Diffusion of a massive particle in a periodic potential: Application to adiabatic ratchets

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We generalize a theory of diffusion of a massive particle by the way in which transport characteristics are described by analytical expressions that formally coincide with those for the overdamped massless case but contain a factor comprising the particle mass which can be calculated in terms of Risken's matrix continued fraction method (MCFM). Using this generalization, we aim to elucidate how large gradients of a periodic potential affect the current in a tilted periodic potential and the average current of adiabatically driven on-off flashing ratchets. For this reason, we perform calculations for a sawtooth potential of the period L with an arbitrary sawtooth length ($l < L$) instead of the smooth potentials typically considered in MCFM-solvable problems. We find nonanalytic behavior of the transport characteristics calculated for the sharp extremely asymmetric sawtooth potential at $l \to 0$ which appears due to the inertial effect. Analysis of the temperature dependences of the quantities under study reveals the dominant role of inertia in the high-temperature region. In particular, we show, by the analytical strong-inertia approach developed for this region, that the temperature-dependent contribution to the mobility at zero force and to the related effective diffusion coefficient are proportional to $T^{-3/2}$ and $T^{-1/2}$, respectively, and have a logarithmic singularity at $l \to 0$.

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I. INTRODUCTION

Diffusion of a massive particle is described by the Klein-Kramers equation [1,2], the analytical solutions of which are restricted to the cases of simple potentials corresponding to a linear coordinate dependence of the force [3]. That is why a number of results of the reaction-rate theory [4–6] as well as the calculated particle velocity in a tilted periodic potential [7] were obtained in the approximation of high potential barriers (compared to the thermal energy) when the vicinities of potential extrema are only important and can be considered for smooth potentials as parabolic. The Klein-Kramers equation for arbitrary potentials is solvable only by various numerical methods [8–15], among which the Risken's matrix continued fraction method (MCFM) [3,16,17] occupies a particular place [3,18–21]. This method allows the particle current to be formally expressed in terms of concentration so that analytical relations can be found in some particular cases [22].

One of the most exciting applications of diffusion transport is a Brownian motor which models the drift of a Brownian particle in a fluctuating periodic potential. It is usually considered in the overdamped regime when the inertial term is negligible compared to the damping one [23–25]. A deep insight into the motion-inducing mechanism was given by Parrondo [26], who considered, as an elementary act of directed motion, a particle move resulting from a fast transition (a jump) from one periodic potential profile to another. He also calculated the net fraction of particles crossing some point in a certain direction over a long period of time (the integrated current) as a pivotal characteristic of adiabatic transport (Parrondo's lemma). Some further development of this overdamped adiabatic approach can be found in Refs. [27,28]. A generalization of Parrondo's lemma to include small inertial corrections has been proposed recently [29,30]. A notable observation made in these studies is that even small inertial corrections may help to overcome some of the symmetry restrictions inherent to the zero-mass limit and thus to produce otherwise prohibited directed motion.

In the present paper we investigate the effect of large gradients in a potential profile on the transport of a massive particle. More specifically, we study Brownian motion in a periodic sawtooth potential for arbitrary inertia with a special emphasis on the limiting cases where jumps in the potential profile make it extremely asymmetric. It is important to note that, at present, a sawtooth potential is not only a theoretical idealization, but can be realized experimentally. We exemplify, following Ref. [31], such a realization by the experimental scheme of a Brownian ratchet that manipulates charged components within supported lipid bilayers. One side of the patterned bilayers was of a sawtooth shape (a planar surface was the opposite side), the asymmetry of which controlled the amount of effect. Particularly, the maximum effect was reached for the extremely asymmetric case of the side of the pattern. The same regularity for inertialess particles in a sawtooth potential was found theoretically in Refs. [32–34].

Dynamics of a Brownian particle differs essentially in a sharp and smooth potential (with and without jumps, respectively), the physics behind this being quite transparent. The

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energy conservation law dictates a strict relationship between the particle velocities on two sides of the potential jump and its height. Thus, a discontinuity in the velocity distribution arises in the vicinity of the jump point. We recall that in the overdamped regime the velocity distribution is Maxwellian and the potential jumps are easily taken into account by the jump conditions for the particle position probability density [3]. This is why sharp potentials are acceptable in solving overdamped diffusion problems but make impossible numerical treatment of underdamped Brownian motion. In view of this fact, the approach developed here appears uniquely helpful to study diffusion of a massive particle in a sharp periodic potential.

Another aim of the paper is to describe inertial adiabatic transport in terms of equations resembling those in the overdamped approach. For the stationary current in a tilted periodic potential and for the integrated current arising from a changing periodic potential [26], we derive analytical expressions that formally coincide with those for the overdamped approach. The expressions contain a factor (accounting for inertia effects) which can be calculated by MCFM. Applying this approach to adiabatic ratchets, we obtain explicit formulas for the average velocity of adiabatically driven on-off flashing and rocking ratchets with inertial effects included. Thus we suggest a unified inertia-relevant description of both ratchet types. A clear mathematical structure of the approach proposed makes the problem analytically treatable provided the inertia factor is analytically expressible. This is demonstrated in Sec. VI by considering the problem at high temperatures when the potential amplitude is small compared to the thermal energy.

The structure of the paper is as follows. In Secs. II and III we define the transport characteristics under study and derive equations containing the above-mentioned inertia-dependent factor. The scheme for calculating this factor, both in general operator notation and in terms of matrix Fourier-transformed equations, is given in Sec. IV. Findings concerning diffusion in a sawtooth potential are presented and discussed in Sec. V with the observation that the quantities concerned lose analyticity in the vicinity of the extremely asymmetric limit of the potential. The latter fact is corroborated in Sec. VI using the high-temperature approximation. In addition, the high-temperature asymptotics for the effective mobility and diffusivity are obtained in this section. The results are summarized in Sec. VII.

II. THE INTEGRATED CURRENT

Consider a Brownian particle moving along x in the spatially periodic potential $V(x)$ with the period L during the large time interval T sufficient for the equilibrium state in this potential to be established. The initial state is assumed equilibrium in some other potential $V_0(x)$. Following Parrondo [26], we are interested in finding the net fraction of particles $\Phi(x)$ crossing point x to the right for time T which determines the main characteristics of adiabatic transport. This quantity is defined as the reduced current $J(x,t)$ integrated over the large time interval T,

$$\Phi(x) = \int_0^T J(x,t)dt. \tag{1}$$

The continuity equation connecting the reduced probability density $\rho(x,t)$ and the corresponding current $J(x,t)$,

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial J(x,t)}{\partial x} = 0, \tag{2}$$

gives the interrelation between values $\Phi(x)$ at points x and x_0,

$$\Phi(x) = \Phi(x_0) - \int_{x_0}^{x} dy[\rho(y) - \rho_0(y)], \tag{3}$$

where $\rho(x) = \rho(x,T)$ and $\rho_0(x) = \rho(x,0)$ are the equilibrium probability densities in the states with potentials $V(x)$ and $V_0(x)$ [$\int_0^L dx\ \rho(x) = 1$ and the same for $\rho_0(x)$]. Thus the difference of $\Phi(x)$ values at two points is simply the difference of the probabilities to find the particle between these points in the initial and final distributions.

Note that Eqs. (1)–(3) are valid for both the overdamped (massless) description and the inertial one. In the first case, the integration constant $\Phi(x_0)$ is easily found since $J(x,t)$ is directly expressible in terms of $\rho(x,t)$, $J(x,t) = (\beta\zeta)^{-1}\exp[-\beta V(x)](\partial/\partial x)\exp[\beta V(x)]\rho(x,t)$, where ζ and $\beta = (k_B T)^{-1}$, respectively, denote the friction coefficient and the inverse thermal energy (k_B is the Boltzmann constant and T is the absolute temperature). This additional equation, together with Eqs. (1) and (3), leads to Parrondo's result [26]. In the second inertial case, the determination of $\Phi(x_0)$ requires the probability density $\rho(x,v,t)$ to find an inertial particle at point x with the velocity v at time t to be known. This probability density obeys the Klein-Kramers equation [1,2],

$$\frac{\partial}{\partial t}\rho(x,v,t) = \left[-\frac{\partial}{\partial x}v + \frac{1}{m}\frac{\partial}{\partial v}\left(\zeta v + V'(x) + \frac{\zeta}{m\beta}\frac{\partial}{\partial v}\right)\right] \times \rho(x,v,t), \tag{4}$$

where m is the particle mass and $V'(x)$ is the first spatial derivative of the potential $V(x)$. Then the reduced functions $\rho(x,t)$ and $J(x,t)$ are the zero and first moments of $\rho(x,v,t)$,

$$\rho(x,t) = \int_{-\infty}^{\infty} dv\ \rho(x,v,t), \quad J(x,t) = \int_{-\infty}^{\infty} dv\ v\rho(x,v,t). \tag{5}$$

These functions, respectively, coincide (up to constant factors) with the two first coefficients $c_n(x,t)$ [$\rho(x,t) = c_0(x,t)$, $J(x,t) = v_{\text{th}}c_1(x,t)$, where $v_{\text{th}} = (m\beta)^{-1/2}$ is the thermal velocity] of the expansion $\rho(x,v,t)$ over orthogonal Hermitian polynomials [3]. Equations for $c_n(x,t)$ follow from Eq. (4) and can be written in the form [30]

$$\left(n + \tau_v\frac{\partial}{\partial t}\right)c_n(x,t) = \varepsilon\sqrt{n}\,\hat{J}(x)c_{n-1}(x,t) - \varepsilon\sqrt{n+1}\,\partial_x c_{n+1}(x,t), \tag{6}$$

where

$$\hat{J}(x) = -e^{-\beta V(x)}\partial_x e^{\beta V(x)} = -\partial_x - \beta L V'(x) \tag{7}$$

is the dimensionless current operator in the overdamped limit, $\partial_x = L\,\partial/\partial x$ is the short notation for the dimensionless differential operator, $\tau_v = m/\zeta$ is the velocity relaxation time, and the dimensionless parameter $\varepsilon = \sqrt{\tau_v/\tau_D}$ characterizes the strength of inertia ($\tau_D = \beta\zeta L^2$ is the diffusion time). Equation (6) can be easily rewritten for the time-independent quantities $\varphi_n(x) = \int_0^T dt\, c_n(x,t)$, that gives Eq. (3) at $n = 0$ [taking into account that $\Phi(x) = v_{\rm th}\varphi_1(x)$] and returns us to Eq. (6) with $c_n(x,t)$ substituted by $\varphi_n(x)$ and without the term containing $\partial/\partial t$ at $n \geqslant 1$.

The MCFM developed in Refs. [3,16,17] (and discussed in Sec. IV of this paper) allows one to write down the following recurrent relation: $\varphi_{n+1}(x) = \hat{S}_n(x)\varphi_n(x)$, where the $\hat{S}_n(x)$ matrix is defined at $n = 0$ as $\hat{S}_0(x) = \varepsilon\hat{G}_0(x)\hat{J}(x)$ with $\hat{G}_0(x)$ as determined by the recursive procedure which can be properly implemented in the Fourier representation scheme [see Eqs. (28) and (35) below]. Thus $\varphi_0(x)$ and $\varphi_1(x)$ are related by the equation

$$e^{\beta V(x)}\hat{G}_0^{-1}(x)\varphi_1(x) = -\varepsilon\, \partial_x e^{\beta V(x)}\varphi_0(x). \tag{8}$$

In view of the periodicity of $V(x)$ and $\varphi_n(x)$, integration of Eq. (8) over the spatial period gives

$$\int_0^L dx\, e^{\beta V(x)}\hat{G}_0^{-1}(x)\Phi(x) = 0. \tag{9}$$

Then, substitution of Eq. (3) into Eq. (9) leads to the equality

$$\Phi(x_0) = \frac{\int_0^L dx\, e^{\beta V(x)}\hat{G}_0^{-1}(x)\int_{x_0}^x dy\, [\rho(y) - \rho_0(y)]}{\int_0^L dx\, e^{\beta V(x)}\hat{G}_0^{-1}(x)}. \tag{10}$$

Let us define the operator $\hat{q}(x)$ generalizing the quantity $q(x) = e^{\beta V(x)}/\int_0^L dx\, e^{\beta V(x)}$ commonly used in the overdamped case,

$$\hat{q}(x) = Z_{\rm in}^{-1}q(x)\hat{G}_0^{-1}(x), \quad Z_{\rm in} = \int_0^L dx\, q(x)\hat{G}_0^{-1}(x). \tag{11}$$

Then Eq. (10) takes the final form

$$\Phi(x_0) = \int_0^L dx\, \hat{q}(x)\int_{x_0}^x dy\, [\rho(y) - \rho_0(y)]. \tag{12}$$

It is worthy to note that this expression is exact for an arbitrary particle mass. In the overdamped limit $\hat{G}_0(x)$ is the unit operator, so $\hat{q}(x)$ coincides with $q(x)$ and Eq. (12) reduces to the known Parrondo result [26] [denoted below as $\Phi_{m=0}(x_0)$] as it should be. It is expedient to introduce an inertial correction,

$$\begin{aligned}\Delta\Phi &= \Phi(x_0) - \Phi_{m=0}(x_0)\\ &= \int_0^L dx[\hat{q}(x) - q(x)]\int_{x_0}^x dy[\rho(y) - \rho_0(y)],\end{aligned} \tag{13}$$

since it is position independent due to the identity $\int_0^L dx[\hat{q}(x) - q(x)] = 0$ (in accordance with the conclusions of Ref. [30]). Therefore the position-dependent contribution to $\Phi(x_0)$ is determined solely by the known inertialess expression $\Phi_{m=0}(x_0)$. For further consideration, we can set $x_0 = 0$ without loss of generality and introduce the average value of $\Phi(x)$,

$$\begin{aligned}\bar{\Phi} &= L^{-1}\int_0^L \Phi(x)dx = \bar{\Phi}_{m=0} + \Delta\Phi,\\ \bar{\Phi}_{m=0} &= \Phi_{m=0}(0) + \Delta\bar{x}/L,\end{aligned} \tag{14}$$

where $\Delta\bar{x} = \bar{x} - \bar{x}_0 = \int_0^L dx\, x[\rho(x) - \rho_0(x)]$ is the distance between the average particle positions in the equilibrium states with potentials $V(x)$ and $V_0(x)$. If $V_0(x) = 0$ and hence $\rho_0(x) = L^{-1}$, the expression for $\Delta\bar{x}/L$ coincides with the net fraction of particles $\Phi(0)$ crossing point $x = 0$ after switching off the potential $V(x)$. That is why the average velocity $\langle v\rangle$ of particle motion arising due to a dichotomic process (with period τ) of switching on and switching off the potential $V(x)$ (so-called on-off ratchet) can be found by the formula $\langle v\rangle = (L/\tau)\,\bar{\Phi}$, where $\bar{\Phi}$, introduced in Eq. (14), takes the form

$$\bar{\Phi} = \int_0^L dx[\hat{q}(x) - L^{-1}]\int_0^x dy[\rho(y) - L^{-1}]. \tag{15}$$

III. STATIONARY CURRENT IN A TILTED PERIODIC POTENTIAL

Consider a massive Brownian particle in the periodic potential $V(x)$ that is driven away from equilibrium by a static force F. At long times, one of the main characteristics of the particle motion in the tilted periodic potential $U(x) = V(x) - Fx$ is the stationary current $J(F)$. The position independence of this quantity follows from the time-independent version of Eq. (2). In order to handle contribution of inertia to $J(F)$ one typically uses MCFM (see, e.g., Refs. [3,18–21]). Using the F-dependent $\hat{S}_0(x;F)$ matrix and the identities $\rho(x,t) = c_0(x,t)$ and $J(x,t) = v_{\rm th}c_1(x,t)$, we have the equality $c_0(x) = \hat{S}_0^{-1}(x;F)c_1$ which, with the normalization condition $\int_0^L c_0(x)dx = 1$ taken into account, immediately gives the result [3],

$$J(F) = v_{\rm th}\left[\int_0^L dx\, \hat{S}_0^{-1}(x;F)\right]^{-1}. \tag{16}$$

The aim of this section is to write the current in the form similar to that known from the studies of the overdamped case, which allows to calculate the mobility μ at zero external force using the same matrix $\hat{G}_0(x)$ as in Sec. II. We start from Eq. (8) in which $\varphi_0(x)$, $\varphi_1(x)$, and $V(x)$ should be replaced by $c_0(x)$, $c_1(x)$, and $U(x)$, respectively, and $\hat{G}_0^{-1}(x) = \hat{G}_0^{-1}(x;F)$ is F dependent. Integration over x of the thus modified Eq. (8) gives

$$c_0(x) = e^{-\beta U(x)}\left[A - (\varepsilon L)^{-1}\int_0^x dy\, e^{\beta U(y)}\hat{G}_0^{-1}(y;F)c_1\right]. \tag{17}$$

The two constants A and c_1 are determined by the normalization condition $\int_0^L c_0(x)dx = 1$ and the periodicity condition $c_0(0) = c_0(L)$. Therefore the resulting expression for $J(F)$ takes the form

$$J(F) = (\beta\zeta)^{-1}\frac{1 - e^{-\beta FL}}{\int_0^L dx\, e^{-\beta U(x)}\int_0^L dx\, e^{\beta U(x)}\hat{G}_0^{-1}(x;F) - (1 - e^{-\beta FL})\int_0^L dx\, e^{-\beta U(x)}\int_0^x dy\, e^{\beta U(y)}\hat{G}_0^{-1}(y;F)}. \tag{18}$$

This expression, just like Eq. (12), is exact for an arbitrary particle mass and turns into the known Stratonovich formula [35] in the overdamped case. The success in obtaining this generalized expression is provided by introducing the formal relation between the particle concentration and the corresponding current which is, together with the continuity Eq. (2), equivalent to the description in terms of the Klein-Kramers Eq. (4) [22].

The expansion coefficients of the average velocity $\langle v(F)\rangle = J(F)L$ over F are easily obtainable from Eq. (18), namely,

$$\langle v(F)\rangle = \mu F + \chi F^2 + \cdots, \tag{19}$$

where

$$\mu = \zeta^{-1}L^2\left[\int_0^L dx\, e^{-\beta V(x)}\int_0^L dx\, e^{\beta V(x)}\right]^{-1} Z_{\rm in}^{-1} \tag{20}$$

is the mobility μ (at zero external force) and

$$\chi = \beta L\mu\left\{\int_0^L dx[\rho(x)-L^{-1}]\int_0^x dy[\hat{q}(y)-L^{-1}] + (\beta L Z_{\rm in})^{-1}\int_0^L dxq\,(x)\left[\partial_F G_0^{-1}(x;F)\right]_{F=0}\right\} \tag{21}$$

is the coefficient (the nonlinear response) which defines the average velocity of rocking ratchets adiabatically driven by a small force with zero average value. Note that Eq. (20) is the generalization to the inertial case of the Lifson-Jackson formula for the effective diffusion coefficient $D_{\rm eff}$ of an overdamped Brownian particle in the periodic potential (related to μ by the Einstein relation $D_{\rm eff} = k_B T\mu$) [36].

Using the persymmetry of the matrix corresponding to the operator $\hat{q}(x)$ in Fourier representation [see Eq. (38) below], it is possible to change the order of integration,

$$\int_0^L dx[\rho(x)-L^{-1}]\int_0^x dy[\hat{q}(y)-L^{-1}] = -\int_0^L dx[\hat{q}(x)-L^{-1}]\int_0^x dy[\rho(y)-L^{-1}] \tag{22}$$

(where the identity $\int_0^L dx[\hat{q}(x)-L^{-1}]=0$ has been used), and we arrive at the following expression:

$$\chi = -\beta L\mu\left\{\bar{\Phi} - (\beta L Z_{\rm in})^{-1}\int_0^L dx\, q(x)\left[\partial_F \hat{G}_0^{-1}(x;F)\right]_{F=0}\right\}, \tag{23}$$

where $\bar{\Phi}$ is given by Eq. (15) for the on-off ratchet. The quantity $[\partial_F \hat{G}_0^{-1}(x;F)]_{F=0}$ requires additional MCFM calculations [see Eqs. (30) and (31) below] from which it follows that this quantity does not contribute to the inertia correction linear in the particle mass. Thus, for small inertia, the average velocities of rocking and on-off flashing ratchets are determined by the same quantity $\bar{\Phi}$, which is in full agreement with the conclusions of Refs. [29,30].

IV. APPLICATION OF THE MATRIX CONTINUED FRACTION METHOD

The MCFM was developed by Risken [3] and Risken and Vollmer [16,17] on the basis of the theory of continued fractions considered in Ref. [37] (see also Refs. [38,39]). Application of this approach to different problems is discussed in the literature, e.g., in Refs. [18–21,40–43]. The MCFM is based on the formal solution of a system of equations

$$-\hat{P}_n^-(x)c_{n-1}(x) + c_n(x) + \hat{P}_n^+(x)c_{n+1}(x) = 0,\quad n = 1,2,\ldots, \tag{24}$$

where $\hat{P}_n^\pm(x)$'s are known differential operators and $c_n(x)$'s are unknown functions to be found. The solution of Eq. (24) is looked for in the form

$$c_{n+1}(x) = \hat{S}_n(x)c_n(x). \tag{25}$$

Substitution of Eq. (25) into (24) gives the recurrence relation,

$$\hat{S}_n(x) = [\hat{1} + \hat{P}_{n+1}^+(x)\hat{S}_{n+1}(x)]^{-1}\hat{P}_{n+1}^-(x), \tag{26}$$

which enables expressing $\hat{S}_n(x)$ through $\hat{S}_{n+1}(x)$. It is assumed that one can set $\hat{S}_{N+1}(x)=0$ at a sufficiently large value of $n=N$ so that all $\hat{S}_n(x)$'s with $n \leqslant N$ can be found from Eq. (26). This allows finding the functions $c_n(x)$ from Eq. (25) if one of them is determined by some additional condition.

By comparison of Eq. (24) with the time-independent Eq. (6) for $c_n(x,t) = c_n(x)$ or its analog for $\varphi_n(x)$ at $n \geqslant 1$, the explicit forms for $\hat{P}_n^\pm(x)$ can be written as

$$\hat{P}_n^-(x) = \frac{1}{\sqrt{n}}\varepsilon \hat{J}(x), \qquad \hat{P}_n^+(x) = \frac{\sqrt{n+1}}{n}\varepsilon\partial_x. \tag{27}$$

The insertion of Eq. (27) into (26) and introducing the new operator $\hat{G}_n(x)$ by the relation $\hat{S}_n(x) = \hat{G}_n(x)\hat{P}_{n+1}^-(x)$ give the recurrence relation connecting operators $\hat{G}_{n-1}(x)$ and $\hat{G}_n(x)$,

$$\hat{G}_{n-1}(x) = [\hat{1} + \varepsilon^2 n^{-1}\partial_x\hat{G}_n(x)\hat{J}(x)]^{-1}. \tag{28}$$

In the presence of the biasing force F, $V(x)$ should be replaced by $U(x) = V(x) - Fx$. Then, the dimensionless current operator and the operator $\hat{G}_n(x)$ become F dependent and equal to $\hat{J}(x) + \beta F L$ [where $\hat{J}(x)$ is given by Eq. (7)] and $\hat{G}_n(x;F)$, respectively. Thus, the recurrence relation for the operator $\hat{G}_n(x;F)$ takes the form

$$\hat{G}_{n-1}(x;F) = [\hat{1} + \varepsilon^2 n^{-1}\partial_x\hat{G}_n(x;F)\hat{J}(x) + \varepsilon^2 n^{-1}\beta F L\,\partial_x\hat{G}_n(x;F)]^{-1}. \tag{29}$$

This relation is needed for the calculation of $\hat{G}_0^{-1}(x;F)$ that is contained in Eq. (18) for $J(F)$.

It follows from Eq. (29) that:

$$\left[\partial_F\hat{G}_{n-1}^{-1}(x;F)\right]_{F=0} = \varepsilon^2 n^{-1}\{\partial_x[\partial_F\hat{G}_n(x;F)]_{F=0}\hat{J}(x) + \beta L\,\partial_x\hat{G}_n(x)\}, \tag{30}$$

where $\hat{G}_n(x) = \hat{G}_n(x;0)$ and $[\partial_F\hat{G}_n(x;F)]_{F=0}$ can be found from the following recurrence relation:

$$[\partial_F\hat{G}_{n-1}(x;F)]_{F=0} = -\varepsilon^2 n^{-1}\hat{G}_{n-1}(x)\{\partial_x[\partial_F\hat{G}_n(x;F)]_{F=0} \times \hat{J}(x) + \beta L\,\partial_x\hat{G}_n(x)\}\hat{G}_{n-1}(x). \tag{31}$$

Equations (30) and (31) allow the calculation of the quantity $[\partial_F\hat{G}_0^{-1}(x;F)]_{F=0}$ needed for determining the nonlinear response [see Eq. (23)].

Note that the above relations give small-inertia corrections [taking into account the contributions linear in ε^2 and setting $\hat{G}_1(x) = \hat{1}$] which were derived and discussed in Ref. [30].

For arbitrary inertia (characterized by the parameter ε), the recurrence procedure [presented by Eq. (28)] should be limited to a definite value of $n = N$ at which $\hat{G}_N(x) = \hat{1}$. The more inertia, the larger value of N should be taken. At the same time, the formal solutions obtained in Secs. II and III become computationally treatable by using the Fourier representation in which operator equations become matrix ones. Due to the periodicity of the potential $V(x)$ and, as consequence, all functions of x in Eqs. (1)–(15) and (20)–(23), we define the matrix elements of an arbitrary operator $\hat{A}(x)$ composed by the product of the differential operators ∂_x and x-dependent periodic functions as

$$A_{pp'} = L^{-1}\int_0^L dx\, e^{-ik_p x}\hat{A}(x)e^{ik_{p'}x},\\ p,p' = 0,\pm 1,\pm 2,\ldots;\; k_p = 2\pi L^{-1}p. \tag{32}$$

With this notation, the matrix elements of the operators $\partial_x = L\,\partial/\partial x$ and $\hat{J}(x)$ [defined by Eq. (7)] take the form

$$(\partial_x)_{pp'} = iLk_p\delta_{pp'},\\ J_{pp'} = -iL\sum_{p''}k_{p''}(E^{-1})_{p-p''}E_{p''-p'}\\ = -iL(k_p\delta_{pp'} + \beta k_{p-p'}V_{p-p'}), \tag{33}$$

where

$$E_p = L^{-1}\int_0^L dx\, e^{\beta V(x)-ik_p x},\\ (E^{-1})_p = L^{-1}\int_0^L dx\, e^{-\beta V(x)-ik_p x}. \tag{34}$$

Thus each recurrence step in Eq. (28) corresponds to solving the system of linear equations,

$$\sum_{p''}\left[\delta_{pp''} + iL\varepsilon^2 n^{-1}k_p\sum_{p'''}(\hat{G}_n)_{pp'''}J_{p'''p''}\right](\hat{G}_{n-1})_{p''p'} = \delta_{pp'}. \tag{35}$$

Of course, for computational procedure, the allowed values of p should be limited by a definite value p_m so that $p = 0,\pm 1,\ldots,\pm p_m$ and the number of equations in Eq. (35) equals $2p_m + 1$. Parameters N and p_m should be chosen properly to provide the required accuracy of the results (see Sec. V).

The expression for the main quantity of interest $\bar{\Phi}$, given by Eq. (15), contains the integral $r(x) = \int_0^x dy\,[\rho(y) - L^{-1}]$, which can be expanded into Fourier series due to the periodicity condition $r(L) = r(0) = 0$. Since the Fourier components of $\rho(x)$ are given by $\rho_p = (E^{-1})_p/L(E^{-1})_0$, the Fourier components of $r(x)$ equal

$$r_p \underset{p\neq 0}{=} -i[L(E^{-1})_0]^{-1}k_p^{-1}(E^{-1})_p,\\ r_0 = i[L(E^{-1})_0]^{-1}\sum_{p\neq 0}k_p^{-1}(E^{-1})_p. \tag{36}$$

Thus Eq. (15) takes the form

$$\bar{\Phi} = L\sum_{p\neq 0}q_{0p}r_p = -i(E^{-1})_0^{-1}\sum_{p\neq 0}q_{0p}k_p^{-1}(E^{-1})_p, \tag{37}$$

where

$$q_{pp'} = (Z_{\rm in}E_0L)^{-1}\sum_{p''}E_{p-p''}\left(\hat{G}_0^{-1}\right)_{p''p'},\\ Z_{\rm in} = (E_0)^{-1}\sum_{p''}E_{-p''}\left(\hat{G}_0^{-1}\right)_{p''0}, \tag{38}$$

and we have used the equality $q_p = E_p/LE_0$ for the Fourier components of $q(x)$.

Let us now prove the identity (22). The left side of Eq. (22) contains the integral $Q(x) = \int_0^x dy\,[\hat{q}(y) - L^{-1}]$, the Fourier components of which are equal to $Q_p = -iq_{p0}/k_p$ so that

$$\int_0^L dx[\rho(x) - L^{-1}]\int_0^x dy[\hat{q}(y) - L^{-1}]\\ = i(E^{-1})_0^{-1}\sum_{p\neq 0}q_{-p0}k_p^{-1}(E^{-1})_p. \tag{39}$$

Comparing Eqs. (37) and (39), we conclude that the identity (22) is true if $q_{-p0} = q_{0p}$. The more general equality $q_{pp'} = q_{-p',-p}$ defines a property of persymmetry (the symmetry with respect to the reverse diagonal) [44]. Thus we need to prove that the matrix $q_{pp'}$ really possesses this property. It is convenient to introduce the operator $\hat{q}_n(x) = q(x)\hat{G}_n^{-1}(x)$ so that $\hat{q}(x) = Z_{\rm in}^{-1}\hat{q}_0(x)$. Using Eq. (28), it is easy to show that $\hat{q}_n(x)$ satisfies the following recurrence relation:

$$\hat{q}_{n-1}(x) = q(x) - \varepsilon^2 n^{-1}q(x)\partial_x[\hat{q}_n(x)]^{-1}\partial_x q(x), \tag{40}$$

which corresponds to the following relation for matrix elements:

$$(\hat{q}_{n-1})_{pp'} = (LE_0)^{-1}E_{p-p'} - \varepsilon^2 n^{-1}(LE_0)^{-2}\\ \times\sum_{p'',p'''}E_{p-p''}k_{p''}\left(\hat{q}_n^{-1}\right)_{p''p'''}k_{p'''}E_{p'''-p'}. \tag{41}$$

Since any matrix $A_{pp'}$ describing multiplication by periodic function $A(x)$ is expressed through its Fourier component $A_{p-p'}$ and belongs to persymmetric matrices, the matrix $(\hat{q}_N)_{pp'} = q_{p-p'}$ is a persymmetric one. Let us assume that the matrix $(\hat{q}_n)_{pp'}$ is also persymmetric, and therefore the same property is true for the matrix $(\hat{q}_n^{-1})_{pp'}$ of the reverse operator $\hat{q}_n^{-1}$ [44]. Substitution of $(\hat{q}_n^{-1})_{p''p'''} = (\hat{q}_n^{-1})_{-p''',-p''}$ to Eq. (41) and changing the summation indices p'' to $-p'''$ and p''' to $-p''$ lead to the equality $(\hat{q}_{n-1})_{pp'} = (\hat{q}_{n-1})_{-p',-p}$ which completes the proof of persymmetry of the matrix $(\hat{q}_n)_{pp'}$ by the mathematical induction method. Since $q_{pp'} = Z_{\rm in}^{-1}(\hat{q}_0)_{pp'}$, the equality $q_{p0} = q_{0,-p}$ follows from $(\hat{q}_n)_{pp'} = (\hat{q}_n)_{-p',-p}$ at $n = 0$ and $p' = 0$. Thus, the identity (22) has been proved.

V. APPLICATION TO A SAWTOOTH POTENTIAL

A sawtooth potential is commonly used in theoretical studies due to its piecewise-linear structure that allows analytical calculations. For our purposes, using this potential gives a possibility to elucidate how a large gradient of a periodic potential affects the characteristics under study (Secs. II and III). Besides, this allows us to operate with analytical expressions for matrix elements entering into the numerical scheme discussed above. On the other hand, the presence of large gradients requires the summation over many harmonics of the potential and a large value of the limiting parameter p_m

(for prescribed accuracy to be reached) unlike, for example, the simple case of cosine potential where p_m can be taken small enough [3].

It is convenient to choose a coordinate system in which the Fourier components of the quantities under study have the simplest form. Of course, such a choice has no influence on the final results. If A_p is a Fourier component in the initial coordinate system, the Fourier component $\tilde{A}_p$ in the new coordinate system shifted along the x axis by a can be found by the formula $\tilde{A}_p = \exp(ik_p a)A_p$. One can check that the factor $\exp(ik_p a)$ does not contribute to the quantities under study. We introduce dimensionless units for length and energy so that the length is measured in units of the potential period L and the energy in units of the potential barrier V. A sawtooth potential can be parametrized in the main period by the following odd function: $V(x) = x/l$ for $-l/2 < x < l/2$ and $V(x) = (\pm 1/2 - x)/(1-l)$ for the intervals $l/2 < x < 1/2$ and $-1/2 < x < -l/2$, respectively, where l and $1-l$ are the sawtooth lengths $(0 < l < 1)$. The Fourier components of the potential gradient $f(x) = V'(x)$ are written as $f_p = \sin(\pi p l)/[\pi p l(1-l)]$. Figure 1(a) presents the dependence f_p on p for several values of l. The smaller l (or $1-l$), the more harmonics should be taken into account in the calculation scheme. The number of sum terms p_m required for calculations can be estimated as $p_m \sim l^{-1}$ at $l \to 0$. On the other hand, $f_p \to 1$ (for arbitrary p) at $l \to 0$ (or $1-l \to 0$) so that we can expect the singular behavior of quantities of interest in the case of an extremely asymmetric sawtooth potential.

As pointed out above, the advantage of the sawtooth potential is that it provides analytical expressions, including the expression for E_p defined by Eq. (34),

$$E_p = \frac{2u\,\sinh[(u - ik_p l)/2]}{u^2 + i(1-2l)uk_p + l(1-l)k_p^2},\qquad u = \beta V,\quad k_p = 2\pi p \tag{42}$$

The expression for $(E^{-1})_p$ is obtained by the replacement of u by $-u$ in Eq. (42). The dimensionless parameter u specifies the ratio of the potential barrier V to the thermal energy $k_B T$ and serves as the dimensionless inverse temperature. In addition to E_p and $(E^{-1})_p$, we need the matrix $(\hat{G}_0^{-1})_{pp'}$ for the quantities $\bar{\Phi}$, Z_{in}, and μ to be calculated from Eqs. (37), (38), and (20). It can be found from the recurrence procedure,

$$\sum_{p''=-p_m}^{p_m} \left\{ \delta_{pp''} + \varepsilon^2 n^{-1} k_p \left[k_{p''}(\hat{G}_n)_{pp''} - iu \sum_{p'''=-p_m}^{p_m} (\hat{G}_n)_{pp'''} f_{p'''-p''} \right] \right\} (\hat{G}_{n-1})_{p''p'} = \delta_{pp'}. \tag{43}$$

Note that in the overdamped case the explicit analytical expressions for $\bar{\Phi}$ and μ (marked with subscript $m = 0$ below) are known for a sawtooth potential [29,30],

$$\bar{\Phi}_{m=0} = (1/2 - l)[\coth(u/2) + (u/2)/\sinh^2(u/2) - 4/u],$$
$$\mu_{m=0} = \zeta^{-1}(E^{-1})_0^{-1} E_0^{-1} = \zeta^{-1}(u/2)^2/\sinh^2(u/2). \tag{44}$$

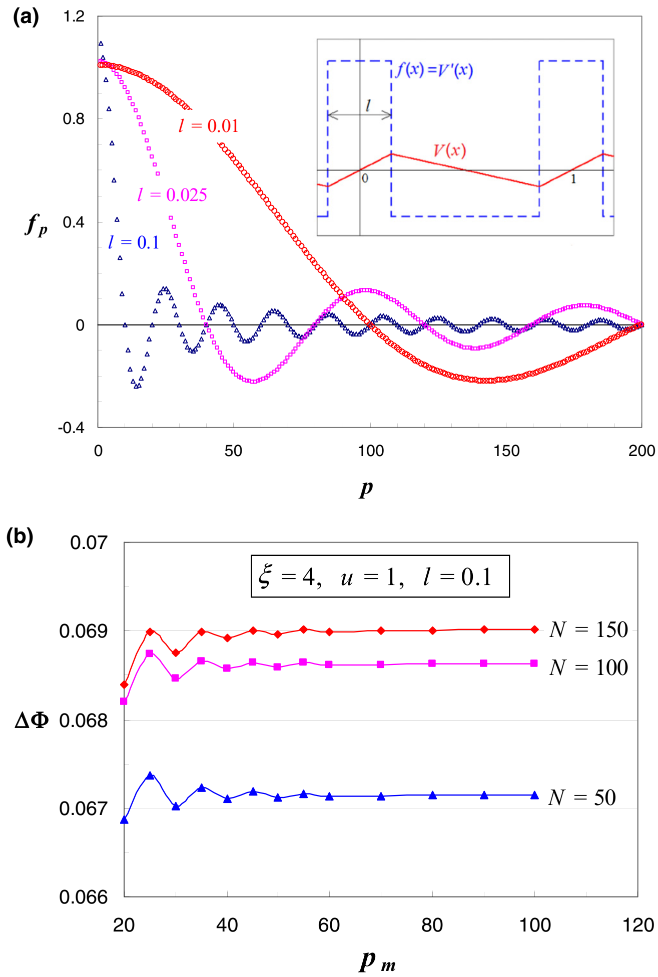

FIG. 1. (Color online) (a) The Fourier components f_p of the gradient of the sawtooth potential $V(x)$ (depicted in the top right frame) for several sawtooth lengths l. (b) The dependence of the inertial correction $\Delta\Phi$ calculated by MCFM on the limiting parameter p_m for several values N.

Thus the mobility μ (at $F = 0$) can be calculated as $\mu = \mu_{m=0}/Z_{\text{in}}$ and the correction $\Delta\Phi$ as $\bar{\Phi} - \bar{\Phi}_{m=0}$ from Eq. (14).

It is convenient to characterize inertia by the temperature-independent parameter,

$$\xi = \varepsilon^2 u = \tau_v/\tau_L = mV/\zeta^2 L^2, \tag{45}$$

which is the ratio of the velocity relaxation time τ_v to the sliding time $\tau_L = \zeta L^2/V$ on the distance L in the overdamped regime. Figure 1(b) provides insight into the values of the limiting parameters N and p_m which ensure the required calculation accuracy. In a wide range of values of ξ, u, and $0.01 < l < 0.99$, an accuracy of up to three significant figures can be reached at $N = 100$ and $p_m = 100$. It is worthy to mention that MCFM calculations with the cosine potentials require much lower values of N and p_m (namely, $N \approx 20$ and $p_m \approx 12$ for the same accuracy) [3].

Figures 2(a) and 2(b) demonstrate the l dependences of $\bar{\Phi}$ and μ for several values of ξ calculated at $u = 1$, $N = 100$, and $p_m = 100$. The point $l = 0.5$ is the center of symmetry for $\bar{\Phi}(l)$ in the interval $0 < l < 1$ [so that $\bar{\Phi}(l) < 0$ at $0.5 < l < 1$] and determines the position of the symmetry axis for

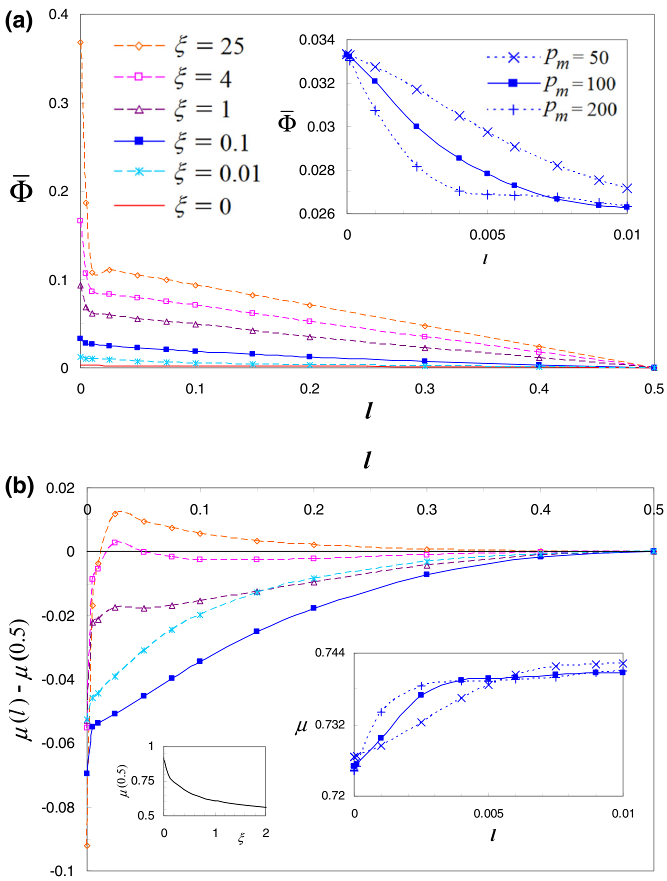

FIG. 2. (Color online) (a) The l dependences of the average integrated current after switching on the sawtooth potential and (b) the shift of the particle mobility $\mu(l)$ (at zero external force) relative to its value $\mu(0.5)$ at the central point $l = 0.5$. The calculations have been performed by MCFM at $u = 1$, $N = 100$, and $p_m = 100$. The detailed l dependences near the point $l = 0$ for different p_m's are given in the corresponding frames. The curves in panel (b) are marked as in panel (a). The dependence of $\mu(0.5)$ on ξ is presented in the bottom left frame in panel (b).

$\mu(l)$ in the same interval. In other words, $\bar{\Phi}$ and μ are odd and even functions of the asymmetry parameter $\kappa = 1 - 2l$. These dependences exhibit a jumplike behavior near the point $l = 0$ (or $l = 1$). The more detailed behavior near this point is depicted in the insets of Fig. 2. The greater the value of p_m, the closer the smooth portion of the curve approaches the y axis. One can say that there is such a value of p_m at which the calculated value of $\bar{\Phi}$ or μ belongs to the smooth portion of the corresponding curve. This is true for an arbitrarily small but nonzero l. On the other hand, the calculation of $\bar{\Phi}$ and μ at $l = 0$ (when $f_p = 1$ for all p) does not require large values of p_m, and the result can differ from that of $l \to 0$. This means that the function $A(l)$ ($\bar{\Phi}$ or μ in our case) satisfies the inequality: $\lim_{l\to 0} A(l) \neq A(0)$. An attempt to explain the physical cause of such a nonanalytic behavior is given in Sec. VI where we develop an analytical approach valid in the high-temperature region.

The mobility $\mu_{m=0}$ (at $F = 0$) of an inertialess particle in a sawtooth potential does not depend on the sawtooth lengths l and $1 - l$ [see Eq. (44)]. It is impressive that such

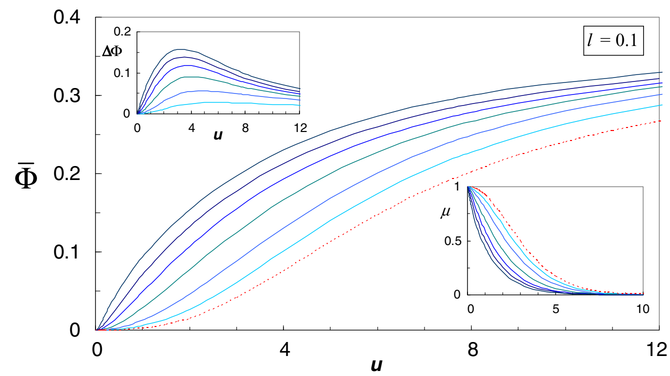

FIG. 3. (Color online) The inverse temperature dependences of the average integrated current after switching on the sawtooth potential. The corresponding dependences of the inertial correction $\Delta\Phi$ are depicted in the top left frame. The curves, from bottom to top, are in the order of increasing the inertial parameter ξ from $\xi = 0$ (the inertialess case, the dotted curve) to $\xi = 0.01, 0.05, 0.25, 1, 4$, and 25 (the solid curves). The inverse temperature dependences of the particle mobility μ (at zero external force) are presented in the bottom right frame. The curves, from top to bottom, correspond to the same increasing order of ξ values. The calculations have been performed by MCFM at $l = 0.1$, $N = 100$, and $p_m = 100$.

a dependence arises in the inertial case. The dependences presented in Fig. 2(b) show that the mobility decreases monotonically with increasing the asymmetry parameter κ for $\xi < 4$ with maximum deviation at $\xi \sim 0.1$. For strong inertia (the underdamped case) at $\xi > 4$, the dependences become nonmonotonic.

It follows from the inverse temperature dependences presented in Fig. 3 that inertia has the opposite effect on the average integrated current $\bar{\Phi}$ and the particle mobility μ: The former increases, and the latter decreases with increasing inertia. In Ref. [29] we have proved such a behavior of μ for arbitrary periodic potentials but only by consideration of small inertia corrections linear in ξ. In this approximation, $\bar{\Phi}$ increases with the increase in inertia at all temperatures for a sawtooth potential and, at high temperatures, for simple periodic potentials described by the first two harmonics. The high-temperature asymptotics of $\bar{\Phi}$ is proportional to T^{-3} for the overdamped case ($\bar{\Phi} = \bar{\Phi}_{m=0}$) [34,45–47] and to T^{-2} when the inertia is small [29,30]. For strong inertia, the linearlike dependence of $\bar{\Phi}$ is observed in Fig. 3 at small u (but not belonging to the very narrow area near $u = 0$ considered in Sec. VI) so that $\bar{\Phi} \propto T^{-1}$. Although $\bar{\Phi}$ dominates $\bar{\Phi}_{m=0}$ at high temperatures, the deviation $\bar{\Phi}$ from $\bar{\Phi}_{m=0}$ is maximal at $u \sim 4$.

VI. HIGH-TEMPERATURE BEHAVIOR

The high-temperature approximation is a fruitful analytical approach which allowed us to obtain a number of useful regularities both for inertialess ratchets [34,45–47] and for the ratchets with the small inertia [29,30]. That is why it is reasonable to apply this approximation to the strong-inertia case considered in this paper. The small parameter is $u = \beta V$, where V is the maximum potential change on its spatial period. At $u \ll 1$, the inertia parameter ε can be arbitrarily chosen (more precise inequalities are given at the end of this section after the final expressions are derived). With this approximation, it is convenient to rewrite Eqs. (37) and (38) for the quantities of interest as follows:

$$Z_{\rm in} = 1 + u\varepsilon^2 (E_0)^{-1} \sum_{p,p'\neq 0} k_p k_{p'} E_{-p} (\hat{G}_1)_{pp'} V_{p'}, \qquad (46)$$

$$\bar{\Phi} = Z_{\rm in}^{-1} \bar{\Phi}_{m=0} - i\varepsilon^2 Z_{\rm in}^{-1} (E_0)^{-1} (E^{-1})_0^{-1} \times \Bigg[\sum_{p,p'\neq 0} k_p E_{-p} (E^{-1})_{p'} (\hat{G}_1)_{pp'} + u \sum_{p,p'\neq 0, p''(\neq p)} k_p^{-1} k_{p'} k_{p''-p} E_{-p'} (E^{-1})_p (\hat{G}_1)_{p'p''} V_{p''-p} \Bigg], \qquad (47)$$

where

$$\bar{\Phi}_{m=0} = -i (E_0)^{-1} (E^{-1})_0^{-1} \sum_{p\neq 0} k_p^{-1} E_{-p} (E^{-1})_p \qquad (48)$$

is the inertialess contribution and $k_p = 2\pi p$. Since E_p and $(E^{-1})_p$ are of order u at $p \neq 0$, the lowest approximation in u requires the matrix elements $(\hat{G}_1)_{pp'}$ to be independent of u for $Z_{\rm in}$ and to contain the linear correction in u for $\bar{\Phi}$. Since the matrices $(\hat{G}_n)_{pp'}$ are diagonal at $u = 0$, the matrix $(\hat{G}_1)_{pp'}$ can be written in the approximate form

$$(\hat{G}_1)_{pp'} \approx g_p^{(1)} \delta_{pp'} + u g_{pp'}^{(1)}. \qquad (49)$$

Here $g_p^{(1)}$ and $g_{pp'}^{(1)}$ define diagonal and nondiagonal [see Eq. (52) below] contributions, respectively.

As follows from Eqs. (28) and (35), the continued fraction $g_p^{(1)}$ is determined by the recurrence relation,

$$g_p^{(n-1)} = \left[1 + \frac{\varepsilon^2 k_p^2}{n} g_p^{(n)} \right]^{-1}, \quad n = 2,3,\ldots,N, \qquad g_p^{(N)} = 1, \quad N \gg 1, \qquad (50)$$

and, in accordance with Ref. [3], is analytically representable,

$$\xi_p \equiv g_p^{(1)} \underset{p\neq 0}{=} \int_0^l dz \, \exp\left[-\varepsilon^2 k_p^2 (z - 1 - \ln\, z)\right] \underset{\varepsilon > 1}{\approx} \sqrt{\frac{\pi}{2}} \frac{1}{\varepsilon |k_p|}, \quad g_0^{(1)} = 1. \qquad (51)$$

Then, the nondiagonal contribution $g_{pp'}^{(1)}$ can be found by the following procedure:

$$g_{pp'}^{(1)} = k_{p'}^{-1} k_{p-p'} V_{p-p'} \xi_{-p,p'}, \quad \xi_{pp'} = \sum_{n=2}^{N} g_p^{(n)} A_{pp'}^{(n)}, \qquad A_{pp'}^{(n)} = \prod_{n'=2}^{n} a_{pp'}^{(n')}, \quad a_{pp'}^{(n)} = \frac{\varepsilon^2}{n} k_p g_p^{(n-1)} k_{p'} g_{p'}^{(n-1)}. \qquad (52)$$

Expanding E_p and $(E^{-1})_p$ in powers of u in Eqs. (46)–(48) and using Eqs. (49), (51), and (52), we arrive at the following general relations:

$$Z_{\rm in} = 1 + u^2 \varepsilon^2 \sum_{p\neq 0} k_p^2 \xi_p |V_p|^2 + O(u^3) \underset{\varepsilon > 1}{\approx} 1 + \sqrt{2\pi} u^2 \varepsilon \sum_{p=1}^{\infty} k_p |V_p|^2 + O(u^3), \qquad (53)$$

$$\bar{\Phi} = i u^3 \sum_{\substack{p,p'\neq 0 \\ (p+p'\neq 0)}} k_p^{-1} [1 + \varepsilon^2 k_{p'} (k_{p'+p} \xi_{p'p} + k_{p'+2p} \xi_{p'})] \times V_p V_{p'} V_{-p-p'} + O(u^4). \qquad (54)$$

These relations in the case of small inertial corrections ($\varepsilon \ll 1$, $\xi_p = 1$, and $\xi_{pp'} = 0$) are reduced to those obtained in Ref. [30]. Since $u \propto T^{-1}$ and $\varepsilon \propto T^{1/2}$, we can see from Eq. (53) that $(Z_{\rm in} - 1) \propto T^{-1}$ for a small inertia and $\propto T^{-3/2}$ for a strong one. We cannot exactly determine the high-temperature asymptotics of $\bar{\Phi}$ since the temperature dependence of $\xi_{p'p}$ is unknown in the general case. Nevertheless, one can state that $\bar{\Phi} \propto T^{-\alpha}$ where $\alpha \subset (2,5/2)$.

The comparison between the exact and the approximate l dependences of $(Z_{\rm in} - 1)/u^2$ and $\bar{\Phi}/u^3$ for the sawtooth potential [when $V_p = -i f_p / k_p$ in Eqs. (53) and (54)] is given in Figs. 4(a) and 4(b). The agreement is good when l is not too small. The cause of the discrepancy lies in the fact that the expansion of E_p in u depends on whether there is a region of rapidly changing potential or not. Indeed, the expansion of Eq. (42) for the sawtooth potential in powers of u ($u \ll 1$) is different for $u \ll |k_p| l$ and $u \gg |k_p| l$. Since $|k_p| = 2\pi |p| \geqslant 2\pi$, the inequality $u \ll |k_p| l$ is valid in the wide region of l, $l \gg u/2\pi$ where the expansions (53) and (54) are justified, whereas the validity of the inequality $u \gg |k_p| l$ at $u \ll 1$ depends on k_p. The numerical procedure limits the maximal value of $|k_p|$ (the parameter p_m) so that, strictly speaking, the region of small l values with $u \gg |k_p| l$ and $u \ll 1$ is narrowed to the point $l = 0$. This is an explanation of the nonanalytic behavior which we observe at small l.

In the case of the sawtooth potential and strong inertia ($\varepsilon > 1$), the summation in Eq. (53) can be carried out analytically [22], which leads to the following expressions for the quantity $Z_{\rm in}$ and the high-temperature mobility μ (at zero external force):

$$Z_{\rm in} \underset{\varepsilon > 1}{\approx} 1 - \frac{2u^2 \varepsilon}{\sqrt{2\pi} l^2 (1-l)^2} \int_0^l dx (l - x) \ln(2\, \sin\, \pi x) \underset{l\to 0}{\to} 1 - \frac{u^2 \varepsilon}{\sqrt{2\pi}} \left[\frac{3}{2} + \ln(2\pi l) \right],$$

$$\zeta \mu \approx (1 - u^2/12) Z_{\rm in}^{-1} \underset{l\to 0 (\varepsilon > 1)}{\to} 1 + \frac{u^2 \varepsilon}{\sqrt{2\pi}} \left[\frac{3}{2} + \ln(2\pi l) \right]. \qquad (55)$$

As we mentioned above, the approximation used is valid for $l \gg u/2\pi$ so that the logarithmic divergence at $l \to 0$ must be eliminated by setting $2\pi l \sim u$ in the logarithmic argument. Thus we obtain the following nonanalytic behavior at the point $l = 0$ and at $u \to 0$: $Z_{\rm in} \to 1 - (2\pi)^{-1/2} \varepsilon u^2 \ln(u)$ ($\varepsilon > 1$), which is in qualitative agreement with the exact results

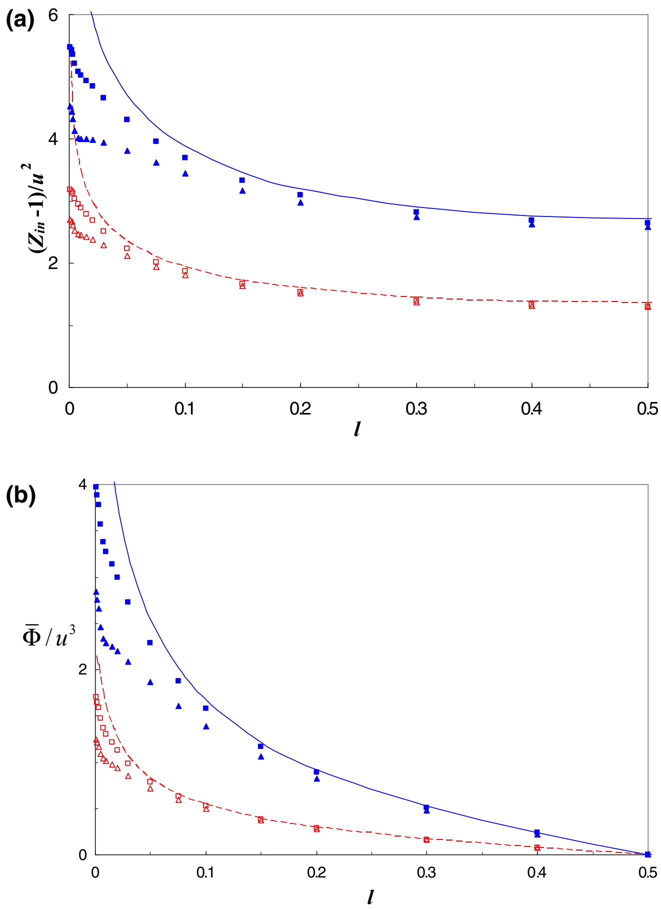

FIG. 4. (Color online) The comparison of the exact (markers) and high-temperature approximate (lines) l dependences of the normalized quantities (a) $(Z_{\rm in} - 1)/u^2$ and (b) $\bar{\Phi}/u^3$ calculated for the sawtooth potential. The dashed and solid curves as well as the open and filled markers correspond to $\varepsilon = 2$ and $\varepsilon = 4$, respectively. The square and triangle markers correspond to $u = 0.05$ and $u = 0.1$.

presented in Fig. 4(a): The smaller u, the larger $(Z_{\rm in} - 1)/u^2$ at $l = 0$. The corresponding high-temperature dimensionless mobility $\zeta\mu$ decreases from the value of $\zeta\mu \approx 1 - 0.68\varepsilon u^2$ at $l = 1/2$ to the asymptotic value of $\zeta\mu \to 1 + 0.40\varepsilon u^2 \ln(u)$ at $l = 0$. Since the high-temperature contribution is assumed to be small, the inertial parameter ε is majorized by the inequality $\varepsilon \ll u^{-1}$.

The high-temperature analysis allows us to conclude that the presence of large gradients in a periodic potential (in the region of the width l) leads to the nonanalytic behavior of the quantities of interest at $l \to 0$. For small inertia, the quantities diverge as l^{-1} [29,30], whereas for strong inertia they diverge as $-\ln\ l$ [see Eq. (55)]. One can say that the nonanalytic area contracts to a point with increasing inertia. In fact, the smallness of l is limited by the smallness of u so that we can expect that the quantities of interest have the logarithmic singularity $-\ln\ u$ at small u. This is true, in particular, for the effective diffusion coefficient since it is related to the effective mobility μ (at zero external force) by the Einstein relation. In addition, we have actually shown that the high-temperature asymptotics of the inertial contribution to the mobility and the effective diffusion coefficient are proportional to $T^{-3/2}$ and $T^{-1/2}$, respectively, for strong inertia.

VII. CONCLUSIONS

We have developed a theory of inertial adiabatic transport in which the main transport characteristics are described by analytical expressions formally coinciding with known ones for the overdamped massless case but containing a factor which just includes all information about inertia and can be calculated in terms of Risken's MCFM. One of the important transport characteristics is the average integrated current $\bar{\Phi}$ arising after switching on a periodic potential which determines the average velocity of an adiabatic on-off flashing ratchet. The second characteristic is the stationary current arising in a tilted periodic potential. In contrast to the traditional computational MCFM scheme [3], our expression for this current formally coincides with the Stratonovich formula [35] which is generalized to the case of inertial particles. Such representation has allowed us to obtain the coefficients of expansion over the small force, namely, the mobility μ (at zero external force) and the effective diffusion coefficient as well as the nonlinear response which determines the average velocity of adiabatically driven rocking ratchets.

Unlike the commonly considered in MCFM cosinelike potentials, the sawtooth potential has been chosen as an example. This choice has allowed us to elucidate how a large gradient of a periodic potential affects the characteristics under study. We have revealed nonanalytic (jump) behavior of the transport characteristics for a stepwise potential when the width l of the steps tends to zero. In contrast to the overdamped case in which the mobility μ (at zero external force) and the effective diffusion coefficient in a sawtooth potential do not depend on l, they decrease with increasing the asymmetry parameter $\kappa = 1 - 2l/L$ when inertia is not very strong and have nonmonotonic behavior for strong inertia. Analysis of the temperature dependences $\mu(T)$ and $\bar{\Phi}(T)$ (determining the average particle velocity of the on-off ratchet) revealed the dominant role of inertia in the high-temperature region. In this region, we have developed an analytical approach which allows us to conclude that the temperature-dependent contribution to the mobility μ is proportional to $T^{-3/2}$ for strong inertia and has the logarithmic singularity $-\ln\ l$ at $u < l \to 0$ changing to the singularity $-\ln\ u$ at $l \ll u \to 0$.

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