

Quantum particle in a V-shaped well of arbitrary asymmetry. Brownian motors

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Abstract. The dependence of the energy spectrum of a quantum particle in an infinite V-shaped potential well on its asymmetry parameter is analyzed. The relationship between the occurrence of this dependence and different depths of quantum particle penetration into classically forbidden regions under the well walls is shown. In particular, an estimate of the energy spectrum using the Bohr–Sommerfeld quantization rule, which does not take into account the particle penetration into subbarrier regions, shows that there is no dependence on the well asymmetry parameter. An exception is the transition to the case of a vertical wall, when the semiclassical approach is characterized by a special boundary condition. The obtained results are illustrated by the dependence of the tunnel current of a Brownian motor (ratchet) with an applied fluctuating force on the asymmetry of the sawtooth potential. With a certain selection of ratchet parameters, considering zero-point oscillations describes the occurrence of a particle flow in the direction opposite to that obtained without such consideration.

Keywords: energy spectrum, asymmetric systems, Airy functions, Brownian motors, ratchets

1. Introduction

The most fruitful method of controlling the energy spectrum of designed electronic devices is the use of an external electric

field. The energy spectrum of such systems is calculated by solving the time-independent Schrödinger equation, which describes the state of a particle in a given potential (reflecting the structure of the designed device) and a DC electric field [1]. As is known, the contribution of this field to the potential relief is linear. On the other hand, the piecewise linear form of the potential profile allows an analytical solution of the Schrödinger equation in the form of a superposition of Airy functions [2]. A simple version of a piecewise linear function is a V-shaped dependence. The energy spectrum of an infinite triangular well is in demand in various applications and, in addition, it has a number of features that distinguish this spectrum from the energy spectra of particles in smooth potential profiles. A smooth potential well near its minimum is approximated well by a quadratic function, and its lower energy levels are close to the equidistant structure of the energy spectrum of a harmonic oscillator [3]. A fundamentally different spectrum arises for a particle in a triangular potential well, since its minimum has a cusp and cannot be approximated by a quadratic function.

According to literature data, the analysis of the energy spectrum of quantum particles was carried out only for two extreme special case of the symmetry of triangular potential wells: a well with one vertical wall and a symmetric well described by a function proportional to $|x|$ [2]. In this article, these known results are extended to the case of a triangular potential well of arbitrary symmetry, characterized by an asymmetry coefficient κ equal to zero for the symmetric well and equal to one for the extremely asymmetric well with one vertical wall. Representation of the energy spectrum as a function of the parameter κ allows identifying a number of interesting features associated with different depths of penetration of a quantum particle into classically forbidden regions under the walls of the well. Since a quantum particle cannot penetrate behind a vertical infinite wall, the dependence of the energy level on κ is characterized by the singular behavior of the first derivative near the extremely asymmetric well with $\kappa \rightarrow 1$.

The applications of the problem considered in this paper are diverse. We will cite some of them. For example, the tunneling of electrons from a perfectly conducting flat surface

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induced by an electric field occurs through an energy barrier close to a triangular one and is described by the Fowler–Nordheim theory [4, 5]. The Schrödinger equation with potential energy in the form of a triangular barrier and its inverse triangular well have exact solutions in terms of Airy functions. Knowledge of the bound states of the potential indicates a way to find quasinormal sub-barrier modes, which are eigenmodes of dissipative systems. These modes are the poles of the scattering matrix (Green’s function) of waves of a different nature on the scattering center [6]. Their characteristics are related to the problem of the passage of quantum particles through a potential barrier and their reflection from it, if we assume that the incident particle flux is absent. This corresponds to decaying waves moving away on both sides of the barrier. Quasinormal modes arise naturally as a perturbation of the classical gravitational background involving black holes or as excitation of nanoresonators [6–8]. Quasinormal modes of the barrier correspond in a certain way to the bound states of the potential inverse to a given barrier [9]. By replacing variables and parameters, the eigenfunctions of the potential are transformed into quasinormal modes with a complex wave vector. This method was used to obtain quasinormal modes of a symmetric triangular potential barrier [10].

In the theory of Brownian motors, a sawtooth potential is widely used as a model periodic potential profile characterized by a minimal set of parameters (energy barrier and asymmetry) [11–16]. In addition, the sawtooth shape of the potential can be easily realized experimentally [14]. Particularly, in numerous experiments on the directed motion of colloidal particles in ratchet systems, sawtooth potential shapes are created using electrodes deposited on glass by photolithographic methods (see, e.g., [15, Ch. 7]). In experiments on the manipulation of charged components inside lipid bilayers on a substrate [16], such a potential is created by a patterned bilayer, one side of which has a sawtooth shape and the other a flat surface. The ratchet effect of quantum Brownian motors is determined by the energy spectrum of quantum particles in sawtooth potentials, the unit cell of which is a triangular well of finite height [11, 17–23]. Since this effect is inherent only in symmetric systems, the study of the influence of the triangular well asymmetry on the energy spectrum is a fundamentally important task in the physics of quantum ratchet systems.

The purpose of these methodological notes is to clarify the dependence of the energy spectrum of a quantum particle in an infinite V-shaped potential well on the asymmetry parameter of the latter. Since it turns out that this dependence is quite nontrivial and arises only with a rigorous quantum-mechanical description, for methodological purposes, it is reasonable to begin the discussion with clear semiclassical relations that use the classical approach to determine the oscillation frequency independent of the asymmetry of the triangular well (Section 2), and only then proceed to a rigorous quantum-mechanical consideration that reveals such a dependence (Section 3). The dependence on the asymmetry parameter is due to its effect on the depth of particle penetration into classically forbidden regions under the walls of the potential well (Section 3).

On the other hand, as shown in Section 4, the tunneling of a particle through a triangular barrier does not depend on its asymmetry, since the barrier height and the tunneling path are invariant with respect to the asymmetry coefficient. However,

the tunneling current of a ratchet with a sawtooth potential (containing triangular barriers and wells) and an applied fluctuating force (the so-called rocking ratchet) depends on the asymmetry coefficient, since this force distorts the shape of the barriers and changes the energy of zero-point oscillations. The results of the performed consideration of the influence of the symmetry of V-shaped potentials on the energy spectrum of particles and the ratchet effect are summarized in Section 5.

2. Quasiclassical approximation

The quasiclassical approximation is valid when the de Broglie wavelength of a particle is small compared to the distance at which its potential energy changes significantly. This approximation allows us to trace the connection between classical and quantum mechanics. For a finite motion, this connection manifests itself in the correspondence principle, according to which, for large quantum numbers n , the separation between adjacent energy levels E_n is determined by the classical frequency of the motion $\omega_0 = 2\pi/T$ (T is the oscillation period), namely $dE_n/dn = \hbar\omega_0$, where \hbar is Planck’s constant [3, 24, 25].

An interesting and important feature of the semiclassical approximation is that it provides reasonable results even in cases where the condition of applicability of such an approximation is seemingly not satisfied. It is usually believed that states related to the discrete energy spectrum are well described by this approximation only for large values of the ordinal number of the state n , coinciding with the number of nodes of the corresponding wave function, since the distance between neighboring nodes is precisely estimated by the de Broglie wavelength. Nevertheless, given that the accuracy of the energy spectrum obtained within the framework of the quasiclassical approximation is not determined by the value of n^{-1} , but by $(\pi n)^{-2}$, which is small enough already for $n = 1$, this approximation describes the energy of the ground and first excited states quite well [25], which is associated with the effective use of this approximation in solving many problems [26–28].

Thus, it is advisable to start the methodological notes with visual semiclassical relations, which will allow us to outline the properties that permit a classical description and, against their background, to vividly present phenomena that in principle cannot be understood within the framework of the classical approach. Such phenomena include the penetration of a quantum particle into classically forbidden regions behind the walls of a potential well. In this section, the efficiency of the semiclassical approximation will be demonstrated by applying the Bohr–Sommerfeld quantization rule to three example problems: a particle in a rectangular box with infinitely high walls and in the Morse potential, as well as an estimate of the energy spectrum of a quantum particle in a V-shaped well of arbitrary asymmetry. The first two problems exactly reproduce the energy spectra that follow from analytical solutions of the Schrödinger equation. The third is considered in detail in the present methodological notes; however, as we shall see, the calculation of the classical frequency of motion will show its invariance with respect to the asymmetry of the V-shaped well and, consequently, the invariance of the energy spectrum in the semiclassical approximation. This circumstance will serve as a convincing argument in favor of the necessity of a rigorous quantum-mechanical consideration, carried out in Section 3.

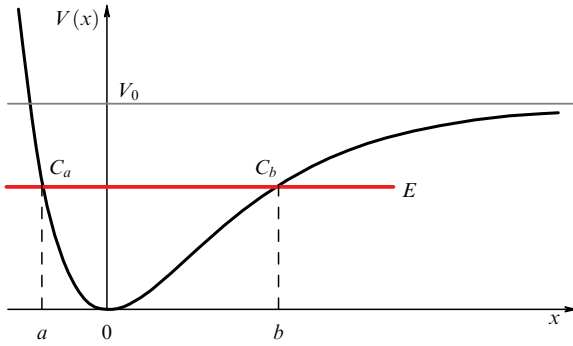


Figure 1. Particle with energy E in Morse potential $V(x)$ with potential well depth V_0 . Classically admissible region is bounded by points a and b , at which the values of constants C_a and C_b , included in Eqn (3), are determined by the course of potential curves.

The Bohr–Sommerfeld quantization rule is formulated for the adiabatic invariant [29]

$$I(E) \equiv \frac{1}{2\pi} \oint p(x) dx = \frac{1}{\pi} \int_a^b p(x) dx. \quad (1)$$

In definition (1), $p(x) = \sqrt{2m[E - V(x)]}$ is the momentum of a particle with total energy E and potential energy $V(x)$, and integration is carried out over the entire region of coordinate variation during the period of the particle motion $T(E)$, which is related to the adiabatic invariant as

$$T(E) = 2\pi \frac{\partial I(E)}{\partial E} = \sqrt{\frac{m}{2}} \oint \frac{dx}{\sqrt{E - V(x)}}, \quad (2)$$

so that the derivative $\partial I(E)/\partial E$ is the inverse cyclic frequency ω_0 . If we introduce the concept of a classically admissible region as one bounded by stopping points a and b , where $V(x) = E$ (Fig. 1), then the integrals in Eqns (1) and (2) over the entire region of coordinate variation over the period are equal to double the integrals over the region $a < x < b$.

Let us write the Bohr–Sommerfeld quantization rule in the general form [25],

$$I(E) = \hbar(n + C_a + C_b), \quad (3)$$

in which the values of the constants C_a and C_b are determined by the slope of the potential curves at stopping points a and b : if the derivative $dV(x)/dx$ at a stopping point is finite (a sloping curve), then the corresponding constant is equal to $1/4$, but if it is infinite (the vertical tangent at a stopping point), then it is equal to $1/2$. For $n \gg 1$, we can assume that n is a continuous variable, which makes differentiation of the left and right parts of Eqn (3) with respect to n viable, and this is precisely what gives the correspondence principle $dI(E_n)/dn = [\partial I(E_n)/\partial E_n] dE_n/dn = \omega_0^{-1} dE_n/dn = \hbar$.

For a rectangular potential well with infinitely high walls $C_a = C_b = 1/2$, and $I(E) = \pi^{-1} L \sqrt{2mE}$. Therefore, the energy spectrum is determined by the formula $E_n = \pi^2 \hbar^2 (n + 1)^2 / (2mL^2)$, which coincides with the solution of the Schrödinger equation [3, 25].¹

¹The resulting formula also implies the principle of correspondence $dE_n/dn = \hbar\omega_0$ if we take into account that $dE_n/dn = \pi^2 \hbar^2 (n + 1) / (mL^2)$, but, on the other hand, $\omega_0 = 2\pi\sqrt{E_n}/(2mL^2) = \pi^2 \hbar (n + 1) / (mL^2)$.

A harmonic oscillator is usually considered another canonical example of the coincidence between a semiclassical solution and an exact one. Let us consider an example that more convincingly demonstrates the effectiveness of the semiclassical approximation—the calculation of the energy spectrum of a particle in the Morse potential (see Fig. 1),

$$V(x) = V_0(1 - \exp(-\alpha x))^2, \quad (4)$$

which, unlike the parabolic one, is more realistic and describes a potential well of finite depth. For small x , this potential is reduced to that of a harmonic oscillator, characterized by a cyclic frequency $\omega_0 = \sqrt{V''(0)}/m = \alpha\sqrt{2V_0}/m$, which is a much more convenient parameter (compared to α) for representing the results obtained.

For potential (4), calculating the integral in Eqn (1) yields $I(E) = (2V_0/\omega_0)(1 - \sqrt{1 - E/V_0})^2$. Since the potential curve at the stopping points is inclined, $C_a = C_b = 1/4$ and the quantization rule (3) leads to the result

$$E_n = \hbar\omega_0 \left(n + \frac{1}{2} \right) \left[1 - \frac{\hbar\omega_0}{4V_0} \left(n + \frac{1}{2} \right) \right], \quad (5)$$

$$n + \frac{1}{2} < \frac{4V_0}{\hbar\omega_0},$$

coinciding with the analytical solution of the Schrödinger equation (see problem 4 after §23 of [3]). As far as we know, the coincidence between the result of the semiclassical approximation and the exact one for the Morse potential is noted here for the first time.

The inequality in (5) means the finiteness of the number of levels in the discrete spectrum. If this inequality becomes strong, that is,

$$\frac{\hbar\omega_0}{4V_0} \left(n + \frac{1}{2} \right) \ll 1, \quad (6)$$

then Eqn (5) gives the energy spectrum of the harmonic oscillator

$$E_n = \hbar\omega_0 \left(n + \frac{1}{2} \right). \quad (7)$$

It is clear that since relation (5) is obtained both by means of the semiclassical approximation and by an exact consideration of the spectrum in the Morse potential, its special case, relation (7) for the harmonic oscillator, also serves as an example of the coincidence of the results of the two approaches.

Note that the strong inequality (6) allows two interpretations. First, $V_0 \rightarrow \infty$ (with $\alpha = \omega_0 \sqrt{m/(2V_0)} \rightarrow 0$) corresponds to the passage from the Morse potential to the limit of a harmonic oscillator potential, characterized by the equidistant spectrum (7) for any n . Second, for limited values of V_0 but for $\hbar\omega_0/4V_0 \ll 1$,³ strong inequality (6) is valid only

² According to relation (2), the period of classical oscillation in the Morse potential is $T(E) = 2\pi\omega_0^{-1}(1 - E/V_0)^{-1/2}$, which coincides with the period of oscillation of the harmonic oscillator at $E \rightarrow 0$ and tends to infinity as $E \rightarrow V_0$.

³ This inequality can be rewritten as a quasi-classicality condition $\lambda_{dB} \equiv 2\pi\hbar/(2mV_0)^{1/2} \ll \alpha^{-1}$ (the de Broglie wavelength of a particle λ_{dB} expressed through the momentum of the particle $(2mV_0)^{1/2}$ at the maximum depth of the potential well is much smaller than its characteristic width α^{-1}). Thus, the quasi-classicality condition allows approximating the low-energy levels of a particle in a potential well of finite depth by the spectrum of the corresponding infinite well.

for the lower levels, i.e., for the region of the approximately equidistant spectrum, for which the curve describing the Morse potential near its minimum can be approximated by a parabola. Since a parabolic approximation is admissible near the local minimum of any smooth potential profile and not only the Morse potential, Eqn (7) with $n = 0$ can be used to estimate the energy of zero-point oscillations in an arbitrary smooth profile. In this regard, we note a certain universality of the zero-point oscillation energy in the form $E_0 = \hbar\omega_0/2$. It can also be considered to result from the Heisenberg uncertainty relation, the most precise formulation of which is

$$\langle \Delta p \rangle^2 \langle \Delta x \rangle^2 \geq \frac{\hbar^2}{4}. \tag{8}$$

Indeed, the state with the minimum uncertainty (the equality sign in Eqn (8)) and the zero mean values of coordinates and momentum corresponds to the Gaussian wave function

$$\psi_0(x) = (2\pi \langle \Delta x^2 \rangle)^{-1/4} \exp\left(-\frac{x^2}{4\langle \Delta x^2 \rangle}\right), \tag{9}$$

which is precisely the wave function of a harmonic oscillator with $\langle \Delta x^2 \rangle = \hbar/(2m\omega_0)$ (see problems 2 and 3 after §23 in Ref. [3]).

The V-shaped potential profile, which is the main object of consideration in these methodological notes, does not belong to smooth functions. Therefore, it is unacceptable to use the relation $E_0 = \hbar\omega_0/2$ for it, and it is necessary to perform a strict quantum-mechanical description, which we will turn to in Section 3. Here, to continue the discussion of the semiclassical approximation, it seems important and interesting to show what its use for such a profile will lead to.

So, let us consider a V-shaped (infinite triangular) potential well, the sides of which have arbitrary slopes F_l and F_r (Fig. 2). The expression of the coordinate dependence of the potential energy has the form

$$V(x) = \begin{cases} F_r x, & x > 0, \\ F_l x, & x < 0. \end{cases} \tag{10}$$

To analyze the asymmetry of the potential well (10), we introduce auxiliary parameters: an arbitrary energy parameter V_0 and the widths of the sections l to the right and $L - l$

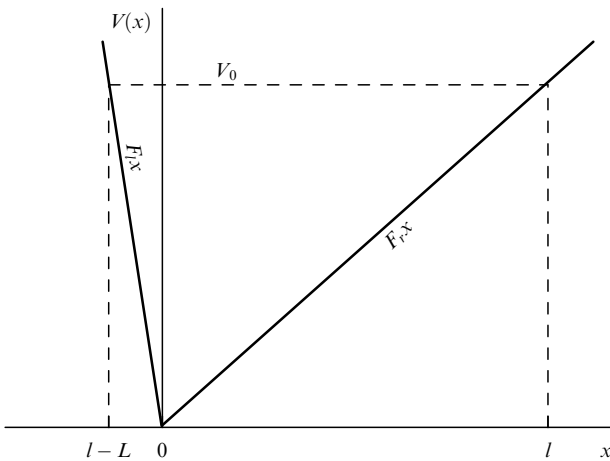


Figure 2. Infinite triangular potential well of arbitrary asymmetry, characterized by asymmetry parameter $\kappa = 2l/L - 1$ (at $\kappa = 0$, well is symmetric; at $\kappa = 1$, left wall is vertical).

to the left of the origin of coordinates, cut off from the potential energy $V(x)$ by the energy level V_0 (see Fig. 2). Then, the forces F_r and F_l are related to the auxiliary parameters by the expressions

$$F_r = \frac{V_0}{l} > 0, \quad F_l = \frac{V_0}{l-L} < 0, \tag{11}$$

so that the asymmetry of the well can be characterized by the parameter

$$\kappa = \frac{2l}{L} - 1 = \frac{|F_l| - F_r}{|F_l| + F_r}. \tag{12}$$

According to the physical meaning of the asymmetry parameter, it is equal to zero for the symmetric well (when $l = L/2$) and to one for the extremely asymmetric well, in which the left wall is vertical (when $l = L$). The dimensionless parameter κ , together with the new dimensional parameter, the effective force

$$F_* \equiv \frac{V_0}{L} = \frac{|F_l|F_r}{|F_l| + F_r}, \tag{13}$$

unambiguously characterizes the original pair of parameters F_r and F_l . The physical meaning of the quantity F_* follows from definition (13) for $|F_l| \rightarrow \infty$: $F_* = F_r$, i.e., the effective force F_* of a triangular well of arbitrary asymmetry is determined by the value of the gentle slope of the potential relief corresponding to the extremely asymmetric well. In turn, F_r and F_l are related to F_* and κ as $F_r = (2F_*)/(\kappa + 1)$, $F_l = (2F_*)/(\kappa - 1)$.

Calculating the integral in Eqn (1) leads to the result

$$I(E) = \frac{2\sqrt{2m}}{3\pi F_*} E^{3/2}, \tag{14}$$

which does not depend on the asymmetry parameter κ .⁴ In order to apply the Bohr–Sommerfeld quantization rule (3), it should be taken into account that, for the chosen parameterization, the right wall of the well cannot be vertical, so that $C_b = 1/4$, and the value of the constant C_a depends on the value of κ , namely $C_a = 1/2$ for $\kappa = 1$ and $C_a = 1/4$ for $\kappa < 1$.⁵ Thus, substituting (14) into (3) and then solving the resulting equation with respect to E_n yields

$$E_n = \left[\frac{3\pi}{2} \left(n + C_a + \frac{1}{4} \right) \right]^{2/3} E_*, \tag{15}$$

where the parameter E_* , having the dimension of energy, is defined by the relation

$$E_* \equiv \left(\frac{\hbar^2 F_*^2}{2m} \right)^{1/3}. \tag{16}$$

⁴ According to relation (2), the period of classical oscillation of a particle in a triangular potential well is $T(E) = (2/F_*)\sqrt{2mE}$ and tends to zero as $E \rightarrow 0$. This differs the behavior of a classical particle in a triangular well from its behavior in a parabolic well, for which the period does not depend on energy.

⁵ The semiclassical approximation for the energy spectrum of a particle in a triangular well with $\kappa = 1$ was considered in problem 119 from [30], where $C_a = 1/4$ was mistakenly used, just as it was for $\kappa < 1$. This resulted in an incorrect formula (119.5), which should have had $n + 3/4$ instead of $n + 1/2$ (which the editor pointed out in their footnote on p. 323). Only after such a correction can the incident of the formula (119.7) with the asymptotic expression (40.14) (problem 40) from [30] be achieved.

Table. Energy spectrum $E_n(\kappa)$ (in units $E_* \equiv (\hbar^2 F_*^2/2m)^{1/3}$) of a particle in an infinite triangular potential well, calculated for different values of asymmetry parameter ($\kappa = 0$ — symmetric well, $\kappa = 1$ — extremely asymmetric well) in semiclassical approximation and by solving the Schrödinger equation.

n	$E_n(\kappa)/E_*$			
	Semiclassical approximation (Eqn (15))		Exact values [2, 30]	
	$\kappa < 1$	$\kappa = 1$	$\kappa = 0$	$\kappa = 1$
0	1.771	2.320	1.617	2.338
1	3.683	4.082	3.712	4.088
2	5.178	5.517	5.156	5.521
3	6.479	6.784	6.489	6.787

Actually, the zero-point energy of the system under consideration depends on the asymmetry parameter for $\kappa < 1$. This will become clear from the results of the exact solution to the problem, carried out in the next section. Here in the Table, we present a comparison of the results of the semiclassical description with the results of solving the Schrödinger equation for the special cases of $\kappa = 0$ and $\kappa = 1$ available in the literature [2, 30]. For example, for the ground state, expression (15) with $n=0$ and $C_a=1/4$ yields $E_0/E_* \approx 1.771$, while the exact value for $\kappa = 0$ is 1.617. For $\kappa = 1$, we have $C_a = 1/2$, and Eqn (15) yields $E_0/E_* \approx 2.320$, while the exact value is 2.338. For $\kappa < 1$, with increasing quantum number n , the results of the semiclassical treatment quickly approach the exact result corresponding to $\kappa = 0$. This means that E_n does not depend on κ for large quantum numbers, when the correspondence principle is valid and the distances between neighboring levels are determined by the classical frequency of motion, independent of the asymmetry parameter (see Eqns (2), (14)). The Table demonstrates excellent agreement of the results both for $\kappa < 0$ and $\kappa = 1$. However, the differences between the results for $\kappa < 1$ and $\kappa = 1$ remain for large n . In the semiclassical treatment, this is due to the different boundary condition and the value of the constant C_a . The exact treatment carried out in Section 3 for arbitrary values of κ will reveal the nonanalyticity of the behavior for $\kappa \rightarrow 1$ (see Eqn (26) below).

3. Quantum mechanical consideration

Let us write the Schrödinger equation for a particle with mass m and energy E in potential (10) for the left and right half-spaces (negative and positive values of x):

$$\frac{d^2\psi_j(x)}{dx^2} + \frac{2m}{\hbar^2} (E - F_j x) \psi_j(x) = 0, \quad j = l, r. \tag{17}$$

The general solutions of differential equations (17) in each half-space contain two arbitrary constants, which, like the energy parameter E , can be uniquely determined from the normalization condition and four boundary conditions:

$$\int_{-\infty}^0 dx |\psi_l(x)|^2 + \int_0^{\infty} dx |\psi_r(x)|^2 = 1, \quad \psi_l(-\infty) = 0, \tag{18}$$

$$\psi_r(\infty) = 0, \quad \psi_l(-0) = \psi_r(+0), \quad \psi_l'(-0) = \psi_r'(+0).$$

Equations (17) in the new variables

$$y_r = \left(\frac{2mF_r}{\hbar^2}\right)^{1/3} \left(x - \frac{E}{F_r}\right),$$

$$y_l = -\left(\frac{2m|F_l|}{\hbar^2}\right)^{1/3} \left(x + \frac{E}{|F_l|}\right) \tag{19}$$

are reduced to the equations

$$\frac{d^2\tilde{\psi}_j(y_j)}{dy_j^2} - y_j\tilde{\psi}_j(y_j) = 0, \quad j = l, r \tag{20}$$

for the new wave functions $\tilde{\psi}_j(y_j) = \psi_j(x)$ ($x < 0$ when $j = l$ and $x > 0$ when $j = r$). The general solutions of Eqns (20) are expressed through the Airy functions of the first and second kind [2, 31],

$$\tilde{\psi}_j(y_j) = C_j \text{Ai}(y_j) + D_j \text{Bi}(y_j), \quad j = l, r, \tag{21}$$

where C_j and D_j are arbitrary constants. Since $y_j \rightarrow \infty$ at $x \rightarrow \pm \infty$ and $\text{Bi}(\infty) \rightarrow \infty$, the boundary conditions $\tilde{\psi}_j(\infty) = 0$ (see (18)) are satisfied at $D_j = 0$ due to the equality $\text{Ai}(\infty) = 0$. The constants C_j are found from the normalization conditions and the continuity of the solution at the point $x = 0$, while the quantization of the energy variable E follows from the continuity condition for the first derivatives of the wave functions at the same point, which, taking into account Eqns (18), (19), and (21), can be written as

$$-|F_l|^{1/3} \frac{\text{Ai}'(y_l)}{\text{Ai}(y_l)} \Big|_{y_l = -\frac{E}{|F_l|} \left(\frac{2m|F_l|}{\hbar^2}\right)^{1/3}} = F_r^{1/3} \frac{\text{Ai}'(y_r)}{\text{Ai}(y_r)} \Big|_{y_r = -\frac{E}{F_r} \left(\frac{2mF_r}{\hbar^2}\right)^{1/3}}, \tag{22}$$

where $\text{Ai}'(y)$ is the derivative of the function $\text{Ai}(y)$.

We introduce the dimensionless variable

$$\gamma \equiv \frac{y_l}{y_r} = \left(\frac{F_r}{|F_l|}\right)^{2/3} = \left(\frac{1 - \kappa}{1 + \kappa}\right)^{2/3}, \tag{23}$$

which is equal to the ratio of the values of the variable y substituted into Eqn (22) and is determined by the asymmetry coefficient κ . If we denote y_r by y , then Eqn (22) takes the form

$$\frac{\text{Ai}'(\tilde{y})}{\text{Ai}(\tilde{y})} \Big|_{\tilde{y} = \gamma y} + \sqrt{\gamma} \frac{\text{Ai}'(y)}{\text{Ai}(y)} = 0. \tag{24}$$

This equation has an infinite number of solutions. We assign the index $n = 0$ to the smallest absolute negative value of y , and number the remaining solutions with the integer index $n = 1, 2, \dots$ as $|y|$ increases. Then, the desired energy spectrum E_n will be determined by the relation

$$E_n = -E_* \left(\frac{2}{1 + \kappa}\right)^{2/3} y_n, \quad n = 0, 1, 2, \dots, \tag{25}$$

where the dimensional energy parameter E_* is given by Eqns (13), (16).

Note that, when the sign of the asymmetry coefficient is reversed, $\kappa \rightarrow -\kappa$, the parameter γ defined by Eqn (23) becomes equal to its reciprocal value, $\gamma \rightarrow \gamma^{-1}$. In this case, it follows from the structure of Eqn (24) that, since y_n is a

function of the parameter γ , and hence the asymmetry parameter κ , $y_n = y_n(\kappa)$, we have $y_n(-\kappa) = \gamma y_n(\kappa)$. Therefore, when replacing $\kappa \rightarrow -\kappa$, the transformation $E_n(-\kappa) = E_n(\kappa)$ takes place, as should follow from the symmetry condition.

Let us proceed to the analysis of the solution of Eqn (24). When $\kappa = 0$, it follows from relation (23) that $\gamma = 1$, so that y_n are the roots of the equation $\text{Ai}'(y) = 0$. Using the tabular values of these roots and multiplying them by $2^{2/3}$, according to Eqn (25), we arrive at the values presented for $E_n(0)/E_*$ in the penultimate column of the Table, corresponding to the exact values at $\kappa = 0$. At $\kappa = 1$, we have $\gamma = 0$. Since the ratio $\text{Ai}'(0)/\text{Ai}(0) \approx -0.7290$ is not equal to zero, the roots of Eqn (24) can only be the roots of the equation $\text{Ai}(y) = 0$. Denoting these roots by z_n , we find that, according to (25), $E_n(1)/E_* = -y_n = -z_n$. The numerical values at $\kappa=1$ are presented in the last column of the Table. To clarify the asymptotic behavior of the function $E_n(\kappa)$ at $\kappa \rightarrow 1$, we expand the function $\text{Ai}(y)$ in a series in $y - z_n$ and use the approximate equality $\text{Ai}(y) \approx \text{Ai}'(z_n)(y - z_n)$. Substituting it into Eqn (24), we obtain $y_n \approx z_n - [\text{Ai}(0)/\text{Ai}'(0)]\sqrt{\gamma}$, whence, taking into account (25), we obtain

$$\begin{aligned} \frac{E_n(\kappa)}{E_*} \underset{\kappa \rightarrow 1}{\approx} & \frac{E_n(1)}{E_*} - 2^{-1/3} \frac{\text{Ai}(0)}{\text{Ai}'(0)} (1 - \kappa)^{1/3} \\ & \approx -z_n + 1.089 (1 - \kappa)^{1/3}. \end{aligned} \quad (26)$$

It follows from this expression that the energy spectrum $E_n(\kappa)$ is characterized by an infinite derivative $E_n'(\kappa)$ at $\kappa \rightarrow 1$.

For numerical calculation of the dependence of the energy spectrum on the asymmetry parameter of the potential well, it is necessary to determine the boundaries of possible values of the roots of Eqn (24) for different values of κ from the interval $(0, 1)$. It is clear that these roots y_n are negative and are bounded by the values of z_n and z_n/γ , at which the Airy functions $\text{Ai}(y)$ and $\text{Ai}(\gamma y)$ vanish. For example, the value of y_0 is bounded by the interval $(z_0, 0)$ at any κ , and y_1 falls into the interval $(z_0/\gamma, z_0)$ at $\kappa < 0.3961$ and into the interval (z_1, z_0) at $\kappa > 0.3961$. As the quantum number n increases, the number of intervals bounded by different values of z_n and z_n/γ increases. The calculations performed showed that the functions $E_n(\kappa)$ change slowly with changing κ , except for a narrow region near the value $\kappa = 1$. Since the values of $E_n(\kappa)$ change significantly with changes in the quantum number n compared to the changes following changes in κ (see Table), it is reasonable to represent the dependences $E_n(\kappa)$ as measured from $E_n(0)$ (Fig. 3). The dependence of the energy of the ground state E_0 on the asymmetry parameter κ is monotonically increasing, whereas the dependences $E_n(\kappa)$ for $n=1, 2, 3$ are described by nonmonotonic functions. In this case, the curve corresponding to $n = 1$ has two nonmonotonic regions, to $n = 2$, three regions, and to $n = 3$, four regions. In accordance with formula (26), near the point $\kappa = 1$, the functions $E_n(\kappa)$ have a first derivative tending to infinity.

Expressions for the wave functions $\psi_n(x)$ in each half-space follow from relations (18)–(21), (23)–(25):

$$\psi_n(x) = \begin{cases} C_n \text{Ai}\left(\left(\frac{2}{1+\kappa}\right)^{1/3} \left(\frac{x}{x_*}\right) + y_n\right), & x > 0, \\ C_n \frac{\text{Ai}(y_n)}{\text{Ai}(\gamma y_n)} \text{Ai}\left(-\left(\frac{2}{1-\kappa}\right)^{1/3} \left(\frac{x}{x_*}\right) + y_n\right), & x < 0. \end{cases} \quad (27)$$

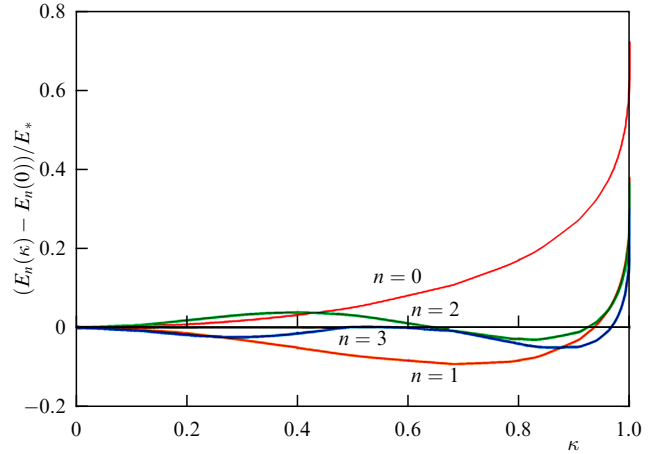


Figure 3. Relative changes in spectrum $E_n(\kappa)$ as functions of asymmetry parameter κ .

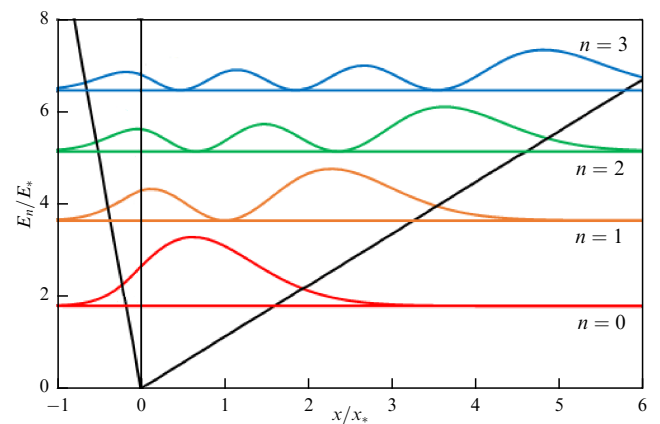


Figure 4. Energy levels E_n and corresponding probability densities of detecting a particle at point x in states with $n = 0, 1, 2, 3$ at $\kappa = 0.8$.

Here,

$$x_* \equiv \frac{E_*}{F_*} = \left(\frac{\hbar^2}{2mF_*} \right)^{1/3}, \quad (28)$$

and the constant C_n is easily found from the normalization conditions in (18):

$$C_n = x_*^{-1/2} \left(\frac{1+\kappa}{2} \right)^{1/3} [\text{Ai}'^2(y_n) - y_n \text{Ai}^2(y_n)]^{-1/2}, \quad (29)$$

which takes into account the identity

$$\int_y^\infty d\xi \text{Ai}^2(\xi) = \text{Ai}'^2(y) - y \text{Ai}^2(y), \quad (30)$$

following from the differential equation (20).

The energy levels E_n and the probability densities of finding a particle at point x in states with $n = 0, 1, 2, 3$ at $\kappa = 0.8$ are shown in Fig. 4. The probabilities of finding a particle in the left and right sub-barrier regions depend on the slopes of the sides of the triangular well. This explains the occurrence of dependences of E_n on the asymmetry parameter κ . For a mathematical justification of this statement, we calculate, for example, the dependence of the probabilities of finding a particle in the left and right sub-barrier regions on the asymmetry parameter κ at

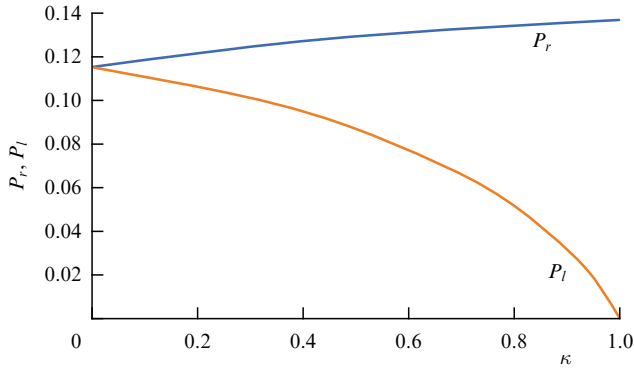


Figure 5. Probabilities of finding a particle in left and right subbarrier regions as functions of asymmetry parameter κ at $n = 0$.

$n = 0$:

$$P_r \equiv \int_{x_r}^{\infty} dx |\psi_0(x)|^2 = \frac{1 + \kappa}{2} \frac{\text{Ai}'^2(0)}{\text{Ai}'^2(y_0) - y_0 \text{Ai}^2(y_0)},$$

$$\frac{P_l}{P_r} = \sqrt{\gamma} \frac{\text{Ai}^2(y_0)}{\text{Ai}^2(\gamma y_0)}. \quad (31)$$

The dependences of P_r and P_l on κ are plotted in Fig. 5. It follows that the probability of penetrating the barrier becomes greater as the slope of the linear function describing this barrier becomes smaller. The probabilities of penetrating the left and right barriers are the same for the symmetric case $\kappa = 0$ and differ most in the extremely asymmetric case $\kappa = 1$, when the particle cannot pass through the vertical barrier ($P_l = 0$).

Let us return to the analysis of Fig. 3. For excited levels $n = 1, 2, 3$, a new factor appears that influences the degree of particle penetration into the sub-barrier region—the proximity to it of one of the wave function zeros, whose position depends on the asymmetry parameter κ . Since the number of zeros of the wave function coincides with the level number n , the probabilities of particle penetration under the barriers become dependent on n . Therefore, in the dependence of the energy spectrum on κ , one can expect the emergence of nonmonotonic regions, the number of which is equal to the level number n . This is observed in Fig. 3. In addition, with increasing n , the dependence of the energy levels on κ becomes less pronounced, which agrees with the correspondence principle, according to which the separations between neighboring levels, determined by the classical frequency of motion, do not depend on κ .

4. Application of the obtained results to ratchet systems

The most popular model potential used to describe ratchet systems is the periodic sawtooth potential (let the widths of its sections be l and $L - l$, L being the period) [11–16, 20]. It is for such a potential that the asymmetry (by the parameter $\kappa \equiv 2l/L - 1$), which is the main parameter of ratchet systems, is most easily specified. Each period of the sawtooth potential contains a triangular well and a triangular barrier. For clarity, let us imagine that Fig. 2 depicts such a well of depth V_0 , which simultaneously determines the barrier height. In Section 2, using the Morse potential as an example, it was shown that, when the energy quantum $\hbar\omega_0$ is small compared to the potential well depth, the positions of

the lower energy levels are determined by the shape of the potential curve near its minimum. For a smooth curve, such a shape is a parabola with sufficient accuracy, and the lower energy levels at $\hbar\omega_0/4V_0 \ll 1$ are described by expression (7) for the spectrum of a harmonic oscillator. It is clear that, for a V-shaped well of depth V_0 , the lower levels at $E_* \ll V_0$ (where E_* is defined by the relations (13), (16))⁶ should be described by the energy spectrum of an infinite V-shaped well (25).

Since the parameter V_0 is the height of the sawtooth potential barrier, the condition $E_* \ll V_0$ simultaneously ensures the possibility of using Gamow's formula [32–35] to describe the tunneling current arising in a ratchet system with such a potential at zero temperature (a rigorous proof of this formula and corrections to it are given in Ref. [36]). It turns out that the result of calculating the tunneling current does not depend on the parameter l and, therefore, on the barrier asymmetry. Only the barrier height V_0 and the tunneling path L determine the tunneling current:

$$J = A \exp\left(-\frac{4L\sqrt{2mV_0}}{3\hbar}\right). \quad (32)$$

The pre-exponential factor A can be omitted if only the exponential behavior of fluxes is of interest.⁷ The absence of a dependence on the barrier asymmetry in Eqn (32) once again points to the determining role of the length of particle penetration into the sub-barrier region as a factor that characterizes the ratchets under discussion.

In [22, 23], the tunnel flux of particles arising in a sawtooth periodic potential under the action of adiabatic dichotomous fluctuations of a homogeneous external force was calculated based on formula (32). As mentioned above, systems with a mechanism for the occurrence of directed motion due to fluctuations of the applied force with a zero mean value are classified as so-called ‘rocking ratchets.’ A modern classification of ratchets can be found in review [20]. The functioning of ratchets of this type is ensured by the asymmetry of the steady-state periodic potential profile $V(x)$, modified by dichotomous fluctuations of the external force $\pm F$. Then, for $F > 0$, in a state of duration τ_+ in the inclined potential profile $U_+(x) = V(x) - Fx$, a positive particle flux $J(F)$ arises. In a state of duration τ_- in the potential profile $U_-(x) = V(x) + Fx$ with the opposite slope, the negative particle flux $J(-F)$ arises. For a symmetric dichotomous process with equal state durations ($\tau_+ = \tau_-$), the time average value of the applied force is zero, but the average flux $J = [J(F) + J(-F)]/2$ may be nonzero. This situation arises if the function $V(x)$ does not belong to the class of spatially symmetric periodic functions, the strict definition and the properties of which are presented in [37]. Tunneling currents of different signs can also arise at low temperatures in ratchets of another type, functioning due to fluctuations of the periodic potential profiles themselves, not belonging to the class of spatially symmetric ones [38].

⁶ This inequality can also be rewritten as a quasi-classicality condition (see footnote 3) $\lambda_{\text{dB}} \equiv 2\pi\hbar/(2mV_0)^{1/2} \ll x_*$, where x_* is the characteristic width of the triangular well at the zero-point energy level, determined by relation (28).

⁷ It is known that the pre-exponential factor changes its value when the potential energy curve becomes vertical, but the exponent in (32) does not depend on this. Therefore, the transmission coefficient through a triangular potential barrier with a vertical wall (see problem 1 after § 50 in [3]) has the same form, although expression (32) is obtained for a triangular barrier of arbitrary symmetry.

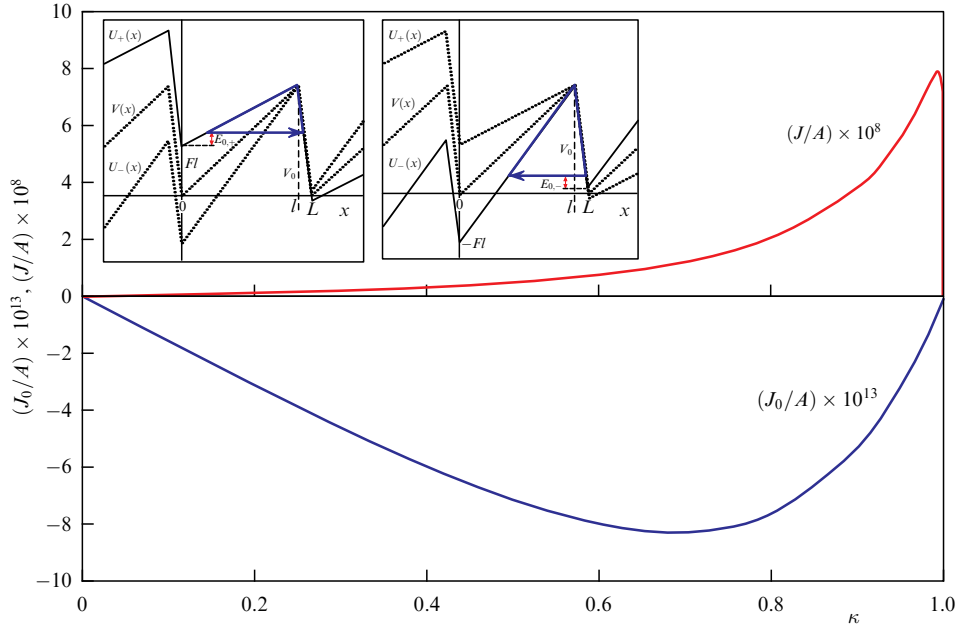


Figure 6. Dependences of tunneling current of a ratchet with fluctuating force on asymmetry parameter $\kappa = 2l/L - 1$ of sawtooth potential, calculated without (lower curve J_0) and with (upper curve J) zero-point oscillations at $FL/V_0 = 0.618$ and $E_*/V_0 = 0.1$. Insets show changes in the shape of asymmetric sawtooth potential caused by applied forces and leading to changes in energy barriers and tunneling paths (shown by arrows). Due to zero-point oscillations with energy levels E_0 , heights of barriers that particle overcomes during tunneling are smaller than initial barriers measured relative to bottom of potential wells.

Since in this paper we discuss piecewise linear forms of potential profiles, we will continue the analysis of sawtooth potentials $V(x)$. While the tunneling current through any barrier of an unperturbed sawtooth potential $V(x)$ does not depend on its asymmetry, fluxes through barriers of potentials $U_{\pm}(x)$ perturbed by applied forces $\pm F$ become dependent on it, for two reasons. The first is the change in the slopes of the rectilinear sections of the sawtooth potential and the values of its minima by the applied forces. Indeed, the values of the minima of the initial function $V(x)$ are the same, whereas the minima of the functions $U_{\pm}(x)$ closest to any maximum become different: one of them is higher and the other is lower than the initial one (see the insets in Fig. 6). Therefore, the application of forces lowers one of the barriers surrounding the potential well, and it is through this barrier that the tunnel current flows. Since due to the asymmetry of the initial profile $V(x)$ the values of the barriers and tunnel paths in the potentials $U_{+}(x)$ and $U_{-}(x)$ are different, the tunnel fluxes in them will be different in absolute value and opposite in direction. Therefore, when averaging, there is no compensation of fluxes; a nonzero average flux arises, which indicates the presence of the ratchet effect (rectification of nonequilibrium fluctuations due to the asymmetry of the system).

Thus, the first reason for the dependence of tunnel currents on the asymmetry coefficient is the different distortion of the shape of the initial periodic potential profile $V(x)$ with symmetric fluctuations of the acting force due to its spatial asymmetry. Assuming for simplicity that tunneling occurs from the minima of the potential profiles $U_{\pm}(x)$, it is easy to calculate the average tunneling current using formula (32). In this case, the barrier and tunneling path will differ from the parameters V_0 and L , by taking into account the distortions introduced by the applied forces $\pm F$. Since such distortions are different for different barrier asymmetries

characterized by the parameter l , the average tunneling current will also depend on l . The results of the described calculation are presented in [22] to show that the reversal of the direction of the tunneling current arising at low temperatures relative to the thermally activated flux at high temperatures, theoretically predicted in [39] and experimentally confirmed in [40, 41], can occur only at relatively small values of the fluctuating force F . In Figure 6, the lower curve displays the dependence of the flux J_0 on the asymmetry parameter $\kappa = 2l/L - 1$ (here, L is the period of the sawtooth potential $V(x)$) for the boundary value of the force $FL/V_0 = (\sqrt{5} - 1)/2 \approx 0.618$, at which $J_0 < 0$ for all κ except for the limiting values $\kappa = 0$ and $\kappa = 1$. An increase in F relative to this boundary value leads to an alternating dependence of J_0 on κ in the range $0.618 < FL/V_0 < 2/3 \approx 0.667$, and at $FL/V_0 > 0.667$ to positive J_0 for any κ , as in the case of thermally activated overcoming the barriers.

The second reason for the dependence of tunnel fluxes on the asymmetry coefficient is the dependence of the particle energy spectrum on it. Within the same approximation $E_* \ll V_0$, the lower energy levels of a particle in the sawtooth potential approximately coincide with the levels in an infinite triangular well of the same asymmetry. Therefore, to describe tunneling from the lower levels of zero-point oscillations of the potential $U_{\pm}(x)$, we can use the results of the previous section, in particular, Eqn (25) with $n = 0$. The tunnel paths in these potentials are shown by arrows in the insets to Fig. 6. In Ref. [23], the contribution of zero-point oscillations to the boundary values of the fluctuating force was analyzed. Here, the dependence of J on κ is presented, corresponding to the above-mentioned boundary value of the fluctuating force ($FL/V_0 \approx 0.618$) but considering the contribution of the energy of zero-point oscillations (the upper curve in Fig. 6).

Let us compare the upper and lower curves in Fig. 6. First of all, we note that taking into account zero-point oscillations

during tunneling significantly increases the values of the tunneling current. This result is well known and is explained by the fact that the energy barrier measured from the levels of zero-point oscillations is smaller than the one measured from the bottom of the potential well. Although such a change is small compared to the barrier height, the exponential dependence of the tunneling current on the barrier value can make the contribution of this change to the tunneling current value quite large [42]. An additional increase in the current values is due to the fact that the ratchet effect, as a consequence of compensation of differently directed particle fluxes in two states of the dichotomous process, is very sensitive even to small changes in the system parameters [20].

The most impressive difference between the curves under discussion is that they correspond to dependences of the opposite sign, so taking into account zero-point oscillations not only significantly increases the ratchet effect but can also reverse the direction of tunneling. In this case, the contribution to the flux due to the dependence of the energy spectrum on the asymmetry of the potential profile dominates the contribution due to the simple distortion of the barrier shape by the applied field. Indeed, the nonmonotonic function $J_0(\kappa)$ with a minimum at $\kappa \approx 0.7$ has no singularities, whereas the dependence $J(\kappa)$ is characterized by an infinite derivative at $\kappa \rightarrow 1$, which is a consequence of the particle not penetrating through the vertical potential barrier.

5. Conclusion

In these methodical notes, the problem of the energy spectrum of a quantum particle in an infinite triangular (V-shaped) potential well with an arbitrary asymmetry coefficient κ varying from zero (for the symmetric well) to unity (for the extremely asymmetric well) is exactly solved. The relationship between the obtained dependence of the energy spectrum on the asymmetry coefficient and the depth of penetration of a quantum particle into classically forbidden regions is shown. The evaluation of the energy spectrum from the Bohr–Sommerfeld quantization rule using the classical approach for determining the oscillation frequency does not take into account the penetration of particles into subbarrier regions. Therefore, the dependence on the well asymmetry parameter is absent for any geometry, except the special case of the vertical wall, $\kappa = 1$, for which the semiclassical approach is characterized by a special boundary condition.

The results obtained for the energy spectrum of a particle in an infinite triangular well within the semiclassical approximation are also valid for a well of finite depth if we are interested in the spectrum only near well's bottom. This circumstance, as well as the use of the Gamow formula, allows us to calculate the tunneling current of ratchet systems of the 'rocking' type, operating in a sawtooth potential (containing both triangular potential wells and triangular barriers) under the action of a fluctuating homogeneous force. The dependence of the ratchet tunneling current on the potential asymmetry coefficient is due to two mechanisms: the distortion of the shape of the original asymmetric triangular barrier by symmetric fluctuations of the force and the dependence of the energy spectrum of a particle in triangular wells of the sawtooth potential profile on this coefficient, with the second mechanism dominating the first. It is shown that, with a certain selection of parameters of the Brownian ratchet, considering the second mechanism can not only significantly increase the ratchet effect, but also reverse the direction of motion of tunneling particles.

Especially noted should be the role of the regions of subbarrier penetration of a particle in the formation of the dependence of its energy spectrum on the asymmetry of the V-shaped potential well. Considering such a dependence is extremely important in studying the characteristics of quantum Brownian motors, the properties of which are determined by the asymmetry of the potential profile.

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