\|D(E) - D^N(E)\right\| = \max_E \left|D(E) - D^N(E)\right|$$

was used in evaluating the convergence of the method; the dependence of this norm on the number of partition points N was numerically studied. The norm was calculated in the $0 < (E/V_0) < 2$ energy range. In Fig. 1 we show the values of $f(N)$ for a barrier with $s = 0.3$. The method was shown by tests to have satisfactory convergence for barriers with various values of the characteristic parameter s.

However, the piecewise linear approximation approach may result in computational instability due to an exponentially large second order Airy function [5] (for example, in simulating structures with a potential slowly varying in space).

To circumvent these difficulties, we have constructed a hybrid algorithm that approximates the potential by constant or linear elements depending on its geometry. The selection of the approximation method is determined on the basis of the absolute value of the slope of the secant of the graph for the potential F_j. Namely, we approximate by constants if $|F_j| < p$; otherwise, use is made of a piecewise linear approximation. In terms of program implementation, at each iteration, we calculate the transfer matrix, whose form depends on the value of $|F_j|$, which are subsequently multiplied according to a procedure similar to (5).

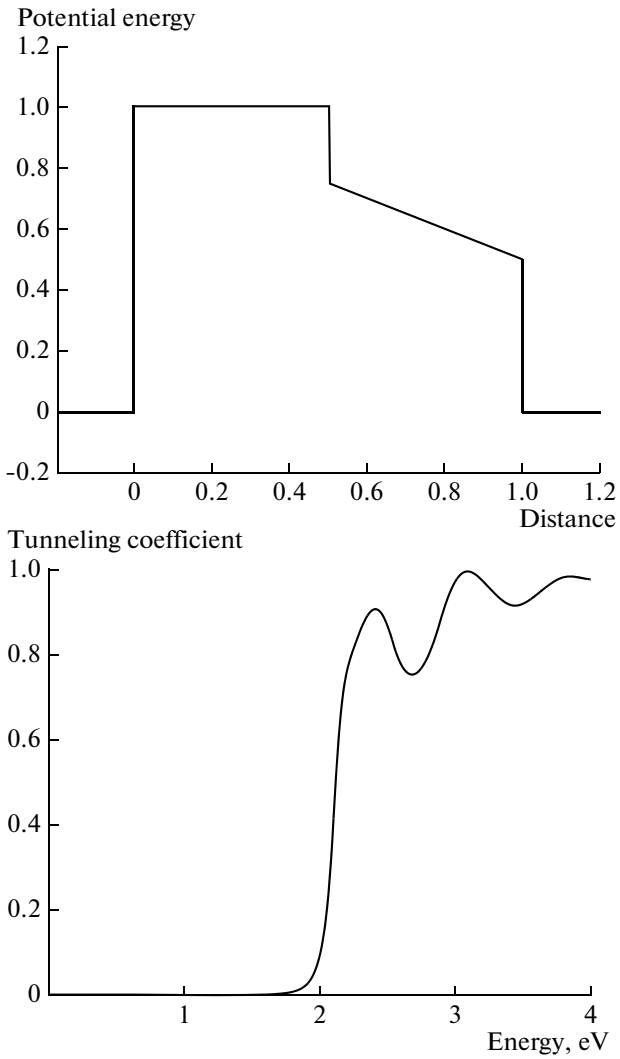

Fig. 2. A combined barrier (a) and the tunneling coefficient across it (b) used in the test.

The hybrid method was tested through the use of a composite barrier (in dimensionless variables, see Fig. 2a):

$$V(x) = \begin{cases} 1, & x \in [0, 0.5], \\ 1 - 0.5x, & x \in [0.5, 1]. \end{cases}$$

Calculations are shown in Fig. 2b. For reasons referred to above, the use of just one of the above approximation methods for such a barrier is inefficient.

Thus, the proposed transfer matrix method for solving the tunneling transfer problem applies to potentials of arbitrary configuration and enables one to perform calculations to any degree of accuracy. In addition, this method features a simple algorithmic structure, which simplifies its computer implementation.

3. THE MATRIX METHOD BASED ON THE ADAMS DIFFERENCE SCHEME

A more efficient matrix method can be built on the basis of the implicit one-step Adams second-order approximation scheme [11]. An equivalent dimensionless formulation of Eq. (1) is given by the following system:

$$\begin{cases} \dfrac{d}{dx}\psi = p, \\ \dfrac{d}{dx}p = -k(x)\psi; \quad k(x) = \dfrac{2mV_0a^2}{\hbar^2}[E - V(x)]. \end{cases} \tag{7}$$

Here, V_0 is the height of the potential structure.

Applying the above Adams method to (7) gives the following recursion relations to determine the values of the functions sought on a new layer:

$$\psi_{j+1} = \psi_j + \frac{h}{2}(p_{j+1} + p_j), \quad p_{j+1} = p_j - \frac{h}{4}(k_{j+1} + k_i)(\psi_{j+1} + \psi_j), \quad j = 0, \ldots, N.$$

As a corollary of these relations, we obtain a matrix equation that links the values of the functions $\psi(x)$ and $p(x)$ on layers j and $j + 1$:

$$\begin{pmatrix} 1 & -\dfrac{h}{2} \\ \dfrac{h}{4}(k_{j+1} + k_j) & 1 \end{pmatrix} \begin{pmatrix} \psi_{j+1} \\ p_{j+1} \end{pmatrix} = \begin{pmatrix} 1 & \dfrac{h}{2} \\ -\dfrac{h}{4}(k_{j+1} + k_j) & 1 \end{pmatrix} \begin{pmatrix} \psi_j \\ p_j \end{pmatrix} \Leftrightarrow \begin{pmatrix} \psi_{j+1} \\ p_{j+1} \end{pmatrix} = Q_{j+1} \begin{pmatrix} \psi_j \\ p_j \end{pmatrix}. \tag{8}$$

Then, the relation between the values of the functions at the boundary points of the region in question will be given by

$$\begin{pmatrix} \psi_N \\ p_N \end{pmatrix} = \prod_{j=1}^{N} Q_j \begin{pmatrix} \psi_0 \\ p_0 \end{pmatrix} = Q \begin{pmatrix} \psi_0 \\ p_0 \end{pmatrix}.$$

Taking into account the boundary conditions, we obtain the following system of linear equations

$$\begin{pmatrix} T \\ ik_L T \end{pmatrix} = Q \begin{pmatrix} 1 + R \\ ik_R(1 - R) \end{pmatrix}, \tag{9}$$

which can be easily solved for T.

Analysis of the stability of this method suggests that the partitioning step h should be chosen so that the coefficient matrix Q in the right-hand side of the system (9) would exist (the solvability condition). In addition, this condition must be satisfied for all the values $0 \le h < h_0$. The first requirement ensures the solvability of the numerical problem for a given partition, while the second one guarantees the monotonic convergence of the difference solution to the differential solution within the specified range of steps. If each of the matrices Q_j from the product Q satisfies these two conditions, this will be sufficient for them to hold for the problem globally.

Comparison of run-time costs for the above methods to calculate D

Form of barrier	Time, s	
Square barrier	5.4	34.0
Triangular barrier	5.4	109.5
Trapezoidal barrier	5.5	75.4
Parabolic barrier	5.4	100.4
Parabolic well	5.5	95.6
Square well	5.6	35.2

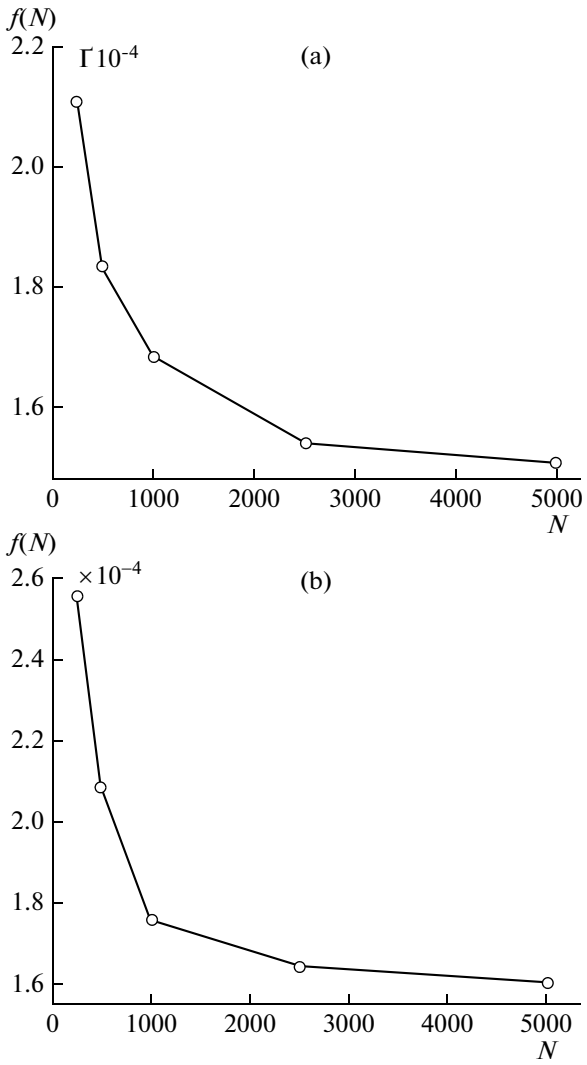

Fig. 3. Absolute error of the matrix method using the Adams scheme for a square (a) and trapezoidal (b) barriers.

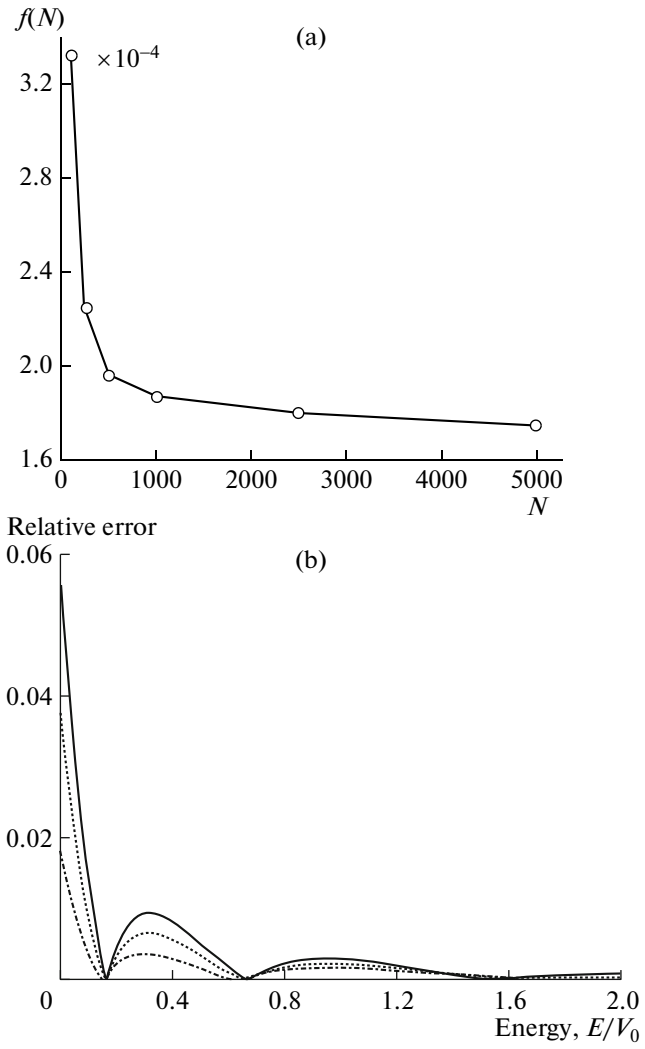

Fig. 4. Absolute (a) and relative (b) errors of the matrix of the Adams method.

The condition for the existence of the matrix Q follows from its definition:

$$Q_j = \frac{1}{1+\frac{h^2}{8}(k_j+k_{j-1})}\begin{pmatrix} 1-\frac{h^2}{8}(k_j+k_{j-1}) & h \\ -\frac{h}{2}(k_j+k_{j-1}) & 1-\frac{h^2}{8}(k_j+k_{j-1}) \end{pmatrix}.$$

It is easily verified that if the sufficient condition

$$1-\frac{h^2}{8}|k_j+k_{j-1}|>0, \quad j=1,\ldots,N \tag{10}$$

is satisfied, then each of Q_j exists, because $\Delta = 1+\frac{h^2}{8}(k_j+k_{j-1})$ is a priori positive. Condition (10) not only guarantees that matrix Q_j exists but also ensures that its diagonal elements and the determinant

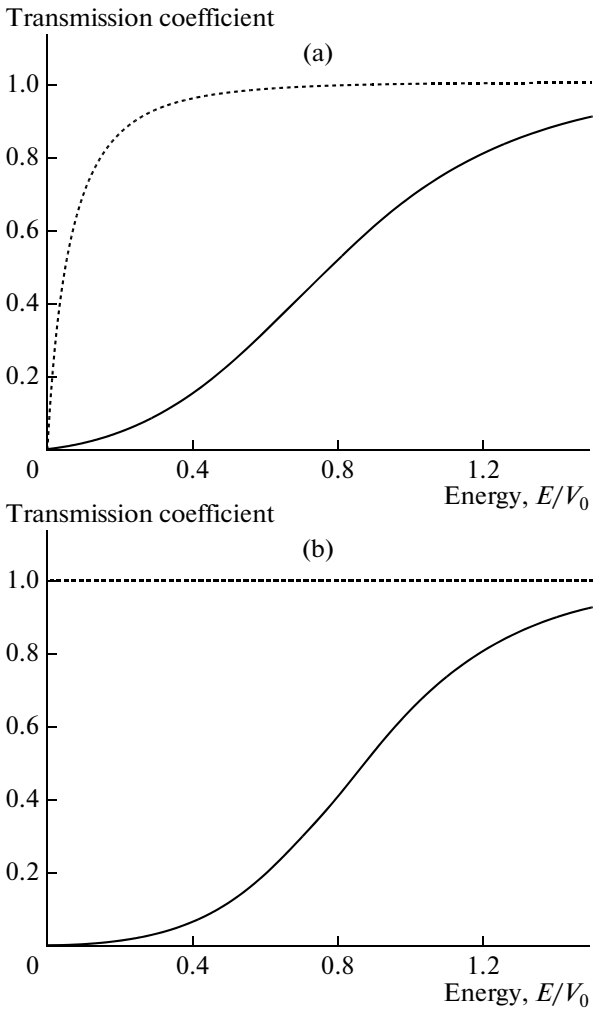

Fig. 5. The transmission coefficient for the Péschl–Teller potential; (a) $s = 0.6$; (b) $s = 0.99$, the dashed line is the well, the solid line is the barrier.

(which in turn also has value Δ) are all positive for all $h < h_0 = \sqrt{\frac{k_j + k_{j-1}}{8}}$. This ensures that the convergence is monotone. In addition, condition (10) shows that it is not necessary to uniformly partition the interval of integration. Use may also be made of nonuniform partitions subject to restriction (10). Then, the convergence of the method is also guaranteed.

We also note that the method proposed is capable of simultaneously determining both the wave function and its derivative, and thus may be used to calculate the tunneling transfer also by using the tunnel BCS Hamiltonian method [12].

Our approach does not have the disadvantages present in the matrix method based on a piecewise constant or piecewise linear approximation, and is shown by analysis as being capable of significantly reducing the number of calculations compared to the hybrid method; this is achieved chiefly by removing the "expensive" calculations of the Airy functions. In Table 1, we show the values of calculation times for the detection of the distribution of the tunneling coefficient over the energy on an Intel® Core™ 2 Duo 1.86 GHz processor in 53-bit arithmetic. The program was compiled using version 6.6 of the HP Visual Fortran Compiler. The number of partition points over the energy range (spatial coordinate) was 2500 ($N = 5 \times 10^3$, respectively). The data were obtained using the Adams method (first column) and the hybrid method (the second column).

The matrix method based on the Adams scheme was shown by numerical analysis on simple barriers (square and trapezoidal) to possess good convergence (see Figs. 3a, 3b).

The method was also tested on the Péschl–Teller barrier (6); the results for $s = 0.3$ are shown in Fig. 4.

In this case too, as is apparent from the picture, the matrix method based on the Adams scheme shows fairly good convergence to the exact solution; moreover, the convergence behaves similarly to that given in Fig. 3. Also, the convergence is fairly uniform over the whole range of particle energies (Fig. 4b). Comparison with Fig. 1 shows that this method gives, among other things, smaller values of the absolute error as compared to the method based on a piecewise linear approximation (one of the reasons for this is the accumulation of errors in the course of the approximate calculation of Airy functions).

The matrix method also renders it possible to simulate the scattering of electrons over a potential well. The comparative results of the calculation of the transmission coefficient for the Péschl–Teller barrier ($V_0 > 0$) and well ($V_0 < 0$) (6) are shown in Fig. 5. In the latter case, for specific values of the depth of the well (for a shallow well), a peculiar quasi-resonance effect may occur [6]: a particle flies past a well practically without reflection. In this case, at low energies the following approximate expression

$$D \approx \frac{k^2}{k^2 + \beta^2 (s-n)^2} \tag{11}$$

is valid for the transmission coefficient; where, $k = \sqrt{\frac{2mE}{\hbar^2}}$, E is the energy of a particle, n is a nonnegative integer, and $s = \frac{1}{2}\left[\sqrt{1 + \frac{8m|V_0|\beta^2}{\beta^2\hbar^2}} - 1\right]$.

This effect is general and manifests itself for a potential well of arbitrary form. It also occurs when a particle flies past over a potential barrier of fairly short height (for $s \sim \frac{2mV_0}{\beta^2\hbar^2} \ll 1$); in this case, the resonance occurs in *virtual* level [6]. The transmission coefficient in this case is also described by formula (11) with $n = 0$:

$$D \approx \frac{k^2}{k^2 + \frac{1}{\beta^2}\left(\frac{2mV_0}{\hbar^2}\right)^2} = \frac{(E/V_0)}{(E/V_0) + s}. \qquad (12)$$

It is worth noting that the height of the barrier may not necessarily be small in comparison with the energy of the particle.

The energy dependences of the transmission coefficient for various values of parameter s, as given in Figs. 5 and 6, show that the method developed is capable of adequately reproducing these subtle features.

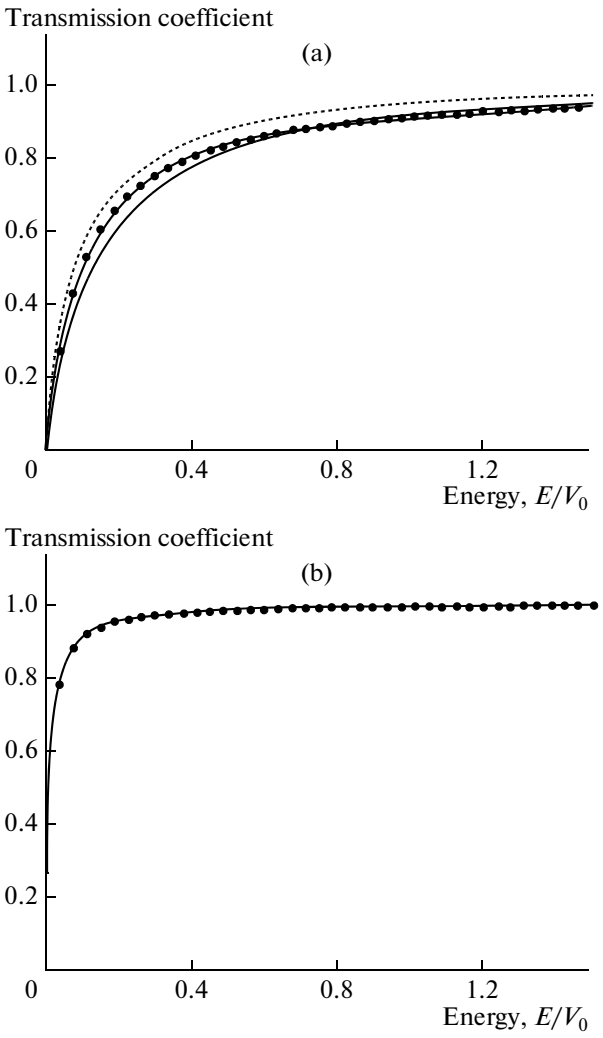

Fig. 6. The transmission coefficient for the Péschl–Teller potential; (a) $s = 0.1$, the dashed line is the well, the solid line is the barrier; (b) $s = 0.01$, the dashed line is the well, the solid line is the barrier; the bulleted line in both figures is curve (12); in (b), all the curves practically coincide.

4. FIELD EMISSION

Our method has been used to simulate field emission [13]. When simulating the field emission from a semiconductor there is a need to accurately calculate the tunneling coefficient over a wide energy range [14, 15]. A common calculation method is the Fowler–Nordheim formula based on the quasi-classical approximation (see, e.g., [13–15]):

$$D(E) = \begin{cases} \exp\left[-\frac{8\pi\sqrt{2m}|\chi - E|^{\frac{3}{2}}}{3hF}\theta\left(\frac{e\sqrt{eF}}{|\chi - E|}\right)\right], & E < \chi, \\ 1, & E > \chi, \end{cases}$$

$$\theta(x) \approx 0.95 - 1.03x^2, \quad x < 0.7;$$

here F is the electric field intensity near the emitter surface and χ is the energy of the electron affinity of a semiconductor ($\chi \approx 4$ eV for silicon).

However, as we have already pointed out, the quasi-classical approximation is strictly limited in its validity, and in many cases is incapable of providing sufficient accuracy, especially for small energies and when the argument of $\theta(x)$ is close to unity. In Fig. 7, we show comparative graphs of the tunneling coefficient calculated by the Fowler–Nordheim formula and through the use of the transfer matrix method.

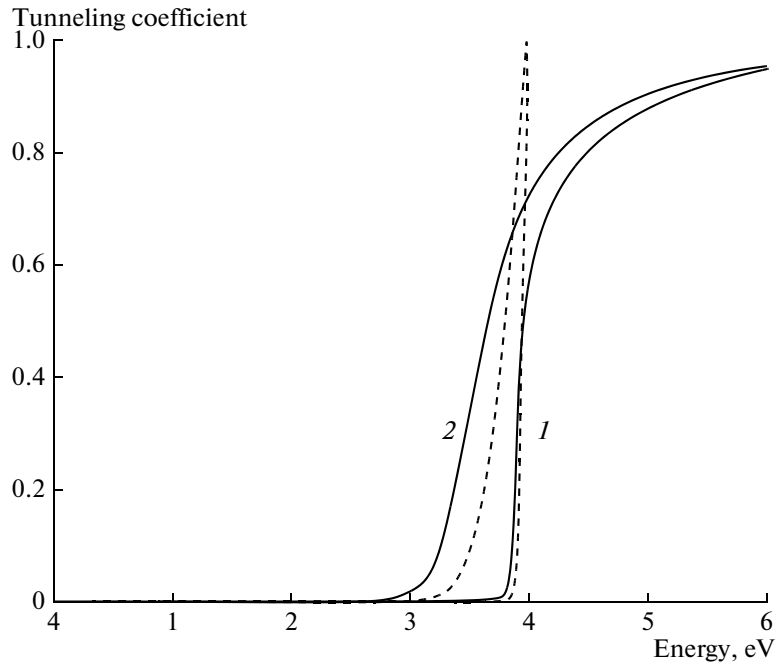

Fig. 7. Coefficient of tunneling from silicon into vacuum in an electric field: (*1*) $F = 10^6$ V/cm; (*2*) $F = 107$ V/cm; the dashed line corresponds to the quasi-classical calculation.

It is apparent from Fig. 7 that the use of the transfer matrix method considerably refines the calculation data.

CONCLUSIONS

The matrix algorithm developed here is an efficient way of modeling the stationary tunneling transfer for the spectrum of problems with fairly arbitrary one-dimensional scattering potential. The virtue of the algorithm in question is that it does not require the calculation of the wave function itself in the region of localization of the potential.

The matrix method of the Adams scheme makes it possible to model the scattering of a quantum particle over an arbitrary one-dimensional potential. The advantage of the matrix method using the Adams difference scheme is that it reduces the length of the calculation. This is extremely important in solving two- or three-dimensional dynamical problems: usually, the transmission coefficient at each point can be calculated within the quasi-one-dimensional model, but this necessitates its calculation over a large array of points at each time layer.

ACKNOWLEDGMENTS

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