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A Monte Carlo investigation of noise and diffusion of particles exhibiting asymmetric exclusion processes

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Abstract
The relation between noise and Fick's diffusion coefficient in barrier limited transport associated with hopping or tunnelling mechanisms of particles exhibiting the asymmetric simple exclusion processes (ASEP) is physically assessed by means of 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.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The inter-relation between noise and diffusion in charge transport is a pillar of non-equilibrium kinetics [1–5]. The existence of such inter-relations proved to be of relevant interest for determining the diffusion coefficient, a kinetic coefficient difficult to obtain, through a noise measurement. For a kinetics 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 using analytical models [1, 3, 5] to numerical solutions of the appropriate kinetic equations [2, 4]. 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 [6–8]. By contrast, a few seminal works have tackled the problem of noise in hopping systems [9, 10] and that of diffusion in both tunnelling and hopping systems [11–13]. 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 [14–19]. 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 tunnelling transport mechanisms. Here, diffusion was investigated by analytical means [14, 20], and current noise with Monte Carlo simulations [9, 10]. 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, and 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 a microscopic interpretation [9, 10, 21].

The aim of the present work is to address this issue by using 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 inter-relation are thus quantitatively assessed on kinetic physical grounds.

2. Theory

We take a one-dimensional physical system consisting of a number N_w of hopping sites, separated by a constant distance l, whose total length is $L = N_w l$. Each site is adjacent to two other sites but, in analogy with [14], we assume that tunnelling events can occur only between nearest neighbours and only in the forward direction. The transition rate is assumed to have a constant value Γ. By imposing a current determined by a rate of transition $\Gamma = 10^{13}$ s^{-1} onto a structure with $l = 3.2$ nm (these 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 $\rho = \langle N\rangle/N_w$, where $\langle N\rangle$ is the average number of carriers inside the sample. We introduce correlations between carriers by imposing a maximum occupation number ν for each site. In particular, when $\nu = 1$ if a site is occupied by one carrier then no other carrier can jump to this site, and thus carriers are strongly correlated. In this case the interaction is known in the literature [14] as the asymmetric simple exclusion process (ASEP). When $\nu \to \infty$ a site can be occupied by an arbitrary number of carriers, and thus carriers are totally uncorrelated.

The instantaneous current $I(t)$ is calculated as [22]

$$I(t) = \frac{e}{L}\sum_{i=1}^{N(t)} v_i(t) = \frac{e}{L}N(t)v_{\mathrm{d}}(t), \tag{1}$$

where e is the unit charge, $N(t)$ the instantaneous number of carriers inside the structure, $v_i(t)$ the instantaneous velocity of the ith carrier, $v_{\mathrm{d}}(t)$ the instantaneous drift velocity of the carrier ensemble. For a steady state, $I(t)$ is a stochastic variable that accounts for fluctuations in carrier number and velocity. In particular, for our discrete system $v_i(t) = l\delta\xi_i/\delta t$, with ξ_i the position index of the ith particle [11]. For the (longitudinal) diffusion coefficient D, following Fick's law we make use of its definition as a spatial spreading quantity [23],

$$D = \frac{1}{2}\frac{\delta\langle(\Delta z(t))^2\rangle}{\delta t}, \tag{2}$$

where $\Delta z(t)$ is the distance between the final and the initial hopping sites, brackets mean average over a statistical ensemble (up to 10^3) of identical systems. The time derivative is carried out in a time domain sufficiently long for extrapolating the long time limit, for which D is found to be independent of time. The spectral density of current fluctuations at zero frequency is [22]

$$S_I = 4\int_0^\infty \mathrm{d}t\,\langle \delta I(0)\delta I(t)\rangle = S_I^{v_\mathrm{d}} + S_I^N + S_I^{Nv_\mathrm{d}} + S_I^{v_\mathrm{d}N}, \tag{3}$$

where $S_I^{v_\mathrm{d}}$, S_I^N and $(S_I^{Nv_\mathrm{d}} + S_I^{v_\mathrm{d}N})$ 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 $\gamma = S_I/(2e\langle I\rangle)$.

3. Results and discussion

We now consider alternatively periodic boundary (closed ring) or open boundary (linear chain) conditions.

3.1. Ring (periodic system)

The periodic boundary conditions adequate to this structure consist in imposing that, for a finite number of sites, the last site is directly connected to the first one by the same hopping rate Γ. Let us consider the case of correlated carriers ($\nu = 1$). For a given carrier concentration and for large N_w, analytical theory [14, 9] gives the following predictions: for the average current

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

and for the diffusion coefficient Δ_1 in the long time limit (the symbol Δ follows the notation of [14] with subscript 1 labelling the case of the ring geometry),

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

(We suppose that in general the value of Δ_1 can differ from that of D in equation (2).) The results of the simulations for the diffusion coefficient are reported in figure 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

$$S_I \equiv S_I^{v_\mathrm{d}} = \frac{4e^2}{l^2}\rho^2\Delta_1, \tag{6}$$

with the corresponding Fano factor (figure 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 [1, 2, 24–26]. The diffusion and noise suppression going 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 [9]

$$\langle I\rangle_0 = e\Gamma\rho, \tag{8}$$

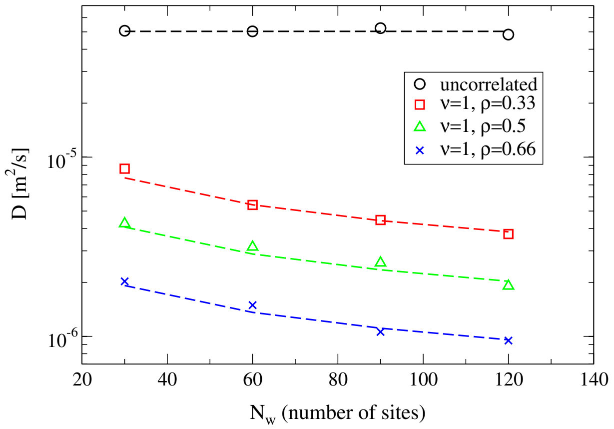

Figure 1. Closed ring. Comparison between the analytical diffusion coefficient in equations (5) and (9) (dashed lines) and that obtained from simulations (symbols).

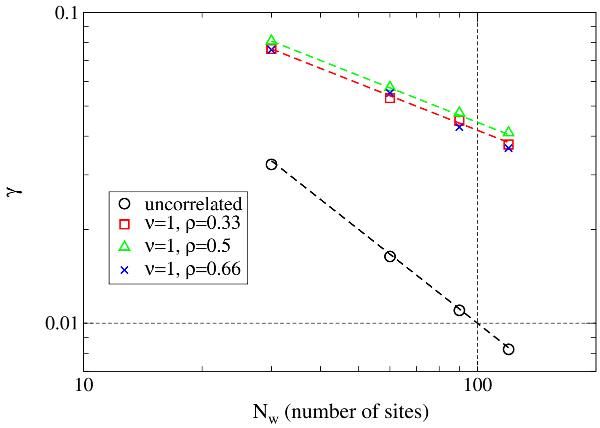

Figure 2. Closed ring. Comparison between the analytical Fano factor in equations (7), (11) (dashed lines) and that obtained from simulations (symbols).

for the diffusion coefficient [12]

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

(with the subscript 0 labelling the case of uncorrelated particles) and for the current noise the standard Nyquist–Einstein relation holds [22]:

$$S_I \equiv S_I^{v_d} = \frac{4e^2}{l^2} \rho^2 \frac{D_0}{N}, \tag{10}$$

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 curve uncorrelated in figure 1), and the Fano factor decreases as $1/N_w$ (see the curve uncorrelated in figure 2).

It is reasonable that, in the case of correlated particles, the diffusion is less than in the free dynamics, since, in the former case, the motion of the particle ensemble is limited by the periodic boundary condition.

In all the cases considered here (even when $\nu = 1$ so that the non-passing constraint is obeyed) the time evolution of the variance in space of the carrier ensemble is found to be linear, contrary to the suggestion of a subdiffusive (and thus sublinear) behaviour [14].

The good agreement between the results of the simulations and analytical predictions is taken as a validation of the numerical approach developed here.

3.2. Open linear chain

The boundary conditions adequate to this structure consist in connecting the two terminals of the device to two reservoirs, where $\Gamma_{\text{in}} \times \Gamma$ and $\Gamma_{\text{out}} \times \Gamma$ are the rates of transition 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 $\Gamma_{\text{in(out)}}$ are taken in the range between 0 and 1, being equivalent respectively to the α and β parameters in [14, 20] and to f_{L} and $(1 - f_{\text{R}})$ in [9].

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 as equation (4). The diffusion coefficient of the linear chain Δ_2 (obtained as Δ_1 with the subscript 2 labelling the case of the open linear chain) takes the forms [20]: if $\Gamma_{\text{in}}+\Gamma_{\text{out}} = 1$,

$$\Delta_2 = \begin{cases} \dfrac{l^2\Gamma}{2}\Gamma_{\text{in}}\Gamma_{\text{out}}|\Gamma_{\text{in}} - \Gamma_{\text{out}}| & \text{when } \Gamma_{\text{in}} \neq \Gamma_{\text{out}} \\ \dfrac{l^2\Gamma}{2}\dfrac{1}{4(\pi N_w)^{1/2}} & \text{when } \Gamma_{\text{in}} = \Gamma_{\text{out}} \end{cases} \tag{12}$$

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

$$\Delta_2 = \frac{l^2\Gamma}{2}\frac{3(2\pi^{1/2})}{64N_w^{1/2}}. \tag{13}$$

(Again we suppose that in general the value of Δ_2 can differ from that of D in equation (2).) The different analytical expressions for Δ_2 are a consequence of the different values taken by $\Gamma_{\text{in,out}}$ and, in turn, by ρ in the steady state. Indeed, the tuning of the $\Gamma_{\text{in,out}}$ controls the strength of the correlation among carriers induced by ASEP and thus the particle density ρ inside the device, as summarized in the phase diagram reported in figure 2 of [14]. Figure 3 shows 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 $\Gamma_{\text{in}} + \Gamma_{\text{out}} = 1$, the value of the diffusion coefficient is well described by the relation

$$D = \frac{l^2\Gamma}{2}\Gamma_{\text{out}} = \frac{l^2\Gamma}{2}(1 - \rho). \tag{14}$$

We notice that in the above expression, D becomes vanishingly small for $\Gamma_{\text{out}} \to 0$ 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 Δ_2 and D describe different microscopic processes. To shed some light on the physical reason for this difference, figure 4 reports the results of the simulations for the current noise (in this case due to the sum

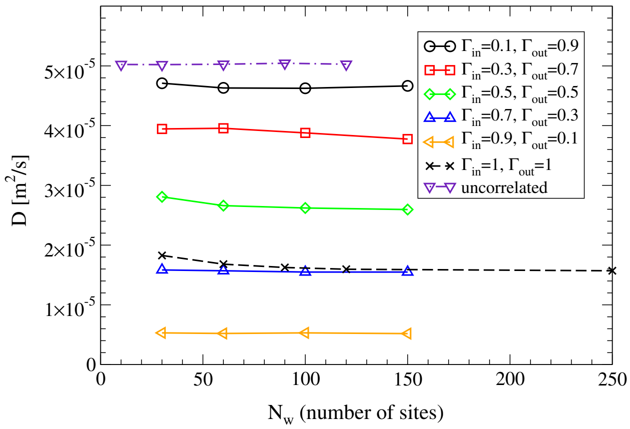

Figure 3. Linear chain. Spreading diffusion coefficient obtained from simulations in the presence of ASEP and for different input and output rates. The value for uncorrelated carriers is reported for comparison. Curves are guides to the eyes.

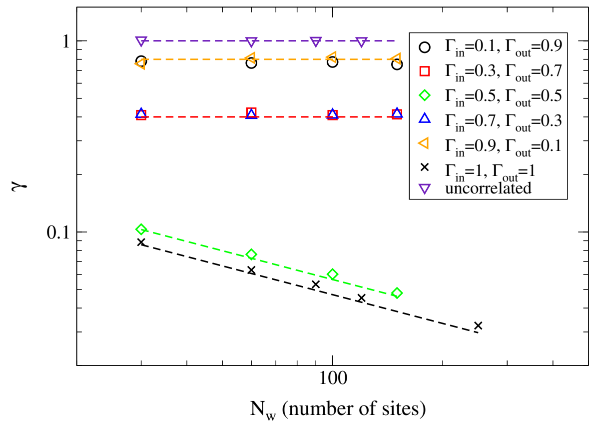

Figure 4. Linear chain. Comparison between analytical Fano factors in equation (16) and full shot noise (dashed lines), with those obtained from simulations (symbols).

of all the contributions in equation (3)) in terms of the Fano factor. From simulations, within numerical uncertainty we find

$$S_I \equiv S_I^{v_d} + S_I^N + S_I^{Nv_d} + S_I^{v_d N} = \frac{4e^2}{l^2}\Delta_2 \tag{15}$$

with the corresponding Fano factor satisfying the relation

$$\gamma = \frac{2\Delta_2}{\Gamma l^2 \rho(1-\rho)}. \tag{16}$$

For example, if $\Gamma_{out} \to 0$, the exit of the particles is highly suppressed, the device will reach high density and, since particles are correlated, the motion of the ensemble in the device will be mostly coherent, with low diffusion. From the above expressions we conclude that Δ_2 describes the total current noise instead of Fick's diffusion process. Indeed, Δ_2 is found to agree well with available analytical expressions, as predicted by equation (15), in full agreement with the results of [20]. By contrast, the quantity D is found: (i) to depend upon the degree of

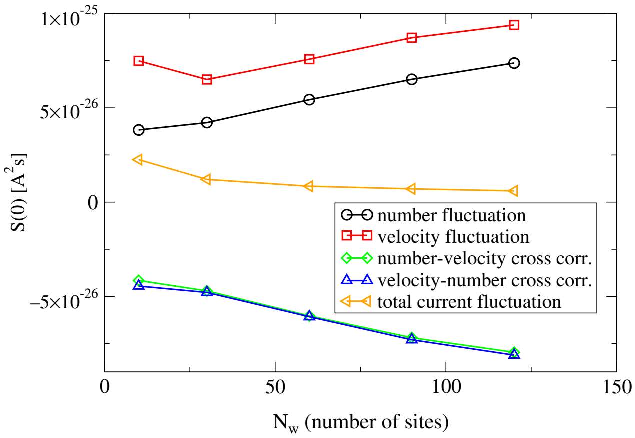

Figure 5. Different contributions and total noise power for the case of ASEP in the open linear case with $\Gamma_{in} = \Gamma_{out} = 1$. Curves are guides to the eyes.

correlation, (ii) to be independent of the number of sites, and (iii), when $\Gamma_{in} + \Gamma_{out} = 1$, to be proportional to Γ_{out}.

Since Δ_2 is related to the 'number of particles that entered the device up to time t' [20], it is possible to show that this stochastic quantity accounts for both velocity and number fluctuations, being thus related to total current noise.

By turning off the ASEP correlation, for a given carrier concentration, analytical theories give: (i) for the average current equation (8), (ii) for the diffusion coefficient equation (9), and (iii) for the current noise (full shot noise is expected)

$$S_I \equiv S_I^N = \frac{2e^2}{L^2}\langle v_d\rangle^2\langle N\rangle\tau_{TR} = 2e\langle I\rangle \tag{17}$$

which follows from a correlation function with triangular shape vanishing at the transit time $\tau_{TR} = L/\langle v_d\rangle$. As a consequence $\gamma = 1$, as confirmed by the results of the simulations reported in figure 4.

Finally, we have investigated separately the contributions to the total current noise which come from velocity, number, and their cross-correlations in the presence of ASEP. From the results in figure 5 we can see that different contributions are comparable in magnitude with the cross-terms that, being negative, are responsible for shot noise suppression. We further notice that the comparison between the two uncorrelated current noise levels belonging to the closed ring (figure 2) and to the open linear chain (figure 3) shows that shot noise of the linear chain exceeds the velocity noise of the closed ring for the ratio L/l, as expected.

4. Conclusions

We have carried out a simulative investigation of the inter-relations between noise and diffusion in barrier limited transport for the ASEP condition. For the case of the closed ring, since the number of particles is fixed, only the noise related to velocity fluctuations is present. Here, the diffusion coefficient obtained from the 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 vice versa. The correlations introduced by ASEP are found to be responsible for 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 no longer 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. In this case, owing to the open boundaries, the number of particles is not constant through the simulation, and the charge density can fluctuate in time.

Finally, we remark that analytical results concerning $\Delta_{1,2}$ in the presence of ASEP [14, 20] are correctly interpreted only if $\Delta_{1,2}$ are related to the variance in the number of carriers that entered up to time t into the system from a given cross-sectional area [20] and not to a diffusion constant.

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