Simultaneous control of multi-species particle transport and segregation in driven lattices

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We provide a generic scheme to separate the particles of a mixture by their physical properties like mass, friction or size. This selective transport is achieved by controlling the late-time nonlinear particle dynamics, via the attractors embedded in the phase space and their bifurcations. To illustrate the spectrum of possible applications of the scheme, we exemplarily demonstrate the separation of polydisperse colloids and mixtures of cold thermal alkali atoms in optical lattices.

Introduction The controlled separation, or spatial sorting, of particle mixtures based on their physical properties like mass, size, shape or mobility presents major challenges cutting across disciplines from biomedical problems such as the separating of malignant circulating tumour cells from leucocytes in the bloodstream [1] to technological problems on colloidal and granular scales [2]. Following these challenges, much effort has been devoted to develop innovative separation schemes complementing traditional techniques such as filtration, distillation or evaporation of mixtures. For example, to separate heterogeneous granular particle mixtures in geological and biological systems, it has been shown that a periodically shaken substrate [3–5] allows to separate two species by size. To separate particles on colloidal scales which are significantly affected by Brownian noise, it has been shown that suitable external forcing may be sufficient to separate mixtures [2, 6–8].

One important class of innovative separation schemes employs so-called Brownian ratchets in which thermal Brownian motion combined with external time-dependent driving generates directed particle motion [2, 9, 10]. Based on an appropriate design of such ratchets, the direction of the emerging particle current may depend on ‘internal’ particle properties such as mass, radius or mobility. This dependence can be exploited to simultaneously transport two different particle species in opposite direction, i.e. for separating them (Fig. 1a, upper panel). Based on this idea, it has been possible to establish a rich set of schemes to separate two component particle mixtures, including a massively parallel particle filter [11] serving as an artificial microsieve with potential biomedical applications [2] and schemes allowing to separate mixtures of cellular membrane associated molecules that differ in electrophoretic mobility and diffusion coefficient [12]. Further examples of ratchet based separation devices allow for the size-sorting of superparamagnetic particles using periodically switching magnetic fields [13], of active and passive particles using active ratchet systems [14, 15] and heterogeneous cell mixtures using microfluidic funnel ratchets [16]. Finally, we note that ratchets in superlattices also allow to separate particles by the type of their motion (ballistic/chaotic) and allow to sort (or filter) them by velocity [17, 18].

These examples illustrate the rich versatility of ratchet-based separation schemes which, in the following respects, seems to be somewhat advantageous over traditional techniques like sieving or filtration: (i) they may operate on many technologically relevant scales ranging from granular and colloidal sizes down to the nanoregime [2] and even to the size of single atoms [19], (ii) the particle current underlying particle separation can be controlled with an external field [20], even in real time [21, 22], and (iii) they allow to separate particles with respect to all kinds of physical properties from size and mass to charge and mobility. However these advantageous, ratchet-based schemes seem to have one striking disadvantage: unlike sieves which can be easily stacked to sort many-component mixtures by size, most (if not all) ratchet-based schemes are restricted to the separation of only two species, based on forward transport of one species and reverse transport of the other one. Since combinations of several ratchets, each separating two species, would be rather sophisticated to design and produce, it would be desirable to know a mechanism allowing for a simultaneous separation of many species.

Here we propose such a mechanism unifying the above advantages of ratchet-based separation schemes with the ability to efficiently separate multi-species mixtures (Fig. 1a) based on their physical properties like mass,
friction or size. To develop this scheme, we use a periodically shaken two-dimensional dissipative lattice, which can be produced for example based on optical molasses and counterpropagating laser beams using oscillating mirrors or acousto-optic modulators (AOMs) [19], and establish a new route to simultaneously control the angular-specific transport of many species which can be applied to separate or sort multi-species mixtures. Initializing particles representing mixtures, of say, polydisperse colloids differently located in the friction they experience, we demonstrate that each colloidal species travels in an individual direction through the lattice allowing for their collection with an angular detector (or a reservoir). The segregation scheme should apply more generally to particles on atomic and nano scales up to colloids and granular particles. In particular, contrasting many other ratchet-based separation schemes, the present one does not hinge on Brownian noise (but is robust against it) and should hence apply for granular particles which are too large to experience a significant effect from Brownian noise and in principle also for the extreme case of a mixture of cold thermal atoms with different masses in purely optical setups [19], where a noise-providing medium is practically absent.

**Setup** We consider a mixture of \( N \) non-interacting classical particles in a two-dimensional lattice defined by a periodic potential \( V(x, y) = V \cos k_x x (1 + \cos k_y y) \) which is driven via external bi-harmonic driving forces \( f_{x,y}(t) = d_{x,y}(\cos \omega t + 0.25 \cos(2\omega t + \pi/2)) \) acting in both \( x \) and \( y \) directions and breaking parity \( x \rightarrow -x + \chi \) and time-reversal \( t \rightarrow -t + \tau \) symmetry, with additional constant spatial and temporal shifts, to allow for a directed particle transport [20, 23]. Here, \( d_x, d_y \) denote the respective driving amplitudes in the two directions, \( k_x, k_y \) and \( \omega \) the respective wave numbers and \( \omega \) is the frequency of the external driving force. The system thus has spatial and temporal periodicities of \( L_{x,y} = 2\pi/k_{x,y} \) and \( T = 2\pi/\omega \). Such a two-dimensional lattice potential can be created for example in cold atom setups by using two sets of counter-propagating laser beams of non-orthogonal polarizations between mirrors and the driving can be implemented with standard techniques like acousto-optical modulators and radio frequency generators leading to a lateral oscillation of the mirrors and hence of the lattice [24]. Here, the damping can be realized using optical molasses [25].

Introducing dimensionless variables \( x' = k_x x, y' = k_y y \) and \( t' = \omega t \) and dropping the primes for simplicity, the equation of motion for a single particle of mass \( m \) located at position \( \mathbf{x} \) with momentum \( \mathbf{p} \) in such a setup reads

\[
\ddot{\mathbf{x}} = U_x \sin x (1 + \cos y) \mathbf{e}_x + U_y \cos x \sin y \mathbf{e}_y + (\cos t + 0.25 \cos(2t + \pi/2)) \mathbf{F} - \Gamma \dot{\mathbf{x}} - \dot{\mathbf{F}}(t)
\] (1)

where \( \mathbf{e}_x = (1, 0) \) and \( \mathbf{e}_y = (0, 1) \). The parameter space of this model has five essential dimensions with \( U_{x,y} = V \kappa^2/\mu \) comparing the velocity of a particle in a static lattice with the velocity of the oscillating lattice,
first allow the colloids to equilibrate in a static lattice for a region $L \approx 10^3$ since for e.g., a CO$_2$ laser, the interaction between the colloids and the lattice potential depends on their surrounding solvent. While $\Gamma = \frac{\gamma}{m\omega^2 \bar{u}^2}$ varying radii initialized at the potential minima may generally also affect Brownian noise in most of our simulations assuming low temperatures in the case of cold atoms or large particle masses as e.g. for granular particles or large underdamped colloids. Our main results are all robust against typical noise as we detail further below.

Simultaneous control of directed transport and particle segregation

Before detailing the general working principle of the scheme, we first illustrate its application to a polydisperse mixture of $N = 2 \times 10^4$ underdamped colloidal particles with continuously and uniformly distributed random radii $r \in [0.2, 0.5]$. We assume that the only effect that the radii has is that it governs both the colloidal mass ($m = \frac{4}{3} \pi \rho r^3$) and the dissipation coefficient ($\gamma = 6 \pi r \eta$) which the colloids experience in the surrounding solvent. While $r$ may generally also affect the interaction between the colloids and the lattice potential, we treat them as point like for our computation since for e.g., a CO$_2$ laser, the lattice spacing would be $10^3 - 10^5$ times larger than typical colloidal sizes.

We initialize the particles randomly within a square region $L_x \times L_y$ of the lattice and give them small random velocities. To mimic potential experimental scenarios, we first allow the colloids to equilibrate in a static lattice for a time $1000T$ (Fig. 1a, lower panel; left). Now switching on the driving, and waiting until $\sim 5 \times 10^4T$ we observe ballistic particle jets (‘rays’), radially moving away from their initial positions at different angles (Fig. 1b). Strikingly, most of these ‘rays’ have an almost uniform color (Fig. 1b), meaning that they involve only colloids with very similar radii and separate them from the rest of the mixture. The figure shows the simultaneous separation of four ‘species’ by radius, while the rays at $0$ and $180$ degrees, as well as the particle cloud around the origin, still contain a mixture of particles with different radii which may be considered as ‘losses’. When analyzing the general working principle of our scheme below, it will become clear that the presented segregation is not at all limited to the four specific radii intervals separated so far, but that it is tunable and can be applied to separate particles with a desired set of radii from the mixtures.

Discussion

We now analyze the working principle underlying the observed particle separation. The separation principle can be best understood on the level of the invariant manifolds in the five dimensional phase space $(x, y, px, py, t)$ of the system. In dissipative systems like the one described here, the asymptotic $t \to \infty$ dynamics depends on the set of attractors (stable invariant manifolds) in the phase space and the associated sets of all initial conditions which asymptotically end up in an attractor i.e. the basin of attraction. For the present periodically driven system, there are two relevant classes of attractors: chaotic attractors and limit cycles, representing chaotic and periodic motion respectively. Generally, the set of attractors and their basins of attraction depend on the parameters of the system, including particle-related parameters such as their mass.

The idea here is to tune the set of attractors such that the late-time dynamics of particles with different properties is governed by species-dependent limit cycles which transport particle to species-specific directions. Generally, limit cycle attractors transport particles in a well-defined direction and with a characteristic (quasi)periodic velocity with average $\bar{v} \equiv \langle \bar{v}_x, \bar{v}_y \rangle = \left( \frac{n_x L_x}{m \omega T}, \frac{n_y L_y}{m \omega T} \right)$ where $n_x, m_x, n_y, m_y$ are attractor specific integers. Hence at a large distance from the centre of the square region $L_x \times L_y$ where the particles were initialized (which we henceforth refer to as ‘origin’), particles following the dynamics of a limit cycle attractor can be collected by placing a suitable collector (detector or reservoir) at an angle $\theta = \tan^{-1} \frac{\bar{v}_y}{\bar{v}_x} = \tan^{-1} \frac{m_y n_x L_x}{m_x n_y L_y}$. Thus, if we manage to tune the limit cycle attractors and their basins of attraction in the phase space such that particles with e.g. different radii end up in different limit cycle attractors they will be automatically separated (Fig. 1b). The size of the detectors would depend on the angular spreading $\Delta \theta$ of the particle ‘jets’, which for this setup (Fig. 1b) was found to be of the order of 0.01 degrees. Hence, if one places the detectors at a radial distance of $R = 10^5$ from the origin, their required sizes would be determined by the arc length $R \Delta \theta \sim 4L_x$. Such detec-
tion and tracking of colloidal particles are routinely done using high resolution optical tracking and holographic microscopy [26, 27]. The chaotic particles, owing to their diffusive nature, stay much closer to the origin and as a result do not interfere with the segregation process.

In order to predict whether a particle would end up in a chaotic attractor or a limit cycle we compute the ‘bifurcation diagram’ associated with the particle velocity as a function of its radius. To do this, we initialize particles of different radii and after an initial transient time stroboscopically monitor (at multiples of $T$) the velocity as a function of the radius. The resulting bifurcation diagrams (Fig. 2) shows that particles can be either attracted to chaotic attractors, period 1 limit cycles or multi-periodic limit cycles. Hence for a given set of parameters, one can predict from such bifurcation diagrams the angles to which particles of different radii would travel.

To make the segregation scheme more flexible and separate particles of a varying range of sizes we use the lattice potential height $V$ as a control parameter. Using similar concept as above, one can construct a two parameter bifurcation diagram of the particle velocity $v_\theta = \tan^{-1} \, \frac{\bar{v}_r}{\bar{v}_x}$ (in the angular coordinates) showing whether a particle of radius $r$ ends up in a limit cycle attractor or a chaotic attractor for a given lattice potential height $V$ (Fig. 3a).

For our segregation scheme, we choose those values of $V$ and $r$ for which the particle dynamics is asymptotically governed by the limit cycle attractors. Depending on the average velocity $\bar{v}$ of these limit cycles, particles of a given radius might be trapped ($\bar{v} = 0$) in the lattice or fly out ballistically at certain angles ($\bar{v} \neq 0$). The asymptotic direction of flight $\theta = \tan^{-1} \, \frac{\bar{v}_r}{\bar{v}_x}$ for these ballistic particles as a function of $V$ and $r$ (Fig. 3b) predicts a priori at which angle a particle of a given radius would travel for a chosen lattice height $V$. At this stage, the segregation protocol becomes very simple: given a set of particles with different radii, the task is to simply choose a value of $V$ from Fig. 3b for which the different species travel ballistically at different angles. One can in principle repeat this process with a different value of $V$ in order to also separate the cloud of ‘lost’ particles, which owing to their diffusive motion, remain close to the origin.

The segregation scheme mentioned here works not just for colloidal particles with a continuous size distribution but for example also for a mixture of particles differing only in mass. We now demonstrate this using a mixture of three cold thermal alkali atoms which can be treated classically in the regime of microkelvin temperatures [19, 28]. Such a scheme can be tested of course also with two species only and also applies to isotopic mixtures of the same atom (see [29, 30] for details on simultaneous trapping). In Fig. 4, we show how our scheme can be adapted to simultaneously separate three species of commonly used alkali atoms of different masses from a mixture. It shows that after $t = 5 \times 10^4 T$, particle rays containing mostly one species emerge at different angles. A detector positioned e.g. at $\theta \approx 320^\circ$ would collect only Na atoms whereas a detector at $\theta \approx 270^\circ$ would see mostly Cs atoms. Such a scheme may be realized using state of the art cold atom experimental setups with optical lattices driven by phase modulation of the laser beams using acousto-optical modulators and radio frequency generators [19, 31–33].

One advantage of our scheme compared to many other ratchet based segregation schemes is that is does not depend on noise and should be applicable to e.g. granular

![Figure 3. (a) Bifurcation diagram of $v_\theta$ (in colour) as a function of lattice potential height $V$ and particle radius $r$. The yellow regions denote period 1 limit cycles, green: period 2 limit cycles, red: period 3 limit cycles and black denotes more than three limit cycle attractors. (b) Asymptotic direction of flight $\theta$ (in the angular coordinates) of the particles ending up in limit cycle attractors (corresponding to yellow, green and red regions of Fig. 3a) with average velocity $\bar{v} \neq 0$ for different values of $V$ (in the radial coordinates) and $r$ (in colorbar). Hence, one can predict a priori that a lattice with a potential height of e.g. $V = 0.6$ can separate particles with radii in the intervals $0.26 \lesssim r \lesssim 0.3$ to $\theta \approx 90^\circ$ and analogously $0.12 \lesssim r \lesssim 0.16$ to $\theta \approx 27^\circ$ and $0.36 \lesssim r \lesssim 0.33$ to $\theta \approx 227^\circ, 333^\circ$. Remaining parameters are $\eta = 0.05$, $d_x = d_y = 1$, $\omega = 1$ and $2k_x = k_y = 2$.](image-url)
which may allow to transfer the scheme even to the pure Hamiltonian regime based on e.g. a mass-selective accumulation of particles in the regular structures of the Hamiltonian phase space [35]. Interaction effects may add to the species-selective directed transport [36].

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Figure 4. Snapshot of particle positions at $t = 5 \times 10^4 T$ (in the radial $R$ and angular $\theta$ coordinates) showing segregation of 3 different masses 0.23 (red), 0.87 (green) and 1.33 (blue) corresponding to atoms Na, Rb and Cs with masses 23, 87 and 133 respectively commonly used in cold atom experiments. Remaining parameters are $\gamma = 0.01$, $d_x = d_y = 3$, $\omega = 1$, $2k_x = k_y = 2$ and $V = 0.1679$. Since in our setup the dimensionless parameters depend on the ratios $\frac{V}{m}$, $\frac{d_x, d_y}{m}$ and $\frac{\gamma}{m}$, the parameters $V$, $d_x$, $d_y$ and $\gamma$ can be scaled up by the same factor as the atomic mass to correspond to relevant experimental setups.

particles which are too heavy to allow Brownian noise to play a significant role and are often underdamped. However, as noise always accompanies dissipation, and may play a significant role for particles on colloidal scales, we have tested the robustness of the present scheme against white noise of strength typical for experiments corresponding to underdamped colloidal ratchets [2] and cold atoms [34]. It adds only minor fluctuations around the average velocity of the limit cycle attractor which broadens the angular particle streams without essentially affecting the overall functionality of our segregation mechanism.

Conclusions We have presented a scheme allowing to separate, or sort, particles from a mixture based on different selection criteria like radius-dependent frictional forces or particle mass. This scheme exploits the strong nonlinearity of driven lattices to control the late-time particle dynamics species selectively on the phase space level. This contrasts standard segregation schemes based on overdamped ratchet setups and allows us to overcome their key limitation of segregating more than two species. Owing to its deterministic character, our new control mechanism can be applied to particle mixtures on an unusually broad range of scales ranging from atoms to granular particles. The segregation scheme can be tested, for example, using polydisperse colloids or mixtures of cold thermal alkali atoms using ac-driven optical lattices. As a perspective, further studies may account for localized perturbations of the ideal periodic potential employed
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