Ratchet transport for a chain of interacting charged particles

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We study analytically and numerically the overdamped, deterministic dynamics of a chain of *charged*, interacting particles driven by a longitudinal alternating electric field and additionally interacting with a smooth ratchet potential. We derive the equations of motion, analyze the general properties of their solutions and find the drift criterion for chain motion. For ratchet potentials of the form of a double-sine and a phase-modulated sine it is demonstrated that both, a so-called integer and fractional transport of the chain, can occur. Explicit results for the directed chain transport for these two classes of ratchet potentials are presented.

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I. INTRODUCTION

During the last decade, much attention was devoted to the study of the so-called ratchet effect, i.e., the rectifying of nondirectional stochastic or deterministic driving forces into directional motion of (quasi-)particles (for comprehensive reviews, see, for example, Refs. [1–5]). This phenomenon is of prominent practical importance and constitutes a theoretical basis for Brownian motors [4,5], particle segregation [6,7], reduction of a vortex density [8], smoothing of a crystalline surface [9–11], and many others [1,2,5].

There exists a large variety of systems that exhibit the ratchet effect. Those of them where transported particles are exposed to a driving force and move in an asymmetric periodic (ratchet) potential form a class of so-called rocking ratchets [12]. In turn, stochastic and deterministic rocking ratchets are distinguished, depending on whether they are driven only deterministically, or whether they are subjected also to stochastic forces. The fluctuating noise component in turn allows for activated escape events [13] even at subthreshold driving. The stochastic situation has been studied for both noninteracting [12,14,15] and interacting [16–19] particles, and the strong influence of the interparticle interactions was revealed. In contrast, the deterministic case has been investigated primarily for noninteracting particles [20–24]. At variance with earlier work [25] focusing on the transport of driven linear defects (i.e., elastic chains) which diffuse on asymmetric substrates at finite temperatures, the objective of this study is to investigate the transport properties of a chain of *charged*, interacting particles in deterministic rocking ratchets. This model can be used for the investigation of one-dimensional crystals in carbon nanotubes [26] and ion transport through synthetic nanopores [27].

The paper is organized as follows. In Sec. II, we derive the reduced system of two equations that describes the deterministic, overdamped motion of a chain. We carry out the general analysis of this system in Sec. III. Specifically, we introduce a class of its steady-state solutions, analyze the chain dynamics in the inverted potential, and derive the drift criterion of a chain. In Sec. IV, we study analytically and numerically the overdamped transport of a chain in the double-sine ratchet potential. Concluding remarks are contained in Sec. V, and the phase-modulated sine potential is introduced in the Appendix.

II. EQUATIONS OF MOTION

We study a chain of charged particles of identical masses M that interact among each other via the Coulomb interaction, a repulsive interaction, and additionally with a (substrate) ratchet potential $V(x)$ having the period d. Moreover, the particles are driven by a longitudinal alternating electric field $E(t)$ of a temporal period $2T$. Therefore, the total potential energy of a chain V_{tot} includes the interaction energy V_{int} and the potential energies V_{r} and V_{el} formed by a ratchet potential and an electric field, respectively. Assuming that any neighboring particles have opposite charges, i.e., $q_{i+1}=-q_i$ and $|q_i|=q$, and a repulsive interaction depends on the interparticle distance as $|x_i-x_j|^{-r}$ [$x_i=x_i(t)$ is the coordinate of the ith particle, $r>1$ since it prevents the unbounded contraction of a chain], these three parts of the total energy can be written as follows:

$$V_{\text{int}} = \frac{1}{2}\sum_{i,j}{}' \frac{q_i q_j}{|x_i - x_j|} + \frac{b}{2}\sum_{i,j}{}' \frac{1}{|x_i - x_j|^r},$$
$$V_r = \sum_i V(x_i), \quad V_{\text{el}} = -\sum_i q_i x_i E(t). \tag{2.1}$$

Here b is a dimensioned parameter characterizing the strength of the repulsive interaction, and the primes on the summation signs imply that $i \neq j$.

Along with the potential force $-\partial V_{\text{tot}}/\partial x_i$ on the ith particle a friction force $-\lambda \dot{x}_i$ (λ is a damping coefficient) is also acting. Then the equation of motion of each, individual particle reads

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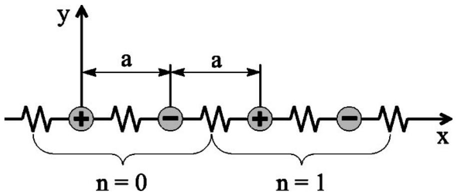

FIG. 1. Schematic representation of the ionic chain.

$$M\ddot{x}_i + \lambda\dot{x}_i + \frac{\partial V_{\text{int}}}{\partial x_i} = q_i E(t) + f(x_i), \qquad (2.2)$$

where $f(x)=-V'(x)$ (here and below, the prime denotes the derivative with respect to the argument of the function) is a force field generated by a ratchet potential. The set of equations (2.2) is very complicated for a detailed analysis of the chain motion because they are coupled and contain the nonlinear terms $\partial V_{\text{int}}/\partial x_i$ and $f(x_i)$. Nevertheless, the problem of coupled ratchets does possess a very rich behavior, such as anomalous hysteresis, self-oscillations, absolute negative mobility, etc. [28], and thus is demanding to analyze. Since our aim is to study a ratchet mechanism of the chain transport, the nonlinear nature of the ratchet force $f(x_i)$ must be taken into account, while the nonlinearity of the interaction force $\partial V_{\text{int}}/\partial x_i$ seemingly is not so essential. Therefore, in order to partially simplify the problem, we restrict ourselves to a harmonic approximation for V_{int}. This approximation is valid if during the period $2T$ of the action of the electric field $E(t)$ the particle displacements are much less than the equilibrium distance a [at $V(x)=0$ and $E(t)=0$] between the nearest particles.

According to the findings in [29], a periodic chain with equidistant particles exists only if $r>r_2\approx 2.799$; in the opposite case the minimum of V_{int} occurs for a chain with infinite period. Assuming that the condition $r>r_2$ holds, it is convenient to introduce the coordinates $2na+x_n^+$ and $(2n+1)a+x_n^-$ [$n(n=0,\pm1,\ldots)$ numbers the chain cells which contain two particles (see Fig. 1)] of positive and negative charges, respectively. The equations of motion for the displacements $x_n^+=x_n^+(t)$ and $x_n^-=x_n^-(t)$ of these particles from the equilibrium positions follow from Eq. (2.2). Using the harmonic approximation for V_{int} [29] and the notations $E(t)=Eh(t)$ and $f(x)=f_0 g(x)$, where E is the amplitude of $E(t)$, $f_0=|\min f(x)|$, and $h(t)$ and $g(x)$ are the dimensionless electric and ratchet force fields, respectively, the equations of motion assume the form

$$\ddot{x}_n^+ + 2\Omega_\lambda \dot{x}_n^+ + \Omega^2 \sum_m \tilde{B}_{2(n-m)-1}(x_n^+ - x_m^-) + \Omega^2 \sum_{m\neq n} \tilde{B}_{2(n-m)}(x_n^+ - x_m^+) = Ah(t) + Rg(x_n^+),$$

$$\ddot{x}_n^- + 2\Omega_\lambda \dot{x}_n^- + \Omega^2 \sum_m \tilde{B}_{2(n-m)+1}(x_n^- - x_m^+) + \Omega^2 \sum_{m\neq n} \tilde{B}_{2(n-m)}(x_n^- - x_m^-) = -Ah(t) + Rg(x_n^-). \qquad (2.3)$$

Here $\Omega_\lambda=\lambda/2M$, $\Omega^2=q^2/Ml^3$, $l=(b/q^2)^{1/(r-1)}$ is the length scale, $A=qE/M$, $R=f_0/M$,

$$\tilde{B}_n = \frac{1}{\gamma_1^3(r)}\left[2\frac{(-1)^n}{|n|^3} + \frac{(r+1)\ln 2}{\zeta(r)|n|^{r+2}}\right], \qquad (2.4)$$

$\gamma_1(r)=[r\zeta(r)/\ln 2]^{1/(r-1)}$, $a=l\gamma_1(r)$, and $\zeta(r)=\Sigma_{n=1}^{\infty} n^{-r}$ is the Riemann zeta function. Note that Eqs. (2.3) are valid if the condition $|x_n^\pm - x_m^\pm| \ll a$ holds for all n and m. It provides the applicability of the harmonic approximation and, as can be shown readily, it does not prohibit the existence of unbounded (at $t\to\infty$) solutions of these equations that describe the chain transport.

The system of equations (2.3) constitutes a theoretical basis for the study of ratchet transport of ionic chains within the harmonic approximation for the interparticle interactions. Unfortunately, at present there are no methods to find and analyze its unbounded solutions. Since this system contains an infinite number of coupled nonlinear equations, the development of such methods is a very complicated problem which, in general, can be solved only approximately. However, we will show that, in a particular case, the chain transport can be studied in detail without approximations.

More specifically, we consider the case when the equilibrium chain period a in absence of the ratchet potential $V(x)$ is a whole integer of the potential period d, i.e., $a=Ld$, where L is a natural number. Although this commensurability assumption is rather restrictive (small discrepancy between a and Ld violates the chain periodicity in presence of the ratchet potential), it permits us to reduce the infinite system (2.3) to the system of only two equations. Indeed, if the initial conditions $x_n^\pm(0)=x_\pm$ and $\dot{x}_n^\pm(0)=v_\pm$ ($x_\pm$ and $v_\pm$ are the initial displacements and velocities of the positive and negative charges) hold for all n, then all positively charged particles and all negatively charged particles move identically. Designating in this case $x_n^\pm=x^\pm$, from Eqs. (2.3) we get

$$\ddot{x}^+ + 2\Omega_\lambda\dot{x}^+ + \frac{1}{2}\omega^2(1)(x^+ - x^-) = Ah(t) + Rg(x^+),$$

$$\ddot{x}^- + 2\Omega_\lambda\dot{x}^- + \frac{1}{2}\omega^2(1)(x^- - x^+) = -Ah(t) + Rg(x^-), \qquad (2.5)$$

where $\omega^2(1)=2\Omega^2\Sigma_m\tilde{B}_{2m-1}$ is the squared frequency of optical vibrations of chain particles that corresponds to the dimensionless wave number $\kappa=1$ [29]. Note that Eqs. (2.5) are derived from Eqs. (2.3) without approximations and they precisely describe the chain dynamics in the examined case. However, since a nonlinear oscillator driven by a periodic force can exhibit chaotic behavior that is characterized by strong sensitivity to initial conditions [30], the chain dynamics governed by Eqs. (2.3) and (2.5) can be quite different if the corresponding initial conditions slightly differ. With increasing damping constant the chaotic domain in the parameter space is reduced, therefore we expect (and this is confirmed by simulations) that it vanishes in the overdamped limit ($\Omega_\lambda\to\infty$). In other words, the chain dynamics in this limit is expected to be regular and predictable.

Introducing the dimensionless time $\tau=t/2T$ and the dimensionless particle displacements $w\equiv w(\tau)=x^+(2T\tau)/d$ and

$u \equiv u(\tau) = x^{-}(2T\tau)/d$, from Eqs. (2.5) we obtain in the overdamped limit

$$\chi \frac{dw}{d\tau} = \phi H(\tau) - \frac{1}{2}(w-u) + \mu G(w),$$
$$\chi \frac{du}{d\tau} = -\phi H(\tau) - \frac{1}{2}(u-w) + \mu G(u). \quad (2.6)$$

Here $\chi = \Omega_\lambda / T\omega^2(1)$ and $\phi = A/d\omega^2(1)$ are the dimensionless parameters characterizing the electric field frequency and amplitude, respectively, $H(\tau) = h(2T\tau)$, $\mu = R/d\omega^2(1)$ is the dimensionless parameter characterizing the ratchet force amplitude, $G(\overline{x}) = g(d\overline{x})$, $\overline{x} = x/d$ is the dimensionless coordinate, and according to Eq. (2.4)

$$\omega^2(1) = \Omega^2 \left(\frac{\ln 2}{r\zeta(r)} \right)^{3/(r-1)} \times \left[4 \ln 2(1 - 2^{-r-2})(r+1)\frac{\zeta(r+2)}{\zeta(r)} - 7\zeta(3) \right]. \quad (2.7)$$

Assuming that all particles at $t=0$ are in equilibrium (their equilibrium positions are those in absence of the ratchet potential), the initial conditions for Eqs. (2.6) are written as $w(0) = u(0) = 0$. The system of equations (2.6) provides a very useful tool for studying the transport properties of ionic chains. Indeed, on the one hand, it is a rather simple set of only two coupled, ordinary differential equations of first order and, on the other hand, it accounts for the interparticle interactions and the action of the ratchet force.

By the definitions, the functions $H(\tau)$ and $G(\overline{x})$ have unit periods, $H(\tau+1) = H(\tau)$ and $G(\overline{x}+1) = G(\overline{x})$, and zero mean values, $\int_0^1 H(\tau) d\tau = 0$ and $\int_0^1 G(\overline{x}) d\overline{x} = 0$. The latter condition shows that the total work, delivered by the ratchet force field $f(x)$ on any interval of length d, equals zero. In general, the functions $H(\tau)$ and $G(\overline{x})$ can be both, continuous and discontinuous. But here, to simplify the numerical solution of Eqs. (2.6), we consider them as smooth, differentiable functions.

In what follows, to find the drift criterion of a chain, we shall use the dimensionless potential energy $U = U(w,u,\tau)$ that reduces Eqs. (2.6) to the form

$$\chi \frac{dw}{d\tau} = -\frac{\partial}{\partial w} U, \quad \chi \frac{du}{d\tau} = -\frac{\partial}{\partial u} U. \quad (2.8)$$

Introducing the representation $V(x) = V_0 W(\overline{x})$, where $V_0 > 0$ and $W(\overline{x})$ is the dimensionless ratchet potential, and by use of the definitions of $f(x)$ and f_0, we get $f_0 = (V_0/d) \max W'(\overline{x})$ and

$$G(\overline{x}) = -W'(\overline{x}) / \max W'(\overline{x}). \quad (2.9)$$

Finally, from the inspection of the right-hand sides of Eqs. (2.6) and (2.8) we obtain

$$U = -\phi \sin(2\pi\tau)(w-u) + \frac{1}{4}(w-u)^2 + \mu[W(w) + W(u)] / \max W'(\overline{x}). \quad (2.10)$$

III. GENERAL RESULTS

A. Periodicity analysis

In order to exclude from consideration transient processes, we need to examine the asymptotic, steady-state solutions of Eqs. (2.6). These solutions depend on many factors, such as the form of a ratchet potential, characteristics of a chain, initial conditions, etc., and consequently can be studied in detail only numerically. However, using the periodicity of $H(\tau)$ and $G(\overline{x})$, it is possible to introduce different classes of the steady-state solutions. One particular such class is generated by those periodic solutions of Eqs. (2.6) that asymptotically $\tau \to \infty$ obey

$$w(\tau+k) = w(\tau) + K, \quad u(\tau+k) = u(\tau) + K, \quad (3.1)$$

where k and K are natural and integer numbers, respectively, that have no common factors. In this case, the periodicity and increment of the functions $w(\tau)$ and $u(\tau)$ are described by the pair $\{k, K\}$ which at $K \neq 0$ corresponds to the drift state of a chain. Since the reduced chain displacement $\Delta w = \lim_{\tau\to\infty}[w(\tau+k) - w(\tau)]/k$ that occurs during one period of $H(\tau)$ is given by $\Delta w = K/k$ (note that the harmonic approximation is valid if $|K|/k \ll L$), we shall term the chain transport characterized by the pair $\{k, K\}$ as "integer" if $k=1$, and "fractional" if $k \geqslant 2$.

According to the conditions (3.1), the average velocity of a chain or drift velocity $v = (d/2T)\lim_{\tau\to\infty} w(\tau)/\tau [= (d/2T)\lim_{\tau\to\infty} u(\tau)/\tau]$ is reduced to

$$v = \frac{d}{2T} \lim_{\tau\to\infty} \frac{w(\tau+k) - w(\tau)}{k}, \quad (3.2)$$

which, in turn, yields $v = v_0 \overline{v}$, where $v_0 = d\omega^2(1)/2\Omega_\lambda$ and $\overline{v} = \chi K/k$ is the dimensionless drift velocity. Taking into account that the periodicity and drift parameters k and K depend, in general, on all parameters of Eqs. (2.6), we conclude that $\overline{v}$ is a discontinuous linear function of χ.

We emphasize that this class does not exhaust all the steady-state solutions of Eqs. (2.6). Moreover, the symmetry approach does not permit us to find their unique steady-state solution in each concrete case. Therefore, to study the transport properties of a chain, it is necessary to numerically find the solution of Eqs. (2.6) (with zero-valued initial conditions) and examine its long-time behavior depending on the form of a ratchet potential, the electric field characteristics, and the chain parameters.

B. Chain dynamics in the inverted potential

We now consider the chain dynamics in the inverted potential $V_{\mathrm{in}}(x) = V(-x)$ that generates the reduced force field $G_{\mathrm{in}}(\overline{x})$. According to Eqs. (2.6), in such a potential the displacements $w_{\mathrm{in}}(\tau)$ and $u_{\mathrm{in}}(\tau)$ of positively and negatively charged particles from their equilibrium positions are governed by the equations of motion

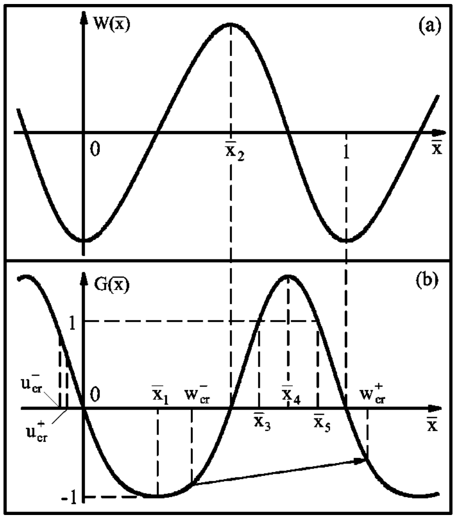

FIG. 2. Form of the reduced ratchet potential $W(\overline{x})$, part (a), and the corresponding force field $G(\overline{x})$, part (b), that are under consideration in this work.

$$\chi\frac{dw_{\rm in}}{d\tau} = \phi H(\tau) - \frac{1}{2}(w_{\rm in} - u_{\rm in}) + \mu G_{\rm in}(w_{\rm in}),$$
$$\chi\frac{du_{\rm in}}{d\tau} = -\phi H(\tau) - \frac{1}{2}(u_{\rm in} - w_{\rm in}) + \mu G_{\rm in}(u_{\rm in}) \tag{3.3}$$

$[w_{\rm in}(0)=u_{\rm in}(0)=0]$. Taking into account that $G_{\rm in}(-\overline{x})=-G(\overline{x})$, one can show from Eqs. (2.6) and (3.3) that $w_{\rm in}(\tau)=-u(\tau)$ and $u_{\rm in}(\tau)=-w(\tau)$. This implies that if the chain dynamics is known for the ratchet potential $V(x)$, then it is also known for the corresponding inverted potential $V_{\rm in}(x)$ as well. In particular, if a chain in the potential $V(x)$ drifts along the x-axis, then in the inverted potential $V_{\rm in}(x)$ it drifts in the opposite direction with the same average velocity, i.e., $v_{\rm in}=-v$. We emphasize that in reflection-symmetric potentials the drift state of a chain, i.e., a chain state with $v\neq 0$, does not exist. Indeed, as it is shown above, the general condition $v_{\rm in}=-v$ must hold. On the other hand, if $V(-x)=V(x)$, then $V_{\rm in}(x)=V(x)$ and so the condition $v_{\rm in}=v$ also must hold. It is obvious that both conditions are met simultaneously only if $v=0$.

The above mentioned features of the chain dynamics permit us to study the overdamped transport of ionic chains only in those ratchet potentials that induce the chain drift, say, with positive velocity v. In the following we consider the simple-structured ratchet potentials. We assume that the reduced potentials $W(\overline{x})$ and the corresponding force fields $G(\overline{x})$ have only one maximum and one minimum on unit period and, in addition, max $G(\overline{x})>1$, (see Fig. 2).

C. Drift criterion

To find the conditions that lead to the drift state of a chain, we rewrite Eqs. (2.6) as

$$\chi\frac{dw}{d\tau} = \phi H(\tau) - \frac{1}{2}(w - u) + \mu G(w),$$
$$\chi\frac{d}{d\tau}(w + u) = \mu[G(w) + G(u)], \tag{3.4}$$

where the second equation is obtained by summing (2.6). If $\mu/\chi\to 0$, then it reduces to the equation $d(w+u)/d\tau=0$, which with $w(0)=u(0)=0$ yields $w(\tau)=-u(\tau)$. Using this relation and the condition that $\mu/\chi\to 0$, the first equation in (3.4) takes the form $\chi dw/d\tau+w=\phi H(\tau)$. Its solution

$$w(\tau) = \frac{\phi}{\chi}\int_0^\tau H(\tau-\tau')e^{-\tau'/\chi}d\tau' \tag{3.5}$$

shows that

$$w(\tau+1) = w(\tau) + \frac{\phi}{\chi}e^{-\tau/\chi}\int_0^1 H(-\tau')e^{-\tau'/\chi}d\tau', \tag{3.6}$$

and so $w(\tau+1)=w(\tau)$ for $\tau\to\infty$. This means that the drift state of a chain does not exist if $\mu/\chi\to 0$. Since the parameter χ is proportional to the electric field frequency, its decrease leads to an increase of the maximal particle displacements, yielding $v|_{\chi>0}=0$ if $v|_{\chi=0}=0$. The last condition is violated if the amplitude parameter ϕ is large enough. Therefore, to find the drift criterion of a chain, we need to consider its dynamics as $\chi\to 0$.

According to Eqs. (3.4), in the stationary regime $(\chi\to 0)$ the chain dynamics is described by the system of nonlinear equations

$$\phi H(\tau) - \frac{1}{2}(w - u) + \mu G(w) = 0,$$
$$G(w) + G(u) = 0. \tag{3.7}$$

If for each time the chain energy U has a minimum value, i.e., if in virtue of Eqs. (3.7) the conditions

$$\frac{\partial^2 U}{\partial w^2} > 0, \quad \frac{\partial^2 U}{\partial w^2}\frac{\partial^2 U}{\partial u^2} - \left(\frac{\partial^2 U}{\partial w\partial u}\right)^2 > 0 \tag{3.8}$$

hold, then $v|_{\chi=0}=0$. The latter condition in (3.8), $G'(w)+G'(u)-2\mu G'(w)G'(u)<0$, is weaker than the former, $2\mu G'(w)-1<0$. Hence, it is violated first under increasing of the parameter ϕ. Let $\phi_{\rm cr}$ be the critical value of the parameter ϕ such that, for $\phi=\phi_{\rm cr}$, the latter inequality in (3.8) is reduced to equality at some instant of time. It is obvious that this occurs for the first time at $\tau=\tau_1$, where $\tau_1(<1)$ is the minimal solution of the equation $H(\tau_1)=1$. Then, using the first equation in (3.7), we obtain

$$\phi_{\rm cr} = \frac{1}{2}(w_{\rm cr}^- - u_{\rm cr}^-) - \mu G(w_{\rm cr}^-), \tag{3.9}$$

where $w_{\rm cr}^-=w(\tau_1-0)$ and $u_{\rm cr}^-=u(\tau_1-0)$ are defined by the system of equations

$$G'(w_{\rm cr}^-) + G'(u_{\rm cr}^-) - 2\mu G'(w_{\rm cr}^-)G'(u_{\rm cr}^-) = 0,$$
$$G(w_{\rm cr}^-) + G(u_{\rm cr}^-) = 0. \qquad (3.10)$$

At $\phi=\phi_{\rm cr}$ and $\tau=\tau_1+0$ the chain particles instantly move to the new equilibrium positions $w_{\rm cr}^+ = w(\tau_1+0)$ and $u_{\rm cr}^+ = u(\tau_1+0)$, which are defined by another system of equations

$$\phi_{\rm cr} - \frac{1}{2}(w_{\rm cr}^+ - u_{\rm cr}^+) + \mu G(w_{\rm cr}^+) = 0,$$
$$G(w_{\rm cr}^+) + G(u_{\rm cr}^+) = 0. \qquad (3.11)$$

As Fig. 2 illustrates, in this case the positively charged particles pass into the next potential wells, while the negatively charged particles do not leave their own wells. A detailed analysis shows that during the second and each following period of $H(\tau)$ both types of particles instantly move into the next potential wells twice. In other words, during each period of an alternating electric field a chain in the steady-state regime is displaced by two periods of a ratchet potential.

Thus, the drift criterion of a chain, that leads to the condition $v|_{\chi=0} \neq 0$, has the form $\phi > \phi_{\rm cr}$. As $\phi \to \phi_{\rm cr}$ and $\chi \to 0$ a chain exhibits the integer transport with the drift parameter $K=2$ and with an average velocity $\overline{v}=2\chi$. According to Eqs. (3.9) and (3.10), to calculate $\phi_{\rm cr}$ it is necessary to know the explicit form of a ratchet potential. However, taking into account that for $w=\overline{x_1}$ and $u=\overline{x_5}-1$ the conditions $G(w)+G(u)=0$ and $v|_{\chi=0}=0$ hold, we find the general condition

$$\phi_{\rm cr} > \frac{1}{2}(\overline{x_1} - \overline{x_5} + 1) + \mu, \qquad (3.12)$$

which can be used for approximate estimation of $\phi_{\rm cr}$.

Note also that, because for noninteracting particles the chain energy (2.10) does not contain the term $(w-u)^2/4$, the drift criterion of free particles assumes the form $\phi > \mu$. The main distinction between the drift states of interacting and noninteracting particles thus is the result that in the latter case $K \to \infty$ as $\chi \to 0$.

IV. DOUBLE-SINE POTENTIAL

A. Analytical results

We examine the chain dynamics in the asymmetric ratchet potential composed of two spatial harmonics [12]. This so-called double-sine potential is defined as $V_{\rm d}(x)=V_{0\rm d}W_{\rm d}(\overline{x})$, where $V_{0\rm d}$ is a positive constant and

$$W_{\rm d}(\overline{x}) = -\sin[2\pi(\overline{x}+\overline{x_{\rm d}})] - \eta_{\rm d}\sin[4\pi(\overline{x}+\overline{x_{\rm d}})]. \qquad (4.1)$$

Here, the parameter $\eta_{\rm d}(>0)$ characterizes the form of the reduced potential $W_{\rm d}(\overline{x})$, and the parameter $\overline{x_{\rm d}}=x_{\rm d}/d$ defines the positions of its extrema. The function $W_{\rm d}(\overline{x})$ and the corresponding reduced force field $G_{\rm d}(\overline{x})=-W'_{\rm d}(\overline{x})/\max W'_{\rm d}(\overline{x})$ $[f_{\rm d}(x)=f_{0\rm d}G_{\rm d}(\overline{x}), f_{0\rm d}=(V_{0\rm d}/d)\max W'_{\rm d}(\overline{x})]$ both have qualitatively the same forms as those depicted in Fig. 2, i.e., they have only two extrema per unit period and $\min W_{\rm d}(\overline{x}) = W_{\rm d}(0)$, if $\eta_{\rm d} < \eta_{0\rm d} = \frac{1}{8}$ and

$$\overline{x_{\rm d}} = \frac{1}{2\pi}\arccos\frac{\sqrt{1+32\eta_{\rm d}^2}-1}{8\eta_{\rm d}}. \qquad (4.2)$$

[Yet another ratchet potential that possesses the same properties as $V_{\rm d}(x)$ is introduced in the Appendix.] For these conditions, we find that $\max W'_{\rm d}(\overline{x})=2\pi(1-2\eta_{\rm d})$, $\min W'_{\rm d}(\overline{x}) = -2\pi(1+2\eta_{\rm d})$, $f_{0\rm d}=2\pi(1-2\eta_{\rm d})V_{0\rm d}/d$,

$$G_{\rm d}(\overline{x}) = \{\cos[2\pi(\overline{x}+\overline{x_{\rm d}})] + 2\eta_{\rm d}\cos[4\pi(\overline{x}+\overline{x_{\rm d}})]\} \times (1-2\eta_{\rm d})^{-1}, \qquad (4.3)$$

$G_{\rm d}(\overline{x_1})=\min G_{\rm d}(\overline{x})=-1$ if $\overline{x_1}=\frac{1}{2}-\overline{x_{\rm d}}$, $G_{\rm d}(\overline{x_2})=G_{\rm d}(0)=0$ if $\overline{x_2} = 1-2\overline{x_{\rm d}}$, $G_{\rm d}(\overline{x_4})=\max G_{\rm d}(\overline{x})=(1+2\eta_{\rm d})/(1-2\eta_{\rm d})$ if $\overline{x_4} = 1-\overline{x_{\rm d}}$, and $G_{\rm d}(\overline{x_3})=G_{\rm d}(\overline{x_5})=1$ if

$$\overline{x}_{3,5} = 1 - \overline{x_{\rm d}} \mp \frac{1}{2\pi}\arccos\frac{\sqrt{1+16\eta_{\rm d}}-1}{8\eta_{\rm d}}, \qquad (4.4)$$

where the upper and lower signs correspond to the indexes 3 and 5, respectively.

To calculate $\phi_{\rm cr}$, we proceed as follows. First, instead of the second equation in (3.10), we introduce the two equations $G(w_{\rm cr}^-)=-\rho$ and $G(u_{\rm cr}^-)=\rho(-1\leqslant\rho\leqslant 1)$. Then, taking into account the conditions $\overline{x_1}<w_{\rm cr}^-<\overline{x_3}$ and $\overline{x_5}-1<u_{\rm cr}^-<\overline{x_1}$, we find their solutions

$$\begin{pmatrix} w_{\rm cr}^- \\ u_{\rm cr}^- \end{pmatrix} = \frac{1\pm 1}{2} - \overline{x_{\rm d}} \mp \frac{1}{2\pi}\arccos\frac{Z(\pm\rho)-1}{8\eta_{\rm d}}, \qquad (4.5)$$

where $Z(\rho)=\sqrt{1-16\eta_{\rm d}\rho+32\eta_{\rm d}^2(1+\rho)}$, and, using Eqs. (4.3) and (4.5), we reduce the first equation in (3.10) to the form

$$\sum_\sigma \frac{\sigma\eta_{\rm d}(1-2\eta_{\rm d})}{Z(\sigma\rho)\sqrt{64\eta_{\rm d}^2-[Z(\sigma\rho)-1]^2}} = \frac{\pi}{2}\mu \qquad (4.6)$$

$(\sigma=\pm 1)$. Since the left-hand side of Eq. (4.6), $L(\rho)$, is a monotonic odd function and $L(\rho)\to\infty$ as $\rho\to 1$, this equation always has a unique solution with respect to ρ. If that solution is known, then from Eqs. (3.9) and (4.5) we get the desired formula

$$\phi_{\rm cr} = \frac{1}{2} + \mu\rho - \frac{1}{4\pi}\sum_\sigma \arccos\frac{Z(\sigma\rho)-1}{8\eta_{\rm d}}. \qquad (4.7)$$

According to Eqs. (4.6) and (4.7), $\phi_{\rm cr}$ is a universal function of μ and $\eta_{\rm d}$. A corresponding 3-D plot, obtained via the numerical solution of Eq. (4.6), shows (see Fig. 3) that $\phi_{\rm cr}$ is an almost linear function of these variables.

An analytical solution of Eq. (4.6) is possible only in some special cases. Specifically, if $\eta_{\rm d}\to 0$, then, calculating the leading term of $L(\rho)$, Eq. (4.6) gives

$$\frac{\rho(3-2\rho^2)}{(1-\rho^2)^{3/2}} = \pi\frac{\mu}{\eta_{\rm d}}. \qquad (4.8)$$

At $\mu/\eta_{\rm d}\to\infty$ its approximate solution reads $\rho=1-(\eta_{\rm d}/\pi\mu)^{2/3}/2$, and Eq. (4.7) yields $\phi_{\rm cr}=\frac{1}{4}+\mu$. Another example corresponds to the limit $\mu\to 0$. Because $L(0)=0$, the solution of Eq. (4.6) tends to zero as $\mu\to 0$, and so $\phi_{\rm cr}=\frac{1}{2}-\overline{x_{\rm d}}$. We emphasize that the cases $\eta_{\rm d}=0$ and $\mu=0$ are degenerate. This means that for $\eta_{\rm d}=0$ and $\mu=0$ the drift state of a

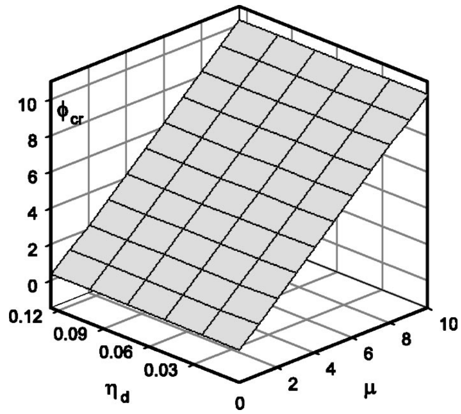

FIG. 3. 3-D plot of $\phi_{\rm cr}$ as a function of μ and $\eta_{\rm d}$.

chain never exists, while for $\eta_{\rm d}\neq 0$ and $\mu\neq 0$ it is realizable. The reason lies in the breakdown of the spatial symmetry.

B. Numerical results

We solved Eqs. (2.6) with zero initial conditions by the fourth-order Runge-Kutta method for $H(\tau)=\sin(2\pi\tau)$ and $G(\overline{x})=G_d(\overline{x})$. The analysis shows that each steady-state solution of Eqs. (2.6) satisfies the conditions (3.1). At $\phi>\phi_{\rm cr}$, the typical dependence of the dimensionless chain displacement Δw on χ is depicted in Fig. 4(a). The changes of Δw occur in a very narrow intervals (χ_1^s,χ_2^s) (the index s labels these intervals) of the χ-axis. We found that if the parameter χ does not belong to these intervals, then $k=1$, and the chain dynamics is characterized by the pairs $\{1,K\}$. According to our terminology, a chain exhibits an integer transport if $K\neq 0$. Its main features are as follows. First, the chain velocity $\overline{v}=K\chi$ is a piecewise linear function of χ that has a number of local maxima [see Fig. 4(b)]. These maxima occur due to the discrete character of the drift parameter K. Second, $K|_{x=0}$ is an increasing, step-like function of ϕ that equals zero if $\phi<\phi_{\rm cr}$ and takes even numbers if $\phi>\phi_{\rm cr}$. Specifically, in

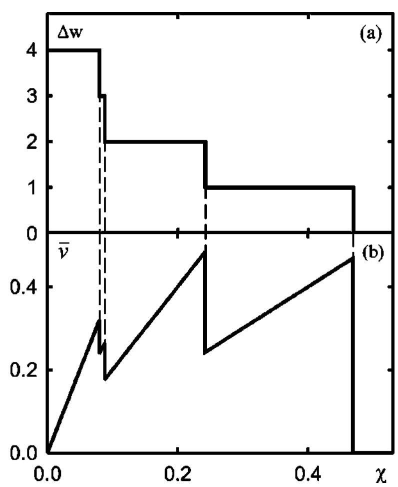

FIG. 4. Plots of Δw, part (a), and $\overline{v}$, part (b), vs χ for $\phi=3$ and $\mu=2$. The intervals (χ_1^s,χ_2^s) $(s=1,\ldots,4)$ are not visible on this scale.

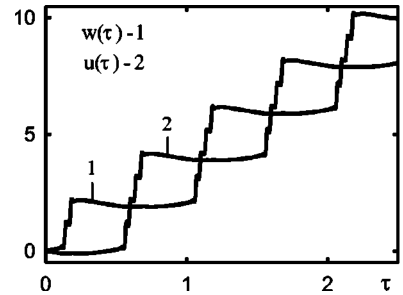

FIG. 5. Plots of the particle displacements $w(\tau)$ and $u(\tau)$ for $\phi=3$, $\mu=2$, and $\chi=10^{-4}$.

accordance with the analytical results, $K|_{\chi=0}=2$ at $\phi\approx\phi_{\rm cr}$. To illustrate for $\chi\ll 1$ the chain dynamics in the drift state, the time dependence of the particle displacements $w(\tau)$ and $u(\tau)$ and the phase trajectory of the chain motion are shown in Figs. 5 and 6 for $\phi=3$ and $\mu=2$. Since a chain reaches the steady state only if $\tau\gg\chi$ (the relaxation time is of the order of χ), the functions $w(\tau)$ and $u(\tau)$ represent the steady-state solution of Eqs. (2.6), which satisfy the conditions $w(\tau+1)=w(\tau)+4$ and $u(\tau+1)=u(\tau)+4$, at $\tau\gtrsim 1$. Finally, the increase of χ leads to the stepwise decrease of K and a smoothing of $w(\tau)$ and $u(\tau)$.

Solving Eqs. (2.6) for $\chi\in(\chi_1^s,\chi_2^s)$, we discovered that the chain dynamics is characterized by the pairs $\{k,K\}$ with $k\geqslant 2$ and $K\neq 0$. In this case a fractional transport of a chain is realized. The number of the intervals (χ_1^s,χ_2^s) equals $K|_{\chi=0}$ $(s=1,2,\ldots,K|_{\chi=0})$ and their width grows with s. Within each such interval the chain displacement $\Delta w=K/k$ assumes a stepwise function of χ that satisfies the condition $K_s-1<K/k<K_s$, where $K_s=K|_{\chi=0}-s+1$ is the drift parameter to the left of the interval (χ_1^s,χ_2^s). If χ approaches its boundaries on the inside, then k is strongly increased, $K/k\to K_s$ as $\chi\to\chi_1^s$, and $K/k\to K_s-1$ as $\chi\to\chi_2^s$. Table I illustrates these properties for the case represented in Fig. 4 at $\chi\in(\chi_1^4,\chi_2^4)$, where $\chi_1^4\approx 0.4693877$ and $\chi_2^4\approx 0.4732787$. To illustrate the chain dynamics at $\chi\in(\chi_1^4,\chi_2^4)$, the time dependence of the particle displacements $w(\tau)$ and $u(\tau)$ and the phase trajectory of the chain motion are depicted in Figs. 7 and 8, respectively. If $\chi>\chi_2^4$, then a drift of the chain does not exist and the phase trajectory explores a finite region of the phase plane.

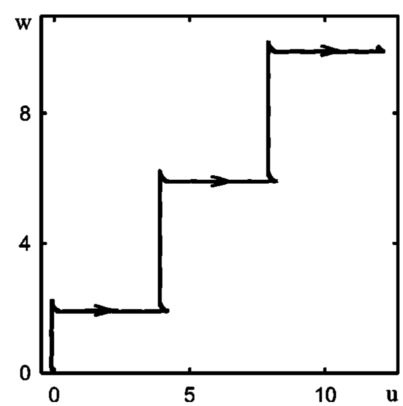

FIG. 6. Phase trajectory of the chain motion for the same parameters as in Fig. 5.

TABLE I. The numbers k and K vs. χ for $\chi \in (\chi_1^4, \chi_2^4)$.

χ	k	K	χ	k	K
0.46938773	135	134	0.472	2	1
0.4693878	39	38	0.473	9	2
0.469388	21	20	0.4732	8	1
0.46939	7	6	0.47327	47	2
0.4694	3	2	0.473278	82	1
0.47	3	2	0.4732785	150	1

The fractional transport occurs also for noninteracting particles. But the χ-intervals, where such a transport exists, are much more narrow as compared to those observed in the interacting case. In particular, according to the above results $\chi_2^4 - \chi_1^4 \approx 3.9 \times 10^{-3}$, while for noninteracting particles the width of the corresponding interval approximately equals 1.4×10^{-4}.

Note that in the phase-modulated sine potential, introduced in the Appendix, the ionic chain exhibits qualitatively the same features. We expect, therefore, that the results of the overdamped ionic chain dynamics are typical and robust for the considered class of ratchet potentials.

V. CONCLUSIONS

We have investigated the overdamped transport of a chain of charged, interacting particles driven by a longitudinal alternating electric field that additionally interact with a smooth, nonsymmetric, periodic ratchet potential. Assuming that the equilibrium particle positions coincide with the minima of a ratchet potential, we have reduced the infinite system of equations that describes the dynamics of each chain to the system of two equations which effectively describe the dynamics of only two, positively and negatively charged, representative particles. The reduced system of equations (2.6) has the advantage of being particularly simple because it consists of two ordinary differential equations of first order, which are driven by the external force.

Using the time-periodicity of an alternating electric field and the space-periodicity of a ratchet potential, we have introduced a wide class of corresponding steady-state solutions of Eqs. (2.6). The mathematical structure corresponds to the drift state of the ionic chain. Particularly, all the steady-state solutions of Eqs. (2.6) obtained numerically in the cases of the double-sine and phase-modulated sine potentials belong to this class. Studying the chain dynamics in the original ratchet potential and in its inverted realization, we have shown that, depending on the parameter regime, a chain either does not drift at all for both realizations, or it has a finite drift velocity v which is opposite in value, and correspondingly $-v$, for the inverted ratchet potential. Considering the chain dynamics in the stationary regime, we have derived the drift criterion of a chain. Accordingly, the drift state of a chain takes place if during the first half-period of an alternating electric field the chain particles perform stick-slip transitions.

Applying analytical and computational methods for analysis of the chain dynamics in the double-sine and phase-modulated sine ratchet potentials, we have shown that the chain displacement, which occurs during one full period of an alternating electric field, is a monotonically decreasing, stepwise function of the electric field frequency. This function, scaled by the ratchet potential period, takes on only integer and fractional values. Therefore, only two types of the chain transport, namely integer and fractional, do exist. Both types occur for tailored frequency intervals; the frequency intervals, however, that correspond to the fractional transport are much more narrow than those corresponding to the integer transport.

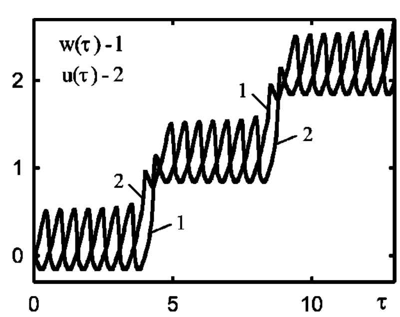

FIG. 7. Plots of the particle displacements $w(\tau)$ and $u(\tau)$ for $\phi=3$, $\mu=2$, and $\chi=0.473$.

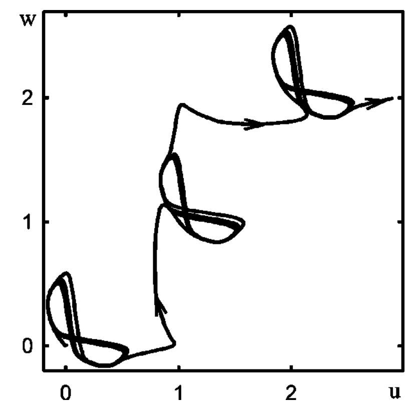

FIG. 8. Phase trajectory of the chain motion for the same parameters as in Fig. 7.

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APPENDIX: PHASE-MODULATED SINE POTENTIAL

We define a new ratchet potential $V_p(x)$, which we call the phase-modulated sine potential, as $V_p(x) = V_{0p} W_p(\overline{x})$, where V_{0p} is a positive constant and

$$W_p(\overline{x}) = -\sin\{2\pi(\overline{x} + \overline{x}_p) + \eta_p \sin[2\pi(\overline{x} + \overline{x}_p)]\}. \quad \text{(A1)}$$

The dimensionless potential $W_{\rm p}(\overline{x})$ and the corresponding dimensionless force $G_{\rm p}(\overline{x})=-W'_{\rm p}(\overline{x})/\max W'_{\rm p}(\overline{x})$ $[f_{\rm p}(x)=f_{0\rm p}G_{\rm p}(\overline{x}), f_{0\rm p}=(V_{0\rm p}/d)\max W'_{\rm p}(\overline{x})]$ both have only two extrema on the unit period if the phase amplitude $\eta_{\rm p}(>0)$ satisfies the condition $\eta_{\rm p}<\eta_{0\rm p}\approx 0.31767$, and $\min W_{\rm p}(\overline{x})=W_{\rm p}(0)$ if the parameter $\overline{x_{\rm p}}$ $[\overline{x_{\rm p}}\in(0,\frac{1}{4})]$ is a solution of the equation

$$2\pi\overline{x_{\rm p}} + \eta_{\rm p}\sin(2\pi\overline{x_{\rm p}}) = \pi/2. \tag{A2}$$

In this case, $\max W'_{\rm p}(\overline{x})=2\pi(1-\eta_{\rm p})$, $\min W'_{\rm p}(\overline{x})=-2\pi(1+\eta_{\rm p})$, $f_{0\rm p}=2\pi(1-\eta_{\rm p})V_{0\rm p}/d$,

$$G_{\rm p}(\overline{x}) = \cos\{2\pi(\overline{x}+\overline{x_{\rm p}}) + \eta_{\rm p}\sin[2\pi(\overline{x}+\overline{x_{\rm p}})]\} \times\{1+\eta_{\rm p}\cos[2\pi(\overline{x}+\overline{x_{\rm p}})]\}(1-\eta_{\rm p})^{-1}, \tag{A3}$$

$G_{\rm p}(\overline{x_1})=-1$ if $\overline{x_1}=\frac{1}{2}-\overline{x_{\rm p}}$, $G_{\rm p}(\overline{x_2})=G_{\rm p}(0)=0$ if $\overline{x_2}=1-2\overline{x_{\rm p}}$, and $G_{\rm p}(\overline{x_4})=\max G_{\rm p}(\overline{x})=(1+\eta_{\rm p})/(1-\eta_{\rm p})$ if $\overline{x_4}=1-\overline{x_{\rm p}}$.

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