

Thermally induced directed currents in hard rod systems

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Abstract We study the non equilibrium statistical properties of a one dimensional hard-rod fluid undergoing collisions and subject to a spatially non uniform Gaussian heat-bath and periodic potential. The system is able to sustain finite currents when the spatially inhomogeneous heat-bath and the periodic potential profile display an appropriate relative phase shift, ϕ . By comparison with the collisionless limit, we determine the conditions for the most efficient transport among inelastic, elastic and non interacting rods. We show that the situation is complex as, depending on shape of the temperature profile, the current of one system may outperform the others.

Keywords Seebeck ratchets · One dimensional systems · Granular systems

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1 Introduction

Recently there has been an upsurge of interest in the understanding of non equilibrium systems which even in the absence of an applied bias can generate currents. Typical examples are the thermal ratchets and Seebeck ratchet [1], where an asymmetric potential and a non Gaussian noise generate a directed motion.

Several authors [2,3] showed that a class of geometrically asymmetric elastic objects undergoing some holonomic constraint and coupled to heat baths at different temperatures can rectify thermal fluctuations and thus produce work. The absence of a time-reversal symmetry invalidates the standard detailed balance [4,5]. The directed motion of microscopic systems of somehow different nature was also studied several years ago by Landauer [6,7] who considered a bistable potential with an hot heat reservoir placed at one side of the potential peak and a cold reservoir on the other side and predicted a directed current of particles toward the colder side. This is the so-called the *blowtorch effect* which has been exploited in [8,9] to produce directed currents in periodic non-isothermal systems.

In this paper, we study how the presence of interactions, such as excluded volume and inelastic collisions among Brownian particles, affects the blowtorch transport mechanism. To the best of our knowledge only the case of overdamped independent particles has been analyzed in detail [10,11].

2 Model

The model consists of N impenetrable hard-rods of mass, m , size σ and position $x_i(t)$ ($i = 1, \dots, N$) evolving on a segment of length L according to the dynamics [12,13]

$$m \frac{d^2 x_i}{dt^2} = -m\gamma \frac{dx_i}{dt} - \frac{dV(x_i)}{dx_i} + \sqrt{2m\gamma T(x_i)} \xi_i(t) + \sum_j f_{ij}. \tag{1}$$

We assume cyclic boundary conditions, so that particles crossing with positive velocity the point $x = L$ reenter at the point $x = 0$ and vice-versa.

Equation (1) is based on the assumption that four kind of forces act on the rods. These are:

- (i) the frictional force, $-m\gamma dx_i/dt$, proportional to the velocity;
- (ii) the gradient of a time-independent spatially periodic potential $V(x) = V_0 \cos(2\pi x/w)$ of period w , tending to confine the particles near its minima;
- (iii) the stochastic driving force, mimicking the action of a heath bath with a spatially non uniform temperature profile, has an intensity $T(x) = T_c + T_h s(x)$ with $s(x) = (1 + \tanh[\mu \sin(2\pi/wx - \phi)])/2$ a periodic smooth step-like function between 0 and 1, which alternates cold T_c and warm $T_c + T_h$ regions of size w in $[0, L]$. The values T_c, T_h characterize the temperature jump amplitude and $\phi = 2\pi x_0/w$ determines the mutual shift of $T(x)$ and $V(x)$. All temperatures are measured in units such that the Boltzmann constant is $k_B = 1$. As usual, $\xi_i(t)$ is a zero mean and Gaussian noise with auto-correlation $\langle \xi_i(t)\xi_j(s) \rangle = \delta_{ij}\delta(t-s)$;
- (iv) finally, the term $\sum_j f_{ij}$ indicates the resultant of contact impulsive forces acting on i due to the particles $j \neq i$. namely, the rods experience mutual inelastic collisions occurring at contact $|x_{i+1} - x_i| = \sigma$. After each collision the velocities of a pair (i, j) change according to the rule $v'_i = v_i - (1 + \alpha)(v_i - v_j)/2$ and $v'_j = v_j + (1 + \alpha)(v_i - v_j)/2$, where the prime indicates post-collisional values and α is the coefficient of restitution.

3 Theory

In the limit $\gamma \rightarrow \infty$ and $m\gamma = \text{const}$, the multiple time scale analysis of [14, 15] can be extend to the present case to derive the evolution of the one-particle density $\rho(x, t)$ from the Kramers equation for the phase-space distribution function $f(x, v, t)$ [16]:

$$\frac{\partial \rho(x, t)}{\partial t} + \frac{\partial J(x, t)}{\partial x} = 0 \tag{2}$$

where the associated current reads:

$$J(x, t) = -\frac{1}{m\gamma} \left\{ \frac{\partial}{\partial x} \left[T_g(x)\rho(x, t) \right] - F(x)\rho(x, t) + \frac{(1 + \alpha)}{2} \rho(x, t) \left[T_g(x + \sigma)g_2(x, x + \sigma) \rho(x + \sigma, t) - T_g(x - \sigma)g_2(x, x - \sigma)\rho(x - \sigma, t) \right] \right\} \tag{3}$$

The first term represents the single particle contribution to the current, whereas the second term, non linear in the density, accounts for the excluded volume effect. It contains the pair correlation function $g_2(x, x')$ evaluated at contact, the coefficient of restitution α and the granular (or kinetic) temperature T_g of particles related to the heat bath temperature by

$$T_g(x) = T(x) \left\{ 1 - \frac{1 - \alpha^2}{2\gamma} \sqrt{\frac{T(x)}{m\pi}} \left[g_2(x, x + \sigma)\rho(x + \sigma) + g_2(x, x - \sigma)\rho(x - \sigma) \right] \right\}. \tag{4}$$

In the high density limit, the above equations indicate that inelasticity, temperature and density itself result intimately connected to determine the system transport properties. On the other hand, in the opposite limit, the latter term in Eq. (3) can be neglected and analytical expressions of current J and particle density $\rho(x)$ can be explicitly worked out. We remark that the system of non interacting particles provides a meaningful comparison as it constitutes the low-density regime extrapolation of interacting particle behavior. The non interacting system admits two types of stationary solutions: those corresponding to vanishing and non vanishing current J respectively. The key quantity determining the presence of a systematic flux is the ‘‘entropy’’ integral

$$S(x) = \int_0^x d\xi \frac{V'(\xi)}{T(\xi)}.$$

Using the periodicity of the system, we obtain the stationary current J_0

$$J_0 = \frac{1}{m\gamma} \frac{1 - e^{S(w)}}{ac - b[1 - e^{S(w)}]} \tag{5}$$

in terms of three constants a, b, c related to $S(x)$ by

$$a = \int_0^w dx \frac{e^{-S(x)}}{T(x)}, \quad b = \int_0^w dx \frac{e^{-S(x)}}{T(x)} \int_0^x d\xi e^{S(\xi)}, \tag{6}$$

$$c = \int_0^w dx e^{S(x)}.$$

It can be easily verified that, when $V(L) = V(0)$ (zero external load) and $T(x)$ is constant or $\phi = 0$, the current automatically vanishes. It is instructive to discuss how the current of the non-interacting system depends on the temperature scales

T_c and T_h . The current, for T_c fixed, grows as the temperature step T_h increases, for the jumps over the barrier to become more probable. On the other hand, if T_h is fixed, J does not depend monotonically on the temperature T_c . Indeed, in the limit $T_c \rightarrow 0$, the particles have a small probability to escape from the potential minima, so that the current must vanish. In the opposite limit $T_c \gg V_0$, the confining effect of the energy barriers becomes negligible and the current must vanish too. For intermediate values of T_c , a maximum in the current is expected at a T_c -value which runs to zero as V_0 is reduced.

4 Numerical results

The case of interacting particles is not so fortunate as not amenable to analytic solution, therefore our study will be based mainly on numerical simulations. The picture, indeed, remains qualitatively but not quantitatively similar to that of the non interacting case and reveals some interesting features.

When considering interacting systems, two main effects come into play which may lead to a behavior deviating from the non interacting system. First, the mutual repulsion between particles induces dynamical correlations, either promoting the exit from a potential well via energetic collisions or forbidding a jump towards a too crowded well. A meaningful parameter commonly used to take into account the crowding degree of a granular system is the packing fraction $\eta = N\sigma/L$ ($0 \leq \eta \leq 1$). Second, the granular temperature of an inelastic system is generally lower than the temperature of the elastic counterpart. Thus, thermally activated transport is expected to be less efficient when dissipative collisions are at work.

One may wonder on the specific influence of the model parameters T_c/V_0 , T_h/V_0 , ϕ , the packing η and inelasticity α on the transport properties of the inelastic system (Inel). For sake of shortness, here we discuss only temperature effect choosing $\phi = \pi$ (which optimizes the current) and we explore some significant regimes in η and α . Moreover we compare the results of the inelastic system with the elastic (El, $\alpha = 1$) and non-interacting (NI, $\eta \rightarrow \sigma/L$) ones, by also analyzing the conditions for the efficient transport.

It is convenient to start the discussion by considering first the stationary density profiles shown in Fig. 1. The inspection of profiles, indeed, provides a first indication on the way particles react to parameter variation and how they distribute over the effective landscape generated by the potential and temperature profiles. In the NI case, with $T_h \ll V_0$ and $T_c \ll V_0$, the combined effect of temperature and potential profiles preferentially confines the particles in the narrow region determined by the minimum of the potential and the nearest colder temperature zone; in other words, the phase difference between the minima of $T(x)$ and $V(x)$ produces a sort of “cage” trapping the particles with small momenta. This feature is clearly noticeable in the $\rho_{NI}(x)$ structure of

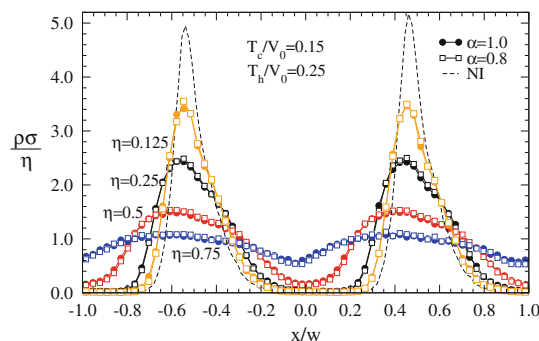


Fig. 1 (Color online) Density profiles of the systems at constant $T_c/V_0 = 0.15$, $T_h/V_0 = 0.25$ and increasing packing fraction $\eta = 1/8$ (orange), $\eta = 1/4$ (black), $\eta = 1/2$ (red) and $\eta = 3/4$ (blue). The dashed curve corresponds to the NI system, while the closed circles and open squares correspond to the interacting systems with $\alpha = 1$ and $\alpha = 0.8$ respectively. The other parameters are the following: $m = 1$, $\sigma = 1$, $\mu = 4.0$ and $\phi = \pi$

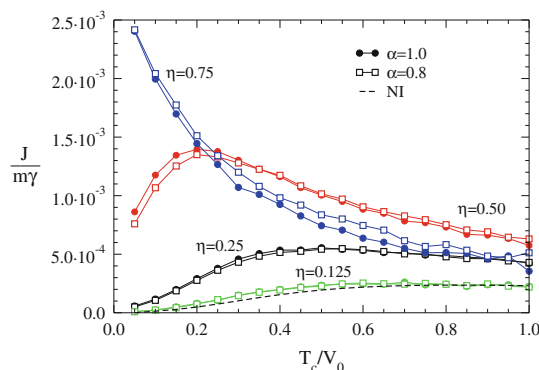


Fig. 2 (Color online) Particle current versus the rescaled temperature T_c/V_0 for four different values of the packing fraction $\eta = 1/8$ (green), $\eta = 1/4$ (black), $\eta = 1/2$ (red) and $\eta = 3/4$ (blue). Open and full symbols refer to inelastic and elastic system, respectively. For sake of comparison to the low η regime also the NI current is plotted (dashed curve)

Fig. 1 which develops peaks in the cage-region. The large preferential confinement of the NI system is however impossible to particles with excluded volume interaction whose density profiles become soon broader and flatter on increasing the average packing fraction η , see Fig. 1. This corresponds to an effective decreasing of the barriers seen by the interacting rods and such differences in the density profiles translates into different transport properties.

We study thus the dependence of the currents J_{NI} , J_{El} , J_{Inel} on T_c (see Fig. 2) at different packing η and $T_h/V_0 = 0.25$ fixed. At low values of $\eta = 0.125$, the current of the interacting systems (green symbols) behaves like the non interacting one (dashed black) as expected. Increasing η , the currents J_{El} and J_{Inel} while remaining very similar to each other, strongly deviate from the corresponding J_{NI} obtained by multiplying for the appropriate number of particles, N , the single particle current J_1 . The currents of the interacting systems start developing a maximum at lower T_c (around

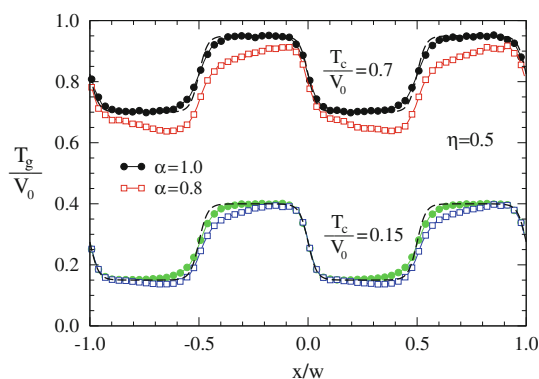


Fig. 3 (Color online) Granular temperature profiles of the systems for two different value of T_c/V_0 : 0.7 (top) and 0.15 (bottom). Open and full symbols correspond to inelastic and elastic system, respectively. The dashed curve is the temperature profile for a NI system. $T_h/V_0 = 0.25$ and the other parameters are the same as in Fig. 1

$T_c/V_0 \simeq 0.5$ for $\eta = 0.25$ or $T_c/V_0 \simeq 0.2$ for $\eta = 0.5$). This behavior can be explained by means of the excluded volume effect that reduces the effective height of the barriers as the mean packing of the wells increases. As a consequence the maximum of the current versus T_c curve is located at smaller temperatures with respect to the corresponding NI case. However, as the packing becomes sufficiently high a second effect come into play which changes the above scenario. In this regime, the effective barriers \tilde{V}_0 become enough small to be of the same order as the temperature step T_h and the particles can escape from the potential well even if $T_c \rightarrow 0$. The currents J_{El} and J_{Inel} , for $\eta = 0.75$, show in fact a finite values for small value of T_c/V_0 (see blue symbols in Fig. 2). Moreover, increasing T_c , the particles become more energetic and the rectifying effect is reduced determining a monotonically decreasing trend of the currents.

Another aspect to consider is the influence of inelasticity on the transport. The curves in Fig. 2 show that, for η sufficiently high (e.g. $\eta = 0.5$), the inelastic system (open symbols) becomes more efficient than the elastic one (closed symbols) as long as $T_c/V_0 > 0.4$. On the other hand, increasing η , J_{Inel} is larger than J_{El} for all values of T_c (blue symbols). This behavior can be explained analyzing the kinetic temperature fields of the two systems. In Fig. 3, we show these fields for $\eta = 0.5$ and two different values of T_c/V_0 .

While the elastic and non-interacting profiles of $T(x)$ are very close, the effective value of the temperature, in the inelastic case, decreases near the potential minima. This indicates that the ratio T_c/\tilde{V}_0 is smaller if $\alpha < 1$. The inelastic system can thus be approximately considered as the elastic one, but with a lower temperature T_c , i.e. $J_{Inel}(T_c) \approx J_{El}(T_c - \delta T_c)$ for a fixed T_c . Such decreasing of T_c helps to rectifying the fluctuations when the energy is enough for the activated thermal process, i.e. for $\eta = 0.75$ or $\eta = 0.5$ and $T_c/V_0 > 0.4$, or it reduces the transport when $T_c + T_h \ll \tilde{V}_0$ (i.e. for $\eta = 0.5$ and $T_c/V_0 < 0.4$).

5 Concluding remarks

In this work, we have shown that contrary to intuition, one-dimensional systems with hard-core interactions can display a more efficient “blowtorch” effect than a non interacting one. Our simulations show this efficiency inversion to be correlated to the resistance of hard-rods to localize in narrow regions. Under some conditions, the inelasticity makes the transport more efficient by reducing the average kinetic energy.

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