Brownian motors in nonlinear diffusive media

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We investigate the performance of Brownian motors in environments governed by the "porous medium" equation $\partial_t\rho = D\partial_x(\rho^{\nu-1}\partial_x\rho)$, where ρ is the density and D and ν positive constants. This nonlinear equation yields anomalous diffusion when $\nu \neq 1$: subdiffusion for $\nu > 1$ and superdiffusion for $\nu < 1$. The thermal ratchet is modeled by an overdamped Brownian particle subject to a one-dimensional, spatially periodic, asymmetric potential, modulated by time-periodic fluctuations. We scrutinize the transport properties in the adiabatic limit. The superdiffusive regime, in comparison with the normal one, exhibits transport enhancement for small amplitudes of the temporal fluctuations. Meanwhile, the subdiffusive regime displays more strident features: The flux may become forbidden in one or in both directions. As a consequence, when the blockade is unidirectional, purely directed transport occurs.

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I. INTRODUCTION

Brownian motors, machines in the molecular scale, have sparked great scientific interest, giving rise to extensive theoretical and experimental research, mainly since the 1990s [1], due to biophysical motivations [2] and also because of potential nanotechnological applications [3].

A Brownian motor can be modeled by an overdamped Brownian particle moving under the effect of a one-dimensional (1D) periodic asymmetric potential and unbiased nonequilibrium fluctuations. Depending on the type of correlated fluctuations, many variants have been studied in the literature [4]. Basically, they belong to two main classes according on whether either the potential or the forces fluctuate in time, regularly or not. Time oscillations of the diffusion coefficient (or the temperature), for instance, can be mapped onto a model of the fluctuating potential class [5]. In any case, the breakdown of spatial symmetry together with temporal correlations gives rise to net directed transport, despite forces being null in temporal as well as in spatial average.

Concerning the thermal environment in which the ratchet is immersed, typically it is characterized by normal diffusive motion—that is, with the mean quadratic displacement growing linearly with time t. However, it is well known that there are media signaled by a t^γ growth of the squared dispersion, with $\gamma \neq 1$—e.g., porous [6], granular [7] (sublinear), or turbulent [8,9] (superlinear) ones—being sub (super) diffusive depending on whether $\gamma < (>) 1$ [10]. The phenomenology of anomalous transport may be described through simple generalizations of the usual diffusion equation. Some of them are based in the introduction of fractionary derivatives (in time and/or in space) [7,10,11], others in the introduction of nonlinearities [6–8]. Among the latter, an important class is given by the "porous medium" equation [6], which, in the 1D problem and in the absence of external forces, can be cast in the form

$$\partial_t\rho = D\partial_x(\rho^{\nu-1}\partial_x\rho), \tag{1}$$

where ρ is the density of the diffusing substance, $\nu \geq 0$, and $D > 0$ is a generalized diffusion constant. For $\nu > 1/3$, the mean quadratic deviation follows the law $\langle x^2\rangle \propto t^{2/(\nu+1)}$ and, outside that interval, although the variance is divergent, the scaling law $x^2 \sim t^{2/(\nu+1)}$ still holds [12], implying sub (super) diffusion when $\nu > (<) 1$.

The nonlinear equation (1) represents an important case of diffusive processes with density-dependent diffusion coefficient, where the functional dependence is given by a power law. It has already been considered for describing diverse subdiffusive transport processes (such as percolation of gases in porous media [13], dispersion of biological populations [14], and grain segregation [7]), as well as superdiffusive ones (e.g., fluxes in plasma [8]). It has been studied also in connection with "nonextensive statistics" [15,16]. Although generalizations of the diffusion equation of the fractionary type, in the presence of ratchet potentials, is currently under investigation [17], the performance of thermal ratchets in media governed by Eq. (1) has not been investigated yet.

Moreover, underlying the functioning of Brownian motors is Kramers' problem. When diffusion is normal, the mean first-passage (or escape) time $\mathcal{T}$ follows, in the low-temperature regime, the well-known Arrhenius law $\mathcal{T} \propto \exp(\Delta V/kT)$, where ΔV is the barrier height, k is the Boltzmann constant, and T is the temperature. The generalization of the Arrhenius law for $\nu \neq 1$ was obtained some years ago [18]. Briefly, in the superdiffusive regime $\mathcal{T}$ saturates as T decreases, while in the subdiffusive region, $\mathcal{T}$ is divergent below a certain critical value of T. The observation of these peculiar behaviors for escaping from a potential well over a barrier suggests that nonlinear diffusion may have relevant consequences on the performance of Brownian machines.

Motivated by this whole scenario, our task will be to investigate the behavior and transport properties of molecular motors in media where diffusive motion is governed by Eq. (1). Let us mention that anomalous diffusion has been reported in deterministic inertial ratchets [19]. In that case, anomalous diffusion arises as a consequence of the Newtonian dynamics driven by deterministic forces. Differently, in the present study, the noisy influence of the environment is taken into account through the nonlinear term in the right-hand side of Eq. (1), in addition to ratchet and other deterministic forces. That is, nonlinear anomalous diffusion is a characteristic of the interaction with the thermal environment and not a consequence of the ratchet operation.

The remainder of this paper is organized as follows. In Sec. II, the specific implementation of a thermal ratchet that will be used as a paradigm is presented. In Sec. III, we will quantify transport in each anomalous diffusive regime, focusing on the adiabatic limit. Basically, we will see that the more superdiffusive the environment is, the more the transport is enhanced for arbitrarily small amplitude of temporal fluctuations. Meanwhile, in subdiffusive environments, the nonlinearity yields peculiar features and purely directed fluxes may arise. Finally, Sec. IV contains concluding remarks.

II. THERMAL RATCHET

Let us consider the problem of a Brownian particle, in a 1D environment, subject to a deterministic force $F(x,t)$, whose overdamped dynamics is associated with the nonlinear diffusion equation (NDE)

$$\partial_t \rho(x,t) + \partial_x j(x,t) = 0, \tag{2}$$

where the probability current is

$$j(x,t) = [F(x,t) - D\rho^{\nu-1}(x,t)\partial_x]\rho(x,t). \tag{3}$$

Moreover, $F(x,t)=f(x)+g(t)$, where $g(t)$ oscillates periodically in time with null average and $f(x)=-\partial_x V(x)$, $V(x)$ being an asymmetric spatially periodic potential. For concreteness, we will choose simple forms for $g(t)$ and $V(x)$: (i) $g(t)$ is a square wave with amplitude f_0 and period τ, and (ii) $V(x)$ is sawtooth shaped with spatial period λ, defined in the interval $[0,\lambda)$ by

$$V(x) = \begin{cases} V_0 x/\lambda_1, & 0 \leqslant x < \lambda_1 \text{ (region 1)}, \\ V_0[\lambda - x]/\lambda_2, & \lambda_1 \leqslant x < \lambda \text{ (region 2)}, \end{cases} \tag{4}$$

where $\lambda_1+\lambda_2=\lambda$. Notice that the spatial average of the force $f(x)$ is null. Moreover, for $\alpha \equiv \lambda_2/\lambda_1 < 1$ ($\alpha=1$ for the symmetric potential), a net flux is expected to occur in the positive x direction, since the slope of the well is steeper to the left.

To quantify transport, we will determine the time-averaged current

$$\bar{J} = \frac{1}{\tau}\int_0^\tau j(x,t)dt. \tag{5}$$

If the period of the oscillations, τ, is much longer than the relaxation time [adiabatic or quasistatic (QS) regime], then the density will be given by steady solutions of the NDE (2), for each half-period (HP) in which $g(t)$ remains constant [20]. Moreover, in the QS regime, one has $\rho(x,t+\tau) = \rho(x,t)$; then, from Eqs. (2) and (5), the mean current does not depend on x.

III. ADIABATIC APPROXIMATION

Let us restrict our analysis to the QS regime. From the stationary NDE ($\partial_t \rho=0$), it results $\partial_x j=0$; then, from Eq. (3), in each HP one has

$$[f(x)+g]\rho(x) - D\rho^{\nu-1}(x)\frac{d\rho(x)}{dx} = J, \tag{6}$$

where the current J is constant and $g=\pm f_0$.

In order to integrate Eq. (6), we must also take into account the continuity conditions

$$\rho_1(0) = \rho_2(\lambda) \equiv y_0, \tag{7}$$

$$\rho_1(\lambda_1) = \rho_2(\lambda_1) \equiv y_1, \tag{8}$$

where ρ_i is the probability density function (PDF) in region i, together with the normalization restraint over one spatial period,

$$\int_0^\lambda dx\rho(x) = \int_0^{\lambda_1} dx\rho_1(x) + \int_{\lambda_1}^{\lambda} dx\rho_2(x) = 1. \tag{9}$$

The currents associated with each HP, $J_+ \equiv J(g=f_0)$ and $J_- \equiv J(g=-f_0)$, allow us to obtain, following Eq. (5), the average current over a full period: namely, $\bar{J}=(J_+ + J_-)/2$. The possible unbalance between the two currents will determine the existence of net directed transport.

In most cases, if $J \neq 0$, only an implicit expression for $\rho_i(x)$ can be extracted from Eq. (6). However, from this implicit solution together with Eqs. (7)–(9), we can derive a system of equations on (y_0, y_1, J), which, for the piecewise linear potential, reads

$$(b_2 - b_1)(y_1^\nu - y_0^\nu)/\nu + J(b_2\lambda_1 + b_1\lambda_2)/D = b_1 b_2, \tag{10}$$

$$y_0^\nu \mathcal{F}_\nu(Db_1y_0/J) - y_1^\nu \mathcal{F}_\nu(Db_1y_1/J) = \lambda_1 J/D, \tag{11}$$

$$y_0^\nu \mathcal{F}_\nu(Db_2y_0/J) - y_1^\nu \mathcal{F}_\nu(Db_2y_1/J) = -\lambda_2 J/D, \tag{12}$$

where $b_i \equiv (f_i+g)/D$ (f_i being the force in region i) and $\mathcal{F}_\nu(z) \equiv F_2^1(\nu,1,\nu+1,z)/\nu$, with F_2^1 the hypergeometric function. The solution of this nonlinear system provides, in particular, the current J. A value of ν for which the problem admits an exact solution is $\nu=1$ (normal diffusion), already studied in the literature [20]. For the marginal case $\nu=0$, the nonlinear system can be reduced to a single equation on J and $\rho(x)$ can be found explicitly. In general cases, we will numerically solve the nonlinear system (10)–(12), or its reduced form, by means of the Newton-Raphson method [21].

The case $J=0$ deserves a separate treatment and will be discussed later. Now, we will analyze separately superdiffusive and subdiffusive environments.

A. Superdiffusion and normal diffusion ($\nu \in [0,1]$)

For $\nu \leqslant 1$, the boundary conditions (7) and (8), applied to the solutions for null current, imply $b_1\lambda_1 + b_2\lambda_2 = 0$, which, in turn, means $g=0$. Reciprocally, if $g \neq 0$, necessarily it must be $J \neq 0$. Then, null current solutions are discarded in superdiffusive environments, as soon as $g \neq 0$.

Let us analyze first the case described by $\nu=0$. Partially solvable analytically, it constitutes a marginal but nontrivial case that allows us to illustrate the superdiffusive behavior. When $\nu=0$, the solution to Eq. (6), in each region i of the piecewise linear potential is given by

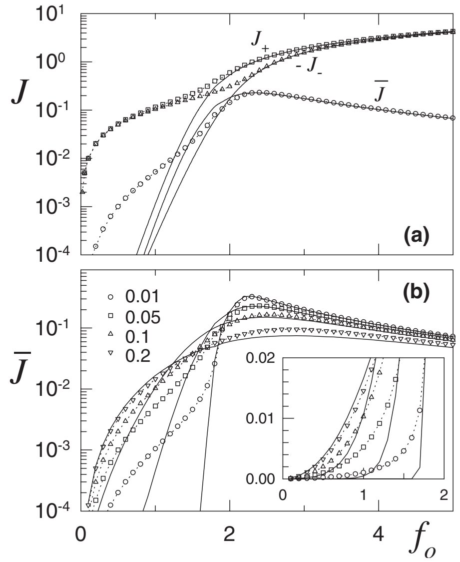

FIG. 1. Superdiffusive case $\nu=0$ (symbols) and normal diffusion (solid lines). (a) Steady currents J_+ (squares) and $-J_-$ (triangles) and average current $\bar{J}$ (circles) as a function of the intensity of the external force f_0, for $D=0.05$. (b) Average current as a function of the amplitude f_0 for different values of the diffusion coefficient indicated in the figure. Inset: close-up of the low-f_0 region. In this and subsequent figures, the potential is defined by $V_0=\lambda=1$, $\alpha=0.8$. In all cases, symbols correspond to $\nu=0$, with dotted lines as guides to the eyes, while solid lines correspond to $\nu=1$ (normal diffusion).

$$\rho_i(x) = J/[Db_i + A_i D(b_2 - b_1)\exp(Jx/D)], \tag{13}$$

where, from the continuity at the boundaries given by Eqs. (7) and (8),

$$A_1 = \frac{1 - z^{\alpha}}{1 - z^{\alpha+1}}, \qquad A_2 = \frac{1 - z^{-1}}{1 - z^{\alpha+1}},$$

where $z=\exp(J\lambda_1/D)$ $(z\neq 1)$. By substitution of A_1 and A_2 into Eq. (9), we obtain the following equation for z (hence for J):

$$\gamma(z^{\alpha+1} - 1)[\kappa z^{\gamma(\alpha+1)+1} - 1] + z(z^{\alpha} - 1)[\kappa z^{\gamma(\alpha+1)} - 1] = 0, \tag{14}$$

where $\gamma=b_1/(b_2-b_1)$ and $\kappa=\exp\{V_0 b_1 b_2/[D(b_1-b_2)]\}$. Clearly, Eq. (14) can also be obtained by elimination of y_0 and y_1 from the system of equations (10)–(12), after taking the limit $\nu\to 0$.

Numerically solving Eq. (14) with $g=\pm f_0$, we obtain the currents in each HP. The plot of Fig. 1(a) presents the currents J_+, J_-, and $\bar{J}$, as a function of f_0, for an arbitrary value of the diffusion constant. The observed behavior may be understood as follows. Keeping D fixed, for small values of f_0 ($f_0 \ll < V_0/\lambda_1$, assuming $\alpha<1$), in each HP, the particle faces similar effective barriers ($V_0 \mp \lambda_1 f_0$ $V_0 \pm \lambda_2 f_0$). So the currents $J_\pm$ are small and, although opposite in sign, are very close in absolute value. Consequently, the resultant flux is reduced. In the opposite extreme, for large values of f_0 ($f_0 \gg V_0/\lambda_2$), the ratchet can slip both forth and back. Since the structure of the potential becomes irrelevant in such a case, the currents $J_\pm$, although large, are also very close in absolute value. Therefore, in both extreme cases, flux and reflux being almost equal, the net current tends to vanish. Meanwhile, there is an intermediate range of force amplitudes that corresponds approximately to the interval $V_0/\lambda_1 < f_0 < V_0/\lambda_2$, within which the asymmetry is crucial and the net flux is maximized.

The effect of varying the diffusion constant can be observed in Fig. 1(b), which presents the average current as a function of f_0, for different values of D. For large amplitudes f_0, diffusion reduces directed transport and the net current diminishes monotonically as the diffusion constant increases. Meanwhile, for f_0 below the maximum, there is an optimal value of D that maximizes $\bar{J}$.

For comparison, we present in Fig. 1 the corresponding curves for normal diffusion [20]. Succinctly, the solution of Eq. (6) for $\nu=1$ is

$$\rho_i(x) = \frac{J}{Db_i}\left(1 + B_i b_i \frac{b_1 - b_2}{b_1 b_2}\exp(b_i x)\right), \tag{15}$$

with

$$B_1 = \frac{1 - e^{-b_2\lambda_2}}{e^{b_1\lambda_1} - e^{-b_2\lambda_2}}, \quad B_2 = \frac{1 - e^{b_1\lambda_1}}{(e^{b_1\lambda_1} - e^{-b_2\lambda_2})e^{-b_2\lambda}},$$

where J can be obtained explicitly by requiring the normalization condition (9).

The cases $\nu=0$ (ballistic superdiffusion) and $\nu=1$ (normal diffusion) define the extrema of the superdiffusive region. We observe that they yield essentially the same qualitative features and even a quantitative agreement for large f_0 at moderate values of D. At large f_0, diffusion always spoils directed transport, although this effect is weaker in the superdiffusive case (see Fig. 1). Nevertheless, the main quantitative differences occur at f_0 below the maximum, where transport can be optimized by a finite value of D. The currents in each HP are generically larger in the superdiffusive environment [Fig. 1(a)]. This is an effect that can be explained by the fact that, at a given D, much larger fluctuations, which are crucial at small f_0, can occur for $\nu<1$. But superdiffusion has consequences also for the average current that decays with f_0 and also with D less abruptly than in the normal regime. However, notice that there is an intermediate range of amplitudes f_0 for which net currents are lower in the superdiffusive case. In that range, the superdiffusing particle, being able to perform large jumps in both directions, loses sensitivity to the asymmetry of the potential.

The transport behavior for $\nu\in[0,1]$ is presented in Fig. 2. The figure exhibits the currents as a function of exponent ν, for fixed values of f_0 and D, obtained by numerically solving the system of equations (10)–(12). One observes monotonic behaviors within the interval $\nu\in[0,1]$. For large and moderate values of the amplitude f_0, currents do not depend significantly on ν. But $\bar{J}$ decreases with ν for large enough f_0, while this tendency is reversed for intermediate forcings. Differences become significant when both f_0 and D are small enough. In this case all fluxes decay monotonically as ν increases (faster than exponentially, as shown in the inset of

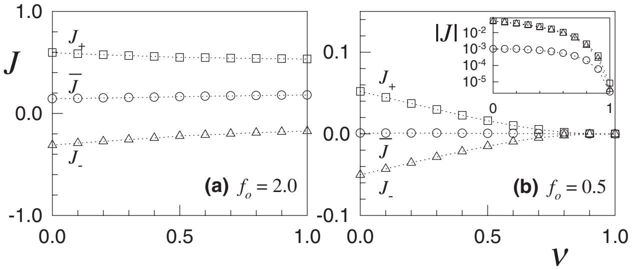

FIG. 2. Superdiffusive regime: currents J_+ (squares), J_- (triangles), and $\bar{J}$ (circles) as a function of parameter ν, for D=0.05 and (a) f_0=2.0 and (b) f_0=0.5. Inset in (b): semilogarithmic representation of the absolute value of the same data plotted in the main frame. In all cases dotted lines are guides to the eye.

Fig. 2) and superdifussion enhances directed transport.

Finally, let us look at the steady-density profiles. Typical shapes for ν=0 and ν=1, at different values of f_0, are illustrated in Fig. 3 (first and second rows, respectively). The scale is log-linear in order to focus on the behavior at the top of the potential barrier. The PDFs are given by Eqs. (13) and (15), respectively. As expected, the density is maximal at the borders, which correspond to the bottom of the potential well. At the top, it is minimal but non-null, agreeing with a nonvanishing circulation J.

B. Subdiffusion (ν>1)

As we have seen, solutions of null current are not admissible in superdiffusive environments for $g \neq 0$. However, notice from Eq. (6) that, if ν>1 (subdiffusion), then it is possible to have regions with $\rho(x)$=0, consistent with J=0, even if $g \neq 0$. In this case, in each region i of the potential given by Eq. (4), the following solutions apply:

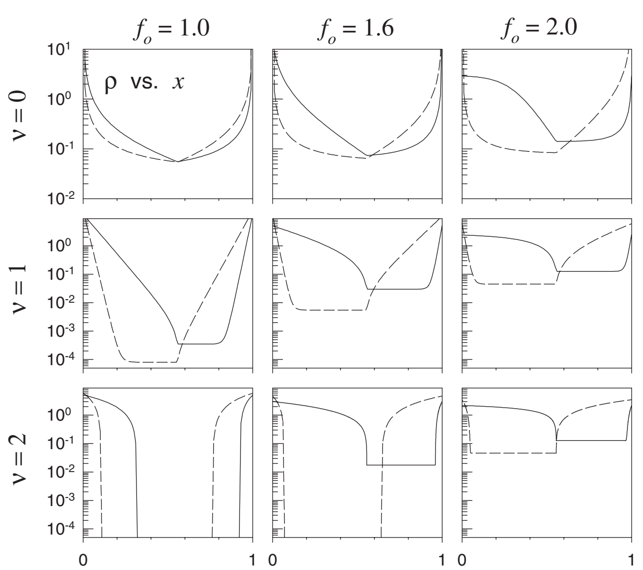

FIG. 3. Steady density profiles $\rho(x)$: for D=0.05 and different values of f_0, in the half-periods when the applied force is f_0 (solid line) and $-f_0$ (dashed line). Superdiffusion (ν=0, first row), normal diffusion (ν=1, second row), and subdiffusion (ν=2, third row).

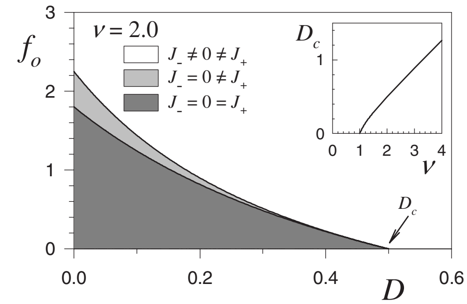

FIG. 4. Subdiffusive regime: Diagram in the f_0-D plane for which the different classes of regimes indicated on the figure occur for ν=2. Inset: critical diffusion constant D_c as a function of ν.

$$\rho_i(x) = [C_i + (\nu-1)b_i x]_+^{1/(\nu-1)}, \tag{16}$$

where C_i is a constant and the subscript "+" indicates that the function vanishes when the expression between brackets is negative. We obtain $C_1 = y_0^{\nu-1}$ and $C_2 = y_0^{\nu-1} - (\nu-1)\lambda b_2$, where, from normalization, $y_0 = [\nu b_1 b_2/(b_1 - b_2)]^{1/\nu}$. Moreover, $\rho(x)$=0 at

$$x_1 = -\frac{y_0^{\nu-1}}{(\nu-1)b_1}, \quad x_2 = \lambda - \frac{y_0^{\nu-1}}{(\nu-1)b_2}, \tag{17}$$

which must obey the inequalities

$$0 \leqslant x_1 \leqslant \lambda_1 \leqslant x_2 \leqslant \lambda. \tag{18}$$

These kinds of solutions are possible only when ν>1 and have the shape illustrated in Fig. 3 (ν=2 and f_0=1.0). Within each spatial period, there are intervals around the top of the barrier where the PDF is strictly zero. Since the probability of a Brownian particle visiting the vicinity of the barrier top is null, then there is no current.

Depending on the values of the parameters, solutions with $J \neq 0$ are also possible. In this case, the PDF must be non-null in the whole interval $[0,\lambda)$ and the solution can be found by the same procedure as that for $\nu \leqslant 1$. Then, different patterns may arise: (i) The current may vanish in both HPs—i.e., J_-, J_+=0. (ii) Only the current in one HP (hence in one direction) vanishes—that is, J_-=0 while $J_+ \neq 0$. (iii) As for superdiffusion, J_-, $J_+ \neq 0$ may also occur. These three cases are illustrated for ν=2 in the third row of Fig. 3, for f_0=1.0, 1.6, and 2.0, respectively. The class of solutions can be determined by the existence, or not, of allowed values of x_1 and x_2, defined by Eqs. (17) and (18). A diagram of the different behaviors in the f_0-D plane is illustrated in Fig. 4, for ν=2. The domains are qualitatively similar for other values of ν>1. The two critical values of f_0, in the limit of small D, correspond to V_0/λ_2 and V_0/λ_1, respectively, independent of ν. Meanwhile, the critical value of the diffusion constant, D_c, depends on ν as illustrated in the inset of Fig. 4. When $\nu \to 1$, then $D_c \to 0$; therefore, the domains of null current solutions collapse and only non-null flux solutions are allowed.

In sum, we observe the following scenario. For large enough values of f_0 and/or D, we have J_-, $J_+ \neq 0$. In this case the transport features are qualitatively similar to those observed for $\nu \leqslant 1$. However, in the limits of small f_0 and D, the main differences occur. In approaching those limits, the currents tend to zero but remain non-null for finite values of the parameters when $\nu \leqslant 1$, whereas for $\nu > 1$, there exist threshold values below which currents become strictly null. For instance, for $\nu=2$, the currents J_- and J_+ as a function of f_0 tend asymptotically to zero, at $f_0=1.5$ and 1.8, respectively. Then, for very low values of f_0 and/or D, for which the current in each HP breaks down, there is no transport ($\bar{J}=0$). Meanwhile, for intermediate values current blockade occurs only in one HP. Thus, in this case the efficiency is maximized since there is no reflux (i.e., $2\bar{J}/J_+=1$).

These observations can also be explained by the possibility of divergence of the average first passage time in the subdiffusive regime, depending on the height of the effective potential barriers, for given D [18]. When f_0 is large, even before reaching the overdriven regime when the ratchet can slip forth and back, the effective barriers in each HP are low, below the critical value. In the opposite case of sufficiently small f_0, complete blockade occurs when the lower effective barrier is larger than the critical value. For an intermediate range of f_0, however, blockade occurs only in the HP that drives the ratchet against the steepest side of the well; hence, transport is purely directed.

IV. FINAL REMARKS

In order to investigate ratchets working in nonlinear diffusive media, we have chosen a particular implementation of a ratchet that allows analytical calculations. In particular, the piecewise-linear shape of the potential is not expected to be restrictive. On the other hand, although the validity of our results is limited to the QS or adiabatic approximation, some of the observed features may hold or, at least, leave fingerprints, in more general conditions.

It is known that, in the sole presence of a periodic potential, for certain (periodic) forms of the spatial dependence of the diffusion coefficient (or the temperature) [22], directed transport may occur, even in the absence of a time-correlated fluctuating force. In the present case, the diffusion coefficient, being proportional to a power of the steady solution, represents a particular case of spatially inhomogeneous diffusion coefficient. This spatial dependence implies the existence of thermal gradients; however, its periodic shape is in phase with the potential, so that there cannot be net transport in the absence of extra correlated fluctuations [22]. In other words, in nonlinear diffusive media, as well as in normal ones, the asymmetry of the potential together with the presence of correlated fluctuations, is necessary for getting directed currents, of course, when macroscopic forces or gradients are absent.

As illustration of the transport properties in the superdiffusive regime, we considered in detail the case $\nu=0$, which, despite being a marginal case, is representative of $\nu \in [0,1)$. In comparison with the normal case, the net current is enhanced in the limits of small f_0 and/or D, although normal diffusion yields larger net currents for intermediate values of those parameters. Therefore, directed transport is not generically favored by superdiffusion. Transport enhancement for small amplitude of the fluctuations has also been observed in media where thermal fluctuations are non-Gaussian [23] and also in normal diffusive media as soon as the oscillatory square force is substituted by Brownian noise [20]. In our case, correlations are provided by the diffusion mechanism. The common feature of these systems is that large jumps, either allowed with non-negligible probability or accumulated through positive correlations, promote the escape of the Brownian particle. In the subdiffusive regime, we have seen that there are marked differences with the normal one, as soon as transport may be completely suppressed in one or in both half-periods of the oscillating external force.

We have also qualitatively interpreted the observed features on the basis of previous results for the escape time [18]. For superdiffusion, the escape time increases more slowly than exponentially as $1/D$ increases, indicating non-negligible escape probabilities even in the limit of low thermal agitation. On the other hand, for subdiffusion, the escape time is divergent for D below a critical value, in agreement with the flux blockade observed in the present context.

Finally, let us note that our results may give insights into potential applications—e.g., particle separation—in systems where the phenomenology of diffusive motion follows Eq. (1).

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