Stochastic exclusion processes versus coherent transport

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Abstract. Stochastic exclusion processes play an integral role in the physics of non-equilibrium statistical mechanics. These models are Markovian processes, described by a classical master equation. In this paper, a quantum mechanical version of a stochastic hopping process in one dimension is formulated in terms of a quantum master equation. This allows the investigation of coherent and stochastic evolution in the same formal framework. The focus lies on the non-equilibrium steady state. Two stochastic model systems are considered: the totally asymmetric exclusion process and the fully symmetric exclusion process. The steady-state transport properties of these models are compared to the case with additional coherent evolution, generated by the $XX$ Hamiltonian.
1. Introduction

Stochastic exclusion processes have been studied in statistical mechanics for a long time [1, 2]. These are simplified one-dimensional (1D) hopping models that allow the study of non-equilibrium phenomena in many-particle systems. The exclusion processes are modeled by a classical master equation that determines the time evolution of the probability distribution. The steady state of the master equation exhibits an interesting non-equilibrium behavior, such as the presence of current, non-equilibrium phase transitions and entire phases with a diverging correlation length [3, 4]. The presence of currents, such as the current of particles, energy or momentum, is a common feature of non-equilibrium steady states and can have profound effects on the correlations present in the system [5, 6]. Non-equilibrium systems can develop long-range correlations in the presence of a high current.

The totally asymmetric exclusion process (TASEP) as well as the symmetric simple exclusion process (SSEP) are prime examples of such model systems [3, 7]. These processes describe the hopping of hard-core particles in a 1D chain, only driven by the inflow and outflow of particles at the boundaries of the chain. Here one considers open boundary conditions, where particles are injected at the first site and are removed at the last site N of the chain. The steady-state properties are entirely determined by the inflow and the outflow. The dynamics of the particles in the bulk are given by translationally invariant hopping rates, which can be chosen asymmetrically. This generic case is then referred to as the asymmetric exclusion process (ASEP). This process has two limiting cases: either when the hopping is restricted to occur only in a single direction (TASEP) or when the hopping rates in both directions are equal (SSEP).

The transport properties of open, quantum mechanical systems, on the other hand, have been subjected to research activities in recent years. There is a general interest in how external noise, generated by the environment, affects the coherent transport in the system. It was found that the presence of noise in the quantum mechanical systems can actually aid the transport process of excitations through heterogeneous environments [8, 9], such as bio-molecules.
An optimal ratio between coherent transport and dephasing noise can be found. The dynamics of open quantum systems are generally formulated in terms of a Markovian Lindblad master equation that describes the time evolution of the density matrix [10].

In this paper, we want to investigate the interplay between stochastic transport processes and coherent transport present in the same system. Here, we consider only the steady-state properties of the system. To treat both processes on an equal footing, we incorporate the classical hopping terms into the quantum master equation. The stochastic hopping is modeled by appropriately chosen quantum jump operators. Such a construction has also been used to find quantum master equations that describe a quantization of kinetic Ising models [11]. These models obey detailed balance and allow for an exact solution. Considering hopping models in this more general quantum framework allows now for additional quantum transport, so to speak, on top of the classical hopping evolution. We can choose an arbitrary, particle number-conserving Hamiltonian to mediate the coherent transport and investigate the effect this quantum perturbation has on the classical hopping process. It is important to point out that this embedding of the classical process into the framework of quantum mechanical master equations is different from the standard classical to quantum mapping; see, for instance, [12–14], where a mapping of the classical Liouvillian to a quantum mechanical XXZ Hamiltonian has been found.

Our paper is organized as follows. Firstly, in section 2, we introduce the hopping model and formulate the problem as a quantum master equation. In different instances we choose either the TASEP or the SSEP as the underlying stochastic process. Secondly, in section 3 the SSEP is considered. The two-point correlation functions of the SSEP can be calculated exactly in the steady state, and we investigate the scaling of the current density for larger lattice sizes. Then, in section 4, the quantum analogue of the TASEP is treated numerically in the framework of matrix product density operators (MPDO). The master equation is evolved in time, for different system sizes, until the steady state is reached. The current, the particle density, as well as the particle density–density correlations, are computed. The conclusions are presented in section 5.

### 2. Formulation of the quantum master equation

We study a system of hard-core particles in a 1D chain of length $N$, where each site ($1 \leq k \leq N$) can be either occupied or empty. This can be cast into the formulation of a spin-1/2 chain. In the spin chain picture this corresponds to either spin up $|1\rangle$ (occupied) or spin down $|0\rangle$ (empty). At the boundary $k = 1$, we allow for an inflow with a rate $\alpha$ and at $k = N$ for an outflow of particles, given by a rate $\beta$. The particles at each site are allowed to hop stochastically to the left with a rate $\varphi_L$ and to the right with $\varphi_R$, see figure 1 for a comparison. In this paper,
we consider only two cases: firstly, the fully symmetric case (SSEP), where both hopping rates are equal, \( \varphi_L = \varphi_R = \varphi \). The stochastic hopping rates in the bulk are in this case completely symmetric. The only asymmetry that can generate driving in this model is due to the biased in- and out-flow at the boundary. In turn, the fully asymmetric case (TASEP) is obtained by setting \( \varphi_R = \varphi \) and \( \varphi_L = 0 \).

We seek to formulate the classical stochastic processes in terms of a quantum Lindblad master equation of the form (3). The stochastic particle jumps, which correspond to the classical stochastic exclusion process, can be formulated in terms of the Lindblad operators \( L_\mu \). As was already discussed, these operators govern the incoherent evolution of the quantum master equation and are typically responsible for the damping or decoherence of the quantum system. In our model, however, these terms generate the classical non-equilibrium dynamics. It is possible to formulate these jumps in terms of spin-flip operations:

\[
L_1 = \sqrt{\alpha} \sigma_1^+ \quad \text{and} \quad L_{R,k,k+1}^R = \sqrt{\varphi_R} \sigma_k^- \otimes \sigma_{k+1}^+ ,
\]

\[
L_N = \sqrt{\beta} \sigma_N^- \quad \text{and} \quad L_{L,k,k+1}^L = \sqrt{\varphi_L} \sigma_k^+ \otimes \sigma_{k+1}^- .
\]

Here, the \( \sigma^\pm \) correspond to the Pauli raising and lowering operators.

In this generalized framework, we can now also allow for an additional coherent evolution of the system by choosing an appropriate Hamiltonian. The \( XX \) Hamiltonian

\[
H_{XX} = \frac{\lambda}{2} \sum_{k=1}^{N-1} \sigma_k^x \otimes \sigma_{k+1}^x + \sigma_k^y \otimes \sigma_{k+1}^y ,
\]

(2)

gives rise to the free coherent evolution of the hard-core particles. Furthermore, we will see that this coherent evolution has the property to conserve the total number of hard-core particles, since it satisfies a continuity equation. The full quantum master equation \( \partial_t \rho = \mathcal{L}(\rho) \), including both coherent and stochastic evolution, can be written as

\[
\partial_t \rho = -i [\rho, H_{XX}] + \sum_\mu L_\mu \rho L_\mu^\dagger - \frac{1}{2} \{ L_\mu^\dagger L_\mu ; \rho \} ,
\]

(3)

To simplify notation we write for the individual Lindblad operators defined in (1) the general expression \( L_\mu \). The sum over \( \mu \) has to therefore be read as a total sum over the boundary operators \( L_1, L_N \) indexed by 1, \( N \) and for all the bulk operators \( L_{R,k,k+1}^R \) and \( L_{L,k,k+1}^L \), where \( k = 1, \ldots, N - 1 \).

The master equation without the presence of a Hamiltonian, i.e. \( \lambda = 0 \), reproduces exactly the classical stochastic behavior of the ASEP, when one restricts to initial density matrices which are diagonal in the basis \( |i_1 \cdots i_N \rangle \). Let us therefore consider density matrices of the form \( \rho = \sum_\sigma p(\sigma) |\sigma\rangle \langle \sigma| \), where \( \sigma = i_1 \cdots i_N \) corresponds to a particular spin configuration and \( p(\sigma) \) is the associated probability. Without the presence of the Hamiltonian the master equation (3) is diagonal preserving, i.e. the diagonal elements and the off-diagonal elements do not couple. Therefore, the dynamics \( \partial_t \rho = \mathcal{L}(\rho) \) can be expressed only in terms of the diagonal elements which obey the classical rate equation

\[
\partial_t p(\sigma) = \sum_{\sigma'} w(\sigma \rightarrow \sigma') p(\sigma') - w(\sigma \rightarrow \sigma') p(\sigma).
\]

(4)
The rates $w(\sigma' \to \sigma)$ are given by

$$w(\sigma' \to \sigma) = \sum_{k=1}^{N-1} \varphi_L \ t^k (01 \to 10) + \varphi_R \ t^k (10 \to 01) + \alpha \ t^k (0 \to 1) + \beta \ t^k (1 \to 0),$$

where we have defined $t^k(ab \to cd) = \delta_{k,i_1} \cdots \delta_{k,i_d} \delta_{k+1,j_1} \cdots \delta_{k+1,j_e}$ to simplify the notation. This rate equation corresponds exactly to the classical ASEP [2]. The fact that the diagonal elements do not couple to the off-diagonal elements is due to the particular form of the Lindblad operators $L_\mu$. For a general density matrix it is easy to see that the off-diagonal elements evolve independently and decay exponentially, so that at the later stages of the evolution only the diagonal dynamics are relevant. However, this behavior changes as soon as the Hamiltonian transport is switched on. Then, the dynamics of the diagonal and the off-diagonal elements can no longer be considered to be independent.

The central observables are the particle density $n_k = \sigma_k^+ \sigma_k^-$ and the current $j_k$ of particles. To find the right expression for the particle current, we consider the continuity equation for the density $n_k$. The continuity equation is obtained in the Heisenberg picture, when the adjoint of $\mathcal{L}$ is acting on $n_k$

$$\partial_t n_k = \mathcal{L}^\dagger [n_k] = -i [H, n_k] + \sum_\mu L_\mu^\dagger n_k L_\mu - \frac{1}{2} [L_\mu^\dagger L_\mu; n_k].$$

If we compute the time evolution of the density operator $n_k$ with respect to the full master equation (3) for all sites $k = 2, \ldots, N - 1$, we can cast the equation in the following form:

$$\partial_t n_k + (j_{k-1,k}^{\text{co}} + j_{k,k+1}^{\text{st}}) - (j_{k,k+1}^{\text{co}} + j_{k+1,k}^{\text{st}}) = 0.$$  

This equation is the standard form of a discrete continuity equation. The additional coherent evolution with respect to the $H_{XY}$ Hamiltonian can thus be seen to be particle number preserving. Furthermore, we can now interpret the sum of the terms $j_{k,k+1} = j_{k,k+1}^{\text{co}} + j_{k,k+1}^{\text{st}}$ given by

$$j_{k,k+1}^{\text{co}} = \frac{\lambda}{t} (\sigma_k^+ \sigma_{k+1}^- - \sigma_k^- \sigma_{k+1}^+),$$

$$j_{k,k+1}^{\text{st}} = \varphi_R (n_k (1 - n_{k+1})) - \varphi_L ((1 - n_k)n_{k+1})$$

as the total current density of the system. Note that there are two different contributions to the current, the coherent part $j^{\text{co}}$ due to the dynamics generated by the Hamiltonian and the stochastic contribution $j^{\text{st}}$ originating from the hopping induced by the Lindblad operators. We observe that the stochastic contribution to the current corresponds exactly to the current present in the classical model [3, 15]. The continuity equation leads to a further conclusion. For the steady state of the master equation we have that $\partial_t \langle n_k \rangle = 0$; thus we can infer that the total current density has to be constant throughout the system. Hence, $\langle j_{k-1,k} \rangle = \langle j_{k,k+1} \rangle$ and therefore no spacial variations of the current are allowed. Here, we have defined the average with respect to the non-equilibrium steady state of the system. We will see later, however, that the individual contributions to the total current density themselves actually do exhibit a spacial dependence in the steady state.
### 3. The symmetric exclusion process

Let us now consider a specific choice of the classical hopping rates that makes the model solvable, that is, a choice for which we can compute the ground-state particle density and current density exactly. If we allow for stochastic hopping in both directions with an equal rate \( \varphi = \varphi_L = \varphi \) and turn off the coherent evolution, the model describes the classical symmetric exclusion process. The symmetric exclusion process is known to possess only a single classical phase \([7]\) that is determined by the current \( j \), which vanishes in the thermodynamic limit \( N \to \infty \). We would like to see whether a quantum perturbation to the system changes this behavior. Note that now, since the classical hopping rates are equal, the quantum-jump operators are related via \( L_{k,k+1}^R = L_{k,k+1}^L \equiv L_{k,k+1} \). This allows us to rewrite the full master equation as

\[
\begin{align*}
\partial_t \rho &= -i \{ \rho, H \} + \sum_{k=1}^{N-1} \left[ [L_{k,k+1}; \rho], L_{k,k+1}^+ \right] + \left[ \left[ L_{k,k+1}^+, \rho \right], L_{k,k+1} \right] \\
&\quad + L_1 \rho L_1^+ - \frac{1}{2} \{ L_1^+, L_1; \rho \} + L_N \rho L_N^+ - \frac{1}{2} \{ L_N^+, L_N; \rho \}.
\end{align*}
\]

Note that the dissipative terms in the bulk are now given by the sum of two double commutators. It is therefore possible to calculate the nearest-neighbor two-point correlation functions exactly. To achieve this, we first transform the Pauli raising and lowering operators, \( \sigma^+ \) and \( \sigma^- \), into fermionic modes by means of the Jordan–Wigner transformation \([16]\). The resulting fermionic creation and annihilation operators read then as

\[
a_k^+ = -\left( \bigotimes_{i=1}^{k-1} \sigma^+ \right) \sigma_k^+ \quad \text{and} \quad a_k = -\left( \bigotimes_{i=1}^{k-1} \sigma^- \right) \sigma_k^-.
\]

One can verify that these modes now obey the fermionic anti-commutation relations \( \{ a_k, a_j^\dagger \} = \delta_{k,j} \) and \( \{ a_k, a_j \} = \{ a_k^\dagger, a_j^\dagger \} = 0 \). It is possible to calculate the evolution of the fermionic two-point function \( \langle a_k^\dagger a_m \rangle \) from the master equation (9) via \( \partial_t \langle a_k^\dagger a_m \rangle = \text{tr} \{ H_k a_k^\dagger a_m \} \). Here, not only the Hamiltonian, but also the terms comprising the Lindblad operators get transformed to fermionic modes and read

\[
\begin{align*}
H &= -\lambda \sum_{k=1}^{N-1} a_k^\dagger a_k + a_k^\dagger a_k^\dagger a_k + a_k a_k^\dagger, \\
L_{k,k+1} &= \sqrt{\varphi} a_k a_{k+1}^\dagger, \\
L_1 &= -\sqrt{\alpha} a_1^\dagger \quad \text{and} \quad L_N = -\sqrt{\beta} \left( \prod_{k=1}^{N-1} (2a_k^\dagger a_k - 1) \right) a_N.
\end{align*}
\]

Since the commutator of two pairs of fermionic modes is again an operator made up of two fermionic modes, we see that the time evolution of the fermionic two-point functions again only depends on two-point functions. Hence, the dynamical functions for the two-point correlation functions can be stated in a closed form, which can be solved exactly. The equations for the correlation functions read

\[
\begin{align*}
\partial_t \langle a_m^\dagger a_l \rangle &= \frac{\alpha}{2} \left( \delta_{m,1} + \delta_{l,1} \right) \langle a_1^\dagger a_l \rangle - \frac{\beta}{2} \left( \delta_{m,N} + \delta_{l,N} \right) \langle a_m^\dagger a_l \rangle \\
&\quad - \varphi \left( \langle a_{m+1}^\dagger a_m^\dagger a_{m+1} \rangle - \langle a_{m+1}^\dagger a_m \rangle - \langle a_{m-1}^\dagger a_{m+1} \rangle + \langle a_{m-1}^\dagger a_m \rangle \right) \delta_{l,m} \\
&\quad + 2\left[ \langle a_m^\dagger a_l \rangle - \langle a_m^\dagger a_l \rangle \right] - i\lambda \left( \left[ \langle a_{m+1}^\dagger a_{l+1} \rangle + \langle a_m^\dagger a_{l-1} \rangle \right] - \left[ \langle a_{m+1}^\dagger a_{l+1} \rangle + \langle a_m^\dagger a_{l-1} \rangle \right] \right),
\end{align*}
\]

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and similarly for the correlation function $\langle a_m^\dagger a_l^\dagger \rangle$, we obtain

$$
\partial_t \langle a_m^\dagger a_l^\dagger \rangle = -\frac{\alpha}{2} \left( \delta_{1,m} + \delta_{1,l} \right) \langle a_m^\dagger a_l^\dagger \rangle - \frac{\beta}{2} \left( \delta_{1,N} + \delta_{m,N} \right) \langle a_l^\dagger a_m^\dagger \rangle \\
- \phi \left( \left[ \delta_{l+1,m} \langle a_l^\dagger a_{l+1}^\dagger \rangle - \delta_{m+1,l} \langle a_m^\dagger a_{m+1}^\dagger \rangle \right] + 2 \langle a_m^\dagger a_l^\dagger \rangle \right) \\
+ i\lambda \left( \langle a_m^\dagger a_{l-1}^\dagger \rangle + \langle a_m^\dagger a_{l+1}^\dagger \rangle + \langle a_{m-1}^\dagger a_l^\dagger \rangle + \langle a_{m+1}^\dagger a_l^\dagger \rangle \right).
$$

The other correlation functions are related to the correlation functions considered above by the identities imposed due to the anti-commutation relations of the fermionic modes; thus $\langle a_m^\dagger a_l^\dagger \rangle = (a_m a_l)^*$ and $\langle a_l^\dagger a_m^\dagger \rangle = \delta_{l,m} - (a_l a_m)^*$. We are only interested in the steady-state correlations here, which can be computed from equations (12) and (13) by requiring that $\partial_t \langle a_m^\dagger a_l^\dagger \rangle = \partial_t \langle a_m a_l \rangle = 0$. This leads to a set of difference equations. The current density as well as the particle number density can be expressed in terms of these correlators. One finds for the particle number density that $\langle n_k \rangle = \langle a_k^\dagger a_k \rangle$ and the two contributions to the current read

$$
j_{k,k+1}^{st} = \varphi \left( \langle n_k \rangle - \langle n_{k+1} \rangle \right),
$$

$$
j_{k,k+1}^{co} = \frac{\lambda}{i} \left( \langle a_{k+1}^\dagger a_k \rangle - \langle a_k^\dagger a_{k+1} \rangle \right).
$$

Note that the stochastic current now only depends on the difference of the densities at adjacent sites and thus greatly simplifies with respect to (8). With these definitions at hand it is possible to compute the current density as well as the particle number density explicitly. We only need to restrict ourselves to equations (12) for the choices $l = m = k$ and $m = k, l = k + 1$ as well as $m = k + 1, l = k$ and we obtain the following difference equations:

$$
\alpha \delta_{k,1} \left( 1 - \langle n_k \rangle \right) + j_{k-1,k}^{st} + j_{k-1,k}^{co} = \beta \delta_{k,N} \langle n_k \rangle + j_{k,k+1}^{st} + j_{k,k+1}^{co},
$$

$$
\alpha \delta_{k,1} j_{k,k+1}^{co} + 4\phi j_{k,k+1}^{st} = 4\frac{\lambda^2}{\varphi} j_{k,k+1}^{st} - \beta \delta_{k+1,N} j_{k,k+1}^{co}.
$$

Recently, the time evolution of the fermionic two-points function was investigated in a strongly related system [17]. This system had the same bulk transport properties, i.e. Hamiltonian transport in addition to the stochastic hopping of the SSEP form. However, rather than considering driving by the Lindblad operators at the boundaries proportional to $\alpha$ and $\beta$, the author considered closed, periodic boundary conditions. For such a model, the matrix of the Liouvillian becomes Hermitian and hence the non-equilibrium steady state is given by the total mixture. The boundary terms in the open boundary model considered here break hermiticity and therefore give rise to a non-trivial non-equilibrium steady state.

The behavior of equations (15) and (16) changes dramatically, depending on presence or absence of the stochastic transport in the bulk. We therefore consider two distinct scenarios.

### 3.1. Simultaneous stochastic and coherent transport in the bulk

Let us first consider the scenario when $\varphi > 0$. Thus, we have to take into account the full set of equations. Combining equations (15) and (16) with the density dependence of the stochastic
current (14), one sees that in the bulk, i.e. \( k \in \{2, \ldots, N-1\} \), the density has to satisfy the difference equation

\[
\langle n_{k+1} \rangle - 2 \langle n_k \rangle + \langle n_{k-1} \rangle = 0.
\]  

(17)

We see that the assignment

\[
\langle n_k \rangle = c_1 + k c_2
\]  

(18)

satisfies this equation. We need to determine the two constants based on the boundary conditions, i.e. \( k = 1, N \). We obtain a linear system of equations that is easily soluble, and we obtain

\[
c_1 = \frac{\alpha \beta \psi N + \alpha \psi \left( \psi + \frac{4 \lambda^2}{\beta + 4 \psi} \right)}{\alpha \beta \varphi (N-1) + \alpha \psi \left( \psi + \frac{4 \lambda^2}{\beta + 4 \psi} \right) + \beta \psi \left( \psi + \frac{4 \lambda^2}{\alpha + 4 \psi} \right)},
\]  

(19)

\[
c_2 = -\frac{\alpha \beta \psi}{\alpha \beta \varphi (N-1) + \alpha \psi \left( \psi + \frac{4 \lambda^2}{\beta + 4 \psi} \right) + \beta \psi \left( \psi + \frac{4 \lambda^2}{\alpha + 4 \psi} \right)}.
\]

Note that \( c_2 < 0 \), so the density is a line that decreases from some fixed value \( c_1 > 0 \) on the left to \( c_1 - N |c_2| \) on the right. From the density, we can immediately deduce the stochastic contribution to the current in the bulk, which reads \( j^\text{st}_{k,k+1} = -\psi c_2 \). Due to the second equation (16) we can also infer the coherent contribution, which is \( j^\text{co}_{k,k+1} = -\frac{\lambda^2}{\psi} c_2 \). We now consider the thermodynamic limit \( N \gg 1 \). In this limit both the coherent contribution and the stochastic contribution behave as

\[
j^\text{st} \approx \frac{\psi}{N} \quad \text{and} \quad j^\text{co} \approx \frac{\lambda^2}{\psi N}.
\]  

(20)

We recall that the SSEP without any further driving, i.e. \( \alpha = \beta = 0 \), obeys the detailed balance condition and thus does not support a steady-state current. When one allows for an external driving of the particles at the boundaries, as we do in our example, a current is induced in the SSEP steady state. This current, however, vanishes as \( \sim 1/N \) in the system size \( N \). As we have shown, this behavior does not change on adding the coherent evolution on top. Both the coherent and the stochastic contribution to the current vanish in the same fashion. Furthermore, neither \( c_1 \) nor \( c_2 \) depends strongly on \( \lambda \). The coherent evolution seems to play a role only for smaller system sizes, i.e. small \( N \). We deduce from this that for all finite \( \psi \) the quantum perturbation does not lead to a qualitatively different behavior of the system’s transport properties. However, whether the quantum perturbation is completely irrelevant cannot be inferred from considering the steady-state density and the current alone. One would need to also take into account higher-order correlations, such as for instance the current–current correlation function at unequal times.

3.2. Vanishing stochastic transport in the bulk

Equations (15) and (16) do exhibit a phase transition, albeit quite a naive transition, upon choosing \( \psi = 0 \). It is easy to see that for this value the system behavior changes abruptly. The model that is obtained by setting \( \psi = 0 \) corresponds to a limiting case of another model for quantum transport that was investigated recently \([18, 19]\). This model only has coherent
transport in the bulk, and stochastic driving only occurs at the boundaries. The equations immediately yield that the current density \( j_{k+1}^{co} = j^B \), as well as the particle density \( \langle n_k \rangle = n^B \), is constant in the bulk and only deviates at the boundaries from this constant value. With this at hand, the set of equations simplify greatly and turn into a set of algebraic equations. The resulting particle density and current in the bulk are given by

\[
n^B = \frac{\alpha (\beta^2 + 4 \lambda^2)}{\beta (\alpha^2 + 4 \lambda^2) + \alpha (\beta^2 + 4 \lambda^2)}, \quad j^B = \frac{4 \alpha \beta \lambda^2}{\beta (\alpha^2 + 4 \lambda^2) + \alpha (\beta^2 + 4 \lambda^2)}.
\] (21)

The boundary densities \( n_1 \) and \( n_k \) turn out to be different from the density in the bulk. For these densities, we obtain

\[
n_1 = \frac{\beta \alpha^2 + \alpha (\beta^2 + 4 \lambda^2)}{\beta (\alpha^2 + 4 \lambda^2) + \alpha (\beta^2 + 4 \lambda^2)}, \quad n_N = \frac{4 \alpha \lambda^2}{\beta (\alpha^2 + 4 \lambda^2) + \alpha (\beta^2 + 4 \lambda^2)}.
\] (22)

We see that the current as well as the particle density are independent of the lattice size \( N \).

This model with only coherent transport has a non-vanishing current in the thermodynamic limit.

4. The asymmetric exclusion process

We now turn to a description of the steady state of the master equation (3) when we choose the stochastic hopping parameters to resemble those of the TASEP; that is, we choose \( \varphi_L = 0 \) and \( \varphi_R = \varphi \). The steady state of the TASEP, without any additional quantum evolution, i.e. \( \lambda = 0 \), can be calculated exactly [15] (see also the appendix) and its solution can be written in terms of an MPDO [20]. The general form of an MPDO is given by

\[
\rho = \sum_{i_1, \ldots, j_N=0}^{d-1} \left| \langle i_1, j_1, \ldots, M_{i_N, j_N} | r \rangle \right\rangle \otimes_{k=1}^{N} \left| i_k \right\rangle \left\langle j_k \right|,
\] (23)

where \( d \) denotes the dimension of the local Hilbert space and \( M_{i_N, j_{N+1}} \) are \( D_k \times D_{k+1} \) dimensional matrices. For the chain we consider here we have of course \( d = 2 \).

In the case of the TASEP, the steady-state solution to the master equation is given by the choice (see the appendix for a derivation):

\[
\langle l \rangle = \sum_{k=0}^{N} \frac{1}{\alpha^k} \langle k \rangle, \quad M_{1,0} = M_{0,1} = 0, \quad M_{0,0} = \sum_{k=1}^{N} |k \rangle \langle k-1 |, \quad M_{1,1} = \sum_{n=0}^{N} \frac{1}{\beta} |0 \rangle \langle n | + \sum_{n=1}^{N} \sum_{m=1}^{n} |m \rangle \langle n |, \quad |r \rangle = |0 \rangle,
\] (24)

which is an MPDO with a matrix dimension of \( D = N + 1 \). In [15], the classical phase diagram with respect to \( \alpha \) and \( \beta \) has been found (figure 2). In general, there are three phases, the low-density phase LD, the high-density phase HD and the maximum-current phase MC. These phases are separated by non-equilibrium phase transitions. The coexistence line (CL) separating the LD from the HD phase terminates in a critical point, which is shared by two other phase transitions. We label the transition from the HD phase to the MC phase as HDMC, whereas the transition from the LD phase to the HD phase is labeled as LDMC.
The TASEP possesses three phases: the LD (low-density), HD (high-density) and the MC (maximum-current) phases. The simulation was performed for four different points in the classical phase diagram. These points are depicted as blue dots, which correspond to different values of $(\alpha, \beta)$. For the coexistence line (CL) we have $(1/4, 1/4)$. For the MC phase we have $(3/4, 3/4)$, and for the HD and LD phases, we have $(1/2, 1/4)$ and $(1/4, 1/2)$, respectively.

The three phases exhibit different behaviors in the current and density. The statistical current and the corresponding density in the large $N$ limit are given by

$$
\begin{array}{c|ccc}
  & \text{LD} & \text{HD} & \text{MC} \\
  n & \alpha & 1 - \beta & 1/2 \\
 \eta & \alpha(1 - \alpha) & \beta(1 - \beta) & 1/4 \\
\end{array}
$$

as has been calculated in [15]. In this paper, we want to understand the system’s response to a quantum mechanical perturbation at distinct points in the phase diagram.

Note that there is a special line in the classical phase diagram marked by $\alpha + \beta = 1$. Along this line the density operator for the classical probabilities factorizes, and mean-field theory becomes exact (see the appendix). This domain is depicted in the phase diagram of the TASEP by the blue dashed line (see figure 2). If we now add the quantum perturbation, we see that the state

$$
\rho = \bigotimes_{k=1}^{N} \begin{pmatrix} \beta & 0 \\ 0 & \alpha \end{pmatrix}
$$

is still the steady state of the system for arbitrary values of $\lambda$. In the appendix, we argue that coherence in the steady-state density matrix can build up only when the steady state is already classically correlated. That is, we see that when the system is classically uncorrelated the quantum perturbation has no effect on the system.

### 4.1. The dynamical matrix product operator approach to open quantum systems

In order to see whether, in the regime where the stochastic steady state is correlated, the coherent evolution alters the steady state, we need to calculate the steady state of the system numerically by time-evolving the density matrix, until we reach the steady state. The numerical simulations
of the real-time evolution are performed by making use of an algorithm for the propagation of MPDOs [20, 21]. This algorithm works as follows. Starting from the initial density matrix $\rho_0$ given as an MPDO, we apply the trace-preserving completely positive map (tcp-map) $\mathcal{E}(\mathcal{L}, t) = \exp(t\mathcal{L})$ for a small time step $\Delta t$ and approximate the resulting density operator, which has now an increased bond dimension, with an MPDO that has a bond dimension $D_k$ corresponding to that of the original MPDO. The approximation of the operator $\rho(t + \Delta t) = \mathcal{E}(\mathcal{L}, \Delta t) \rho(t)$ is chosen in such a way that the Frobenius norm $\|\rho(t + \Delta t) - \rho_{\text{new}}\|_F^2 = \text{tr} \left[ (\rho(t + \Delta t) - \rho_{\text{new}})^2 \right]$ is minimized. This optimization can be performed efficiently by sweeping from left to right over the individual sites and optimizing the matrices $M_{k, j}$ locally. For the application of the tcp-map to be computable, we perform a second-order Trotter expansion of the tcp-map as follows:

$$\mathcal{E}(\mathcal{L}, \Delta t) \approx \mathcal{E}(\mathcal{L}_c, \Delta t/2) \mathcal{E}(\mathcal{L}_o, \Delta t/2),$$

(26)

where $\mathcal{L} = \mathcal{L}_c + \mathcal{L}_o$ corresponds to a splitting of the Liouvillian into commuting terms which act on the sites $(2k, 2k + 1)$ and $(2k - 1, 2k)$, respectively. The resulting MPDO $\rho_{\text{new}}$ is then chosen as the initial condition for the next step and the procedure is repeated. For a more detailed description of the algorithm, see [20, 21].

As the initial state for the evolution we chose the classical steady state (24). The matrices of the steady state can thus be chosen with a bond dimension of $D = N + 1$. We then changed the value of $\lambda = 0$ to $\lambda = 1$ and $\lambda = 2$, and evolved the MPDO, until the steady state was reached, i.e. until all considered observables did not change any more. Negative values of $\lambda$ were also simulated and led to the same results. We conclude from this that the system’s response only depends on the absolute value of $\lambda$. The simulations were done for different lattice sizes with $N = 20, 40, 60, 80, 100$ sites. The matrix bond dimension of the MPDO was chosen as $D = 40, 40, 60, 120, 150$, respectively, and we chose Trotter steps $\Delta t$ between $10^{-3}$ and $10^{-4}$. To get a better understanding of how the system responds to the quantum perturbation in each of the different phases, we computed the steady state at different values of $\alpha$ and $\beta$, which correspond to points lying in different phases.

Four different points were selected (see figure 2). Note that the different phases in the diagram are related by a simple symmetry transformation, which essentially amounts to a particle–hole transformation with a subsequent exchange of the driving parameters $\alpha$ and $\beta$. It therefore suffices to only simulate four points to understand the system’s response to the perturbation. The first point which was chosen to lie on the coexistence line (CL), where $\alpha = \beta$ and $\beta + \alpha \leq 1$, was chosen as $\alpha = \beta = 1/4$. Furthermore, we chose a point on the transition between the LD phase and the maximum-current (MC) phase (LDMC) with $\alpha = 1/2$ and $\beta = 3/4$. This point is related to the point depicted in figure 2 on the HDMC line by the previously mentioned symmetry transformation. In the MC phase, with $\alpha > 1/2$ and $\beta > 1/2$ we chose $\alpha = \beta = 3/4$. For the HD phase, we chose $\alpha = 1/2, \beta = 1/4$. This phase is related to the LD phase by symmetry as well.

The observable we considered first was the density distribution $\langle n_k \rangle = \text{tr} [n_k \rho]$ as a function of the lattice site $k$ (figure 3). Furthermore, we calculated the values of the two-point correlation functions, of the densities $n_k = \sigma_k^+ \sigma_k^-$ for all pairs $(l, m)$ of sites

$$\langle n_l n_m \rangle' = \langle n_l n_m \rangle - \langle n_l \rangle \langle n_m \rangle.$$

(27)

The expectation values are taken with respect to the system’s steady state. In figures 4(a)–(b) and 5(c)–(d), the correlation functions are compared with the different contributions to the current $j^{\text{tot}}$ defined in (8), for different values of $\lambda = 0, 1, 2$. The first observation to be made is that the individual contributions to the total current are no longer
Figure 3. Density distribution $\langle n_k \rangle$ for the different points $(\alpha, \beta)$, (a) CL $(1/4, 1/4)$, (b) LDMC $(1/2, 3/4)$ and (c) MC $(3/4, 3/4)$, as well as (d) HD $(1/2, 1/4)$. The black solid line corresponds to $\lambda = 0$, i.e. the classical solution. The red dashed line corresponds to a quantum perturbation with $\lambda = 1$, and the blue dashed-dotted line to a perturbation $\lambda = 2$. The plots show the density distribution for a system size of $N = 80$.

constant throughout the lattice. They show a dependence on the lattice site. The total current, however, i.e. $j^{\text{tot}} = j^{\text{co}} + j^{\text{st}}$, is still constant at each site of the lattice, as is required, since the system is in a steady state.

One observes that the quantum perturbation $\lambda > 0$ modifies the density distribution only slightly for the chosen parameter values and a system size of $N = 80$. This effect is stronger for smaller system sizes. We note that the quantum perturbation leads to a smoothing of the sharper density profiles present in the classical distribution.

4.2. The coexistence line and the low-density–maximum-current transition

The two points at CL and LDMC are depicted in figures 4(a) and (b), respectively. These points correspond to the non-equilibrium phase transitions of the system. Even though the total current $j^{\text{tot}}$ assumes a constant value throughout the system, as is required by stationarity and the presence of a continuity equation, we observe that the individual contributions $j^{\text{co}}$ and $j^{\text{st}}$ can vary spatially. This phenomenon can be observed in all simulations. The existence of coherent transport is an indicator of the fact that coherence is present in the steady-state density matrix, departing from the classical behavior present at $\lambda = 0$. As expected this effect becomes stronger with increasing $\lambda$. In turn, we realize that the presence of coherent perturbation actually decreases the magnitude of the correlations present in the system.

If we turn to the current density distribution at CL, we see that the coherent evolution allows for a flow opposite to the boundary driving, thus reducing the total current carried by the system. This effect is strongest in the bulk of the system. The backflow of the coherent transport is partially compensated for by an increased stochastic current in the bulk as well. The effect is reduced at the boundaries of the chain. As pointed out earlier, the plot indicates that the magnitude of correlations is actually reduced by onset of the coherent evolution.

The value of the total current $j^{\text{tot}}$ at the LDMC transition is only slightly affected by the presence of coherent transport. The coherent contribution to the current $j^{\text{co}}$ is increased at the
right boundary of the chain, which is matched by a decrease in stochastic current density. For increased values of $\lambda$ the density–density correlation almost vanishes completely.

4.3. The maximum-current and high-density phases

In the classical process, the MC phase, see figure 5(c), corresponds to the maximum amount of current the system can carry. Allowing for a quantum perturbation, the system makes use of the additional transport capacity and increases its total current. For these boundary conditions the stochastic as well as the coherent contributions flow in the same direction. This effect is strongest in the bulk of the chain. The classical correlation function initially assumes negative values close to the boundaries. The onset of the quantum perturbation also reduces the magnitude of the correlations in this phase, even though the total amount of current is increased.

In the HD phase depicted in figure 5(d), the additional coherent transport does not alter the total current significantly. We observe that at the right boundary, where the particles are
injected, the coherent transport leads to a flow in the direction opposite to the driving of the system, which is almost entirely compensated for by an increased stochastic flow of the particles in accordance with the driving. Again, we observe a further decrease in magnitude of the correlations. However, note that even though smaller, the correlations seem to be longer ranged. We expect, however, that this effect is only present in systems of finite size.

4.4. The dependence of the current on the system size

We now turn to the dependence of the current density as a function of the system size. We depict the scaling of the different fractions of the current as well as the total current with chain length \( N \), see figure 6. The plot shows in each column from (a) to (d) the different contributions for each simulated point to the current as a function of the system size, ranging from \( N = 20 \) to...
Figure 6. Scaling behavior of the currents $j_{\text{co}}$, $j_{\text{st}}$ and $j_{\text{tot}}$ with $N$ for different values of $\lambda = 0, 1, 2$ at the link $(N/2, N/2 + 1)$. Here, the black solid line corresponds to $\lambda = 0$, whereas $\lambda = 1$ is shown as the red dashed line. The blue dashed-dotted line depicts the current for $\lambda = 2$. The first row depicts the total current $j_{\text{tot}}$. The subsequent rows depict $j_{\text{st}}$ and $j_{\text{co}}$, respectively. All plots are given in dependence of the system size $N$.

$N = 100$ sites. The quantum effects exhibit a strong dependence on the system size. We see that the coherent contribution in all the four cases decays as the system size increases. The curves suggest that coherent transport vanishes in the bulk completely in the limit of large $N$. This is actually already the case in the HD phase with a quantum perturbation of $\lambda = 1$ (figure 6(d)). Comparing the numerical values of the stochastic current with those of the coherent current, we see that at all the points we have investigated in the phase diagram, the stochastic current is significantly larger than the coherent transport, even though the two parameters $\lambda$ and $\phi$ are of the same magnitude. We conclude from this that the quantum evolution does not modify the system’s stochastic transport properties significantly. It therefore seems that the decoherence, which is induced by the stochastic hopping of the particles, strongly suppresses the coherent transport for larger system sizes.
5. Conclusions

We have investigated a quantum perturbation to the dynamics of the simple symmetric exclusion process as well as to the TASEP. We find that we can rephrase the stochastic master equation as a quantum equation that fully reproduces the classical dynamics. The quantum perturbations modify the steady-state behavior and allow for two different types of currents, which, each on their own, can vary as a function of the site. The analytical solution for the symmetric exclusion process shows that the transport behavior for large system sizes is not modified by the coherent perturbation, since both the stochastic and the coherent contributions to the steady-state current vanish in the limit of large system sizes. The system’s behavior only changes abruptly when the stochastic evolution is switched off, and there is only coherent transport in the bulk. The TASEP numerical simulations of the full master equation indicate that the underlying classical phase-diagram is respected. The steady state responds to driving due to the boundary terms with a different behavior in current and density. This change, however, vanishes for increasing system sizes. We therefore conclude that the transport behavior of the exclusion processes is not modified significantly by the coherent evolution. It is, however, not possible to conclude that the coherent evolution leaves the system’s steady state entirely unaffected, since higher-order correlations may play an important role. A further step would be to investigate the current–current correlation function of the SSEP, to see whether the quantum perturbation has an effect on the current fluctuations.

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Appendix. Derivation of the steady-state algebra

An exact solution to the steady state of the classical model has been found by Derrida et al in [15] already. As an ansatz for the steady state a translationally invariant matrix product state was chosen and algebraic relations for the matrices were derived. This ansatz can, of course, also be generalized to matrix product operators (MPOs). We define a translationally invariant density matrix with open boundary conditions, i.e. we choose the matrices site independent, and write

$$\tilde{\rho} = \langle l | (G B A E) \otimes^N | r \rangle,$$

where we have to require that $A = \tilde{B}$ and $G, E$ are real due to Hermiticity. It is now possible to impose similar algebraic constraints on the MPO that were imposed for the matrix product states [15]. That is, if we split the master equation (3) into individual summands that constitute only two-body interactions and write

$$\mathcal{L}[\rho] = \mathcal{L}_1[\rho] + \sum_{k=1}^{N-1} \mathcal{L}_{k,k+1}[\rho] + \mathcal{L}_N[\rho],$$

$$\text{(A.2)}$$
we can require that the matrices $A, B, E, G$ together with some ancilla matrices that we mark by $\hat{A}, \hat{B}, \ldots$ have to satisfy the constraints

$$L_{k,k+1} \left( \frac{G}{A} \frac{B}{E} \otimes \frac{G}{A} \frac{B}{E} \right) = \left( \frac{\hat{G}}{\hat{A}} \frac{\hat{B}}{\hat{E}} \right) \otimes \left( \frac{G}{A} \frac{B}{E} \right) - \left( \frac{G}{A} \frac{B}{E} \right) \otimes \left( \frac{\hat{G}}{\hat{A}} \frac{\hat{B}}{\hat{E}} \right). \quad (A.3)$$

Furthermore, we require that the single-site operators at the boundaries have to satisfy

$$\langle l | L_1 \left[ \left( \frac{G}{A} \frac{B}{E} \right) \right] = -\langle l | \left( \frac{\hat{G}}{\hat{A}} \frac{\hat{B}}{\hat{E}} \right),$$

$$L_N \left[ \left( \frac{G}{A} \frac{B}{E} \right) \right] | r \rangle = \left( \frac{\hat{G}}{\hat{A}} \frac{\hat{B}}{\hat{E}} \right) | r \rangle. \quad (A.4)$$

We see that the total sum (A.2) telescopes to zero and $\tilde{\rho}$ is the steady-state solution of the equation. For a suitable decomposition into two-body terms that correspond to $H_{k,k+1} = \frac{1}{2}(\sigma_k^x \otimes \sigma_{k+1}^x + \sigma_k^y \otimes \sigma_{k+1}^y)$ and the Lindblad operators $L_{k,k+1}$ with the two boundary terms $L_1, L_2$, we can derive the following algebra for the steady state. The eight matrices need to satisfy 16 equations in the bulk (A.3). First, all matrices have to commute with their ancilla counterpart, that is, $[A, \hat{A}] = [B, \hat{B}] = [E, \hat{E}] = [G, \hat{G}] = 0$. The remaining equations are then as follows:

$$-\frac{2\lambda}{i} BG - \frac{\varphi}{2} GB = \hat{G} B - G \hat{B} \quad \text{and} \quad -\frac{2\lambda}{i} GB = \hat{B} G - B \hat{G}, \quad (A.5)$$

$$-\frac{2\lambda}{i} E A - \frac{\varphi}{2} A E = \hat{A} E - A \hat{E} \quad \text{and} \quad -\frac{2\lambda}{i} AE = \hat{E} A - E \hat{A}, \quad (A.6)$$

as well as

$$\frac{2\lambda}{i} AG - \frac{\varphi}{2} GA = \hat{G} A - G \hat{A} \quad \text{and} \quad \frac{2\lambda}{i} GA = \hat{A} G - A \hat{G}, \quad (A.7)$$

$$\frac{2\lambda}{i} GE - \frac{\varphi}{2} BE = \hat{B} E - B \hat{E} \quad \text{and} \quad \frac{2\lambda}{i} BE = \hat{E} B - E \hat{B}, \quad (A.8)$$

and finally we have also

$$\frac{2\lambda}{i} [A, G] - \varphi GE = \hat{G} E - G \hat{E} = E \hat{G} - \hat{E} G, \quad (A.9)$$

$$-\frac{2\lambda}{i} [G, B] - \frac{\varphi}{2} BA = \hat{B} A - B \hat{A} \quad \text{and} \quad (A.10)$$

$$\frac{2\lambda}{i} [G, E] - \frac{\varphi}{2} AB = \hat{A} B - A \hat{B}. \quad (A.11)$$

We furthermore need to satisfy the constraints set by the boundary terms that govern the inflow and outflow of the particles. The edge algebra derived from (A.4) then reads

$$\langle l | \left( \begin{array}{c} E \\ A \\ B \\ E \end{array} \right) = \langle l | \left( \frac{-1}{a} \frac{\hat{G}}{\hat{A}} \frac{2}{a} \frac{\hat{B}}{\hat{E}} \right),$$

$$\left( \begin{array}{c} G \\ A \\ B \\ G \end{array} \right) | r \rangle = \left( \frac{-1}{b} \frac{\hat{G}}{\hat{A}} \frac{2}{b} \frac{\hat{B}}{\hat{E}} \right) | r \rangle. \quad (A.12)$$
As one can see, this algebra becomes significantly more complex in the quantum setting and it appears to be very challenging to find an algebraic representation for the eight matrices. However, let us briefly consider the classical case setting $\lambda = 0$. Then the algebra simplifies greatly and we can set $A = \hat{A} = B = \hat{B} = 0$. Choosing furthermore $-\hat{G} = \hat{E} = 1$, we recover the classical algebra $GE = E + G$ and $\langle l | E = 1/\alpha \langle l |$ as well as $G |r\rangle = 1/\beta |r\rangle$. For this a representation can be found [15], such as for example the Fock representation

$$\langle l | = \sum_{k=0}^{\infty} \frac{1}{\alpha^k} |k\rangle \quad \text{and} \quad |r\rangle = |0\rangle,$$

$$E = \sum_{k=1}^{\infty} |k\rangle \langle k - 1| \quad \text{and} \quad G = \sum_{n=0}^{\infty} \frac{1}{\beta} |0\rangle \langle n| + \sum_{n=1}^{\infty} \sum_{m=1}^{n} |m\rangle \langle n|,$$

which is a representation that is infinite dimensional. In fact, one can show easily that all representations have to be infinite dimensional unless $\alpha + \beta = 1$. From this representation, the normalization, or partition function, can be computed as $Z = \text{tr}[\hat{\rho}]$ as was done in [15]. Note that since we are dealing with a Fock representation here, it is possible to reproduce the steady state with a finite matrix dimension, even though the algebra is not satisfied exactly. It is straightforward to see that truncating the dimension of the matrices to $D = N + 1$ reproduces the same contraction values.

We would like to point out that recently a similar method has been used to construct the steady state of a driven, interacting quantum spin chain [22]. The author was able to construct an algebra and find the corresponding representation for the matrices of the steady state which depended on three, rather than two sites.

Note that the line $\alpha + \beta = 1$ is special. For this case one can easily show that a 1D representation of $E = \alpha^{-1}$ and $G = \beta^{-1}$ suffices, since in this case $\alpha^{-1} + \beta^{-1} = (\alpha \beta)^{-1}$. The matrices $E$ and $G$ commute, and we can set the matrices $B = A = 0$. We see that coherence can build up only when $E$ and $G$ no longer commute. That is, we have that when the system is classically uncorrelated, the quantum perturbation has no effect on the system.

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