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Note: On the relation between Lifson-Jackson and Derrida formulas for effective diffusion coefficient

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The language of lattice random walks or hopping models is widely used to describe different kinetic and transport processes in physics, chemistry, and biology. Examples range from hopping transport in semiconductors to single-molecule enzyme kinetics and intracellular transport by molecular motors.[1–10] When (1) the random walk occurs on a periodic lattice and (2) the observation time is sufficiently long so that a typical displacement exceeds the lattice period, one can use a coarse-grained description of the motion. In this description, all information about the underlying random walk is packed into the effective drift velocity, V_{eff}, and diffusion coefficient, D_{eff}. The goal of the theory is to establish the relation between V_{eff} and D_{eff} and the parameters of the underlying random walk.

For a Markovian nearest-neighbor random walk in one dimension,

$$\ldots \underset{\beta_{n-1}}{\overset{\alpha_{n-2}}{\rightleftarrows}} n-1 \underset{\beta_n}{\overset{\alpha_{n-1}}{\rightleftarrows}} n \underset{\beta_{n+1}}{\overset{\alpha_n}{\rightleftarrows}} n+1 \underset{\beta_{n+2}}{\overset{\alpha_{n+1}}{\rightleftarrows}} \ldots, \tag{1}$$

where α_n and β_n are the rate constants for transitions from site n to sites $n+1$ and $n-1$, respectively, which are assumed to be periodic functions of n with period N, $\alpha_{n+N} = \alpha_n$, and $\beta_{n+N} = \beta_n$, such a theory was developed by Derrida[11] (see also the analysis of a special case in Ref. 12). In the absence of the effective drift velocity, $V_{eff} = 0$, the Derrida (D) formula for D_{eff} takes the form (see Eqs. (46), (47), and (50) from Ref. 11),

$$D_{eff}^{(D)} = \frac{N}{\left(\sum_{n=1}^{N} r_n\right)^2} \sum_{n=1}^{N} \alpha_n u_n r_n, \tag{2}$$

where

$$r_n = \frac{1}{\alpha_n}\left(1 + \sum_{i=1}^{N-1}\prod_{j=1}^{i}\frac{\beta_{n+j}}{\alpha_{n+j}}\right) \tag{3}$$

and

$$u_n = \frac{1}{\alpha_n}\left(1 + \sum_{i=1}^{N-1}\prod_{j=1}^{i}\frac{\beta_{n-j+1}}{\alpha_{n-j}}\right). \tag{4}$$

In this Note we show that the Derrida formula, Eq. (2), can be interpreted as a discretized version of the Lifson-Jackson formula for the effective diffusion coefficient.[13] The latter provides the effective diffusion coefficient for a particle diffusing in an arbitrary one-dimensional periodic potential $U(x)$, $U(x+L) = U(x)$, where L is the period. Assuming that the particle position-dependent diffusion coefficient $D(x)$ is also a periodic function of x, $D(x+L) = D(x)$, the Lifson-Jackson (LJ) formula for D_{eff} can be written as

$$D_{eff}^{(LJ)} = \frac{1}{\langle e^{-\beta U(x)}\rangle\langle e^{\beta U(x)} / D(x)\rangle}. \tag{5}$$

Here the angular brackets denote averaging over the period, $\langle f(x)\rangle = (1/L)\int_0^L f(x)dx$, and $\beta = (k_BT)^{-1}$, where k_B and T are the Boltzmann constant and absolute temperature. It is convenient to introduce the equilibrium probability density, $p_{eq}(x)$, normalized to unity on the period L,

$$p_{eq}(x) = e^{-\beta U(x)} \Big/ \int_0^L e^{-\beta U(x)}dx. \tag{6}$$

Using this probability density we can write $D_{eff}^{(LJ)}$ in Eq. (5) as

$$D_{eff}^{(LJ)} = \frac{L^2}{\int_0^L \frac{dx}{D(x)p_{eq}(x)}}. \tag{7}$$

To transform the Derrida formula, Eq. (2), to the form similar to that of the Lifson-Jackson formula, Eq. (7), we introduce the equilibrium distribution function, P_n^{eq}, for the hopping dynamics, Eq. (1), normalized to unity on the period N,

$$\sum_{n=1}^{N} P_n^{eq} = 1. \tag{8}$$

This distribution function is periodic, $P_{n+N}^{eq} = P_n^{eq}$, and satisfies the detailed balance condition,

$$\alpha_n P_n^{eq} = \beta_{n+1} P_{n+1}^{eq}. \tag{9}$$

Using Eqs. (8) and (9) we find that r_n and u_n are given by

$$r_n = P_n^{eq}\sum_{i=1}^{N}\frac{1}{\alpha_i P_i^{eq}}, \qquad u_n = \frac{1}{\alpha_n P_n^{eq}}. \tag{10}$$

Substituting these expressions into Eq. (2), we obtain

$$D_{eff}^{(D)} = \frac{N^2}{\sum_{n=1}^{N} \frac{1}{\alpha_n P_n^{eq}}} = \frac{N^2}{\sum_{n=1}^{N} \frac{1}{\beta_n P_n^{eq}}}, \tag{11}$$

where the detailed balance condition, Eq. (9), and the periodicity have been taken into account in writing the second equality.

The effective diffusion coefficient, Eq. (11), can be written in the form symmetric about the rate constants α_n and β_n,

$$D_{eff}^{(D)} = \frac{N^2}{\sum_{n=1}^{N} \frac{\alpha_n+\beta_n}{2\alpha_n\beta_n} \frac{1}{P_n^{eq}}}. \tag{12}$$

It is convenient to introduce the mean lifetime of the random walk on site n, τ_n,

$$\tau_n = (\alpha_n + \beta_n)^{-1} \tag{13}$$

and the probabilities $w_n^{(\pm)}$ that the random walk jumps from site n to sites $n+1$ and $n-1$, respectively,

$$w_n^{(+)} = \alpha_n \tau_n \ , \qquad w_n^{(-)} = \beta_n \tau_n. \tag{14}$$

Then we can write $D_{eff}^{(D)}$ in Eq. (12) as

$$D_{eff}^{(D)} = \frac{N^2}{\sum_{n=1}^{N} \frac{\tau_n}{2w_n^{(+)}w_n^{(-)}} \frac{1}{P_n^{eq}}}. \tag{15}$$

When comparing the Derrida and Lifson-Jackson formulas for the effective diffusion coefficient, we take that the neighboring lattice sites are separated by distance l, so that $L = Nl$.

With this in mind, the comparison of the expressions for D_{eff} given in Eqs. (7), (12), and (15) show that $D_{eff}^{(D)}$ can be considered as a discretized version of $D_{eff}^{(LJ)}$, Eq. (7), in which the local diffusion coefficient is $D(x = nl) = l^2 D_n$, where D_n is defined as

$$D_n = \frac{2\alpha_n\beta_n}{\alpha_n + \beta_n} = \frac{2w_n^{(+)}w_n^{(-)}}{\tau_n}. \tag{16}$$

Note that for a symmetric random walk, $\alpha_n = \beta_n$ and hence $w_n^{(+)} = w_n^{(-)} = 1/2$, Eq. (16) leads to the conventional expression, $D(x = nl) = l^2/(2\tau_n)$.

Finally, we take advantage of Eq. (11) to derive an expression which gives $D_{eff}^{(D)}$ in terms of the rate constants α_n and β_n. To do this we first find a solution for P_n^{eq}, using the detailed balance and normalization conditions, Eqs. (8) and (9), respectively. The solution is given by

$$P_n^{eq} = P_1^{eq} \prod_{j=2}^{n} \frac{\alpha_{j-1}}{\beta_j} \ , \qquad n = 2, 3, \ldots, N, \tag{17}$$

where P_1^{eq} is

$$P_1^{eq} = \frac{1}{1 + \sum_{n=2}^{N} \prod_{j=2}^{n} \frac{\alpha_{j-1}}{\beta_j}}. \tag{18}$$

Substituting this solution for P_n^{eq} into Eq. (11), we arrive at

$$D_{eff}^{(D)} = \frac{\alpha_1 N^2}{\left(1 + \sum_{n=2}^{N} \prod_{j=2}^{n} \frac{\alpha_{j-1}}{\beta_j}\right)\left(1 + \sum_{n=2}^{N} \prod_{j=2}^{n} \frac{\beta_j}{\alpha_j}\right)}. \tag{19}$$

One might think that $D_{eff}^{(D)}$ in Eq. (19) depends on how we choose site 1. However, this is not true because the solution for P_n^{eq} is unique, and we substitute this unique solution, Eqs. (17) and (18), into Eq. (11), according to which $D_{eff}^{(D)}$ is independent of how the sites are enumerated.

In summary, we have established the relation between the Derrida and Lifson-Jackson formulas for the effective diffusion coefficient. The latter gives this quantity for a particle diffusing in a periodic potential, while the former provides the effective diffusion coefficient when the underlying dynamics is described as an unbiased nearest-neighbor Markovian random walk on a periodic lattice. We showed that the Derrida formula can be considered as a discretized version of the formula obtained by Lifson and Jackson with correctly chosen position-dependent diffusion coefficient. Although the existence of such a relation between the Derrida and Lifson-Jackson formulas does not seem surprising, the expression in Eq. (16), which gives the discretized position-dependent diffusion coefficient in terms of the rate constants, is not so obvious.

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