Reliability of rectified transport: Coherence and reproducibility of transport by open-loop and feedback-controlled Brownian ratchets

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Brownian ratchets are small-scale systems which rectify thermal fluctuations to produce a net current of particles. They have inspired many models of molecular motors that perform transport in the noisy environment of living cells. For the most common ratchet systems, this rectification is achieved by means of the switching of a periodic and spatially asymmetric potential (flashing ratchets) or by means of a rocking force (rocking ratchets). The rectification mechanism can be applied without information on the state of the system (open-loop ratchets) or using information on the state of the system (feedback or closed-loop ratchets). In order to characterize the transport, the most used quantity is the mean velocity of the center of mass of the system. However, another important transport attribute that has not received much attention is its quality. Here we analyze the quality of transport by studying the coherence and reproducibility of the transport induced by several representative open- and closed-loop rectification protocols under the maximum mean velocity conditions. We find that for few-particle systems, the best protocol is the rocked feedback protocol, producing the transport of particles with the highest coherence and reproducibility per distance traveled at the maximum mean velocity, while for larger systems it is overtaken by its open-loop counterpart. Our results also show that protocols with similar maximum mean velocities can have quite different coherences and reproducibilities. This highlights the importance of studying the reliability of rectified transport to develop performant synthetic rectification devices. These contributions to the emerging field of reliable transport in noisy environments are expected also to provide insight into the performance of natural molecular motors.

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I. INTRODUCTION

Great advances have been witnessed in the field of stochastic processes since the discovery of so-called Brownian motion [1]. For a long time, the unavoidable presence of noise in a system was supposed to play a destructive role [2–5]. Recently, however,many situations have arisen in which noise can lead to a constructive effect [6,7].

An interesting application deals with transport phenomena: noise can be used in order to obtain directed motion, i.e., one can rectify unbiased fluctuations caused by the thermal environment obtaining a net current in the system [1]. This mechanism is known in the literature as the Brownian motor or ratchet. Basically, it consists of a small-scale system subjected to thermal fluctuations which are rectified through some sort of asymmetry, either spatial or temporal, present in the system. This transport effect is known as the ratchet effect. Generally, it is achieved by means of a periodic and spatially asymmetric potential, called the ratchet potential. The ratchet mechanism not only is important from a theoretical point of view, but also is of relevance in biology. For example, ratcheting has been proposed as an effective model to describe the stepping motion of the two-headed kinesin [8], protein biosynthesis on the ribosome is suggested to occur through a ratchet mechanism [9–12], and models of Brownian ratchets have been employed to simulate the action of RNA and DNA polymerases during RNA and DNA replication [13–16].

In most cases, the system to be controlled is modeled as a collection of Brownian particles undergoing Langevin dynamics and subjected to control actions (that is, a rectification mechanism implemented by applying random or deterministic time-dependent perturbations to the particles). In this context, one can distinguish two types of ratchets: (i) open-loop ratchets, which apply a rectifying control action independently of the state of the system to be controlled [1,5]; (ii) and closed-loop or feedback ratchets, whose rectification action on a system has an explicit dependence on that system's evolution in time [4,17,18].

When one studies the motion of ratchets, the most important transport quantity is the mean stationary velocity of the motor [1,19]. The mean velocity describes how much time a particle needs to overcome a given distance in the long-time state. In open-loop ratchets, the mean velocity is independent of the number of particles, because the Langevin equations for the particles' positions are decoupled from each other. A significant increase in the mean velocity in a ratchet can be obtained if feedback on the state of the system is used by the protocol that switches on and off the ratchet potential [1,17,20]. One of the main ratchet types is the flashing ratchet, which operates by switching a spatially periodic asymmetric potential on and off [1]. For one-particle flashing ratchets,

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the optimal operation is a protocol that maximizes the instant velocity of the system [21]. However, in the limit of an infinite number of particles, no advantage over open-loop strategies is achieved by using any feedback in the system for flashing ratchets [21]. In contrast, rocked flashing feedback ratchets, which add a periodic driving force to the feedback-operated flashing potential, perform much better than any previously considered open-loop or feedback ratchet [22]. In Sec. II, we briefly review these results on mean velocity [17,20–22].

The mean velocity, however, is not the only transport attribute, since its quality (i.e., coherence and reproducibility) also plays a crucial role. It is well known that there will be a spread in the distances over which the motor carries out transport. The dispersion gives information about the spreading in the space position at a fixed time. Thus, the particles travel coherently together when the dispersion is small or the particles spread out as time goes by when the dispersion is large [4,23,24]. Furthermore, the transport of particles is reproducible if, for many realizations, the particles move similar distances in a given time or irreproducible if the dispersion of the final positions of the particles for different realizations is large. Here, we characterize the quality of the transport of particles achieved with different open-loop and feedback control protocols, and we use this information together with previous results on the mean velocity to analyze the performance of the generated transport.

In Sec. III, we compute for the different control protocols the diffusion coefficients of the transport, the loss of coherence and reproducibility of the transport of particles per unit of time. Furthermore, for some practical applications, the optimal control protocol may be the one that coherently and reproducibly moves all the particles a target distance. Thus, the most relevant quality traits may be the loss of coherence and reproducibility not per unit of time but per unit of distance traveled. In Sec. IV we compare the coherence and reproducibility of the transport with the mean velocity, through the Péclet number. The Péclet number is defined as the quotient of the characteristic displacement and dispersal. Large values of the Péclet number mean that ordered and directed motion dominates, whereas small values of the Péclet number indicate that random motion prevails [4,25,26]. Hence, with the computed Péclet numbers we characterize the quality of the transport for different representative control protocols. Finally, in Sec. V we show that the main results are independent of the ratchet potential height, and in Sec. VI we summarize the main conclusions of this work.

II. MEAN VELOCITY

We consider the one-dimensional motion of N Brownian particles, whose dynamics are governed by the overdamped Langevin equations

$$\gamma\,\dot{x}_i(t) = \alpha(t)\,F[x_i(t)] + \xi_i(t) \quad (i = 1, \ldots, N), \tag{1}$$

where the overdot denotes the time derivative, γ is the friction coefficient, $x_i(t)$ is the position of particle i at time t, and $\xi_i(t)$ are the thermal noises with zero mean and cross-covariances $\langle \xi_i(t)\,\xi_j(t')\rangle = 2\,\gamma\,k_B\,T\,\delta_{ij}\,\delta(t-t')$, with k_B the Boltzmann constant and T the temperature of the system. $F[x_i(t)]$ is the ratchet force acting on particle i at time t, caused by a ratchet potential $V(x)$: $F[x_i(t)] = -V'[x_i(t)]$, where the prime denotes derivatives with respect to the position. This ratchet potential depends solely on the particle position, is spatially periodic, and has broken symmetry $x \to -x$. Finally, the function $\alpha(t)$ is a control parameter that can switch on and off the ratchet potential to optimize the process. In the present study, we consider the ratchet potential [1]

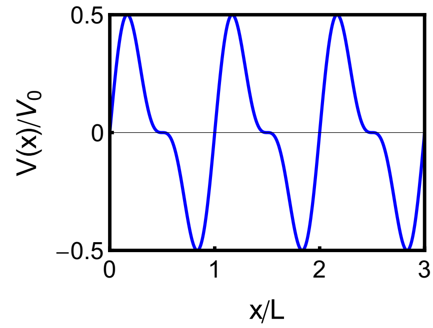

FIG. 1. Ratchet potential, defined in Eq. (2), as a function of the position. This potential is periodic, $V(x) = V(x+L)$, and has broken symmetry, $x \to -x$.

$$V(x) = \frac{2\,V_0}{3\sqrt{3}}\left[\sin\left(\frac{2\,\pi\,x}{L}\right) + \frac{1}{2}\,\sin\left(\frac{4\,\pi\,x}{L}\right)\right], \tag{2}$$

with potential height V_0 and spatial period L (see Fig. 1).

Throughout this study, we consider a series of representative control protocols for the ratchets. On one hand, control protocols may be divided into two major categories, closed loop and open loop, depending on whether or not they use information about the state of the system in the rectification of thermal fluctuations. On the other hand, ratchets are often subdivided into pulsating and tilting ratchets, paradigmatic examples of each of these two categories are the flashing and the rocking ratchets, respectively. In flashing models, the rectification is obtained by the switching of a ratchet potential, whereas in rocking ratchets it is achieved by the addition of a rocking force. As a representative example of an open-loop flashing ratchet we use the periodic ratchet, which periodically switches the ratchet potential on and off. For closed-loop flashing ratchets, we consider two examples: the instant maximization of the velocity protocol, which switches on the potential if and only if the net force per particle is positive; and the threshold protocol, which switches on and off the potential if and only if the net force per particle is above and below certain thresholds. Additionally, we consider control protocols that add a rocking force to the flashing potential, a mixture of flashing and rocking ratchets that has been determined to improve the performance of simple flashing ratchets [21]. A summary of the considered control protocols is given in Table I. The center-of-mass (CM) mean velocity

TABLE I. Summary of the studied control protocols.

	Open-loop control	Closed-loop control
Flashing ratchet	Periodic	Instant maximization threshold
Rocked flashing ratchet	Rocked flashing	Rocked feedback flashing

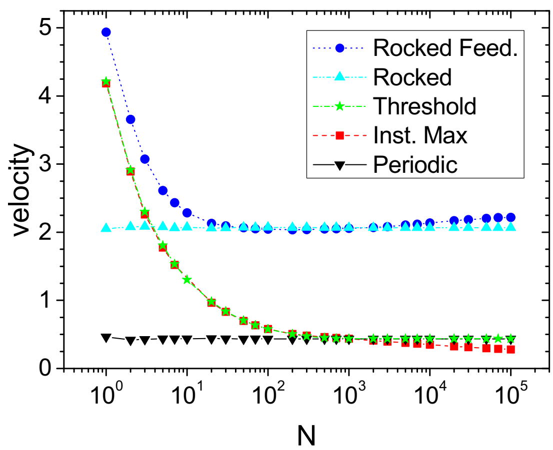

FIG. 2. CM mean velocity as a function of the number of particles in the system, N, for the different control protocols with the optimal parameter values (Table II). The ratchet potential considered for all protocols is that given by Eq. (2), with $V_0 = 5$. (Analogous figures for potential heights $V_0 = 2$ and 10 are shown in Fig. S1 of the Supplemental Material [27].) Units: $L = \gamma = k_B T = 1$.

is defined as the average CM velocity over different transport realizations. Previous works have characterized the CM mean velocity achieved with these control protocols [17,20–22]. In this section, we review these results.

Historically, the periodic protocol was the first switch-control protocol studied. This is an open-loop protocol and just involves periodic switching on and off of the ratchet potential [1,2,17,20]. The control parameter is then defined as

$$\alpha(t + \tau_{\rm on} + \tau_{\rm off}) = \alpha(t) = \begin{cases} 1 & \text{if } t \in [0, \tau_{\rm on}), \\ 0 & \text{if } t \in [\tau_{\rm on}, \tau_{\rm on} + \tau_{\rm off}). \end{cases} \quad (3)$$

The potential is switched on during a time interval $\tau_{\rm on}$ and switched off during an interval $\tau_{\rm off}$, with $\tau_{\rm on} + \tau_{\rm off}$ the time period of the protocol.

The rocked flashing control protocol is another open-loop protocol, which also switches the ratchet potential on and off periodically but, additionally, introduces a periodic oscillating force. The equations of motion that describe the particle dynamics are

$$\gamma\, \dot{x}_i(t) = \alpha(t)\, F[x_i(t)] + A\cos(\Omega t + \varphi_0) + \xi_i(t) \\ (i = 1, \dots, N), \quad (4)$$

where A is the amplitude of the rocking force, Ω its frequency, φ_0 an initial phase, and the control parameter $\alpha(t)$ is given by Eq. (3). The optimal CM mean velocity for the rocked flashing protocol is higher than that for the periodic protocol (Fig. 2). Note that for these open-loop protocols the CM mean velocity is independent of the number of particles. This is a consequence of the fact that for open-loop protocols the equation for each particle is decoupled from all the others, and thus the number of particles is irrelevant. Computations of the CM mean velocity

TABLE II. Optimal protocol parameters maximizing the CM mean velocity in the large number of particles limit for all considered control protocols (Table I), for the potential heights $V_0 = 2$, 5, and 10. Units: $L = \gamma = k_B T = 1$.

Control protocol	Protocol parameter	Optimal $V_0 = 2$	Optimal $V_0 = 5$	Optimal $V_0 = 10$
Periodic	$\tau_{\rm on}$	0.15	0.06	0.04
	$\tau_{\rm off}$	0.05	0.05	0.04
Threshold	$u_{\rm on}$	0.06	0.54	1.4
	$u_{\rm off}$	−0.04	−0.3	−1.1
Rocked flashing	$\tau_{\rm on}$	0.15	0.06	0.04
	$\tau_{\rm off}$	0.05	0.05	0.04
	A	8	20	40
	Ω	31	57	79
	φ_0	$\pi/2$	$\pi/2$	$\pi/2$
Rocked feedback flashing[a]	A	8	20	40
	Ω	31	57	79

[a]For the rocked feedback flashing control protocols, the initial phase φ_0 does not affect either the CM mean velocity, the coherence, or the reproducibility of the transport.

are done for the optimal parameter values maximizing this CM mean velocity (Table II).

In contrast to open-loop protocols, closed-loop or feedback protocols use information about the state of the system in order to operate. For the instant maximization protocol, the control policy depends on the sign of the net force per particle at each instant in time [17]. The ratchet potential is switched on if the average net force per particle with the potential 'on,'

$$f(t) = \frac{1}{N}\sum_{i=1}^{N} F[x_i(t)], \quad (5)$$

is positive. Otherwise, the ratchet potential is switched off. Thus, the control parameter can be defined as

$$\alpha(t) = \Theta[f(t)] = \begin{cases} 1 & \text{for } f(t) \geqslant 0, \\ 0 & \text{for } f(t) < 0, \end{cases} \quad (6)$$

where Θ is the Heaviside step function. The CM mean velocity obtained with this protocol decreases significantly with the number of particles in the system (see Fig. 2). Reference [17] shows that for a large number of particles the system gets trapped with the potential 'on' or 'off.' The reason behind this behavior is that for an infinite number of particles the mean force $f(t)$ goes to 0 only asymptotically and is never exactly 0. For a finite but large number of particles, the picture is similar but with fluctuations of amplitude $1/\sqrt{N}$, which make $f(t)$ cross 0, inducing a switching. This means that with increasing N the switches become more and more rare, and the system tends to get trapped, as previously commented. This trapping starts to occur earlier (for lower numbers of particles) for higher ratchet potential heights (Fig. S1, Supplemental Material [27]).

In order to avoid the trapping, the threshold protocol was introduced [20,21]. For the threshold protocol, the control parameter is described as

$$\alpha(t) = \begin{cases} 1 & \text{for } f(t) \geqslant u_{\rm on} \quad \text{or} \quad u_{\rm off} < f(t) < u_{\rm on} \quad \text{and} \quad \dot{f}_{\rm exp} \geqslant 0, \\ 0 & \text{otherwise}, \end{cases} \quad (7)$$

with $\dot{f}_{\exp}(x_i)$ an estimator for the time derivative of $f(t)$ (see Ref. [17]),

$$\dot{f}_{\exp}(t) \equiv \frac{1}{\gamma N} \sum_{i=1}^{N} \alpha(t)\, F[x_i(t)]\, F'[x_i(t)] + \frac{k_B T}{\gamma N} \sum_{i=1}^{N} F''[x_i(t)]\,. \tag{8}$$

For this protocol, the ratchet potential is switched on when the net force per particle with the potential on, $f(t)$, is above the positive threshold, $u_{\rm on}$, but also when $f(t)$ is between the two positive and negative thresholds, if the mean slope of $f(t)$ is nonnegative. Conversely, the ratchet potential is switched off if $f(t)$ is below the negative threshold, $u_{\rm off}$, or is between the two thresholds and the mean slope of $f(t)$ is negative. These thresholds induce earlier potential switches, which prevent the trapping of the system. As the number of particles increases, the fluctuations are reduced and the switching time becomes more and more deterministic, leading to a behavior analogous to that in the periodic protocol. If the optimal values of the threshold are set (Table II), the CM mean velocity obtained with the threshold protocol beats both the instant maximization and the periodic protocols (see Fig. 2). However, for a large number of particles, the threshold protocol is not able to beat the open-loop rocked flashing protocol.

Finally, for the rocked feedback flashing protocol [22], the particle dynamics is given by Eq. (4), while the control parameter α is operated as in the instant maximization protocol, Eq. (6). If optimal parameter values are set, with the rocked feedback flashing protocol we obtain higher CM velocities than with any of the previously referenced protocols, for any number of particles (see Fig. 2): for a low number of particles, this protocol generates a higher flux than the threshold or the instant maximization protocol, while for larger systems, this protocol and its open-loop counterpart produce the highest fluxes. This result is summarized as the "CM mean velocity" in Table III.

III. COHERENCE AND REPRODUCIBILITY DIFFUSION COEFFICIENTS

For practical applications, the CM mean velocity is not the only relevant characteristic of particle transport. The quality of the transport, i.e., its coherence and reproducibility, is also critical to evaluate the performance of a given ratchet.

TABLE III. Best control protocols for different criteria. Protocol parameters are optimized for the maximum CM mean velocity (Fig. 2). The protocol in parentheses is as good as the other specified protocol, but only for the specified system size.

	Few particles	Many particles
CM mean velocity	Rocked feedback	Rocked feedback (Rocked flashing)
Coherence (Pe_C)	Rocked feedback	Rocked feedback (Rocked flashing)
CM position reproducibility ($\mathrm{Pe}_{R,\mathrm{CM}}$)	Rocked feedback (Instant maximization threshold)	Rocked flashing
Particle position reproducibility (Pe_R)	Rocked feedback	Rocked feedback (Rocked flashing)

We say that a transport is coherent when all the particles travel close to their CM position $\bar{x} \equiv \frac{1}{N}\sum_{i=1}^{N} x_i$. Hence, the coherence of the transport can be characterized by the dispersion

$$\sigma_C^2(t) \equiv \langle\, \overline{(x(t) - \overline{x(t)})^2}\,\rangle = \langle\, \overline{x(t)^2}\,\rangle - \langle\, \overline{x(t)}^2\,\rangle, \tag{9}$$

where we denote the average over the number of particles $\bar{\cdot}$ and the average over realizations $\langle\cdot\rangle$. The coherence gives the average squared distance between a particle and the CM.

Apart from the coherence, another magnitude related to the quality of the transport is its reproducibility. A transport is reproducible when the particles travel similar distances during a given time for different realizations. First, we can characterize the reproducibility of the motion of the CM of the system through the dispersion

$$\sigma_{R,\mathrm{CM}}^2(t) \equiv \langle\, (\overline{x(t)} - \langle\overline{x(t)}\rangle)^2 \rangle = \langle\, \overline{x(t)}^2 \rangle - \langle\, \overline{x(t)}\,\rangle^2. \tag{10}$$

The motion of the CM will be reproducible if the CM travels similar distances in a given time interval for different realizations or, equivalently, if for different realizations the final positions of the CM are close to each other, leading to a small dispersion of the CM positions.

Additionally, we can study the reproducibility of the motion of all the particles in the system. This reproducibility of the transport of particles is given by the dispersion

$$\sigma_R^2(t) \equiv \langle\, \overline{(x(t) - \langle\, \overline{x(t)}\,\rangle)^2}\, \rangle = \langle\, \overline{x(t)^2}\,\rangle - \langle\, \overline{x(t)}\,\rangle^2. \tag{11}$$

If, for different realizations, all the particles travel similar distances in the same time, this dispersion will be small. We say then that the transport of particles is reproducible. In contrast, if the transport of particles is not reproducible, the final positions for different transport events of the same duration will greatly differ.

It is important to note that the reproducibility of the particle transport is determined by the reproducibility of the CM transport and the coherence, through the relation

$$\sigma_R^2(t) = \sigma_{R,\mathrm{CM}}^2(t) + \sigma_C^2(t)\,, \tag{12}$$

which can be derived from the definitions in Eqs. (9)–(11). A graphical interpretation of the meaning of these three dispersions is given in Fig. 3.

In systems with inertia, rocking ratchets has been reported to produce long transients of anomalous diffusion [28,29]. However, in our systems without inertia, our simulations with all control protocols show normal diffusion, with dispersions $\sigma_R^2(t)$, $\sigma_{R,\mathrm{CM}}^2(t)$, and $\sigma_C^2(t)$ increasing linearly with time t. Thus, we define the coherence and reproducibility diffusion coefficients

$$D_C \equiv \frac{\sigma_C^2(t)}{2t}, \quad D_{R,\mathrm{CM}} = \frac{\sigma_{R,\mathrm{CM}}^2(t)}{2t}, \quad D_R = \frac{\sigma_R^2(t)}{2t}, \tag{13}$$

which do not depend on the final time of evolution t. Therefore, these coherence D_C, CM reproducibility $D_{R,\mathrm{CM}}$, and particle reproducibility D_R diffusion coefficients (see Fig. 4) characterize how rapidly coherence and reproducibility are lost per unit of time during the transport induced by a given protocol.

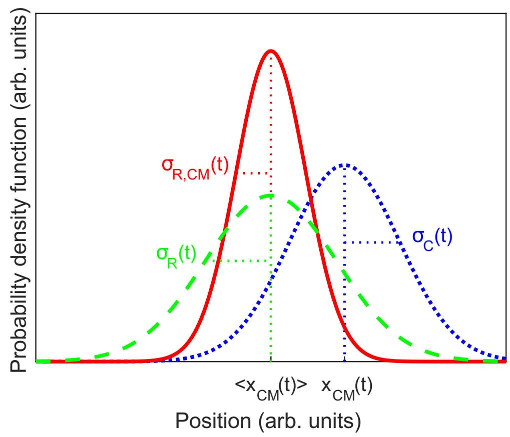

FIG. 3. Graphical interpretation of the different dispersion definitions for a given transport event. Solid red line: Probability density function (PDF) of the CM positions after a given time t for different realizations. The CM PDF is centered at the mean CM position, with standard deviation $\sigma_{R,\mathrm{CM}}(t)$ [Eq. (10)]. Dashed green line: PDF of the positions of the particles after a time t for different realizations. This PDF is also centered at the mean CM position, with standard deviation $\sigma_R(t)$ [Eq. (11)]. Dotted blue line: PDF of particles' positions after a time t for a given realization. It is centered at the CM position for this realization, with standard deviation $\sigma_C(t)$ [Eq. (9)]. The squared standard deviations of these three distributions increase linearly with time and verify Eq. (12). All PDFs are computed assuming that all particles were initially located in the same position.

In general, for all control protocols, the coherence diffusion coefficient D_C [Fig. 4(a)] increases with the number of particles, until reaching a constant finite value in the many-particle limit. This indicates that the coherence is lost more rapidly for many-particle systems than for few-particle systems and that, in the many-particle limit, the rate of loss of coherence is independent of the number of particles. An exception occurs for the instant maximization protocol, under which the coherence diffusion D_C has a maximum for systems of 10–100 particles. The higher values of D_C (i.e., the fastest loss of coherence) correspond with the rocked flashing and rocked feedback flashing protocols. Conversely, the lower values of D_C (slower loss of coherence) occur with the periodic and the instant maximization protocols, for systems of small and large numbers of particles, respectively.

The CM reproducibility diffusion coefficient $D_{R,\mathrm{CM}}$ [Fig. 4(b)] decreases with the number of particles. That is, the loss of CM reproducibility is higher for few-particle systems than for many-particle systems. The rocked feedback flashing protocol produces transports with higher values of $D_{R,\mathrm{CM}}$, i.e., with faster loss of CM reproducibility. On the contrary, the lower values of $D_{R,\mathrm{CM}}$ (i.e., with slower loss of CM reproducibility) are achieved with the open-loop protocols and the threshold protocol.

Finally, higher values of the particle reproducibility diffusion coefficient D_R [Fig. 4(c)] occur for systems of few particles, going to a nearly constant value for large numbers of particles (except in the instant maximization protocol, for which D_R continues to decrease). Thus, faster losses of particle reproducibility with time are expected for few-particle systems than for many-particle systems. Furthermore, excluding systems of one or two particles, the rocked flashing and rocked feedback flashing control protocols display the largest values of D_R.

IV. COHERENCE AND REPRODUCIBILITY LOST PER DISTANCE TRAVELED: PÉCLET NUMBERS

In Sec. III, while studying the coherence and reproducibility coefficients, we found that the rocked feedback flashing protocol leads to the fastest loss of coherence and reproducibility in the transport of particles. Hence, one might naively think that this control protocol produces low-quality transport. However, in Sec. II we have shown that this protocol maximizes the CM mean velocity. That is, while the quality of transport per unit of time is the lowest, the average distance traveled by the CM in that time is the largest. Therefore, if we compute the transport per unit of distance instead of time, this protocol may present a higher quality of transport than the others.

This leads us to postulate that, for many practical applications, the quality of transport should be defined through its loss of coherence and reproducibility per unit of distance traveled. Henceforth, one has to study and compare both the CM mean velocity of the directed motion (Sec. II) and the spread of the particles of the diffusive motion (Sec. III). A parameter that incorporates both velocity and spread is the dimensionless Péclet number, borrowed from fluid dynamics. The Péclet number is a measure of linear transport compared to diffusion, and it is defined as [4]

$$\mathrm{Pe} = \frac{v\, l}{D}, \tag{14}$$

where l is the length over which the transport is observed, v is the CM mean velocity, and D is the corresponding diffusion coefficient [Eq. (13)]. l is simply a reference length, usually set to a characteristic length of the system; we take here the period of the ratchet potential, $l = L$. For each diffusion coefficient defined in Sec. III, we define its respective Péclet number, representing the indicated quality of the transport per unit of characteristic distance traveled.

The coherence Péclet number Pe_C [Fig. 5(a)] allows us to compare how coherently the particles travel the characteristic distance l. For a highly coherent transport, all the particles will be located near the CM, and Pe_C will be large. On the contrary, for an incoherent transport the particles will present a high dispersion when the CM travels this reference distance l, and Pe_C will be small. In general, the coherence decreases with the number of particles of the system regardless of the control protocol, but there is a stable minimum coherence level reached for large enough systems (except for the instant maximization control protocol). For few-particle systems, the most coherent transports are achieved with the closed-loop protocols, especially with the rocked feedback flashing protocol. For systems with more particles, the coherence of the transport is decreased, and both the instant maximization of the velocity and the threshold control protocols are surpassed by the open-loop rocked flashing protocol, which equals the coherence of its feedback counterpart.

The CM reproducibility Péclet number $\mathrm{Pe}_{R,\mathrm{CM}}$ [Fig. 5(b)] represents the reproducibility of the motion of the CM of the system. For all the protocols, the reproducibility of the motion

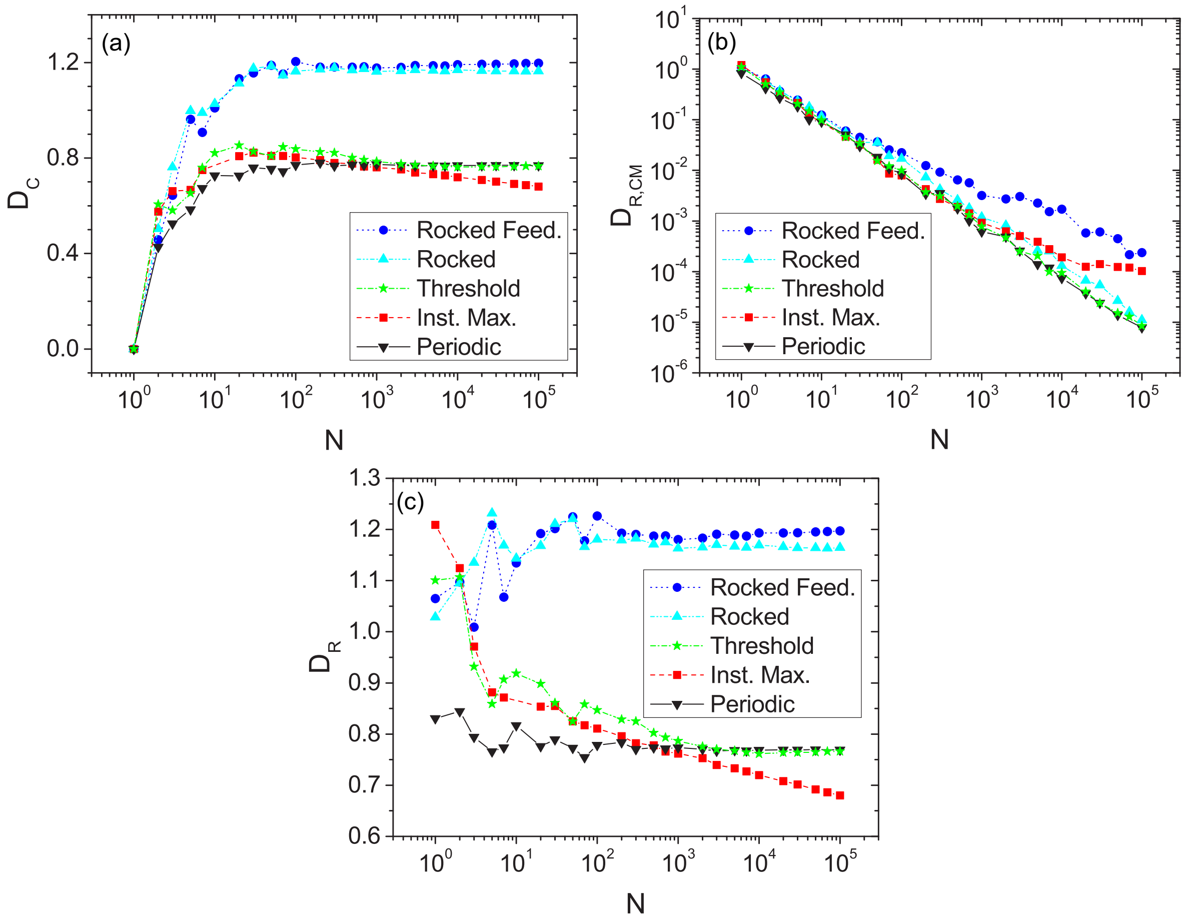

FIG. 4. (a) Coherence diffusion coefficient D_C, (b) CM reproducibility diffusion coefficient $D_{R,\mathrm{CM}}$, and (c) particles' reproducibility diffusion coefficient D_R, as functions of the number of particles N for the different control protocols with the optimal parameter values maximizing the CM mean velocity (Table II). The ratchet potential considered for all protocols is that given by Eq. (2), with $V_0 = 5$. (The analogous figures for potential heights $V_0 = 2$ and 10 are shown in Figs. S2–S4 of the Supplemental Material [27].) Units: $L = \gamma = k_B T = 1$.

of the CM increases with the number of particles. For few-particle systems, the most reproducible motions of the CM are obtained with the closed-loop protocols, while for larger systems they are obtained with the open-loop rocked flashing protocol.

The particle reproducibility Péclet number Pe_R, which represents the reproducibility of the transport of all the particles of the system, is related to the coherence of the transport and to the reproducibility of the motion of the CM. If the transport is very coherent and the motion of the CM is very reproducible, then the reproducibility of the motion of all the particles will also be high. In fact, from Eq. (12), we can see that

$$\frac{1}{\mathrm{Pe}_R} = \frac{1}{\mathrm{Pe}_C} + \frac{1}{\mathrm{Pe}_{R,\mathrm{CM}}}. \tag{15}$$

For few-particle systems, the most reproducible transport of particles is obtained with the closed-loop control protocols and, more specifically, with the rocked feedback flashing protocols [Fig. 5(c)]. For larger systems, the most reproducible particle transports are achieved with the open-loop and the closed-loop rocked flashing protocols.

V. DEPENDENCE OF THE RESULTS ON THE RATCHET POTENTIAL HEIGHT

In Secs. II–IV we show how different open-loop and closed-loop control protocols can produce transports of particles with different average fluxes and qualities (defined in terms of the coherence and reproducibility). The optimal protocol parameters have been computed as those which maximize the CM mean velocity for systems with a large number of particles, N. These optimal parameters for $V_0 = 5k_BT$ have been computed numerically and the results for the different protocols are listed in Table II. Note that for the rocked flashing control protocol, the optimal rocking force is synchronized with the periodic switching of the ratchet potential, i.e., the rocking frequency is $\Omega = 2\pi/(\tau_{\mathrm{on}} + \tau_{\mathrm{off}})$. The same amplitude and frequency of the rocking force are also found for its closed-loop version, the rocked feedback flashing protocol.

One relevant question is whether, from the optimal parameter values listed in Table II for $V_0 = 5k_BT$, we can estimate the optimal parameter values for other ratchets' potential heights. Let us start with the periodic control protocol, which operates by turning the ratchet potential alternately on and off during time periods τ_{on} and τ_{off}, respectively. When the potential is turned off, the dynamics does not depend on V_0, so we can

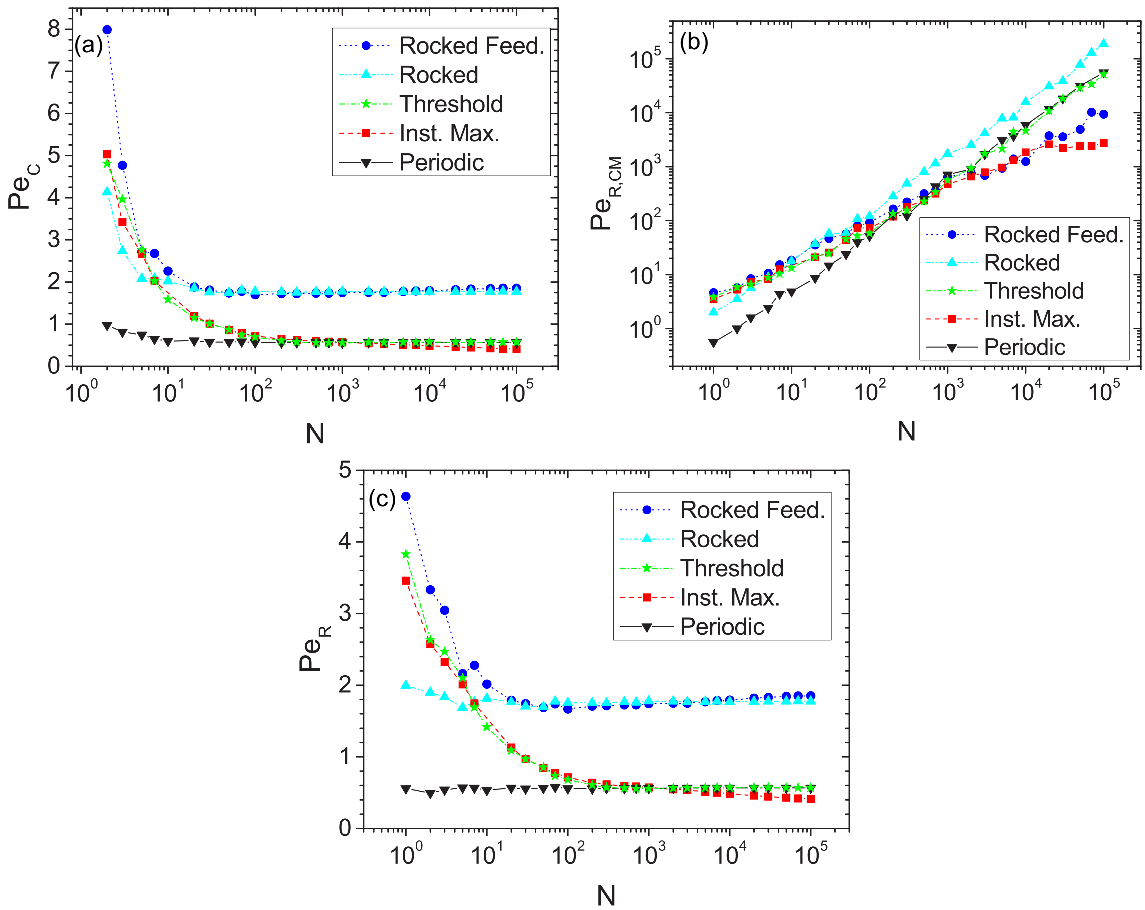

FIG. 5. (a) Coherence Péclet number Pe_C, (b) CM reproducibility Péclet number $\mathrm{Pe}_{R,\mathrm{CM}}$, and (c) particle reproducibility Péclet number Pe_R as a function of the number of particles N for the different control protocols with the optimal parameter values maximizing the CM mean velocity (Table II). The potential considered for all protocols is that given by Eq. (2), with $V_0 = 5$. (The analogous figures for potential heights $V_0 = 2$ and 10 are shown in Figs. S5–S7 of the Supplemental Material [27].) Units: $L = \gamma = k_B T = 1$.

assume that the off period does not depend on V_0 either. On the contrary, when the ratchet potential is turned on, the forces acting on the particles are proportional to V_0, so the time needed for the particles to move to the potential minimum scales as V_0^{-1}. Thus, we expect

$$\tau_{\mathrm{on}}(V_0) \propto \frac{1}{V_0}, \quad \tau_{\mathrm{off}}(V_0) \propto 1. \tag{16}$$

For the rocked flashing protocol, the optimal rocking frequency is expected to coincide with the frequency of the periodic protocol (as we observed for $V_0 = 5k_BT$). The amplitude of the rocking force should be proportional to the ratchet potential height, in order to maintain the effectiveness of the rocking force over that potential, while the phase is expected to be independent of V_0. That is,

$$A(V_0) \propto V_0, \quad \Omega(V_0) = \frac{2\pi}{\tau_{\mathrm{on}}(V_0) + \tau_{\mathrm{off}}(V_0)}, \quad \varphi_0(V_0) \propto 1. \tag{17}$$

Optimal parameter values have been computed numerically for $V_0 = 2k_BT$ and $10k_BT$ and are listed in Table II. They approximately verify relations given in Eqs. (16) and (17). Using these optimal parameter values, one can compute the CM mean velocity, the diffusion coefficients, and the Péclet numbers of the transport of particles for the different potential heights (Figs. S1–S7 of the Supplemental Material [27]). Qualitative behavior for these potential heights are analogous to the results discussed here for $V_0 = 5k_BT$. In particular, the best control protocols for the different criteria do not depend on V_0 (Table III). Different potential heights simply imply an increase in the speed of all the protocols with V_0 (in a similar proportion) and a slight change in the number of particles which separates the few-particle and the many-particle behaviors.

VI. CONCLUSIONS

We have compared the velocity and the quality of the transport of particles generated by different representative open-loop and closed-loop control protocols (Table I). The rocked feedback flashing protocol produces flux of particles with a higher center-of-mass (CM) mean velocity (Fig. 2), independently of the number of particles in the system. Nevertheless, the open-loop rocked flashing protocol gives a similar flux for large numbers of particles.

We have described the quality of transport comparing the directed and the diffusive motions, using three Péclet numbers. These Péclet numbers are related to the coherence, the CM position reproducibility, and the particle position reproducibility. The coherence quantifies how close the set of particles travels with respect to their CM. The reproducibility quantifies the dispersal in the times it takes to travel a certain distance in different realizations by the CM or by a particle.

For the transport coherence and the particle position reproducibility, the results are similar to those for the CM mean velocity. The most coherent and particle reproducible transport is achieved with the rocked feedback flashing protocol (Table III). However, for many-particle systems, its open-loop counterpart, the rocked flashing protocol, also has a high coherence and particle reproducibility performance [Figs. 5(a) and 5(c)].

The rocked feedback protocol is also the best protocol for CM reproducibility, but only for few-particle systems. For many-particle systems, the protocol with the best CM reproducibility is the rocking flashing protocol (its open-loop counterpart). [See also Table III and Fig. 5(b).]

Thus, the rocked feedback flashing protocol is the best control protocol for few-particle systems, since it produces the highest flux of particles, with the highest coherence and reproducibility. However for many-particle systems, the open-loop rocked flashing protocol may prove to be more suitable, since it provides similar average fluxes, levels of coherence, and levels of reproducibility for the transport of the particles, but with higher reproducibility levels for the center-of-mass motions.

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