Interaction-induced current-reversals in driven lattices

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Abstract. Long-range interactions are shown to cause, as time evolves, consecutive reversals of directed currents for dilute ensembles of particles in driven lattices. These current reversals are based on a general mechanism that leads to an interaction-induced accumulation of particles in the regular regions of the underlying single-particle phase space and to a synchronized single-particle motion as well as enhanced efficiency of Hamiltonian ratchets. Suggestions for experimental implementations using ionized mesoscopic clusters in micromechanical lattices or dipolarly interacting colloidal particles in ac-driven optical lattices are provided.

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1. Introduction

Ratchets involve nonequilibrium dynamical processes, which make it possible to realize the old desire of converting thermal fluctuations into directed currents (dcs) and therefore usable work. According to their generality and their relevance for devices such as Brownian [1–3] and molecular motors [4], but also for biophysical problems such as the migration of bacteria [5] or cell mobility in cancer metastasis [6], the need for an understanding of the detailed properties and prospects of the mechanisms of ratchets has given rise to the development of a highly active research field. This ranges from the theoretical analysis of the generating mechanism of dcs [7–10] to the remarkable realizations of ratchets in setups as different as semiconductor nanostructures [11], Josephson junction arrays [12] and optical lattices [13–15] (see also the review [16]). Recently, it was demonstrated that lattices with spatially dependent driving imply a tunable phase space [17] and enrich the physics of dcs with mechanisms allowing for the creation of traveling density waves [18] and designable patterned particle deposition [19].

All of the above investigations do not focus on particle interactions and indeed most works on interacting ratchets concentrate either on the stochastic or the overdamped deterministic case [20–23], leaving a gap in the literature concerning the microscopic analysis of interacting (deterministic) ratchets. In this context, a topic of particular interest is the so-called current-reversals [11, 17, 24–28], i.e. the tunability of the orientation of dcs via system parameters or particle density. Very recently, a current reversal occurring in the time evolution was achieved by a time-dependent modulation of the asymmetry of the ratchet potential [29].

In this work, we demonstrate that long-range interactions in a dilute particle ensemble cause self-driven current reversals without requiring time-dependent modulations of external parameters. We analyze this surprising phenomenon to be the expression of a more general mechanism based on the interplay of two-body collisions and the underlying driven single-particle dynamics. As a consequence, we obtain synchronized single-particle motion as well as an increase of dcs.

2. Setup

We consider a system of $N$ equally charged particles in a one-dimensional lattice of laterally oscillating Gaussian potential barriers with amplitude $a$, frequency $\omega$, height $V$ and equilibrium distance $L$ described by the Hamiltonian

$$ H = \sum_{i=1}^{N} \left[ \frac{p_i^2}{2m} + V \sum_{j=-\infty}^{\infty} e^{-\beta \left[ x_i - a f_j(t) - j \cdot L \right]^2} + \sum_{k=1}^{i-1} \frac{\alpha}{\left| x_i - x_k \right|} \right], $$

(1)

Therein $x_i$, $p_i$ and $m$ denote the position, momentum and mass of the $i$th particle, respectively, $f_j(t)$ is the driving law of the barrier with equilibrium position $j \cdot L$ and $\alpha := q^2 / 4\pi \varepsilon$ represents the interaction coefficient, where $q$ is the charge of the particles and $\varepsilon$ is the permittivity. After performing the scaling transformations $(x, t, m) \mapsto (x' := x/a, t' := \omega t, m' := m \omega^2 a^2 / V)$, we may set $a = \omega = V = 1$ without loss of generality. For the remaining parameters, we choose $m = \beta = 1; L = 10$ and simulate 125 ensembles each consisting of $N = 80$ interacting particles by numerical integration of the corresponding Hamiltonian equations of motion. Large-scale numerical computations have been performed for the integration of the resulting 160 coupled,
nonlinear ordinary differential equations for $t/T = 2 \times 10^5$ periods of the driving law. Even though our results are essentially independent of the initial conditions, our focus is on dilute ensembles whose initially stored interaction energy and kinetic energy is small in comparison to $V$ (for simplicity all particles are placed equidistantly with a spacing $L_0 := x_{i+1} - x_i$). The total energy concerning the interactions of the $i$th particle with the others reads $V_{ia}(x_i) = (\alpha/L_0)\left[H_{i-1} + H_{N-i}\right]$ where $H_k = \sum_{i=1}^k (1/i)$ is the $k$th harmonic number. Choosing $L_0 = 15L$ and $\alpha \leq 8.0$, we have $V_{ia}(x_i) \lesssim 0.06\alpha < V$. The initial particle velocities are randomly chosen in the low-velocity region of the chaotic sea of the corresponding single-particle phase space (SPPS) resulting from equation (1) for $N = 1$. For $f_i(t)$, we choose a harmonic driving law and in order to break the symmetries necessary to obtain a dc \cite{8}, phase shifts of period three $(\phi_1, \phi_2, \phi_3) = (0, 2\pi/3, 4\pi/3)$, $\phi_{i+3} = \phi_i$ are applied \cite{17}. It is important to note that the observed effects and the underlying mechanism are generally valid and therefore not restricted to a specific driving as long as the relevant symmetries are broken.

3. Current reversals and fast ratchets

We now explore the impact of long-range interactions on the directed transport. Figures 1(a)–(d) show the time evolution of the mean position and velocity of the ensemble of particles for three different interaction strengths, which can be adjusted according to the above-mentioned scaling behavior of the system. In figure 1(a), which shows the long-time behavior for $\alpha = 0$, we observe a directed particle current with a negative transport velocity $v_T \sim -0.28$. In the presence of interactions, we first note that the directed transport persists. Surprisingly, for the interaction strength $\alpha = 0.8$ the direction of transport is inverted. For $\alpha = 8.0$, the dc again points in the
Figure 2. Stroboscopic PSOS of the SPPS \((N = 1)\) at times \(t/T \in \mathbb{N}\). Parameters, \(a = \omega = V = \beta = 1\) and \(L = 10\). Blue dots: chaotic sea. Red lines: regular orbits.

same direction as for the noninteracting case. Figure 1(b) shows that in the noninteracting case a constant transport velocity is reached already after a short time \(t \sim 10^2\). In contrast with this, for \(\alpha = 0.8\) the dc initially points in the same direction as for \(\alpha = 0\) and possesses a similar velocity for several hundreds of periods of the driving law, but for longer times the particle current continuously slows down and reverses its direction. Furthermore, we observe a magnitude of the reversed transport velocity that is larger than for the noninteracting case (figure 1(c)). Thus, we encounter two phenomena: an interaction-induced current reversal and an increase of the ratchet efficiency (‘fast ratchet’). For \(\alpha = 8.0\), two current reversals can be observed (figures 1(a) and (b)). The dc deviates earlier from its noninteracting counterpart than for \(\alpha = 0.8\), but inverts its direction for a second time. Most clearly, the situation is reflected in figure 1(d): due to their small initial velocities the particles remain for the first few collisions on their lattice sites and are shaken according to the force provided by the driving law, so that their mean velocity simply follows the latter. Then, for \(\alpha = 0.8\) and \(\alpha = 8.0\) the mean velocity increasingly deviates from its noninteracting counterpart. We remark that, in spite of the significant computational effort leading to the results, shown in figure 1, the asymptotic behavior for long times is not yet reached. Indeed, below we will argue why the asymptotic states are reached only for such long times.

4. The particle accumulation mechanism

We now derive the mechanism that is responsible for the current reversals. The backbone of our analysis is the single-particle dynamics in the absence of all interactions. Since our many-particle system is dilute, the impact of the Coulomb interaction on the dynamics represents, most of the time, a small perturbation of the interaction-free dynamics. However, as we shall see, there are events, namely two-body collisions, for which the Coulomb interaction plays a significant role and which are responsible for the observed phenomena. Let us therefore first analyze the structure of the SPPS via the stroboscopic single-particle Poincaré surface of section (PSOS) shown in figure 2. The phase space is mixed, i.e. we encounter a large chaotic sea at low
velocities with embedded elliptic islands and invariant spanning curves confining the chaotic sea. The elliptic islands correspond to synchronized particle-barrier motion in configuration space. Islands crossing the \( v = 0 \) line belong to particles that are trapped between two of the Gaussian potential barriers, whereas the others belong to particles ballistically moving in a given spatial direction. The first invariant spanning curve (FISC) limits the energy which is maximally achievable for chaotic trajectories. Motion on these invariant spanning curves involves energies which allow the ballistically flying particles to traverse the barriers for any phase of the motion of the latter. We observe an apparent asymmetry w.r.t. \( v = 0 \) in the PSOS (figure 2), which reflects the breaking of the relevant symmetries [8] and is responsible for the occurrence of directed transport in the noninteracting system.

For the interacting many-particle system, it is not possible to visualize the underlying high-dimensional phase space, and we focus on specific observables to analyze and understand the time-evolution. Let us first inspect the time evolution of the velocity distributions. For \( \alpha = 0 \) (figure 3(a)) we encounter a uniform distribution in regions where we have no relevant elliptic islands in the phase space (figure 2) and dips at velocities where large islands are located. The sharp decrease at \( v \sim 3.0 \) and \( v \sim -2.7 \), for times \( t > 100 \) when the SPPS is occupied uniformly, reflects the velocity-borders of the FISCs. The occurrence of a directed transport with negative velocity is predominantly due to the strongly reduced density for velocities \( v \gtrsim 1.9 \) corresponding to the large elliptic islands centered at \( v \sim 2.5 \) (figure 2).

For \( \alpha = 0.8 \) (figure 3(b)) and for short times, the velocity distribution is similar to the corresponding distribution for \( \alpha = 0 \), reflecting the observed equality of the transport velocity in both cases. Subsequently, the fine structure of the SPPS, i.e. the dips in the velocity distribution, dies out continuously. Simultaneously, the particles start to accumulate at velocities \( v \sim 2-3 \) and around \( v \sim -2.5 \). Since the accumulation of particles around \( v \sim 2.5 \) is dominant for large times, we obtain a dc pointing in the opposite direction as for \( \alpha = 0 \), i.e. a current reversal is encountered. For \( \alpha = 8.0 \) (figure 3(c)) a faster broadening of the velocity distribution compared to \( \alpha = 0.8 \) is observed. From \( t \sim 200 \) on, particle accumulation develops in the velocity region \( v \sim 2-3 \) (first current reversal) and spreads out up to \( v \sim 3.9 \). Subsequently, a second particle accumulation sets in for \( v \sim (-3.5, -2.8) \), which becomes dominant (second current reversal). The key observation to understand the above-discussed effects is that the velocity regime \( (v \sim 2-3) \) for which the particle accumulation occurs in the case of the first current reversal matches the velocity regime of the large elliptic islands of the SPPS (figure 2). The additional above-mentioned particle accumulations occur for velocities which are directly above/below the FISC velocities of the SPPS. These observations indicate that the structure of the phase space of the corresponding single-particle system is still of crucial importance for the many-particle dynamics. To verify the particle accumulation in certain (regular) parts of the underlying SPPS we lay the PSOS (figure 2) and the position velocity distribution of the ensemble for large times \( (t/T \sim 2 \times 10^5) \) on top of each other. For \( \alpha = 0 \) (figure 4(a)), all particles are situated in the chaotic sea of the SPPS and the regular parts are unoccupied. The same holds also for the short-time behavior \( (t < 10^5 T) \) for \( \alpha = 0.8 \) (not shown). Considering the case \( \alpha = 0.8 \) at \( t = 2 \times 10^5 T \) we observe a vital accumulation of particles in both large elliptic islands centered at \( v \approx 2.5 \). This accumulation spreads out into the region of the invariant spanning curves of the SPPS. A further accumulation occurs directly below the lower FISC. Since the one in the large islands for positive velocities is dominant, the average velocity has become positive. We therefore conclude that both the current reversal and the high velocity of the dc for \( \alpha = 0.8 \) are caused by particle accumulation in the regular islands of the corresponding SPPS which
are inaccessible for chaotic trajectories in the noninteracting case. For $\alpha = 8.0$, the particle accumulation in the large regular islands takes place for earlier times and it is responsible for the first reversal of the dc. Figure 4(c) shows the corresponding superposition for long times ($t/T \sim 2 \times 10^5$) and exhibits a dominant accumulation below the lower FISC of the SPPS, which illuminates the second current reversal with the dc pointing finally in the negative direction.

Let us explore the doorway process into the regular parts of the SPPS and the subsequent trapping for long times. A typical island-entering event is shown for $N = 2$, $\alpha = 0.8$ in figure 5. Before the two particles encounter a close collision ($t \sim 3.57 \times 10^4$; see figure 5(b)) their dynamics is chaotic. Thereafter one particle is inside the regular island and the other particle exhibits chaotic motion. The regular motion persists until a further collision occurs: then the particle inside the island (red) can either penetrate deeper into the island or it might exit the

Figure 3. Time evolution of the velocity distribution for 125 ensembles of 80 particles. The number of particles (color) is shown as a function of time (logarithmically) and velocity. (a) $\alpha = 0$, (b) $\alpha = 0.8$ and (c) $\alpha = 8.0$. Ensemble and parameters are as in figure 1.
island and proceed with chaotic motion again. The interaction-induced doorway to the regular parts of the SPPS is therefore inherently a two-particle process. Note that contact interactions instead of long-range interactions would only yield the exchange of the velocities of both particles and no island-entering events would take place.

5. Discussion

It is important to note that the localization onto the elliptic islands of the SPPS induces a synchronized ballistic particle-barrier motion which is stable with respect to small perturbations. This mechanism combined with the tunability of the regular structures of the SPPS and their possible change in time via external parameters \[17, 19, 30\] provides the perspective for controlling the time evolution of the direction and magnitude of \(\alpha\).

Let us address the question of the balance of entrance and exit processes concerning the regular parts of the SPPS in order to illuminate the particle accumulation process.
For a dilute system the mean interaction energy is small in comparison with the mean kinetic energy of the particles. As long as the particles are largely separated in configuration space, their Coulomb interaction provides only a weak perturbation to the single-particle dynamics resulting, in general, in only a weak perturbation of the regular motion. For the case of two-particle collisions however, their strong interaction destroys the tori of the SPPS for a short transient time. A random perturbation could, in principle, change the single-particle dynamics with equal probability for into- and out-of-island processes. The crucial difference is, that a chaotic trajectory can approach, in line with the single-particle dynamics, the border of any elliptic island embedded in the chaotic sea, but particles confined to orbits inside elliptic islands possess a minimal nonzero distance to this border in phase space. Consequently, small perturbations can be sufficient to bring a particle across the border inside an elliptic island, but in order for a particle which is deep inside an elliptic island of the SPPS to leave it, a whole sequence of adjusted perturbations is necessary. For this reason, on average more particles enter the regular parts of the SPPS than are leaving them. We have confirmed this by additional simulations for weaker interactions $\alpha = 0.08$ for which also the smaller regular islands of the SPPS possess an enhanced occupation. The imbalance of entrance and exit currents into regular structures of the SPPS is supported by the spreading of the ensemble in configuration space: ballistic particles at the outermost parts of the ensemble can only be overtaken by faster ballistic particles and rarely by chaotic ones, yielding an accumulation of fast ballistic particles in these regions. Since the average distance between the repulsively interacting particles increases with increasing time, the collisional interaction energy decreases and the doorway process to the islands becomes less efficient, which is in line with the decrease of the acceleration of the dc observed in figure 1(d). Figure 5(c) shows that the collisional rate increases for short times but thereafter decreases rapidly, reaching approximately one collisional event per $10^5$ particles and period $T$ at $t = 2 \times 10^5$. For long times the decrease is well described by a $t^{-1.2}$-fit, i.e. it is slightly faster than linear. The latter leads to a stabilization of the particle accumulation for very long time scales, probably also in the asymptotic regime.
Let us finally briefly discuss the timescales of the dynamics. The ergodic filling of the SPPS \( (t \ll 10^2; \text{figure} \ 3) \), current-reversals \( (t \sim 10^3-2 \times 10^4; \text{figure} \ 1) \) and the decay of the collisional rate \( (t \sim 3 \times 10^4; \text{figure} \ 5(\text{c})) \) happen at separate timescales. As the incoming particle current into a regular region of the SPPS notably increases with the surface of the latter (i.e. the corresponding particle density increases with the fraction surface/volume), we obtain particle accumulations first for the small islands, followed by the large islands and then beyond the FISC (figures \( 3(\text{b}) \) and \( 3(\text{c}) \)). This current increases with \( \alpha \) and the population of the small and the large islands (figure \( 3(\text{b}) \) and \( 3(\text{c}) \)) as well as the first current reversal happen earlier for \( \alpha = 8.0 \) compared to \( \alpha = 0.8 \). After reaching saturation of the island occupation, the relatively slow occupation of the regular regions below the lower FISC (smaller surface) can become dominant and lead to the observed second reversal.

We emphasize that the mechanism of particle accumulation in the regular regions of the SPPS is solely based on the very general requirements of an underlying mixed SPPS and the presence of weak interactions interrupted by short collisional events that lead to a temporary breakup of the SPPS. Then, the imbalance of entrance and exit currents into the regular structures of the SPPS, i.e. the self-driven synchronization of the particle dynamics, occurs automatically and current reversals can take place, if the symmetries that suppress dcs [8] are broken. Therefore, no fine-tuning of parameters is required. In contrast with the generality of the process, the quantitative relation between the dependence of the timescales of island occupation and current reversals on the system parameters is very difficult to establish: a statistical description, e.g. of the island accumulation process would require not only a modeling of the structure of the SPPS but also of the collision rates as a function of SPPS position and total time. In order to describe the island exit currents, even the spatially and energetically resolved correlation function for the time-dependent collision rates would be needed. However, it is of course possible to predict and design current reversals qualitatively via the structure of the SPPS and the interaction strength.

In the following, we provide two possible experimental realizations of the above-analyzed setup and processes. The first one is mesoscopic particles carrying a charge in a micromechanical lattice. Exemplarily, one could use colloids or (spherical) clusters consisting of \( \sim 10^7 \) atoms and a lattice with amplitude \( a = 0.1 \) mm, site distance \( L = 1.0 \) mm, driving frequency \( \omega = 10 \) Hz and a barrier height of \( h = 0.1 \) \( \mu \)m/\( \alpha \). An optical lattice-based experimental realization is possible for dipolar \( (\alpha/|x_i - x_k|^3 \text{ in equation (1)}) \) instead of Coulomb interactions (the same parameters but \( \alpha = 10 \) for one and \( \alpha = 100 \) for two current-reversals). This implies slowly moving electrically dipolar clusters in phase modulated (or biharmonically driven) optical lattices using acousto-optical modulators. For clusters with mass \( 2.1 \times 10^{-17} \) kg (solid spheres with radius \( \sim 100 \) nm) and an electric dipole moment of \( Z \) Debye we require \( a = L/10 = 0.52 \) \( \mu \)m, \( \omega = 0.34 \text{Hz} \sqrt{Z/\alpha} \) (scaling \( \omega \propto 1/\sqrt{m} \)) and a laser potential of \( V = (Z^2/\alpha) \times 4.0 \times 10^{-12} \text{eV} \). In all cases current reversals and the subsequent growth of synchronized motion will occur on a timescale determined by \( 10^3/\omega - 10^5 \omega \).

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