Granular Brownian ratchet model

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We show by numerical simulations that a nonrotationally symmetric body, whose orientation is fixed and whose center of mass can slide along a rectilinear guide, under the effect of inelastic collisions with a surrounding gas of particles, displays directed motion. We present a theory which explains how the lack of time reversal induced by the inelasticity of collisions can be exploited to generate a steady average drift. In the limit of a heavy ratchet, we derive an effective Langevin equation whose parameters depend on the microscopic properties of the system and obtain a fairly good quantitative agreement between the theoretical predictions and simulations concerning effective friction, diffusivity, and average velocity.

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I. INTRODUCTION

The striking contrast between the simplicity of models or experimental setups and the richness and complexity of the observed phenomena has contributed to generate much interest toward the physics of granular media over the past two decades [1]. A series of reasons, such as the macroscopic nature of grains, their inelastic collisions and the lack of true thermodynamic equilibrium represent an obstacle to a straightforward application of standard methods of statistical mechanics. Dilute granular systems, the so-called granular gases [2], today are a privileged theoretical and experimental benchmark to test the fundaments of kinetic theory and of nonequilibrium statistical mechanics in general [3].

This paper is inspired to a recent numerical experiment [4] where a Brownian ratchet, i.e., a mechanical device able to rectify thermal fluctuations [5], is obtained in a nonequilibrium system with energy conserving dynamics. As shown by Van den Broeck, this rectification can be obtained by coupling the ratchet to two thermal reservoirs at different temperatures without violating the second principle of thermodynamics. We underline that in order to generate a Brownian ratchet, two symmetries must be broken: The time reversal symmetry (detailed balance) and rotational invariance of the object.

We depart from this work by proposing an even simpler device, the granular ratchet, which contains the minimal ingredients necessary to obtain directed motion. It is designed to achieve a nonequilibrium stationary regime using the inelasticity and the consequent lack of detailed balance [6] together with the broken rotational symmetry to extract work from a single source.

II. MODEL

The granular ratchet model, sketched in Fig. 1, consists of a triangular particle (the ratchet) of mass M, shaped as an isosceles triangle with base l and angle opposite to the base $2\theta_0$ and surrounded by a gas of N disks of diameter $\sigma=1$ and mass $m=1$. The ratchet can only slide, without rotating, along the direction x, perpendicular to its base and the whole system is enclosed in a squared box of side L with periodic boundary conditions. The $N+1$ particles undergo binary instantaneous collisions described by the rule

$$\mathbf{v}_i = \mathbf{v}_i' - (1+\alpha_{ij})c_{ij}[(\mathbf{v}_i' - \mathbf{v}_j')\cdot\hat{\mathbf{n}}]\hat{\mathbf{n}}, \tag{1}$$

where $\mathbf{v}$ and $\mathbf{v}'$ are the postcollisional and precollisional velocities, respectively. The quantity $\alpha_{ij}\leqslant 1$ is the coefficient of restitution for that particular collision, taking value α_d if both objects are disks or value α_r if the ratchet is involved, $\hat{\mathbf{n}}$ is the outward-pointing unit vector normal, in the contact point, to the surface of particle i, and c_{ij} is a coefficient which takes, in the different collisions, the values

$$c_{ij} = \begin{cases} 1/2 & \text{if objects are both disks,} \\ 1/(1+\epsilon^2\hat{n}_x^2) & \text{if } j \text{ is the triangle,} \\ \epsilon^2/(1+\epsilon^2\hat{n}_x^2) & \text{if } i \text{ is the triangle,} \end{cases} \tag{2}$$

where $\epsilon^2=m/M$. Because of the constraint the vertical velocity of the ratchet is always 0. The collision rule (1) conserves the total momentum if i and j are disks, and conserves the x

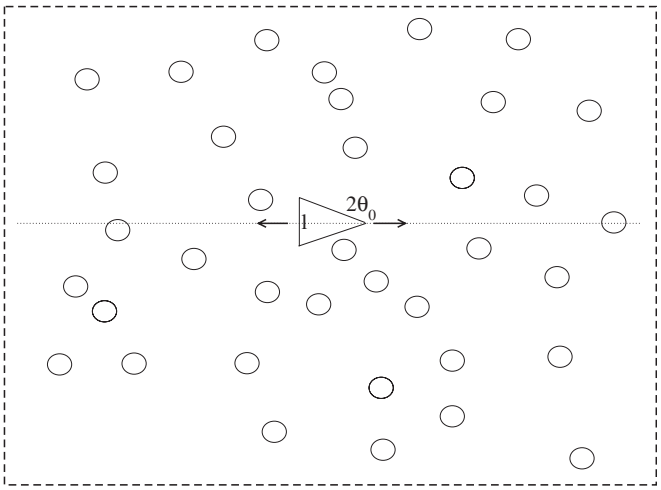

FIG. 1. Sketch of the 2D model. The triangle is constrained to move only in the $\hat{x}$ (left-right) direction, while its orientation is fixed, i.e., it cannot rotate. Gas particles collide against it and occasionally receive energy from an external bath, in the form of uncorrelated isotropic random kicks.

component of the momentum only, when the triangle is involved. If $\alpha_{ij}=1$ the total kinetic energy is also conserved. Three possible cases may be considered: (i) A pure elastic gas where $\alpha_d=\alpha_r=1$, (ii) a mixed gas where $\alpha_d=1$ and $\alpha_r<1$, and (iii) a pure inelastic gas where $\alpha_d<1$ and $\alpha_r<1$. In both cases (ii) and (iii) an external driving mechanism is needed to attain a stationary state and avoid indefinite cooling of the system. Here, we use a homogeneous random driving because it is the simplest and most studied in theoretical literature [7,8]. In particular, our simulation implements the nonviscous version of this thermostat: all disks receive, at a constant frequency, independent random Gaussian accelerations with zero average and $T_b=1$ variance. In experiments one may easily reproduce such a thermostat by placing the grains upon a horizontal plate vibrating at a high frequency [9]. The system is simulated by means of an event driven molecular dynamics algorithm. The triangle is "smoothed" by approximating its three vertexes with arcs of circle, with the condition of tangent continuity along the perimeter.

III. RESULTS AND DISCUSSION

The gas is initialized (at $t=0$) by assigning to the disks nonoverlapping random positions and Maxwellian velocities with zero average and unitary variance. The system forgets its initial configuration and attains a stationary state. In the pure elastic case the total energy $E=\frac{1}{2}\Sigma_i m_i v_i^2$ (where $m_i=m$ if i is a disk and $m_i=M$ if i is the triangle) is strictly conserved, while in the inelastic case, due to the action of the thermostat, it reaches a stationary value depending on all the control parameters (frequency of the thermostat, collision frequency, coefficients of restitution, masses, etc.). Numerical simulations indicate that the probability distribution function (pdf) for the velocity of gas particles and of the ratchet are close to a Maxwellian. In the following we will indicate as T_g the stationary values of the gas temperature and T_r the ratchet temperature. The cases $\alpha_d<1$ and $\alpha_d=1$ differ for the stationary temperature T_g, which is smaller in the inelastic gas case. Other differences are negligible if the setup is kept dilute. For this reason we reduce the number of free parameters and restrict our simulations to cases (i) and (ii), that is keep $\alpha_d=1$ and vary the inelasticity of the triangle α_r only. The molecular dynamics (MD) simulations have been performed using $N=1000$, $L=500$ (i.e., covered volume fraction $\sim 4\times 10^{-3}$), $\theta_0=\pi/6$, $l=10$, and giving random accelerations to each gas particles at times separated by an interval 32τ, where $\tau=\sqrt{m/T_b}/(4\rho\sigma)$, and $\rho=N/L^2$.

We focus here on the statistical behavior of the ratchet, whose position and velocity at time t are denoted as $X(t)$ and $V(t)$, respectively. Trajectories are averaged over 1000 realizations starting with different random configurations and discarding the initial transient. Averaged trajectories for two particular choices of the parameters are displayed in the top frame of Fig. 2, showing that when the system is totally elastic no average motion occurs for the triangle. On the contrary, when inelasticity is switched on, i.e., $\alpha_r<1$, even if the external driving mechanism acts through random isotropic accelerations and without any privileged direction, the triangle drifts with average velocity $\langle V\rangle\neq 0$. In all our MD simulations we always observed a negative velocity: The triangle on average moves toward its base. We also studied the tracer self-diffusion, measuring the quantity

$$d_2(t)=\langle(d(t)-\langle d(t)\rangle)^2\rangle, \tag{3}$$

with $d(t)=X(t)-X(0)$ the displacement of the tracer with respect to a starting time $t=0$, taken when the whole system has become stationary. This measure is presented in the bottom frame of Fig. 2, rescaled following the theory discussed below. The usual Brownian behavior with a ballistic first stage and diffusive asymptotics is observed.

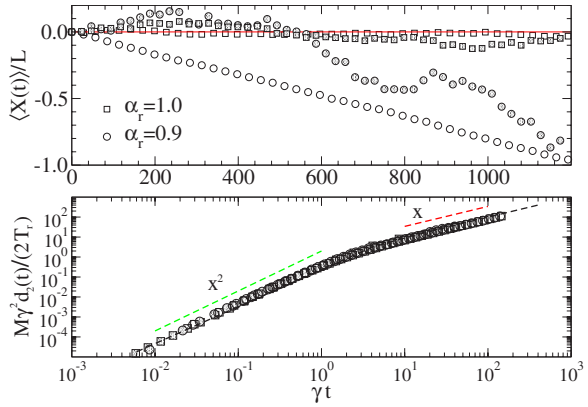

FIG. 2. (Color online) Top frame: Averaged trajectory of the tracer in MD (full symbols) and DSMC (empty symbols) with $M=10$. Bottom frame: Rescaled mean squared displacement $d_2(t)$ (see text) for the same choices of parameters. The power law $\sim x$ and $\sim x^2$ are drawn for reader's convenience (dotted straight lines).

In Fig. 3 the average velocities and energies of the tri-

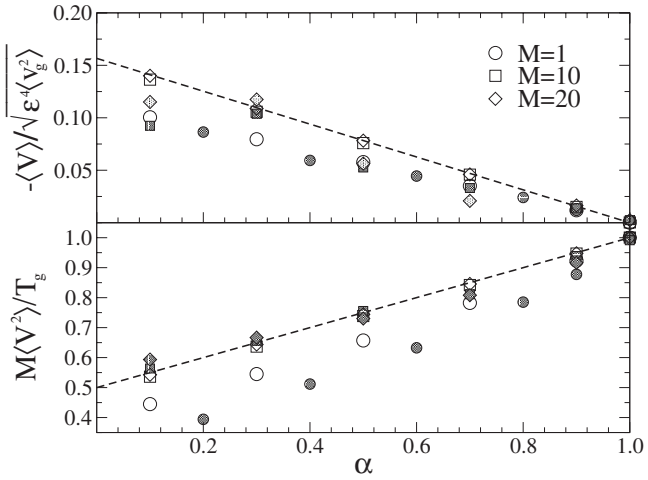

FIG. 3. Rescaled average velocities and energies of the tracer, both from MD (full symbols) and DSMC (empty symbols) simulations. Averages have been obtained with 10^3 MD dynamics and 10^4 DSMC dynamics. Gas particles have always $m=1$. In MD, $T_g=m\langle v_g^2\rangle/2$ changes when changing the parameters (α and M), in DSMC it is always $T_g=1$. The dashed line represents the theorical predictions obtained from Langevin theory.

angle, measured in MD (gray symbols), are shown. The absolute value of the average velocity of the tracer increases as elasticity is reduced, showing the origin of the effect. As the partial collapse suggests, the ratchet velocity is proportional to the thermal velocity of the gas $\sqrt{2T_g/m}$ and to m/M. The bottom frame of Fig. 3 illustrates the decrease of the average ratchet energy, with respect to T_g, with increasing inelasticity. For smaller ratchet masses the effect is stronger. We have also considered different values of θ_0 (not shown in figure): It appears that reducing this angle is a way to increase the ratchet effect, i.e., $|\langle V\rangle|$ increases. This is consistent with the fact that nonzero motion of the triangle has origin in its asymmetry. Our next step is obtaining some analytical predictions to be compared with numerical observations.

In the dilute gas limit, it is reasonable to study the ratchet dynamics by means of a linearized Boltzmann equation for its velocity pdf, $P(V,t)$, which can be written as a master equation (ME) for a Markov process [4]:

$$\frac{\partial P(V,t)}{\partial t} = \int dV'[W(V|V')P(V',t) - W(V'|V)P(V,t)], \tag{4}$$

where the transition rate is

$$W(V|V') = \int_0^{2\pi} d\theta\, SF(\theta) \int_{-\infty}^{\infty} dv_x' \int_{-\infty}^{\infty} dv_y' \rho\phi(v_x', v_y') \times (\vec{V}' - \vec{v}') \cdot \hat{\mathbf{n}}\Theta[(\vec{V}' - \vec{v}') \cdot \hat{\mathbf{n}}] \cdot \delta[V - V_{\text{post}}(V', \vec{v}', \alpha_r, \epsilon)], \tag{5}$$

with V_{post} the postcollisional ratchet velocity [see Eq. (1)], Θ the Heaviside step function, S the perimeter length, $\hat{\mathbf{n}} = (\sin\theta, -\cos\theta)$ and for the triangle

$$SF(\theta) = \frac{l}{2\sin\theta_0}\{2\sin\theta_0 \delta(\theta - 3\pi/2) + \delta(\theta - \theta_0) + \delta[\theta - (\pi - \theta_0)]\}. \tag{6}$$

Following numerical evidence we approximate the velocity pdf of the gas, $\phi(\mathbf{v})$, by a Maxwellian with zero mean and variance T_g. Expression (5) is equivalent to a master equation (ME) describing a Markov process. It is straightforward to verify that detailed balance, in the form

$$P(V)W(V'|V) = P(-V')W(-V|-V'), \tag{7}$$

holds if $\alpha_r = 1$. In a real system, as well as in MD simulation, inhomogeneities around the ratchet cannot be ruled out. We have verified that in our setup, which is very dilute, such inhomogeneities are small and do not prevent the above assumptions to be valid.

As our numerical results suggest the ME describes a driven-diffusive process. In order to gain a deeper insight it is convenient to approximate the ME by a Fokker-Planck equation (FPE), from which we can extract the analytical expression of the drift and diffusion terms. This is achieved by expressing the right-hand side of Eq. (4) by means of the Kramers-Moyal (KM) expansion

$$\frac{\partial P(V,t)}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!}\left(\frac{d}{dV}\right)^n [j_n(V)P(V,t)], \tag{8}$$

where $j_n(V) = \int dV'(V'-V)^n W(V'|V)$. By retaining only the first two terms we obtain the sought FPE, which can be still simplified by expanding these terms in the small parameter ϵ. The resulting expressions suggest a simple physical picture, which can be illustrated with the help of the Langevin equation associated with the FPE:

$$\dot{V}(t) = -\gamma V(t) + \frac{F}{M} + \Gamma(t), \tag{9}$$

with noise

$$\langle \Gamma(t)\Gamma(t')\rangle = \frac{2\gamma T_r}{M}\delta(t-t'), \quad \langle \Gamma(t)\rangle = 0. \tag{10}$$

The quantities γ and F are effective parameters related to the original parameters by

$$\gamma = 4\eta\rho l\epsilon\sqrt{\frac{T_g}{2\pi M}}(1+\sin\theta_0), \tag{11}$$

$$\frac{F}{M} = -\rho l\frac{T_g}{M}\epsilon^2(1-\sin^2\theta_0)\eta(1-\eta), \tag{12}$$

$$1-\eta = 1 - \frac{T_r}{T_g} = \frac{1-\alpha_r}{2}. \tag{13}$$

Hence, for $\alpha_r < 1$, the ratchet drifts with an average negative velocity

$$\langle V(t)\rangle = \frac{F}{M\gamma} = -\frac{1-\alpha_r}{8}\sqrt{\frac{2\pi T_g}{M}}\epsilon(1-\sin\theta_0). \tag{14}$$

Indeed, the net velocity vanishes linearly with $\epsilon \to 0$ and is very tiny for massive ratchets. It is of interest to observe that in virtue of Eq. (13) the net driving force is proportional to the temperature difference $T_g - T_r$, so that the tracer and the gas temperatures play role analogous the two reservoir temperatures of the Brownian ratchet model. In principle it is possible that for a purely inelastic system [case (iii)], for some choice of inelasticity and masses, the difference $T_g - T_r$ can change sign, implying a change of sign of the average ratchet velocity.

From Eqs. (9)–(13) it is also possible to estimate the signal to noise ratio:

$$\sqrt{\frac{\langle V(t)\rangle^2}{\langle V^2(t)\rangle - \langle V(t)\rangle^2}} \simeq \sqrt{2\pi}\frac{1-\alpha_r}{8}\epsilon(1-\sin\theta_0). \tag{15}$$

The measure of $\langle V\rangle$ can be blurred by thermal noise in the limit of large M/m, a fact that can be avoided with a large number of independent trajectories.

Equations (9) and (10) indicate that a fluctuation-dissipation relation (FDR) holds, because the noise correlation function appearing in Eq. (10) is proportional to the effective temperature T_r and to the effective friction γ.

This is in contrast with the small violations of FDR reported in studies of different models of granular tracers [10].

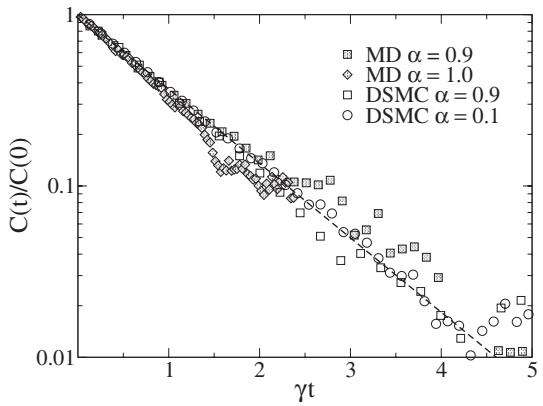

FIG. 4. Rescaled self-correlation functions of the tracer velocity with different choices of parameters, elastic and inelastic, from MD and DSMC, against rescaled time γt. The bold dashed line is the theoretical prediction coming from Eq. (11).

Indeed, the validity of the FDR in our case is an effect of the truncation of the KM expansion and of the small ϵ approximation considered here.

As anticipated in Figs. 2 and 3 the validity of the analytical theory has been also tested against direct simulation Monte Carlo (DSMC [11]) which enforces the molecular chaos assumption, used to derive Eq. (4), but in principle not verified in MD. In addition, DSMC allows to fix the desired form of $\phi(\mathbf{v})$ at our will, while in MD this depends on the control parameters of the system. Figure 3 displays a good agreement between theory and DSMC for both observables, when $\epsilon > 1$. Even for $\epsilon = 1$ the deviations are not very large. The comparison with MD results is fair but, as α_r is reduced, systematic corrections appear. When ϵ decreases MD, DSMC and theoretical predictions show a satisfactory agreement and in particular the results for $M\langle V^2\rangle$ match better than those for the average velocity. The latter, in fact, originates from a higher order term in the ϵ expansion, and therefore is subject to a stronger relative noise.

The tracer velocity self-correlation

$$C(t) = \langle (V(t) - \langle V\rangle)(V(0) - \langle V\rangle)\rangle, \tag{16}$$

displayed in Fig. 4 together with the theoretical prediction $T_r/M \exp(-\gamma t)$, gives a direct measure of γ and agrees well with the theory for low inelasticity. For larger inelasticities, at large time, $C(t)$ shows a slightly fatter tail, a feature observed in previous studies of granular gases [12]. In our opinion this could explain the lack of perfect agreement with the estimates of $\langle V\rangle$. Nevertheless, the exponential decay of $C(t)$ is consistent with the observed diffusive behavior at large times, as shown in Fig. 2. In particular, from Eq. (9) one can predict a diffusion coefficient $D = T_r/(M\gamma)$ and a general formula for the mean squared displacement which reads: $d_2(t)\gamma/2D = z - [1 - \exp(-z)]$ where $z = \gamma t$. This prediction is fairly confirmed by MD and DSMC simulation; see again Fig. 2, bottom frame.

IV. CONCLUSIONS

We are now in a position to draw conclusions and discuss perspectives. Our main result is the unveiling of an effect unknown, to the best of our knowledge, in granular gases: a directed motion driven by undirected fluctuations, exploiting only the time irreversibility of inelastic collisions. Experimental verification of such a phenomenon may easily be achieved: only technical problems (such as keeping the tracer in contact only with the gas and far from the external driving, in order to reduce noise, e.g., constraining it on a suspended guide) must be solved. Predictions can be made for different ratchets: for instance, we can consider a symmetrically shaped tracer, such as a piston or a disk, but with sides (say left-right) made of different materials, which correspond to different inelasticities, α_1 and α_2, respectively. The theory predicts (at first order in ϵ) a drift velocity,

$$\langle V\rangle = \sqrt{2\pi mkT}(u-1)(M/m + \eta - 1)/[4M(u+1)], \tag{17}$$

with $u = (1+\alpha_1)/(1+\alpha_2)$. Moreover, other kinds of external drivings can be used: A typical setup, for example, receives energy from the boundaries. In this case a box is vibrated and the tracer should be constrained to be in contact with the gas, but free to move on a $1d$ guide.

We conclude pointing out that the main analytical results presented here have been independently obtained in [13], submitted for publication at the same time of our manuscript. Nevertheless, here we have also reported the agreement of these predictions with molecular dynamics simulations of a driven gas of inelastic hard disks, and with the same system in the molecular chaos approximation (DSMC), together with a discussion of the validity of the fluctuation-dissipation relation, the measurement of diffusion and velocity self-correlations and the average velocity prediction for a disk with two sides of different inelasticities.

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[1] H. M. Jaeger, S. R. Nagel, and R. P. Behringer, Rev. Mod. Phys. **68**, 1259 (1996) and references therein.
[2] *Granular Gases*, edited by T. Pöschel and S. Luding, Lecture Notes in Physics Vol. 564 (Springer, Berlin, 2001).
[3] A. Puglisi, F. Cecconi, and A Vulpiani, J. Phys.: Condens. Matter **17**, S2715 (2005) and references therein.
[4] C. Van den Broeck, R. Kawai, and P. Meurs, Phys. Rev. Lett. **93**, 090601 (2004).
[5] M. v. Smoluchowski, Phys. Z. **13**, 1069 (1912); R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics I* (Addison-Wesley, Reading, MA, 1963), Chap. 46; M. Levanon and D. C. Rapaport, Phys. Rev. E **64**, 011304

(2001); D. van der Meer, P. Reimann, K. van der Weele, and D. Lohse, Phys. Rev. Lett. **92**, 184301 (2004).
[6] A. Puglisi, P. Visco, E. Trizac, and F. van Wijland, Phys. Rev. E **73**, 021301 (2006).
[7] A. Puglisi, V. Loreto, U. Marini Bettolo Marconi, and A. Vulpiani, Phys. Rev. Lett. **81**, 3848 (1998); Phys. Rev. E **59**, 5582 (1999).
[8] D. R. M. Williams and F. C. MacKintosh, Phys. Rev. E **54**, R9 (1996); T. P. C. van Noije, M. H. Ernst, E. Trizac, and I. Pagonabarraga, *ibid.* **59**, 4326 (1999).
[9] J. S. Olafsen and J. S. Urbach, Phys. Rev. E **60**, R2468 (1999).
[10] A. Puglisi, A. Baldassarri, and V. Loreto, Phys. Rev. E **66**, 061305 (2002); A. Barrat, V. Loreto and A. Puglisi, Physica A **334**, 513 (2004); V. Garzó, *ibid.* **343**, 105 (2004).
[11] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Clarendon, Oxford, 1994); J. M. Montanero and A. Santos, Granular Matter **2**, 53 (2000).
[12] T. P. C. van Noije, M. H. Ernst, and R. Brito, Physica A **251**, 26683 (1998).
[13] B. Cleuren and C. Van den Broeck, Europhys. Lett. **77**, 50003 (2007).