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# Single-Vacancy Induced Motion of a Tracer Particle in a Two-Dimensional Lattice Gas

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We study the random motion of a tracer particle in a two-dimensional dense lattice gas. Repeated encounters of a *single* vacancy displace the tracer particle from its initial position by a vector $\mathbf{y}$ of which we calculate the time-dependent distribution $P_t(\mathbf{y})$. On an infinite lattice and for large times

$$P_t(\mathbf{y}) \simeq \frac{2(\pi-1)}{\ln t} K_0\left(\left(\frac{4\pi(\pi-1)}{\ln t}\right)^{1/2} y\right)$$

where $K_0$ is a modified Bessel function. The same problem is studied on a finite $L \times L$ lattice with periodic boundary conditions; there $P_t(\mathbf{y})$ is shown to be a Gaussian on a time scale $L^2 \ln L$. On an $\infty \times L$ strip and for large times, $P_t(\mathbf{y})$ is an explicitly given (but nonelementary) function of the scaling variable $\xi = y_1/t^{1/4}$, identical to the function occurring in the problem of a random walker on a random one-dimensional path.

**KEY WORDS:** Tracer diffusion; two-dimensional lattice gas; correlated Brownian motion; vacancy.

## 1. INTRODUCTION

We consider a square lattice of which each site *except one* is filled with a particle. The empty site is referred to as the "hole." The particles carry out Brownian motion, subject to the condition that each site can be at most singly occupied. More specifically, we stipulate that at each instant of time $t = 1, 2, 3,...$ one particle, selected with probability 1/4 from among the four particles adjacent to the hole, will move into it. Then the hole obviously performs a simple random walk.

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We now select and "tag" one particle, the "tracer particle," whose motion we want to follow. This motion depends on the trajectory of the hole in a complicated way: the tagged particle can move only when it is encountered by the hole, and its successive moves will be correlated. Evidently, from the point of view of the tagged particle, the hole is more likely to return for its next encounter from the direction in which it has left than from a perpendicular or opposite direction. On a two-dimensional lattice, the tagged particle will, with probability 1, make an infinite number of steps, even in the presence of just one vacancy. In this work we calculate the probability $P_t(\mathbf{y})$ that at time $t$ the tagged particle be displaced a distance $\mathbf{y} = (y_1, y_2)$ from its initial position.

This problem can also be formulated for a three-dimensional lattice. However, the properties of the three-dimensional simple random walk ensure that, with probability 1, the hole will wander off to infinity only a finite number of encounters with the tagged particle, so that in an effectively finite time $P_t(\mathbf{y})$ tends to an equilibrium distribution $P_\infty(\mathbf{y})$ with a spatial decay length of only a few lattice sites. A rapidly converging method for calculating this distribution (subject to the condition that there be an initial encounter between the vacancy and the tagged particle) has been given by Sholl.[1] On a three-dimensional lattice with a *finite but very small* vacancy *density*, a tracer particle will be met by new vacancies at a constant average rate, and $P_\infty(\mathbf{y})$ then is the essential ingredient in calculating its diffusion constant.[1,2] This problem is known in the literature as the tracer diffusion problem. A general theory for tracer diffusion in three dimensions has been given by Kehr *et al.*,[3] who also present results of Monte Carlo calculations.

In one dimension the tracer diffusion problem has a long history, which was reviewed by Van Beijeren *et al.*,[4] who report Monte Carlo calculations and present an approximate theory. The Green–Kubo relation between the diffusion constant and the velocity autocorrelation function of the tracer particle was exploited by Van Beijeren and Kehr.[5]

In this work we deal exclusively with the interaction between a tracer particle and a *single* vacancy in two dimensions. Since this interaction extends infinitely in time, a correct understanding of it is a necessary prerequisite for the study of finite vacancy densities. We summarize our results. On an infinite two-dimensional lattice, studied in Section 3, it appears that in the limit of large $t$ and large $y$ the distribution $P_t(\mathbf{y})$ is a function only of the scaling variable

$$\eta = y/(\ln t)^{1/2} \tag{1.1}$$

Most surprisingly, however, the scaling function *is not a Gaussian* but a modified Bessel function $K_0$. Its precise form, and the conditions under which it is obtained, are given in Section 3.2.1. The deviation from Gaussian behavior indicates that even when separated by long time intervals, successive steps of the tagged particle cannot be considered as effectively uncorrelated.

Second, we consider in Section 4 the same problem on a square lattice of $L \times L$ sites with periodic boundary conditions. In this case it is clear that for sufficiently large $L$ there is an initial time scale where the hole does not notice that the lattice is finite and the analysis of the infinite lattice applies. At times $t \sim L^2$, however, the hole is likely to explore the full periodic lattice, after which it will return to the tagged particle from a completely uncorrelated direction. Since in two dimensions the time needed by a random walker to return to a specified lattice point a distance $\sim L$ away is $\sim L^2 \ln L$, we expect a subsequent time scale $t \gg L^2 \ln L$ on which the tagged particle performs diffusive motion and $P_t(\mathbf{y})$ is Gaussian. This is indeed what we find, and the corresponding diffusion constant is

$$D_L = \frac{1}{4(\pi - 1)\, L^2} \tag{1.2}$$

This behavior is followed by a crossover to a final time scale on which $P_t(\mathbf{y})$ flattens out to the stationary value $1/L^2$ on each site; clearly the time scale for this to happen is $t \sim L^4$. In Section 4.3 we comment on our finite lattice calculation, and also make contact with work by Palmer,[6] who has proposed the same system within the framework of the study of constrained dynamics.

Third, we study in Section 5 the same problem on a strip of finite width, i.e., an array of $\infty \times L$ sites. It there appears that in the limit of large $t$ and large $|y_1|$ the distribution function $P_t(\mathbf{y})$ depends only on the scaling variable

$$\xi = \frac{y_1}{t^{1/4}} \tag{1.3}$$

and again *is not a Gaussian.* Its precise form and the details of the calculation are given in Section 5.2. In Section 5.3 we comment on the strip calculation, and observe in particular that our result for the distribution function is identical, in the scaling limit, to what was found by Kehr and Kutner[7] for a random walker on a one-dimensional random path!

## 2. FORMULATION OF THE PROBLEM

### 2.1. The Distribution Function $P_t(\mathbf{y})$

The three lattice geometries to be considered are all special cases of a square lattice of $L_1 \times L_2$ sites labeled by integer coordinates $\mathbf{x} \equiv (x_1, x_2)$, where

$$x_i = 0, 1, 2, \ldots, L_i - 1, \qquad i = 1, 2 \tag{2.1}$$

We shall impose periodic boundary conditions so that the origin is a site equivalent to all others. We introduce the two unit vectors

$$\mathbf{e}_1 = (1, 0), \qquad \mathbf{e}_2 = (0, 1) \tag{2.2}$$

For the initial ($t = 0$) position of the tagged particle we take the origin, and we denote the initial position of the hole by $\mathbf{x}_0 \neq \mathbf{0}$.

One approach to the motion of the tagged particle would be to write down the master equation for the joint distribution $P_t^{(2)}(\mathbf{y}, \mathbf{x})$ of the tagged particle position $\mathbf{y}$ and the hole position $\mathbf{x}$. Finding the relaxation modes and eigenvalues of this equation amounts to an $L_1 L_2 (L_1 L_2 - 1)$-dimensional matrix problem which, although perhaps not untractable, does not appear easy. Since, moreover, the information about the motion of the hole is redundant for our purpose, we shall focus directly upon the quantity of interest, viz. the reduced distribution function for the tagged particle position alone,

$$P_t(\mathbf{y}) \equiv \sum_{\mathbf{x}(\neq \mathbf{y})} P_t^{(2)}(\mathbf{y}, \mathbf{x}) \tag{2.3}$$

This distribution no longer satisfies a master equation. It is nevertheless possible to derive an expression for it from which all desired information can be extracted.

### 2.2. The Return Probabilities $W_\tau(\boldsymbol{\delta}, \boldsymbol{\delta}')$

In tracer diffusion problems a key role is played by a set of conditional return probabilities (also called waiting time distributions) $W_\tau(\boldsymbol{\delta}, \mathbf{x})$, where $\boldsymbol{\delta}$ is one of the unit vectors $\pm\mathbf{e}_1$, $\pm\mathbf{e}_2$. For all $\mathbf{x} \neq \mathbf{0}$ we define $W_0(\boldsymbol{\delta}, \mathbf{x}) \equiv 0$; and, for $\tau = 1, 2, \ldots$, we define $W_\tau(\boldsymbol{\delta}, \mathbf{x})$, as the probability that a simple random walker initially at $\mathbf{x} \neq 0$, (i) hits the origin for the first time at time $\tau$, *and* that, (ii) its position at $\tau - 1$ was $\boldsymbol{\delta}$. Continuous-time equivalents of these quantities occur, e.g., in refs. 1, 3, and 5.

If for the simple random walker we take the hole initially at $\mathbf{x}_0 \neq \mathbf{0}$, and if the tagged particle is initially at the origin, then $W_\tau(\boldsymbol{\delta}, \mathbf{x}_0)$ is the probability that at time $\tau$ the tagged particle will make its first step, and that this step is in the direction $\boldsymbol{\delta}$. But then at time $\tau$ the hole is at a distance $-\boldsymbol{\delta}$ from the tagged particle, and the probability that the next step of this particle will take place at time $\tau+\tau'$ and be in the direction $\boldsymbol{\delta}'$ is $W_{\tau'}(\boldsymbol{\delta}', -\boldsymbol{\delta})$. We can continue in this way and, clearly, once the first step of the tagged particle has taken place, the 16 time-dependent quantities $W_\tau(\boldsymbol{\delta}, \boldsymbol{\delta}')$ (with $\boldsymbol{\delta}$, $\boldsymbol{\delta}'$ nearest neighbor vectors) suffice to describe the motion of the tagged particle. From time-reversal invariance of the Brownian paths we have the symmetry property

$$W_\tau(\boldsymbol{\delta}, \boldsymbol{\delta}') = W_\tau(\boldsymbol{\delta}', \boldsymbol{\delta}), \qquad \tau = 0, 1, 2,... \tag{2.4}$$

Taking also into account the other symmetries of the problem, we find that, for each $\tau$, there are only five independent quantities, for which it will be convenient to introduce separate symbols,

$$\begin{aligned} A_\tau &\equiv W_\tau(\mathbf{e}_1, \mathbf{e}_1) \\ A'_\tau &\equiv W_\tau(\mathbf{e}_2, \mathbf{e}_2) \\ B_\tau &\equiv W_\tau(-\mathbf{e}_1, \mathbf{e}_1) \\ B'_\tau &\equiv W_\tau(-\mathbf{e}_2, \mathbf{e}_2) \\ C_\tau &\equiv W_\tau(\mathbf{e}_2, \mathbf{e}_1) \end{aligned} \tag{2.5}$$

The quantities $A_\tau$ and $A'_\tau$, $B_\tau$ and $B'_\tau$, and $C_\tau$ describe the probability of a first return (after a time $\tau$) from directions which are opposite, equal, and perpendicular, respectively, to the direction of departure. In a square geometry (an $L \times L$ or an $\infty \times \infty$ lattice) the additional invariance under rotations over $\pi/2$ reduces the number of independent quantities to three, since then $A'_\tau = A_\tau$ and $B'_\tau = B_\tau$. In view of our calculation for a finite strip (Section 5), we shall pursue the general case here; the simplifications valid for a square geometry will be listed in Section 2.6.

A number of quantities well known in the study of simple random walks can be expressed immediately in terms of the $W_\tau$. First,

$$F_\tau(\mathbf{x}) \equiv \sum_{\boldsymbol{\delta}} W_\tau(\boldsymbol{\delta}, \mathbf{x}), \qquad \tau = 0, 1, 2,..., \mathbf{x} \neq \mathbf{0} \tag{2.6}$$

is the probability that a simple random walker initially at $\mathbf{x} \neq \mathbf{0}$ will hit the origin for the first time at time $\tau$, regardless (for $\tau \geqslant 1$) of its position at time $\tau - 1$. Consequently, $1 - \sum_{\tau=0}^{t} F_\tau(\mathbf{x})$ is the probability that a simple random walker initially at $\mathbf{x}$ has not yet reached the origin at time $t$. In Section 2.4 we shall employ the well-known relation between the generating functions of $F_\tau(\mathbf{x})$ and those of the simple random walk. With the aid of (2.5) two particular instances of (2.6) can be written as

$$\begin{aligned} F_\tau(\mathbf{e}_1) &= A_\tau + B_\tau + 2C_\tau \\ F_\tau(\mathbf{e}_2) &= A'_\tau + B'_\tau + 2C_\tau, \qquad \tau = 0, 1, 2,... \end{aligned} \tag{2.7}$$

Second, let $R_\tau$ be the probability that a simple random walker initially at the origin will return there for the first time after $\tau$ steps. From the fact that the walker's first step is with equal probability to any of the neighbors $\boldsymbol{\delta}$ of the origin, and from relation (2.7), we have that

$$\begin{aligned} R_\tau &= \frac{1}{4} \sum_{\boldsymbol{\delta}} F_{\tau-1}(\boldsymbol{\delta}) \\ &= \frac{1}{2} (A_{\tau-1} + A'_{\tau-1} + B_{\tau-1} + B'_{\tau-1} + 4C_{\tau-1}), \qquad \tau = 1, 2,... \end{aligned} \tag{2.8}$$

Spitzer[8] has shown that $R_\tau$ decays very slowly with $\tau$. Explicitly,

$$R_\tau \simeq [1 + (-1)^\tau] \frac{\pi}{\tau \ln^2 \tau} \qquad \text{as} \quad \tau \to \infty \tag{2.9}$$

Finally, since in two dimensions it is certain that a simple random walker will eventually arrive at a specified lattice site adjacent to its point of departure, we have the relation

$$\sum_{\tau=0}^{\infty} \sum_{\boldsymbol{\delta}} W_\tau(\boldsymbol{\delta}, \boldsymbol{\delta}') = 1 \tag{2.10}$$

Two things have to be done now: (i) we have to express $P_t(\mathbf{y})$ in terms of the $W_\tau(\boldsymbol{\delta}, \boldsymbol{\delta}')$ and $W_\tau(\boldsymbol{\delta}, \mathbf{x}_0)$; and (ii) we have to express the $W_\tau$ in terms of the simple random walk generating function.

## 2.3. Expressing $P_t(\mathbf{y})$ in the $W_\tau$

From the definition of the $W_\tau(\boldsymbol{\delta}, \boldsymbol{\delta}')$ and the discussion in the preceding subsection it is clear that one can find an expression for $P_t(\mathbf{y})$ by summing over the number of steps $n$ of the tagged particle, over the step directions $\boldsymbol{\delta}_1, \boldsymbol{\delta}_2,..., \boldsymbol{\delta}_n$, and over the lengths of the time intervals $\tau_2,..., \tau_n$ separating the steps, as well as the time intervals $\tau_1$ preceding the first step and $\tau_{n+1}$ elapsed since the last step. Since at the initial time the hole is at

$\mathbf{x}_0$, the expression for $P_t(\mathbf{y})$ depends on $\mathbf{x}_0$. We find, remembering the definition (2.6) of $F_\tau(\mathbf{x})$,

$$P_t(\mathbf{y}) = \delta_{\mathbf{y},\mathbf{0}} \left[ 1 - \sum_{\sigma=0}^{t} F_\sigma(\mathbf{x}_0) \right]$$
$$+ \sum_{n=1}^{\infty} \sum_{\tau_1=1}^{\infty} \cdots \sum_{\tau_n-n=1}^{\infty} \sum_{\tau_{n+1}=0}^{\infty} \delta_{\tau_1+\cdots+\tau_{n+1},t} \sum_{\boldsymbol{\delta}_1} \cdots \sum_{\boldsymbol{\delta}_n} \left[ 1 - \sum_{\sigma=0}^{\tau_{n+1}} F_\sigma(-\boldsymbol{\delta}_n) \right]$$
$$\times \delta_{\boldsymbol{\delta}_1+\cdots+\boldsymbol{\delta}_n,\mathbf{y}} W_{\tau_n}(\boldsymbol{\delta}_n, -\boldsymbol{\delta}_{n-1}) \cdots W_{\tau_n}(\boldsymbol{\delta}_2, -\boldsymbol{\delta}_1) W_{\tau_1}(\boldsymbol{\delta}_1, \mathbf{x}_0) \quad (2.11)$$

where in the $n=1$ term it is to be understood that $-\boldsymbol{\delta}_0 = \mathbf{x}_0$. The first term in (2.11) represents the event that at time $t$ the tagged particle has not stepped yet.

We now define for any time-dependent quantity $X_t$ the (discrete) Laplace transform (or: generating function)

$$\hat{X}(z) \equiv \sum_{t=0}^{\infty} z^t X_t \quad (2.12)$$

Furthermore, we define for any space-dependent quantity $X(\mathbf{y})$ the Fourier transform

$$X^*(\mathbf{q}) \equiv \sum_{\mathbf{y}} [\exp(i\mathbf{q}\cdot\mathbf{y})]\, X(y) \quad (2.13)$$

where the sum runs through the whole lattice and $\mathbf{q}$ takes the values

$$q_i = 2\pi k_i/L_i, \qquad k_i = 0, 1,..., L_i - 1, \quad i = 1, 2 \quad (2.14)$$

The Fourier–Laplace transform of Eq. (2.11) for $P_t(\mathbf{y})$ is

$$\hat{P}^*(\mathbf{q}; z) = \frac{1 - \hat{F}(\mathbf{x}_0; z)}{1-z}$$
$$+ \frac{1}{1-z} \sum_{\boldsymbol{\alpha}} \sum_{\boldsymbol{\beta}} [1 - \hat{F}(-\boldsymbol{\alpha}; z)]\, I - \hat{T}(\mathbf{q}; z)^{-1}_{\boldsymbol{\alpha},\boldsymbol{\beta}}\, \hat{T}_{\boldsymbol{\beta},-\mathbf{x}_0}(\mathbf{q}; z)$$

where $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ run through $\pm\mathbf{e}_1$, $\pm\mathbf{e}_2$, we have defined

$$\hat{T}_{\boldsymbol{\alpha},\mathbf{x}}(\mathbf{q}; z) \equiv [\exp(i\mathbf{q}\cdot\boldsymbol{\alpha})]\, \hat{W}(\boldsymbol{\alpha}, -\mathbf{x}; z) \quad (2.16)$$

and $[I - \hat{T}(\mathbf{q}; z)]^{-1}$ is the matrix inverse of the $4\times 4$ block with matrix elements $\delta_{\boldsymbol{\alpha},\boldsymbol{\beta}} - \hat{T}_{\boldsymbol{\alpha},\boldsymbol{\beta}}(\mathbf{q}; z)$. The $\hat{F}(\mathbf{x}; z)$ can be eliminated from (2.15) with the aid of the Laplace transform of (2.6) and of (2.16), which together give

$$\hat{F}(\mathbf{x}; z) = \sum_{\boldsymbol{\delta}} [\exp(-i\mathbf{q}\cdot\boldsymbol{\delta})]\, \hat{T}_{\boldsymbol{\delta},-\mathbf{x}}(\mathbf{q}; z), \qquad \mathbf{x} \neq \mathbf{0} \quad (2.17)$$

Substituting this in Eq. (2.15) and using that $I + \hat{T}(I-\hat{T})^{-1} = (I-\hat{T})^{-1}$, we obtain

$$\hat{P}^*(\mathbf{q}; z) = \frac{1}{1-z}\left\{1 + \sum_{\alpha}\sum_{\beta}[1-\exp(-i\mathbf{q}\cdot\boldsymbol{\alpha}) \times [I-\hat{T}(\mathbf{q}; z)]^{-1}_{\alpha,\beta}\,\hat{T}_{\beta,-\mathbf{x}_0}(\mathbf{q}; z)\right\} \tag{2.18}$$

From (2.5), (2.12), and definition (2.16) of $\hat{T}_{\alpha,\mathbf{x}}(\mathbf{q}; z)$ we have

$$\hat{T}(\mathbf{q}; z) = \begin{pmatrix} e^{iq_1}\hat{B}(z) & e^{iq_1}\hat{A}(z) & e^{iq_1}\hat{C}(z) & e^{iq_1}\hat{C}(z) \\ e^{-iq_1}\hat{A}(z) & e^{-iq_1}\hat{B}(z) & e^{-iq_1}\hat{C}(z) & e^{-iq_1}\hat{C}(z) \\ e^{iq_2}\hat{C}(z) & e^{iq_2}\hat{C}(z) & e^{iq_2}\hat{B}'(z) & e^{iq_2}\hat{A}'(z) \\ e^{-iq_2}\hat{C}(z) & e^{-iq_2}\hat{C}(z) & e^{-iq_2}\hat{A}'(z) & e^{-iq_2}\hat{B}'(z) \end{pmatrix} \tag{2.19}$$

where the rows and columns correspond to the lattice vectors $\mathbf{e}_1$, $-\mathbf{e}_1$, $\mathbf{e}_2$, and $-\mathbf{e}_2$, respectively. We define

$$\mathscr{D}(\mathbf{q}; z) \equiv \det[I - \hat{T}(\mathbf{q}; z)] \tag{2.20}$$

Evaluating this determinant, we find

$$\mathscr{D}(\mathbf{q}; z) = (1 - 2\hat{B}\cos q_1 + \hat{B}^2 - \hat{A}^2)[1 - 2\hat{B}'\cos q_2 + (\hat{B}')^2 - (\hat{A}')^2] + 4\hat{C}^2(\hat{B} - \hat{A} - \cos q_1)(\hat{B}' - \hat{A}' - \cos q_2) \tag{2.21}$$

where, for notational simplicity, the $z$ dependence of $\hat{A}$,..., $\hat{C}$ is indicated only implicitly by the caret. We shall simplify Eq. (2.18) further with the aid of the definition

$$\hat{U}_{\beta}(\mathbf{q}; z)\,\mathscr{D}^{-1}(\mathbf{q}; z) \equiv \sum_{\alpha}[1-\exp(-i\mathbf{q}\cdot\boldsymbol{\alpha})][I-\hat{T}(\mathbf{q}; z)]^{-1}_{\alpha,\beta}\exp(i\mathbf{q}\cdot\boldsymbol{\beta}) \tag{2.22}$$

The expression (2.18) for $\hat{P}^*(\mathbf{q}; z)$ then takes the form

$$\hat{P}^*(\mathbf{q}; z) = \frac{1}{1-z}\left[1 + \mathscr{D}^{-1}(\mathbf{q}; z)\sum_{\beta}\hat{U}_{\beta}(\mathbf{q}; z)\,\hat{W}(\boldsymbol{\beta}, \mathbf{x}_0; z)\right] \tag{2.23}$$

A straightforward but tedious calculation yields

$$\begin{aligned}\hat{U}_{\mathbf{e}_1}(\mathbf{q}; z) &\equiv V(q_1, q_2; \hat{A}, \hat{A}', \hat{B}, \hat{B}', \hat{C}) \\ &= [(\hat{A}')^2 - (\hat{B}')^2 + 2\hat{B}'\cos q_2 - 1][\hat{B} + e^{iq_1}(\hat{A}-1)](1-e^{-iq_1}) \\ &\quad - 2\hat{C}(\hat{A}' - \hat{B}' - 1)(\hat{B} - \hat{A} - e^{iq_1})(1 - \cos q_2) \\ &\quad - 4i\hat{C}^2(\hat{A}' - \hat{B}' + \cos q_2)\sin q_1\end{aligned} \tag{2.24}$$

and from this we have by symmetry

$$\begin{aligned} \hat{U}_{-\mathbf{e}_1}(\mathbf{q}; z) &= V(-q_1, q_2; \hat{A}, \hat{A}', \hat{B}, \hat{B}', \hat{C}) \\ \hat{U}_{\mathbf{e}_2}(\mathbf{q}; z) &= V(q_2, q_1; \hat{A}', \hat{A}, \hat{B}', \hat{B}, \hat{C}) \\ \hat{U}_{-\mathbf{e}_2}(\mathbf{q}; z) &= V(-q_2, q_1; \hat{A}', \hat{A}, \hat{B}', \hat{B}, \hat{C}) \end{aligned} \tag{2.25}$$

Equation (2.23) for $\hat{P}^*(\mathbf{q}; z)$, together with the expressions (2.24) and (2.25) for $\hat{U}$ and (2.21) for $\mathscr{D}$, constitutes the final result of this section, and with this we have completed the first of the two tasks set at the end of Section 2.2.

## 2.4. Expressing the $W_\tau$ in the Simple Random Walk Generating Function

The second task is to find an expression for the $W_\tau$ in terms of the simple random walk generating function. We shall need the following definitions and properties, which can all be found in any introductory discussion of random walks.[8–12] Let $G_t(\mathbf{x})$, for $t = 0, 1,...$ and $\mathbf{x}$ arbitrary, denote the probability of finding a simple random walker at time $t$ on lattice site $\mathbf{x}$, given that at $t = 0$ it started at $\mathbf{x} = \mathbf{0}$. Then

$$\hat{G}(\mathbf{x}; z) = \frac{1}{L_1 L_2} \sum_{\mathbf{p}} \frac{\exp(-i\mathbf{p} \cdot \mathbf{x})}{1 - 1/2z(\cos p_1 + \cos p_2)} \tag{2.26}$$

where the wavevector $\mathbf{p} = (p_1, p_2)$ runs through the same values as $\mathbf{q}$ in Eq. (2.14). This function satisfies

$$\frac{z}{4} \sum_{\boldsymbol{\delta}} \hat{G}(\mathbf{x} + \boldsymbol{\delta}; z) - \hat{G}(\mathbf{x}; z) = -\delta_{\mathbf{x},\mathbf{0}} \tag{2.27}$$

from which, upon putting $\mathbf{x} = \mathbf{0}$ and using that $\hat{G}(\mathbf{x}; z) = \hat{G}(-\mathbf{x}; z)$, we have

$$1/2z[\hat{G}(\mathbf{e}_1; z) + \hat{G}(\mathbf{e}_2; z)] = \hat{G}(\mathbf{0}; z) - 1 \tag{2.28}$$

Another useful relation is[9,11,12]

$$\hat{F}(\mathbf{x}; z) = \hat{G}(\mathbf{x}; z)/\hat{G}(\mathbf{0}; z), \qquad \mathbf{x} \neq \mathbf{0} \tag{2.29}$$

where we used that $F_t(-\mathbf{x}) = F_t(\mathbf{x})$. The function

$$\mathscr{G}(\mathbf{x}; z) \equiv \hat{G}(\mathbf{x}; z) - \hat{G}(\mathbf{0}; z) \tag{2.30}$$

has the property that, whereas $\lim_{z \uparrow 1} \hat{G}(\mathbf{x}; z) = \infty$, the *lattice Green* *function* $\mathscr{G}(\mathbf{x}; 1)$ is finite for all $\mathbf{x}$, as is easily seen with the aid of (2.26). For the infinite lattice it has the asymptotic behavior[8]

$$\mathscr{G}(\mathbf{x}; 1) \simeq -\frac{2}{\pi} \ln x, \qquad x \to \infty \tag{2.31}$$

In order to obtain an equation from which we can solve $W_\tau(\boldsymbol{\delta}, \mathbf{x})$ we shall follow a procedure similar to the one that leads to (2.29). We first observe that the probability for a simple random walker (starting at $t=0$ at the origin) to be at time $t-1$ at $\mathbf{x}+\boldsymbol{\delta}$ *and* at time $t$ at $\mathbf{x}$ (with $\mathbf{x} \neq \mathbf{0}$ and $t=1, 2,\ldots$) is given by $\frac{1}{4}G_{t-1}(\mathbf{x}+\boldsymbol{\delta})$. We next write this quantity as the probability that the visit at time $t$ to the site $\mathbf{x}$ was the *first* visit to that site, *plus* the sum on $t'$ of the probability $F_{t'}(\mathbf{x})$ that the first visit to $\mathbf{x}$ has taken place at some earlier time $t'$ multiplied by the probability $\frac{1}{4}G_{t-1-t'}(\boldsymbol{\delta})$ of going from $\mathbf{x}$ to $\mathbf{x}+\boldsymbol{\delta}$ after $t-1-t'$ steps, and to $\mathbf{x}$ after $t-t'$ steps. Explicitly,

$$\frac{1}{4} G_{t-1}(\mathbf{x}+\boldsymbol{\delta}) = W_t(\boldsymbol{\delta}, -\mathbf{x}) + \frac{1}{4} \sum_{t'=0}^{t-1} F_{t'}(\mathbf{x})\, G_{t-1-t'}(\boldsymbol{\delta}) \tag{2.32}$$

$$t=1, 2,\ldots, \qquad \mathbf{x} \neq \mathbf{0}$$

We multiply this equation by $z^t$, sum on $t$ from 1 to $\infty$, and obtain, using (2.29),

$$\hat{W}(\boldsymbol{\delta}, -\mathbf{x}; z) = \frac{z}{4}\left[\hat{G}(\mathbf{x}+\boldsymbol{\delta}; z) - \frac{\hat{G}(\mathbf{x}; z)\, \hat{G}(\boldsymbol{\delta}; z)}{\hat{G}(\mathbf{0}; z)}\right], \qquad \mathbf{x} \neq \mathbf{0} \tag{2.33}$$

This is the desired expression for $\hat{W}$ in terms of the simple random walk generating function $\hat{G}$, and with this we have completed the second task set at the end of Section 2.2. We specialize it first of all to the case that $\mathbf{x}$ is a nearest neighbor vector. From (2.33) and the Laplace transforms of the definitions (2.5) we find

$$\begin{aligned}
\hat{A}(z) &= \frac{z}{4}\left[\hat{G}(\mathbf{0}; z) - \frac{\hat{G}^2(\mathbf{e}_1; z)}{\hat{G}(\mathbf{0}; z)}\right] \\
\hat{B}(z) &= \frac{z}{4}\left[\hat{G}(2\mathbf{e}_1; z) - \frac{\hat{G}^2(\mathbf{e}_1; z)}{\hat{G}(\mathbf{0}; z)}\right] \\
\hat{C}(z) &= \frac{z}{4}\left[\hat{G}(\mathbf{e}_1+\mathbf{e}_2; z) - \frac{\hat{G}(\mathbf{e}_1; z)\, \hat{G}(\mathbf{e}_2; z)}{\hat{G}(\mathbf{0}; z)}\right]
\end{aligned} \tag{2.34}$$

The expressions for $\hat{A}'(z)$ and $\hat{B}'(z)$ are found from those for $\hat{A}(z)$ and $\hat{B}(z)$, respectively, by replacing $\mathbf{e}_1$ with $\mathbf{e}_2$. Equivalent relations occur in refs. 1, 3, and 5 and were apparently first derived by Benoist *et al.*[13] From (2.7) together with (2.12), (2.29), and (2.30) we have the useful relations

$$\begin{aligned}\hat{A}(z)+\hat{B}(z)+2\hat{C}(z)&=\hat{F}(\mathbf{e}_1;z)=1+\frac{\mathscr{G}(\mathbf{e}_1;z)}{\hat{G}(\mathbf{0};z)}\\ \hat{A}'(z)+\hat{B}'(z)+2\hat{C}(z)&=\hat{F}(\mathbf{e}_2;z)=1+\frac{\mathscr{G}(\mathbf{e}_2;z)}{\hat{G}(\mathbf{0};z)}\end{aligned} \tag{2.35}$$

In particular, in view of the finiteness of $\mathscr{G}(\mathbf{x};1)$ for all $\mathbf{x}$ and the fact that $\lim_{z\uparrow 1}\hat{G}(\mathbf{x};z)=\infty$, we find from (2.35)

$$\begin{aligned}\hat{A}(1)+\hat{B}(1)+2\hat{C}(1)&=1\\ \hat{A}'(1)+\hat{B}'(1)+2\hat{C}(1)&=1\end{aligned} \tag{2.36}$$

Since $\hat{A}(1)=\sum_{\tau=0}^{\infty}A_\tau$, etc., these relations just tell us that a two-dimensional random walk is recurrent.

### 2.5. The Effective Propagator $\mathscr{D}$

We now have to calculate the inverse Fourier and Laplace transform

$$P_t(\mathbf{y})=\frac{1}{L_1L_2}\sum_{\mathbf{q}}\exp(-i\mathbf{q}\cdot\mathbf{y})\frac{1}{2\pi i}\oint\frac{dz}{z^{t+1}}\hat{P}^*(\mathbf{q};z) \tag{2.37}$$

where the integral is around the origin of the complex $z$ plane. Hence our task will be to determine the analytic structure of $\hat{P}^*(\mathbf{q};z)$. The main structure is entirely contained in the denominator $\mathscr{D}(\mathbf{q};z)$ in (2.21), which plays the role of an effective propagator, analogous to the denominator in the integrand of the expression (2.26) for the simple random walk.

It is not possible to determine the zeros of $\mathscr{D}(\mathbf{q};z)$ exactly. We shall therefore make a long-time expansion, for which the only knowledge required is the behavior of $\mathscr{D}(\mathbf{q};z)$ around its singular point nearest to $z=0$. When $\mathbf{q}=\mathbf{0}$ this is the point $z=1$. One readily verifies this from (2.21), which gives

$$\begin{aligned}\mathscr{D}(\mathbf{0};1)&=[1-\hat{B}(1)+\hat{A}(1)][1-\hat{B}'(1)+\hat{A}'(1)]\\ &\quad\times\{[1-\hat{B}(1)-\hat{A}(1)][1-\hat{B}'(1)-\hat{A}'(1)]-4\hat{C}^2(1)\}\\ &=0\end{aligned} \tag{2.38}$$

where the second equality follows from the relations (2.36) between $\hat{A}(1)$, $\hat{A}'(1)$,..., $\hat{C}(1)$. For $\mathbf{q}$ different from zero this singularity shifts to $z$ values larger than 1. Hence, our small-$(z-1)$ expansion has to be accompanied by a small-$\mathbf{q}$ expansion. This will be done separately for the three lattice geometries of interest in Sections 3–5.

### 2.6. Simplified Formulas for a Square Geometry

In Sections 3 and 4 we shall specialize to square geometries (an $\infty \times \infty$ lattice and an $L \times L$ lattice, respectively). The extra invariance under rotations over $\pi/2$ then allows us to simplify the formulas derived above in the following way. We have

$$\begin{aligned} A'_\tau &= A_\tau, & B'_\tau &= B_\tau \\ \hat{A}'(z) &= \hat{A}(z), & \hat{B}'(z) &= \hat{B}(z) \end{aligned} \tag{2.39}$$

It is now useful to define

$$G(z) \equiv \hat{G}(\mathbf{0}; z) \tag{2.40a}$$

$$g(z) \equiv -\tfrac{1}{2}[\hat{G}(2\mathbf{e}_1; z) - \hat{G}(\mathbf{0}; z)] \tag{2.40b}$$

Equation (2.28) then reduces to

$$\hat{G}(\pm\mathbf{e}_i; z) = \frac{1}{z}[G(z) - 1] \tag{2.41}$$

and, upon using (2.27) for $\mathbf{x}$ equal to a nearest neighbor vector, we find

$$\hat{G}(\pm\mathbf{e}_1 \pm \mathbf{e}_2; z) = \left(\frac{2}{z^2} - 1\right) G(z) - \frac{2}{z^2} + g(z) \tag{2.42}$$

Using the general results (2.34), one then obtains the simplified expressions

$$\begin{aligned} \hat{A}(z) &= \frac{1}{4z}\left[2 - \frac{1}{G(z)} - (1 - z^2)\, G(z)\right] \\ \hat{B}(z) &= \frac{1}{4z}\left\{2[1 - z^2 g(z)] - \frac{1}{G(z)} - (1 - z^2)\, G(z)\right\} \\ \hat{C}(z) &= \frac{1}{4z}\left[z^2 g(z) - \frac{1}{G(z)} + (1 - z^2)\, G(z)\right] \end{aligned} \tag{2.43}$$

These show that the two functions $G(z)$ and $g(z)$ contain all important information.

## 3. INFINITE LATTICE

### 3.1. Expansion of $\hat{P}^*(\mathbf{q}; z)$ for Small q and $z-1$

We shall now evaluate expression (2.37) for $P_t(\mathbf{y})$ for an infinite lattice. We first expand $\hat{P}^*(\mathbf{q}; z)$ for small $\mathbf{q}$ and $z-1$. If we let $K$ denote the elliptic integral of the first kind, then for the infinite square lattice we have from Eqs. (2.40a), (2.40b), and (2.26)

$$\begin{aligned} G(z) &= \frac{1}{(2\pi)^2} \iint_{-\pi}^{\pi} d\mathbf{q} \, \frac{1}{1-\frac{1}{2}z(\cos q_1 + \cos q_2)} \\ &= \frac{2}{\pi} K(z^2) \\ &= \frac{1}{\pi} \ln\left(\frac{8}{1-z}\right) - \frac{1}{2\pi}(1-z)\ln(1-z) + \mathcal{O}(1-z), \qquad z \to 1 \end{aligned} \tag{3.1}$$

(see ref. 14) and

$$\begin{aligned} g(z) &= \frac{1}{(2\pi)^2} \iint_{-\pi}^{\pi} d\mathbf{q} \, \frac{\sin^2 q_1}{1-\frac{1}{2}z(\cos q_1 + \cos q_2)} \\ &= \left(2 - \frac{4}{\pi}\right) + \frac{2}{\pi}(1-z)\ln(1-z) + \mathcal{O}(1-z), \qquad z \to 1 \end{aligned} \tag{3.2}$$

[cf. McCrea and Whipple,[15] who calculated $g(1)$]. Using these expansions in the formulas (2.43) for $\hat{A}(z)$, $\hat{B}(z)$, and $\hat{C}(z)$, one finds

$$\begin{aligned} \hat{A}(z) &= \frac{1}{2} - \frac{\pi}{4\ln[8/(1-z)]} + \frac{1}{2\pi}(1-z)\ln(1-z) + \mathcal{O}(1-z) \\ \hat{B}(z) &= \left(\frac{2}{\pi} - \frac{1}{2}\right) - \frac{\pi}{4\ln[8/(1-z)]} - \frac{1}{2\pi}(1-z)\ln(1-z) + \mathcal{O}(1-z) \\ \hat{C}(z) &= \left(\frac{1}{2} - \frac{1}{\pi}\right) - \frac{\pi}{4\ln[8/(1-z)]} + \mathcal{O}(1-z) \end{aligned} \tag{3.3}$$

From Eq. (3.3) we see that the motion of the tagged particle is strongly anticorrelated; the probability for the particle to step in the direction *opposite* to its previous move is $\hat{A}(1) = 0.5$; the probability to step in a *perpendicular* direction is $\hat{C}(1) = 0.1816...$; and the probability to step once more in the *same* direction is $\hat{B}(1) = 0.1366....$ The leading correction terms in Eq. (3.3) can be used to find the long-time behavior of $A_t$, $B_t$, and $C_t$:

$$X_t \simeq [1 + (-1)^{t+1}] \frac{\pi}{4t \ln^2 t}, \qquad t \to \infty, \qquad X = A, B, C \tag{3.4}$$

Clearly $\sum_{t=0}^{\infty} X_t$ is finite, as it should be. Furthermore, the long-time behavior is compatible with the asymptotic result (2.9) for $R_t$.

After these preliminaries we are able to expand $\hat{P}^*(\mathbf{q}; z)$ around $(\mathbf{q}; z) = (\mathbf{0}; 1)$. To this end we first consider Eq. (2.21) for $\mathscr{D}(\mathbf{q}; z)$ and find

$$\mathscr{D}(\mathbf{q}; z) = \frac{1}{4} g \left(1 - \frac{1}{4} g^2\right) q^2 + \pi g \left(1 + \frac{1}{2} g\right)^2 \frac{1}{\ln[8/(1-z)]} + \dots, \qquad q \to 0, \quad z \to 1 \tag{3.5}$$

where the dots indicate terms of higher order in $q^2$ and/or in $1/\ln[8/(1-z)]$, and where

$$g \equiv g(1) = 2 - 4/\pi \tag{3.6}$$

The first two terms in this expansion can be controlled independently and become of comparable magnitude when

$$q^2 \sim \frac{1}{\ln[8/(1-z)]} \tag{3.7}$$

This relation will serve to compare orders of $q$ to orders of $1/\ln[8/(1-z)]$ and will eventually determine how distance scales with time in $P_t(\mathbf{y})$.

Considering Eqs. (2.24) and (2.25) for the four $\hat{U}_{\boldsymbol{\beta}}(\mathbf{q}; \mathbf{z})$, we find, upon expanding these expressions in powers of $q_1$ and $q_2$, that the coefficients of the linear terms become proportional to $1/\ln[8/(1-z)]$ for $z \to 1$. But hence, by Eq. (3.7), they are effectively of third order in $q$. The coefficients of the quadratic terms, however, tend to finite values as $z \to 1$, and we get explicitly

$$\hat{U}_{\boldsymbol{\beta}}(\mathbf{q}; z) \simeq -\frac{1}{4} g \left(1 - \frac{1}{4} g^2\right) q^2, \qquad q \to 0, \quad z \to 1 \tag{3.8}$$

which is independent of $\boldsymbol{\beta}$. It remains to evaluate

$$\begin{aligned} \sum_{\boldsymbol{\beta}} \hat{W}(\boldsymbol{\beta}, \mathbf{x}_0; z) &= \hat{F}(\mathbf{x}_0; z) \\ &= 1 + \mathscr{G}(\mathbf{x}_0; z)/G(z) \\ &= 1 + \pi \mathscr{G}(\mathbf{x}_0; 1)/\ln\left(\frac{8}{1-z}\right) + \dots, \qquad z \to 1 \end{aligned} \tag{3.9}$$

where we have used, successively, (2.6), (2.29), (2.30), (2.40a), and (3.1). From the asymptotic expression (2.31) we see that the first term in (3.9) dominates the remainder if the initial hole position $\mathbf{x}_0$ satisfies

$$2 \ln x_0 \ll \ln\left(\frac{8}{1-z}\right) \tag{3.10}$$

We shal henceforth consider only $\mathbf{x}_0$ for which this condition holds. Upon using (3.5), (3.8), and (3.9) in (2.23), we obtain

$$\hat{P}^*(\mathbf{q}; z) \simeq \frac{1}{(1-z)\{1+fq^2 \ln[8/(1-z)]\}}, \qquad q \to 0, \quad z \to 1 \quad (3.11)$$

where we have defined

$$f \equiv \frac{1}{4\pi} \frac{2-g}{2+g} = \frac{1}{4\pi(\pi-1)} \quad (3.12)$$

Equation (3.11) is the final result of the expansion of $\hat{P}^*$ for small $\mathbf{q}$ and $(1-z)$.

### 3.2. Results for $P_t(\mathbf{y})$

Now (3.11) has to be substituted in (2.37) and the $z$ and $\mathbf{q}$ integrals have to be carried out. The quantity $\ln(1-z)$ occurring in (3.11) causes the integrand to have a branch cut, starting at $z=1$, which we may take along the positive real axis. Due to the factor $z-1$ in the denominator of the integrand in (3.11), the leading contributions to the integral come, for $t \to \infty$, from the neighborhood of $z=1$. We may therefore fold the contour around the branch cut and integrate the discontinuity of the integrand. This gives

$$P_t(\mathbf{y}) \simeq \frac{1}{(2\pi)^2} \iint_{-\pi}^{\pi} d\mathbf{q} \exp(-i\mathbf{q}\cdot\mathbf{y}) \times \int_1^\infty \frac{dz}{z^{t+1}} \frac{1}{z-1} \frac{fq^2}{\{1+fq^2 \ln[8/(z-1)]\}^2 + (fq^2\pi)^2}, \qquad t \to \infty \quad (3.13)$$

In terms of new integration variables $\boldsymbol{\kappa}$ and $w$ defined by

$$\mathbf{q} \equiv (\ln t)^{-1/2} \boldsymbol{\kappa} \quad (3.14a)$$

$$z \equiv 1 + 8/t^w \quad (3.14b)$$

the expression for $P_t(\mathbf{y})$ becomes

$$P_t(\mathbf{y}) \simeq \frac{1}{\ln t} \frac{1}{(2\pi)^2} \iint_{-\pi(\ln t)^{1/2}}^{\pi(\ln t)^{1/2}} d\boldsymbol{\kappa} \exp\left[-i\boldsymbol{\kappa}\cdot\frac{\mathbf{y}}{(\ln t)^{1/2}}\right] \times \int_{-\infty}^{\infty} \frac{dw}{(1+8/t^w)^{t+1}} \frac{f\kappa^2}{(1+f\kappa^2 w)^2 + (f\kappa^2\pi/\ln t)^2}, \qquad t \to \infty \quad (3.15)$$

Although in the derivation of this formula the $y_i$ ($i=1, 2$) were assumed to take only integer values, the formula itself can also be used for noninteger values for the $y_i$. We now discuss two cases.

**3.2.1. The Scaling Limit: $y/(\ln t)^{1/2}$ Fixed, $t \to \infty$, $y \to \infty$.** In this limit one finds from (3.15), with $\boldsymbol{\eta} = \mathbf{y}/(\ln t)^{1/2}$,

$$\begin{aligned} P_t(\mathbf{y}) &\simeq \frac{1}{\ln t}\frac{1}{(2\pi)^2}\iint_{-\infty}^{\infty} d\boldsymbol{\kappa}\,[\exp(-i\boldsymbol{\kappa}\cdot\boldsymbol{\eta})]\,f\kappa^2\int_1^{\infty}\frac{dw}{(1+fw\kappa^2)^2} \\ &= \frac{1}{\ln t}\frac{1}{(2\pi)^2}\iint_{-\infty}^{\infty} d\boldsymbol{\kappa}\,\frac{\exp(-i\boldsymbol{\kappa}\cdot\boldsymbol{\eta})}{1+f\kappa^2} \\ &= \frac{1}{\ln t}\frac{1}{(2\pi)^2}\iint_{-\infty}^{\infty} d\boldsymbol{\kappa}\,\exp(-i\boldsymbol{\kappa}\cdot\boldsymbol{\eta})\int_0^{\infty} d\lambda\,\exp[-\lambda(1+f\kappa^2)] \end{aligned} \tag{3.16}$$

The integrals on $\boldsymbol{\kappa}$ are Gaussian and easily carried out. The remaining integral on $\lambda$ is found to represent the modified Bessel function $K_0$, and the final result is

$$P_t(\mathbf{y}) \simeq \frac{2(\pi-1)}{\ln t}K_0\left(\left(\frac{4\pi(\pi-1)}{\ln t}\right)^{1/2} y\right), \quad \frac{\mathbf{y}}{(\ln t)^{1/2}} \text{ fixed}, \quad y, t \to \infty \tag{3.17}$$

Hence $P_t(\mathbf{y})$ is *non-Gaussian*! With the aid of the integral (ref. 16, p. 388)

$$\int_0^{\infty} dx\, x^{1+2\nu}K_0(x) = 2^{2\nu}\Gamma^2(\nu+1) \tag{3.18}$$

one easily verifies that $P_t(\mathbf{y})$ is properly normalized and that

$$\langle y^2 \rangle = \frac{\ln t}{\pi(\pi-1)} \tag{3.19}$$

The main features of the behavior of (3.17) follow from the properties[17]

$$K_0(x) \simeq \begin{cases} -\ln x, & x \downarrow 0 \\ (\pi/2x)^{1/2}\,e^{-x}, & x \to \infty \end{cases} \tag{3.20}$$

A particularity is that $P_t(\mathbf{y})$ has a logarithmic singularity when $\mathbf{y}/(\ln t)^{1/2}$ becomes small. This provides a reason for also studying a second limit.

**3.2.2. The limit $t \to \infty$ at Fixed $\mathbf{y}$.** Upon employing in (3.13) expression (3.14b), but not (3.14a), we get

$$\begin{aligned} P_t(\mathbf{y}) \simeq{}& \frac{1}{\ln t}\frac{1}{(2\pi)^2}\iint_{-\pi}^{\pi} d\mathbf{q}\,\exp(-i\mathbf{q}\cdot\mathbf{y}) \\ &\times \int_{-\infty}^{\infty}\frac{dw}{(1+8/t^w)^{t+1}}\,\frac{fq^2}{(1/\ln t + fq^2w)^2 + (fq^2\pi/\ln t)^2}, \quad t \to \infty \end{aligned} \tag{3.21}$$

We now first observe that, for $t \to \infty$ and for all $w < 1$, $(1 + 8t^{-w})^{-(t+1)}$ tends to zero faster than any power of $t$. Hence, we may let the $w$ integration run from 1 to $\infty$. If in the integrand we then set $t = \infty$, it reduces to $1/fw^2q^2$, and the $\mathbf{q}$ integral diverges in the origin. Therefore, more care is required near $\mathbf{q} = \mathbf{0}$, and we now employ the scaling (3.14a) in (3.21). Also using that, for $w > 1$, $(1 + 8t^{-w})^{-(t+1)} \sim \exp(-8t^{1-w}) \to 1$ as $t \to \infty$, we find

$$P_t(\mathbf{y}) \simeq \frac{1}{\ln t} \frac{1}{(2\pi)^2} \iint_{-\pi(\ln t)^{1/2}}^{\pi(\ln t)^{1/2}} d\boldsymbol{\kappa} \exp\left[ - \frac{i\boldsymbol{\kappa} \cdot \mathbf{y}}{(\ln t)^{1/2}} \right] \times \int_1^\infty dw \frac{f\kappa^2}{(1 + fw\kappa^2)^2 + (f\kappa^2\pi/\ln t)^2} \tag{3.22}$$

We can set $t = \infty$ in the integrand of (3.22) without creating any divergences. This yields

$$P_t(\mathbf{y}) \simeq \frac{1}{\ln t} \frac{1}{(2\pi)^2} \iint_{-\pi(\ln t)^{1/2}}^{\pi(\ln t)^{1/2}} d\boldsymbol{\kappa} \frac{1}{1 + f\kappa^2} \tag{3.23}$$

For $t \to \infty$ the integral diverges at large $\kappa$. Since we are only interested in the leading behabvio, we can write, using the value (3.12) for $f$,

$$\begin{aligned} P_t(\mathbf{y}) &\simeq \frac{2(\pi - 1)}{\ln t} \int^{\pi(\ln t)^{1/2}} d\kappa \frac{1}{\kappa} \\ &\simeq (\pi - 1) \frac{\ln \ln t}{\ln t}, \qquad \mathbf{y} \text{ fixed}, \quad t \to \infty \end{aligned} \tag{3.24}$$

This expression shows how near the origin the distribution function $P_t(\mathbf{y})$ decays to zero. It should be contrasted with the decay

$$G_t(\mathbf{y}) \simeq 1/\pi t, \qquad \mathbf{y} \text{ fixed}, \quad t \to \infty \tag{3.25}$$

which follows from (2.26) for a simple random walk.

Finally we recall that both results (3.17) and (3.24) hold subject to the condition that the hole is initially not too far away from the particle; explicitly, we should have

$$2 \ln x_0 \ll \ln t \tag{3.26}$$

as may be deduced from (3.10), (3.14b), and the fact that the $w$ integrals in (3.16) and (3.22) do not get any significant contributions from the region $w < 1$.

## 4. $L \times L$ LATTICE

In this section we evaluate the expression (2.37) for $P_t(\mathbf{y})$ for a square lattice of $L \times L$ sites with periodic boundary conditions. Since we are again dealing with a square geometry, we can express $\hat{A}(z)$, $\hat{B}(z)$, and $\hat{C}(z)$ in terms of $G(z)$ and $g(z)$ with the aid of the simplified formulas of Section 2.6. The only difference with the calculation of Section 3 is that $G(z)$ and $g(z)$ are now given not by integrals but by sums on $\mathbf{q}$; we indicate this explicitly by writing these functions now as $G_L(z)$ and $g_L(z)$, respectively. The following calculation will be for strictly finite $L$.

### 4.1. Expansion of $\hat{P}^*(\mathbf{q}; z)$ for Small q and $z-1$

We must again expand $G_L(z)$ and $g_L(z)$ around the point $z=1$. In this case, too, the expansion of $G_L(z)$ in powers of $(1-z)$ is known[18,19]:

$$G_L(z) = \frac{1}{L^2(1-z)} + a_0(L) - a_1(L)(1-z) + \mathcal{O}[(1-z)^2], \qquad z \to 1 \tag{4.1}$$

where $a_0(L)$ and $a_1(L)$ have been given by Den Hollander and Kasteleyn[19] (but see also ref. 18) as

$$\begin{aligned} a_0(L) &= (2/\pi)\ln L + \mathcal{O}(L^0) \\ a_1(L) &= 0.06187...\, L^2 + \mathcal{O}(\ln L), \qquad L \to \infty \end{aligned} \tag{4.2}$$

From (4.1) we see that as $z \to 1$, the first term in the expansion for $G_L(z)$ will dominate the remainder only if

$$1 - z \ll \begin{cases} 1/L^2 a_0(L), & L \text{ fixed, arbitrary} \\ 1/L^2 \ln L, & L \text{ fixed, large} \end{cases} \tag{4.3}$$

where for the lower inequality (4.2) has been used. The $1-z$ expansion of $g_L(z)$ is easily found from (2.40b):

$$g_L(z) = g_L + [g_L - \tfrac{1}{2} a_0(L)](1-z) + \mathcal{O}[(1-z)^2], \qquad z \to 1 \tag{4.4}$$

where

$$\begin{aligned} g_L &\equiv g_L(1) \\ &= \left(2 - \frac{4}{\pi}\right) - \frac{2}{L^2} + \mathcal{O}\left(\frac{1}{L^4}\right), \qquad L \to \infty \end{aligned} \tag{4.5}$$

Substituting the expansions (4.1) and (4.4) of $G_L(z)$ and $g_L(z)$ in the formulas (2.43) for $\hat{A}(z)$, $\hat{B}(z)$, and $\hat{C}(z)$, one obtains for $z \to 1$

$$\hat{A}(z) = \frac{1}{2}\left(1 - \frac{1}{L^2}\right) - \frac{1}{4}\left[L^2 + 2a_0(L) - 2 + \frac{1}{L^2}\right](1-z) + \mathcal{O}[(1-z)^2]$$

$$\hat{B}(z) = \frac{1}{2}\left(1 - \frac{1}{L^2} - g_L\right) - \frac{1}{4}\left[L^2 + a_0(L) - 2 + \frac{1}{L^2}\right](1-z) + \mathcal{O}[(1-z)^2]$$

$$\hat{C}(z) = \frac{1}{4}\left(g_L + \frac{2}{L^2}\right) - \frac{1}{4}\left[L^2 - \frac{3}{2}a_0(L) - \frac{1}{L^2}\right](1-z) + \mathcal{O}[(1-z)^2] \qquad (4.6)$$

Just as in Eq. (3.3), the quantities $\hat{A}(1)$, $\hat{B}(1)$, and $\hat{C}(1)$ represent the correlations between two successive step directions, but now corrected for finite-size effects. We make an expansion of $\mathscr{D}$ for small $\mathbf{q}$ as well as for small $z-1$ by substituting these results in (2.21) and obtain

$$\mathscr{D}(\mathbf{q}; z) = \frac{1}{4}\left(g_L + \frac{2}{L^2}\right)\left(1 - \frac{1}{4}g_L^2\right)q^2 + (L^2 - 1)\left(1 + \frac{1}{2}g_L\right)^2 \times \left(g_L + \frac{2}{L^2}\right)(1-z) + \cdots \qquad (4.7)$$

where the dots indicate terms of higher order in $q^2$ and/or $1-z$. This expansion is valid for

$$q^2 \ll 1, \qquad 1 - z \ll \frac{1}{L^2 a_0(L)}, \qquad L \text{ fixed} \qquad (4.8)$$

We see from it that in the case of a finite lattice the proper scaling relation between $q^2$ and $1-z$ is

$$q^2 \sim L^2(1-z), \qquad L \text{ fixed} \qquad (4.9)$$

instead of (3.7). We now argue as in the case of the infinite lattice that for large $t$ the important term in $\hat{U}_{\boldsymbol{\beta}}$ is the one quadratic in the $q_i$. From this we find

$$\hat{U}_{\boldsymbol{\beta}}(\mathbf{q}; z) \simeq -\frac{1}{4}\left(g_L + \frac{2}{L^2}\right)\left(1 - \frac{1}{4}g_L^2\right)q^2 \qquad (4.10)$$

valid under condition (4.8). Since, just as happened in Eq. (3.8), this result is to lowest order independent of $\boldsymbol{\beta}$, the third quantity in Eq. (2.23) which we have to expand is

$$\sum_{\boldsymbol{\beta}} \hat{W}(\boldsymbol{\beta}, \mathbf{x}_0; z) = 1 + \mathscr{G}(\mathbf{x}_0; z)/G_L(z)$$
$$= 1 + L^2(1-z)\,\mathscr{G}(\mathbf{x}_0; 1) + \mathcal{O}[(1-z)^2], \qquad z \to 1 \qquad (4.11)$$

where we used successively Eqs. (2.6), (2.29), (2.30), and (4.1). Upon using for $\mathscr{G}(\mathbf{x}; 1)$ the large-$x$ expression (2.31), we see that we can replace expression (4.11) by unity if

$$1 - z \ll \frac{1}{L^2 \ln x_0} \tag{4.12}$$

an inequality which in view of (4.8) and (4.3) is certainly satisfied. Hence the results that we shall obtain will be independent of the starting position $\mathbf{x}_0$ of the hole. Substituting the relations (4.7), (4.10), and (4.11) in Eq. (2.23) for $\hat{P}^*(\mathbf{q}; z)$, we find

$$\hat{P}^*(\mathbf{q}; z) \simeq \frac{1}{(1-z) + D_L q^2} \tag{4.13}$$

which is valid under condition (4.8) and where we have defined

$$D_L \equiv \frac{1}{4(L^2-1)} \frac{2-g_L}{2+g_L} \tag{4.14}$$

Equation (4.13) is the finite-lattice analogue of Eq. (3.11).

## 4.2. Results for $P_t(\mathbf{y})$

Expression (4.13) for $\hat{P}^*(\mathbf{q}; z)$ has to be substituted in (2.37) and we have to carry out the inverse Laplace and Fourier transformations. The integrand has only a simple pole at $z = 1 + D_L q^2$, and if we shift the integration contour around this pole, condition (4.3) leads to

$$D_L q^2 \ll \begin{cases} 1/L^2 a_0(L), & L \text{ fixed, arbitrary} \\ 1/L^2 \ln L, & L \text{ fixed, large} \end{cases} \tag{4.15}$$

After performing the $z$ integration we obtain

$$P_t(\mathbf{y}) \simeq \frac{1}{L^2} \sum_{\mathbf{q}} \frac{\exp(-i\mathbf{q}\cdot\mathbf{y})}{(1 + D_L q^2)^{t+1}} \tag{4.16}$$

For $t = \infty$ only the term with $\mathbf{q} = \mathbf{0}$ contributes, so that $P_\infty(\mathbf{y}) = 1/L^2$, as it should be. Since the denominator of the summand in (4.16) has been derived in a small-$q$ expansion, we can relate the scales of $t$ and $q$ as

$$t \sim 1/D_L q^2 \tag{4.17}$$

In view of condition (4.15), this means that the times to be considered are

$$t \gg \begin{cases} L^2 a_0(L), & L \text{ fixed, arbitrary} \\ L^2 \ln L, & L \text{ fixed, large} \end{cases} \tag{4.18}$$

Hence, for large $t$ we have

$$P_t(\mathbf{y}) \simeq \frac{1}{L^2} \sum_{\mathbf{q}} \exp(-i\mathbf{q} \cdot \mathbf{y} - D_L q^2 t) \tag{4.19}$$

subject to the conditions in Eqs. (4.17) and (4.18). This expression shows that the time and space scales are connected by

$$y^2 \sim D_L t \tag{4.20}$$

Equation (4.19) is precisely the probability distribution for a simple random walker which diffuses on a square lattice with diffusion constant $D_L$. Using (4.14) and (4.5), we find

$$D_L = \frac{1}{4(\pi - 1) L^2} \left[ 1 + \frac{\pi^2 + 2\pi - 2}{2(\pi - 1) L^2} + \cdots \right] \quad \text{as} \quad L \to \infty \tag{4.21}$$

of which the first term is the result (1.2).

In the large-$L$ limit we obtain from (4.19) the Gaussian distribution

$$P_t(\mathbf{y}) = \frac{(\pi - 1) L^2}{\pi t} e^{-(\pi - 1) L^2 y^2 / t} \tag{4.22}$$

which, if we combine the conditions (4.18) and (4.20), is valid for

$$t \gg L^2 \ln L, \qquad y^2 \gg \ln L, \qquad L^2 y^2 / t \text{ finite} \tag{4.23}$$

and subject to the obvious condition $t \ll L^4$, which ensures that the distribution is not yet affected by the periodic boundaries of the lattice.

## 4.3. Discussion

**4.3.1. A Heuristic Argument.** This exact finite-lattice calculation gives support to the following heuristic argument. When the hole is near the tagged particle at site $\mathbf{y}$, it needs $\tau_1 \sim L^2$ steps before it reaches one of the periodic boundaries (with respect to the particle) situated at $x_1 = y_1 \pm L/2$ and $x_2 = y_2 \pm L/2$. While executing these steps, it will cause the tagged particle to undergo a mean square displacement $\Delta y^2$, which, on the basis of the infinite-lattice calculation, is given by

$$\Delta y^2 \sim \ln \tau_1 \sim \ln L \tag{4.24}$$

After it crosses one of the two boundaries, the hole will return to the particle from a completely uncorrelated direction (with respect to one of the two Cartesian directions). The time $\tau_2$ needed, after crossing, to return for its next visit to the tagged particle is

$$\tau_2 \sim L^2 \ln L \tag{4.25}$$

(This is because the number of new sites visited by the hole after the instant of crossing increases as $\sim \tau_2/\ln \tau_2$, see refs. 20 and 21; and this number should equal $L^2$ if the tagged particle is to have a reasonable probability to have been visited again.) Hence, the motion of the tagged particle can be decomposed into uncorrelated time intervals of length $\tau_1 + \tau_2 \sim \tau_2 \sim L^2 \ln L$ during each of which it accumulates a mean square displacement $\Delta y^2 \sim \ln L$. Its total mean square displacement after a time $t$ therefore is

$$y^2 \sim (t/\tau_2)\,\Delta y^2 \sim L^{-2} t \tag{4.26}$$

Not only is this in full agreement with the exact result (4.22), but it also explains the conditions of validity (4.23).

**4.3.2. Correlation Factor.** If one is just interested by the result (4.14) for the diffusion constant of the tracer particle, the following shortcut is possible. The diffusion constant of a random walk with correlations between successive jumps can be written[22–24] as the diffusion constant of a corresponding walk with the same jump frequency but uncorrelated jumps, times a correction factor $f_{\text{corr}}$. For the latter one can derive[23,24]

$$f_{\text{corr}} = \frac{1 + \langle \cos\theta \rangle}{1 - \langle \cos\theta \rangle} \tag{4.27}$$

where $\theta$ is the angle between two successive jump vectors and $\langle \cdots \rangle$ is the average over all pairs of successive jumps.

In our specific case we therefore have

$$D_L = D_L^0 f_{\text{corr}} \tag{4.28}$$

where $D_L^0$ refers to the corresponding uncorrelated walk. Both $f_{\text{corr}}$ and $D_L^0$ are easily calculated. First, from the definition of $\hat{A}(z)$, $\hat{B}(z)$, $\hat{C}(z)$, and the small-$(z-1)$ expansion (4.6) we find that

$$\langle \cos\theta \rangle = \hat{B}(1) - \hat{A}(1) = -\tfrac{1}{2} g_L \tag{4.29}$$

For $L \to \infty$ the result for $f_{\text{corr}}$ for the infinite square lattice, as was evaluated by Schoen and Lowen,[25] is recovered. Second, $4D_L^0$ is equal to the jump frequency of the tracer particle, i.e., to the fraction of all time steps for which the hole displaces the tracer particle. In a moving coordinate system in which the tracer particle is at rest, the hole will occupy the $L^2 - 1$ remaining lattice sites with equal probability. From four of these it can make, with probability 1/4, a jump across the tracer particle, so that in the original coordinate frame the tracer jump frequency, and hence $4D_L^0$, is given by

$$4D_L^0 = 1/(L^2 - 1) \tag{4.30}$$

Upon combining Eqs. (4.27)–(4.30), one arrives directly at the expression (4.14) for $D_L$.

**4.3.3. Constrained Dynamics.** The problem of Brownian motion on a finite $L \times L$ lattice with only one vacancy was proposed by Palmer[6] as a microscopic model of constrained dynamics. Such models are of great interest, since constrained dynamics is held responsible for "slow" (i.e., slower than exponential) relaxation in many physical systems (e.g., in spin glasses and ordinary glasses). One slow decay law that has received a great deal of attention is the "stretched exponential decay" $X(t) \sim \exp[-(t/t_0)^p]$, with $0 < p < 1$. Such decay is known to occur, in particular in microscopic diffusion models that possess quenched randomness[12] or in relaxation models with hierarchical constraints.[26] It would be extremely interesting to know if translationally invariant (as opposed to hierarchical) lattice models like the one studied here, which is constrained by the single occupancy condition at each site, can also produce stretched exponential decay. Computer simulation[6] of the model of this section for values of $L$ up to $L = 64$ preliminarily suggested an approximate stretched exponential behavior in the main decay regime. For the Manhattan distance $|y_1| + |y_2|$ considered in ref. 6 we predict, however [indicating the average with respect to the distribution (4.22) by angular brackets]

$$\langle |y_1| + |y_2| \rangle^2 = \frac{4t}{\pi(\pi - 1)\, L^2} = 0.5945... \left(\frac{t}{L^2}\right) \tag{4.31}$$

valid in the regime (4.23), for large $L$, and as long as $t \ll L^4$. Hence, this purely diffusive behavior (albeit on a time scale $L^2$) excludes the appearance of stretched exponentials.

## 5. STRIP OF WIDTH $L$

In this section we study the $t \to \infty$ limit of the probability distribution $P_t(\mathbf{y})$ on a strip of finite width $L$ in the $y_2$ direction and which is infinite in the $y_1$ direction. We proceed again via an expansion of the expression (2.23) for $\hat{P}^*(\mathbf{q}; z)$ for small $q_1, q_2$, and $1 - z$. In this section we shall denote the function $\hat{G}(\mathbf{x}; z)$ of Eq. (2.26) as $\hat{G}_L(\mathbf{x}; z)$, so that

$$\hat{G}_L(\mathbf{x}; z) = \frac{1}{L} \sum_{k=0}^{L-1} \frac{1}{2\pi} \int_{-\pi}^{\pi} dq_1 \frac{\exp(-iq_1 x_1 - 2\pi i k x_2/L)}{1 - \frac{1}{2} z[\cos q_1 + \cos(2\pi k/L)]} \tag{5.1}$$

From the general expressions (2.34) for $\hat{A}(z)$, $\hat{A}'(z)$, $\hat{B}(z)$, $\hat{B}'(z)$, and $\hat{C}(z)$ we see that we need $\hat{G}_L(\mathbf{x}; z)$ for $\mathbf{x} = \mathbf{0}$, $\mathbf{e}_1$, $\mathbf{e}_2$, $2\mathbf{e}_1$, $2\mathbf{e}_2$, $\mathbf{e}_1 + \mathbf{e}_2$. We can, for all these cases, perform the $q_1$ integration in (5.1) and find, for $L \geqslant 2$,

$$\begin{aligned}
\hat{G}_L(\mathbf{0}; z) &= C_{L,0}(z) \\
\hat{G}_L(\mathbf{e}_1; z) &= \frac{2}{z}\,[C_{L,0}(z) - 1] - C_{L,1}(z) \\
\hat{G}_L(\mathbf{e}_2; z) &= C_{L,1}(z) \\
\hat{G}_L(2\mathbf{e}_1; z) &= -\frac{8}{z^2} + \left(\frac{8}{z^2} - 1\right) C_{L,0}(z) - \frac{8}{z}\, C_{L,1}(z) + 2C_{L,2}(z) \\
\hat{G}_L(2\mathbf{e}_2; z) &= 2C_{L,2}(z) - C_{L,0}(z) \\
\hat{G}_L(\mathbf{e}_1 + \mathbf{e}_2; z) &= \frac{2}{z}\, C_{L,1}(z) - C_{L,2}(z)
\end{aligned} \tag{5.2}$$

where we have used the abbreviation

$$C_{L,n}(z) \equiv \frac{1}{L} \sum_{k=0}^{L-1} \frac{\cos^n(2\pi k/L)}{\{[1 - \frac{1}{2} z \cos(2\pi k/L)]^2 - z^2/4\}^{1/2}}, \qquad n = 0, 1, 2 \tag{5.3}$$

As a check, one may verify that the expressions (5.2) satisfy Eq. (2.27) for $\mathbf{x} = \mathbf{0}$, $\mathbf{e}_1$, $\mathbf{e}_2$.

### 5.1. Expansion of $\hat{P}^*(\mathbf{q}; z)$ for small $\mathbf{q}$ and $z - 1$

Expanding the expressions (5.2) in powers of $1 - z$ is straightforward, and we obtain

$$\begin{aligned}
\hat{G}_L(\mathbf{0}; z) &= \frac{1}{L(1-z)^{1/2}} + S_{L,-1} + \mathcal{O}(1-z) \\
\hat{G}_L(\mathbf{e}_1; z) &= \frac{1}{L(1-z)^{1/2}} + S_{L,-1} + 2S_{L,1} - 2 + \frac{2}{L}\,(1-z)^{1/2} + \mathcal{O}(1-z) \\
\hat{G}_L(\mathbf{e}_2; z) &= \frac{1}{L(1-z)^{1/2}} + S_{L,-1} - 2S_{L,1} + \mathcal{O}(1-z) \\
\hat{G}_L(2\mathbf{e}_1; z) &= \frac{1}{L(1-z)^{1/2}} + S_{L,-1} + 8S_{L,1} + 8S_{L,3} - 8 \\
&\quad + \frac{8}{L}\,(1-z)^{1/2} + \mathcal{O}(1-z) \\
\hat{G}_L(2\mathbf{e}_2; z) &= \frac{1}{L(1-z)^{1/2}} + S_{L,-1} - 8S_{L,1} + 8S_{L,3} + \mathcal{O}(1-z) \\
\hat{G}_L(\mathbf{e}_1 + \mathbf{e}_2; z) &= \frac{1}{L(1-z)^{1/2}} + S_{L,-1} - 4S_{L,3} + \frac{2}{L}\,(1-z)^{1/2} + \mathcal{O}(1-z)
\end{aligned} \tag{5.4}$$

where we introduced the sums

$$S_{L,n} \equiv \frac{1}{L} \sum_{k=1}^{L-1} \frac{\sin^n(\pi k/L)}{[1+\sin^2(\pi k/L)]^{1/2}}, \qquad n = -1, 1, 3 \tag{5.5}$$

for which a large-$L$ expansion gives

$$\begin{aligned} S_{L,-1} &= (2/\pi) \ln L + \mathcal{O}(L^0) \\ S_{L,1} &= 1/2 + \mathcal{O}(L^{-1}) \\ S_{L,3} &= 1/\pi + \mathcal{O}(L^{-1}) \end{aligned} \tag{5.6}$$

By substituting (5.4) in (2.34), we find the small-$(1-z)$ expansion

$$\begin{aligned} \hat{A}(z) &= 1 - S_{L,1} - \left[ (1-S_{L,1})^2 + \frac{1}{L^2} \right] L(1-z)^{1/2} + \mathcal{O}(1-z) \\ \hat{A}'(z) &= S_{L,1} - S_{L,1}^2 L(1-z)^{1/2} + \mathcal{O}(1-z) \\ \hat{B}(z) &= S_{L,1} + 2S_{L,3} - 1 - \left[ (1-S_{L,1})^2 - \frac{1}{L^2} \right] L(1-z)^{1/2} + \mathcal{O}(1-z) \\ \hat{B}'(z) &= -S_{L,1} + 2S_{L,3} - S_{L,1}^2 L(1-z)^{1/2} + \mathcal{O}(1-z) \\ \hat{C}(z) &= \frac{1}{2} - S_{L,3} - S_{L,1}(1-S_{L,1}) L(1-z)^{1/2} + \mathcal{O}(1-z) \end{aligned} \tag{5.7}$$

The quantities $\hat{A}(1),..., \hat{C}(1)$ represent again the correlations between two successive step directions; horizontal and vertical steps are clearly inequivalent now. Substituting the expansions (5.7) in the formula (2.21) for $\mathscr{D}(\mathbf{q}; z)$, one finds

$$\begin{aligned} \mathscr{D}(\mathbf{q}; z) \simeq\ & 2(1-2S_{L,3})(3-2S_{L,1}-2S_{L,3})(1+2S_{L,1}-2S_{L,3}) L(1-z)^{1/2} \\ & + (1+2S_{L,1}-2S_{L,3})(1-2S_{L,3})(S_{L,1}+S_{L,3}-1/2) q_1^2 \\ & + (3-2S_{L,1}-2S_{L,3})(1-2S_{L,3})(S_{L,3}-S_{L,1}+1/2) q_2^2 \\ & \text{as} \quad q \to 0, \quad z \to 1 \end{aligned} \tag{5.8}$$

Hence, between the scales of the $q_i$ and of $1-z$ we now have the relation

$$q_i^2 \sim L(1-z)^{1/2}, \qquad L \text{ fixed} \tag{5.9}$$

Taking this relation into account, we find once again that the leading terms in the expansion of $\hat{U}_{\beta}(\mathbf{q}; z)$ around $(\mathbf{q}; z) = (\mathbf{0}; 1)$ are the ones quadratic in the $q_i$. Explicitly,

$$\begin{aligned} \hat{U}_{\beta}(\mathbf{q}; z) \simeq\ & -(1-2S_{L,3})(1+2S_{L,1}-2S_{L,3})(S_{L,1}+S_{L,3}-1/2) q_1^2 \\ & -(1-2S_{L,3})(3-2S_{L,1}-2S_{L,3})(-S_{L,1}+S_{L,3}+1/2) q_2^2 \\ & q \to 0 \quad \text{and} \quad z \to 1 \end{aligned} \tag{5.10}$$

which is independent of the index $\boldsymbol{\beta}$. Furthermore, one can check that

$$\sum_{\boldsymbol{\beta}} \hat{W}(\boldsymbol{\beta}, \mathbf{x}_0; z) = 1 + \mathcal{O}[h(\mathbf{x}_0)(1-z)^{1/2}], \qquad z \to 1 \tag{5.11}$$

where $h(\mathbf{x}_0)$ is a function behaving $\sim |x_{0,1}|$ for large $x_{0,1}$. We shall therefore continue our calculation supposing

$$|x_{0,1}| \, (1-z)^{1/2} \ll 1 \tag{5.12}$$

Upon substituting the results (5.8), (5.10), and (5.11) in Eq. (2.23) we find after some algebra that

$$\begin{aligned} \hat{P}^*(\mathbf{q}; z) \simeq & \left[ (1-z)^{1/2} + \frac{S_{L,1} + S_{L,3} - 1/2}{2(3 - 2S_{L,1} - 2S_{L,3})} \frac{q_1^2}{L} \right. \\ & \left. + \frac{1/2 - S_{L,1} + S_{L,3}}{2(1 + 2S_{L,1} - 2S_{L,3})} \frac{q_2^2}{L} \right]^{-1} \\ & \times \frac{1}{(1-z)^{1/2}} \qquad \text{for} \quad q \to 0, \quad z \to 1 \end{aligned} \tag{5.13}$$

## 5.2. Results for $P_t(\mathbf{y})$

The inverse Fourier and Laplace transform (2.37) reads in this case

$$P_t(\mathbf{y}) = \frac{1}{L} \sum_{q^2} \frac{1}{2\pi} \int_{-\pi}^{\pi} dq_1 \, [\exp(-i\mathbf{q} \cdot \mathbf{y})] \frac{1}{2\pi i} \oint \frac{dz}{z^{t+1}} \hat{P}^*(\mathbf{q}; z) \tag{5.14}$$

The main contribution to this integral will once again come from the region $(\mathbf{q}, z) \approx (\mathbf{0}, 1)$. Since $q_2$ takes discrete values separated by $2\pi/L$, Eqs. (5.8) and (5.9) now show that when $(1-z)^{1/2} \ll L^{-3}$, the expression for $\mathscr{D}$ can become $\ll L^{-3}$ only for $q_2 = 0$. We shall abbreviate

$$\gamma_L \equiv \left( \frac{S_{L,1} + S_{L,3} - 1/2}{3 - 2S_{L,1} - 2S_{L,3}} \right)^{1/2} \tag{5.15}$$

which for large $L$ becomes

$$\gamma_L \simeq \frac{1}{[2(\pi - 1)]^{1/2}} \tag{5.16}$$

Using $\hat{P}^*(\mathbf{q}; z)$ from Eq. (5.13) in (5.14), keeping only the $q_2 = 0$ term, and deforming the integration contour in the complex $z$ plane in the same way as was done for the infinite lattice, one finds

$$P_t(\mathbf{y}) \simeq \frac{1}{L}\frac{1}{2\pi}\int_{-\pi}^{\pi} dq_1 \exp(-iq_1 y_1) \times \frac{1}{\pi}\int_1^{\infty} \frac{dz}{z^{t+1}} \frac{2L\gamma_L^2 q_1^2}{4L^2(z-1)^{3/2}+\gamma_L^4 q_1^4 (z-1)^{1/2}}, \qquad t\to\infty \quad (5.17)$$

After scaling

$$z \equiv 1 + x^2/t \quad (5.18a)$$

$$q_1 \equiv \kappa/t^{1/4} \quad (5.18b)$$

we get, with $\xi \equiv y_1/t^{1/4}$ fixed and for $t\to\infty$,

$$\begin{aligned} P_t(\mathbf{y}) &\simeq \frac{\gamma_L^2}{2\pi^2 L^2 t^{1/4}} \int_{-\infty}^{\infty} d\kappa\, \kappa^2 e^{-i\kappa\xi} \int_0^{\infty} dx \frac{e^{-x^2}}{x^2+\gamma_L^4\kappa^4/4L^2} \\ &= \frac{\gamma_L^2}{2\pi^2 L^2 t^{1/4}} \int_{-\infty}^{\infty} d\kappa\, \kappa^2 e^{-i\kappa\xi} \\ &\quad \times \int_0^{\infty} d\lambda\, e^{-\lambda(\gamma_L^4\kappa^4/4L^2)} \int_0^{\infty} dx\, e^{-(1+\lambda)x^2} \end{aligned} \quad (5.19)$$

Now carrying out the integration on $x$ and changing the variable $\lambda$ to $\mu \equiv \frac{1}{2}\gamma_L^2\kappa^2[(\lambda+1)^{1/2}-1]$, we find

$$\begin{aligned} P_t(\mathbf{y}) &\simeq \frac{1}{\pi^{3/2} L t^{1/4}} \int_{-\infty}^{\infty} d\kappa \exp(-i\kappa\xi) \int_0^{\infty} d\mu \exp\left[-\left(\mu^2+\mu\frac{\gamma_L^2\kappa^2}{L}\right)\right] \\ &= \frac{2}{\pi L^{1/2} t^{1/4}\gamma_L} \int_0^{\infty} du \exp(-u^4) \exp\left(-\frac{\xi^2 L}{4\gamma_L^2}\frac{1}{u^2}\right) \\ &\quad t\to\infty, \qquad \xi = \frac{y_1}{t^{1/4}} \text{ fixed} \end{aligned} \quad (5.20)$$

where in the last step we have performed the integration on $\kappa$ and set $\mu = u^2$. Instead, we could have done the $\kappa$ integration in (5.19) first to find (ref. 27, p. 409)

$$\begin{aligned} P_t(\mathbf{y}) &\simeq \frac{2\sqrt{2}}{\pi L^{1/2} t^{1/4}\gamma_L} \int_0^{\infty} du \left[\exp(-u^4) \exp\left(-u\frac{|\xi|\sqrt{L}}{\gamma_L}\right)\right] \\ &\quad \times \cos\left(\frac{\pi}{4} + u\frac{|\xi|\sqrt{L}}{\gamma_L}\right) \\ &\quad t\to\infty, \qquad \xi = y_1/t^{1/4} \text{ fixed} \end{aligned} \quad (5.21)$$

where we have put $x = u^2$. Neither of the integral representations (5.20) or (5.21) of $P_t(\mathbf{y})$ can, to our knowledge, be evaluated analytically. However, both show that $P_t(\mathbf{y})$ has the scaling form

$$P_t(\mathbf{y}) \simeq \frac{2}{\pi L^{1/2} t^{1/4} \gamma_L} \mathscr{F}\left(\frac{|y_1| L^{1/2}}{\gamma_L t^{1/4}}\right)$$

$$|y_1|, t \to \infty, \qquad \frac{y_1}{t^{1/4}} \text{ fixed}, \quad L \text{ fixed} \tag{5.22}$$

It is again easy to verify, especially via (5.20), that $P_t(\mathbf{y})$ is properly normalized and that its variance in the $y_1$ direction is given by

$$\langle y_1^2 \rangle = \frac{2}{\sqrt{\pi}} \frac{\gamma_L^2}{L} t^{1/2} \simeq \frac{t^{1/2}}{\pi^{1/2}(\pi - 1) L}, \qquad L \to \infty \tag{5.23}$$

Both (5.20) and (5.21) are useful for making asymptotic expansions. With $s \equiv |\xi| \sqrt{L}/\gamma_L$ one easily finds from (5.20)

$$\mathscr{F}(s) = \int_0^\infty du \exp\left[-\left(u^4 + \frac{s^2}{4u^2}\right)\right] \simeq \left(\frac{\pi}{6}\right)^{1/2} s^{-1/3} \exp\left(-\frac{3}{4} s^{4/3}\right), \qquad s \to \infty \tag{5.24}$$

and from (5.21)

$$\mathscr{F}(s) = \sqrt{2} \int_0^\infty du\, e^{-(u^4 + su)} \cos\left(\frac{\pi}{4} + su\right)$$

$$\simeq \Gamma\left(\frac{5}{4}\right) - \frac{1}{2} s \sqrt{\pi} + \frac{1}{4} s^2 \Gamma\left(\frac{3}{4}\right), \qquad s \downarrow 0 \tag{5.25}$$

These relations determine the scaling behavior of $P_t(\mathbf{y})$ for large and small values of the combination $|y_1|\, t^{-1/4}$. In particular, $P_t(\mathbf{y})$ has a kink at $y_1 t^{-1/4} = 0$. Furthermore, since the calculation is also valid for $t \to \infty$ at fixed $\mathbf{y}$, we immediately find

$$P_t(\mathbf{y}) \simeq \frac{2}{\pi L^{1/2} t^{1/4} \gamma_L} \Gamma\left(\frac{5}{4}\right), \qquad \mathbf{y} \text{ fixed and } t \to \infty \tag{5.26}$$

## 5.3. Discussion

Root-mean-square displacements increasing with time as $t^{1/4}$ are known to occur in several one-dimensional systems. An example is the reptation model introduced by de Gennes[28] to describe the motion of a polymer chain in a melt or dense solution. An example closer to the model of this section is a strictly one-dimensional chain (a strip of width $L = 1$) on which impenetrable particles execute Bownian motion in the presence of a *finite density* of vacancies. (See ref. 4 for a survey of work on this problem.) It was shown by Harris[29] that in such a system the rms displacement of a tagged particle increases as $t^{1/4}$, and, moreover, that its distribution function approaches a *Gaussian* for long times. For these $t^{1/4}$ dependences several heuristic explanations are known (see, e.g., ref. 30). In our case the heuristic argument runs as follows. With respect to the hole, the tagged particle position $\mathbf{y}$ may be considered in good approximation as an immobile origin. In a time $t$ the hole, performing a simple random walk, will cross the vertical axis $x_1 = y_1$ a number of times $\sim\sqrt{t}$. But on each crossing, since the strip has a width $L \geqslant 2$, the hole will miss the tagged particle with a finite probability, which will destroy the correlation between previous and later horizontal displacements of the particle. Hence, the particle will undergo $\sim\sqrt{t}$ uncorrelated horizontal displacements, which directly leads to the $t^{1/4}$ law. Finally, a model for which this law is immediately evident is the random walker on a random one-dimensional path studied by Kehr and Kutner.[7] Moreover, although there is no direct connection with our model, these authors find the same scaling function (5.20).

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