Inertial effects in adiabatically driven flashing ratchets

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(Received 19 December 2013; published 19 May 2014)

We study analytically the effect of a small inertial correction on the properties of adiabatically driven flashing ratchets. Parrondo's lemma [J. M. R. Parrondo, Phys. Rev. E **57**, 7297 (1998)] is generalized to include the inertial term so as to establish the symmetry conditions allowing directed motion (other than in the overdamped massless case) and to obtain a high-temperature expansion of the motion velocity for arbitrary potential profiles. The inertial correction is thus shown to enhance the ratchet effect at all temperatures for sawtooth potentials and at high temperatures for simple potentials described by the first two harmonics. With the special choice of potentials represented by at least the first three harmonics, the correction gives rise to the motion reversal in the high-temperature region. In the low-temperature region, inertia weakens the ratchet effect, with the exception of the on-off model, where diffusion is important. The directed motion adiabatically driven by potential sign fluctuations, though forbidden in the overdamped limit, becomes possible due to purely inertial effects in neither symmetric nor antisymmetric potentials, i.e., not for commonly used sawtooth and two-sinusoid profiles.

DOI: 10.1103/PhysRevE.89.052131

PACS number(s): 05.40.-a, 05.60.Cd, 82.20.-w, 87.16.Nn

I. INTRODUCTION

Nonequilibrium fluctuations can cause a net particle drift along periodic structures lacking reflection symmetry, even without any macroscopic bias force. This phenomenon is known as the ratchet effect [1–3]. Predictive model systems for such nonequilibrium transport, called ratchets or Brownian motors, have been discussed in various contexts, especially in relation to studies of the physics of protein motors [4,5] and nanoscale artificial engines [3,6]. Systems of this kind are usually driven out of equilibrium either by pulsing the potential (flashing ratchets) [7–9] or by rocking it back and forth (rocking ratchets) [10,11].

Most of works on the ratchet effect consider Brownian motion in the overdamped regime, where friction dominates inertia, so the finiteness of the mass is neglected. In many cases, such as in biological applications, this approximation can be well justified on physical grounds [2,12]. However, finite inertia effects are important in many experimental situations and have attracted some recent attention [3,13–20]. For example, particle masses are of significance in experiments on microscopic particle separation [3]. In thermal ratchets, the decay of the massive particle current at short noise-correlation times behaves in a more complicated manner than previously reported in the overdamped limit and the direction of transport may depend on the particle mass [14]. Rocking ratchets are well studied in the overdamped limit [10–12,21,22] and also in the opposite limit, where inertial effects are strong and

can lead to motion reversal as well as to chaotic dynamics in the absence of noise (inertia ratchets) [13,15,16]. With the appropriate noise level, the inertia ratchets provide efficient mass-sensitive scenarios for particle separation [3,17,18]. As shown in Ref. [19], a small inertia correction always decreases the particle mobility in a stationary periodic potential, but enhances the rocking ratchet effect at high temperatures. The inertial effects in the flashing mechanism have been less frequently investigated, but their significance can be seen from the following observation: Directed motion induced by shifting dichotomic fluctuations of a symmetric potential is impossible in the overdamped regime [23,24] but occurs in the underdamped regime, as numerical simulations have shown [20].

The goal of the present paper is to study analytically the influence of finite inertia in the particle dynamics on the flashing ratchet mechanism. In order to make the problem analytically tractable, we invoke two simplifying assumptions: (i) The inertia corrections are small and (ii) the potential variation is adiabatic. These simplifications allow us to stress essential physical points made in this paper.

While the overdamped Brownian motion in a potential is governed by the Smoluchowski equation [25], containing no information about the particle mass and velocity, the rigorous treatment of a Brownian particle with finite mass involves time evolution of the particle probability in the phase space, which satisfies the much more complicated Klein-Kramers equation [26,27], analytically solvable only in a few special cases [28]. So to handle inertial effects in the particle dynamics, one usually invokes approximate approaches. The most well known and commonly used is the high-friction expansion of the Klein-Kramers equation [28–31]. In this way, the Klein-Kramers equation can be reduced to a Smoluchowski-like

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one-dimensional form [32] containing a series of corrections, so that the mapped equation respects inertia, although working in coordinate space. In the lowest order of such approximate dimension reduction, the mapped equation takes the form of the Smoluchowski equation with the current operator [28–32]

$$\hat{J}(x) = \left[1 + \frac{m}{\zeta^2} V''(x)\right] \hat{J}(x),$$

$$\hat{J}(x) = -De^{-\beta V(x)} \frac{\partial}{\partial x} e^{\beta V(x)},$$
(1)

where m, ζ , $D = (\beta \zeta)^{-1}$, and $\beta = (k_B T)^{-1}$ respectively denote the particle mass, the friction coefficient, the diffusion coefficient, and the inverse thermal energy $(k_B$ is the Boltzmann constant and T is the absolute temperature), V(x)and V''(x) are the potential and its second spatial derivative, and $\hat{J}(x)$ is the current operator in the overdamped limit (the Smoluchowski current operator). The factor $[1 + mV''(x)/\zeta^2]$ can be associated with the position dependence of the diffusion coefficient (or mobility) [32]. It would seem that one could use the results obtained in early studies of ratchet systems [33-36], with the position-dependent particle mobility (or the friction coefficient), to account for the inertial correction in the present case. A position-dependent mobility can lead to net transport, provided the system is driven out of equilibrium and there is a phase shift between equiperiodic mobility and potential, which can even be symmetric [35]. In our case, however, there is no phase shift between the potential and the mobility associated with the inertial correction. Thus the effect of the inertial correction (depending on the second spatial derivative of the periodic potential) on the ratchet properties requires separate detailed consideration carried out in this paper.

The second simplifying assumption, adiabatic fluctuations, is based on Parrondo's lemma [37]. It allows a massless particle movement on a large time interval, resulting after a fast transition from one periodic potential profile to another, to be described in terms of the equilibrium probability distributions of the particle in these profiles. The lemma determines the average velocity of directed motion arising from the periodically repeated fast transitions between longlived states (adiabatic dichotomic process). The simplicity of the adiabatic approach permits formulation of symmetry properties of adiabatically driven flashing ratchets operating in the overdamped regime [24]. In Sec. II Parrondo's lemma is generalized to include the inertial effects, thus affording an explicit expression for the particle velocity, which is analyzed with sawtooth potentials. As found for these potentials, the inertial correction leads to the increased velocity at all temperatures, but the quantities of interest behave unphysically in the low-temperature region. The symmetry properties and the high-temperature expansion of the particle velocity are obtained in Sec. III for arbitrary potential profiles. A discussion of the results exemplified by the potentials of different symmetry and shape is presented in Sec. IV. A summary is given in Sec. V.

II. ADIABATICALLY DRIVEN INERTIAL PARTICLE TRANSPORT

Consider a particle moving in a potential that undergoes periodically repeated fast transitions between two long-lived spatially periodic profiles. This setup is a deterministic analog of the two-state model that is widespread in studies of flashing ratchet systems [2]. We assume that the potential is changed adiabatically (adiabatic dichotomic process), i.e., the interstate transitions occur instantaneously and the state lifetimes are so long that equilibrium is achieved before each transition. Following Parrondo [37], the calculation of the average particle velocity can be based on determining the time-integrated current over the lifetime of each state. The explicit expression for this quantity obtained in the overdamped limit constitutes Parrondo's lemma [37]. In this section we generalize Parrondo's lemma to the case of inertial particles and on this basis obtain inertial corrections to the velocity of directed motion induced by the adiabatic dichotomic process. First, we briefly review the diffusion dynamics of inertial particles to make further consideration self-contained. Then we derive the time-integrated current for the general state of the problem with arbitrary inertia, assuming the nonequilibrium initial and final distributions. The current derived is further adapted to small inertial corrections and the equilibrium initial and final distributions. Finally, the generalized Parrondo lemma is exploited to treat analytically the case of sawtooth potentials.

A. Diffusion dynamics of inertial particles

The probability density $\rho(x, v, t)$ to find an inertial particle at point x with the velocity v at time t obeys the Klein-Kramers equation [26,27]

$$\frac{\partial}{\partial t}\rho(x,v,t) = \left[-\frac{\partial}{\partial x}v + \frac{1}{m}\frac{\partial}{\partial v}\left(\zeta v + V'(x) + \frac{\zeta}{m\beta}\frac{\partial}{\partial v}\right)\right] \times \rho(x,v,t).$$
(2)

It is convenient to search for the solution of Eq. (2) as a series [28]

$$\rho(x,v,t) = \sqrt{\frac{m\beta}{2\pi}} \exp(-q^2) \sum_{n=0}^{\infty} \frac{1}{\sqrt{2^n n!}} c_n(x,t) H_n(q), \quad (3)$$

where orthogonal Hermitian polynomials $H_n(q)$ are defined by

$$H_{n}(q) = (-1)^{n} \exp(q^{2}) \frac{d^{n}}{dx^{n}} \exp(-q^{2}),$$

$$\int_{-\infty}^{\infty} dq \exp(-q^{2}) H_{n}(q) H_{n'}(q) = 2^{n} n! \sqrt{\pi} \delta_{n,n'},$$
(4)

and $q = v \sqrt{m\beta/2}$ is the dimensionless velocity $[(m\beta)^{-1/2}$ is the thermal velocity]. The equation for the coefficients $c_n(x,t)$ can be obtained by substitution of Eq. (3) into Eq. (2) [28]:

$$\left(n+\tau_{v}\frac{\partial}{\partial t}\right)c_{n}(x,t) = (m\beta)^{1/2}\sqrt{n}\,\hat{J}(x)c_{n-1}(x,t)$$
$$-(m\beta)^{-1/2}\tau_{v}\sqrt{n+1}\frac{\partial}{\partial x}c_{n+1}(x,t),$$
(5)

where $\hat{J}(x)$ is the current operator in the overdamped limit defined in Eq. (1) and $\tau_v = m/\zeta$ is the velocity relaxation time. The reduced distribution function and current are defined as the zero and first moments of the distribution function $\rho(x, v, t)$ over velocity v,

$$\rho(x,t) = \int_{-\infty}^{\infty} dv \,\rho(x,v,t), \quad J(x,t) = \int_{-\infty}^{\infty} dv \,v\rho(x,v,t).$$
(6)

Using the equalities $H_0(q) = 1$, $H_1(q) = 2q$, and Eq. (3), one can make sure that $\rho(x,t) = c_0(x,t)$ and $J(x,t) = (m\beta)^{-1/2}c_1(x,t)$. For n = 0, Eq. (5) reduces to the continuity equation

$$\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial J(x,t)}{\partial x} = 0.$$
 (7)

B. Parrondo's lemma including inertia

Consider Brownian particles moving in the spatially periodic potential V(x) with period L during the time interval (0, T). For generality, the initial and final reduced distribution functions $\rho(x,0)$ and $\rho(x,T)$ are considered as nonequilibrium ones. The reduced current integrated over the time interval (0, T),

$$\Phi(x) = \int_0^T J(x,t)dt,$$
(8)

defines the net fraction of particles $\Phi(x)$ crossing point *x* to the right for time *T*. Integrating over *t* the continuity equation (7) and solving the obtained differential equation, we arrive at the following relation, which connects $\Phi(x)$ at *x* and x_0 :

$$\Phi(x) = \Phi(x_0) + \int_{x_0}^x dy [\rho(y,0) - \rho(y,T)].$$
(9)

By integrating Eq. (5) over *t* in the range (0, *T*), we obtain the equation for the quantities $\varphi_n(x) = \int_0^T dt c_n(x,t)$:

$$n\varphi_{n}(x) + \tau_{v}[c_{n}(x,T) - c_{n}(x,0)]$$

= $(m\beta)^{1/2}\sqrt{n} \hat{J}(x)\varphi_{n-1}(x) - (m\beta)^{-1/2}$
 $\times \tau_{v}\sqrt{n+1}\frac{d}{dx}\varphi_{n+1}(x).$ (10)

Termwise multiplication of this equation by $\exp[\beta V(x)]$ with subsequent integration over the spatial period gives, at $n \ge 1$,

$$\int_{0}^{L} dx \ e^{\beta V(x)} \varphi_{n}(x) = n^{-1} \tau_{v} \int_{0}^{L} dx \ e^{\beta V(x)} [c_{n}(x,0) - c_{n}(x,T)]$$
$$- n^{-1} \sqrt{n+1} \tau_{v}(m\beta)^{-1/2}$$
$$\times \int_{0}^{L} dx \ e^{\beta V(x)} \frac{d}{dx} \varphi_{n+1}(x). \tag{11}$$

In this transformation, we have used the spatial periodicity of V(x) and $c_n(x,t)$ provided the equality $\int_0^L dx \exp[\beta V(x)] \times \hat{J}(x)\varphi_{n-1}(x) = 0$. Taking into account that $\Phi(x) = (m\beta)^{-1/2}\varphi_1(x)$ and using Eq. (9), we obtain the following result from Eq. (11) at n = 1:

$$\Phi(x_0) = \int_0^L dx \, q(x) \int_{x_0}^x dy \left[\rho(y,T) - \rho(y,0)\right] - \sqrt{2}D \int_0^L dx \, q(x) \frac{d}{dx} \varphi_2(x) + \tau_v \int_0^L dx \, q(x) [J(x,0) - J(x,T)], \quad (12)$$

where we have introduced the quantity

$$q(x) = \frac{\exp[\beta V(x)]}{\int_0^L dx \exp[\beta V(x)]}.$$
 (13)

Let us discuss the important consequences of Eq. (12).

In the overdamped limit $(m \to 0, \tau_v \to 0), \varphi_n(x) \to 0$ at $n \ge 2$ and only the first term on the right-hand side of Eq. (12) exists. This term depends on the position x_0 and coincides with the corresponding expression for $\Phi(x_0)$ of Parrondo's lemma [37] if the final probability density $\rho(x,T)$ corresponds to the equilibrium distribution in the potential V(x) and the initial one $\rho(x,0)$ represents the equilibrium distribution in some other potential. On the other hand, inertial contributions given by the second and third terms do not depend on x_0 . The third term describes relaxation processes taking place for the nonequilibrium initial and final states and vanishes when they are equilibrium ones. The second term is the sole contribution of inertia for the equilibrium initial and final states and essentially depends on the potential V(x); it equals zero if the potential is absent since q(x) = 1 and $\varphi_2(x)$ is a periodic function. Thus, at V(x) = 0, inertial effects contribute nothing to the net fraction of particles $\Phi(x_0)$ crossing $x = x_0$ during time T and this fraction is determined only by the equilibrium distribution functions in the initial and final states.

There are two important characteristic times of Brownian motion in a periodic potential V(x) with period L: the diffusion time $\tau_D = L^2/D$ over the distance L and the sliding time $\tau_s = \zeta l^2/V$ in the overdamped regime on the length l, where l < L is the length of the steepest part of the potential V(x)where it varies over V. Inertial effects can be considered small if $\tau_v \ll \tau_D$ and $\tau_v \ll \tau_s$. For $V < k_B T$ and $l \sim L$, diffusion dominates the sliding motion ($\tau_D < \tau_s$), and the second and third terms on the right-hand side of Eq. (12) can be estimated as τ_v/τ_s and τ_v/τ_D , respectively. For $V > k_B T$ ($\tau_D > \tau_s$), the second term is again of order τ_v/τ_s . Thus, when initial and final states are equilibrium ones, the sole inertial correction is given by the second term, which is of order τ_v/τ_s .

Hereinafter, the probability densities $\rho(x,0)$ and $\rho(x,T)$ will be considered as equilibrium distribution functions (in different potentials), so $c_n(x,0) = c_n(x,T) = 0$ at $n \ge 1$. For calculation of inertial corrections of order τ_v/τ_s , one can use Eq. (10) with n = 0, 1, 2 and the identity

$$\hat{J}(x)\frac{\partial}{\partial x} - \frac{\partial}{\partial x}\hat{J}(x) = \frac{1}{\zeta}V''(x)$$
(14)

for the expressions arising after substituting $\varphi_2(x)$ in the equation for $\varphi_1(x)$. By neglecting the term with $\varphi_3(x)$, which gives contributions to $\Phi(x)$ of order $(\tau_v/\tau_s)^2$, we get the following representation for $\Phi(x)$:

$$\Phi(x) = \tilde{J}(x)\varphi_0(x) + O((\tau_v/\tau_s)^2),$$
(15)

where $\tilde{J}(x)$ is given by Eq. (1) and O(z) denotes terms of order z. Then we equate the right-hand sides of Eqs. (9) and (15) and eliminate the term with $\varphi_0(x)$ by multiplying all terms by the factor $\exp[\beta V(x)]/[1 + mV''(x)/\zeta^2]$ with subsequent integration over the spatial period. This leads us to the result

$$\Phi(x_0) = \int_0^L dx \, \tilde{q}(x) \int_{x_0}^x dy [\rho(y,T) - \rho(y,0)] + O((\tau_v/\tau_s)^2),$$
(16)

where

$$\tilde{q}(x) = \frac{\exp[\beta V(x)]/[1 + mV''(x)/\zeta^2]}{\int_0^L dx \exp[\beta V(x)]/[1 + mV''(x)/\zeta^2]} \approx q(x) \left\{ 1 - \frac{m}{\zeta^2} \left[V''(x) - \int_0^L dy \, V''(y)q(y) \right] \right\}$$
(17)

[the approximate connection between $\tilde{q}(x)$ and q(x) is obtained by the linear expansion over $mV''(x)/\zeta^2$].

Note that Eq. (15) [as well as Eqs. (16) and (17) following from it] could be obtained directly from Eq. (8) by substituting the flow of particles in the form $J(x,t) = \hat{J}(x)\rho(x,t)$ with $\hat{J}(x)$ given by Eq. (1). In fact, we have derived the inertial correction in terms of the sought quantity $\Phi(x)$. In this way, we have obtained the exact representation given by Eq. (12), which allows us to discuss the influence of arbitrary particle mass on the net fraction of particles $\Phi(x_0)$ crossing $x = x_0$.

Using the result given by Eq. (16), consider now the adiabatic dichotomic process with periodically repeated fast transitions between two long-lived spatially periodic potential profiles. Let $V_a(x)$ and $V_b(x)$ denote these potential profiles and τ_a and τ_b are their lifetimes. If τ_a and τ_b are much larger than τ_D and τ_s , the distribution function before transitions relaxes to the equilibrium ones $\rho_a(x)$ or $\rho_b(x)$:

$$\rho_i(x) = \frac{\exp[-\beta V_i(x)]}{\int_0^L dx \exp[-\beta V_i(x)]}, \quad i = a, b.$$
(18)

Then the quantity $\Phi(x_0)$ given by Eq. (16) with $\rho(x,T) = \rho_b(x)$, $\rho(x,0) = \rho_a(x)$, and $q(x) = q_b(x)$ [where $q_b(x)$ is given by Eq. (13) with $V(x) = V_b(x)$] can be considered as the net fraction of particles $\Phi_{ab}(x_0)$ crossing $x = x_0$ during time τ_b . The quantity $\Phi_{ba}(x_0)$ can be written similarly. The average particle velocity for the adiabatic dichotomic process with period $\tau = \tau_a + \tau_b$ is defined through the quantities $\Phi_{ab}(x_0)$ and $\Phi_{ba}(x_0)$,

$$\begin{aligned} \langle v \rangle &= \frac{L}{\tau} \tilde{\Phi}, \quad \tilde{\Phi} = \tilde{\Phi}_{ab}(x_0) + \tilde{\Phi}_{ba}(x_0) \\ &= \int_0^L dx [\tilde{q}_b(x) - \tilde{q}_a(x)] \int_{x_0}^x dy [\rho_b(y) - \rho_a(y)], \quad (19) \end{aligned}$$

and does not depend on x_0 in view of $\int_0^L dx [\tilde{q}_b(x) - \tilde{q}_a(x)] = 0$. Hereinafter, all the quantities with a tilde denote the quantities depending on the particle mass.

For further discussion, we can set $x_0 = 0$ without loss of generality and present $\tilde{\Phi}_{ab}(0)$ as a sum of contributions depending and not depending on the particle mass. By using Eqs. (16) and (17) and the identities

$$q'(x) = \beta V'(x)q(x),$$

$$V''(x)q(x) = \beta^{-1}q''(x) - \beta [V'(x)]^2 q(x),$$
 (20)

we get the final result

$$\tilde{\Phi}_{ab}(0) = \left\{ 1 - \frac{m\beta}{\zeta^2} \int_0^L dx [V_b'(x)]^2 q_b(x) \right\} \Phi_{ab}(0) - \frac{m}{\zeta^2} \int_0^L dx V_b'(x) q_b(x) \rho_a(x)$$

$$+\frac{m\beta}{\zeta^2}\int_0^L dx [V_b'(x)]^2 q_b(x)\int_0^x dy [\rho_b(y) - \rho_a(y)],$$
(21)

where

$$\Phi_{ab}(0) = \int_0^L dx \, q_b(x) \int_0^x dy [\rho_b(y) - \rho_a(y)].$$
(22)

Note that if $V_a(x)$ and $V_b(x)$ differ only by amplitude [that is, $V_b(x)/V_a(x) = \text{const}$], the second term on the right-hand side of Eq. (21) equals zero. Let us compare the expression in the large curly brackets of the first term with the expression for the particle mobility in the potential V(x) [19]:

$$\tilde{\mu} = \mu \left[1 - \frac{m\beta}{\zeta^2} \int_0^L dx [V'(x)]^2 q(x) \right],$$

$$\mu = \zeta^{-1} L^2 \left\{ \int_0^L dx \exp[\beta V(x)] \int_0^L dx \exp[-\beta V(x)] \right\}^{-1}.$$
(23)

The ratio of the particle mobilities $\tilde{\mu}$ and μ (with and without inertial corrections, respectively) is always less than unity, which proves that inertial corrections decrease the particle mobility in the periodic potential [19]. The same factor enters the first term in Eq. (21), which leads to decreasing its absolute value.

C. Sawtooth potentials

For the widely used sawtooth potentials

$$V_{a,b}(x) = \begin{cases} V_{a,b}x/l, & 0 < x < l\\ V_{a,b}(L-x)/(L-l), & l < x < L, \end{cases}$$
(24)

only the first term on the right-hand side of Eq. (21) contributes to $\tilde{\Phi}_{ab}(0)$, so by taking the corresponding integrals in Eqs. (21) and (22) and using Eq. (19) we obtain

$$\tilde{\Phi}_{ab}(0) = \frac{1}{2} \kappa \left[1 - \frac{4mb^2}{\beta \zeta^2 l(L-l)} \right] \\ \times \left[\frac{b}{\sinh^2 b} - \frac{a}{a-b} \frac{\sinh(a-b)}{\sinh a \sinh b} \right], \quad (25)$$

$$\tilde{\Phi} = \frac{1}{2}\kappa \left[f(a,b) + \frac{4m}{\beta\zeta^2 l(L-l)}g(a,b) \right],$$

$$f(a,b) = \frac{a}{\sinh^2 a} + \frac{b}{\sinh^2 b} - \frac{a+b}{a-b}\frac{\sinh(a-b)}{\sinh a\sinh b},$$
(26)
$$(a,b) = \frac{a^3}{a^3} + \frac{b^3}{ab(a+b)} +$$

$$g(a,b) = -\frac{a}{\sinh^2 a} - \frac{b}{\sinh^2 b} + \frac{ab(a+b)}{a-b} \frac{\sinh(a-b)}{\sinh a \sinh b},$$

where $a = \beta V_a/2$, $b = \beta V_b/2$, and $\kappa = 1 - 2l/L$ is the asymmetry parameter. Though $1 - 4mb^2/[\beta \zeta^2 l(L-l)] < 1$, it makes sure that the inertial correction always increases the absolute value of the quantity $\tilde{\Phi}$ defining the average particle velocity. This follows from expressions (26) in which f(a,b) > 0 and g(a,b) > 0 at a > |b|, both taking zero value at a = |b| (see Fig. 1). For the on-off flashing ratchet, b = 0, $f(a,0) = \coth a + a/\sinh^2 a - 2/a$, $g(a,0) = a[1 - (a/\sinh a)^2]$, and we arrive at the result of Ref. [19]. In the following sections we show that inertial corrections in



FIG. 1. Functions (a) f(a,b) and (b) g(a,b) determining the main contribution and the inertial correction to the average particle velocity in Eq. (26) for the sawtooth potentials (24).

the case of arbitrary potentials (in contrast to that seen above for the sawtooth potential) do not always increase the absolute value of the particle velocity.

Note that the mass-dependent contribution proportional to g(a,b) diverges at $T \rightarrow 0$ [see Fig. 1(b)] because of the existence of the potential cusps, so the results obtained for the sawtooth potentials have unphysical behavior in the low-temperature limit. On the other hand, when the potential profiles are smooth (described by differentiable functions), the mass-dependent contribution always tends to zero at $T \rightarrow 0$. Indeed, one can make sure that the substitution $q(x) = \delta(x - x_{\text{max}})$ (where x_{max} is the position of the maximum of the potential) nullifies all inertial corrections.

To elucidate the effect of smoothing on the inertial corrections at low temperatures, consider the rounding of the upper cusp point x = l in Eq. (24) with the curvature parameter $-\omega$. Assuming the continuity of the function V(x) and its first derivative V'(x) at the points $x = l \pm \delta$, we obtain the relationship $\omega = V_0 L/[2\delta l(L-l)]$ (with $V_0 = V_{a,b}$) so that $\omega \to \infty$ at $\delta \to 0$. The potential near the point x = l assumes the smooth shape $V(x) = V(x_{\text{max}}) - (1/2)\omega(x - x_{\text{max}})^2$, where $V(x_{\text{max}}) = V_0(1 - \delta/L)$ and $x_{\text{max}} = l + \delta \kappa$. This narrow smooth part of the potential gives the main Gaussian-like contribution to the function q(x) in the low-temperature region $T \ll k_B^{-1} V_0^2 L^{-2} \omega^{-1}$. Then the inertial

correction to q(x) defined by Eq. (17) takes the form

$$\tilde{q}(x)/q(x) - 1 \approx (2\pi)^{-1/2} [mV_0/(\zeta L)^2] (k_B T/V_0)^{1/2} \times [V_0/(\omega L^2)]^{-3/2}.$$

Thus the rounding of the cusp point leads to the disappearance of inertial corrections at temperatures satisfying the stronger inequality $T \ll k_B^{-1} V_0^4 L^{-6} \omega^{-3}$.

III. SYMMETRY PROPERTIES AND HIGH-TEMPERATURE EXPANSION

We start our consideration of symmetry properties with the analysis of the reflection symmetry transformation of $\tilde{\Phi}_{ab}(0)$. The quantity $\tilde{\Phi}_{ab}(0)$ is the functional of the potential functions $V_a(x)$ and $V_b(x)$, which will be denoted in this section by $\tilde{\Phi}_{ab}\{V_{a,b}(x)\}$. Introducing new integration variables x' = L - x and y' = L - y in Eqs. (21) and (22) and taking into account that $V_{a,b}(L - x) = V_{a,b}(-x)$, it is easy to show that

$$\tilde{\Phi}_{ab}\{V_{a,b}(x)\} = -\tilde{\Phi}_{ab}\{V_{a,b}(-x)\}.$$
(27)

This suggests that $\tilde{\Phi}_{ab}\{V_{a,b}(x)\} = 0$ for symmetric periodic potentials with $V_{a,b}(-x) = V_{a,b}(x)$ by an appropriate choice of the origin of coordinates. There is another important type of potential widely used in the description of flashing ratchets, namely, antisymmetric periodic potentials, for which $V_{a,b}(-x) = -V_{a,b}(x)$ by an appropriate choice of the origin of coordinates. An asymmetric sawtooth potential and a potential composed of the sum of two sinusoids (with their periods differing by a factor of 2) are typical representatives of this type. Equation (27) suggests that $\tilde{\Phi}_{ab}\{-V_{a,b}(x)\} = -\tilde{\Phi}_{ab}\{V_{a,b}(x)\}$ is an odd functional of the potential. It is evident that these properties are also valid for $\tilde{\Phi}\{V_{a,b}(x)\} = \tilde{\Phi}_{ab}\{V_{a,b}(x)\} + \tilde{\Phi}_{ba}\{V_{a,b}(x)\}$, which defines the particle velocity [see Eq. (19)].

Note that, in accordance with Ref. [24], the particle velocity is an odd functional of any type of potential in the overdamped limit. This follows from the structure of Eq. (19) with $\tilde{q}_a(x) = q_a(x)$ and $\tilde{q}_b(x) = q_b(x)$ as well as from the fact that q(x) and $\rho(x)$ differ by the sign of the potentials [compare Eqs. (13) and (18)]. The direct consequence of this is that directed motion induced by adiabatic potential sign fluctuations $[V_a(x) = -V_b(x)]$ is impossible for massless particles. With the inertial correction in Eq. (19), $\tilde{\Phi}\{V_{a,b}(x)\}$ is no longer an odd functional of the potentials since now $\tilde{q}_a(x) \neq q_a(x)$ and $\tilde{q}_b(x) \neq q_b(x)$. Thus we arrive at the important conclusion that the directed motion adiabatically driven by potential sign fluctuations, though forbidden in the overdamped limit, becomes possible due to purely inertial effects. Such directed motion is, however, impossible for the commonly used sawtooth potentials and potentials composed of the sum of two sinusoids. It exists for potentials not belonging to symmetric or antisymmetric classes. An example of this kind is discussed further.

The other symmetry properties of the particle velocity follow from the invariance of Eq. (19) under the interchange $a \leftrightarrow b$. By introducing the functions $u(x) = (1/2)[V_a(x) + V_b(x)]$ and $w(x) = (1/2)[V_a(x) - V_b(x)]$ instead of $V_{a,b}(x)$, we can make sure that this invariance leads to the equality

$$\tilde{\Phi}\{u(x), -w(x)\} = \tilde{\Phi}\{u(x), w(x)\},$$
(28)

i.e., the velocity is an even functional of w(x). For massless particles or for inertial particles in antisymmetric periodic potentials, the velocity is an odd functional of u(x) and vanishes at u(x) = 0. In the general case, $\tilde{\Phi}\{-u(x), w(x)\} \neq -\tilde{\Phi}\{u(x), w(x)\}$, which provides the possibility to have directed motion induced by the potential sign fluctuations when u(x) = 0.

Many useful conclusions have been made for hightemperature flashing ratchets working in the overdamped limit [23,24,38,39]. Here we generalize the high-temperature expansion of the particle velocity presented in Ref. [24] to the case where inertial corrections are taken into account. Because we consider the case of adiabatically driven flashing ratchets, the high-temperature expansion valid for $V_{a,b} \ll k_B T$ [where $V_{a,b}$ are the characteristic amplitudes of the potentials $V_a(x)$ and $V_b(x)$] is significantly simplified at $\tau_v \ll \tau_s \ll \tau$. Introducing the Fourier components u_q and w_q (q is integer) of the functions u(x) and w(x), the result can be written in the form

$$\begin{split} \tilde{\Phi} &= \tilde{\Phi}_{3} + \tilde{\Phi}_{4} + O((\beta V_{a,b})^{4}), \\ \tilde{\Phi}_{3} &= \frac{4i}{\pi} \beta^{3} \sum_{\substack{q,q' \neq 0 \\ (q+q'\neq 0)}} \frac{1}{q} \left[1 + \frac{4\pi^{2}m}{\beta\zeta^{2}L^{2}} (q^{2} + q'^{2} + qq') \right] \\ &\times u_{q'} w_{q} w_{-q-q'}, \\ \tilde{\Phi}_{4} &= 4\pi i \frac{m\beta^{3}}{\zeta^{2}L^{2}} \left\{ \sum_{\substack{q,q',q''\neq 0 \\ (q+q'+q''\neq 0)}} \frac{w_{q} w_{q'}}{q} [q'^{2} w_{q''} w_{-q-q'-q''} + (q'^{2} + 2q''^{2} - q^{2}) u_{q''} u_{-q-q'-q''}] \\ &+ (2\pi^{2} + 2q''^{2} - q^{2}) u_{q''} u_{-q-q'-q''} \right\}. \end{split}$$

$$(29)$$

The terms $\tilde{\Phi}_3$ and $\tilde{\Phi}_4$ include the contributions of third and fourth order over u_q and w_q . One can see that $\tilde{\Phi}$ is the even function of w_q , while $\tilde{\Phi}_3$ and $\tilde{\Phi}_4$ are the odd and even functions of u_q , respectively. That is why the sum of $\tilde{\Phi}_3$ and $\tilde{\Phi}_4$, the quantity $\tilde{\Phi}$, does not refer to both the odd and even functions of u_q . In terms of Fourier components, symmetric and antisymmetric potentials V(x)are characterized by the equalities $V_{-q} = V_q$ and $V_{-q} = -V_q$, respectively. The structure of the expressions (29) is that the interchange $q, q', \ldots \rightarrow -q, -q', \ldots$ changes the signs of subexpressions containing q, q', \ldots . Thus $\tilde{\Phi}$ is always equal to zero for symmetric potentials and $\tilde{\Phi}_4$ is equal to zero for antisymmetric potentials, so $\tilde{\Phi}$ becomes the odd function of u_q in the latter case. For the adiabatic potential sign fluctuations $[u(x) = 0, w_q = V_q]$, the only $\tilde{\Phi}_4$ equal to

$$\tilde{\Phi}_4 = 4\pi i \frac{m\beta^3}{\zeta^2 L^2} \sum_{\substack{q,q',q'' \neq 0\\(q+q'+q''\neq 0)}} \frac{q'^2}{q} w_q w_{q'} w_{q''} w_{-q-q'-q''} \quad (30)$$

gives the pure effect of directed motion due to solely inertial corrections. Certainly, all these conclusions agree with the general symmetry analysis presented at the beginning of this section.

Note that the summation in Eq. (29) is simplified in the particular case of the on-off flashing ratchet for which one of the potential profiles is absent and $u_q = w_q$. In this case, using the identity

$$\int_{0}^{L} dx \frac{d}{dx} [V(x) - \langle V \rangle]^{n}$$

= $2\pi in \sum_{\substack{q_{1}, \dots, q_{n-1} \neq 0 \\ (q_{1} + \dots + q_{n-1} \neq 0)}} q_{1} V_{q_{1}} \cdots V_{q_{n-1}} V_{-q_{1} - \dots - q_{n-1}} = 0,$
(31)

where $\langle V \rangle = L^{-1} \int_0^L dx \ V(x) = V_0$, the terms $\tilde{\Phi}_3$ and $\tilde{\Phi}_4$ in Eq. (29) take the form

$$\tilde{\Phi}_{3} = \frac{4i}{\pi} \beta^{3} \sum_{\substack{q,q'\neq 0\\(q+q'\neq 0)}} \frac{1}{q} \left(1 + \frac{4\pi^{2}m}{\beta\zeta^{2}L^{2}} q'^{2} \right) u_{q'} u_{q} u_{-q-q'},$$

$$\tilde{\Phi}_{4} = 16\pi i \frac{m\beta^{3}}{\zeta^{2}L^{2}} \sum_{\substack{q,q',q''\neq 0\\(q+q'+q''\neq 0)}} \frac{q'^{2}}{q} u_{q} u_{q'} u_{q''} u_{-q-q'-q''}. \quad (32)$$

Returning to Eq. (29), we note that the inertial corrections make contributions to $\tilde{\Phi}_3$ and $\tilde{\Phi}_4$ of order $m\beta^2 V_{a,b}^3/(\zeta L)^2$ and $m\beta^3 V_{a,b}^4/(\zeta L)^2$, respectively. Since the main contribution corresponding to the case of m = 0 is of order $(\beta V_{a,b})^3$, the inertial correction of order $m\beta^2 V_{a,b}^3/(\zeta L)^2$ in $\tilde{\Phi}_3$ can be larger than the main contribution at sufficiently large temperatures and at $u(x) \neq 0$. If the signs of these contributions are opposite, the motion reversal can appear. On the other hand, the factor $q^2 + q'^2 + qq'$ in $\tilde{\Phi}_3$ is always positive and the opposite signs of the contributions can occur only at different signs of $\text{Im}(u_{q'}w_qw_{-q-q'})$. To clarify this, consider a potential composed of the first three harmonics with $q = \pm 1, \pm 2, \pm 3$. Then the expression for $\tilde{\Phi}_3$ can be written as

$$\tilde{\Phi}_{3} = -\frac{4}{\pi}\beta^{3} \operatorname{Im}\left(u_{1}w_{1}w_{2}^{*} + 2u_{2}^{*}w_{1}^{2}\right) \\ \times \left[1 + \frac{1}{3}\Lambda + \frac{12\pi^{2}m}{\beta\zeta^{2}L^{2}}\left(1 + \frac{7}{9}\Lambda\right)\right], \\ \Lambda = \frac{\operatorname{Im}(u_{1}w_{2}w_{3}^{*} + 4u_{2}w_{1}w_{3}^{*} + 9u_{3}^{*}w_{1}w_{2})}{\operatorname{Im}\left(u_{1}w_{1}w_{2}^{*} + 2u_{2}^{*}w_{1}^{2}\right)}.$$
 (33)

For a widely used potential composed of the sum of two sinusoids or for more general case of a two-harmonics potential ($u_3 = w_3 = 0$), parameter Λ equals zero and the inertial correction can only increase the absolute value of the average velocity. When the shape of potential profiles becomes more complicated (more extrema on the spatial period), the possibility of motion reversal arises. One can see that the main contribution and the inertial correction have the same sign except for the narrow region $-3 < \Lambda < -9/7$. For potentials with parameters belonging to this region, the motion reversal appears at the temperature $T = -(2\pi)^{-2}(\zeta^2 L^2/mk_B)(3 + \Lambda)/(9 + 7\Lambda)$. This conclusion generalizes the previously obtained result in Ref. [19] where the particular case of an on-off flashing ratchet with a three-sinusoidal potential has been considered.

By collecting the first three harmonics in Eq. (30), we get the expression

$$\tilde{\Phi}_4 = -\frac{\pi}{3} \frac{m\beta^3}{\zeta^2 L^2} \operatorname{Im} \left(16w_1^3 w_3^* + 9w_1 w_2^{*2} w_3 \right), \qquad (34)$$

from which it follows that the directed motion is impossible for the adiabatic sign fluctuations of simple potentials composed only of the first two harmonics. It can be checked that this conclusion is valid not only in the high-temperature region, but also at all temperatures. Thus, a complex potential shape is necessary to visualize inertial effects.

IV. DISCUSSION

In this section we estimate the inertial correction and show that, despite its smallness for nano-objects, it can have a major impact on the emergence of the directed motion. Then we present a few illustrative examples.

As shown in Sec. II B, the significance of the inertial effect can be characterized by the ratio of two characteristic times τ_v and τ_s . To quantify the strength of the effect, we introduce the dimensionless parameter $\varepsilon = (2\pi)^2 \tau_v / \tau_s$, which is $(2\pi)^2 \approx$ 40 times larger than τ_v / τ_s [due to the more accurate estimate of the second derivative of a periodic function V(x) of the simplest form $V \cos(2\pi x/L)$: $V''(x) \sim (2\pi/L)^2 V$ instead of $V''(x) \sim V/L^2$]. Then, for a spherical particle of density ρ and radius *R* moving in a medium with viscosity η , we have

$$\varepsilon = (2\pi)^2 \frac{\tau_v}{\tau_s} = (2\pi)^2 \frac{mV}{\zeta^2 L^2} = \frac{4\pi}{27} \frac{\rho RV}{\eta^2 L^2} \sim \frac{\rho}{\eta^2} \frac{V}{L}.$$
 (35)

(Here we have used that $m = (4\pi/3)\rho R^3$, $\zeta = 6\pi R\eta$, and finally set $R \sim L$). For the dynamical viscosity of water $\eta \approx$ 10^{-3} kg/(m s) , $\rho \sim 10^3 \text{ kg/m}^3$, $V \sim 5 k_B T \approx 20 \text{ pN nm}$ (at T = 300 K), and $L \sim 1 \text{ nm}$, we obtain $\tau_v \approx 2 \times 10^{-13} \text{ s}$, $\tau_s \approx$ 10^{-9} s , and $\varepsilon \sim 10^{-2}$, so inertial corrections are not extremely small and can be taken into account as needed.

The value of the inertial correction can be significantly increased if the effective mass *m* of a carrier is modified by picking up a cargo of large mass *M*. In accordance with Eq. (33) at $-3 < \Lambda < -9/7$, it is possible that the unloaded carrier with mass *m* goes to the right while the loaded carrier with mass *m* + *M* goes to the left. Such a carrier can be used to transfer the cargo from one point to another like in the molecular shuttle model [14]. One more way to increase the inertial correction is to enhance potentials in narrow regions. Narrow corrugated channels can be described by an effective entropic potential in which large entropic barriers correspond to narrow pore widths. That is why inertial corrections cannot be neglected as long as the channel bottlenecks are narrower than the appropriate particle diffusion length [40,41].

What is even more important is that the inertial corrections, despite their smallness, may assist in overcoming some of the symmetry restrictions inherent in the overdamped limit and hence in producing the directed motion otherwise forbidden. Based on this impressive observation, we suggest a relevant thought experiment illustrating the qualitative significance of the inertial effect. Unlike the experiment [42], where the potential is switched on and off, we propose to alternate the potential



FIG. 2. Average particle velocity (in units of the dimension parameter $v_0 = mV/\zeta^2 L \tau$) versus the dimensionless parameter V/k_BT for the purely inertial effect under adiabatic sign fluctuations of the potential (36). The solid, dot-dashed, and dashed curves correspond to $A_2 = 0.25$, 0.6, and 1.0 at $A_3 = -0.5$ in Eq. (36) [see the corresponding curves in Fig. 3(a), where the potential profiles V(x) are depicted].

energy sign either by changing the sign of the potential applied to a charged particle (e.g., switching the electrode polarities) or by sign fluctuations of particle characteristics (the charge, dipole moment, etc.). In the proposed experiment, the directed motion results from purely inertial effects (and is forbidden for massless particles). Of course, as explained in Sec. III, the potential in this experiment should be asymmetric, but in no way antisymmetric, so the most common potential profiles, such as sawtooth and double-sine ones, are not suitable in this case.

For illustrative purposes, let us choose the potential

$$V(x) = V[\sin(2\pi x/L) + A_2 \sin(4\pi x/L) + A_3 \cos(6\pi x/L)]$$
(36)

and assume that $V(x) \equiv V_a(x) = -V_b(x)$. The numerically calculated dependence of the quantity $\tilde{\Phi}$ on the dimensionless parameter V/k_BT [see Eq. (19)] is shown in Fig. 2. The potential consists of the first three harmonics with $V_1 = -V_1^* =$ V/2i, $V_2 = -V_2^* = VA_2/2i$, and $V_3 = V_3^* = VA_3/2$, so the high-temperature region of the dependence is described by Eq. (34) with $w_q = V_q$. In the definite region of the parameters $(A_2 > 0.6 \text{ and } A_3 = -0.5)$, the average velocity (determined by $\tilde{\Phi}$) can change its sign, which leads to the current reversal. Figure 3(a) illustrates that this effect is connected with the appearance of additional potential extrema of V(x).

In principle, many ratchet properties depend on the extremum positions of the potentials $V_a(x)$ and $V_b(x)$. If the extrema are appropriately shifted relative to each other, Brownian motion is not involved in the transport generation [9] and the ratchet efficiency is more than an order of magnitude larger than for the models involving diffusion [43,44]. The role of the shape of the potentials (and, in particular, their extrema) becomes crucial as soon as the inertial effects come into play. This follows from the fact that the inertial correction in Eq. (1) is determined by the second derivative of V(x). That is why the inertial properties of ratchets with smooth potentials containing few or many extrema in the period are different. The



FIG. 3. Potential profiles V(x)/V defined by (a) Eq. (36) with $A_2 = 0.25$, 0.6, and 1.0 at $A_3 = -0.5$ (the solid, dot-dashed, and dashed curves, respectively) and (b) Eq. (37) with A = 0, -9/14, and -27/98 (the solid, dot-dashed, and dashed curves, respectively). The dotted curve in (b) corresponds to the sawtooth potential inscribed in the two-sinusoid potential (37) at A = 0 by the least-squares method.

high-temperature analysis shows that the periodic potentials consisting of the first three harmonics provide the motion reversal if the ratio of harmonic amplitudes obeys a definite relationship.

Consider the potential

$$V(x) = V[\sin(2\pi x/L) + (1/4)\sin(4\pi x/L) + A\sin(6\pi x/L)]$$
(37)

as an example. As follows from Eq. (33), the net drift in the on-off flashing ratchet exhibits the motion reversal in the high-temperature region if the parameter $A = (3/14)\Lambda$ belongs to the interval (-9/14, -27/98). As Fig. 3(b) indicates, the boundaries of this interval approximately correspond to the appearance of additional potential extrema of the potential described by Eq. (37). The exact conditions for the appearance of additional extrema are A = -1/2 and -1/6.

An even greater sensitivity of inertial corrections to the potential shape is manifested in the cases where potential extrema are described by cusps rather than by twicedifferentiable functions. The two-sinusoid potential profile defined by Eq. (37) with A = 0 and the appropriate shifted sawtooth potential defined by Eq. (24) can be approximately superposed with good accuracy by the least-squares method at $V_{a,b} \equiv V_0 = 2.517V$ and l = 0.3309L [compare the solid and dotted curves in Fig. 3(b)]. The difference in the character of the extrema leads to the different behavior of the velocity in the low-temperature region. Indeed, while the temperature dependences of the sawtooth and two-sinusoid potentials



FIG. 4. Average particle velocity (in units of the dimension parameter $v_0 = L/\tau$) versus the dimensionless parameter V_a/k_BT for the sawtooth (curves with markers) and two-sinusoid (curves without markers) potentials, the amplitudes of which take the values (a) V_a and $V_b = 0$ (on-off flashing ratchet) and (b) V_a and $V_b = -V_a/3$. The sawtooth potentials are inscribed in the corresponding two-sinusoid potentials by the least-squares method. The solid and dashed curves correspond to the calculations with $(mV/\zeta^2L^2 = 0.005)$ and without (m = 0) inertial effects.

are qualitatively the same in the high-temperature region, they essentially differ in the low-temperature region (compare the curves with and without markers in Fig. 4). We can see that the inertial correction contribution tends to zero at $T \rightarrow 0$ for the two-sinusoid potentials, whereas the sawtooth potentials demonstrate saturation for the on-off flashing ratchet [Fig. 4(a)] and divergence for the flashing ratchet with $V_b(x) = -V_a(x)/3$ [Fig. 4(b)]. An interesting peculiarity is that the inertial correction increases the velocity at all temperatures with the exception of the low-temperature region for ratchets with nonzero smooth (two-sinusoid) potentials in both states.

The main quantity determining the properties of adiabatically driven ratchets is the net fraction of particles $\tilde{\Phi}_{ab}(x_0)$ crossing $x = x_0$ over a long time after a fast transition from a periodic potential profile $V_a(x)$ to $V_b(x)$. In Sec. II B, both exact and approximate expressions for $\tilde{\Phi}_{ab}(x_0)$, being a generalization of Parrondo's lemma to include the inertia term, have allowed us to conclude that inertial contributions to $\tilde{\Phi}_{ab}(x_0)$ do not depend on x_0 and exist only if $V_b(x) \neq 0$. In Sec. III the explicit expressions for $\tilde{\Phi}_{ab}(x_0)$ obtained for the case of small inertial corrections have allowed us to reveal the symmetry properties and to find the high-temperature expansion of the average particle velocity [see Eq. (19) as a definition] for adiabatic dichotomic process. It is worth mentioning that the quantity $\tilde{\Phi}_{on-off} = \tilde{\Phi}_{ab}(x_0) + \tilde{\Phi}_{ba}(x_0)$ determining the average velocity for an adiabatically driven on-off flashing ratchet [$V_a(x) = V(x), V_b(x) = 0$] also determines the average velocity for the rocking ratchet adiabatically driven by symmetric dichotomic fluctuations of potentials $V(x) \pm Fx$ at small force F [19]:

$$\langle v \rangle_{\rm rock} = -\beta L F^2 \tilde{\mu} \, \tilde{\Phi}_{\rm on-off} + O((\beta F L)^4),$$
 (38)

where mobility $\tilde{\mu}$ is given by Eq. (23). Thus, the average velocity is proportional to product of the mobility and the main characteristic of the on-off flashing ratchet taken with opposite sign.

V. CONCLUSIONS

To summarize, we have demonstrated that the inertial correction enhances the flashing ratchet effect in the

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high-temperature region for simple potential profiles represented by the first two harmonics. With the special choice of potentials represented by at least the first three harmonics, the correction gives rise to the motion reversal in the hightemperature region. In the low-temperature region, inertia decreases the absolute value of the average velocity with the exception of the on-off flashing ratchet, where diffusion is important. One notable observation is that the directed motion adiabatically driven by potential sign fluctuations, forbidden in the adiabatic limit, becomes possible due to purely inertial effects for potentials not belonging to symmetric and antisymmetric profiles.

ACKNOWLEDGMENTS

This work was supported by National Chiao Tung University and Academia Sinica. V.M.R. thanks the Complex Program for Basic Research of the National Academy of Sciences of Ukraine for partial support (Grant No. 3/14-H). Yu.A.M. thanks the Russian Foundation for Basic Research for partial support (Grant No. 14-03-00343). V.M.R. and Yu.A.M. gratefully acknowledge the kind hospitality received from the Institute of Atomic and Molecular Sciences.

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