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Force-dependent motion reversal in quantum rocking ratchets

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Abstract
It is well known that at low temperatures, the direction of motion for a quantum rocking ratchet in an asymmetric periodic potential (with a period L and an energy barrier V_0), driven by an external fluctuating force F ($\langle F \rangle = 0$), can be opposite to the direction for the analogous classical ratchet operating at high temperature (Reimann et al, Phys. Rev. Lett. **1997**, 79, 10). In the present work, within the semiclassical approximation and taking into account zero-point fluctuations of a quantum particle in the minima of a sawtooth potential of an arbitrary asymmetry at the temperature of absolute zero, we obtain analytical expressions for the tunneling current in the rocking ratchet. These expressions allowed us to obtain the dependencies of the ratio FL/V_0, at which the motion direction is reversed, on the asymmetry parameter and other parameters of the system. Similar results are obtained for a particle in a two-sinusoidal potential.

KEYWORDS
Brownian motors, motion reversal, quantum ratchet systems, sawtooth potential, symmetry

1 | INTRODUCTION

At present, much attention is paid to nanosystems, in which unbiased nonequilibrium disturbances of various natures can lead to a directional motion of nanoparticles when the spatial and/or temporal symmetry of the system is broken. Such nanosystems are normally called Brownian motors or ratchets.[1–6] The main parameter influencing the direction of a Brownian-motor motion is the asymmetry of potential energy landscape characterizing the nanoparticles.[5,7–10] In addition to the asymmetry and other features of the potential landscape, various dynamic effects can significantly influence the direction of motion.[11] More possibilities for controlling nanotransport arise for nanoparticles of sufficiently large or small mass, when

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inertial or quantum effects, respectively, should also be considered.[3,5]

Accounting for quantum effects in the functioning mechanisms of microscopic ratchets often leads to fundamentally new physics that does not appear in a classical description.[3] In a quantum mechanical description, the critical factor is the temperature under which particles surmount potential barriers. As is well known (see, for example,[12,13] and the references therein), at a certain temperature, there occurs a transition from the low-temperature tunneling regime to the classical regime, in which the particles move above the barrier. In other words, there exists a temperature criterion, depending on the barrier parameters and on the particle mass, at which the mechanism of the particle transport alters. In particular, this result applies to the quantum rocking ratchet described in the pioneering work[14]: At sufficiently high temperatures, the ratchet effect led to a one-directional particle motion (analogous to the motion of a classical ratchet), while at low temperatures, when the tunneling mechanism prevails over the classical one, the particles moved in the opposite direction. That theoretical result was confirmed experimentally in[15] (see also Ref. [16] for more details).

Note that a rigorous description of quantum ratchets should be based on the known principles of driven quantum tunneling.[17] It uses various approaches that take into account, to some extent, quantum fluctuations and friction.[18] For example, strong friction at relatively low temperatures for an adiabatic rocking ratchet driven by a dichotomous process (nonthermal two-state noise) was taken into account in[19,20] using the modified quantum Smoluchowski equation. The reverse conditions were also considered to analyze the quantum ratchet with low friction[21] or at high temperatures.[22] The developed quantum theory provides the key to understanding the properties of real quantum ratchets.[23–25]

In the present work, using the semiclassical approximation and taking into account zero-point fluctuations of a quantum particle we developed analytical expressions for the tunneling current of a rocking ratchet in a sawtooth periodic potential of an arbitrary asymmetry at the temperature of absolute zero. This made it possible to determine the limited range of model parameters responsible for reversing the motion direction. To involve in our description the zero-point fluctuations of the quantum particle in the minima of a sawtooth potential, which mathematically are cusp points, it was necessary to solve an auxiliary problem, represented in the Appendix 1. As a result, in Section 2, we show that the motion of the quantum rocking ratchet at low temperatures and the motion of the corresponding classical ratchet at high temperatures can be oppositely directed only in a certain region of the parameter space determined by the value of the barrier height V_0, the particle mass, the magnitude of the external fluctuating force F, the period L, and the asymmetry l/L of the sawtooth potential profile with the widths of its linear sections l and $L-l$. In Section 3, we discuss the dependence of the direction of the ratchet motion on the asymmetry of the potential and emphasize that the significant contribution to the appearance of this dependence is given by the energy of zero-point vibrations, which was not taken into account before. The value FL/V_0 at which the motion direction reverses decreases when zero vibrations are taken into account if the sawtooth profile does not belong to extremely asymmetric ones ($l/L \neq 0,1$). A similar result is obtained for the motion of the rocking ratchet when choosing the two-sinusoidal form of the potential, the same as was considered in Ref. [14].

2 | FORCE-DEPENDENT MOTION OF ROCKING RATCHETS

A rocking ratchet is a system in which the directed motion of a particle in an asymmetric periodic potential profile $V(x)$ with a period length L [i.e., $V(x+L)=V(x)$] is forced by the action of a zero-mean time-dependent external force $F(t)$, $\langle F(t)\rangle=0$. As a rule, a dichotomous time dependence $F(t)$ is considered, in which the force takes on two values, F_+ and F_-, during alternating time intervals, τ_+ and τ_-, (a deterministic process) or these two values (two states) are switched in a random way with known frequencies γ_+ and γ_- (a stochastic process with average state durations $\langle\tau_\pm\rangle=\gamma_\pm^{-1}$). In this (dichotomous) case, the equality $\langle F(t)\rangle=0$ is ensured by the relations $F_+\tau_+ + F_-\tau_- = 0$ and $F_+/\gamma_+ + F_-/\gamma_- = 0$ in the first and the second cases, respectively. In a particular case $\tau_+=\tau_-$, we set $F_\pm=\pm F$ ($F>0$), and the total potential energy of a nanoparticle at a position x is given by

$$U_\pm(x)=V(x)\mp F\times(x-l), \tag{1}$$

where the parameter $l\subset(0,L)$ specifies the location of the potential maximum in the main domain $(0,L)$. It should be noted that the contribution $\pm Fl$ to the potential energy (1) does not affect the dynamics of the particle motion and is introduced here only for the convenience of geometrical representation of the origin of the applied-force fluctuations. We choose $V(x)$ as a sawtooth potential with a potential barrier V_0 and the widths of the linear sections l and $L-l$; it is defined in the main domain by the following function:

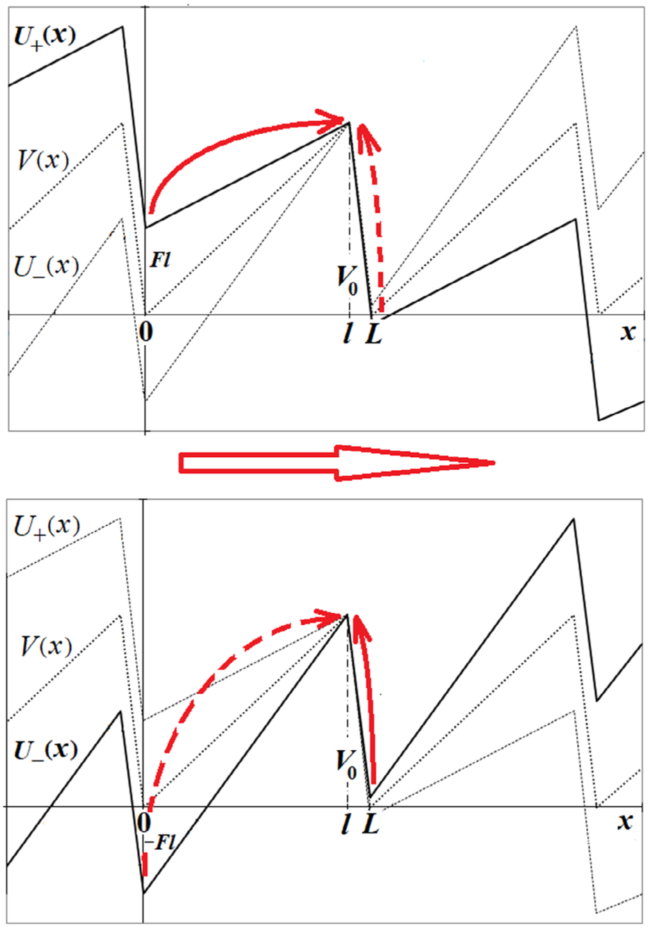

FIGURE 1 The mechanism of the appearance of a directed motion in a rocking-ratchet system at high temperatures, caused by over-barrier thermally activated transitions, according to the Arrhenius law (4). The solid and dashed arrows (red online) depict major and minor transitions in the alternating states with potential profiles (1). Since the direct major transition in the "+" state is more probable than the reverse major transition in the "–" state (due to the different heights of the potential barriers), Brownian particles will move to the right at high temperatures

$$V(x) = V_0 \times \begin{cases} x/l, & 0 < x < l, \\ (L-x)/(L-l), & l < x < L. \end{cases} \tag{2}$$

Note that at $l = 0$ or $l = L$, the sawtooth potential becomes extremely asymmetric, and a Brownian ratchet with such potential has a number of unique properties due to the presence of the jump in the potential shape.[26–28] In the case of the quantum ratchet, such a potential in the presence of a weak oscillating field and within a semiclassical approximation was considered, for example, in Ref. [29].

The applied force F tilts the potential profiles $U_\pm(x)$ (tilted periodic potential, washboard potential), invoking a stationary particle current $J_\pm$ for each of these profiles. In the adiabatic approximation, with the lifetimes $\tau_\pm$ of both states significantly exceeding characteristic relaxation times of the system (the times during which initial conditions become forgotten and the currents become stationary), the average current J for the symmetric dichotomic process ($\tau_+ = \tau_-$) is determined by the arithmetic mean of the currents $J_\pm$:

$$J = (J_+ + J_-)/2. \tag{3}$$

The classical description in the high-barrier approximation (corresponding to the energy barriers large in comparison with the thermal energy $k_B T$ of the system) allows one to calculate the particle current in the state with the potential profile $U_\pm(x)$ using the Arrhenius law,

$$\begin{aligned} J_\pm^{(\mathrm{cl})} &= C\left[e^{-\beta(V_0 - U_\pm(0))} - e^{-\beta(V_0 - U_\pm(L))}\right] \\ &= Ce^{-\beta V_0}\left[e^{\pm\beta Fl} - e^{\pm\beta F(L-l)}\right]. \end{aligned} \tag{4}$$

Here, the first and second terms correspond to the currents of particles that surmount the barrier from left to right and from right to left, respectively (see Figure 1), $\beta = (k_B T)^{-1}$, and the pre-exponential factor C describes the frequency with which the particles hit the barrier. By averaging expression (4) using formula (3), we find the total current

$$J^{(\mathrm{cl})} = 2Ce^{-\beta V_0} \sinh(\beta FL/2) \sinh[\beta F(2l - L)/2]. \tag{5}$$

From this, it follows that the current is positive when $l > L/2$ (Figure 1), that is the particles will move from the potential barrier to the nearest potential well. Note that analytical expressions for the velocity of the adiabatic rocking ratchet with a sawtooth potential profile, not limited to the case of high potential barriers, have been obtained in Ref. [30,31]. Formula (5) is a particular case of these expressions. Since in this article our aim is only to clarify the mechanisms responsible for the occurrence of currents in classical and quantum ratchets to a certain, one or another, direction, the high-potential-barrier approximation should suffice.

A rigorous quantum treatment of the particle motion in a periodic potential under the action of the homogeneous static force F should take into account the presence of Bloch bands at sufficiently small F[32] and the appearance of Wannier ladders with gaps FL at large F.[33,34] For sufficiently large barriers V_0 of the potential profile, one may use the semiclassical approximation (the quantitative condition for the validity of this approximation is given below by inequality (7)), in which the main mechanism of the motion is tunneling from the lower levels of the zero-point vibrations. If, however, the inequality $FL < V_0$ holds true, then the presence of the Wannier ladders does not prevent the use of that semiclassical approximation. Within the adiabatic approximation, described above, with $\tau_+ = \tau_-$ the semiclassical approximation will be used for two values of the applied forces, F and $-F$.

At zero temperature, there are no thermally activated contributions to the current, and the only motion mechanism corresponds to quantum tunneling. From the semiclassical approximation, the tunneling current is proportional to the rate constant of overcoming the potential barrier, which is determined by the following expression:

$$J_\pm^{(\mathrm{qm})} = Ae^{-S_\pm/\hbar},\ S_\pm = 2\left|\int_{x_{0,\pm}}^{x_{1,\pm}} dx\sqrt{2m[U_\pm(x) - U(x_{0,\pm})]}\right|, \tag{6}$$

where A is the pre-exponential factor, $\hbar$ is the Planck constant, and $S_\pm$ is the action in the Gamow formula[35–37] (a rigorous proof of this formula and the corrections to it are given in Ref. [38]), in which m is the particle mass, and we integrate over the sub-barrier range of the potential profile $U_\pm(x)$ with the entry and exit points $x_{0,\pm}$ and $x_{1,\pm}$, respectively (the modulus sign is necessary when $x_{0,\pm} > x_{1,\pm}$). The coordinates of the entry and exit points satisfy the equations $U_\pm(x_{0,\pm}) = U_\pm(x_{1,\pm}) = E_\pm$, where $E_\pm$ are particle energies in the potentials $U_\pm(x)$; in the limit of low temperatures, they correspond to the energy levels of zero-point vibrations. The validity of the semiclassical approximation is ensured by the smallness of the following dimensionless parameter

$$\varepsilon \equiv \frac{\hbar^2}{2mV_0L^2} << 1 \tag{7}$$

(the smallness of the ratio of the de Broglie wavelength of the particle to the characteristic size of the system, determined by the quantity $\sqrt{\varepsilon}$). Within this approximation, the tunneling currents are exponentially small, and the energy levels $E_\pm$ are close to the minima of the potential wells.

For a sawtooth potential, the sub-barrier region has a triangular shape, so the integral in expression (6) containing the piecewise linear function can be expressed in elementary terms:

$$I \equiv \int_{x_0}^{x_1} dx\sqrt{y(x)} = \frac{2}{3}\sqrt{h}|x_1 - x_0|, \tag{8}$$

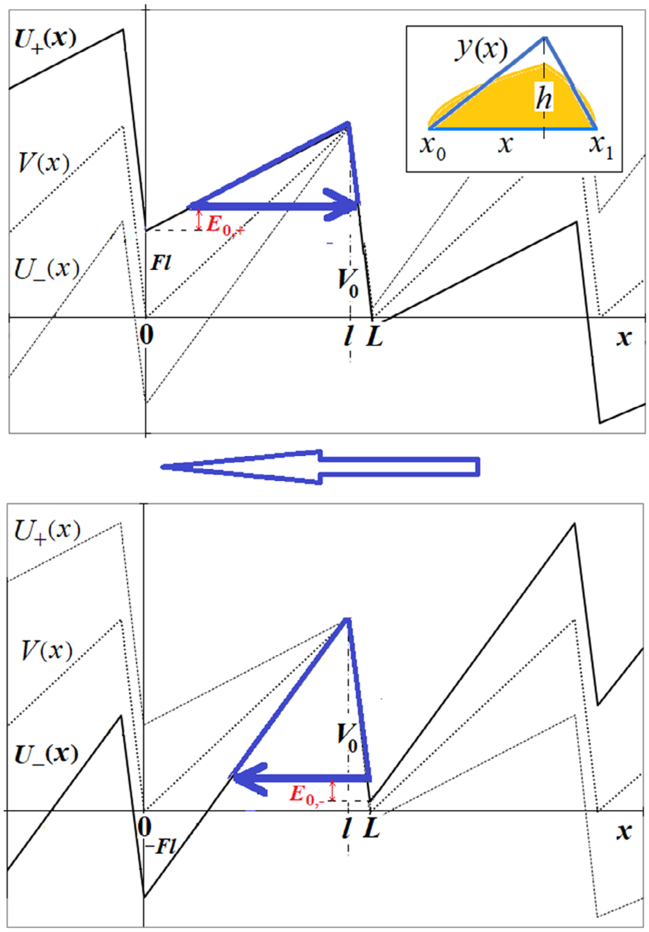

FIGURE 2 The mechanism of the appearance of a directed motion in a rocking ratchet at low temperatures, caused by tunneling. Arrows (blue online) represent tunneling trajectories in the alternating states with potential profiles (1). The inset shows a triangular-shaped sub-barrier region and the corresponding integral value (shaded) described by formula (8) for a sawtooth potential. For relatively weak forces F, the characteristic height of the barrier region under which tunneling occurs (blue online profile) is approximately the same in both states; hence, the smaller the tunneling path, the greater the probability of tunneling transitions. Due to this, at low temperatures, a Brownian particle will move to the left, that is, in the direction opposite to the direction of its motion at high temperatures

where $y(x)$ is the piecewise linear function that corresponds to the top of the triangle, h is the triangle height, and $|x_1 - x_0|$ is the length of its base (see the inset in Figure 2). For the potential $U_+(x)$, the sub-barrier region is determined as follows. Tunneling can occur from any potential well only to the right. Assuming that tunneling occurs from the minimum of the potential well (that is $E_+ = U_{\min,+} = Fl$), then $h_+ = V_0 - Fl$ and $x_{1,+} = V_0L/[V_0 + F(L - l)]$. Similarly, for the potential

$U_-(x)$, tunneling can only occur to the left, from the point $x_{0,-} = L$ (with $E_- = U_{\min,-} = F(L-l)$), so that $h_- = V_0 - F(L-l)$ and $x_{1,-} = FLl/(V_0 + Fl) < x_{0,-}$. If, however, we take into account that the energy level $E_\pm$ of the tunneling particle is separated from the bottom of the considered potential well $U_{\min,\pm}$ by the value of the energy of zero-point vibrations $E_{0,\pm}$, so that $E_\pm = U_{\min,\pm} + E_{0,\pm}$ (see Figure 2), then the height $h_\pm$ and the base $|x_{1,\pm} - x_{0,\pm}|$ of the triangle will change by a factor of $(1 - E_{0,\pm}/h_\pm)$. Therefore, the modified value of the integral (8) (accounting for the zero-point energy) will be related to the original relation by the equality $I' = (1 - E_{0,\pm}/h_\pm)^{3/2} I$.

It is convenient to define the dimensionless parameters, characterizing the applied force F, the asymmetry of the potential profiles, and the zero-point energy:

$$\alpha \equiv \frac{FL}{V_0},\ \xi \equiv \frac{l}{L},\ z_\pm \equiv \frac{E_{0,\pm}}{h_\pm}. \tag{9}$$

With them, the expressions for the actions $S_\pm$ defined by formula (6) take on the following form:

$$S_+/\hbar = \frac{4}{3}\varepsilon^{-1/2}\varphi_\alpha(\xi)\left[1 - z_+(\alpha,\ \xi)\right]^{3/2},\ S_-/\hbar = \frac{4}{3}\varepsilon^{-1/2}\varphi_\alpha(1-\xi)\left[1 - z_-(\alpha,\ \xi)\right]^{3/2}, \tag{10}$$

where

$$\varphi_\alpha(\xi) \equiv \frac{\sqrt{1 - \alpha\xi}}{1 + \alpha(1-\xi)}. \tag{11}$$

Deriving the expressions for the parameters that take into account the zero-point energy requires special treatment since the minimum of the sawtooth potential is at its cusp point. These expressions are derived in Appendix 1 and have the following approximate form:

$$z_+(\alpha,\ \xi) = -\varepsilon^{1/3}\frac{y(\gamma_+)}{\left[\xi^2(1-\alpha\xi)\right]^{1/3}},\ z_-(\alpha,\ \xi) = -\varepsilon^{1/3}\frac{y(\gamma_-)}{1-\alpha(1-\xi)}\left(\frac{1-\alpha\xi}{\xi}\right)^{2/3}, \tag{12}$$

where

$$\gamma_\pm = \gamma_\pm(\alpha,\ \xi) = \left\{\frac{(1 \mp \alpha\xi)(1-\xi)}{\left[1 \pm \alpha(1-\xi)\right]\xi}\right\}^{2/3}. \tag{13}$$

Here, the functions $y(\gamma)$ are the smallest in magnitude negative roots of equation (A1.10), which comprises the Airy functions, changing from -2.338 to -1.019 when γ runs from 0 to 1. Note that the parameters $z_\pm$ are small, they are proportional to the small value $\varepsilon^{1/3}$.

To determine the sign of the average quantum mechanical current (3), we represent it in the following form:

$$J^{(\mathrm{qm})} = Ae^{-S_+/\hbar}\left\{1 - \exp\left[-\frac{4}{3}\varepsilon^{-1/2} f_\alpha(\xi)\right]\right\},$$
$$f_\alpha(\xi) \equiv \varphi_\alpha(1-\xi)\left[1 - z_-(\alpha,\ \xi)\right]^{3/2} - \varphi_\alpha(\xi)\left[1 - z_+(\alpha,\ \xi)\right]^{3/2}, \tag{14}$$

from which we find that the sign of $J^{(\mathrm{qm})}$ will be the same as the sign of the function $f_\alpha(\xi)$. From its definition (14) and from the identity $z_\mp(\alpha, 1-\xi) = z_\pm(\alpha, \xi)$, which is a consequence of the Eq. (A1.11), the equality $f_\alpha(1-\xi) = -f_\alpha(\xi)$ follows; hence it suffices to study the behavior of $f_\alpha(\xi)$, say, on the interval $1/2 < \xi < 1$ on which the classical current (5) is positive. The absence of the current at $\xi = 1/2$ ($f_\alpha(1/2) = 0$) is consistent with the fact that the ratchet effect is absent for a symmetric potential.

The graph of the function $f_\alpha(\xi)$ for several values of α is presented in Figure 3. The dashed and solid curves show the dependences obtained without and with considering zero fluctuations. For small α values, the function $f_\alpha(\xi)$ will be negative, while for large α values, it is positive. At $\xi \to 1$, we have the following approximate equalities: $\gamma_\pm \approx \left[(1 \mp \alpha)(1-\xi)\right]^{2/3}$, $z_+(\alpha, \xi) \approx -\varepsilon^{1/3}(1-\alpha)^{-1/3} y(\gamma_+)$, and $z_-(\alpha, \xi) \approx -\varepsilon^{1/3}(1-\alpha)^{2/3} y(\gamma_-)$, so that with (A1.12),

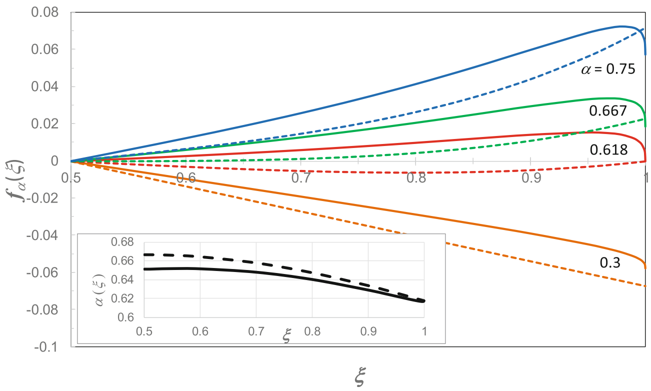

FIGURE 3 Family of functions $f_\alpha(\xi)$ (Equation (14)) that describe the tunneling current of the quantum rocking ratchet in a sawtooth potential. The parameters $\xi = l/L$ and $\alpha = FL/V_0$ are the asymmetry of the sawtooth potential and the magnitude of the applied fluctuating force, respectively. The inset shows the dependences $\alpha(\xi)$ and $\alpha_0(\xi)$ (Equation (17) with $\varepsilon = 0.001$ and $\varepsilon = 0$, respectively), which correspond to the stopping points of the ratchet. The dashed and solid curves show the dependences without ($\varepsilon = 0$) and with ($\varepsilon = 0.001$) taking into account the zero-point energy

we come to the conclusion that, at $\xi \to 1$, the derivatives $\partial z_{\pm}(\alpha, \xi)/\partial \xi$ diverge according to the law $(1-\xi)^{-2/3}$. Due to this, the solid curves in Figure 3 have an infinite derivative at $\xi = 1$.

Let us find the roots of equation $f_\alpha(\xi) = 0$. Substituting (11) into expression (14) for $f_\alpha(\xi)$, we obtain an equation of the form

$$\left(1-\xi+\xi^2\right)\alpha^2 + \alpha - 1 = \varepsilon^{1/3}\Lambda(\alpha, \xi). \tag{15}$$

Because of the smallness of the parameter ε, an approximate solution to this equation can be sought by assuming that the value of the variable α belonging to $\Lambda(\alpha, \xi)$ is equal to the value of the positive root $\alpha_0 = \alpha_0(\xi)$ of Equation (15) with $\varepsilon = 0$. Therefore, it suffices for us to give here only an explicit expression for the quantity $\Lambda(\alpha_0, \xi)$:

$$\Lambda(\alpha_0, \xi) = 3\frac{\{(1-\alpha_0\xi)[1+\alpha_0(1-\xi)]\}^{2/3}(1+\alpha_0\xi)^2}{\alpha_0(1-2\xi)}\Delta(\alpha_0, \xi),$$
$$\Delta(\alpha_0, \xi) = \frac{y(\gamma_+)}{[1+\alpha_0(1-\xi)]^{2/3}} - \frac{y(\gamma_-)}{[1-\alpha_0(1-\xi)]^{2/3}}. \tag{16}$$

The solution of equation (15) with $\alpha > 0$ has the form

$$\alpha = \frac{\sqrt{5-4\xi(1-\xi)-4\varepsilon^{1/3}\Lambda(\alpha_0, \xi)\left(1-\xi+\xi^2\right)}-1}{2\left(1-\xi+\xi^2\right)}, \tag{17}$$

where the value α_0 is defined by the same equation (17) with $\varepsilon = 0$. On the inset in Figure 3, the dependences $\alpha(\xi)$ and $\alpha_0(\xi)$ are depicted by the solid and dashed curve, respectively. Using the approximate equalities $\gamma_{\pm} \approx [(1 \mp \alpha)(1-\xi)]^{2/3}$ and (A1.12), it is easy to show that at $\xi \to 1$, we have $\Lambda(\alpha_0, \xi) \approx -0.615(1-\xi)^{1/3}$. Therefore, first, $\Lambda(\alpha_0, 1) = 0$ and $\alpha(1) = \alpha_0(1) = \left(\sqrt{5}-1\right)/2 \approx 0.618$, and second, near the value $\xi = 1$ and at $\varepsilon \neq 0$, the first derivative of the function $\alpha(\xi)$ is infinite (we observe it in the inset to Figure 3). Thus, zero vibrations do not make any contribution to the location of the stopping point of the quantum rocking ratchet in the extremely asymmetric sawtooth potential with $\xi = 1$. Note that the boundary value $F \approx 0.618\,V_0/L$ was given in the review [1] within the semiclassical consideration of the rocking ratchet in the extremely asymmetric potential but without taking into account the zero vibrations. Note also that the expression for $\Lambda(\alpha_0, \xi)$ in (16) takes a finite value at the point $\xi = 1/2$ due to the identities $\gamma_{\pm}(\alpha, 1/2) = \gamma_{\mp}^{-1}(\alpha, 1/2)$ and $y(\gamma_{\pm}) = \gamma_{\mp} y(\gamma_{\mp})$ (the latter follows from the first identity in (A1.11)) and due to the fact that the factor $\Delta(\alpha_0, \xi)$ vanishes at the same point.

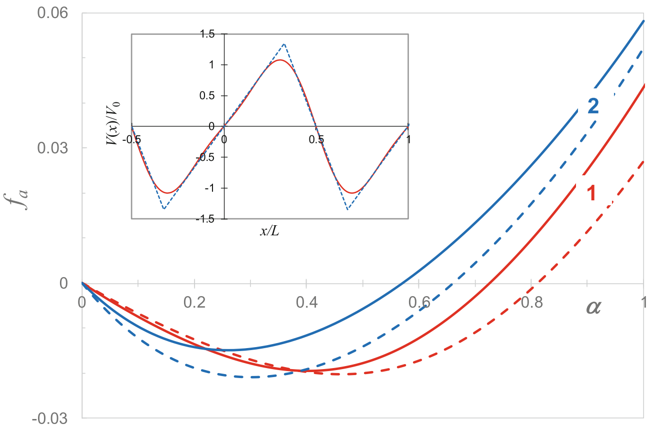

FIGURE 4 Dependence of the function f_α that describes the tunneling current for the potential profiles (18) (curves 1, red online) and (2) (curves 2, blue on-line) on the parameter α. The two-sinusoid potential (18) and the sawtooth potential (2) which is the least-square fit of the potential (11) with parameters $V_0 \approx 2.50\widetilde{V}_0$ and $\xi \approx 0.655$ are shown by the corresponding curves in the inset. The dashed and solid curves show the dependences without ($\varepsilon = 0$) and with ($\varepsilon = 0.001$) taking into account the zero-point energy

It should be noted that the dependence of the motion direction of a quantum rocking ratchet on the magnitude of the applied force is typical not only for the sawtooth potential. In [14], the periodic potential profile was chosen as the following sum of two sinusoids:

$$V(x) = \widetilde{V}_0[\sin(2\pi x/L) - 0.22\sin(4\pi x/L)], \tag{18}$$

and only the force value F corresponded to the modified parameter $\widetilde{\alpha} \approx FL/\widetilde{V}_0 = 0.4\pi$. It is easy to show that the function (18) is best approximated by the sawtooth potential with $V_0 \approx 2.50\widetilde{V}_0$ and $\xi \approx 0.655$ (see the inset in Figure 4). Since $\alpha \equiv FL/V_0 \approx 0.4\widetilde{\alpha}$, then the value $\widetilde{\alpha} \approx 0.4\pi$ from [14] corresponds to $\alpha \approx 0.503 < \alpha_1$, so that $f_\alpha(\xi) < 0$, and indeed the quantum current will be in the direction opposite to the classical current. The direction of the average quantum current (14) for the potential profile (18) can also be analyzed in terms of the function $f_\alpha(\xi)$. Since the second equality of Equation (14) is applicable to a sawtooth case only, we estimated $f_\alpha(\xi)$ implicitly, by solving the first equation of Equation (14) for $f_\alpha(\xi)$ at known $J^{(\mathrm{qm})}$, which in turn was obtained by computing numerically the integrals in (6). Accounting for zero-point vibrations for the potential of two sinusoids is carried out in a standard way (the energy of the zero-point vibrations is equal to $\hbar\omega/2$, where $\omega = \sqrt{U''_{\min}/m}$ is the frequency of classical vibrations of a particle of mass m near the minimum of the potential well with a curvature

$U''_{\min}$). A comparison of the numerical result with the analytical one obtained for the corresponding sawtooth approximation of the potential (curves 1 and 2 in Figure 4) shows that both dependences behave in a similar fashion. The boundary values α, at which the functions $f_{\alpha}(\xi)$ change their signs, are shifted for the two-sinusoid potential by about 0.15 upward relative to the sawtooth potential.

3 | DISCUSSION AND CONCLUSIONS

The cause for the reversal in the motion direction of a rocking ratchet at lower temperatures, corresponding to the transition from the classical to quantum regime, lies in different mechanisms—thermal activation and tunneling, respectively—for overcoming the potential barrier. In the first case, only the height of the barrier to be surmounted is important; in the second case, the length of the tunneling path in the sub-barrier region also comes into play. The choice of a sawtooth potential to develop a model capable of reproducing these dynamic effects turned out to be reasonable. The model gave analytical dependences of currents on the applied fluctuating force, as well as allowed us to visualize and explain the conditions under which the tunneling can dominate over the thermal-activation mechanism (that is, when the decrease in the tunneling path dominates over the barrier height decrease). The competition between these two factors arises from the interplay of the asymmetry magnitudes in the periodic potential profile and the applied force F that perturbs it (see Figures 1 and 2). From the analysis of the obtained expressions, it follows that for small values of F, the quantum rocking ratchet moves in the direction opposite to the classical one. That was in full agreement with the results of [14]. The new result is that such a behavior of the quantum ratchet will differ from the known behavior in the region of large F: The quantum ratchet will move in the same direction as the classical one. This result can be understood from the fact that at large F, one of the potential barriers becomes small (see the left barriers on the upper insets of Figures 1 and 2); these changes increase the tunneling current in the direction of the thermally activated current, not only the thermally activated current itself (despite the fact that the tunneling path remains practically unchanged).

We found that for the values of the asymmetry parameter of the sawtooth potential $\xi \equiv l/L$ (l is the width of one of its linear sections and L is its period), which correspond to a positive thermally activated current ($1/2 < \xi \le 1$), there exists such an interval of $\alpha \equiv FL/V_0$ values (V_0 is the energy barrier of the potential) in which the sign of the tunneling current depends on ξ. Without accounting for the zero-point fluctuations, this interval is determined by the boundary values $\alpha \approx 0.618$ and $\alpha \approx 0.667$ at $\xi = 1$ and at $\xi = 1/2$, respectively. Accounting for zero vibrations leads to a decrease in the boundary values of the parameter α for all ξ values except for the case of the extremely asymmetric sawtooth potential with $\xi = 1$ (see the inset in Figure 3). When $\xi \to 1$, the dependence on ξ of both the current and the boundary α value are characterized by infinite derivatives, this fact reflects the jump-like behavior of the potential profile $V(x)$. To analyze the effect of the zero-point vibrations on the properties of the system, in the Appendix 1, we present a solution to the problem of the energy spectrum of a quantum particle in an infinite triangular well of an arbitrary symmetry (reducible, as particular cases, to known solutions in a symmetric triangular well $V(x) \propto |x|$ and a well with its one vertical wall).

Special attention should be paid to the appearance of the dependence of the zero-point energy on the asymmetry of the triangular potential well; this dependence also makes a significant contribution to the boundary values of the parameters corresponding to the stopping points of the quantum ratchet. For a parabolic potential well, the energy of zero vibrations E_0 is related to the cyclic frequency of vibrations ω_0 and the period of vibrations $T_0 = 2\pi/\omega_0$ by the equation $E_0 = \hbar\omega_0/2$, and the classical mechanics formula can be used to calculate the period: $T_0 = \sqrt{m/2}\oint [E - V(x)]^{-1/2} dx$. This approach to estimating the energy of zero-point vibrations gives an accurate result both for a parabolic potential well $V(x) = kx^2/2$, when the formula for the period leads to the known expression $\omega_0 = \sqrt{k/m}$, and for a rectangular infinite well of the width L. In this case $\omega_0 = \pi\sqrt{2E_0/mL^2}$, this result being substituted to the formula $E_0 = \hbar\omega_0/2$ gives an equation for E_0, the solution of which, $E_0 = \pi^2\hbar^2/(2mL^2)$, is also an exact result.

For the asymmetric infinite triangular well, the above approach yields the expression for frequency $\omega_0 = (\pi V/L)(2mE_0)^{-1/2}$, which does not depend on the asymmetry of the well. From this result, the energy of zero-point vibrations turns out to be equal $z = E_0/V = (\pi/2)^{2/3}\varepsilon^{1/3} \approx 1.351\varepsilon^{1/3}$ and also independent of the asymmetry parameter ξ. This z value is significantly less than the exact values obtained in the Appendix 1, which change from 1.618 to 2.338 depending on ξ values. The presence of the dependence E_0 on ξ is explained by the different penetration lengths of the quantum particles under the potential barriers that are formed by the sides of the triangular well. Under the classical description, there is no such penetration at all, and the contributions to the oscillation period from the sections to the left and to the right of the minimum cusp point are compensated. Thus, the accounting for zero-point vibrations and the dependence of their energy on the asymmetry parameter, which was performed in this paper for the first time, are fundamentally important not only from a quantitative point of view but also for the correct description of quantum effects in the sub-barrier regions of the ratchet motion.

The tunneling current has also been estimated using numerical integration for a two-sinusoid potential, with parameters allowing us for modeling it with high accuracy by a sawtooth potential. The results obtained with the potential of two sinusoids also confirmed the conclusion that the motion reversal of the quantum rocking ratchet with respect to the classical one (motion reversal with decreasing temperature) occurs only in the region of small values of α ($\alpha < 0.81$ without the zero-point fluctuations and at less boundary values of α with accounting for them). This allows us to assert that the regularities established here do not depend on the specific choice of the asymmetric periodic profile perturbed by an external fluctuating force and are of a general nature. This conclusion is confirmed by the experimentally observed dependence of the tunneling current J on the applied force F (see figure 2 (B) in [15]): At sufficiently low temperatures, the non-monotonic function $J(F)$ changes its sign at a certain value of F, while at higher temperatures, this function becomes monotonic and sign-constant.

In conclusion, we note that the simple model used in the present work made it possible not only to draw conclusions about the existence of a limited range of system parameters that permit motion reversal but also to quantify the boundaries of this range, which depend on the type of potential profile and asymmetry of the system.

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APPENDIX 1

ZERO-POINT ENERGY FOR AN INFINITE TRIANGULAR WELL OF ARBITRARY ASYMMETRY

Consider an infinite triangular potential well defined by the following expression:

$$V(x)=\begin{cases}F_r x, & x>0,\\ F_l x, & x<0,\end{cases} \tag{A1.1}$$

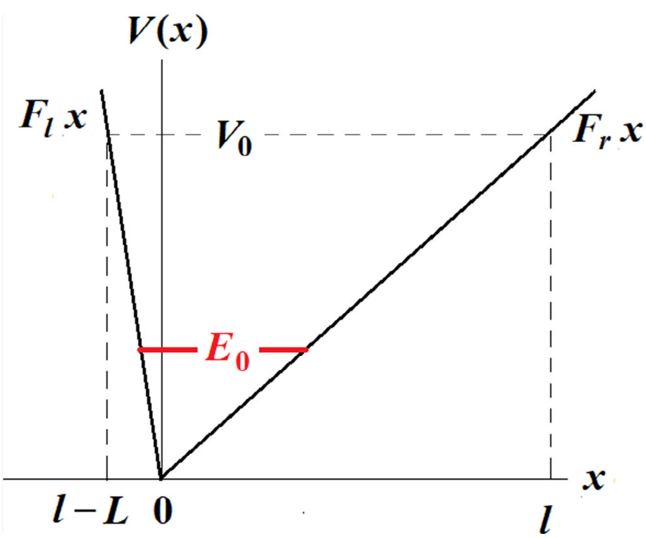

FIGURE 5 An infinite triangular potential well of arbitrary asymmetry, characterized by the ratio $\xi=l/L$ (for $\xi=1/2$, the well is symmetric, and for $\xi=1$, the left wall of the well is vertical)

where the forces F_r и F_l can be set by the energy parameter V_0 and the widths l and $L-l$ of the rightward and leftward links of the triangle, respectively (Figure 5),

$$F_r=\frac{V_0}{l}>0, \quad F_l=\frac{V_0}{l-L}<0, \tag{A1.2}$$

so that the asymmetry of the potential well can be characterized by the parameter $\xi=l/L$ ($\xi=1/2$ corresponds to the symmetric well; $\xi=0$ and $\xi=1$ means the extremely asymmetric well, one of its walls is vertical). The Schrödinger equation for a particle of mass m and energy E in the potential (A1.1) for the leftward and rightward half-space (negative and positive x values) takes on the form,

$$\frac{d^2\psi_j(x)}{dx^2}+\frac{2m}{\hbar^2}(E-F_j x)\psi_j(x)=0, \quad j=l,r. \tag{A1.3}$$

For each half-space, the general solutions of differential equations (A1.3) contain two arbitrary constants, which (together with the energy parameter E) can be determined from the normalization condition and four boundary conditions:

$$\int_{-\infty}^{0} dx|\psi_l(x)|^2+\int_{0}^{\infty} dx|\psi_r(x)|^2=0,\ \psi_l(-\infty)=0,\ \psi_r(\infty)=0,$$
$$\psi_l(-0)=\psi_r(+0),\ \psi_l'(-0)=\psi_r'(+0). \tag{A1.4}$$

In terms of the following new variables:

$$y_r=\left(\frac{2mF_r}{\hbar^2}\right)^{1/3}\left(x-\frac{E}{F_r}\right),\ y_l=-\left(\frac{2m|F_l|}{\hbar^2}\right)^{1/3}\left(x+\frac{E}{|F_l|}\right) \tag{A1.5}$$

equations (A1.3) are reduced to the equations

$$\frac{d^2\tilde{\psi}_j(y_j)}{dy_j^2}-y_j\tilde{\psi}_j(y_j)=0,\ j=l,r. \tag{A1.6}$$

for the new wave functions $\tilde{\psi}_j(y_j)=\psi_j(x)$ ($x<0$ at $j=l$ and $x>0$ at $j=r$). The general solutions to (A1.6) are expressed in terms of Airy functions of the first and second kind [39]:

$$\tilde{\psi}_j(y_j)=C_j\mathrm{Ai}(y_j)+D_j\mathrm{Bi}(y_j),\ j=l,r, \tag{A1.7}$$

were C_j and D_j are arbitrary constants. Since $y_j \to \infty$ at $x \to \pm\infty$, and $\mathrm{Bi}(\infty) \to \infty$, then the boundary conditions $\widetilde{\psi}_j(\infty) = 0$ (see (A1.4)) are satisfied when $D_j = 0$ due to the equality $\mathrm{Ai}(\infty) = 0$. The constants C_j are expressed from the normalization condition and the continuity condition at the point $x = 0$, while the quantization of the energy variable E follows from the condition of continuity of the first derivatives of the wave functions at the same point. The last condition, taking into account equations (A1.4), (A1.5), and (A1.7), can be written as follow:

$$-|F_l|^{1/3}\frac{\mathrm{Ai}'(y_l)}{\mathrm{Ai}(y_l)}\Big|_{y_l=-\frac{E}{|F_l|}\left(\frac{2m|F_l|}{\hbar^2}\right)^{1/3}} = F_r^{1/3}\frac{\mathrm{Ai}'(y_r)}{\mathrm{Ai}(y_r)}\Big|_{y_r=-\frac{E}{F_r}\left(\frac{2mF_r}{\hbar^2}\right)^{1/3}}, \tag{A1.8}$$

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

Define the dimensionless variables

$$\gamma \equiv \frac{y_l}{y_r} = \left(\frac{F_r}{|F_l|}\right)^{2/3} = \left(\frac{1-\xi}{\xi}\right)^{2/3}, \; z \equiv \frac{E}{V_0} = -\varepsilon^{1/3}\xi^{-2/3}y_r; \tag{A1.9}$$

the first one is equal to the ratio of variables being substituted as y in equation (A1.8) and is determined by the asymmetry coefficient $\xi = l/L$, and the second one specifies the ratio of energy E to the barrier value V_0. If we denote y_r by y, then equation (A1.8) takes on the form:

$$\frac{\mathrm{Ai}'(\widetilde{y})}{\mathrm{Ai}(\widetilde{y})}\Big|_{\widetilde{y}=\gamma y} + \sqrt{\gamma}\frac{\mathrm{Ai}'(y)}{\mathrm{Ai}(y)} = 0. \tag{A1.10}$$

Since we are interested in precisely the zero-point energy values E_0, then from the set of solutions to equation (A1.10) (which defines the energy spectrum of the system), we must choose the smallest in magnitude negative value of y and consider it as a function of the parameter γ or asymmetry coefficient ξ. By passing in equation (A1.10) from variable y to variable $\widetilde{y}$ and using the identity $\gamma(1-\xi) = \gamma^{-1}(\xi)$, it is easy to verify the validity of the following identities:

$$y(\gamma^{-1}) = \gamma y(\gamma), \quad z(1-\xi) = z(\xi). \tag{A1.11}$$

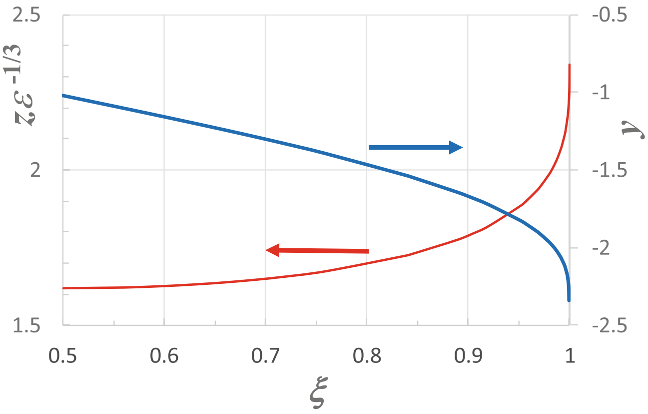

FIGURE 6 The results obtained by numerically solving equation (A1.10) (curve $y(\xi)$, right axis) and the ratio of the zero-point energy to the parameter V_0 (curve $z(\xi)\varepsilon^{-1/3}$, left axis) for different values of the parameter ξ)

The second identity means that the energy spectrum is invariant with respect to the symmetry transformation $x \to -x$. These properties allow us to bound the range of change of the asymmetry parameter ξ by values from 1/2 to 1, and the parameter γ by values from 0 to 1.

The results of the numerical solution of equation (A1.10) for various ξ values are shown in Figure 6. When ξ changes from 1/2 to 1, the function $z(\xi)\varepsilon^{-1/3}$ increases monotonically from 1.618 to 2.338, and the function $y(\gamma^{-1}) = \gamma y(\gamma)$ decreases monotonically from -1.019 to -2.338. These boundary values are the largest roots of the functions $\mathrm{Ai}'(y)$ and $\mathrm{Ai}(y)$ and correspond to the cases of the symmetric triangular well $V(x) \propto |x|$ and the well with a vertical wall which have been considered in [40], respectively. Near the point $\xi = 1$ ($\gamma = 0$), the functions $z(\xi)$ and $y(\gamma)$ have their first derivatives tending to infinity. This follows from the asymptotic solution of equation (A1.10). By expanding the Airy function and its first derivative near the point $y_0 = -2.338$ ($\mathrm{Ai}(y_0) = 0$), $\mathrm{Ai}(y) \approx \mathrm{Ai}'(y_0)(y - y_0)$, and substituting into (A1.10), we obtain an asymptotic solution at $\gamma \to 0$:

$$y(\gamma) \underset{\gamma\to 0}{\approx} y_0 - [\mathrm{Ai}(0)/\mathrm{Ai}'(0)]\sqrt{\gamma} \approx -2.338 + 1.372\sqrt{\gamma}, \tag{A1.12}$$

that is $y'(\gamma) \to \infty$ as $\gamma \to 0$.