Single-file transport in periodic potentials: The Brownian ASEP

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Single-file Brownian motion in periodic potentials is an important process in nature and technology. Often this type of motion is restricted to strongly confined geometries, hindering the particles to overtake each other. In cell biology, examples of such single-file transport are the motion of motor proteins along microtubules or actin filaments [5, 6], ion migration through membrane channels [7, 8], and protein synthesis by ribosomes [4]. With the steadily increasing quality of experimental techniques capable to control and manipulate particle motion on molecular scales, single-file transport in periodic potentials becomes of increasing importance also for applications, as, e.g., transport in carbon nanotubes [9], mesoporous materials [7, 8], and nanofluidic devices [3].

A much investigated and well understood feature in single-file diffusion is the anomalous subdiffusion of a tracer particle in the long-time limit [10]. This was first proven in the mathematical literature [11] and later detected experimentally in zeolites [12, 13] and in nanotubes [14, 15] by using NMR techniques. Further direct observation was possible in colloidal experiments by optical imaging [16]. The aspect of subdiffusion was further elaborated in connection with general theories of anomalous transport [17], including descriptions in terms of fractional Brownian motion [18], effects of initial and boundary conditions [19, 20], external force fields [21], time-varying potentials [22], first-passage time distributions [23, 24], and partial overtaking of particles [25, 26].

As for collective transport properties, single-file motion has been mainly investigated in lattice models, which reflect a periodic structure in a coarse-grained manner. These lattice models can be considered as variants of the so-called asymmetric simple exclusion process (ASEP) and have found applications in the modeling of biological traffic [29, 30], of protein synthesis by ribosomes [4], and of molecular motor motion [31, 32].

The minimal ASEP model, where particles perform nearest-neighbor hops between lattice sites with a bias in one direction and under the constraint that only one particle can occupy a lattice site has become a reference model for studying fundamental questions of statistical physics out of equilibrium [33, 34]. For this model, exact results for microstate distributions in nonequilibrium steady states could be obtained [35]. When coupled to particle reservoirs, three different phases of nonequilibrium steady states appear [36, 37] in dependence of the reservoir densities. Studies with nearest-neighbor interactions between particles showed richer phase diagrams [38, 39]. They led to a clarification of the role of system-reservoir couplings in open systems for the topology of non-equilibrium phase diagrams and of the meaning of particle-hole symmetry [40, 41]. This clarification turned out to be useful also for understanding collective particle dynamics in lattice models with time-varying site energies [42].

Many further interesting results were reported for the ASEP, as, e.g., singularities in large deviation functions for time-averaged currents [43, 44], and condensation transitions for nonuniform currents [45, 46]. More recently, new universality classes in the hydrodynamic limit of nonlinear hydrodynamics were discovered for multi-lane variants of the model [47]. Predictions for long-time tails could be proven for a specific microscopic model [48].

As the hopping transitions in the ASEP can be considered to reflect rare events of thermally activated barrier crossings, one may conjecture the continuous single-file motion in a periodic potential to exhibit similar features...
as the ASEP. However, in a recent study \[50\] we showed that a much richer behavior occurs in continuous Brownian motion because of additional length scales associated with particle-particle interactions. The simplest model is that of hardcore interacting particles, which we referred to as the Brownian asymmetric simple exclusion process (BASEP). In this BASEP, hard rods with diameter \(\sigma\) are driven through a periodic potential with wavelength \(\lambda\) by a constant drag force \(f\).

The BASEP is particularly interesting in connection with recent experiments utilizing advanced techniques of microfluidics and optical and/or magnetic micromanipulation \[51\, 52\], which includes setups where the particles are not driven by a constant drag force but a traveling wave potential \[50\]. This is because the Brownian motion of a particle in a traveling wave potential \(U(x - vt)\) is mapped onto that in a periodic potential \(U(x)\) with a constant drag force \(f = \nu/\sigma\) after a coordinate transformation \(x \to x - vt; \mu\) is the bare mobility of the particles.

Furthermore, the BASEP should allow one to understand under which conditions a coarse-grained description in terms of lattice models will be appropriate. Generally, a more detailed understanding of the connection between the BASEP and corresponding lattice models is necessary to explain why certain effects are seen in one description but not in the other. For example, a current reversal was reported in lattice models \[42\, 57\, 60\], and recently experimentally seen in a rocking Brownian motor \[58\], but it was not found in an analogous setting with continuous-space dynamics \[61\]. Current reversals in space-continuous models were reported earlier for a constant and “flashing” asymmetric sawtooth-shaped external potential \[62\, 63\], and in a recent work with time-discontinuous driving of a single potential barrier along a ring \[64\]. In the BASEP, a barrier reduction and an exchange symmetry effect were identified as decisive mechanisms for the characteristics of single-file transport, but it is yet unclear to which extent these effects have a counterpart in lattice descriptions. In this study, we will provide further insight into this issue.

The main goal of this study is to gain a complete description of the steady-state current in the BASEP and an explicit verification of all phases of nonequilibrium steady states in an open system coupled to particle reservoirs. We believe that this provides a useful basis for further investigations of model variants where further details can be included to capture specific experimental conditions.

As for the completed description of the steady-state current, we note that our results reported in \[50\] focused on a limited regime of particle densities \(\rho \leq 1\), which we defined as the (dimensionless) filling factor of the potential wells. The maximal possible density \(\rho\) is thus equal to \(\lambda/\sigma\), which means that there is a yet unexplored regime of densities in the range \(1 < \rho \leq \lambda/\sigma\). In fact, by making use of a mapping of currents for different particle sizes, we give a description for all particle sizes and densities.

Our extensive simulations are supported by an analytical treatment following the derivations in the supplemental material of Ref. \[50\]. This yields an approximate expression for the current in the linear response regime, which shows qualitative agreement with the simulation results. It is shown that quantitative deviations are mainly due to the neglect of an interaction-mediated effective drift term. We will analyze this term in more detail. Moreover, we investigate the influence of the temperature on the current. In the open BASEP coupled to particle reservoirs, we verify by simulations the phase diagram that contains five possible nonequilibrium phases.

II. BASEP: MODEL AND GENERAL PROPERTIES

A. Model

In the BASEP, the one-dimensional single-file motion of \(N\) hard rods (particles) with diameter \(\sigma\) is considered. These particles perform an overdamped Brownian motion driven by an external force \(f_\text{ext}(x) = f - \partial U(x)/\partial x\), where \(U(x) = U(x + \lambda)\) is a periodic potential and \(f\) a constant drag force. Accordingly, their dynamics are described by the Langevin equations

\[
\frac{dx_i}{dt} = \mu f - \mu \frac{\partial U(x_i)}{\partial x_i} + \sqrt{2D}\eta_i(t) \quad (1)
\]

Here, \(x_i, i = 1, \ldots, N\), are the center positions of the particles, \(\mu\) and \(D = \mu k_B T\) are the bare mobility and diffusion coefficient, and \(k_B T\) is the thermal energy. The \(\eta_i(t)\) are independent and \(\delta\)-correlated Gaussian white noise processes with zero mean and unit variance, \(\langle \eta_i \rangle = 0\) and \(\langle \eta_i(t)\eta_j(t') \rangle = \delta_{ij}\delta(t - t')\). The hardcore interactions imply the boundary conditions \(x_1, x_N \geq \sigma\), i.e. overlaps between neighboring particles are forbidden. We define the density as a (dimensionless) filling factor of the potential wells, i.e. by \(\rho = N/\lambda\); the number density then is \(\rho/\lambda\) and has the upper bound \(1/\sigma\).

In the following we will distinguish between the closed BASEP, where periodic boundary conditions are applied with particle coordinates in sequential order \(x_1 \leq x_2 \leq \ldots \leq x_N \leq \lambda\), and the open BASEP, where the left and right boundaries are coupled to particle reservoirs with in general different densities. In the closed BASEP, the drag force \(f\) leads to a steady state with a constant particle current \(j\) and a \(\lambda\)-periodic local density profile \(\rho(x)\). The dependence of the current on \(\rho\) and \(\sigma\) is denoted explicitly, i.e. \(j = j(\rho, \sigma)\), while other dependencies on \(T\), \(f\) etc. are omitted in the notation. In the open BASEP, specification of the way of how particles are exchanged with the reservoirs is a subtle issue, which will be discussed in sections \[11\] and \[13\].

In simulations of the model, we used numerical algorithms specifically developed for Brownian dynamics of hard-sphere systems \[66\, 69\]. These algorithms use the Euler method and differ in the implementation of the hardcore (excluded volume) constraints. Specifically, we
applied the two algorithms developed in Refs. 68 and 69. Our results are not affected by the choice of any of these algorithms, and they showed agreement with exact analytical findings for specific cases.

B. Equivalence to traveling wave driving

For overdamped Brownian motion of hard rods with coordinates $x_i'$ in a traveling wave potential with wave velocity $v_w$, the Langevin equations read

$$\frac{dx_i'}{dt} = -\mu \frac{\partial U(x_i' - v_w t)}{\partial x_i'} + \sqrt{2\eta(t)},$$

where the hardcore constrains are $|x_i'_{i+1} - x_i'| \geq \sigma$. By the Galilean transformation $x_i' \rightarrow x_i = x_i' - v_w t$ these equations reduce to the Eqs. (1) with the drag force $f = -v_w/\mu$. Hence, the probability of a path $P[x_i(t)]$ in the traveling wave system is equal to the probability $P(\{x_i(t)\})$ of the corresponding path $\{x_i(t)\} = \{x_i'_{i+1} - v_w t\}$ in the BASEP, $P(\{x_i(t)\}) = P(\{x_i(t)\})$ (given the same initial conditions).

For local particle densities and currents in stationary states, this means

$$\rho(x) = \rho'(x + v_w t),$$

$$j(\rho, \sigma) = j'(\rho, \sigma) - \rho v_w,$$

where the primed quantities refer to the traveling wave system and the unprimed quantities to the BASEP, and $\rho = \int_0^L dx \rho(x) = \int_0^L dx' \rho'(x')$. We denote the traveling wave system corresponding to the BASEP with drag force $f = -v_w/\mu$ as TW-BASEP in the following.

C. Continuity equation and stationary current

The local particle density obeys the continuity equation

$$\frac{\partial \rho(x, t)}{\partial t} = -\frac{\partial J(x, t)}{\partial x},$$

where $J(x, t)$ is the local particle current. For arbitrary short-ranged pair interactions $V(x, x')$, this current is given by

$$J(x, t) = \mu[f^{\text{ext}}(x) + f^{\text{int}}(x, t)]\rho(x, t) - D\frac{\partial \rho(x, t)}{\partial x},$$

where $f^{\text{int}}(x, t)$ is the mean force at position $x$ at time $t$ due to the interactions. Denoting by $\rho(x'|x; t)$ the local particle density at position $x'$ at time $t$ under the condition that a particle is at position $x$ at time $t$, this force can be written as

$$f^{\text{int}}(x, t) = \int dx' \left[ -\frac{\partial V(x, x')}{\partial x} \right] \rho(x'|x; t)$$

$$= \frac{1}{\rho(x, t)} \int dx' \left[ -\frac{\partial V(x, x')}{\partial x} \right] \rho^{(2)}(x, x', t)$$

where $\rho^{(2)}(x, x', t)$ is the two-particle density.

For hardcore interactions, a treatment based on the many-particle Smoluchowski equation given in the supplemental material of Ref. 50 leads to an expression for $f^{\text{int}}$ that agrees with the one following from Eq. (4) when formally setting $-\partial V(x, x')/\partial x = k_BT[\delta(x' - (x - \sigma)) - \delta(x' - (x + \sigma))]$. This can be intuitively understood as follows: for a particle at position $x$ there is a positive and a negative force on contacts with other particles at positions $x - \sigma$ and $x + \sigma$ that correspond to the two $\delta$-functions. The amplitude in front of the $\delta$-functions must be an energy on dimensional reasons, for which $k_BT$ is the only relevant scale. Accordingly,

$$f^{\text{int}}(x, t) = k_BT \frac{\rho^{(2)}(x, x - \sigma, t) - \rho^{(2)}(x, x + \sigma, t)}{\rho(x, t)}. \quad (7)$$

In a steady state, the density profile $\rho$ is time-independent and the current homogeneous, $J(x) = j$. For periodic boundary conditions, the $\lambda$-periodicity of the external force $f^{\text{ext}}$ entails that the steady state solution is as well $\lambda$-periodic, i.e. $\rho(x) = \rho(x + \lambda)$. Dividing Eq. (5) by $\rho(x)$ and integrating over one period, we obtain for the steady-state current in the closed BASEP

$$j(\rho, \sigma) = \frac{\mu}{\lambda} \int_0^\lambda dx \frac{\rho^{(2)}}{\rho(x)}$$

where $\rho^{(2)} = (1/\lambda) \int_0^\lambda f^{\text{int}}(x) dx$ is the period averaged mean interaction force.

D. Recurrent dynamics in periodicity intervals of the particle diameter

The complete range of densities $\rho$ and particle diameters $\sigma$ in the BASEP covers the range $0 \leq \sigma < \infty$ and $0 \leq \rho \leq \lambda/\sigma$. In a closed system with periodic boundary conditions, it is sufficient to know the behavior in the reduced range $0 \leq \sigma < \lambda$ because of a recurrent dynamics in successive intervals separated by integer multiples of the diameter, i.e. for $m\lambda < \sigma \leq (m+1)\lambda$, $m = 1, 2, \ldots$ The reason for this is as follows. Let us consider a system with particle diameter $\sigma' > \lambda$ and denote by $m = \text{int}(\sigma'/\lambda)$ the integer number of periods fitting into $\sigma'$. By applying the coordinate transformation $x_i' \rightarrow x_i = x_i' - im\lambda$ to the Langevin equations (11), the external forces remain the same, $f^{\text{ext}}(x_i') = f^{\text{ext}}(x_i' - im\lambda) = f^{\text{ext}}(x_i)$, and the hardcore constraints become $|x_{i+1} - x_i| \geq \sigma' - m\lambda = \sigma$. Moreover, the confinement $(x_N - x_1) < (L' - \sigma')$ transforms into $(x_N - x_1) < L' - (N - 1)m\lambda - \sigma' = (L' - Nm\lambda) - \sigma$, corresponding to a change $L' \rightarrow L = L' - Nm\lambda$ of the system length.

Hence there is a one-to-one mapping of probabilities of paths $\{x_i'(t)\}$ and $\{x_i(t) = x_i'(t) - im\lambda\}$ between a system with $\sigma'$ and $L'$ and a system with $\sigma = \sigma' - m\lambda$
and \( L = L' - N m \lambda \) (for fixed particle number \( N \)),
\[
P[(x_i(t)); L', \sigma'] = P[(x_i(t)); L, \sigma'] .
\]  

(9)

The arguments after the semicolon indicate the respective system length and particle diameter. Knowing the behavior of an observable for diameters \( m \lambda \leq \sigma < (m + 1) \lambda \) and for all densities \( 0 \leq \rho \leq \lambda / \sigma \), one can infer its behavior for any other particle diameter from Eq. (9). Let us note that Eq. (9) is applicable also to time-dependent observables if corresponding initial conditions are used.

In the thermodynamic limit, relations connecting systems at different \( L \) can be rewritten in terms of relations connecting systems at different \( \rho \). The change in system size then transfers into a change \( \rho' = N / L' \rightarrow \rho = N / L = \rho / (1 - \rho / m \lambda) \) of the density. Specifically, for the relevant steady-state quantities considered below, namely the local density \( \varrho(x; \rho, \sigma) \) and the current \( j(\rho, \sigma) \), we obtain [with \( m = \text{int}(\sigma / \lambda) \)]
\[
\varrho(x; \rho', \sigma') = \frac{\rho'}{\rho} \varrho(x; \rho, \sigma)
\]
\[
= (1 - m \lambda \rho') \varrho \left( x; \frac{\rho'}{1 - m \lambda \rho'}, \sigma' - m \lambda \right),
\]
\[
j(\rho', \sigma') = (1 - m \lambda \rho') j \left( \frac{\rho'}{1 - m \lambda \rho'}, \sigma' - m \lambda \right).
\]

(10a)

(10b)

Equation (10) implies a commensurability effect for particle diameters equal to integer multiples of the periodicity length \( \lambda \), where the dynamics becomes reducible to that for \( \sigma = 0 \). In this case of hardcore interacting point particles, it is obvious from Eq. (4) that \( f^{\text{int}} \) vanishes for all \( x \), and Eq. (4) reduces to the Smoluchowski equation for non-interacting particles subject to the external force \( f^{\text{ext}} \). Accordingly, \( j(\rho, m \lambda), m = 0, 1, \ldots \) is equal to the current \( j_0(\rho) \) for non-interacting particles. This current \( j_0(\rho) \) is linearly dependent on the particle density, \( j_0 = v_0 \rho \), where
\[
v_0 = \frac{\lambda}{\lambda - x + \lambda} \frac{D \lambda (1 - e^{-\beta f \lambda})}{\int_0^x dx \int dy \exp[\beta (U(y) - f y - U(x) + f x)]}
\]

(11)

is the mean velocity of a single particle in the steady state.

An alternative way to reason \( j(\rho, 0) = j_0(\rho) \) is to refer to the invariance of collective properties under particle exchange for hardcore interacting point particles \( [22] \). This exchange symmetry can be explained by the consideration of path probabilities: to a path \( P \) in a system \( S \) with hardcore constraints one can assign the set \( \{P' \} \) of all paths \( P' \) in a system \( S' \) of independent particles that result from particle exchanges at all contact points of individual particle trajectories in \( P \). Because the probability for the set \( \{P' \} \) in \( S' \) is equal to the probability of the path \( P \) in \( S \), it follows that averages of collective quantities, like the current, are equal in \( S' \) and \( S \).

E. Current bounds and absence of current reversal

Intuitively, we expect that \( |j(\rho, \sigma)| \) in the BASEP can not be larger than the magnitude \( \mu |f| \geq 0 \) of the current of non-interacting particles in a flat potential \( U(x) = \text{const}. \). This can be shown explicitly for point particles from Eq. (11), while for \( \sigma > 0 \) a proof is still lacking. Interestingly, assuming
\[
j_{a.b.} = \mu |f| \]

(12)

to be an upper bound implies that there can not be a current reversal in a TW-BASEP with wave velocity \( v_w \). This is because when taking the drag force \( f = -v_w / \mu \) in the corresponding BASEP, the magnitude of the current in this BASEP is bounded by \( \rho |v_w| \), i.e. \( -\rho |v_w| \leq j \leq \rho |v_w| \). Then, using Eq. (5b), it follows \( \rho |v_w - \rho |v_w| \leq j' \leq \rho |v_w + \rho |v_w| \), which implies that \( j' \) and \( v_w \) have the same sign (no current reversal in the TW-BASEP). Let us note that an absence of a current reversal in the TW-BASEP has been conjectured also based on an approximate perturbative treatment valid for small \( v_w \) and small \( \sigma \) \( [61, 60] \). By contrast, a current reversal occurs in lattice models that resemble discretized versions of the continuum model \( [42, 60] \).

Using the same type of reasoning, one can furthermore conclude that \( j \) and \( f \) in the corresponding BASEP have the same sign (no current reversal in the BASEP). This is because the magnitude of the mean velocity of a single particle in a TW-BASEP should not exceed \( |v_w| \), i.e. \( |j'| \leq |v_w| \).

Given \( 0 \leq |j| \leq j_{a.b.} \), the period averaged mean interaction force \( f^{\text{int}} \) must always be opposite to the drag force \( \text{sign}(f^{\text{int}}) = -\text{sign}(f) \) and its magnitude smaller than \( |f| \). This follows from Eq. (5) and by taking into account that \( \int_0^\lambda dx [\lambda g(x)]^{-1} \geq \rho \geq 0 \). We believe that the current bounds and associated implications for \( f^{\text{int}} \) are valid also for other particle interactions.

F. Phase transitions in open systems

A striking feature of the ASEP is the occurrence of nonequilibrium phase transitions in open systems coupled to particle reservoirs \( [34, 71] \). These phase transitions manifest themselves as discontinuous changes of the bulk density in dependence of control parameters specifying the coupling to the reservoirs (or jumps in the derivatives of the bulk densities with respect to these control parameters). How these phases change with experimentally tunable control parameters depends on details of the system reservoir couplings \( [40, 41] \). However, all possible phases can be derived from extremal current principles \( [36, 38, 41] \). The arguments leading to these principles are quite general for driven diffusive systems and are valid also for driven Brownian motion.

We focus here on an open BASEP with \( M \) potential wells \( i = 1, \ldots, M \) coupled to reservoirs \( L \) and \( R \) at its
left \((i = 1)\) and right \((i = M)\) end. The period averaged density profile in the stationary state is given by 
\[
\rho_i = \frac{1}{(i-1)\lambda} \int_{(i-1)\lambda}^{i\lambda} \rho(x) \, dx, \quad i = 1, \ldots, M.
\]
In the thermodynamic limit \((M \to \infty)\), this profile exhibits a constant bulk value \(\rho_b\) in the interior of the system, which defines the order parameter of the phase transitions. For finite large \(M\), \(\rho_b\) refers to the density of an extended plateau-like region in the interior of the system. Using the extremal current principles, \(\rho_b\) is given by
\[
\rho_b = \begin{cases} 
\text{argmin} \{ j(\rho, \sigma) \}, & \rho_L \leq \rho_b, \\
\text{argmax} \{ j(\rho, \sigma) \}, & \rho_R \leq \rho_b.
\end{cases}
\quad (13)
\]
Here \(\rho_L\) and \(\rho_R\) can be any densities bounding a monotonically varying region encompassing the plateau part from the left and right side, respectively. For globally monotonic profiles in particular, it is possible to interpret \(\rho_L\) and \(\rho_R\) as reservoir densities.

In general, however, interaction effects lead to density oscillations close to the boundaries, and only a specific coupling called “bulk-adapted” ensures a global monotonic behavior and a controlled generation of all possible phases \([40, 41]\). While such bulk-adapted coupling can be realized in a systematic manner in lattice models, its implementation in Brownian dynamics of interacting particles remains challenging. We will take a pragmatic approach and present in section IV.B a simple coupling scheme of particle injection and ejection for the BASEP for the simulation of the phases.

### III. CURRENT IN CLOSED SYSTEM

We now turn to a specific implementation and demonstrate the transport properties and phase transitions in a BASEP with the periodic potential
\[
U(x) = \frac{U_0}{2} \cos \left( \frac{2\pi x}{\lambda} \right).
\quad (14)
\]
As units we choose \(\lambda\) for length, \(\lambda^2/D\) for time, and \(k_b T\) for energy (and accordingly \((k_b T)/\lambda\) for forces). Unless specified otherwise, we use the following model parameters in these units: the barrier height \(U_0 = 6\), the bare mobility \(\mu = 1\), and the drag force \(f = 1\). The barrier height \(U_0 \gg k_b T\) leads to an effective hopping motion between the potential wells, which resembles the discrete hopping motion in the lattice ASEP. The model is illustrated in Fig. 1 where also a few representative particle trajectories are shown.

In the simulations of the closed BASEP the system length was set to \(L = 100\lambda\) and the time step of the simulation scheme to \(\Delta t = 10^{-4}\lambda^2/D\). We checked that our results are not affected by the finite system length and the chosen time step.

![Fig. 1. Illustration of the Brownian asymmetric simple exclusion process, where hardcore interacting particles of size \(\sigma\) are driven through a \(\lambda\)-periodic potential \(U(x)\) with amplitude \(U_0 \gg k_b T\) by a constant drag force \(f\). The example of eight stochastic trajectories of neighboring particles was obtained from Brownian dynamics simulations in a system with \(\sigma = 0.5\lambda\) at a density \(\rho = 0.8\).](image)

### A. Dependence on particle size and density

As mentioned in the Introduction, we here give a complete description of the current, which includes all particle sizes and also densities \(\rho\) in the range \(\text{int}(\sigma + 1) < \rho < \lambda/\sigma\), i.e. regimes not considered in our previous work \([50]\). Representative examples of current-density relations for several \(\sigma\) are shown in Fig. 2 for the density ranges (a) \(0 \leq \rho \leq 1\) and (b) \(1 \leq \rho \leq 8\).

In the low density limit \(\rho \to 0\) particle interactions become negligible and the current-density relations approach the linear relation \(j_0(\rho) = v_0\rho\) of non-interacting particles [solid black line in Fig. 2(a)], where Eq. (11) yields \(v_0 = 0.043D/\lambda\) for our parameters. Beyond this common asymptotic limit for all \(\sigma\), the form of the current-density relation in the BASEP varies strongly with the particle size. For comparison with the lattice model, the parabolic current-density relations of a corresponding ASEP \(j_{\text{ASEP}}(\rho) = v_0\rho(1 - \rho)\) is shown in Fig. 2(a) also (dashed black line).

The change of the current-density relation with the particle size is due to the interplay of three physical effects \([50]\): a barrier reduction, a blocking and an exchange-symmetry effect. The barrier reduction effect occurs if a potential well is occupied by more than one particle. It leads to a current enhancement compared to \(j_0\), because the particles in the well are pushing each other to regions of higher potential energy and therefore the effective barrier for a transition to the neighboring wells is reduced. In contrast, the blocking effect lowers the current: if a particle attempts a transition to the next potential well, its motion can be blocked by a particle already occupying the neighboring well. The exchange-symmetry effect emerges as a result of the exact invari-
(b). In the limit

\[ \lim_{\rho \to \infty} \frac{j_0(\rho)}{\rho} = v_{\text{bulk}}(1 - \rho) \]

increasing with \( \rho \) high the current approaches \( j_0(\rho) = v_{\text{bulk}} \rho \), and the dashed line the current-density relation \( j_{\text{ASEP}}(\rho) = v_{\text{bulk}}(1 - \rho) \) of a corresponding ASEP. In (b) the dashed black line indicates the upper bound \( j_{\text{ASEP}} = \mu \rho |f| = \rho \) of the current (\( \mu = f = 1 \) in the chosen units).

ance of the current under particle exchange for commensurable diameters \( \sigma = m \lambda \), as explained Sec. 11. It leads to a continuous deformation of the curved current-density relation for \( \sigma \lesssim m \lambda \) towards the linear dependence for \( \sigma = m \lambda \) [see the curve for \( \sigma = 0.99 \lambda \) in Fig. 2(a)]. The exchange symmetry effect thus becomes already notable for \( \sigma \lesssim \lambda \).

To understand how these effects influence \( j(\rho, \sigma) \) in Fig. 2(a), we discuss the curves with increasing particle size. For small \( \sigma \), \( j(\rho, \sigma) \) is monotonically increasing with \( \rho \) and always larger than \( j_0(\rho) \), see the curve for \( \sigma = 0.21 \lambda \) in Fig. 2(a). The enhancement compared to \( j_0(\rho) \) is due to the barrier reduction effect, which prevails for small \( \sigma \) because of a high multi-occupation probability of potential wells. With increasing \( \sigma \), the influence of the blocking effect becomes stronger, which leads to currents smaller than \( j_0(\rho) \) at intermediate \( \sigma \) and not too high \( \rho \). In this regime, \( j(\rho, \sigma) \) is still monotonically increasing with \( \rho \), see the curve for \( \sigma = 0.47 \lambda \) in Fig. 2(a). The strong rise of \( j(\rho, \sigma) \) at larger \( \rho \) values is caused by double occupancies that are propagating through clusters of single occupied wells in a cascade-like manner [51, 72].

Beyond a certain particle size \( \sigma_c \), a local maximum and local minimum appears at \( j(\rho, \sigma) \) at densities \( \rho_{\text{max}} = \rho(\sigma) \) and \( \rho_{\text{min}} = \rho(\sigma) \), see the curves for \( \sigma = 0.61 \lambda \) in Fig. 2(a). When further enlarging \( \sigma \), the blocking effect dominates the behavior for all \( 0 \leq \rho \leq 1 \) and the current-density relations approach \( j_{\text{ASEP}}(\rho) \) as a limiting curve with a maximum at \( \rho \approx 0.5 \). This occurs in the range \( 0.74 \lambda \lesssim \sigma \lesssim 0.82 \lambda \) for our setup. Close to the commensurate diameter \( \sigma = \lambda \), the exchange symmetry effect becomes relevant. As a consequence, the position of the maximum in \( j(\rho, \sigma) \) moves to higher densities and the current approaches \( j_0(\rho) \) from below.

If the number of particles exceeds the number of potential wells, i.e. when \( \rho > 1 \), the particles can not all be localized close to a potential minimum and double or multi-occupied wells are permanently present. This leads to a strong increase of the particle current with \( \rho \) towards values much larger than those seen in Fig. 2(a) for \( \rho < 1 \) [note the different scales of the current axes in Figs. 2(a) and (b)]. The upper bound \( j_{\text{ASEP}} = \mu \rho |f| = \rho \) (see Sec. 11) is shown as the dashed black line in Fig. 2(b). In the limit of complete filling \( \rho \rightarrow \lambda/\sigma \), the curves approach \( j_{\text{ASEP}} \) from below, in agreement with the behavior conjectured in Sec. 11.

How the influence of the barrier reduction, blocking and exchange symmetry effects changes with the particle size becomes particularly transparent when plotting the relative change \( \Delta j(\rho, \sigma) = [j(\rho, \sigma) - j_0(\rho)]/j_0(\rho) \) of the current with respect to \( j_0(\rho) \) as a function of \( \sigma \) for different fixed \( \rho \). Corresponding curves shown in Fig. 3 all display a local maximum at a value \( \sigma_{\text{max}}(\rho) \) and show a plateau-like behavior in an intermediate \( \sigma \) range. For \( \sigma \) below the onset of the plateau-like regime, the barrier reduction and the blocking effect compete with each other, where the barrier reduction and blocking effect govern the change of \( \Delta j \) for \( \sigma < \sigma_{\text{max}} \) and \( \sigma > \sigma_{\text{max}} \), respectively. In the plateau-like regime, the barrier reduction effect becomes almost negligible. For \( \sigma \rightarrow \lambda \) the exchange symmetry effect causes the curves to increase back to \( j_0(\rho) \) which is reached at \( \sigma = \lambda \).

Having fully described the current for all densities \( 0 \leq \rho \leq \lambda/\sigma \) in the range of particle sizes \( 0 \leq \sigma \leq \lambda \), we are able to use the mapping in Eq. 10 to derive the current for diameters \( \sigma > \lambda \) at arbitrary densities. The emerging recurrence pattern in the \( \sigma-\rho \) plane is shown in Fig. 4, where the current values are represented by a color coding. Note that this pattern is not periodic in \( \sigma \), but has a more complicated structure because of the
FIG. 3. Change of the current in the BASEP relative to that of independent particles as a function of the particles diameter for several fixed densities.

necessary rescaling of the density. Due to the prefactor $(1 - m\lambda\rho')$ on the right hand side of Eq. (10b), the currents overall become smaller with increasing recurrence index $m$.

When comparing the current behavior in the BASEP and ASEP, the blocking effect is present in both models, while the barrier reduction effect has no analogue in the lattice model, because multi-occupation of a site is forbidden in the standard ASEP. The exchange-symmetry effect is also absent in lattice models, even if one introduces a generalized $l$-ASEP, where the particles occupy $l$ lattice sites. This is because the particle size is an integer multiple of the lattice constant and accordingly there is no continuous transition towards a commensurate diameter.

Nevertheless, the reasoning in Sec. III D can be taken over to the $l$-ASEP with $l > 1$, $N$ particles, $M$ lattice sites with periodic boundary conditions, and hopping rates $\Gamma_+$ and $\Gamma_-$ in and against bias direction. A transformation $l \to 1$ and $M \to M - N(l - 1)$ corresponds to the transformation considered in Sec. III D for the BASEP with $m = (l - 1)$. Hence from Eq. (10b) and with $j_{\text{ASEP}}(\rho) = (\Gamma_+ - \Gamma_-)\rho(1 - \rho)$ we obtain

$$j_{\text{l-ASEP}}(\rho) = [1 - (l - 1)\rho] j_{\text{ASEP}} \left( \frac{\rho}{1 - (l - 1)\rho} \right) = (\Gamma_+ - \Gamma_-) \rho(1 - l\rho) \frac{1}{1 - (l - 1)\rho}. \quad (15)$$

The reduction from an $l$-ASEP to the standard ($l = 1$) ASEP has been used in the literature before to obtain the current-density relation $f_{\text{ASEP}}$. In contrast to the equality of the current in the BASEP for commensurate $\sigma = m\lambda$, $m = 0, 1, 2, \ldots$, the currents in the $l$-ASEP change with $l$. This is because the current-density relation $j_{\text{ASEP}}(\rho)$ for the smallest length $l = 1$ in the $l$-ASEP is nonlinear, while $j_0(\rho)$ for the smallest length $\sigma = 0$ (point particles) in the BASEP is a linear function of the density.

B. Temperature dependence

With decreasing temperature, the particles become stronger localized at the minima of the potential wells. In the $\sigma$ regime of dominant blocking effect, the current-density relation therefore follows more closely $j_{\text{ASEP}}$. This causes the plateau-like regimes discussed in connection with Fig. 3 to extend and to become extremely flat in the zero temperature (low-noise) limit. However, the stronger localization at the minima of the potential does not mean that the barrier reduction effect disappears for small $\sigma$. In relation to the current $j_0$ of a single particle, double occupancies of wells lead to an enhancement

FIG. 4. Color coded representation of the current $j(\rho, \sigma)$ in the $\sigma$-$\rho$–plane. Values below $10^{-3}D/\lambda^2$ and above $10^{-1}D/\lambda^2$ are indicated in dark blue and red, respectively. The scale bar specifies the color coding for the other values.

in the BASEP.

FIG. 5. Current ratio $j/j_0$ as a function of $U_0/(k_B T)$ at fixed $\rho = 0.52$ and $f\lambda/U_0 = 1/6$ for different particle diameters. The dashed line marks the the low-temperature limit $j_{\text{ASEP}}/j_0$ in the regime of dominating blocking effect.
at arbitrary low temperatures. As the barrier reduction should become almost independent of temperature at low \( T \), \( f / j_0 \) will even be larger for lower temperatures. Hence, when considering the dependence of \( f / j_0 \) on temperature for decreasing \( T \), we expect a decrease for large \( \sigma \) where the blocking effect prevails, and an increase for small \( \sigma \) where the barrier reduction dominates. This is indeed the case and demonstrated in Fig. 5 which shows \( j / j_0 \) as a function of \( U_0/(k_B T) \) for different \( \sigma \) at a fixed density \( \rho = 0.52 \) (and the same ratio \( f \lambda / U_0 = 1/6 \) as considered before).

C. Analytical approaches

The exact expression for the steady state current in Eq. 4 allows for an approximate calculation for small drag forces. In an equilibrium system \(( f = 0 )\), the current disappears and thus the period-averaged mean interaction force vanishes, \( \bar{f}^m = 0 \). In the linear response regime, we thus obtain from Eq. 4

\[
\bar{j}(\rho, \sigma) \sim \frac{\mu (1 + \alpha)}{1 + \lambda \int_0^\lambda dx \frac{1}{\varrho_{eq}(x)}} f, \quad \alpha = \frac{\partial \bar{f}^m}{\partial f} \bigg|_{f=0},
\]

where \( \varrho_{eq}(x) \) is the local density profile in equilibrium. The equilibrium density profile (in the grand-canonical ensemble) is obtained by minimizing the exact density functional

\[
\Omega[\varrho(x)] = \int_0^\lambda dx \varrho(x) \left\{ U(x) - \mu_{ch} - k_B T \left[ 1 - \ln \left( \frac{\varrho(x)}{1 - \eta(x)} \right) \right] \right\}
\]

for hard rods in one dimension [73]. Here, \( \mu_{ch} \) is the chemical potential and

\[
\eta(x) = \int_{x-\sigma}^{x} dy \varrho(y).
\]

Minimizing \( \Omega[\varrho(x)] \) in Eq. 17 yields

\[
0 = \frac{\delta \Omega[\varrho]}{\delta \varrho} \bigg|_{\varrho=\varrho_{eq}} = \ln \left( \frac{\varrho_{eq}(x)}{1 - \eta_{eq}(x)} \right) + \int_{x-\sigma}^{x} dy \frac{\varrho_{eq}(y)}{1 - \eta_{eq}(y)} + \beta[U(x) - \mu_{ch}].
\]

We discretized this equation and solved it numerically under periodic boundary conditions \([\varrho_{eq}(x) = \varrho_{eq}(x + \lambda)]\) to obtain the density profile for a given chemical potential \( \mu_{ch} \) (or density \( \rho \)). Inserting the solution for \( \varrho_{eq}(x) \) in Eq. 16 and setting \( \alpha = 0 \) in Eq. 16, we obtain a linear response approximation (LRA) for \( j(\rho, \sigma) \).

Another approximate approach is to use dynamical density functional theory (DDFT) [75, 76], where the two-particle density at contact appearing in Eq. 7 is related to the single-particle density as in an equilibrium system:

\[
\varrho^{(2)}(x, x + \sigma, t) = \frac{\varrho(x, t) \varrho(x + \sigma, t)}{1 - \eta(x + \sigma, t)} \quad \text{(20a)}
\]

\[
\varrho^{(2)}(x, x - \sigma, t) = \frac{\varrho(x, t) \varrho(x - \sigma, t)}{1 - \eta(x, t)} \quad \text{(20b)}
\]

Here, \( \eta(x, t) \) is given by Eq. 18 with \( \varrho(y) \) replaced by \( \varrho(y, t) \). Combining Eqs. 11, 12, 17 and (20) results in a nonlinear and nonlocal evolution equation for the density:

\[
\frac{\partial \varrho(x, t)}{\partial t} = \frac{\partial}{\partial x} \left\{ D \frac{\partial \varrho(x, t)}{\partial x} - \mu f^{\text{int}}(x) \varrho(x, t) \right\} - D \varrho(x, t) \left\{ \frac{\varrho(x - \sigma, t)}{1 - \eta(x, t)} - \frac{\varrho(x + \sigma, t)}{1 - \eta(x + \sigma, t)} \right\}.
\]

To find its stationary solution we used two methods. First, we propagated an initial density profile into the stationary regime with a forward-time central-space scheme. Secondly, we solved the corresponding stationary equation \((\partial \varrho / \partial t = 0)\) with an iterative scheme. Both methods lead to equivalent results.

Current-density relations obtained with the LRA, DDFT and Brownian dynamics simulations with the algorithms given in Ref. 69 (BDS1) and Ref. 68 (BDS2) are shown in Fig. 6 for three particle diameters \( \sigma = 0.2 \lambda \) (blue), \( \sigma = 0.5 \lambda \) (orange), and \( \sigma = 0.85 \lambda \) (yellow). The DDFT calculation and the Brownian dynamics simulations were performed in the small bias regime at \( f = 0.2 (k_B T) / \lambda \). As it is visible from Fig. 6 the DDFT results are almost indistinguishable from the LRA results for all shown diameters, and the results from BDS1 and BDS2 are in very good agreement. Overall the LRA and DDFT capture the qualitative features of the current-density relations. However, comparing the results of the LRA/DDFT with that of the simulations quantitatively, we observe deviations that become largest for intermediate particle sizes close to \( \sigma = 0.5 \lambda \). The DDFT underestimates the magnitude of the period-averaged mean interaction force \( f^m \), which we determined from BDS1. This force \( f^m \), shown in the inset of Fig. 6 as a function of \( \sigma / \lambda \) for different densities, is always opposite to the bias \( f \), in agreement with our discussion in Sec. 11E. Its minimum shifts slightly to higher \( \sigma \) and becomes more pronounced with increasing \( \rho \).

Closers inspection of the local mean interaction force \( f^{\text{int}}(x) \) in the stationary state reveals that it can be both parallel and anti-parallel to the drag force \( f \) and that it is always small close to the local extrema of the external potential, where \( f^{\text{int}}(x) \approx 0 \). This is demonstrated in Fig. 7 where we show representative profiles \( f^{\text{int}}(x) \) for different \( \rho \) and \( \sigma \). The shape of these profiles changes significantly with the particle diameter. For small \( \sigma = 0.1 \lambda \...
[Fig. 7(a)], a region of negative and positive $f^{\text{int}}(x)$ values occurs next to the minimum of the external potential in ($x \lesssim 0.5$) and against bias ($x \gtrsim 0.5$) direction, respectively. At an intermediate $\sigma = 0.5 \lambda$ [Fig. 7(b)], these regions of negative and positive $f^{\text{int}}(x)$ have shifted to locations close to the potential barriers, and an extended regime of negligible $f^{\text{int}}(x) \simeq 0$ appears around $x = 0.5$. At large $\sigma = 0.9 \lambda$ [Fig. 7(c)], the profile from Fig. 7(a) appears to be kind of inverted, with now a region of positive and negative $f^{\text{int}}(x)$ occurring for $x \lesssim 0.5$ and $x \gtrsim 0.5$, respectively. As for the density dependence, it changes the magnitude of $f^{\text{int}}(x)$ along with a shift of the positions of its local minima and maxima.

Intuitively, one can understand the change of the profiles $f^{\text{int}}(x)$ by noting that for small $\sigma$, a particle located at a position left (right) of the potential minimum collides with other particles in multiple-occupied wells, which more frequently are coming from the right (left). This leads to a mean repulsive force that tends to push the particle further away from the potential minimum, i.e. we obtain $f^{\text{int}}(x) < 0$ for $x \lesssim 0.5$ and $f^{\text{int}}(x) > 0$ for $x \gtrsim 0.5$. At intermediate $\sigma$, multiple occupancies become unlikely and the particles preferentially occupy positions close the potential minima. A particle positioned near a potential minimum then rarely collides with other particles and $f^{\text{int}}(x) \simeq 0$ in a region around the minimum. Particles located close to the potential barriers now interact most strongly with other particles. For large $\sigma$, the blocking effect pushes the particles towards their minima, i.e. we find $f^{\text{int}}(x) > 0$ for $x \lesssim 0.5$ and $f^{\text{int}}(x) < 0$ for $x \gtrsim 0.5$.

IV. PHASE-TRANSITIONS IN OPEN SYSTEM

A. Phases derived from extremal current principles

Application of the extremal current principles \cite{13} to the simulated current-density relations of the closed system yields the phase diagrams for the open BASEP. The change of the shape $j(\rho, \sigma)$ with the particle diameter leads to different types of diagrams. Representative examples are shown in Figs. 8(a)-(d). For $\sigma < \sigma_c$ no phase transitions occur, because the current as a function of density exhibits no local extrema. For $\sigma \gtrsim \sigma_c$, the maximum number of five phases appears, which we labeled I-V in Fig. 8(a). These phases are colored equally in all other panels. Phases I, II and V are boundary-matching with $\rho_b = \rho_c$ in phases I and V, and $\rho_c = \rho_b$ in phase I. Phases II and IV are maximal and minimal current phases with $\rho_b = \rho_{\text{max}}$ and $\rho_b = \rho_{\text{min}}$, respectively ($\rho_{\text{max}}$ and $\rho_{\text{min}}$ are the densities at which the current-density relation has a local maximum and minimum, see Sec. IIIA). First-order transitions between the phases in Figs. 8(a)-(d) are marked by solid lines, and second-order transitions
FIG. 8. Phase diagrams of the open BASEP predicted by the extremal current principles for (a) $\sigma = 0.58\lambda$, (b) $\sigma = 0.62\lambda$, (c) $\sigma = 0.75\lambda$, and (d) $\sigma = 0.98\lambda$. The phases I and V are left-boundary induced phases, phase II is a maximal current phase, phases III is a right-boundary induced phase, and phase IV is a minimal current phase. The phases are equally colored in all panels. Solid lines mark first order phase transitions and dashed lines second order phase transitions.

With increasing $\sigma > \sigma_c$, the phases IV and V shrink [Fig. 8(c)]. This shrinkage continues up to the point where the phase diagram is similar to the one for a corresponding ASEP with three phases [Fig. 8(c)]. Close to the commensurate diameter, the diagram with the three phases becomes asymmetric due to the change of $\rho_{\text{max}}(\sigma)$ [Fig. 8(d)].

B. Simulated phases

To verify the phase diagrams predicted by the extremal current principles in the Brownian dynamics simulations, we used the following method for the exchange of particles with the reservoirs. If the leftmost (rightmost) potential well is empty, a particle is injected with a rate $\alpha_L$ ($\alpha_R$). Injected particles are placed at the maximal distance ($\lambda - \sigma$) away from the boundary, which avoids particle overlaps. Ejection of a particle to a reservoir is implemented by removing them from the system once its center position crosses the left or right boundary.

When varying the injection rates $\alpha_L$ and $\alpha_R$, the period-averaged boundary densities in the leftmost and rightmost potential well change. Hence, each simulation run with given ($\alpha_L$, $\alpha_R$) results in one set of period-averaged boundary and bulk densities ($\rho_L$, $\rho_R$, $\rho_b$) in the nonequilibrium steady state. By performing many simulation runs for different ($\alpha_L$, $\alpha_R$) the various phases can be identified.

Correspondingly simulated data points in a system of length $L = 200\lambda$ for $\sigma = 0.58\lambda$ are shown in Fig. 9 together with the surface $\rho_b = \rho_b(\rho_L, \rho_R)$ obtained from the extremal current principles. As can be seen from the figure, the simulated data are in excellent agreement with the theoretical predictions. In particular, the discontinuous first-order transitions from the left-boundary induced phase I to the minimal current phase IV and to the right-boundary induced phase III are clearly visible, as well as the continuous transitions between phase I and the maximal current phase II. Also the continuous transitions between phases III and IV, and between phases II and III can be seen in the simulated data. As for phase V, our simple injection and ejection method did not generate the very high boundary densities $\rho_L$ in this phase.

V. CONCLUSIONS

The BASEP constitutes a simple model for Brownian single-file transport in periodic structures, which is suitable to explore and understand basic physical mechanisms of nonequilibrium driven motion. We expect that the competition between the barrier reduction, blocking and exchange symmetry effect plays a decisive factor also in systems with other short-ranged interactions. The BASEP can thus serve as a reference for more complicated nonequilibrium systems, similar as the hard-sphere fluid became a useful basis in equilibrium liquid theory.

One remaining challenge is to develop better analytical approaches for the local mean interaction force acting on
a particle. With that at hand, perturbative treatments for interactions beyond hardcore exclusion could be developed.

In this work we have focused on a sinusoidal form of the external potential. In the approximate analytical treatment, arbitrary forms of the periodic potential $U(x)$ can be used by inserting it in the density functional in Eq. (17). Based on our findings for the BASEP, we conjecture that this method will capture the transport behavior on a qualitative level. A better quantitative agreement requires improved theories for the mean interaction force.

As for the connection of the thermally activated transport in the BASEP to the hopping motion in lattice models, one can think of developing extended jump models. The barrier reduction effect, absent in the standard ASEP, can, for example, be incorporated by allowing for different internal states of the particles that correspond to the different occupancies of the potential wells. Another more obvious approach is to discretize the potential energy landscape in space, but earlier results indicate that in such models current reversals, absent in the BASEP, become possible \[42, 60\]. Hence, qualitative features can be different in continuum and related lattice models. A deeper understanding of the correspondence of continuum and discrete models in single-file transport should be sought of in future investigations.

A welcome feature of the BASEP is that it describes physics of biased single-file motion generated by laser or magnetic fields in confined geometries, and by flow fields in microfluidic devices. Our results shall help to interpret experimental findings in such systems. Experimental studies in open systems offer the possibility to investigate nonequilibrium phase transitions predicted by theory under well-controlled conditions. A further interesting aspect, both for experimental and theoretical work, is to study the implications of local disturbances in the periodic structure similar as they were investigated in corresponding lattice models \[78, 79\].

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In most simulations, the period-averaged density profile \( \rho_i = \int_{0}^{L} dx \rho(x)/\lambda \), \( i = 1, \ldots, M \), turned out to be monotonically varying with \( i \). Only for very high \( \alpha_L \) and \( \alpha_R \) small dips appear close to the system boundaries. Then \( \rho_i \) and \( \rho_0 \) were determined from the region of monotonically varying profile in the interior.