A Granular Brownian Ratchet Model

Giulio Costantini,1 Umberto Marini Bettolo Marconi,1 and Andrea Puglisi2

1Università di Camerino, Dipartimento di Fisica, Via Madonna delle Carceri, I-62032 Camerino, Italy
2Università di Roma “La Sapienza”, Dipartimento di Fisica, p.le Aldo Moro 2, I-00185 Roma, Italy

(Dated: March 23, 2022)

We show by numerical simulations that a non rotationally symmetric body, whose orientation is fixed and whose center of mass can only 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 an 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 mobility, diffusivity and average velocity.

PACS numbers: 05.40.-a, 05.70.Ln, 45.70.-n

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 a 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 fundamentals of kinetic theory and of non-equilibrium 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 non-equilibrium 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 non-equilibrium stationary regime using the inelasticity and the consequent lack of detailed balance [4] together with the broken rotational symmetry to extract work from a single source.

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 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:

$$v_i = v_i' - (1 + \alpha_{ij})c_{ij}(v_i' - v_j') \cdot \hat{n}_i \hat{n}_j,$$  \hspace{1cm} (1)

where $v$ and $v'$ are the post-collisional and pre-collisional velocities respectively, $\alpha_{ij} \leq 1$ is the coefficient of restitution for that particular collision, taking value $\alpha_{ij}$ if both objects are disks or value $\alpha_r$ if the ratchet is involved, $\hat{n}$ 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 the value $1/2$ if the objects are both disks, or the value $1/(1 + \epsilon^2 n_i^2)$ if $j$ is the triangle, or the value $\epsilon^2/(1 + \epsilon^2 n_i^2)$ if $i$ is the triangle, 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, but conserves only the $x$-component of the momentum, when the triangle is involved. If $\alpha_{ij} = 1$ the total kinetic energy is also con-
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 \( \alpha_r < 1 \), (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. In particular, our simulation implements the non viscous 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. Since the results are qualitatively the same, we will 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 \( \alpha_r \) only. The system is simulated by means of an event driven Molecular Dynamics algorithm. The triangle is “smoothed” by approximating its three vertices with arcs of circle, with the condition of tangent continuity along the perimeter.

The gas is initialized (at \( t = 0 \)) by assigning to the disks non-overlapping 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 \( E = \sum m_i v_i^2 \) (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. All MD results given hereafter are obtained using \( N = 1000, L = 500 \) (i.e. covered volume fraction \( \sim 4 \times 10^{-3} \)), \( \theta_0 = \pi / 6, l = 10 \), giving random uncorrelated kicks to all gas particles every 2000 seconds (gas collision frequency is observed to be of the order of 1 collision every 20 seconds).

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 ratchet self-diffusion, measuring the quantity \( d_2(t) = \langle (d(t) - \langle d(t) \rangle)^2 \rangle \) 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.

In Fig. 3 the average velocities and energies of the triangle, 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 nice collapse suggests, the ratchet velocity is proportional to the thermal velocity of the gas \( \sqrt{2T_g/m} \) and to 1/\( M \). Therefore, its measure becomes very difficult in the limit of large \( M \), being blurred by thermal noise. 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 \( \theta_0 \) (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 non-zero motion of the triangle has origin in its asymmetry. Our next step is obtaining some analytical predictions to be compared with numerical observation.

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]:

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

where the transition rate is:

\[
W(V|V') = \int_0^{2\pi} d\Theta \int_{-\infty}^{\infty} dv_x' \int_{-\infty}^{\infty} dv_y' \rho(v_x', v_y') \\
\left(\vec{V}' - \vec{v}'\right) \cdot \Theta [\left(\vec{V}' - \vec{v}'\right) \cdot \hat{n}] \cdot \delta[V - V_{\text{post}}(V', \vec{v}', \alpha_r, \epsilon)]
\]

with \( \rho \) the density of the gas, \( V_{\text{post}} \) the post-collisional ratchet velocity (see eq. (11)), \( \Theta \) the Heaviside step function, \( S \) the perimeter length, \( \hat{n} = (\sin \theta, -\cos \theta) \) and for the triangle \( SF(\Theta) = \frac{2\sin \theta_0}{\sin \theta_0} \left(2 \sin \theta_0 \delta(\theta - 3\pi/2) + \delta(\theta - \theta_0) + \delta(\theta - (\pi - \theta_0))\right) \).

Following numerical evidence we approximate the velocity pdf of the gas, \( \phi(v) \), by a Maxwellian with zero mean and variance \( T_g \). It is straightforward to verify that detailed balance, in the form \( P(V)W(V'|V) = P(V')W(-V'|-V) \), holds if \( \phi(v) \) is Gaussian and \( \alpha_r = 1 \).

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 r.h.s. of eq. (2) by means of the Kramers-Moyal (KM) expansion

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

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 \( \epsilon \). The resulting expressions suggest a simple physical picture, which can be illustrated with the help of the Langevin equation associated with the FPE:

\[
\dot{V}(t) = -\gamma V(t) + \frac{F}{M} + \Gamma(t)
\]

The quantities \( \gamma, F, \Gamma(t) \) are effective parameters and are related to the original parameters by

\[
\gamma = 4\eta \rho \epsilon \sqrt{\frac{T_g}{2\pi M}} (1 + \sin \theta_0)
\]

\[
F = -\eta \frac{T_g}{M} \epsilon^2 (1 - \sin^2 \theta_0) \eta (1 - \eta)
\]

\[
\langle \Gamma(t) \rangle = 0
\]

Hence, for \( \alpha_r < 1 \) the ratchet drifts with an average negative velocity \( \langle V(t) \rangle = F/(M\gamma) \). 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. (9) 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.

To corroborate the robustness of the results we went beyond the Maxwellian approximation for the gas pdf and used the so-called first Sonine correction, which is tantamount to assume \( \phi_s(v) = \frac{m}{m(T_g)} \exp\left(-\frac{mv^2}{2T_g}\right) (1 + c_2 S_2(mv^2/2T_g)) \) with \( S_2(x) = \frac{1}{2}x^2 - 2x + 1 \) [10]. In this case one may perform the calculations retrieving a correction to formula (9) of the form \( \eta = \frac{8 + 3c_2}{2\pi\epsilon} \), which makes possible the case \( T_r/T_g > 1 \), i.e. \( \langle V \rangle > 0 \). Note that in the literature \( \eta \), i.e. the ratio between the gas temperature and the tracer temperature, has been calculated also for spherical particles in [11].

Eqs. (9) indicate that a Fluctuation-Dissipation Relation (FDR) holds, in contrast with the small violations of FDR reported in studies of different models of granular tracers [12]. However, the validity of the FDR in our case is an effect of the truncation of the KM expansion and of the small \( \epsilon \) 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) which enforces the Molecular Chaos assumption, used to derive Eq. (2), but in principle not verified in MD. In addition within DSMC it is possible to fix the desired form of \( \phi(v) \) at our will, while in MD this depends on the control parameters of the system. Fig. 4 displays a good agreement between the theory and DSMC results for both observables. When \( \epsilon \sim 1 \) the theoretical results deviate from the DSMC results. The comparison with MD results is fair, but as \( \alpha_r \) decreases systematic corrections appear. In particular when \( M = 1 \) we observe a nice agreement with DSMC results, suggesting that in this case the only source of mismatch with the theory is the high value of \( \epsilon \) rather than
the lack of perfect agreement with the estimates of transport coefficient divergence, very well known for disks shows a fatter tail, which could be the prelude of some $\gamma$ measure of elasticity. For larger inelasticities, at large time, the theoretical prediction $T$ dictates a diffusion coefficient shown in Fig. 2. In particular, from Eq. (5) one can predict with the observed diffusive behavior at large times, as the dashed line is the theoretical prediction coming from Eq. (6)

$$C(t)/C(0) = \langle V(t) - \langle V \rangle \rangle (V(0) - \langle V \rangle)$$

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 $\gamma t$. The bold dashed line is the theoretical prediction coming from Eq. \ref{eq:6}.

The tracer velocity self-correlation $C(t) = \langle (V(t) - \langle V \rangle)(V(0) - \langle V \rangle) \rangle$, displayed in Fig. 3, together with the theoretical prediction $T/\gamma$ (say left/right) made of different materials, which correspond to different inelasticities, $\alpha_1$ and $\alpha_2$, respectively. The theory predicts (at first order in $\epsilon$) a drift velocity, $\langle V \rangle = \sqrt{2\gamma \pi k T(u - 1)(M/m + \eta - 1)/[4M(u + 1)]}$ with $u = (1 + \alpha_1)/(1 + \alpha_2)$. Moreover, other kinds of external driving 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 1$d$ guide. Finally, we cannot rule out that similar mechanisms are at work also in more packed situations and contribute to spontaneous de-mixing phenomena, such as the Brazil Nut Problem \ref{15}.

A. P. acknowledges the Marie Curie grant No. MERIC-021847 and UMBM acknowledges a grant COFIN-MIUR 2005, 2005027808.

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