Brownian asymmetric simple exclusion process

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We study the driven Brownian motion of hard rods in a one-dimensional cosine potential with an amplitude large compared to the thermal energy. In a closed system, we find surprising features of the steady-state current in dependence of the particle density. The form of the current-density relation changes greatly with the particle size and can exhibit both a local maximum and minimum. The changes are caused by an interplay of a barrier reduction, blocking and exchange symmetry effect. The latter leads to a current equal to that of non-interacting particles for a particle size commensurate with the period length of the cosine potential. For an open system coupled to particle reservoirs, we predict five different phases of non-equilibrium steady states to occur. Our results show that the particle size can be of crucial importance for non-equilibrium phase transitions in driven systems. Possible experiments for demonstrating our findings are pointed out.

A minimal model for studying fundamental questions of statistical physics out of equilibrium is the asymmetric simple exclusion process (ASEP) [1, 2], which, due to its simplicity, is sometimes referred to as the ”Ising model of non-equilibrium statistical mechanics” [3]. In this model, particles with exclusion interaction are considered to hop between neighboring sites of a one-dimensional lattice with a bias in one direction. Many intriguing findings were reported for this ASEP, as exact results for microstate distributions in non-equilibrium steady states (NESS) [4], phase transitions of NESS in systems with open boundaries [5, 6] and defects [7], condensation transitions in systems with random [8] and non-Poissonian hopping rates [9], and singular points in rate functions characterizing large deviations of fluctuations in time-averaged currents [10–12].

Most applications of the ASEP are found in the modeling of biological traffic [13, 14], where the model was first introduced to describe protein synthesis by ribosomes [13] and where it is frequently used now in studies of molecular motor motion [16, 17]. Clearly, refinements of the core model are needed for corresponding applications, such as the consideration of inhomogeneous hopping rates, particles occupying several sites, internal states of particles and multi-lane variants [13, 14, 16, 17]. A direct comparison of models and experiments in this area, however, is difficult to realize and hampered by the complexity of biological transport phenomena.

Here, we consider a Brownian motion of particles with the following ingredients resembling features of the ASEP: (i) an exclusion interaction between particles over a range \( \sigma \), (ii) a periodic potential \( U(x) \) with period length \( \lambda \), giving rise to an effective hopping motion of the particles between the potential wells, and (iii) a constant drag force \( f \) acting on the particles. This BASEP is a broadly applicable model of single-file diffusion [18, 19], and can be realized in lab by driving colloids using a combination of microfluidics and optical micro-maniupulation techniques [20, 22]. These recent experiments have a potential to probe and verify fundamental theoretical predictions for non-equilibrium collective phenomena. The lattice ASEP may, due to its discreteness, not be a correct model for corresponding experimental tests.

Indeed, we show in this Letter that the BASEP exhibits surprising features which have no counterpart in the ASEP. These features are a consequence of the length scale \( \sigma \), which enters the problem as a parameter in addition to the particle density \( \rho \). The site blocking effect associated with the exclusion interaction is dominating the steady-state particle current \( j(\rho, \sigma) \) in a limited \( \sigma \) range only. Due to a barrier reduction effect, \( j(\rho, \sigma) \) can be larger than the current \( j_0(\rho) \) of non-interacting particles. An exchange symmetry effect emerges when \( \sigma \) becomes commensurate with the period length \( \lambda \). In this case \( j(\rho, \sigma = \lambda) = j_0(\rho) \), as if there were no interactions. The interplay of the barrier reduction, blocking and exchange symmetry effects leads to changes of the form of the current-density relation with the particle size. This in turn leads to the appearance of five different non-equilibrium phases in open BASEPs coupled to particle reservoirs.

Figure 1 illustrates interacting particles of size \( \sigma \) that are driven by a drag force \( f \) through a cosine potential \( U(x) = (U_0/2) \cos(2\pi x/\lambda) \) with barrier height \( U_0 \). Their center of mass positions \( x_i, i = 1, \ldots, N \), are considered

![FIG. 1. Driven Brownian motion of interacting particles of size \( \sigma \) in a cosine potential with barrier height \( U_0 \) and period length \( \lambda \) under a drag force \( f \).](image-url)
FIG. 2. (Color online) (a) Current-density relations for various fixed particle sizes $\sigma$. The solid and dashed black lines mark the currents $j_0(\rho)$ and $j_{\text{ASEP}}(\rho)$ for non-interacting particles and the corresponding ASEP, respectively. (b) Particle size dependence of the current change $\Delta j(\rho, \sigma) = (j(\rho, \sigma) - j_0(\rho))/j_0(\rho)$ due to hard-core interactions for different fixed densities $\rho$. The inset shows the curve $\sigma_x(\rho)$, which separates the region of current enhancement (blue area) and reduction (red area), and the dependence of $\rho_{\text{ext}}, \rho_{\text{max}}$ and $\rho_{\text{min}}$ on $\sigma$. 

To perform an overdamped Brownian motion according to the coupled Langevin equations

$$\frac{dx_i}{dt} = \mu [f^\text{ext}(x_i) + f^\text{int}] + \sqrt{2D\eta_i(t)},$$

where $f^\text{ext}(x) = f - dU(x)/dx$ is the external force, $f^\text{int} = f^\text{int}(x_1, \ldots, x_N)$ is the interaction force on the $i$th particle, and $\eta_i(t)$ are independent Gaussian white noise processes with zero mean and $\langle \eta_i(t)\eta_j(t'') \rangle = \delta_{ij}\delta(t-t')$; $\mu$ and $D = k_B T \mu$ are the bare mobility and diffusion coefficient, respectively, and $k_B T$ is the thermal energy. In the BASEP, $f^\text{int}$ is solely determined by the hard-core exclusion between neighboring particles, i.e. a contribution upon particle contact. The system size $L$ is taken to be an integer multiple of $\lambda$ and periodic boundary conditions are imposed. As units for length, time, and energy we choose $\lambda, \lambda^2/D$, and $k_B T$, respectively. The density, or filling factor, is $\rho = N/L$. We set $U_0 \gg k_B T$ to generate an effective hopping motion of the particles, and focus first on the case where both $\rho$ and $\sigma$ lie in the range $[0,1]$.

To determine $j(\rho, \sigma)$ in the non-equilibrium steady state (NESS), we have carried out Brownian dynamics simulations, which we corroborate by analytical considerations. The barrier height and the drag force are fixed by setting $U_0 = U_0/(k_B T) = 6$ and $f = f\lambda/(k_B T) = 1$. In most of the simulations we have chosen $L = 100$. For $\rho$ and $\sigma$ close to one, simulations were performed also for larger $L$ to check that our results are not affected by the finite system size. The hard-core interaction force between neighboring particles was simulated according to the algorithm developed in [23]. For $\sigma$ close to one, we also used the method proposed in [24].

For non-interacting particles, the current increases linearly with $\rho$, $j_0 = v_0 \rho$, where $v_0$ is the mean velocity of a single particle and can be calculated analytically for our parameters $v_0 \cong 0.043$. By the hard-core interaction, this linear current-density relation is modified in quite different ways for different particle sizes $\sigma$, as can be seen from Fig. 2(a). As reference curves, we included in this figure the line $j_0 = v_0 \rho$ for non-interacting particles (solid black line) and the corresponding one for the ASEP [1,2], $j_{\text{ASEP}}(\rho) = j_0(\rho)(1-\rho) = v_0 \rho (1-\rho)$ (dashed line). Remarkably, the parabolic curve of the ASEP is resembled in a quite limited $\sigma$ range only.

To understand the nonlinear current-density relation for different particle sizes, it is helpful to first consider the relative current change $\Delta j(\rho, \sigma) = (j(\rho, \sigma) - j_0(\rho))/j_0(\rho)$ due to the interactions as a function of $\sigma$ for several fixed $\rho$. Corresponding curves plotted in Fig. 2(b) show a similar behavior for all $\rho$. For small $\sigma$, $\Delta j$ increases with $\sigma$ up to a maximum and then it decreases until crossing the zero line at a value $\sigma_x(\rho)$. Hence, for $0 < \sigma < \sigma_x(\rho)$, $j(\rho, \sigma)$ becomes enhanced compared to $j_0(\rho)$. When increasing $\sigma$ beyond $\sigma_x(\rho)$, $\Delta j$ first decreases, then remains approximately constant in a plateau-like regime, and eventually increases again, where $\Delta j = 0$ for $\sigma = 1$ and all particle densities $\rho$. Hence, $j(\rho, \sigma)$ becomes reduced compared to $j_0(\rho)$ for $\sigma_x(\rho) < \sigma < 1$, and it becomes equal to $j_0$ for $\sigma = 1$. The crossover value $\sigma_x(\rho)$ increases with $\rho$ and the full curve shown in the inset of Fig. 2(b) divides the $\sigma$-$\rho$-plane in two regions of current enhancement and reduction.

The enhancement of the current is caused by a barrier reduction effect, which occurs if a potential well is occupied by more than one particle [20]. Inside a...
The horizontal dotted lines indicate the positions of the potential minima. In (a) a cascade-like propagation of double-occupancies marked by the circles is demonstrated by the arrows. In (b) potential wells are vacated and filled in a sequential process.

FIG. 3. (Color online) Typical particle trajectories in the BASEP for $\rho = 0.75$, and (a) $\sigma = 0.25$ and (b) $\sigma = 0.75$. The horizontal dotted lines indicate the positions of the potential minima. In (a) a cascade-like propagation of double-occupancies is demonstrated by the potential minima. In (b) potential wells are vacated and filled in a sequential process.

multi-occupied well, the mutually excluding particles exhibit, on average, higher potential energies than a particle in a single-occupied well. They need to surmount a lower barrier for escaping the well, which causes the current enhancement. This enhancement is the stronger the larger $\rho$ [see Fig. 2(b)], because the probability of multi-occupancies rises with increasing $\rho$. Also, clusters of neighboring occupied wells become larger on average. This facilitates a cascade-like propagation of multi-occupancies as demonstrated in Fig. 3(a).

The enhancement effect due to barrier reduction is pronounced at small $\sigma$, because for larger $\sigma$, the formation of double (or higher) occupancies requires larger energies and becomes less likely. For $\sigma > \sigma_c(\rho)$, the blocking effect, known from the ASEP, prevails. It means that an effective hopping of a particle to a neighboring well is suppressed if the target well is occupied. Typical particle trajectories in this regime, as displayed in Fig. 3(b), show that clusters of neighboring particles frequently move in a manner, where wells are sequentially vacated and filled. Hence, when increasing $\sigma$ beyond $\sigma_c(\rho)$, the particle motion becomes similar to a hopping on a lattice with forbidden multi-occupation of sites. The current then is nearly independent of the particle size $\sigma$, as reflected in the plateau-like $\sigma$-intervals in Fig. 2(b).

To understand why the current increases again for large $\sigma$ approaching one, let us consider a coordinate transformation $x_i \rightarrow x'_i = x_i - i\sigma$ in the Langevin equations [1], which for $\sigma = \lambda = 1$ leaves them invariant, because of the $\lambda$-periodicity of $f^{\text{int}}(x)$. After this transformation, the dynamics of the $x'_i$ corresponds to that of point particles. However, for point particles with hard-core interaction, collective properties, like the current, become invariant under particle exchange [27] and accordingly $j(\rho, 1) = j_0(\rho)$ for all $\rho$.

Refining this line of reasoning, we show in the supplemental material [28] that the current for general $\sigma \geq 0$ with $m = \text{int}(\sigma/\lambda)$ fulfills the relation

$$j(\rho, \sigma) = (1 - m\rho) j \left( \frac{\rho}{1 - m\rho}, \sigma - m\lambda \right).$$

(2)

This relation means that the current behavior for $\sigma \geq \lambda$ can be inferred from that for $\sigma < \lambda$. Moreover, it implies: (i) $j(\rho, \sigma) = j_0(\rho)$ for all $\sigma = m\lambda$, $m = 1, 2, \ldots$; (ii) $j(\rho, \sigma)$ can resemble the behavior of an $l$-ASEP [29], where particles occupy $l$ lattice sites.

All results are further supported by analytical calculations when starting from the Smulochowski equation for the joint probability density $p_N(x_1, \ldots, x_N, t)$ of finding the particles at positions $x_1, \ldots, x_N$ at time $t$ [28]. In the NESS, the current $j(\rho, \sigma)$ is given by

$$j(\rho, \sigma) = \left[ \mu(f^{\text{int}}(x) + \langle f^{\text{int}}(x) \rangle) - \frac{d}{dx} \right] \rho_{\text{loc}}(x),$$

(3)

where $\rho_{\text{loc}}(x)$ is the local density and

$$\langle f^{\text{int}}(x) \rangle = k_B T \left[ \psi_-(x) - \psi_+(x) \right].$$

(4)

is the mean interaction force on a particle at position $x$. Here, $\psi_- = \Psi_- / \rho_{\text{loc}}$ and $\psi_+ = \Psi_+ / \rho_{\text{loc}}$ are the conditional probability densities that, given a particle at position $x$, a neighboring particle is in contact (at distance $\sigma$) to it in counterclockwise and clockwise direction, respectively; $\Psi_{\pm}(x)$ are the respective joint probability densities in the NESS. Because $\Psi_-(x) = \Psi_+(x)$ for $\sigma = \lambda$, one obtains $\langle f^{\text{int}}(x) \rangle = 0$ for $\sigma = \lambda = 1$ from Eq. 4, and it follows $j(\rho, 1) = j_0(\rho)$ from Eq. 3.

Moreover, multiplying Eq. 3 with $1 / \rho_{\text{loc}}(x)$ and integrating over one period $\lambda$, we obtain, when utilizing the $\lambda$-periodicity of $\rho_{\text{loc}}(x)$ in the NESS and of $U(x)$ in $f^{\text{int}}(x) = f - dU(x)/dx$, the average interaction force on a particle in the NESS

$$j(\rho, \sigma) = \int \lambda \rho_{\text{loc}}(x) \frac{d}{dx} \right] \rho_{\text{loc}}(x),$$

(5)

where $\bar{f}^{\text{int}} = \lambda^{-1} \int_0^\lambda dx (f^{\text{int}}(x))$ is the period-averaged mean interaction force. The form of this exact expression for the current is fully analogous to the corresponding one for a single particle [29], but here it refers to a many-body system with hard-core interactions, where $\bar{f}^{\text{int}}$ gives an additional contribution to the driving force and is related to the two-particle density in the NESS via Eq. 1. In fact, Eq. 5 is valid also for other interaction forces if the
corresponding mean interaction force is used. We further demonstrate [28] that an approximate analysis of Eq. (5) in the linear response limit reproduces qualitatively the behavior shown in Figs. 2(a) and (b).

Let us now discuss the curves in Fig. 2(a) with increasing $\sigma$. For small $\sigma = 0.25$, $j(\rho, \sigma)$ is larger than $j_0(\rho)$ and increases monotonically due to the barrier reduction effect. Enlarging $\sigma$, the blocking effect becomes more relevant, which causes the curves to approach more and more $j_{\text{NESS}}(\rho)$. First, this leads to a change of curvature of $j(\rho, \sigma)$ from concave to convex at a density $\rho = \rho_{\text{c}}$, see the curve for $\sigma = 0.5$. Then, when $\sigma$ exceeds a critical value $\sigma_{c} \approx 0.55$, a local maximum at $\rho = \rho_{\text{max}}$ and a local minimum at $\rho = \rho_{\text{min}}$ occurs, see the curves for $\sigma = 0.58$ and $\sigma = 0.62$. Upon further increasing $\sigma$, a range of particle sizes appears, where $j(\rho, \sigma) \approx j_{\text{NESS}}(\rho)$. Eventually the exchange symmetry effect becomes noticeable, which causes $j(\rho, \sigma)$ to approach $j_0(\rho)$. Going along with this is a shift of the local maximum $\rho_{\text{max}}$ and of $j(\rho_{\text{max}}, \sigma)$ towards larger values, see the curve for $\sigma = 0.98$. The dependence of $\rho_{\text{c}}$, $\rho_{\text{max}}$ and $\rho_{\text{min}}$ on $\sigma$ is shown in the inset of Fig. 2(b).

The different forms of the current-density relation lead to a versatile emergence of NESS phases in an open BASEP in contact with two particle reservoirs at its left and right end. In this open BASEP, the period averaged densities $\bar{\rho}_i = \lambda^{-1} \int_{(i-1)\lambda}^{i\lambda} dx \rho(x)$ in each well $i = 1, \ldots, L/\lambda$ are no longer equal in the NESS, but approach a constant “bulk value” $\rho_b$ in the system’s interior far from the boundaries. This bulk density $\rho_b$ or its derivative can change abruptly upon variation of the system-reservoir couplings, i.e. the parameters controlling the particle exchange with the reservoirs. The corresponding sets of phase transition points separate NESS phases, in which the order parameter $\rho_b$ varies smoothly with the system-reservoir couplings.

Independent of the details of the couplings, all possible NESS phases can be uncovered from $j(\rho, \sigma)$ by considering just two control parameters $\rho_L, \rho_R \in [0, 1]$, which for bulk-adapted couplings represent the particle densities in the left and right reservoir, respectively [30–32]. The different phases are obtained by applying the extremal current principles [5, 33], which state that $\rho_b$ assumes the value at which $j(\rho, \sigma)$ becomes minimal (for $\rho_L < \rho_b$) or maximal (for $\rho_R < \rho_b$) in the $\rho$-intervals enclosed by $\rho_L$ and $\rho_R$:

$$\rho_b = \begin{cases} \argmin_{\rho_L \leq \rho \leq \rho_R} \{ j(\rho, \sigma) \}, & \rho_L \leq \rho_R, \\
\argmax_{\rho_L \leq \rho \leq \rho_R} \{ j(\rho, \sigma) \}, & \rho_R \leq \rho_L. \end{cases} \quad (6)$$

For $\sigma < \sigma_c$, the extremal current principles in Eq. (6) imply that no phase transitions occur in the open BASEP, because $j(\rho, \sigma)$ exhibits no local minima or maxima. For $\sigma > \sigma_c$, by contrast, phase transitions occur and we show in Figure 4 different examples of phase diagrams of NESS. Dashed and solid lines in these diagrams indicate phase transitions of first and second order, respectively.

In Fig. 4(a), $\sigma = 0.58$ is close to $\sigma_c$ and in total five NESS phases appear. For the left-boundary induced phases I and $\nu$, $\rho_b = \rho_L$, and for the right-boundary induced phase III, $\rho_b = \rho_R$. Phase II is a maximal current phase with $\rho_b = \rho_{\text{max}} \approx 0.60$ and phase IV is a minimal current phase with $\rho_b = \rho_{\text{min}} \approx 0.83$ [see Fig. 4(a)]. With increasing $\sigma$, the phase regions II-IV extend, while the regions I and $\nu$ shrink, see Fig. 4(b). Let us note that the topology of the phase diagrams in Figs. 4(a) and (b) resembles features seen in corresponding phase diagrams of driven lattice gases with repulsive nearest-neighbor interactions [30, 32, 33]. For the phase diagram in Fig. 4(b), we demonstrate the occurrence of different NESS phases in simulations of an open BASEP in the supplemental material [28].

When entering the $\sigma$ regime, where $j(\rho, \sigma) \approx j_{\text{NESS}}(\rho)$, the phase diagram resembles that of the ASEP with the phases I-III, as shown in Fig. 4(c) [34]. Finally, when the exchange symmetry effect causes $\rho_{\text{max}}$ to approach one, the phase regions II and III shrink at the expense of region I, see Fig. 4(d).
To conclude, the interplay of the barrier reduction, blocking, and exchange symmetry effects gives rise to a surprisingly versatile form of the current-density relation in the BASEP in dependence of the particle size. This leads us to predict the appearance of in total five different phases of NESS states in the open BASEP coupled to particle reservoirs. Only for a quite limited range of particle sizes is the behavior of the BASEP resembled by the ASEP.

Similar non-equilibrium phase transitions as in the BASEP are expected to occur for particles with soft repulsive interactions of short range. Indeed, we could identify these in simulations with a Yukawa interaction. For a power-law soft core, just an ASEP-like behavior was reported earlier [38].

Besides its relevance in biology, where confined transport processes through channels with binding sites [39–38] are mediated by driven Brownian motion, we believe that the BASEP is an ideal in-situ tunable model system for an experimental exploration of non-equilibrium phase transitions. Current experimental micro-manipulation techniques allow precise engineering and fine tuning of relevant aspects of the model: the external tilted periodic potential and the confinement. The precise control of the potential may be achieved with high precision using holographic optical tweezers as it was done in a related experimental work [20]. The confinement can be realized within microfluidic chips. Combining microfluidics with optical tweezers already proved to be a realizable method to probe fundamentals of facilitated diffusion in confined spaces [39, 40] and of escape times in single-file transport [41]. Another intriguing recent option is to consider a nanofluidic ratchet [21, 22], where the periodic potential landscape is shaped by the geometry of a nanofluidic slit and an additional electrostatic interaction between particles and walls.

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