General technique of calculating the drift velocity and diffusion coefficient in arbitrary periodic systems

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Abstract. We develop a practical method of computing the stationary drift velocity V and the diffusion coefficient D of a particle (or a few particles) in a periodic system with arbitrary transition rates. We solve this problem in a physically relevant continuous-time approach as well as for models with discrete-time kinetics, which are often used in computer simulations. We show that both approaches yield the same value of the drift, but the difference between the diffusion coefficients obtained in each of them equals $\frac{1}{2}V^2$. Generalization to spaces of arbitrary dimension and several applications of the method are also presented.

1. Introduction

Investigation of diffusive transport is of the highest importance in many areas of physics and related sciences. The most fundamental characteristics of diffusion is provided by two quantities—the diffusion coefficient D and the drift velocity V. Knowledge of the latter is especially important in studies of non-equilibrium phenomena, where usually $V \neq 0$. This includes, among others, diffusion in disordered media subject to an external field [1–7] or the so-called molecular 'pumps' and 'motors' [8–10], responsible for transport of various chemicals in biological cells. However, no universal *and* practical theoretical method of determining V and D for arbitrary systems has been developed, and although many solutions for some particular physical models have been proposed, in more complicated cases one often has to resort to approximations or numerical methods.

The first attempt, to our knowledge, towards determining V and D in an arbitrary system was made by Derrida [11], who considered a one-dimensional, periodic lattice of a period L and arbitrary hopping rates between nearest-neighbour sites. He managed to give exact expressions for the velocity and the diffusion constant as functions of the hopping rates. He then extended his method [12] to a periodic d-dimensional system, but his solution turns out to be rather complicated. An alternative method of calculating V was also developed by Kehr *et al* [5]. Of the two quantities V and D, the latter is, of course, much harder to find. A surprisingly simple formula for one-dimensional systems with transition rates satisfying the

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detailed balance condition was derived by Lyo and Richards [13], and recently independently reinvented by Kutner [14] and Wichmann [15],

$$D = \left(\frac{1}{L^2} \sum_{j=0}^{L-1} \frac{1}{P_j^{\text{eq}} \Gamma_j^{\rightarrow}} \right)^{-1} \tag{1}$$

where L is the period of the lattice, P_j^{eq} denote the equilibrium site occupancy probabilities, and $\Gamma_j^{\rightarrow}$ are the transition rates from site j to $j + 1$. However, this equation is valid only when the random walker hops between nearest-neighbour sites. A method of determining D in arbitrary periodic systems satisfying the detailed balance condition was then proposed by Braun and Sholl [16]. Description of several other techniques, developed for some special types of random environments, can be found in review articles [1–4, 17].

All the above-mentioned methods are based on the following scheme:

(1) Reduce the infinite system to a single elementary cell with periodic boundary conditions.
(2) Write down the master equation.
(3) Using it calculate the steady-state properties of this system; in particular, find the steady-state site occupation probabilities [11, 12, 14–16] or propagators [18].
(4) Given these quantities, find V and D.

The third step is critical and can be carried out explicitly only for relatively small systems or for models possessing some special properties, e.g. one-dimensional lattices with jumps restricted to the nearest-neighbour sites. The main goal of this paper is to develop a simple and, at the same time, general method of calculating V and D explicitly without performing detailed analysis of the steady state. In our approach the third step reads as follows:

(3′) Find the matrix $\Lambda(k)$ representing the Fourier transform of the master equation;

which is a rather straightforward operation. The technique we propose is valid for both equilibrium and non-equilibrium systems. It can also be quite easily implemented in computer-algebra or numerical programming languages.

Following the first step, our considerations will be restricted to periodic systems, such as crystals or molecular motors. A general problem of diffusion in an arbitrary disordered system remains an open question. One might be tempted to treat it by taking the limit $L \to \infty$. This method can sometimes provide a hint about the anomalous type of diffusion in a given aperiodic system [17]. However, except for some simple models [2, 19], it has not been established whether the limits $t \to \infty$ and $L \to \infty$ commute and, thus, whether this approach is generally correct.

We will pay special attention to a one-dimensional system of finite period L with arbitrary jump rates between any of its sites whose distance is less than L. This is perhaps the simplest model of a periodic system where all elements of the transition rate matrix can take on nonzero values. Its investigation can be therefore carried out with relatively simple mathematical formalism. A solution to a general, multi-particle and multi-dimensional problem requires the same mathematical methods, but the notation would have to be complex. What is even more important, any periodic system with a finite number of sites in its elementary cell can be mapped on such a one-dimensional system; the geometry of the original problem is relevant mainly in constructing the matrix $\Lambda(k)$ and can be taken into account quite easily. Once the explicit form of $\Lambda(k)$ has been found, one can compute V and D using the methods we derive here for this simple one-dimensional system.

In our calculations we will use both continuous-time and discrete-time formalisms. One could expect that since we calculate V and D in a stationary state, where all quantities are independent of time, both approaches should yield the same result. However, as was found

by Derrida [11], the form of the diffusion coefficient as a function of the transition rates can depend on whether time flows continuously, or not. This is an important issue, since using discrete-time models belongs to the favourite techniques of computer physics (in particular, cellular-automata [20] and exact-enumeration [3] methods), and one needs to know whether results obtained in this way are correct. Derrida [11] showed that in his (grossly simplified) model the relation between the diffusion constants obtained in the continuous-time (D) and discrete-time (D^D) formalisms reads $D - D^D = \frac{1}{2}V^2$. We will show that this relation is general and will prove it for any periodic system with arbitrary transition rates.

The paper is organized as follows. Using the Fourier transform of the master equation, see [1, 17, 21], in section 2 we analyse a one-dimensional system with arbitrary period L and transition rates Γ_{jl}. We find a simple technique of calculating V and D in terms of the three lowest coefficients of the characteristic polynomial of the Fourier-transformed transfer matrix, $\Lambda(k)$. The most important properties of its spectrum at $k = 0$ have been already described in [21, 22], but only for systems obeying the detailed balance condition. Therefore, in sections 2.1 and 2.2 we analyse in detail the spectrum of $\Lambda(k)$ in a general case, assuming that the time is a continuous or a discrete quantity, respectively. Then, in section 2.3, we compare the two approaches and explain the different forms of diffusion coefficients derived in each of them. In section 3 we generalize our approach to systems in arbitrary space dimension, and in section 4 we present a particularly simple method of calculating V and D for one-dimensional systems with transitions between the nearest-neighbour sites. In section 5 we derive explicit forms of V and D in some commonly used models. In particular, one of the examples studied there explains how to apply our technique to many-body problems. Finally, section 6 is devoted to conclusions.

2. General case of a periodic one-dimensional system

2.1. Continuous-time formalism

Consider a one-dimensional lattice with its sites located at x_n, $n \in \mathcal{N}$. At time $t = 0$ we put a particle at site $x_0 = 0$. The particle can then jump between the lattice sites. Transitions are assumed to represent a continuous (e.g. Poisson) Markov process in time. The (constant in time) transition rate from a site x_n to a site x_m will be denoted by Γ_{mn}. We assume that the system is periodic in space and denote its period by $L \geqslant 1$,

$$\forall_{n,m} \Gamma_{mn} = \Gamma_{m+L,n+L} \qquad x_m - x_n = x_{m+L} - x_{n+L}. \tag{2}$$

Of course transition rates between two different sites cannot be negative; $\Gamma_{mn} \geqslant 0$ if $m \neq n$. For simplicity we also restrict our considerations to the case where direct transitions between sites m and n are allowed only if $|m - n| < L$.

Let $P(n, t)$ denote the probability density of finding the particle at site x_n at time t. The evolution of this quantity is governed by the master equation

$$\frac{\partial P(n, t)}{\partial t} = \sum_m [\Gamma_{nm} P(m, t) - \Gamma_{mn} P(n, t)] \tag{3}$$

and the initial condition reads

$$P(n, 0) = \delta_{n,0}. \tag{4}$$

We can now treat the whole lattice as if it consisted of L sublattices and define the probability densities $P_l(j, t)$ of finding a particle at a given sublattice l at site n at time t as

$$P_l(n, t) \equiv P(n, t)\delta_{n,l}^L \tag{5}$$

where $\delta_{n,l}^L$ is a generalized Kronecker delta, $\delta_{n,l}^L = 1$ if $n = l \pmod L$ and $\delta_{n,l}^L = 0$ otherwise. We can now rewrite (3) as a system of L linear differential equations for $P_l(n, t)$, $l = 0, \ldots, L - 1$,

$$\frac{\partial P_l(n, t)}{\partial t} = \sum_{j=1-L}^{L-1} [\Gamma_{l,l+j} P_{l+j}(n + j, t) - \Gamma_{l+j,l} P_l(n, t)]. \tag{6}$$

The major advantage of (6) as compared with (3) is that its coefficients do not depend on n. Therefore, we can calculate its Fourier transform as

$$\frac{\partial \tilde{P}_l(k, t)}{\partial t} = \sum_{j=1-L}^{L-1} [\Gamma_{l,l+j} e^{ik(x_{l+j} - x_l)} \tilde{P}_{l+j}(k, t) - \Gamma_{l+j,l} \tilde{P}_l(k, t)] \tag{7}$$

where $\tilde{P}_l(k, t) \equiv \sum_n \exp(-ikx_n) P_l(n, t)$.

The system of equations (7) can be written in a compact form using an $L \times L$ matrix $\Lambda_{lj}(k)$,

$$\frac{\partial \tilde{P}_l(k, t)}{\partial t} = \sum_{j=0}^{L-1} \Lambda_{lj}(k) \tilde{P}_j(k, t) \tag{8}$$

where

$$\Lambda_{lj}(k) \equiv \begin{cases} \Gamma_{lj} e^{ik(x_j - x_l)} + \Gamma_{l,j+L} e^{ik(x_{j+L} - x_l)} & j < l \\ \Gamma_{lj} e^{ik(x_j - x_l)} + \Gamma_{l,j-L} e^{ik(x_{j-L} - x_l)} & j > l \\ -\sum_{m \neq l} \Gamma_{ml} & j = l. \end{cases} \tag{9}$$

We will impose only one restriction on the form of transition rates Γ_{lj}. We will demand that $\Lambda(0)$ be irreducible (by a permutation of indices) [23, 24]; i.e., in the stationary state the particle can be found at any of the sublattices defined in (5) with a probability >0. Physically, this condition means that in the long-time limit the system does not split up into several non-interacting subsystems. Mathematically, irreducibility means that $\Lambda(0)$ has exactly one eigenvector whose all components are strictly positive. Our approach is thus quite general— we do not require that the transition rates should satisfy the detailed balance condition, the Fourier-transformed transition rate matrix, $\Lambda(k)$, need not be symmetric or even diagonalizable at $k = 0$, and some of its eigenvalues can be complex.

A general solution to (8) reads [25]

$$\tilde{P}_l(k, t) = \sum_{j=0}^{L-1} T_{lj}(k, t) \exp[\lambda_j(k)t] \qquad l = 0, \ldots, L - 1 \tag{10}$$

where the coefficients $T_{lj}(k, t)$ are polynomials in t and can be determined using the initial condition. The degree of $T_{lj}(k, t)$ is smaller than the multiplicity of $\lambda_j(k)$. We assume that the eigenvalues $\lambda_j(k)$ are ordered in accordance with the descending magnitude of their real parts at $k = 0$; i.e., $j < l \Rightarrow \text{Re}(\lambda_j(0)) \geqslant \text{Re}(\lambda_l(0))$. Since $P(n, t) = \sum_{l=0}^{L-1} P_l(n, t)$, there is $\tilde{P}(k, t) = \sum_{l=0}^{L-1} \tilde{P}_l(k, t)$, and so (10) yields

$$\tilde{P}(k, t) = \sum_{l=0}^{L-1} h_l(k, t) \exp[\lambda_l(k)t] \tag{11}$$

where $h_l(k, t) \equiv \sum_{j=0}^{L-1} T_{jl}(k, t)$ are polynomials in t (actually $h_l(k, t)$ can depend on time only if $\lambda_l(k)$ is degenerated).

In a one-dimensional system the stationary drift velocity V and the diffusion coefficient D are given by

$$V = \lim_{t\to\infty} \frac{\langle x \rangle}{t}$$

$$= \lim_{t\to\infty} i\frac{\frac{\partial \tilde{P}(k,t)}{\partial k}|_{k=0}}{t} \qquad (12)$$

$$D = \lim_{t\to\infty} \frac{\langle x^2 \rangle - \langle x \rangle^2}{2t}$$

$$= \lim_{t\to\infty} \frac{-\frac{\partial^2 \tilde{P}(k,t)}{\partial k^2}|_{k=0} + (\frac{\partial \tilde{P}(k,t)}{\partial k}|_{k=0})^2}{2t} \qquad (13)$$

where $\langle f(x) \rangle \equiv \int f(x) P(x,t)\,dx$. Thus, if we could calculate the eigenvalues of $\Lambda(k)$, we would be able, in principle, to calculate V and D. The diagonalization of $\Lambda(k)$, however, is a formidable task feasible only in some special cases (e.g. for small L or when special relations have been imposed on its elements). Fortunately, as we will see below, if our aim is restricted only to determining V and D as functions of the transition rates Γ_{lj}, we need not calculate explicitly even a single eigenvalue of the transition rate matrix!

Let μ be a constant such that $\forall_j \mu > |\Lambda_{jj}(0)|$ and let Q denote an auxiliary matrix, $Q_{jl} \equiv \Lambda_{jl}(0) + \mu\delta_{jl}$. Since $\Lambda(0)$ is irreducible, so is Q. Moreover, because all elements of Q are non-negative, we can apply to it the Frobenius theorem [23, 24] and conclude that Q has a positive eigenvalue q, which is a simple root of the characteristic equation, and the moduli of all other eigenvalues are at most q. Because the dominant eigenvalue of an irreducible, non-negative matrix lies between the largest and smallest column sums [23, 24], and in our case these sums are all equal to μ, we find that the dominant eigenvalue $q = \mu$. Since the spectrum of Q is shifted, with respect to the spectrum of $\Lambda(0)$, by μ, we conclude that for $k = 0$ the matrix $\Lambda(k)$ has exactly one dominating eigenvalue $\lambda_0(0) = 0$ and the real parts of all other eigenvalues are negative,

$$\lambda_0(0) = 0 > \text{Re}\,(\lambda_1(0)) \geqslant \cdots \geqslant \text{Re}\,(\lambda_{L-1}(0)). \qquad (14)$$

Thus, in the limit $t \to \infty$ this single eigenvalue dominates the sum in the rhs of (10) at $k \approx 0$. In determining the forms of V and D we can therefore employ a simple approximation

$$\tilde{P}(k,t) = h_0(k,t)\exp[\lambda_0(k)t]. \qquad (15)$$

Moreover, since $\sum_n P(n,t) = 1$, there is

$$\forall_{t\geqslant 0} \tilde{P}(0,t) = 1 \qquad (16)$$

which, owing to (14), implies

$$h_0(0,t) = 1. \qquad (17)$$

Upon inserting (15) into (12), (13) and using (14), (17) we conclude that

$$V = i\frac{\partial \lambda_0}{\partial k}\bigg|_{k=0} \qquad (18)$$

$$D = -\frac{1}{2}\frac{\partial^2 \lambda_0}{\partial k^2}\bigg|_{k=0}. \qquad (19)$$

Let $W(x)$ denote the characteristic polynomial of the matrix $\Lambda(k)$. Let $c_i(k)$ denote its coefficients at x^j, $j = 0, \ldots, L$. We thus have

$$\forall_k W(\lambda_0(k)) = \sum_{j=0}^{L} c_j(k)[\lambda_0(k)]^j = 0. \qquad (20)$$

On differentiating it with respect to k and using the first part of (14) we arrive at

$$\left.\frac{\partial \lambda_0}{\partial k}\right|_{k=0} = -\frac{c_0'}{c_1} \tag{21}$$

where we used a shorthand notation $c_j \equiv c_j(0)$ and $c_j' \equiv \partial c_j/\partial k|_{k=0}$. Note that $c_1 \neq 0$, which follows from (14). Differentiating (20) twice yields

$$\left.\frac{\partial^2 \lambda_0}{\partial k^2}\right|_{k=0} = -\frac{c_0'' + 2c_2(\lambda_0')^2 + 2c_1'\lambda_0'}{c_1} \tag{22}$$

where $\lambda_0' \equiv \partial \lambda_0(k)/\partial k|_{k=0}$ and $c_0'' \equiv \partial^2 c_0/\partial k^2|_{k=0}$. We thus finally arrive at our major result

$$V = -i\frac{c_0'}{c_1} \tag{23}$$

$$D = \frac{c_0'' - 2c_2 V^2 - 2ic_1' V}{2c_1}. \tag{24}$$

Functions $c_j(k)$ can depend on k and the transition rates in a very complicated way. We were able to find only two general properties, both following immediately from (14): $c_0 = 0$ and $c_1 \neq 0$. Explicit forms of c_0', c_0'', c_1, c_1' and c_2 for some particular models will be given below, in sections 4 and 5.

2.2. Discrete-time formalism

The discrete-time formulation of the problem is basically similar to the continuous one, but there are some major differences, too. For simplicity we will use the same notation as in the previous section, but one should remember that almost all functions employed in the discrete-time formulation of the problem differ from those we dealt with in section 2.1. Where it will be necessary to compare quantities computed within each approach, we will attach a superscript 'D' to the quantity derived in the discrete-time formalism.

In the discrete-time version of the problem the master equation (expressed in terms of the probabilities $P_l(n, t)$ of finding a particle at time t at a site x_n belonging to a sublattice l) reads

$$P_l(n, t+1) = P_l(n, t) + \sum_{j=1-L}^{L-1} [\Gamma_{l,l+j} P_{l+j}(n+j, t) - \Gamma_{l+j,l} P_l(n, t)] \tag{25}$$

where $l = 0, \ldots, L-1$, and Γ_{lj} are dimensionless probabilities satisfying the usual condition $\forall_{lj}\ 0 \leqslant \Gamma_{jl} \leqslant 1$. Note that in the continuous formulation of the problem Γ_{jl} were unbounded from above, dimensional quantities (of dimension $[T^{-1}]$) and we called them 'transition rates'. Last, but not least, in the present approach time t assumes only integer values.

Upon taking the Fourier transform of (25) we arrive at

$$\tilde{P}_l(k, t+1) = \tilde{P}_l(k, t) + \sum_{j=1-L}^{L-1} [\Gamma_{l,l+j} e^{ik(x_{l+j}-x_l)} \tilde{P}_{l+j}(k, t) - \Gamma_{l+j,l}\tilde{P}_l(k, t)] \tag{26}$$

which can be rewritten using a stochastic matrix $\Lambda_{lj}^{\mathrm{D}}(k)$

$$\tilde{P}_l(k, t+1) = \sum_{j=0}^{L-1} \Lambda_{lj}^{\mathrm{D}}(k) \tilde{P}_j(k, t) \tag{27}$$

where the only difference between Λ^{D} and its continuous-time counterpart Λ lies in their diagonal elements

$$\Lambda_{lj}^{\mathrm{D}}(k) = \Lambda_{lj}(k) + \delta_{lj}. \tag{28}$$

Therefore, the eigenvalues λ_l^{D} of Λ^{D} are related to the eigenvalues λ_l of Λ through a simple formula

$$\lambda_l^{\mathrm{D}}(k) = \lambda_l(k) + 1 \qquad l = 0, \ldots, L-1. \tag{29}$$

Applying the theorem of Frobenius [23,24] to $\Lambda^{\mathrm{D}}(0)$, which is a real, non-negative matrix, we conclude that

$$\lambda_0^{\mathrm{D}}(0) = 1 \tag{30}$$

and the moduli of all other eigenvalues do not exceed one. However, in contrast to the continuous-time formalism, now there can be $s \geqslant 1$ eigenvalues, say $\lambda_{j_m}^{\mathrm{D}}(k), m = 0, \ldots, s-1$, such that $|\lambda_{j_m}^{\mathrm{D}}(0)| = 1$; for convenience we assume that $\lambda_{j_0}^{\mathrm{D}} \equiv \lambda_0^{\mathrm{D}}$. Although this can happen only if all diagonal elements of $\Lambda^{\mathrm{D}}(0)$ vanish [23,24], we do not exclude this exceptional case from our considerations [11]. The Frobenius theorem ensures us that all these dominating eigenvalues are distinct, and so in the normal Jordan representation of $\Lambda^{\mathrm{D}}(k)$ the size of the corresponding Jordan blocks is one. This suffices to assert that for $k \approx 0$ and $t \to \infty$

$$\tilde{P}(k, t) = \sum_{m=0}^{s-1} h_m(k)[\lambda_m^{\mathrm{D}}(k)]^t \tag{31}$$

where h_m are some functions of k.

Because equation (16) is valid both in continuous-time and discrete-time formalisms, upon comparing it with (31) we conclude that except for $h_0(k)$ all other coefficients $h_m(k)$ in (31) must vanish at $k = 0$,

$$h_0(0) = 1 \qquad h_m(0) = 0 \qquad m = 1, \ldots, s-1. \tag{32}$$

Actually, since t is an integer, this is not a trivial statement; a proof is based on the fact that all dominant eigenvalues λ_m^{D} are distinct roots of the equation $x^s = 1$, see [23,24]. Upon inserting (31) into (12) and (13) and then using (30) and (32) we arrive at

$$V^{\mathrm{D}} = \mathrm{i} \frac{\partial \lambda_0^{\mathrm{D}}(k)}{\partial k} \Bigg|_{k=0} \tag{33}$$

$$D^{\mathrm{D}} = -\frac{1}{2} \left[\frac{\partial^2 \lambda_0^{\mathrm{D}}(k)}{\partial k^2} - \left(\frac{\partial \lambda_0^{\mathrm{D}}(k)}{\partial k} \right)^2 \right] \Bigg|_{k=0} - \Psi(0, t) \tag{34}$$

where

$$\Psi(k, t) \equiv \sum_{m=1}^{s-1} \frac{\partial h_m}{\partial k} \left(\frac{\partial \lambda_m^{\mathrm{D}}}{\partial k} - \frac{\partial \lambda_0^{\mathrm{D}}}{\partial k} \lambda_m^{\mathrm{D}} \right) (\lambda_m^{\mathrm{D}})^{t-1}. \tag{35}$$

Note that, by definition, $\Psi(k, t) \equiv 0$ if $s = 1$, i.e., if $\lambda_0^{\mathrm{D}}(0)$ is the only dominating eigenvalue of the transition matrix $\Lambda(0)$. Moreover, because the existence of the diffusion constant is guaranteed by the central limit theorem, $\Psi(0, t)$ must be independent of time, at least in the limit $t \to \infty$, for any s. This, in turn, requires that even if $s > 1$

$$\Psi(0, t) = 0 \tag{36}$$

(see the comment under equation (32)). Therefore, to determine V and D one needs only to investigate the properties of a single eigenvalue $\lambda_0^{\mathrm{D}}(0)$ at $k \approx 0$, i.e. equation (31) can be replaced with

$$\tilde{P}(k, t) = h_0(k)[\lambda_0^{\mathrm{D}}(k)]^t. \tag{37}$$

Finally, using (18), (19), (29), and (33)–(36) we conclude that the drift velocities and diffusion coefficients obtained in continuous and discrete formulations of the problem are related to each other by simple, general formulae

$$V^D = V \tag{38}$$

$$D^D = D - \tfrac{1}{2} V^2. \tag{39}$$

Equation (39) holds, however, only if the interval τ between successive jumps in the discrete formulation of the problem equals one, which has been assumed in our calculations for simplicity. For a general value of τ the relation between D and D^D reads

$$D^D = D - \tfrac{1}{2} \tau V^2 \tag{40}$$

which has a correct dimensional form (all its terms have a dimension $[L^2\,T^{-1}]$).

2.3. Comparison of the two formalisms

Comparing equations (15) and (37) we find that the main mathematical differences between the continuous- and discrete-time formalisms are related to different functional forms of $\tilde{P}(k, t)$ at $k \approx 0$. While in the continuous-time approach this function is given by an exponential, in the discrete-time model we deal with a power function. In particular, notice that $\partial^2 \lambda^t(k)/\partial k^2$ yields a term proportional to $t(t - 1) = t^2 - t$. This gives rise to an additional term linear in t, which is responsible for the difference between (34) and (19), and hence for the term $\tfrac{1}{2}\tau V^2$ in (40).

The presence of the time unit τ in (40) suggests that the key to understanding the physical reasons for the difference between D and D^D lies in the dimensional analysis. In the continuous-time approach the transition rates Γ_{jl} are *dimensional* quantities that scale with time as $[T^{-1}]$. Therefore, multiplying them all by some positive constant $\alpha \neq 1$ corresponds to changing the time unit, and so the resulting diffusion coefficient D_{new} will be equal to the product of α and the original value of the diffusion coefficient, D_{old}. Similarly, $V_{\text{new}} = \alpha V_{\text{old}}$. This explains why in the continuous-time approach we could safely assume $\tau = 1$. However, in the discrete formalism there is no such a simple relation between the time interval τ and the jump probabilities Γ_{jl}, which are *dimensionless*. Suppose, for example, that at times $t = 0, \tau, 2\tau, \ldots$ we toss a coin. Changing the frequency of tossing, or $1/\tau$, will have no impact on the probability of the coin falling heads up. The proper way of taking the continuous-time limit in the discrete-time model is to assume that the jump probabilities Γ_{jl}^D are related to the continuous-time transition rates Γ_{jl} by a simple formula $\Gamma_{jl}^D = \tau \Gamma_{jl}$ and taking the limit $\tau \to 0$. In other words, to get the continuous-time limit, we need to apply the 'alpha-transformation' to the transition probabilities with an infinitesimally small value of α. Equation (40) shows that D^D is actually a sum of two terms—one that scales linearly under the 'α-transformation' (D), and the other one which scales quadratically ($-\tfrac{1}{2}\tau V^2$). In the limit $\tau \to 0$ the continuous-time diffusion coefficient D is thus of order $O(\tau)$, while $-\tfrac{1}{2}\tau V^2$ is of order $O(\tau^2)$ and can be neglected. Consequently, as could be expected, the relative difference between diffusion coefficients calculated within each approach vanishes, $(D - D^D)/D \to 0$ as $\tau \to 0$.

A decrease of the diffusion coefficient in the discrete-time formalism can be also interpreted as a consequence of the fact that a discrete process tends to be 'less random' than a continuous one. This is clearly seen in a limiting case of a one-dimensional lattice (with lattice constant a and time unit τ) where all probabilities of jumping to the left vanish ($\Gamma_j^{\leftarrow} = 0$) and all probabilities of jumping to the right are equal to one ($\Gamma_j^{\rightarrow} = 1$). A discrete process with this choice of probabilities is completely deterministic. At each time interval the diffusing particle with probability one hops to the right, hence the diffusion constant vanishes.

On the other hand, if we consider a continuous-time process with $\Gamma^{\leftarrow} = 0$ and $\Gamma^{\rightarrow} = 1$, we can see that the motion of the particle is now by no means deterministic. Although we know that on average there will be one jump to the right per unit time, we do not know when it will actually occur. This uncertainty introduces randomness to the process, and the corresponding diffusion coefficient equals $a^2/2\tau$.

Note finally that because the left-hand side of (40) represents a diffusion coefficient, it cannot be negative, and so

$$D \geqslant \tfrac{1}{2}\tau V^2. \tag{41}$$

This has several interesting consequences. First, if in a periodic system there is a stationary drift ($V \neq 0$), then the continuous-time diffusion coefficient D is bounded from below. That such a bound exists can indirectly imply bounds on other physical quantities, e.g., the maximal force exerted by a molecular motor [26]. Second, *suppose* that (40), and hence (41), is also valid in *infinite* (aperiodic) random systems. Whenever the diffusion is sublinear, i.e., whenever $\lim_{t\to\infty}(\langle x^2 \rangle - \langle x \rangle^2)/t = 0$, there is $D = 0$. Equation (40) would then imply that $V = 0$, or $\lim_{t\to\infty}\langle x \rangle/t = 0$. This would mean that whenever diffusion is sublinear ('subdiffusion'), the drift is also sublinear ('subdrift') or vanishes altogether. The asymmetric hopping model with bond disorder can serve as an example of an infinite system where such relation is actually observed [2].

3. Diffusion in arbitrary space dimension d

Suppose we want to calculate the drift velocity $\vec{V}$ and the diffusion tensor $\mathbf{D}$ in a system with d Euclidean coordinates. If the system can be divided into a *finite* number of subsystems with constant transition rates between each two of them, our major results (14)–(17) and (37) remain valid irrespective of the geometry of the system. Such division is always possible for periodic systems with a finite number of sites in the elementary cell. The matrix $\Lambda(\vec{k})$ is the most 'sensitive' to the geometry of the system under consideration. In calculating its explicit form one can use an equation similar to (9), remembering, however, that $\vec{k}$ and $\vec{x}_n$ are now vectors in a d-dimensional space. One should also take into account all possible transitions between sublattices, and this can be done by considering all possible jumps starting at any site belonging to some elementary cell and ending in the same cell or in one of its nearest-neighbour cells.

The components of the velocity vector $\vec{V}$ and the diffusion tensor $\mathbf{D}$ are given by

$$V_\mu = \lim_{t\to\infty} \frac{\langle x_\mu \rangle}{t} = \lim_{t\to\infty} i\frac{1}{t} \frac{\partial \tilde{P}(\vec{k},t)}{\partial k_\mu}\bigg|_{\vec{k}=0} \tag{42}$$

$$D_{\mu\sigma} = \lim_{t\to\infty} \frac{\langle x_\mu x_\sigma \rangle - \langle x_\mu \rangle\langle x_\sigma \rangle}{2t} = \lim_{t\to\infty} \frac{1}{2t}\left(-\frac{\partial^2 \tilde{P}(\vec{k},t)}{\partial k_\mu \partial k_\sigma} + \frac{\partial \tilde{P}(\vec{k},t)}{\partial k_\mu}\frac{\partial \tilde{P}(\vec{k},t)}{\partial k_\sigma}\right)\bigg|_{\vec{k}=0}. \tag{43}$$

Using (14)–(17) and (37) we conclude that

$$V_\mu = V_\mu^{\mathrm{D}} = i\frac{\partial \lambda_0}{\partial k_\mu}\bigg|_{\vec{k}=0} \tag{44}$$

$$D_{\mu\sigma} = -\frac{1}{2}\frac{\partial^2 \lambda_0}{\partial k_\mu \partial k_\sigma}\bigg|_{\vec{k}=0} \tag{45}$$

$$D_{\mu\sigma}^{\mathrm{D}} = -\frac{1}{2}\left[\frac{\partial^2 \lambda_0^{\mathrm{D}}}{\partial k_\mu \partial k_\sigma} - \frac{\partial \lambda_0^{\mathrm{D}}}{\partial k_\mu}\frac{\partial \lambda_0^{\mathrm{D}}}{\partial k_\sigma}\right]\bigg|_{\vec{k}=0} \tag{46}$$

where $\mu, \sigma = 1, \ldots, d$. Actually, since $\log \tilde{P}(\vec{k},t) \approx \lambda_0(\vec{k})t$ is a generating function for cumulants of $P(\vec{x},t)$ [22], the first two of the above formulae are a natural consequence of (15) and (17).

Just as in the one-dimensional case, any component of $\vec{V}$ or D can be expressed in terms of derivatives of the three lowest coefficients of the characteristic polynomial of the matrix $\Lambda(k)$ at $k = 0$. In particular,

$$V_\mu = V_\mu^{\mathrm{D}} = -\mathrm{i} \frac{c_0^{(\mu)}}{c_1} \bigg|_{\vec{k}=0} \tag{47}$$

$$D_{\mu\sigma} = \frac{c_0^{(\mu)(\sigma)} - 2c_2 V_\mu V_\sigma - \mathrm{i}(c_1^{(\mu)} V_\sigma + c_1^{(\sigma)} V_\mu)}{2c_1} \bigg|_{\vec{k}=0} \tag{48}$$

$$D_{\mu\sigma}^{\mathrm{D}} = D_{\mu\sigma} - \tfrac{1}{2} V_\mu V_\sigma \tag{49}$$

where we used a shorthand notation $f^{(\mu)} \equiv \partial f / \partial k_\mu$.

4. The nearest-neighbour transition rates

If in a one-dimensional system only transitions to the nearest-neighbours are allowed, and if the distance between nearest-neighbour sites is equal to one, our formulae (23) and (24) can be simplified by noting that in this particular case

$$c_0' = \mathrm{i}L \left(\prod_{j=0}^{L-1} \Gamma_j^{\rightarrow} - \prod_{j=0}^{L-1} \Gamma_j^{\leftarrow} \right) \tag{50}$$

$$c_0'' = L^2 \left(\prod_{j=0}^{L-1} \Gamma_j^{\rightarrow} + \prod_{j=0}^{L-1} \Gamma_j^{\leftarrow} \right) \tag{51}$$

$$c_1' = 0 \tag{52}$$

where $\Gamma_j^{\rightarrow}$ and $\Gamma_j^{\leftarrow}$ are the transition rates to the right and left from site j, respectively; $\Gamma_j^{\rightarrow} \equiv \Gamma_{j+1,j}$ and $\Gamma_j^{\leftarrow} \equiv \Gamma_{j-1,j}$. Thus, to determine V and D we only need to compute the two terms of the characteristic polynomial of $\Lambda(0)$: c_1 and c_2.

Although c_1 and c_2 could be, at least in principle, found by calculating $\det(xI - \Lambda(0))$, I being the identity matrix, this could lead to serious computational overhead even for L of order ten. A more efficient method exploits the fact that c_l are polynomials in $\Gamma_j^{\leftarrow}$ and $\Gamma_j^{\rightarrow}$, $j = 0, \ldots, L - 1$, and can be expressed as

$$c_l = \sum_{\{\gamma_j\}, \{\delta_j\}} \prod_{m,n=0}^{L-1} (\Gamma_m^{\rightarrow})^{\gamma_m} (\Gamma_n^{\leftarrow})^{\delta_n} \psi_l(\{\gamma_j\}, \{\delta_j\}) \tag{53}$$

where $l \in \{1, 2\}$, $\gamma_m \in \{0, 1\}$, $\delta_n \in \{0, 1\}$, and $\psi_l(\{\gamma_j\}, \{\delta_j\}) = 0$ if at least one of the following conditions is satisfied:

$$\sum_{m=0}^{L-1} (\gamma_m + \delta_m) \neq L - l$$
$$\exists_m \gamma_m = \delta_m = 1 \tag{54}$$
$$\exists_m \gamma_m = \delta_{m+1} = 1.$$

Otherwise $\psi(\{\gamma_j\}, \{\delta_j\}) = 1$. For example, for $L = 3$ there is

$$c_1 = \Gamma_2^{\leftarrow}\Gamma_0^{\leftarrow} + \Gamma_2^{\leftarrow}\Gamma_0^{\rightarrow} + \Gamma_2^{\rightarrow}\Gamma_0^{\rightarrow} + \Gamma_1^{\leftarrow}\Gamma_2^{\leftarrow} + \Gamma_1^{\leftarrow}\Gamma_2^{\rightarrow} + \Gamma_1^{\rightarrow}\Gamma_2^{\rightarrow}$$
$$+ \Gamma_0^{\leftarrow}\Gamma_1^{\leftarrow} + \Gamma_0^{\leftarrow}\Gamma_1^{\rightarrow} + \Gamma_0^{\rightarrow}\Gamma_1^{\rightarrow} \tag{55}$$

$$c_2 = \Gamma_0^{\leftarrow} + \Gamma_1^{\leftarrow} + \Gamma_2^{\leftarrow} + \Gamma_0^{\rightarrow} + \Gamma_1^{\rightarrow} + \Gamma_2^{\rightarrow}.$$

Although formally the sum in (53) consists of 2^{2L} terms, in practice only for a few of them do $\psi_l(\{\gamma_j\}, \{\delta_j\}) \neq 0$. In particular, for a given value of L the sum in (53) consists of L^2

non-vanishing terms for c_1 and $(L^4 - L^2)/12$ terms for c_2. Thus it should be possible to calculate D algebraically for L of order of 20, and numerically for L of order at least 100. It is worth noting that since c_l can be computed as sums of positive values, by using (53) rather than calculating the determinant of $xI - \Lambda(0)$ we can avoid large numerical errors which often appear when computing determinants of large matrices.

It is not difficult to show that our general formulae (23) and (24) are consistent with equation (1) derived for a general case of one-dimensional systems at equilibrium with nearest-neighbour transitions. To this end it suffices to notice that the equilibrium site occupation probabilities P_j^{eq} can be expressed in terms of the jump probabilities as

$$\frac{1}{P_j^{\text{eq}}\Gamma_j^{\rightarrow}} = \frac{1}{\Gamma_j^{\rightarrow}} + \frac{\Gamma_j^{\leftarrow}}{\Gamma_j^{\rightarrow}\Gamma_{j-1}^{\rightarrow}} + \cdots + \frac{\Gamma_j^{\leftarrow}\Gamma_{j-1}^{\leftarrow}\cdots\Gamma_{j-L+2}^{\leftarrow}}{\Gamma_j^{\rightarrow}\Gamma_{j-1}^{\rightarrow}\cdots\Gamma_{j-L+1}^{\rightarrow}}. \tag{56}$$

On inserting it into (1) and then taking into account (53) and the trivial condition $V = 0$ one arrives at (24).

Another interesting consequence of (50)–(52) is that diffusion in systems with transitions to nearest neighbours is always normal. To see it note that since $c_1 \neq 0$, D is always finite and thus no superdiffusion is possible. The other type of anomaly, subdiffusion, would require that $D = 0$. Owing to (41) this would imply $V = 0$ which, upon taking into account (24), would require $c_0'' = 0$. However, the explicit form of c_0'', see (51), guarantees that $c_0'' > 0$ except for a degenerated case where the diffusing particle is confined to a finite region of the lattice ($\Gamma_j^{\leftarrow} = \Gamma_l^{\rightarrow} = 0$ for some j and l).

One final remark. Some authors [5, 10, 14], when considering a one-dimensional system with nearest-neighbour transitions, prefer to reduce the problem to diffusion on a finite ring and investigate the probability current J rather than the drift velocity V. The former is defined as $J = P_j\Gamma_j^{\rightarrow} - P_{j+1}\Gamma_{j+1}^{\leftarrow}$ and in the steady state does not depend on the site j it is measured at. For single-particle systems J and V are related to each other through a simple formula $J = V/L$ [11]. In this case our approach can thus be applied for calculating both V and J.

5. Applications

5.1. The case $L = 1$ and $L = 2$

Applying our approach to a particle diffusing in a one-dimensional system with a lattice constant $a = 1$, time unit $\tau = 1$, and the period $L = 1$ we immediately arrive at a well known result:

$$V = \Gamma^{\rightarrow} - \Gamma^{\leftarrow} \tag{57}$$

$$D = (\Gamma^{\rightarrow} + \Gamma^{\leftarrow})/2 \tag{58}$$

$$D^{\text{D}} = [\Gamma^{\rightarrow} + \Gamma^{\leftarrow} - (\Gamma^{\rightarrow} - \Gamma^{\leftarrow})^2]/2. \tag{59}$$

For $L = 2$ we find

$$V = 2\frac{\Gamma_1^{\rightarrow}\Gamma_2^{\rightarrow} - \Gamma_1^{\leftarrow}\Gamma_2^{\leftarrow}}{S} \tag{60}$$

$$D = 2\frac{\Gamma_1^{\rightarrow}\Gamma_2^{\rightarrow} + \Gamma_1^{\leftarrow}\Gamma_2^{\leftarrow}}{S} - \frac{V^2}{S} \tag{61}$$

$$D^{\text{D}} = 2\frac{\Gamma_1^{\rightarrow}\Gamma_2^{\rightarrow} + \Gamma_1^{\leftarrow}\Gamma_2^{\leftarrow}}{S} - \frac{2 + S}{S}\frac{V^2}{2} \tag{62}$$

where $S \equiv \Gamma_1^{\rightarrow} + \Gamma_2^{\rightarrow} + \Gamma_1^{\leftarrow} + \Gamma_2^{\leftarrow}$. Note also that the solution for $L = 3$ can be easily derived using (55).

5.2. The sawtooth potential of arbitrary period in an external field

Consider a one-dimensional system of period L with site energies $E_{nL+j} = j\varepsilon$, where n is an integer, $j = 0, \ldots, L - 1$, and $\varepsilon > 0$ is a constant. Such a pattern is known as a discrete sawtooth potential [5, 9]. We assume that the transition rate from a site j to $j + 1$ is given by

$$\Gamma_j^{\rightarrow} = b \exp(-\beta\varepsilon/2) \tag{63}$$

and the rate of jumping from j to $j - 1$ reads

$$\Gamma_j^{\leftarrow} = \begin{cases} b^{-1} \exp(\beta\varepsilon/2) & j \neq 0 \pmod{L} \\ b^{-1} \exp(\beta\varepsilon(1/2 - L)) & j = 0 \pmod{L} \end{cases} \tag{64}$$

where $\beta \equiv 1/k_B T$ is the Boltzmann factor and $b \equiv \exp(\beta F/2)$ represents a bias due to an external force F. Note that with this choice of the transition rates, for $b = 1$ the system satisfies the detailed balance condition $\Gamma_{j+1}^{\leftarrow} \exp(-\beta E_{j+1}) = \Gamma_j^{\rightarrow} \exp(-\beta E_j)$.

Using (53) and some combinatorics one can prove that for $L > 2$

$$c_0' = iLR^L(b^L - b^{-L}) \tag{65a}$$

$$c_0'' = L^2 R^L(b^L + b^{-L}) \tag{65b}$$

$$c_1 = G^{-L-1}\mathcal{S}_L(G) + R^{2L}G^{L-1}\mathcal{S}_{L-1}(G^{-1}) \tag{65c}$$

$$c_1' = 0 \tag{65d}$$

$$c_2 = G^{2-L}\mathcal{Z}_{L-2}(G) + R^{2L}G^{L-4}\mathcal{Z}_{L-3}(G^{-1}) \tag{65e}$$

where $R \equiv \exp(-\beta\varepsilon/2)$ controls the anisotropy of the potential, $G \equiv Rb$, $\mathcal{S}_m(x) \equiv \sum_{j=1}^{m} jx^{2j} = [x^{2m+2}(1 + m - mx^2) - x^2]/(x^2 - 1)^2$, and $\mathcal{Z}_m(x) \equiv \frac{1}{2}\sum_{j=0}^{m}(m + 1 - j)(j + 1)(j + 2)x^{2j}$. Actually, we were able to prove only (65a)–(65d), and (65e) is a conjecture based on the form of c_2 derived for $L = 2, \ldots, 20$.

The stationary drift velocity V and the diffusion constants D and D^D can be now calculated using (23), (24), and (40). The resulting velocity has already been studied in [5]. The diffusion coefficient D calculated for various values of R and L as a function of the bias b is depicted in figure 1. For $R = 1$ there is $\varepsilon = 0$, and so for any j we have $\Gamma_j^{\rightarrow} = b$ and $\Gamma_j^{\leftarrow} = b^{-1}$. Consequently, the effective period equals one. Using (58) we conclude that $D = \frac{1}{2}(b + b^{-1})$. For $R < 1$ the behaviour of D becomes more complicated. For a large bias to the right, $b \gg 1$, the jumps to the left are so rare that practically they become irrelevant. We thus have $\Gamma_j^{\rightarrow} = bR$, $\Gamma_j^{\leftarrow} \approx 0$, and so $D \approx bR/2$ irrespective of L. For a strong bias to the left, $b \ll 1$, the jumps to the right can be neglected, but the particle has to jump over a large potential barrier located at sites $j = \ldots, -L, 0, L, \ldots$ whose height is proportional to $L - \frac{1}{2}$, see (64). Therefore, in this regime D is a quickly decreasing function of L. These two limiting solutions match in the intermediate regime, which can be roughly described as $1 \leqslant b \leqslant 1/R$.

5.3. Two particles in a sawtooth potential on a ring of length $L = 4$

Consider *two* particles diffusing in a sawtooth potential on a ring of length $L = 4$. We assume that any site j can be occupied by only one of them (the hard-core interaction). For simplicity we also assume that the distance between the particles cannot exceed $L - 1$, so that we can reduce the system to a ring consisting of L sites.

Each state of the system can be described as a pair of integers, (n, m), where $n, m = 0, \ldots, L - 1$ denote the currently occupied sites. As $n \neq m$, there are $L(L - 1)/2 = 6$ different states. Our two-particle system is thus equivalent to a six-state system with one 'virtual' random walker. These states are, in order, $(0, 1)$, $(0, 2)$, $(0, 3)$, $(1, 2)$, $(1, 3)$, $(2, 3)$. The distance between a state (i_1, j_1) and (i_2, j_2) equals $i_2 - i_1 + j_2 - j_1$. For example, the
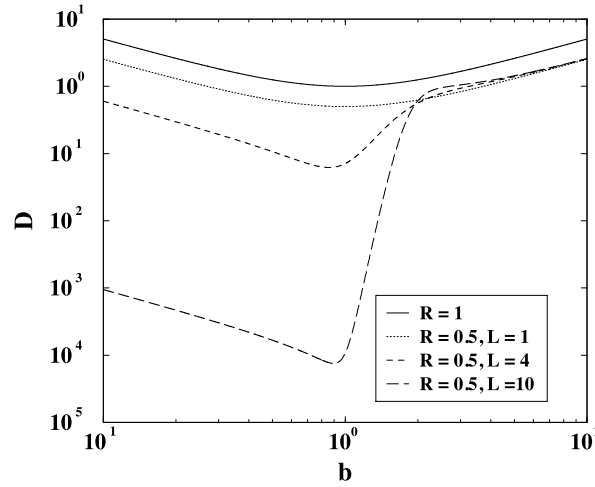
Figure 1. Diffusion coefficient D of a single particle in a sawtooth potential (63) and (64) for various potential periods L and anisotropy parameters R as a function of the bias b. Arbitrary units.

distance from $(0, 1)$ to $(0, 2)$ is one. The transition rate between (i_1, j_1) and (i_2, j_2) vanishes unless $|i_2 - i_1| + |j_2 - j_1| = 1$, and in this case a transition from (i_1, j_1) to (i_2, j_2) corresponds to a single jump of one of two diffusing particles. For example, the transition rate from $(0, 1)$ to $(0, 2)$ is $\Gamma_1^{\rightarrow}$, and from $(0, 1)$ to $(0, 3)$ is zero. Consequently, if the lattice constant $a = 1$, the matrix $\Lambda(k)$ takes on the following form:

$$\Lambda(k) = \begin{bmatrix} -\Gamma_1^{\rightarrow} - \Gamma_0^{\leftarrow} & \Gamma_2^{\leftarrow} e^{ik} & 0 & 0 & \Gamma_3^{\rightarrow} e^{-ik} & 0 \\ \Gamma_1^{\rightarrow} e^{-ik} & -\Gamma_2^{\leftarrow} - \Gamma_2^{\rightarrow} - \Gamma_0^{\rightarrow} - \Gamma_0^{\leftarrow} & \Gamma_3^{\leftarrow} e^{ik} & \Gamma_1^{\leftarrow} e^{ik} & 0 & \Gamma_3^{\rightarrow} e^{-ik} \\ 0 & \Gamma_2^{\rightarrow} e^{-ik} & -\Gamma_3^{\leftarrow} - \Gamma_0^{\rightarrow} & 0 & \Gamma_1^{\leftarrow} e^{ik} & 0 \\ 0 & \Gamma_0^{\rightarrow} e^{-ik} & 0 & -\Gamma_1^{\leftarrow} - \Gamma_2^{\rightarrow} & \Gamma_3^{\leftarrow} e^{ik} & 0 \\ \Gamma_0^{\leftarrow} e^{ik} & 0 & \Gamma_0^{\rightarrow} e^{-ik} & \Gamma_2^{\leftarrow} e^{-ik} & -\Gamma_3^{\rightarrow} - \Gamma_1^{\leftarrow} - \Gamma_3^{\leftarrow} - \Gamma_1^{\rightarrow} & \Gamma_2^{\leftarrow} e^{ik} \\ 0 & \Gamma_0^{\leftarrow} e^{ik} & 0 & 0 & \Gamma_1^{\rightarrow} e^{-ik} & -\Gamma_3^{\rightarrow} - \Gamma_2^{\leftarrow} \end{bmatrix}. \quad (66)$$

The drift velocity V and the diffusion coefficient D can be found for arbitrary transition rates, but the results are *very* lengthy. However, in a particular case of the sawtooth potential the transition rates $\Gamma_j^{\rightarrow}$ and $\Gamma_j^{\leftarrow}$ are given by relatively simple formulae (63) and (64), respectively. Then,

$$c_0' = 8iG^{-6}(G^8 - R^8)(R^8 + 2G^2 + 1)(G^2 + 1)$$
$$c_0'' = 32G^{-6}(G^8 + R^8)(R^8 + 2G^2 + 1)(G^2 + 1)$$
$$c_1 = G^{-5}(G^2 + 1)[12G^8 + 15G^6 + 10G^4 + 5G^2 + 2 + R^8(9G^6 + 13G^4 + 17G^2 + 5)$$
$$\qquad + R^{16}(G^4 + 2G^2 + 5)] \quad (67)$$
$$c_1' = 8iG^{-5}(G^8 - R^8)(R^8 + 4G^2 + 3)$$
$$c_2 = G^{-4}[37G^8 + 69G^6 + 58G^4 + 31G^2 + 9 + R^8(23G^6 + 49G^4 + 53G^2 + 19)$$
$$\qquad + R^{16}(3G^4 + 8G^2 + 9)]$$

where G and R were defined below equation (65).

Just like in the previous example, V, D, and D^D can be now determined using (23), (24), and (40). The properties of the velocity V will be studied in detail elsewhere (see [27]). Here, in figure 2 we present the ratio of the diffusion coefficient calculated for a two-particle system (D_2) to that calculated for a single-particle system (D_1), for $L = 4$, as a function of the bias b. This ratio measures the change of diffusivity due to interactions with the second particle. As could be expected, $D_2 < D_1$, i.e. the presence of the second particle decreases the diffusivity of
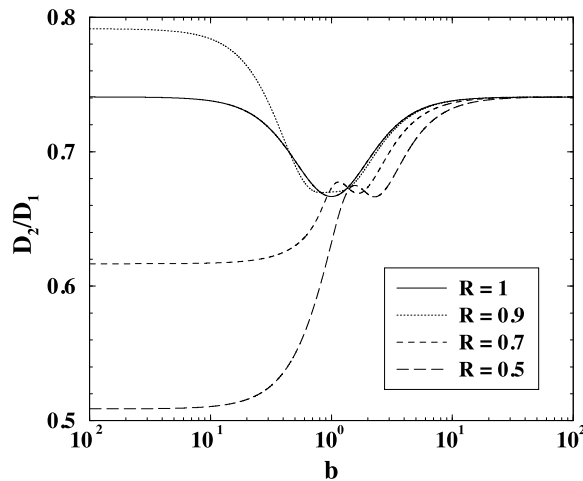
Figure 2. The ratio of the diffusion coefficients D_2 and D_1 calculated for a four-site ring containing two and one particles, respectively, as a function of the bias b, for various values of the anisotropy parameter R. Arbitrary units.

the first one. This effect is not strong, however, for we find that $D_2 \geqslant \frac{1}{2}D_1$. As in the previous example, for large bias b, the ratio D_2/D_1 becomes independent of the potential anisotropy R.

6. Conclusions

We have developed an effective technique of calculating the drift velocity $\vec{V}$ and the diffusion tensor D in arbitrary periodic systems. A novel feature of our approach, as compared with previously proposed methods [11–16], consists in the fact that we need not examine in detail the steady-state properties of the system. In particular, we do not need to solve linear equations of relatively high order to find the stationary probability distribution of the random walker over different sublattices. Instead, we calculate $\vec{V}$ and D directly. The only quantity we really need in order to carry out our calculations is the matrix $\Lambda(k)$. Its explicit form, however, can be found almost trivially; all one needs to know are the transition rates and distances from any site of an elementary cell to any other site in the same or adjacent cell. Once the form of $\Lambda(k)$ has been determined, one should calculate the three lowest terms of its characteristic polynomial. Then $\vec{V}$ and D can be determined using our formulae (47) and (48), respectively.

Our approach is very general and can be applied practically to any periodic system in an arbitrary space dimension. It is particularly well suited for calculations employing computer-algebra systems, e.g., Maple or Reduce, or for numerical analysis. In this context one should also note that the coefficients c_l of the characteristic polynomial of $\Lambda(0)$ can be *always* expressed as polynomials in $\Lambda_{jl}(0)$, $j \neq l$, with *positive* coefficients, and thus can be calculated numerically with extremely high accuracy. While this is not necessarily true in the case of their derivatives, we believe that our approach enables one to calculate $\vec{V}$ and D even for systems where the corresponding steady-state problem is numerically ill-conditioned.

We were able to prove a general relation between the diffusion constants calculated using continuous-time and discrete-time approaches. Our analysis shows that in *any* periodic system (including, for example, lattice gases studied in [6, 7]) they differ by a term $\frac{1}{2}V^2$, where V denotes the steady-state drift velocity along a given direction. Since the limits $t \to \infty$ and $L \to \infty$ were shown to commute, at least in some simple models [2, 19], we expect that this

relation holds also for infinite random systems. It would be interesting to know whether such a simple and apparently universal relation can be applied in contexts other than those studied here.

We also showed how our technique can be applied to a simple many-body problem. While, owing to mathematical complexity, we do not expect that in this way one will be able to calculate explicitly transport coefficients in non-equilibrium systems containing more than a few particles, our conclusion about the universal difference between diffusion coefficients calculated in continuous- and discrete-time models should still hold. This conjecture is based on the fact that diffusion of several particles can be interpreted as diffusion of a single particle in the corresponding multidimensional phase space, and for the latter problem the relation between D and D^{D} has been established rigorously in section 3. Thus, for the future work, two problems are of primary importance: the role of periodic boundary conditions in the limit of asymptotically infinite period, $L \to \infty$, and detailed analysis of possible applications of our method to many-body systems.

Acknowledgments

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