Relationships among coefficients in deterministic and stochastic transient diffusion

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Systems are studied in which transport is possible due to large extensions with open boundaries in certain directions, but the particles responsible for transport can disappear from it by leaving it in other directions, by chemical reaction or by adsorption. The connection of the total escape rate, the rate of the disappearance, and the diffusion coefficient is investigated. It leads to the observation that the diffusion coefficient defined by $\langle x^2 \rangle$ is in general different from the one present in the effective Fokker-Planck equation. The result makes it possible to generalize the Gaspard-Nicolis formula [Phys. Rev. Lett. **65**, 1693 (1990)] to this transient case in deterministic systems. [S1063-651X(99)17005-3]

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I. INTRODUCTION

Randomness and diffusion are common features of extended stochastic and chaotic systems [1–9]. Among deterministic systems, diffusion has been much studied in the Lorentz gas [3,4]. As more simple models, proper one-dimensional (1D) maps [5–8] and a 2D map [9] have been introduced, which were built as chains of maps. Reference [10] showed a relationship between the diffusion coefficient and microscopic quantities, namely, the Liapunov exponent and the Kolmogorov-Sinai entropy referring to the repeller. This was later generalized to other transport coefficients [11] and the case of small external field [12]. The Liapunov exponent was independently calculated for the random Lorentz gas [13].

There are systems in which particles can escape in directions transversal to the extension of the system, raising interesting problems [14] in the field of transient chaos [15], in particular in the critical case [16,17]. A simple example is a channel in a mesoscopic system modeled by a strip of Lorentz gas with open side boundaries (see Fig. 1). Particles in such transiently chaotic or stochastic systems can diffuse in the extended direction or directions for some time, and then escape either through the ends in the extended direction (if the system is finite) or in the other directions or other ways. Therefore, the average period for which they take part in transport is finite, and remains finite even in the limit when the size of the system in the extended direction goes to infinity.

Another example with similar behavior is the Troll-Smilansky model for chaotic scattering, consisting of a 1D infinite periodic array of soft potential valleys, which is a system related to a model of ionization [18,19]. A further example is the motion in an infinite set of resonances in the phase space of Hamiltonian systems when one considers the particle to escape when it leaves the set of chosen resonances [20]. Diffusion has also been investigated on a chaotic saddle in a model for the interaction of a particle with an electrostatic wave packet [21]. In general, particles can also be lost from the point of view of diffusion by absorption or chemical reaction [22], or in other ways.

The aim of the present paper is to generalize the Gaspard-Nicolis formula [10] to the case of the above described transient diffusion in deterministic systems. For this purpose, we study how the total escape rate separates to terms related to the extended direction and the transversal direction. This investigation is made in a general way, leading to interesting results for both deterministic and stochastic systems.

II. DESCRIPTION OF THE SYSTEMS

For simplicity the system is assumed to possess one extended direction with a discrete translational symmetry, and, in most of the considerations here, an inversion symmetry that reverses the extended direction. For the sake of convenience the primitive cells with respect to the translational symmetry shall be labeled by a discrete variable x that is monotonic in the extended direction. The rest of the variables, specifying the state of the particle, shall be assembled in y. It may be helpful to describe the choice of x and y in the case of a strip of Lorentz gas. Here, as generally, it is easier to study the system in discrete instead of continuous time. Taking the union of the surfaces of the disks as a Poincaré surface, the state of the particles on it can be given by the coordinates x, q, α, and β. x is the ordered label of the primitive cells of the structure, and q is a label of the disk inside one primitive cell, as seen in Fig. 1. α is the angle of position on the disk, and β is the angle of reflection. Then y corresponds to the vector (q,α,β).

The general evolution equation for the probability distribution $\phi_t(x,y)$ of the particle can be written as a master equation

$$\phi_{t+1}(x,y)=\sum_{j=-J}^{J}\sum_{y'} w_{j,y,y'}\phi_t(x-j,y'), \tag{1}$$

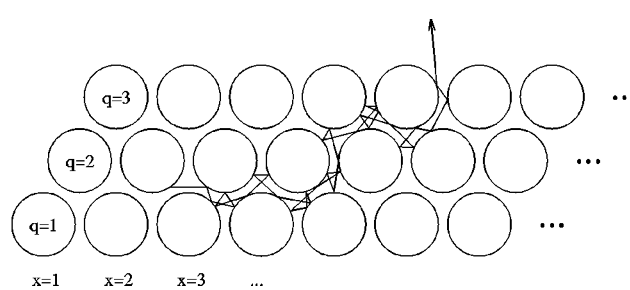

FIG. 1. Sketch of a strip of Lorentz gas.

where, if y contains continuous variables, one can consider the sums as integrals over the continuous components or one can use coarse graining with arbitrary precision. Here $\phi_t=0$ if the argument falls outside the region of the system. The maximal jump J can be assumed to be finite, or the transition probability $w_{j,y,y'}$ to decay quickly in j. The translational symmetry is implied in the form of Eq. (1), while an inversion symmetry can be written as $w_{j,y,y'}=w_{-j,Ty,Ty'}$, where $T^2y=y$ for every y.

Two representative classes of such systems can one keep in mind here. The first is a 2D random walk in a strip, for simplicity assuming no memory, for which

$$\phi_{t+1}(x,y)=\sum_{j=-J}^{J}\sum_{k=-K}^{K}W_{kj}\phi_t(x-j,y-k)\tag{2}$$

applies. This can be considered as a rough description of the Lorentz gas strip. The inversion symmetry can be a point inversion or a line inversion symmetry. 1D walks with memory are taken as a second group of examples. Then Eq. (1) can be used, conceiving y as the memory containing, say, n number of past steps $j_1,j_2,\dots,j_n$, and $w_{j_{n+1},y,y'}=P(j_{n+1}|j_n,j_{n-1},\dots,j_1)$ is the conditional probability of the next step. The inversion symmetry implies

$$P(j_{n+1}|j_n,j_{n-1},\dots,j_1)=P(-j_{n+1}|-j_n,-j_{n-1},\dots,-j_1).$$

The second model was chosen to study the effect of correlation between transitions, which is present in the Lorentz gas but neglected in the first model.

For general considerations we shall return to Eq. (1), taken without restriction to one dimension. For the diffusion process the long time behavior of the system is important. That is governed by the leading eigenvector ϕ of the right hand side of Eq. (1), which means $\phi_t\approx ce^{-\kappa t}\phi$ for large t, where κ is the escape rate. Being an eigenvector, ϕ satisfies the condition that, starting with $\phi_0=\phi$, Eq. (1) gives $\phi_1=e^{-\kappa}\phi$. ϕ shall be called the asymptotic distribution. The boundary of the system should also show the symmetry, so the region of the system should be defined by independent conditions in x and y ($x\in R_x$ and $y\in R_y$). If a particle from a point (x_0,y_0) jumps to a point (x,y), for that $y\notin R_y$, the particle shall be considered to escape in the y direction, while in case $y\in R_y$ but $x\notin R_x$ it escapes in the x direction. Corresponding escape rates κ_x and κ_y are defined in such a way that $e^{-\kappa_x}$ ($e^{-\kappa_y}$) is the probability of escape in the x (y) direction. The condition $y\in R_y$ in the definition of escape in the x direction ensures that $\kappa=\kappa_x+\kappa_y$.

III. SEPARABLE CASES

It is enlightening to study simple cases first. These are the cases in which the asymptotic distribution separates as a product $\phi(x,y)=\psi(x)\omega(y)$. This happens if the transition probability matrix can be written as a sum of dyadic products $w_{jyy'}=\Sigma_s u_j^{(s)}v_{yy'}^{(s)}$ (this may be a single product, as well), such that the following two conditions hold. First, the eigenvalue equations constructed from the u components of $w_{jyy'}$ have a common eigenvector, namely, $\Sigma_j u_j^{(s)}\psi(x-j)=\mu_s\psi(x)$. Second, for every s the eigenvalue μ_s is maximal among the eigenvalues of the latter eigenvalue equation. This property shall be denoted by S_x. It is easy to see that in this case the eigenvalue equation in the y direction, $\Sigma_{y's}v_{yy'}^{(s)}\mu_s\omega(y')=e^{-\kappa}\omega(y)$, determines ω and $e^{-\kappa}$. It is useful to show an example of this property from the class of 2D walks [Eq. (2)], when the condition for $w_{jyy'}$ is simplified as $W_{kj}=\Sigma_s V_k^{(s)}u_j^{(s)}$. The example is a walk on a square lattice $[1,L]\otimes[1,M]$ with transition probability matrix

$$\{W_{kj}\}_{-1,-1}^{1,1}=\begin{pmatrix}0&q&0\\0&r&0\\p&0&p\end{pmatrix}=\begin{pmatrix}q\\r\\0\end{pmatrix}\bigcirc(010)+\begin{pmatrix}0\\0\\p\end{pmatrix}\bigcirc(101),\tag{3}$$

where Eq. (3) also shows how W can be written in terms of dyadic products. The asymptotic distribution reads $\phi=\sin(\pi x/(L+1))2p/q\cos(\pi/(L+1))^{y/2}\sin(\pi y/(M+1))$.

Another possibility is when the eigenmode is common in y direction, i.e., $\Sigma_{y'}v_{yy'}^{(s)}\omega(y')=\nu_s\omega(y)$ (property S_y). Then $\Sigma_{js}u_j^{(s)}\nu_s\psi(x-j)=e^{-\kappa}\psi(x)$ determines ψ and $e^{-\kappa}$. When the properties S_x and S_y are both satisfied, then $e^{-\kappa}=\Sigma_s\mu_s\nu_s$.

One can obtain the asymptotic distribution on a large scale in the x direction in either of the above cases with a separable asymptotic distribution $\phi(x,y)=\psi(x)\omega(y)$. Starting with $\phi_0(x,y)=\phi(x,y)$, one should obtain $\phi_t(x,y)=\psi_t(x)\omega(y)$, where $\psi_t(x)=e^{-\kappa t}\psi(x)$. It is convenient to use the normalization $\Sigma_y\omega(y)=1$, since then $\psi_t(x)=\Sigma_y\phi_t(x,y)$. (Starting from here, $y,y'\in R_y$ is assumed). Using the latter equation and Eq. (1), one obtains

$$\psi_{t+1}(x)=\sum_j\tilde{w}_j\psi_t(x-j),\quad \tilde{w}_j\equiv\sum_{yy'}w_{j,y,y'}\omega(y').\tag{4}$$

It is obvious from Eqs. (4) that the probability that a particle at $x_0=x-j$ does not escape in the y direction in the next step is $e^{-\kappa_y}=\Sigma_j\tilde{w}_j\equiv\Sigma_{jyy'}w_{jyy'}\omega(y')$, which is independent of x_0. One can separate this escape with the substitution $\psi_t(x)=e^{-\kappa_y t}g_t(x)$, which yields $g_{t+1}(x)=\Sigma_j\tilde{w}_je^{\kappa_y}g_t(x-j)$. Since this equation describes a random walk, and the system is extended in the x direction, an effective Fokker-Planck equation $g_{t+1}(x)=g_t(x)+D_{\mathrm{FP}}g_t''(x)$ is valid on large scales. Returning to ψ, it takes the form

$$\psi_{t+1}(x)=\left(1+D_{\mathrm{FP}}\frac{d^2}{dx^2}\right)e^{-\kappa_y}\psi_t(x).\tag{5}$$

Its dominant solution in case of a channel of length L is

$$\psi_t(x)=e^{-\kappa t}\sin\left(\pi\frac{x}{L}\right),\tag{6}$$

and $\kappa=\pi^2D_{\mathrm{FP}}/L^2+\kappa_y+O(1/L^3)$, where the first and third term corresponds to κ_x.

Following Ref. [10] in the case of a deterministic process, the total escape rate can be related to the Liapunov exponents and the Kolmogorov-Sinai entropy of the repeller, namely, $\kappa=\Sigma_{\lambda_i>0}\lambda_i-h_{\rm KS}$ [23,24]. This yields a generalization of the Gaspard-Nicolis formula [10]

$$\sum_{\lambda_i>0}\lambda_i-h_{\rm KS}=\kappa=\frac{\pi^2 D_{\rm FP}}{L^2}+\kappa_y+O\left(\frac{1}{L^3}\right). \tag{7}$$

A further generalization and an alternative form shall be given at the end of Sec. IV.

Note that κ_y may also depend on L, as it does in case of example (3). This can be seen from the values of κ and κ_x, which can be found exactly for any L in this example:

$$e^{-\kappa}=4p\cos\frac{\pi}{L+1}\cos\frac{\pi}{M+1}+r\sqrt{\frac{2p}{q}\cos\frac{\pi}{L+1}}, \tag{8}$$

$$e^{-\kappa_x}=1-2p\left(1-\cos\frac{\pi}{L+1}\right). \tag{9}$$

IV. GENERAL CASES

The general case when $\phi(x,y)\neq\psi(x)\omega(y)$ is more complicated. As we shall see, the main point is that $\kappa_y(x)$, the local probability to escape in the y direction, becomes dependent on x. However, in the case when L, the length of the system in the x direction, is much larger than the size in the other directions, and there is an inversion symmetry, it shall be shown that, apart from the vicinity of the ends of the channel, the deviation of $\kappa_y(x)$ from a value $\kappa_y^{(\infty)}$ is proportional to $f''(x)/f(x)$. Here $f(x)$ is introduced analogously to $\psi(x)$ as $f(x)=\Sigma_y\phi(x,y)$ and $\kappa_y^{(\infty)}$ is the value of κ_y for the homogeneous solution in the case $L=\infty$. This makes it possible to write down a proper effective Fokker-Planck equation.

It is suitable to choose a segment I of the system separated by $x=x_1$ and $x=x_2$ planes, such that its size is still much larger than the transversal size, but much smaller than L. Such a segment ''feels'' values $f(x_1)$, and $f(x_2)$ of f at its ends with a common exponential decay $e^{-\kappa t}$. It is assumed that the diffusion in the system mixes the contribution of sites with different y coordinates. So systems are excluded in which the particles from one site cannot fill the whole system, and thereby different initial distributions can lead to different asymptotic states. With this assumption one can expect that the distribution inside the segment approaches an adiabatic distribution if $f(x)$ changes slowly in x. Then the transversal distribution $\phi(x,y)/f(x)$ also changes slowly. So this adiabatic distribution inside the segment is determined by the values $f(x_1)$ and $f(x_2)$ and the decay rate κ.

Thereby the distribution can have three free parameters. Since the evolution equation (1) is linear in the distribution, the asymptotic distributions ϕ and f can be assumed to have linear combination forms

$$\phi(x,y)=[\phi^{(\infty)}(x-x_0,y)+c_1\phi^{(1)}(x-x_0,y)+c_2\phi^{(2)}(x-x_0,y)]e^{-\kappa t}, \tag{10}$$

$$f(x)=[1+c_1f^{(1)}(x-x_0)+c_2f^{(2)}(x-x_0)]e^{-\kappa t}, \tag{11}$$

where $f^{(k)}(x)=\Sigma_y\phi^{(k)}(x,y)$ for $k=1$ and 2, and x_0 is the center of the segment. Here $\phi^{(\infty)}(x,y)$ is independent of x and equal to the asymptotic distribution in the limit $L\to\infty$. This is just the limit of $\omega(y)$. The corresponding escape rate shall be denoted by $\kappa_y^{(\infty)}$. $\phi^{(1)}$ is the asymptotic solution of Eq. (1) with antisymmetric boundary conditions $f(x_1)=-f(x_2)$. This term is responsible for current through the middle of the segment. Starting with a $\phi^{(\infty)}$ alone and symmetric boundary conditions $f(x_1)=f(x_2)=ae^{-\kappa t}$, one observes in general that ϕ in the middle decays faster or slower than on the boundary depending on the sign of $\kappa-\kappa_y^{(\infty)}$. In the asymptotic state this leads to a hump- or vale-shaped term $f^{(2)}$ in f, which corresponds to some $\phi^{(2)}$. The partial distributions can be approximated as $f^{(1)}(x-x_0)=x-x_0$ and $f^{(2)}(x-x_0)=(x-x_0)^2-b$ in the vicinity of the middle of the segment if $\phi^{(k)}$, $k=1$ and 2 are properly normalized. This means, that the general solution is

$$\begin{aligned}\phi(x,y)&=f(x_0)\phi^{(\infty)}(x-x_0,y)+f'(x_0)\phi^{(1)}(x-x_0,y)\\&\quad+\frac{f''(x_0)}{2}(\phi^{(2)}(x-x_0,y)+b\phi^{(\infty)}(x-x_0,y))\end{aligned} \tag{12}$$

in the vicinity of the point x_0. The local rate of escape $\kappa_y(x_0)$ in the y direction in the middle can be calculated as

$$1-e^{-\kappa_y(x_0)}=\frac{E(x_0)}{f(x_0)}, \tag{13}$$

$$E(x_0)=\sum_y\phi(x_0,y)-\sum_{jyy'}w_{jyy'}\phi(x_0,y'), \tag{14}$$

where $E(x_0)$ is the flow of escape in the y direction at x_0. Then, clearly,

$$E(x_0)=E_\infty f(x_0)+E_1f'(x_0)+\frac{E_2+bE_\infty}{2}f''(x_0), \tag{15}$$

where E_k, $k=\infty,1,2$ are constants characteristic of $\phi^{(k)}$, respectively. It can be shown that $E_1=0$. To see this one can separate Eq. (1) into terms related to a transition from the inside of the chosen segment and a transition from the outside. Conceiving $\phi_t(x,y)$ as a vector $\Phi=\{\Phi_i\}_i$, where any value of the index i corresponds to a point in (x,y) space inside the segment, and assuming the asymptotic state (i.e., $\phi_{t+1}=e^{-\kappa}\phi_t$), one obtains $e^{-\kappa}\Phi_i=\Sigma_j\tilde{w}_{ij}\Phi_j+\chi_i$. Here $\tilde{w}$ describes the transitions from inside, and χ the transitions from outside, and $\tilde{w}$ and χ can be constructed using w and values of ϕ outside but near the boundary of the segment. The solution for Φ is $\Phi=(e^{-\kappa}I-\tilde{w})^{-1}\chi$, where I is the unit matrix. The boundary conditions are antisymmetric for the symmetry transformation T in the state $\phi^{(1)}$; thereby χ is also antisymmetric. w and $\tilde{w}$ are symmetric for T. Consequently Φ corresponding $\phi^{(1)}$ and $\phi^{(1)}$ itself are antisymmetric. Therefore, Eq. (14) yields $E_1=0$. Using Eqs. (13) and (15) one obtains

$$\kappa_y(x) = \kappa_y^{(\infty)} + \eta \frac{f''(x)}{f(x)} + O\left(\frac{1}{L^3}\right), \tag{16}$$

with a suitable constant η, since for large L one expects $f'' = O(L^{-2})$. The above considerations are not valid near the ends of the channel where the middle of the segment cannot be placed. The interval of their validity shall be denoted by V. Then the analog of the effective Fokker-Planck equation (5) in V becomes of the form

$$f_{t+1}(x) = \left(1 + D_{\mathrm{FP}} \frac{d^2}{dx^2}\right) e^{-\kappa_y(x)} f_t(x), \tag{17}$$

or, with substitution of Eq. (16),

$$f_{t+1}(x) = e^{-\kappa_y^{(\infty)}} \left(1 + (D_{\mathrm{FP}} - \eta) \frac{d^2}{dx^2}\right) f_t(x) \tag{18}$$

in the interval V. It is plausible to assume that a distribution corresponding to Eq. (12) sets in earlier in time than the asymptotic state in the extended direction. After some time $f(x)$ is slowly varying in x. Then the considerations in this section are valid replacing κ in Eqs. (10) and (11) with the local decay rate $-\log(f_{t+1}(x)/f_t(x))$. So Eqs. (17) and (18) are also valid for general $f(x)$ distributions which are still not in the asymptotic state but which vary slowly in x. Equation (18) shall be applied later for such a case, but here the asymptotic distribution is important. It is given by

$$f_t(x) = e^{-\kappa t} \cos\left[\sigma\left(\frac{x}{L} - \frac{1}{2}\right)\right], \tag{19}$$

with $\kappa = \kappa_y^{(\infty)} - \log[1 - (D_{\mathrm{FP}} - \eta)\sigma^2/L^2]$, which is valid in V with a possible deviation outside V, such that $f_t(x)$ reaches zero at the ends of the full channel ($x=0$ and $x=L+1$). Thereby σ may slightly differ from π, and Eq. (19) may take a zero value at $\xi \equiv (1-\pi/\sigma)L/2 \neq 0$ and $L+1-\xi \neq L+1$. In the limit $L \to \infty$ the value of ξ becomes constant, since the neighborhood of the end of the channel that is outside V is bounded, and the distribution behaves in it in a well defined way (apart from normalization) in this limit. Therefore, $\sigma = \pi + O(L^{-1})$ and

$$\kappa = \kappa_y^{(\infty)} + \frac{\pi^2 (D_{\mathrm{FP}} - \eta)}{L^2} + O\left(\frac{1}{L^3}\right). \tag{20}$$

Using Eqs. (16) and (19), one can notice that $\kappa_y(x)$ is constant in V. However, the length of the regions outside V is bounded. (This is confirmed by the numerics; see Fig. 2 and Sec. V). Therefore, the value of $\kappa_y(x)$ in V is a typical value, which is

$$\breve{\kappa}_y = \kappa_y^{(\infty)} - \frac{\pi^2 \eta}{L^2} + O\left(\frac{1}{L^3}\right). \tag{21}$$

Note that all escape quantities depend on L except $\kappa_y^{(\infty)}$. From Eqs. (20) and (21) one obtains the relation of the escape rates to the diffusion coefficient

$$\kappa = \frac{\pi^2 D_{\mathrm{FP}}}{L^2} + \breve{\kappa}_y + O\left(\frac{1}{L^3}\right). \tag{22}$$

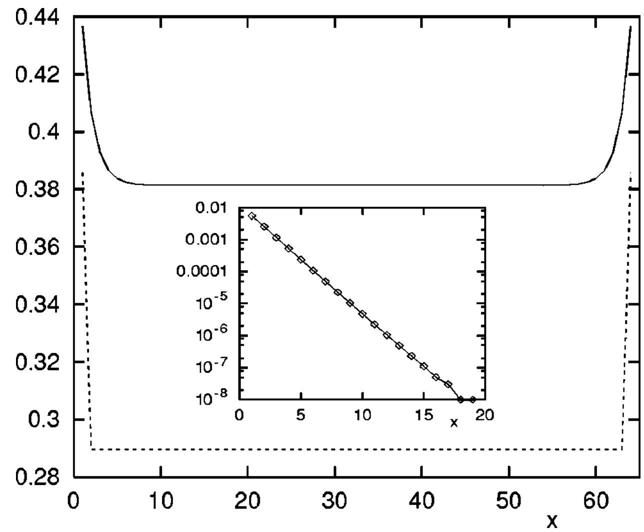

FIG. 2. Values of $\kappa_y(x)$ for models A (solid line) and B (dashed line) with $L=64$. The inset shows the decay of $\kappa_y(x) - \breve{\kappa}_y$ on a logarithmic scale for model A.

Equations (20) and (21) [and thereby Eq. (22)] have been verified numerically; the results are seen in Fig. 3 and explained in Sec. V.

By the same arguments as those above Eq. (7), the latter equation yields the main result of this paper, a further generalization of the Gaspard-Nicolis formula [10]

$$\sum_{\lambda_i > 0} \lambda_i - h_{\mathrm{KS}} = \kappa = \frac{\pi^2 D_{\mathrm{FP}}}{L^2} + \breve{\kappa}_y + O\left(\frac{1}{L^3}\right). \tag{23}$$

Part of Eq. (23) can also be used in the case of stochastic diffusion. Then the right hand side determines how κ separates to a term related to diffusion in the x direction and another term related to the transversal escape.

Comparing with the original Gaspard-Nicolis formula [10], we can see that the transversal escape (or other way of

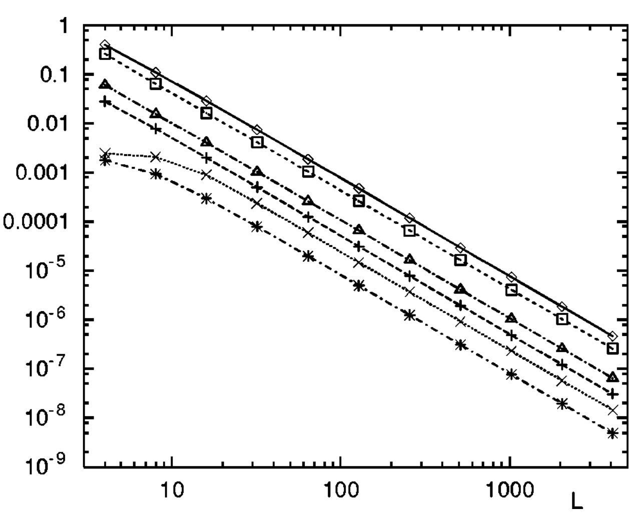

FIG. 3. Test of the L^{-2} decay of escape quantities on a log-log scale. For model A, $+$: $(\kappa - \kappa_y^{(\infty)})/4$; $\times$: $\breve{\kappa}_y - \kappa_y^{(\infty)}$; $*$: $\kappa_y - \kappa_y^{(\infty)}$. For model B, $\diamond$: $2(\kappa - \kappa_y^{(\infty)})$; $\square$: $\breve{\kappa}_y - \kappa_y^{(\infty)}$; $\triangle$: $\kappa_y - \kappa_y^{(\infty)}$. Integer multipliers are used in two cases, when the values are close (but not equal) to other values (namely, to $\breve{\kappa}_y - \kappa_y^{(\infty)}$ for model B).

disappearance of the particles) adds a new term to it. However, this term is in general not the global escape rate (contrary to the separable cases), but a typical value of the x-dependent rate of escape in the y direction. That is an important fact, since the deviation of $\breve{\kappa}_y$ from the corresponding global escape rate κ_y is of the order L^{-2}, which is comparable to the first term on the right hand side of Eq. (23). The difference $\breve{\kappa}_y-\kappa_y$ can be estimated knowing that it comes from the contribution of the end regions to the global escape. Since the asymptotic distribution (19) after normalization has a slope $O(L^{-2})$ at the end regions, these regions give an $O(L^{-2})$ contribution to κ_y. Thereby the above mentioned differences are proportional to L^{-2}, and κ_y shows an L^{-2} decay to $\kappa_y^{(\infty)}$, similarly to Eq. (21), as is confirmed by the numerical tests. Consequently, $\pi^2 D_{\mathrm{FP}}/L^2$ does not correspond to κ_x in general.

One more important question is whether D_{FP} defined as the coefficient in Eq. (17) is equal to the one defined by the mean square deviation of x as $\int f_t(x)(x-x_0)^2 dx/\int f_t(x)dx \propto 2D_{\mathrm{msd}}t$, starting from a state concentrated in a vicinity of x_0. Introducing $g_t(x)=e^{\kappa_y^{(\infty)}t}f_t(x)$ in Eq. (18), one can eliminate the factor containing $\kappa_y^{(\infty)}$. Then the equation becomes an evolution equation of a diffusion process whose diffusion coefficient

$$D_{\mathrm{msd}}=D_{\mathrm{FP}}-\eta \tag{24}$$

is clearly equal to the diffusion coefficient defined for $f_t(x)$ by mean square deviation. So we can see D_{FP} and D_{msd} are in general different.

Using Eqs. (21) and (24), one can obtain another form of Eq. (23) in which D_{msd} and $\kappa_y^{(\infty)}$ are present instead of D_{FP} and $\breve{\kappa}_y$:

$$\sum_{\lambda_i>0}\lambda_i-h_{\mathrm{KS}}=\kappa=\frac{\pi^2 D_{\mathrm{msd}}}{L^2}+\kappa_y^{(\infty)}+O\left(\frac{1}{L^3}\right), \tag{25}$$

for which the comments below Eq. (23) apply analogously.

V. NUMERICAL RESULTS

Numerical calculations have been made to test the validity of Eqs. (17)–(24) in two concrete models. Model A is a 2D random walk on a square lattice $[1,L]\otimes[1,M]$, with

$$\{W_{kj}\}_{-1,-1}^{1,1}=\begin{pmatrix} 0 & 0 & p \\ q & r & q \\ p & 0 & 0 \end{pmatrix}. \tag{26}$$

The numerical parameters are $p=0.1$, $q=0.2$, $r=0.4$, and $M=4$, and L has run over integer powers of 2 from 4 up to 4096.

Model B is a 1D random walk with two step memory such that $P(j_{t+1}|j_t,j_{t-1})=R_{j_t j_{t-1}}Q_{j_{t+1}j_t}$, $R_{+1}=0.45$, $R_{-1}=0.9$, $Q_{+1}=\frac{4}{9}$, and $Q_{-1}=\frac{5}{9}$. To ensure symmetry, Q and R depend only on the product in their subscript. $Q_{+1}+Q_{-1}=1$; therefore, R describes the probability that the particle does not escape in the y direction, and Q describes the relative probability of the steps j_{t+1}. A possibility was given to rest for one step with a probability $g=0.01$ without changing j_t, j_{t-1}. L was also chosen to be a power of 2 from 4 until 4096.

In both models $\kappa_y(x)$ has been found to be constant in a middle region V (see Fig. 2). In the case of model A $\kappa_y(x)$ has been found to decay exponentially to $\breve{\kappa}_y$, reaching the middle region from either side, with an exponent approximately independent of L. In case of model B $\kappa_y(x)$ is constant for $x=2,3,\ldots,L-1$, and has different values only at the endpoints. These support the statement, that the irregular regions outside V are of bounded length with any choice of the precision demanded for the equations in region V.

For both models Fig. 3 shows that κ, $\breve{\kappa}_y$, and κ_y follow the L^{-2} decay according to Eqs. (20) and (21) and the remark below Eq. (23). $D_{\mathrm{msd}}=D_{\mathrm{FP}}-\eta$, η and D_{FP} have been calculated from them. Four-digit precision has already been reached using results for $L=512$ and 1024. This has been improved up to 6 digits fitting a fourth order polynomial of L^{-1} to values for $L=128,\ldots,2048$. The results, in model A—$D_{\mathrm{msd}}=0.207942$, $\eta=0.024545$, and $D_{\mathrm{FP}}=0.232487$—and in model B—$D_{\mathrm{msd}}=0.197183$, $\eta=0.219092$, and $D_{\mathrm{FP}}=0.416275$—agree with the following independent calculations of D_{msd} and D_{FP}. In both models D_{msd} has been determined with five-digit precision measuring $\langle(x-x_0)^2\rangle$ for a well concentrated initial distribution. In the case of model B, D_{FP} has also been calculated by using $i(x)=D_{\mathrm{FP}}(f(x)-f(x+1))e^{-\kappa_y(x)}$, where $i(x)$ is the current between sites at x and $x+1$. Its result matches the above result up to six digits.

VI. SUMMARY

Systems have been studied that are extended in one direction (or more), such that diffusion is possible. If the system is large and finite, particles escape at the ends. In addition to this escape there is another way of disappearance: escape in the transversal direction or disappearance by adsorption or chemical reaction. It was shown that this additional disappearance of particles adds a nontrivial term to the Gaspard-Nicolis formula. This term is in general not a global transversal escape rate, but a typical value of the local escape rate. Also, due to the additional disappearance, the two diffusion coefficients (the one arising in the effective Fokker-Planck equation and the one defined by mean square deviation) are in general different. These effects occur not only in chaotic diffusion, when the Gaspard-Nicolis formula can be used, but also in stochastic diffusion. In the latter case one part of formulas (23) and (25) can be used to relate κ to the diffusion coefficients.

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[1] H. Haken, *Synergetics* (Springer-Verlag, Berlin, 1978).
[2] A. J. Lichtenberg and M. A. Lieberman, *Regular and Stochastic Motion* (Springer-Verlag, Berlin, 1983).
[3] L.A. Bunimovich and Ya. G. Sinai, Commun. Math. Phys. **78**, 247 (1980); **78**, 479 (1980).
[4] J. Machta and R. Zwanzig, Phys. Rev. Lett. **50**, 1959 (1983).
[5] T. Geisel and J. Nierwetberg, Phys. Rev. Lett. **48**, 7 (1982); T. Geisel and J. Nierwetberg, Z. Phys. B **56**, 59 (1984).
[6] M. Schell, S. Fraser, and R. Kapral, Phys. Rev. A **26**, 504 (1982).
[7] S. Grossmann and H. Fujisaka, Phys. Rev. A **26**, 1779 (1982).
[8] R. Klages and J. R. Dorfman, Phys. Rev. Lett. **74**, 387 (1995).
[9] P. Gaspard, J. Stat. Phys. **68**, 673 (1992).
[10] P. Gaspard and G. Nicolis, Phys. Rev. Lett. **65**, 1693 (1990).
[11] J. R. Dorfman and P. Gaspard, Phys. Rev. E **51**, 28 (1995).
[12] T. Tél, J. Vollmer, and W. Breymann, Europhys. Lett. **35**, 659 (1996).
[13] H. van Beijeren, and J. R. Dorfman, Phys. Rev. Lett. **74**, 4412 (1995).
[14] Z. Kaufmann, H. Lustfeld, A. Németh, and P. Szépfalusy, Phys. Rev. Lett. **78**, 4031 (1997).
[15] T. Tél, in *STATPHYS 19*, Proceedings of the 19th IUPAP Conference on Statistical Physics, edited by Hao Bai-Lin (World Scientific, Singapore, 1996), pp. 346–362.
[16] A. Németh and P. Szépfalusy, Phys. Rev. E **52**, 1544 (1995).
[17] H. Lustfeld and P. Szépfalusy, Phys. Rev. E **53**, 5882 (1996).
[18] G. Troll and U. Smilansky, Physica D **35**, 34 (1989).
[19] Y. C. Lai and C. Grebogi, Phys. Rev. E **49**, 3761 (1994).
[20] I. Dana, Phys. Rev. Lett. **64**, 2339 (1990).
[21] I. Dana and T. Kalisky, Phys. Rev. E **53**, R2025 (1996).
[22] *Nonequilibrium Statistical Mechanics in One Dimension*, edited by V. Privman (Cambridge University Press, Cambridge, 1997).
[23] J.-P. Eckmann and D. Ruelle, Rev. Mod. Phys. **57**, 617 (1985).
[24] H. Kantz and P. Grassberger, Physica D **17**, 75 (1985).