Noise and diffusion of particles obeying asymmetric exclusion processes

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The relation between noise and Fick’s diffusion coefficient in barrier limited transport associated with hopping or tunneling mechanisms of particles obeying the asymmetric simple exclusion processes (ASEP) is physically assessed by Monte Carlo simulations. For a closed ring consisting of a large number of barriers the diffusion coefficient is related explicitly to the current noise thus revealing the existence of a generalized Nyquist-Einstein relation. Both diffusion and noise are confirmed to decrease as the square root of the number of barriers as a consequence of the correlation induced by ASEP. By contrast, for an open linear chain of barriers the diffusion coefficient is found to be no longer related to current noise. Here diffusion depends on particle concentration but is independent of the number of barriers.

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The inter-relations between noise and diffusion in charge transport is a pillar of non-equilibrium kinetics since the theoretical interpretation of the Brownian motion by Einstein. For a kinetic described within a continuous transport model, where quasi-particles undergo local scattering events between stochastic free flights, the inter-relation between noise and diffusion was investigated by a number of theoretical approaches ranging from analytical models to numerical solutions of the appropriate kinetic equations. The case of a barrier transport model, dominated by tunnelling and/or hopping processes, is less developed. Here, noise was mostly investigated for the case of single and multiple quantum barriers. By contrast, a few seminal works have tackled the problem of noise in hopping systems and that of diffusion in both tunneling and hopping systems. For the case of a very large number of barriers, the asymmetric simple exclusion process (ASEP) has been widely used in the recent past as a relevant physical model for the description of non-equilibrium dynamics. In this context, two systems of basic interest are the closed ring and the open linear chain consisting of a set of multiple barriers, which are the prototypes of closed and open systems driven by hopping or tunneling transport mechanisms. Here, diffusion was investigated in by analytical means and current noise with Monte Carlo simulations. However, the attempt to interrelate diffusion and current noise in these systems remains a largely unexplored issue. In particular, the dependence or less of diffusion on the number of barriers, as well as the prediction of a partial or complete suppression of shot noise in the presence of a large number of barriers are intriguing features still lacking of a microscopic interpretation. The aim of the present work is to address this issue by first principles Monte Carlo simulations. Accordingly, diffusion is obtained by the calculation of the time evolution of the spreading in space of a particle ensemble and current noise by the calculation of the autocorrelation function of current fluctuations as measured in the outside circuit. The main features of diffusion and noise and their interrelation are thus quantitatively assessed on a kinetic physical ground.

We take a physical system consisting of a number of hopping sites, separated by a constant distance , whose total length is . The tunneling rate between two adjacent site is assumed to have the same value . We then consider alternatively periodic- (closed ring) or open-boundary (linear chain) conditions. By imposing a current determined by a transition rate to a structure with (which are taken as plausible parameters for a real case) we evaluate current, diffusion, and noise making use of an ensemble Monte Carlo simulator. It is convenient to define the dimensionless carrier concentration as , where is the average number of carrier inside the sample. We then introduce correlations between carriers within the ASEP model by imposing a maximum occupation number for each site. In particular, when a site is occupied by one carrier then no other carrier can jump to this site, thus carriers are strongly correlated. When a site can be occupied by an arbitrary number of carriers, thus carriers are totally uncorrelated. The instantaneous current is calculated as

\[ I(t) = \frac{e}{L} \sum_{i=1}^{N(t)} v_{i}(t) = \frac{e}{L} N(t) v_{d}(t), \]  

where is the unit charge, (the instantaneous number of carriers inside the structure, ) the instantaneous velocity of the -th carrier, the instantaneous drift velocity of the carrier ensemble. Under steady state is a stochastic variable that accounts for fluctuations in carrier number and velocity. In particular, for our discrete system , with the position index of the -th particle.

For the (longitudinal) diffusion coefficient , following Fick’s law we make use of its definition as a spatial...
The spectral density of current fluctuations at zero frequency is given by:

\[ S_I = 4 \int_0^\infty dt \langle (\Delta I(t))^2 \rangle = S_I^{vd} + S_I^N + S_I^{vd,N} \tag{3} \]

where \( S_I^{vd} \), \( S_I^N \) and \( S_I^{vd,N} \) refer to the three contributions (drift velocity, number and cross-correlations between them) in which the total spectral density can be decomposed. With Monte Carlo simulations these terms can be calculated separately. The Fano factor is \( \gamma = S_I / (2e\langle I \rangle) \).

A. Closed ring. The periodic boundary conditions adequate to this structure consists in imposing that, for a finite number of sites, the last site is directly connected to the first one by the same hopping rate \( \Gamma \). Let us consider the case of correlated carriers (\( \nu = 1 \)). For a given carrier concentration and for large \( N_w \), analytical theory\(^{15,21}\) gives the following predictions: for the average current

\[ \langle I \rangle_1 = e\Gamma \rho (1 - \rho) \tag{4} \]

and for the diffusion coefficient \( \Delta_1 \) (following \(^21\)), with the subscript 1 labeling the case of the ring geometry,

\[ \Delta_1 = \frac{l^2 \Gamma \sqrt{\pi}}{2} \frac{(1 - \rho)^{3/2}}{(\rho N_w)^{3/2}} \tag{5} \]

[We suppose that in general the value of \( \Delta_1 \) differs from that of \( D \) in Eq.\(^2)\]

The results of the simulations for the diffusion coefficient are reported in Fig. 1. Here, the identity \( \Delta_1 = D \) is confirmed for all the concentrations considered.

For the current noise (in this case due only to velocity fluctuations since the number of carriers is rigorously constant in time) the simulations confirm the relation

\[ S_I = S_I^{vd} = 4e^2 / l^2 \rho^2 \Delta_1 \tag{6} \]

with the corresponding Fano factor (Fig. 2), given by

\[ \gamma = \frac{\sqrt{\pi}}{2} \frac{\rho^{1/2} (1 - \rho)^{1/2}}{N_w^{1/2}} \tag{7} \]

Equation \(^6\), by revealing a strict relation between noise and diffusion, takes the form of a generalized Nyquist-Einstein relation\(^2,7,30\). The reason of diffusion and noise suppression as \( 1 / \sqrt{N_w} \) confirmed by the simulations, is attributed to the strong correlation among carriers. To support this interpretation, we considered also the case of uncorrelated carriers (i.e. in the absence of ASEP) where, for a given carrier concentration, analytical theory gives the following predictions: for the average current\(^{15}\)

\[ \langle I \rangle_0 = e\Gamma \rho \tag{8} \]

for the diffusion coefficient\(^{18,19}\)

\[ D_0 = \frac{l^2 \Gamma}{2} \tag{9} \]

(with the subscript 0 labeling the case of uncorrelated particles) and for the current noise the standard Nyquist relation\(^2\)

\[ S_I = S_I^{vd} = 4e^2 / l^2 \rho^2 D_0 \tag{10} \]

with the corresponding Fano factor

\[ \gamma = \frac{1}{N_w} \tag{11} \]

The result of simulations confirms that, in the absence of ASEP, diffusion becomes independent of \( N_w \) (see the
the expected 1 number of scattering events, which is found to exhibit ASEP is found to be related to a subpoissian variance of
other hand, the suppression of diffusion in the presence of
evolution of the variance in space of the carrier ensem-
ble is found to be linear, contrarily to the suggestion of
between 0 and 1 being equivalent respectively to the
parameters in [21,26] and to

and Γ are the transition rates from the left reser-
in, out
in, out
in, out
in, out

FIG. 3: (Color online) Linear chain. Spreading diffusion co-
efficient obtained from simulations in the presence of ASEP and
for different input and output rates. The value for uncor-
related carriers is reported for comparison. Curves are guide
to the eyes.

FIG. 4: (Color online) Linear chain. Comparison between
analytical Fano factors in Eq. (12) and full shot noise (dashed
lines), with that obtained from simulations (symbols).

curve uncorrelated in Fig. 1, and the Fano factor decreases as $1/N_w$ (see the curve uncorrelated in Fig. 2). In all the cases considered here (even when $\nu = 1$ so that the non-passing constraint is accomplished) the time evolution of the variance in space of the carrier ensemble is found to be linear, contrarily to the suggestion of a sub-diffusive (and thus sublinear) behavior [22]. On the other hand, the suppression of diffusion in the presence of ASEP is found to be related to a subpoissian variance of the number of scattering events, which is found to exhibit the expected $1/\sqrt{N_w}$ behavior.

B. Open linear chain. The boundary conditions adequate to this structure consists in connecting the two terminals of the device with two reservoirs, where $\Gamma_{in} \times \Gamma$ and $\Gamma_{out} \times \Gamma$ are the transition rates from the left reservoir to the first site of the device, and from the last site of the device to the right reservoir, respectively. For convenience, the values of $\Gamma_{in(out)}$ are taken in the range between 0 and 1 being equivalent respectively to the $\alpha$ and $\beta$ parameters in [22,26] and to $f_L$ and $(1 - f_R)$ in [15].

Let us first consider the case of correlated carriers (ASEP model). For a given carrier concentration and for large $N_w$ analytical theory gives for the average current the same expression of Eq. (4). The diffusion coefficient of the linear chain $\Delta_2$ (following [20], with the subscript 2 labeling this specific case) takes the form: if $\Gamma_{in} + \Gamma_{out} = 1$, 

$$\Delta_2 = \left\{ \begin{array}{ll}
\frac{4\sqrt{\rho}}{\pi N_w} \left| \Gamma_{in} - \Gamma_{out} \right| & \text{ when } \Gamma_{in} \neq \Gamma_{out} \\
0 & \text{ when } \Gamma_{in} = \Gamma_{out}
\end{array} \right. $$

(12)

and, if $\Gamma_{in} = \Gamma_{out} = 1$, 

$$\Delta_2 = \frac{\rho^2 \Gamma}{2} \left( 3(2\pi^{1/2}) + 64N_w^{1/2} \right).$$

(13)

[Again $\Delta_2$ is supposed to differ in general from $D$ obtained from Eq. (4).] The different analytical expressions for $\Delta_2$ are a consequence of the different values taken by $\Gamma_{in(out)}$ and, in turn, by $\rho$ in the steady state. Indeed, the tuning of the $\Gamma_{in(out)}$ controls the strength of the correlation among carriers induced by ASEP and thus the particle density $\rho$ inside the device, as summarized in the phase diagram reported in Fig. 2 of [21].

Figure 4 reports the Fick’s diffusion coefficient $D$ obtained from simulations for the case of the linear chain. Here, $D$ is found to be practically independent of $N_w$. Furthermore, in the presence of ASEP the value of $D$ is systematically lower than that of uncorrelated particles $D_0$. For the case $\Gamma_{in} + \Gamma_{out} = 1$, the value of the diffusion coefficient is well described by the relation

$$D = \frac{\rho^2 \Gamma}{2} \Gamma_{out} = \frac{\rho^2 \Gamma}{2} (1 - \rho)$$

(14)

We notice that in the above expression, $D$ becomes vanishing small for $\Gamma_{out} \to 0$ because in this limit spreading and current of carriers through the structure tends to stop. In the presence of ASEP the values of diffusion obtained by simulations are found to differ significantly from those given by analytical expressions, thus implying that the quantities $\Delta_2$ an $D$ describe different microscopic processes.

Figure 4 reports the results of the simulations for the current noise [in this case due to the sum of all the contributions in Eq. (8)] in terms of the Fano factor. From simulations, within numerical uncertainty we find:

$$S_I = S_I^{cw} + S_I^{cN} + S_I^{cw} + S_I^{cN} = \frac{4\sqrt{\rho}}{\rho^2} \Delta_2$$

(15)

with the corresponding Fano factor satisfying the relation

$$\gamma = \frac{2\Delta_2}{\Gamma^2 \rho (1 - \rho)}.$$ 

(16)

From the above expressions we conclude that $\Delta_2$ describes the total current noise instead of the Fick’s diffusion process. The quantity $\Delta_2$ is found to agree well with available analytical expressions, as predicted by Eq. (15), in full agreement with the results of [26]. The quantity $D$ is found to depend upon the degree of correlation, to be independent of the number of sites and, when
The correlations introduced by ASEP are found to be responsible of the dependence of diffusion upon the inverse square root of the device length. For the case of the open linear chain the diffusion coefficient obtained from Fick’s law is explicitly related to current noise, both in the presence and in the absence of the ASEP. Therefore, evidence is provided for the existence of a generalized Nyquist-Einstein relation allowing the determination of diffusion from a noise measurement or viceversa. The correlations introduced by ASEP are found to be responsible of the dependence of diffusion upon the inverse square root of the device length. For the case of the open linear chain the diffusion coefficient obtained from Fick’s law is not related to the current noise, which now contains contributions coming from velocity, number and their cross-correlations. Here the diffusion coefficient is found to be independent of the number of sites but to depend on the strength of the correlation that is ultimately controlled by the carrier density. We remark, that the total current noise is found to be related to a “diffusion constant” (more properly a counting statistics phenomenon), whose analytical expressions are satisfactorily confirmed by simulations.

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