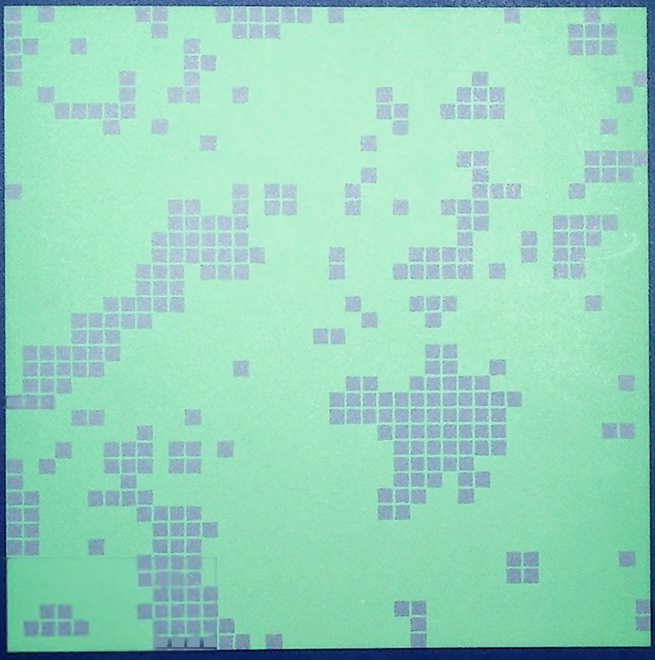
APPLICATIONS OF RANDOM WALK: TRACER DIFFUSION, LATTICE COVERING, AND DAMAGE SPREADING



MARCO BRUMMELHUIS

Kast dissertaties

Cover:

A 40×40 lattice with periodic boundaries that has been partly covered by a simple random walk, as described in chapter 5 of this thesis. The situation depicted corresponds to $\alpha = 0.15$ (cf. chapter 5). The starting point of the random walk is in the middle of the picture.

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PROEFSCHRIFT

TER VERKRIJGING VAN DE GRAAD VAN DOCTOR AAN DE RIJKSUNIVERSITEIT TE LEIDEN, OP GEZAG VAN DE RECTOR MAGNIFICUS DR. L. LEERTOUWER, HOOGLERAAR IN DE FACULTEIT DER GODGELEERDHEID, VOLGENS BESLUIT VAN HET COLLEGE VAN DEKANEN TE VERDEDIGEN OP WOENSDAG 17 APRIL 1991 TE KLOKKE 15.15 UUR

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Ce qui n'est pas clair n'est pas français

Antoine de Rivarol (1753 – 1801)

Chapter 1

Introduction

1.1 Random walks

As one knows from everyday life, a walk is a succession of individual steps. Therefore, the displacement $\vec{R}_n$ after an n-step walk can be written as

$$\vec{R}_n = \vec{r}_1 + \ldots + \vec{r}_n, \tag{1.1}$$

with the $\vec{r}_i$ denoting the separate steps.

This is also true for a random walk, the word "random" being added to denote that the (generally independent) steps constituting the walk are drawn randomly from a given probability distribution, which usually is the same for every step. Obviously, the displacement $\vec{R}_n$ then becomes random too, having a probability distribution of its own. The question as to what this distribution is for given but general n is old; it was apparently first raised in 1905 by Pearson for a walk in a plane, when all the individual steps have the same length and are uniformly distributed with respect to direction [1]. From that same period stem the works by Einstein [2] and Von Smoluchowski [3] on Brownian motion. As is well-known nowadays, there is an intimate connection between the long-time and large-scale behaviour of a random walk with statistically independent steps on the one hand, and Brownian motion on the other. Therefore already [2] and [3] imply that the mean square displacement $\langle R_n^2 \rangle$ of such a random walk eventually grows linearly with n, thus allowing one to define a diffusion constant D as:

$$D \equiv \lim_{n\to\infty} \frac{\langle R_n^2 \rangle}{2dn} \;. \tag{1.2}$$

The factor $1/2d$, where d stands for the dimension of the space in which the random walk takes place, is conventional. Apart from its second moment, $\langle R_n^2 \rangle$, one can in fact in many cases obtain the *full* displacement distribution function for large n. This is because for $n \to \infty$, the *central limit theorem*, loosely stated, asserts that if the successive steps of the walk are "not too strongly" correlated, while the probability distribution they are drawn from is "not too broad", then the distribution function of

$\vec{R}_n$ has a Gaussian as a limiting form. The Gaussian distribution is therefore generic for this kind of problem. (Cf. ref. [4] for a more precise discussion of this point.)

One can think of many (smaller or larger) variations on the random-walk theme sketched above. For example, apart from varying the dimension of the space in which the random walk takes place, one may decide either to put the walk on a lattice, or not. Also, the individual steps may be chosen "random" not only with respect to direction, but also with respect to their lengths. One can furthermore introduce correlations of varying range between the steps of the walk. One may even decide not to consider the random-walk process in its own "time", n, but rather to introduce an external time by demanding that there be a distribution of waiting times between successive steps. In that case, the displacement can be studied as a function of this external time, t. Especially cases where the waiting time distribution does *not* have a finite mean τ are potentially interesting, since then the natural identification $n \leftrightarrow [t/\tau]$ does not exist, and the displacement distribution function need not become Gaussian as $t \to \infty$. In any case, one can obviously conclude that indeed plenty of variations on the random-walk theme are possible.

Of course, in all of those cases, apart from the probability distribution of the displacement, one can also study other quantities related to the specific random walk process under study. For example, for a walk on a lattice one may wonder what the probability is that the random walk after n steps is at its starting point again. Or, for that matter, that it will *ever* return to its starting point at all. (For the continuum case one could ask analogous questions by dividing the space into small cells, say.) In 1921 Pólya showed that a simple random walk on a lattice (i.e., a random walk where the walker can only step to nearest-neighbour sites, with equal probabilities for all of the allowed steps) in one and two dimensions is certain to return to its starting point, whereas this is no longer true for the higher-dimensional case [5]. One could furthermore consider e.g. the question of the "volume" (in one sense or another) traced out by the random walk after n steps. Dvoretzky and Erdős [6], and later Montroll and Weiss [7] using an elegant generating function technique, some 40 years ago studied a lattice version of this problem, counting the number of different sites visited by a simple random walk on several types of lattices and in various dimensions, as a function of n. The results obtained then are still quoted and used today. And these are only two examples of the many random-walk-related quantities that have been studied in the course of time.

What makes it worth to spend so much time studying these random walks in so much detail, I think, are two things. First of all, random walks are just interesting in their own right. They represent time-dependent processes which one *can* master relatively well. Secondly, and in my opinion this is perhaps the most important reason for studying random walks, they form a *tool* which can be used in the study of many other time-dependent systems. What typically happens, namely, is that one starts with a dynamical system with many degrees of freedom, described by a Liouville equation, say, for which the equations of motion are heavily coupled and too hard to solve directly. One then resorts to a coarse-graining approach. On the coarse-grained level, only a limited number (typically one or two) of collective degrees of freedom are retained; their once deterministic couplings to the other many degrees of freedom are now replaced by a postulated or calculated stochastic behaviour that can often be modelled as a random walk through their range of values.

1.2 Summary and outline of this thesis

This thesis is concerned with random walks *and* their applications. More specifically, three different subjects involving random walks are considered: tracer diffusion, lattice covering, and damage spreading.

First of all, in chapters 2, 3, and 4, the so-called *tracer particle problem* is studied. It can basically be described as follows. One starts by taking an infinite, or a finite lattice with periodic boundary conditions, in dimension d. Lattice gas particles are put on the sites of the lattice. Not all of the sites are occupied, though. The sites which are left empty are called the *vacancies*. Via particle-vacancy exchange processes the vacancies perform simple random walks, all taking a step at every unit of time t. One then randomly selects one of the lattice gas particles and "tags" it. This particle is called the *tracer particle*. The questions one can ask about its motion are very similar to the questions already described above for random-walk motion itself. That is to say, one may study its displacement with time. Or the number of different sites it visits in a given time. And so on. Obviously, the tracer particle only has a nonzero probability of moving when at least one of its nearest-neighbour sites is vacant. In the following the density of vacancies ρ will always be so low, that the probability of finding two or more vacancies occupying nearest-neighbour sites of the tracer particle at the same time is negligible. When a vacancy initially adjacent to the tracer particle leaves its nearest-neighbour position, the tracer particle has either to wait for this vacancy to return or for another vacancy to come in before it can make its next step. There thus is a model-generated *distribution of waiting times* between successive steps of the tracer particle. Also, the *motion* of the tracer particle is *strongly anti-correlated*: just after a tracer-particle-vacancy exchange, the tracer particle and the vacancy are still on nearest-neighbour sites, but now in opposite directions. There is then a considerable probability that the tracer particle will step back to its previous position. The interplay of precisely these two effects, waiting times and anti-correlation, makes it interesting to study the tracer particle problem.

In chapter 2 the *two-dimensional* case with *only one vacancy* in the system is studied for several lattice geometries. On a finite square lattice of linear size L and with periodic boundary conditions, the probability $P_t(\vec{y})$ that the tracer particle be displaced by a vector $\vec{y}$ from its initial position at time t is shown to be a Gaussian for times $L^2 \ln L \ll t \ll L^4$. The lower limit of this time scale is set by the rate at which steps of the tracer particle become decorrelated, being due to the vacancy experiencing the periodic boundaries of the lattice. The upper limit comes from the demand that the tracer particle itself must not have seen the periodic boundaries of the lattice yet. The diffusive motion of the tracer particle one finds here is characterized by a diffusion constant D which, to leading order in L, is given by

$$D = \frac{1}{4\,(\pi - 1)\,L^2} \,. \tag{1.3}$$

In this formula the factor $(\pi - 1)^{-1}$ incorporates the effects of the anti-correlation in the tracer particle's motion, while the factor L^2 in the denominator reflects the mean waiting time between two steps of the tracer particle. The behaviour (1.3) was confirmed by simulations by Ajay and Palmer [8].

The results obtained in chapter 2 for the fully infinite two-dimensional square lattice are totally different. This is because the mean waiting time between successive steps of the tracer particle is now infinite, as can be seen from the fact that the probability for the vacancy to return to its initial site for the first time at time t falls off as $1/t \ln^2 t$ for large times t (cf. chapter 2). The divergence of the mean waiting time causes the mean square displacement of the tracer particle eventually to grow like $\ln t$, instead of t. The tracer particle's motion is then no longer diffusive (the diffusion constant being identically zero) and, in fact, $P_t(\vec{y})$ remains non-Gaussian even for very long times. In chapter 2 the functional form of $P_t(\vec{y})$ is calculated explicitly for this case.

Also the case of a strip (i.e., an $\infty \times L$ lattice) is studied. Here, the probability for a first return of the vacancy to its initial site at time t decays as $L/t^{3/2}$, so that the mean waiting time between the tracer particle's successive steps again is infinite. The tracer particle's mean square displacement turns out to grow as $\sqrt{t}/L$, which is consistent with the long-time tail of the waiting-time distribution (cf. ref. [4, (1.31)]). The probability $P_t(\vec{y})$ itself is a complicated, nonelementary, function of the variable $y_1/t^{1/4}$, and is given explicitly in chapter 2. One should realize that both the case of an infinite square lattice with only one vacancy on it, as well as the similar case for the strip, represent strictly $\rho = 0$ cases.

Chapter 3 shows what happens when one introduces a small but *finite density* of vacancies in the aforementioned infinite systems. Obviously, the mean waiting time between two successive steps of the tracer particle then becomes finite again. Also, there will be a decorrelation of the steps of the tracer particle due to its interactions with different, independent, vacancies. One could therefore a priori expect the displacement distribution function of the tracer particle eventually to become Gaussian and the motion diffusive. In fact, up till now this was usually *assumed implicitly*, and it was thought it sufficed to give an expression for the diffusion constant of the tracer particle's motion to describe it completely. In the low density limit one obtained

$$D = \frac{\rho}{4\,(\pi - 1)} \,. \tag{1.4}$$

Formula (1.4) is compatible with (1.3) since a system consisting of one vacancy on a finite lattice of L^2 sites can be looked upon as being a system with a *finite* vacancy density, $1/L^2$. In chapter 3 the mean square displacement of the tracer particle is found to grow linearly with time for all times $t \gg 1$. Nevertheless it is shown that this does not imply that the tracer particle's displacement distribution function is a Gaussian, then. The Gaussian distribution is in fact only obtained for very long times: $t \gg \rho^{-1} \ln \rho^{-1}$ for the infinite square lattice, and $t \gg \rho^{-2}L^{-2}$ for the strip, respectively. Before entering this asymptotic regime, one first sees the effect of the interaction of a *single* vacancy with the tracer particle, described in chapter 2. Chapter 3 now describes the full crossover from this single-vacancy result to the asymptotic limit where the distribution function does become Gaussian.

Chapter 4 is concerned with the calculation of the average number of different sites visited by the tracer particle, a question traditionally asked and answered for the simple random walk. Only the *three- and higher*-dimensional case with a small vacancy density ρ is considered. In these dimensions the displacement distribution function of the tracer particle is easily shown to become Gaussian for large times and distances. The motion is then diffusive. The corresponding diffusion constant D can be written as $2dD = f_{corr}\,\rho$, with the correlation factor f_{corr} taking the anti-correlation effects of the tracer-particle-vacancy exchange mechanism into account, and ρ reflecting the mean waiting time between successive steps of the tracer particle. For what concerns its displacement distribution function, the tracer particle's motion can be described as that of a simple random walk in a "renormalized time". However, as Czech [9] already showed, when calculating the number of different sites visited by the tracer particle, this "renormalization procedure" does not work: just clumping the anti-correlation effects together is too rough a procedure to follow. Instead, he gave an approximate description of the tracer particle's motion in terms of a correlated random walk with a one-step memory, where the probability of a step in a given direction depends only on the direction of the previous step. In chapter 4 it is shown how on the basis of a similar procedure, but using a different correlated random walk model, one can obtain the *exact* result for the number of different sites visited by the tracer particle, in the limit of large times and low vacancy densities. The results obtained are compatible with simulations by Czech [9].

Chapter 5 describes a second problem involving random walk. Namely, the covering process of a d-dimensional periodic hypercubic lattice of N sites by a simple random walk. More specifically, one executes such a random walk on this lattice and colours the sites visited by it. After n steps of the walk, in which n is arbitrary, there obviously are two sets of sites: sites which are coloured, having been visited, and sites which are not. One can then try to answer questions like: "How many sites of the lattice have not been visited yet?", or "What is the structure of the set of sites not yet visited?", as a function of n. Another type of question, not involving n, is: "Which site of the lattice is the last site visited in the covering process?". Especially this last question is a priori hard to answer, since one inquires after an, in general, nonlocal property (except in dimension $d = 1$ where one only has to keep track of the endpoints of the interval of sites already visited) that depends on the whole history of the walk. Nevertheless this question is addressed and answered in chapter 5, and so are the other questions raised above. One there finds for the one-dimensional version of the problem, that the probability $L_N(x)$ for the site x to be visited last in the covering process is *independent* of x, as long as x is not the starting point of the walk. This turns out to be no longer true for the higher-dimensional case. In dimensions higher than two $L_N(\vec{x})$ is found to approach a constant value according to a Coulomb law:

$$L_N(\vec{x}) \simeq \frac{1}{N}\left[1 - \frac{\text{const}}{|\vec{x}|^{d-2}}\right], \tag{1.5}$$

valid for $|\vec{x}|$ small on the scale $N^{1/d}$, while in two dimensions it behaves logarithmically. It is shown that there is in each dimension a characteristic time scale on which the last site is visited. Whereas in three and higher dimensions, on this time scale, the sites not yet visited are essentially distributed randomly through the lattice, in two dimensions the set of these sites is fractal-like.

In chapter 6, a problem nowadays referred to as "damage spreading" is considered. In its most general form this problem consists of taking two copies of the same many variable system differing only slightly in initial configurations, then subjecting them to the *same* Monte Carlo simulation, and subsequently monitoring how the small initial difference between them (the "damage") develops in time. The idea is to learn, through the study of the time evolution of the distance in configuration space, about the properties of the single system. For example, if this system has a critical temperature, then qualitatively different time-dependences of the distance between the two copies of the system are expected above and below the critical temperature. In practice it has proven nontrivial to relate the observed differences in the behaviour of the distance to the properties of the single system. E.g., both in the study of spin glasses and for XY-models, with the damage spreading method, one found critical temperatures not present in the equilibrium phase diagrams of the single systems. It appears (see e.g. the recent Ph.D.-thesis by Golinelli [10] for an overview), that these temperatures are only of a "dynamical" nature. Chapter 6 studies the effects of the introduction of correlations in the time evolutions of two copies s and s' of a one-dimensional Ising chain. It turns out to be possible to adjust continuously the correlations in the dynamics of the individual systems from "none at all" to those used in the damage spreading case. In all cases, the combined system goes to an equilibrium with an unknown Hamiltonian $\mathcal{H}_2$. For a special choice of the spin-flip probabilities it is shown how, despite not knowing $\mathcal{H}_2$, one can find expressions for the equilibrium n-point (interchain) correlation functions. In particular $\langle s_i s'_i s_j s'_k \rangle_{eq}$ is calculated. This then is where random-walk theory comes in again. The reason is that to find $\langle s_i s'_i s_j s'_k \rangle_{eq}$ a set of equations must be solved which can be looked upon as belonging to a special type of random walk on a two-dimensional square lattice.

The solution is obtained in the continuum limit, i.e., in this case, for large distances and low temperatures, where it appears that the discrete difference equations can be replaced by differential equations. It resembles the procedure one usually follows when going from discrete random-walk equations on a lattice to the diffusion equation in continuous space. In the equilibrium state the interchain correlations $\langle s_i s_i' s_j s_k' \rangle_{eq}$ are found to decay in space according to a sum of two or three exponentials (depending on temperature) *plus* an integral on a continuum of decay lengths. From it one can conclude that the Hamiltonian $\mathcal{H}_2$ cannot be of strictly finite range.

1.3 Further reading

As already indicated, random-walk theory itself has been studied quite intensively for many years now, and so have its applications. This has led to such a wealth of results on the subject, that it is virtually impossible even to come close to giving a complete list of references. Let me instead just point out a few good review articles which have appeared in recent years. In particular, I would like to mention the works by Bouchaud and Georges [4], Weiss and Rubin [11], Haus and Kehr [12], and Havlin and Ben Avraham [13], all shedding light on the subject from a different point of view. The classic monograph by Spitzer on the subject [14], which still is something of a standard work, should also be mentioned, while the work by Feller [15], concerned with probability theory in general, always proves to be a rich source of information and reference too. Finally, for material directly related to a subject treated in a given chapter of this thesis, the reader is of course also advised to consult the more extensive list of references in the corresponding chapter.

References

[1] K. Pearson, Nature **72** (1905) 294.

[2] A. Einstein, Ann. Physik **17** (1905) 549.

[3] M. von Smoluchowski, Ann. Physik **21** (1906) 756.

[4] J.P. Bouchaud and A. Georges, *Anomalous diffusion in disordered media: statistical mechanisms, models and physical applications*, Phys. Rep. **195** (1990) 127.

[5] G. Pólya, Math. Ann. **84** (1921) 149.

[6] A. Dvoretzky and P. Erdös in: *Proceedings of the Second Berkeley Symposium*, Vol. 33, (Univ. of California Press, Berkeley, 1951).

[7] E.W. Montroll and G.H. Weiss, J. Math. Phys. **6** (1965) 167.

[8] Ajay and R.G. Palmer, J. Phys. A **23** (1990) 2139.

[9] R. Czech, J. Chem. Phys. **91** (1989) 2498.

[10] O. Golinelli, Ph.D.-thesis, Université Paris VI, 1990.

[11] G.H. Weiss and R.J. Rubin, *Random Walks: theory and selected applications*, Adv. Chem. Phys. **52** (1983) 363.

[12] J.W. Haus and K.W. Kehr, *Diffusion in regular and disordered lattices*, Phys. Rep. **150** (1987) 263.

[13] S. Havlin and D. Ben Avraham, *Diffusion in disordered media*, Adv. Phys. **36** (1987) 695.

[14] F. Spitzer, *Principles of Random Walk* (Van Nostrand, Princeton, 1964).

[15] W. Feller, *An Introduction to Probability Theory and Its Applications*, Vols. 1 and 2 (Wiley, New York, 1950 and 1966).

Chapter 2

Single-vacancy induced motion of a tracer particle in a two-dimensional lattice gas

2.1 Introduction

In this chapter 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 $t = 1, 2, 3, \ldots$ one particle, selected with probability $\frac{1}{4}$ from among the four particles adjacent to the hole, will move into it. Then the hole obviously performs a simple random walk.

We now select and "tag" one particle, the "tracer particle", whose motion we shall 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 one, make an infinite number of steps, even in the presence of just one vacancy. The probability $P_t(\vec{y})$ that at time t the tagged particle be displaced a distance $\vec{y} = (y_1, y_2)$ from its initial position is calculated in this chapter.

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 one, the hole will wander off to infinity after only a finite number of encounters with the tagged particle. In an effectively finite time, $P_t(\vec{y})$ then tends to an equilibrium distribution, $P_\infty(\vec{y})$, 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 $P_\infty(\vec{y})$ 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, Kutner, and Binder [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, Kehr, and Kutner [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 chapter 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, the subject of chapter 3. We summarize our results. On an infinite two-dimensional lattice, studied in section 2.3, it appears that in the limit of large t and large $y\,(\equiv|\vec{y}\,|)$ the distribution $P_t(\vec{y})$ is a function only of the scaling variable

$$\eta = \frac{y}{\sqrt{\ln t}} \,. \tag{2.1}$$

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 2.3.3. The deviation from Gaussian behaviour indicates that even when separated by long time intervals, successive steps of the tagged particle cannot be considered as effectively uncorrelated.

Secondly, we consider in section 2.4 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 $P_t(\vec{y})$ is Gaussian. This is indeed what we find, and the corresponding diffusion constant is

$$D_L = \frac{1}{4(\pi-1)L^2} \,. \tag{2.2}$$

This behaviour is followed by a crossover to a final time scale on which $P_t(\vec{y})$ 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 sections 2.4.3 – 2.4.5 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.

Thirdly, we study in section 2.5 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 $P_t(\vec{y})$ depends only on the scaling variable

$$\xi = \frac{y_1}{t^{\frac{1}{4}}}, \tag{2.3}$$

and again *is not a Gaussian*. Its precise form and the details of the calculation are given in section 2.5.2. In section 2.5.3 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!

2.2 Formulation of the problem

2.2.1 The distribution function $P_t(\vec{y})$

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

$$x_i = 0,\ 1,\ 2,\ \ldots,\ L_i - 1, \qquad i = 1,\ 2\ . \tag{2.4}$$

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

$$\vec{e}_1 = (1,0) \ \text{ and } \ \vec{e}_2 = (0,1)\ . \tag{2.5}$$

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

One approach to the motion of the tagged particle would be to write down the master equation for the joint distribution $P_t^{(2)}(\vec{y}, \vec{x})$ of the tagged particle position $\vec{y}$ and the hole position $\vec{x}$. Finding the relaxation modes and eigenvalues of this equation amounts to an $L_1L_2\,(L_1L_2 - 1)$-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,

$$P_t(\vec{y}) \equiv \sum_{\vec{x}\,(\neq \vec{y})} P_t^{(2)}(\vec{y}, \vec{x})\ . \tag{2.6}$$

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.

2.2.2 The return probabilities $W_\tau(\vec{\nu}, \vec{x})$

In tracer diffusion problems a key role is played by a set of conditional return probabilities (also called waiting time distributions) $W_\tau(\vec{\nu}, \vec{x})$, where $\vec{\nu}$ is one of the unit vectors $\pm\vec{e}_1, \pm\vec{e}_2$. For all $\vec{x} \neq \vec{0}$ we define $W_0(\vec{\nu}, \vec{x}) \equiv 0$; and, for $\tau = 1, 2, \ldots,$ we define $W_\tau(\vec{\nu}, \vec{x})$ as the probability that a simple random walker initially at $\vec{x} \neq \vec{0}$

(i) hits the origin for the first time at time τ, *and* that

(ii) its position at $\tau - 1$ was $\vec{\nu}$.

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 $\vec{x}_0 \neq \vec{0}$, and if the tagged particle is initially at the origin, then $W_\tau(\vec{\nu}, \vec{x}_0)$ is the probability that at time τ the tagged particle will make its first step, and that this step is in the direction $\vec{\nu}$. But then at time τ the hole is at a distance $-\vec{\nu}$ 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 $\vec{\nu}'$ is $W_{\tau'}(\vec{\nu}', -\vec{\nu})$. We can continue in this way and, clearly, once the first step of the tagged particle has taken place, the sixteen time-dependent quantities $W_\tau(\vec{\nu}, \vec{\nu}')$ (with $\vec{\nu}$, $\vec{\nu}'$ nearest-neighbour vectors) suffice to describe the motion of the tagged particle. From time reversal invariance of the Brownian paths we have the symmetry property

$$W_\tau(\vec{\nu}, \vec{\nu}') = W_\tau(\vec{\nu}', \vec{\nu}), \quad \tau = 0, 1, \ldots \,. \tag{2.7}$$

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

$$\begin{aligned} A_\tau &\equiv W_\tau(\vec{e}_1, \vec{e}_1), \\ A'_\tau &\equiv W_\tau(\vec{e}_2, \vec{e}_2), \\ B_\tau &\equiv W_\tau(-\vec{e}_1, \vec{e}_1), \\ B'_\tau &\equiv W_\tau(-\vec{e}_2, \vec{e}_2), \\ C_\tau &\equiv W_\tau(\vec{e}_2, \vec{e}_1) \,. \end{aligned} \tag{2.8}$$

The quantities A_τ and A'_τ, B_τ and B'_τ, and C_τ, describe the probability of a first return (after a time τ) 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 2.5), we shall pursue the general case here; the simplifications valid for a square geometry will be listed in section 2.2.6.

A number of quantities well-known in the study of simple random walks can be expressed immediately in terms of the W_τ. Firstly,

$$F_\tau(\vec{x}) \equiv \sum_{\vec{\nu}} W_\tau(\vec{\nu}, \vec{x}), \quad \tau = 0, 1, \ldots, \quad \vec{x} \neq \vec{0}, \tag{2.9}$$

is the probability that a simple random walker initially at $\vec{x} \neq \vec{0}$ will hit the origin for the first time at time τ, regardless (for $\tau \geq 1$) of its position at time $\tau - 1$. Consequently, $1 - \sum_{\tau=0}^{t} F_\tau(\vec{x})$ is the probability that a simple random walker initially at $\vec{x}$ has not yet reached the origin at time t. In section 2.2.4 we shall employ the well-known relation between the generating functions of $F_\tau(\vec{x})$ and those of the simple random walk. With the aid of (2.8) two particular instances of (2.9) can be written as

$$\begin{aligned} F_\tau(\vec{e}_1) &= A_\tau + B_\tau + 2C_\tau, \\ F_\tau(\vec{e}_2) &= A'_\tau + B'_\tau + 2C_\tau, \qquad \tau = 0,\ 1,\ \ldots\ . \end{aligned} \tag{2.10}$$

Secondly, let R_τ be the probability that a simple random walker initially at the origin will return there for the first time after τ steps. From the fact that the walker's first step is with equal probability to any of the neighbours $\vec{\nu}$ of the origin, and from relation (2.10), we have that

$$\begin{aligned} R_\tau &= \frac{1}{4}\sum_{\vec{\nu}} F_{\tau-1}(\vec{\nu}) \\ &= \frac{1}{2}(A_{\tau-1} + A'_{\tau-1} + B_{\tau-1} + B'_{\tau-1} + 4C_{\tau-1}), \qquad \tau = 1,\ 2,\ \ldots\ . \end{aligned} \tag{2.11}$$

Spitzer [8] has shown that R_τ decays very slowly with τ. Explicitly,

$$R_\tau \simeq (1 + (-1)^\tau)\frac{\pi}{\tau \ln^2 \tau} \qquad \text{as } \tau \to \infty\ . \tag{2.12}$$

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

$$\sum_{\tau=0}^{\infty}\sum_{\vec{\nu}} W_\tau(\vec{\nu}, \vec{\nu}\,') = 1\ . \tag{2.13}$$

Two things have to be done now:

(i) we have to express $P_t(\vec{y})$ in terms of the $W_\tau(\vec{\nu}, \vec{\nu}\,')$ and $W_\tau(\vec{\nu}, \vec{x}_0)$;

(ii) we have to express the W_τ in terms of the simple random walk generating function.

2.2.3 Expressing $P_t(\vec{y})$ in the W_τ

From the definition of the $W_\tau(\vec{\nu}, \vec{\nu}\,')$ and the discussion in the preceding subsection it is clear that one can find an expression for $P_t(\vec{y})$ by summing over the number of steps n of the tagged particle, over the step directions $\vec{\nu}_1, \vec{\nu}_2, \ldots, \vec{\nu}_n$, and over the lengths of the time intervals $\tau_2, \ldots, \tau_n$ separating the steps, as well as the time intervals τ_1 preceding the first step and τ_{n+1} elapsed since the last step. Since at the initial time the hole is at $\vec{x}_0$, the expression for $P_t(\vec{y})$ depends on $\vec{x}_0$. We find, remembering the definition (2.9) of $F_\tau(\vec{x})$,

$$\begin{aligned}
P_t(\vec{y}) \;=\; & \delta_{\vec{y},\vec{0}}[1-\sum_{\sigma=0}^{t} F_\sigma(\vec{x}_0)] \\
& + \sum_{n=1}^{\infty}\sum_{\tau_1=1}^{\infty}\cdots\sum_{\tau_n=1}^{\infty}\sum_{\tau_{n+1}=0}^{\infty} \delta_{\tau_1+\ldots+\tau_{n+1},t}\sum_{\vec{\nu}_1}\cdots\sum_{\vec{\nu}_n}[1-\sum_{\sigma=0}^{\tau_{n+1}} F_\sigma(-\vec{\nu}_n)] \\
& \times \delta_{\vec{\nu}_1+\ldots+\vec{\nu}_n,\vec{y}} W_{\tau_n}(\vec{\nu}_n,-\vec{\nu}_{n-1})\ldots W_{\tau_2}(\vec{\nu}_2,-\vec{\nu}_1)W_{\tau_1}(\vec{\nu}_1,\vec{x}_0), \qquad (2.14)
\end{aligned}$$

where in the $n=1$ term it is to be understood that $-\vec{\nu}_0=\vec{x}_0$. The first term on the right-hand side of (2.14) 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)

$$\widehat{X}(z) \equiv \sum_{t=0}^{\infty} z^t X_t\ . \qquad (2.15)$$

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

$$X^*(\vec{q}) \equiv \sum_{\vec{y}} \exp(i\vec{q}\cdot\vec{y})\, X(\vec{y}), \qquad (2.16)$$

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

$$q_i = 2\pi\frac{k_i}{L_i}, \qquad k_i = 0,\ 1,\ \ldots,\ L_i-1, \qquad i=1,\ 2\ . \qquad (2.17)$$

The Fourier-Laplace transform of equation (2.14) for $P_t(\vec{y})$ is

$$\begin{aligned}
\widehat{P}^*(\vec{q};z) \;=\; & \frac{1-\widehat{F}(\vec{x}_0;z)}{1-z} \\
& + \frac{1}{1-z}\sum_{\vec{\alpha}}\sum_{\vec{\beta}}[1-\widehat{F}(-\vec{\alpha};z)]\left(I-\widehat{T}(\vec{q};z)\right)^{-1}_{\vec{\alpha},\vec{\beta}}\ \widehat{T}_{\vec{\beta},-\vec{x}_0}(\vec{q};z), \qquad (2.18)
\end{aligned}$$

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

$$\widehat{T}_{\vec{a},\vec{x}}(\vec{q};z) \equiv \exp(i\vec{q}\cdot\vec{\alpha})\ \widehat{W}(\vec{\alpha},-\vec{x};z), \qquad (2.19)$$

and where $(I-\widehat{T}(\vec{q};z))^{-1}$ is the matrix inverse of the 4×4 block with matrix elements $\delta_{\vec{\alpha},\vec{\beta}}-\widehat{T}_{\vec{\alpha},\vec{\beta}}(\vec{q};z)$. The $\widehat{F}(\vec{x};z)$ can be eliminated from (2.18) with the aid of the Laplace transform of (2.9) and of (2.19), which together give

$$\widehat{F}(\vec{x};z) = \sum_{\vec{\nu}} \exp(-i\vec{q}\cdot\vec{\nu})\ \widehat{T}_{\vec{\nu},-\vec{x}}(\vec{q};z), \qquad \vec{x}\neq\vec{0}\ . \qquad (2.20)$$

Substituting this in equation (2.18) and using that $I + \widehat{T}(I-\widehat{T})^{-1} = (I-\widehat{T})^{-1}$, we obtain

$$\widehat{P}^{*}(\vec{q};z) = \frac{1}{1-z}[1 + \sum_{\vec{\alpha}}\sum_{\vec{\beta}}(1-e^{-i\vec{q}\cdot\vec{\alpha}})\left(I-\widehat{T}(\vec{q};z)\right)^{-1}_{\vec{\alpha},\vec{\beta}}\,\widehat{T}_{\vec{\beta},-\vec{x}_0}(\vec{q};z)] \,. \qquad (2.21)$$

From (2.8), (2.15), and definition (2.19) of $\widehat{T}_{\vec{\alpha},\vec{x}}(\vec{q};z)$ we have

$$\widehat{T}(\vec{q};z) = \begin{pmatrix} e^{iq_1}\widehat{B}(z) & e^{iq_1}\widehat{A}(z) & e^{iq_1}\widehat{C}(z) & e^{iq_1}\widehat{C}(z) \\ e^{-iq_1}\widehat{A}(z) & e^{-iq_1}\widehat{B}(z) & e^{-iq_1}\widehat{C}(z) & e^{-iq_1}\widehat{C}(z) \\ e^{iq_2}\widehat{C}(z) & e^{iq_2}\widehat{C}(z) & e^{iq_2}\widehat{B'}(z) & e^{iq_2}\widehat{A'}(z) \\ e^{-iq_2}\widehat{C}(z) & e^{-iq_2}\widehat{C}(z) & e^{-iq_2}\widehat{A'}(z) & e^{-iq_2}\widehat{B'}(z) \end{pmatrix}, \qquad (2.22)$$

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

$$\mathcal{D}(\vec{q};z) \equiv \det\left(I - \widehat{T}(\vec{q};z)\right) \,. \qquad (2.23)$$

Evaluating this determinant we find

$$\begin{aligned}\mathcal{D}(\vec{q};z) &= (1-2\widehat{B}\cos q_1 + \widehat{B}^2 - \widehat{A}^2)(1-2\widehat{B'}\cos q_2 + \widehat{B'}^2 - \widehat{A'}^2) \\ &\quad -4\widehat{C}^2(\widehat{B}-\widehat{A}-\cos q_1)(\widehat{B'}-\widehat{A'}-\cos q_2),\end{aligned} \qquad (2.24)$$

where, for notational simplicity, the z-dependence of $\widehat{A},\ldots,\widehat{C}$ is indicated only implicitly by the hat. We shall simplify equation (2.21) further with the aid of the definition

$$\widehat{U}_{\vec{\beta}}(\vec{q};z)\,\mathcal{D}^{-1}(\vec{q};z) \equiv \sum_{\vec{\alpha}}(1-e^{-i\vec{q}\cdot\vec{\alpha}})\left(I-\widehat{T}(\vec{q};z)\right)^{-1}_{\vec{\alpha},\vec{\beta}}\,e^{i\vec{q}\cdot\vec{\beta}} \,. \qquad (2.25)$$

The expression (2.21) for $\widehat{P}^{*}(\vec{q};z)$ then takes the form

$$\widehat{P}^{*}(\vec{q};z) = \frac{1}{1-z}[1 + \mathcal{D}^{-1}(\vec{q};z)\sum_{\vec{\beta}}\widehat{U}_{\vec{\beta}}(\vec{q};z)\,\widehat{W}(\vec{\beta},\vec{x}_0;z)] \,. \qquad (2.26)$$

A straightforward but tedious calculation yields

$$\begin{aligned}\widehat{U}_{\vec{e}_1}(\vec{q};z) &\equiv V(q_1,q_2;\widehat{A},\widehat{A'},\widehat{B},\widehat{B'},\widehat{C}) \\ &= (\widehat{A'}^2 - \widehat{B'}^2 + 2\widehat{B'}\cos q_2 - 1)(\widehat{B} + e^{iq_1}(\widehat{A}-1))(1-e^{-iq_1}) \\ &\quad -2\widehat{C}(\widehat{A'}-\widehat{B'}-1)(\widehat{B}-\widehat{A}-e^{iq_1})(1-\cos q_2) \\ &\quad -4i\widehat{C}^2(\widehat{A'}-\widehat{B'}+\cos q_2)\sin q_1,\end{aligned} \qquad (2.27)$$

and from this we have by symmetry

$$\begin{aligned}\widehat{U}_{-\vec{e}_1}(\vec{q};z) &= V(-q_1,q_2;\widehat{A},\widehat{A'},\widehat{B},\widehat{B'},\widehat{C}), \\ \widehat{U}_{\vec{e}_2}(\vec{q};z) &= V(q_2,q_1;\widehat{A'},\widehat{A},\widehat{B'},\widehat{B},\widehat{C}), \\ \widehat{U}_{-\vec{e}_2}(\vec{q};z) &= V(-q_2,q_1;\widehat{A'},\widehat{A},\widehat{B'},\widehat{B},\widehat{C}) \,.\end{aligned} \qquad (2.28)$$

Equation (2.26) for $\widehat{P}^{*}(\vec{q};z)$, together with the expressions (2.27) and (2.28) for $\widehat{U}$ and (2.24) for $\mathcal{D}$, 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 .

2.2.4 Expressing the W_τ in the simple random walk generating function

The second task is to find an expression for the W_τ 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 [8, 9, 10, 11, 12] of random walks. Let $G_t(\vec{x})$, for $t = 0, 1, \ldots$ and $\vec{x}$ arbitrary, denote the probability of finding a simple random walker at time t on lattice site $\vec{x}$, given that at $t = 0$ it started at $\vec{x} = \vec{0}$. Then

$$\hat{G}(\vec{x}; z) = \frac{1}{L_1 L_2} \sum_{\vec{p}} \frac{\exp(-i\vec{p}\cdot\vec{x})}{1 - (z/2)(\cos p_1 + \cos p_2)}, \tag{2.29}$$

where the wavevector $\vec{p} = (p_1, p_2)$ runs through the same values as $\vec{q}$ in equation (2.17). This function satisfies

$$\frac{z}{4}\sum_{\vec{\nu}} \hat{G}(\vec{x}+\vec{\nu}; z) - \hat{G}(\vec{x}; z) = -\delta_{\vec{x},\vec{0}} \tag{2.30}$$

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

$$\frac{z}{2}[\hat{G}(\vec{e}_1; z) + \hat{G}(\vec{e}_2; z)] = \hat{G}(\vec{0}; z) - 1 \ . \tag{2.31}$$

Another useful relation is [9, 11, 12]

$$\hat{F}(\vec{x}; z) = \frac{\hat{G}(\vec{x}; z)}{\hat{G}(\vec{0}; z)}, \quad \vec{x} \neq \vec{0}, \tag{2.32}$$

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

$$\mathcal{G}(\vec{x}; z) \equiv \hat{G}(\vec{0}; z) - \hat{G}(\vec{x}; z) \tag{2.33}$$

has the property that, whereas $\lim_{z\uparrow 1} \hat{G}(\vec{x}; z) = \infty$, the *lattice Green function* $\mathcal{G}(\vec{x}; 1)$ is finite for all $\vec{x}$, as is easily seen with the aid of (2.29). For the infinite lattice it has the asymptotic behaviour [8]

$$\mathcal{G}(\vec{x}; 1) \simeq \frac{2}{\pi} \ln x, \qquad x \to \infty \ . \tag{2.34}$$

In order to obtain an equation from which we can solve $W_\tau(\vec{\nu}, \vec{x})$ we shall follow a procedure similar to the one that leads to (2.32). 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 $\vec{x}+\vec{\nu}$ *and* at time t at $\vec{x}$ (with $\vec{x} \neq \vec{0}$ and $t = 1, 2, \ldots$) is given by $\frac{1}{4}G_{t-1}(\vec{x}+\vec{\nu})$. We next write this quantity as the probability that the visit at time t to the site $\vec{x}$ was the *first* visit to that site, *plus* the sum on t' of the probability $F_{t'}(\vec{x})$ that the first visit to $\vec{x}$ has taken place at some earlier time t' multiplied by the probability $\frac{1}{4}G_{t-1-t'}(\vec{\nu})$ of going from $\vec{x}$ to $\vec{x}+\vec{\nu}$ after $t-1-t'$ steps, and to $\vec{x}$ after $t-t'$ steps. Explicitly, for $t = 1, 2, \ldots$, and $\vec{x} \neq \vec{0}$

$$\frac{1}{4}G_{t-1}(\vec{x}+\vec{\nu}) = W_t(\vec{\nu},-\vec{x}) + \frac{1}{4}\sum_{t'=0}^{t-1} F_{t'}(\vec{x})G_{t-1-t'}(\vec{\nu}) \ . \tag{2.35}$$

We multiply this equation by z^t, sum on t from 1 to ∞, and obtain, using (2.32),

$$\widehat{W}(\vec{\nu},-\vec{x};z) = \frac{z}{4}[\widehat{G}(\vec{x}+\vec{\nu};z) - \frac{\widehat{G}(\vec{x};z)\widehat{G}(\vec{\nu};z)}{\widehat{G}(\vec{0};z)}], \qquad \vec{x}\neq\vec{0} \ . \tag{2.36}$$

This is the desired expression for $\widehat{W}$ in terms of the simple random walk generating function $\widehat{G}$, and with this we have completed the second task set at the end of section 2.2.2. We specialize it first of all to the case that $\vec{x}$ is a nearest-neighbour vector. From (2.36) and the Laplace transforms of the definitions (2.8) we find

$$\begin{aligned}
\widehat{A}(z) &= \frac{z}{4}[\widehat{G}(\vec{0};z) - \frac{\widehat{G}^2(\vec{e}_1;z)}{\widehat{G}(\vec{0};z)}], \\
\widehat{B}(z) &= \frac{z}{4}[\widehat{G}(2\vec{e}_1;z) - \frac{\widehat{G}^2(\vec{e}_1;z)}{\widehat{G}(\vec{0};z)}], \\
\widehat{C}(z) &= \frac{z}{4}[\widehat{G}(\vec{e}_1+\vec{e}_2;z) - \frac{\widehat{G}(\vec{e}_1;z)\widehat{G}(\vec{e}_2;z)}{\widehat{G}(\vec{0};z)}] \ .
\end{aligned} \tag{2.37}$$

The expressions for $\widehat{A'}(z)$ and $\widehat{B'}(z)$ are found from those for $\widehat{A}(z)$ and $\widehat{B}(z)$, respectively, by replacing $\vec{e}_1$ with $\vec{e}_2$. Equivalent relations occur in [1], [3], and [5] and were apparently first derived by Benoist, Bocquet, and Lefore [13]. From (2.10) together with (2.15), (2.32), and (2.33) we have the useful relations

$$\begin{aligned}
\widehat{A}(z) + \widehat{B}(z) + 2\widehat{C}(z) &= \widehat{F}(\vec{e}_1;z) = 1 - \frac{\mathcal{G}(\vec{e}_1;z)}{\widehat{G}(\vec{0};z)}, \\
\widehat{A'}(z) + \widehat{B'}(z) + 2\widehat{C}(z) &= \widehat{F}(\vec{e}_2;z) = 1 - \frac{\mathcal{G}(\vec{e}_2;z)}{\widehat{G}(\vec{0};z)} \ .
\end{aligned} \tag{2.38}$$

In particular, in view of the finiteness of $\mathcal{G}(\vec{x};1)$ for all $\vec{x}$ and the fact that $\lim_{z\uparrow 1}\widehat{G}(\vec{x};z) = \infty$, we find from (2.38)

$$\begin{aligned}
\widehat{A}(1) + \widehat{B}(1) + 2\widehat{C}(1) &= 1, \\
\widehat{A'}(1) + \widehat{B'}(1) + 2\widehat{C}(1) &= 1 \ .
\end{aligned} \tag{2.39}$$

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

2.2.5 The effective propagator

We now have to calculate the inverse Fourier and Laplace transform

$$P_t(\vec{y}) = \frac{1}{L_1 L_2} \sum_{\vec{q}} e^{-i\vec{q}\cdot\vec{y}} \frac{1}{2\pi i} \oint \frac{dz}{z^{t+1}} \hat{P}^*(\vec{q}; z), \tag{2.40}$$

where the integral is around the origin of the complex z plane. Hence our task will be to determine the analytic structure of $\hat{P}^*(\vec{q}; z)$. The main structure is entirely contained in the denominator $\mathcal{D}(\vec{q}; z)$ in (2.24), which plays the role of an effective propagator, analogous to the denominator in the summand of the expression (2.29) for the simple random walk.

It is not possible to determine the zeros of $\mathcal{D}(\vec{q}; z)$ exactly. We shall therefore make a long-time expansion, for which the only knowledge required is the behaviour of $\mathcal{D}(\vec{q}; z)$ around its singular point nearest to $z = 0$. When $\vec{q} = \vec{0}$ this is the point $z = 1$. One readily verifies this from (2.24), which gives

$$\begin{aligned} \mathcal{D}(\vec{0}; 1) &= \left(1 - \hat{B}(1) + \hat{A}(1)\right)\left(1 - \widehat{B'}(1) + \widehat{A'}(1)\right) \\ &\quad \times \left[\left(1 - \hat{B}(1) - \hat{A}(1)\right)\left(1 - \widehat{B'}(1) - \widehat{A'}(1)\right) - 4\hat{C}^2(1)\right] \\ &= 0, \end{aligned} \tag{2.41}$$

where the second equality follows from the relations (2.39) between $\hat{A}(1)$, $\widehat{A'}(1)$, ..., $\hat{C}(1)$. For $\vec{q}$ different from zero this singularity shifts to z values larger than 1. Our small-$(1-z)$ expansion has to be accompanied by a small-q expansion. This will be done separately for the three lattice geometries of interest in sections 2.3 – 2.5.

2.2.6 Simplified formulas for a square geometry

In sections 2.3 and 2.4 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

$$\begin{aligned} A'_\tau &= A_\tau, & B'_\tau &= B_\tau, \\ \widehat{A'}(z) &= \hat{A}(z), & \widehat{B'}(z) &= \hat{B}(z). \end{aligned} \tag{2.42}$$

It is now useful to define

$$G(z) \equiv \hat{G}(\vec{0}; z), \tag{2.43a}$$

$$g(z) \equiv -\frac{1}{2}[\hat{G}(2\vec{e}_1; z) - \hat{G}(\vec{0}; z)] \, . \tag{2.43b}$$

Equation (2.31) then reduces to

$$\hat{G}(\pm\vec{e}_i; z) = \frac{1}{z}[G(z) - 1], \tag{2.44}$$

and, upon using (2.30) for $\vec{x}$ equal to a nearest-neighbour vector, we find

$$\widehat{G}(\pm\vec{e}_1 \pm \vec{e}_2; z) = (\frac{2}{z^2} - 1)\, G(z) - \frac{2}{z^2} + g(z) \; . \tag{2.45}$$

Using the general results (2.37), one then obtains the simplified expressions

$$\begin{aligned} \widehat{A}(z) &= \frac{1}{4z}\left(2 \qquad - \frac{1}{G(z)} - \left(1 - z^2\right) G(z)\right), \\ \widehat{B}(z) &= \frac{1}{4z}\left(2\,[1 - z^2 g(z)] - \frac{1}{G(z)} - \left(1 - z^2\right) G(z)\right), \\ \widehat{C}(z) &= \frac{1}{4z}\left(z^2 g(z) \qquad - \frac{1}{G(z)} + \left(1 - z^2\right) G(z)\right) . \end{aligned} \tag{2.46}$$

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

2.3 Infinite lattice

2.3.1 Expansion of $\widehat{P}^*(\vec{q}; z)$ for small q and $1 - z$

We shall now evaluate expression (2.40) for $P_t(\vec{y})$ for an infinite lattice. We first expand $\widehat{P}^*(\vec{q}; z)$ for small q $(\equiv |\vec{q}\,|)$ and $1 - z$. If we let K denote the elliptic integral of the first kind, then for the infinite square lattice we have from equations (2.43a), (2.43b), and (2.29)

$$\begin{aligned} G(z) &= \frac{1}{(2\pi)^2} \iint_{-\pi}^{\pi} d\vec{q}\, \frac{1}{1 - (z/2)(\cos q_1 + \cos q_2)} \\ &= \frac{2}{\pi} K(z^2) \\ &= \frac{1}{\pi} \ln(\frac{8}{1 - z}) - \frac{1}{2\pi}(1 - z)\ln(1 - z) + \mathcal{O}(1 - z), \qquad z \to 1, \end{aligned} \tag{2.47}$$

(see [14]) and

$$\begin{aligned} g(z) &= \frac{1}{(2\pi)^2} \iint_{-\pi}^{\pi} d\vec{q}\, \frac{\sin^2 q_1}{1 - (z/2)(\cos q_1 + \cos q_2)} \\ &= (2 - \frac{4}{\pi}) + \frac{2}{\pi}(1 - z)\ln(1 - z) + \mathcal{O}(1 - z), \quad z \to 1 \end{aligned} \tag{2.48}$$

(cf. McCrea and Whipple [15], who calculated $g(1)$). Using these expansions in the formulas (2.46) for $\widehat{A}(z), \widehat{B}(z)$, and $\widehat{C}(z)$, one finds for $z \to 1$

$$\begin{aligned} \widehat{A}(z) &= \frac{1}{2} - \frac{\pi}{4\, \ln(\frac{8}{1-z})} + \frac{1}{2\pi}(1 - z)\ln(1 - z) + \mathcal{O}(1 - z), \\ \widehat{B}(z) &= (\frac{2}{\pi} - \frac{1}{2}) - \frac{\pi}{4\, \ln(\frac{8}{1-z})} - \frac{1}{2\pi}(1 - z)\ln(1 - z) + \mathcal{O}(1 - z), \end{aligned}$$

$$\widehat{C}(z) = (\frac{1}{2} - \frac{1}{\pi}) - \frac{\pi}{4\ln(\frac{8}{1-z})} + \mathcal{O}(1-z) \,. \tag{2.49}$$

From equation (2.49) we see that the motion of the tagged particle is strongly anti-correlated; the probability for the particle to step in the direction *opposite* to its previous move is $\widehat{A}(1) = 0.5$; the probability to step in a *perpendicular* direction is $\widehat{C}(1) = 0.1816\ldots$; and the probability to step once more in the *same* direction is $\widehat{B}(1) = 0.1366\ldots$. The leading correction terms in equation (2.49) can be used to find the long-time behaviour of A_t, B_t, and C_t:

$$X_t \simeq (1 + (-1)^{t+1})\,\frac{\pi}{4t\ln^2 t}, \qquad t \to \infty, \qquad X = A,\ B,\ C \,. \tag{2.50}$$

Clearly $\sum_{t=0}^{\infty} X_t$ is finite, as it should be. Furthermore, the long-time behaviour is compatible with the asymptotic result (2.12) for R_t.

After these preliminaries we are able to expand $\widehat{P}^{*}(\vec{q}; z)$ around $(\vec{q}; z) = (\vec{0}; 1)$. To this end we first consider equation (2.24) for $\mathcal{D}(\vec{q}; z)$ and find

$$\mathcal{D}(\vec{q}; z) = \frac{g}{4}\,(1 - \frac{g^2}{4})\,q^2 + \pi\,g\,(1 + \frac{g}{2})^2\,\frac{1}{\ln(\frac{8}{1-z})} + \ldots, \quad q \to 0, \quad z \to 1, \tag{2.51}$$

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

$$g \equiv g(1) = 2 - \frac{4}{\pi} \,. \tag{2.52}$$

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

$$q^2 \sim \frac{1}{\ln(\frac{8}{1-z})} \,. \tag{2.53}$$

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

Considering equations (2.27) and (2.28) for the four $\widehat{U}_{\vec{\beta}}(\vec{q}; z)$ we find, upon expanding these expressions in powers of q_1 and q_2, that the coefficients of the linear terms become proportional to $1/\ln(\frac{8}{1-z})$ for $z \to 1$. But hence, by equation (2.53), 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

$$\widehat{U}_{\vec{\beta}}(\vec{q}; z) \simeq -\frac{g}{4}(1 - \frac{g^2}{4})\,q^2, \qquad q \to 0, \quad z \to 1, \tag{2.54}$$

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

$$\begin{aligned} \sum_{\vec{\beta}} \widehat{W}(\vec{\beta}, \vec{x}_0; z) &= \widehat{F}(\vec{x}_0; z) \\ &= 1 - \mathcal{G}(\vec{x}_0; z)/G(z) \\ &= 1 - \pi\,\mathcal{G}(\vec{x}_0; 1)/\ln(\frac{8}{1-z}) + \ldots, \qquad z \to 1, \end{aligned} \tag{2.55}$$

where we have used, successively, (2.9), (2.32), (2.33), (2.43a), and (2.47). From the asymptotic expression (2.34) we see that the first term in (2.55) dominates the remainder if the initial hole position $\vec{x}_0$ satisfies

$$2 \ln x_0 \ll \ln(\frac{8}{1-z}) . \tag{2.56}$$

We shall henceforth consider only $\vec{x}_0$ for which this condition holds. Upon using (2.51), (2.54), and (2.55) in (2.26), we obtain

$$\hat{P}^*(\vec{q}; z) \simeq \frac{1}{(1-z)(1+f\,q^2 \ln(\frac{8}{1-z}))}, \qquad q \to 0, \quad z \to 1, \tag{2.57}$$

where we have defined

$$f \equiv \frac{1}{4\pi}\frac{2-g}{2+g} = \frac{1}{4\pi(\pi-1)} . \tag{2.58}$$

Equation (2.57) is the final result of the expansion of $\hat{P}^*$ for small q and $(1-z)$.

2.3.2 An integral representation for $P_t(\vec{y})$

Now (2.57) has to be substituted in (2.40) and the z and $\vec{q}$ integrals have to be carried out. The quantity $\ln[8/(1-z)]$ occurring in (2.57) 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 $1-z$ in the denominator of the integrand in (2.57), the leading contributions to the integral come, for $t \to \infty$, from the neighbourhood of $z=1$. We may therefore fold the contour around the branch cut and integrate the discontinuity of the integrand. This gives for $t \to \infty$

$$P_t(\vec{y}) \simeq \frac{1}{(2\pi)^2} \iint_{-\pi}^{\pi} d\vec{q}\, e^{-i\vec{q}\cdot\vec{y}} \int_1^\infty \frac{dz}{z^{t+1}} \frac{1}{z-1} \frac{f\,q^2}{\left(1+f q^2 \ln\left(\frac{8}{z-1}\right)\right)^2 + (f q^2 \pi)^2} . \tag{2.59}$$

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

$$\vec{q} \equiv \frac{1}{\sqrt{\ln t}} \vec{\kappa}, \tag{2.60a}$$

$$z \equiv 1 + \frac{8}{t^w}, \tag{2.60b}$$

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

$$P_t(\vec{y}) \simeq \frac{1}{\ln t} \frac{1}{(2\pi)^2} \iint_{-\pi\sqrt{\ln t}}^{\pi\sqrt{\ln t}} d\vec{\kappa}\, e^{-i\vec{\kappa}\cdot\frac{\vec{y}}{\sqrt{\ln t}}} \int_{-\infty}^{\infty} \frac{dw}{\left(1+\frac{8}{t^w}\right)^{t+1}} \frac{f\kappa^2}{(1+f\kappa^2 w)^2 + \left(\frac{f\kappa^2\pi}{\ln t}\right)^2} . \tag{2.61}$$

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.

2.3.3 Evaluation of $P_t(\vec{y})$ in the scaling limit

In the scaling limit $t,\ y \to \infty$ with $\vec{\eta} = \vec{y}/\sqrt{\ln t}$ fixed, one finds from (2.61)

$$\begin{aligned}
P_t(\vec{y}) &\simeq \frac{1}{\ln t}\frac{1}{(2\pi)^2}\iint\limits_{-\infty}^{\infty} d\vec{\kappa}\, e^{-i\vec{\kappa}\cdot\vec{\eta}}\, f\kappa^2 \int\limits_{1}^{\infty} \frac{dw}{(1+fw\kappa^2)^2} \\
&= \frac{1}{\ln t}\frac{1}{(2\pi)^2}\iint\limits_{-\infty}^{\infty} d\vec{\kappa}\, \frac{e^{-i\vec{\kappa}\cdot\vec{\eta}}}{1+f\kappa^2} \\
&= \frac{1}{\ln t}\frac{1}{(2\pi)^2}\iint\limits_{-\infty}^{\infty} d\vec{\kappa}\, e^{-i\vec{\kappa}\cdot\vec{\eta}} \int\limits_{0}^{\infty} d\lambda\, e^{-\lambda(1+f\kappa^2)}\,.
\end{aligned} \tag{2.62}$$

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

$$P_t(\vec{y}) \simeq \frac{2(\pi-1)}{\ln t} K_0\left(\sqrt{\frac{4\pi(\pi-1)}{\ln t}}\, y\right), \qquad \frac{\vec{y}}{\sqrt{\ln t}} \text{ fixed}, \quad y,t \to \infty\,. \tag{2.63}$$

Hence $P_t(\vec{y})$ is *non-Gaussian*! With the aid of the integral [16, p. 38?]

$$\int\limits_{0}^{\infty} dx\, x^{1+2\nu} K_0(x) = 2^{2\nu}\,\Gamma^2(\nu+1) \tag{2.64}$$

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

$$\langle y^2\rangle_t \simeq \frac{\ln t}{\pi(\pi-1)}, \tag{2.65}$$

where $\langle\ldots\rangle_t$ denotes the average with respect to the distribution (2.63). The main features of the behaviour of (2.63) follow from the properties [17]

$$K_0(x) \simeq \begin{cases} -\ln x, & x \downarrow 0, \\ \sqrt{\frac{\pi}{2x}}\,e^{-x}, & x \to \infty\,. \end{cases} \tag{2.66}$$

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

2.3.4 The long-time limit at fixed $\vec{y}$

Upon employing in (2.59) expression (2.60b), but not (2.60a), we get

$$P_t(\vec{y}) \simeq \frac{1}{\ln t}\frac{1}{(2\pi)^2}\iint\limits_{-\pi}^{\pi} d\vec{q}\, e^{-i\vec{q}\cdot\vec{y}} \int\limits_{-\infty}^{\infty} \frac{dw}{(1+\frac{8}{t}w)^{t+1}}\, \frac{fq^2}{\left(\frac{1}{\ln t}+fq^2w\right)^2+\left(\frac{fq^2\pi}{\ln t}\right)^2}\,. \tag{2.67}$$

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 ∞. If in the integrand we then set $t = \infty$, it reduces to $1/fw^2q^2$, and the $\vec{q}$ integral diverges in the origin. Therefore, more care is required near $\vec{q} = \vec{0}$, and we now employ the scaling (2.60a) in (2.67). Also using that, for $w > 1$, $(1 + 8t^{-w})^{-(t+1)} \simeq e^{-8t^{1-w}} \to 1$ as $t \to \infty$, we find

$$P_t(\vec{y}) \simeq \frac{1}{\ln t}\frac{1}{(2\pi)^2} \iint_{-\pi\sqrt{\ln t}}^{\pi\sqrt{\ln t}} d\vec{\kappa}\, e^{-i\vec{\kappa}\cdot\vec{y}/\sqrt{\ln t}} \int_1^\infty dw \frac{f\kappa^2}{(1 + fw\kappa^2)^2 + \left(\frac{f\kappa^2\pi}{\ln t}\right)^2} \,. \qquad (2.68)$$

We can set $t = \infty$ in the integrand of (2.68) without creating any divergences. This yields

$$P_t(\vec{y}) \simeq \frac{1}{\ln t}\frac{1}{(2\pi)^2} \iint_{-\pi\sqrt{\ln t}}^{\pi\sqrt{\ln t}} d\vec{\kappa} \frac{1}{1 + f\kappa^2} \,. \qquad (2.69)$$

For $t \to \infty$ the integral diverges at large κ. Since we are only interested in the leading behaviour we can write, using the value (2.58) for f,

$$\begin{aligned} P_t(\vec{y}) &\simeq \frac{2(\pi-1)}{\ln t} \int^{\pi\sqrt{\ln t}} d\kappa \frac{1}{\kappa} \\ &\simeq (\pi - 1)\frac{\ln \ln t}{\ln t}, \qquad \vec{y} \text{ fixed, } t \to \infty \,. \end{aligned} \qquad (2.70)$$

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

$$G_t(\vec{y}) \simeq (1 + (-1)^{t+y_1+y_2})\frac{1}{\pi t}, \qquad \vec{y} \text{ fixed, } t \to \infty, \qquad (2.71)$$

which follows from (2.29) for a simple random walk.

Finally we recall that both results (2.63) and (2.70) hold subject to the condition that the hole is initially not too far away from the particle; explicitly, we should have

$$2 \ln x_0 \ll \ln t, \qquad (2.72)$$

as may be deduced from (2.56), (2.60b), and the fact that the w integrals in (2.62) and (2.68) do not get any significant contributions from the region $w < 1$.

2.4 $L \times L$ lattice

In this section we evaluate the expression (2.40) for $P_t(\vec{y})$ 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 $\widehat{A}(z), \widehat{B}(z)$, and $\widehat{C}(z)$ in terms of $G(z)$ and $g(z)$ with the aid of the simplified formulas of section 2.2.6. The only difference with the calculation of section 2.3 is that $G(z)$ and $g(z)$ are now given not by integrals but by sums on $\vec{q}$; 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.

2.4.1 Expansion of $\widehat{P}^*(\vec{q}; z)$ for small q and $1 - z$

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]:

$$G_L(z) = \frac{1}{L^2(1-z)} + a_0(L) - a_1(L)(1-z) + \mathcal{O}(\,(1-z)^2), \qquad z \to 1, \tag{2.73}$$

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

$$\begin{aligned} a_0(L) &= \frac{2}{\pi} \ln L + \mathcal{O}(L^0), \\ a_1(L) &= 0.06187\ldots\, L^2 + \mathcal{O}(\ln L), \qquad L \to \infty\,. \end{aligned} \tag{2.74}$$

From (2.73) we see that as $z \to 1$, the first term in the expansion for $G_L(z)$ will dominate the remainder only if

$$1 - z \ll \begin{cases} 1/L^2 a_0(L), & L \text{ fixed, arbitrary,} \\ 1/L^2 \ln L, & L \text{ fixed, large,} \end{cases} \tag{2.75}$$

where for the lower inequality (2.74) has been used. The $1 - z$ expansion of $g_L(z)$ is easily found from (2.43b):

$$g_L(z) = g_L + (g_L - \frac{a_0(L)}{2})(1-z) + \mathcal{O}(\,(1-z)^2), \qquad z \to 1, \tag{2.76}$$

where

$$\begin{aligned} g_L &\equiv g_L(1) \\ &= (2 - \frac{4}{\pi}) - \frac{2}{L^2} + \mathcal{O}(\frac{1}{L^4}), \qquad L \to \infty\,. \end{aligned} \tag{2.77}$$

Substituting the expansions (2.73) and (2.76) of $G_L(z)$ and $g_L(z)$ in the formulas (2.46) for $\widehat{A}(z), \widehat{B}(z)$, and $\widehat{C}(z)$, one obtains for $z \to 1$

$$\begin{aligned}
\widehat{A}(z) &= \frac{1}{2}(1-\frac{1}{L^2}) \qquad -\frac{1}{4}(L^2+2a_0(L)-2+\frac{1}{L^2})(1-z)+\mathcal{O}(\,(1-z)^2),\\
\widehat{B}(z) &= \frac{1}{2}(1-\frac{1}{L^2}-g_L)-\frac{1}{4}(L^2+\ a_0(L)-2+\frac{1}{L^2})(1-z)+\mathcal{O}(\,(1-z)^2),\\
\widehat{C}(z) &= \frac{1}{4}(g_L+\frac{2}{L^2}) \qquad -\frac{1}{4}(L^2-\frac{3}{2}a_0(L) \qquad -\frac{1}{L^2})(1-z)+\mathcal{O}(\,(1-z)^2).
\end{aligned} \tag{2.78}$$

Just as in equation (2.49), the quantities $\widehat{A}(1)$, $\widehat{B}(1)$, and $\widehat{C}(1)$ represent the correlations between two successive step directions, but now corrected for finite-size effects. We make an expansion of $\mathcal{D}$ for small q as well as for small $1-z$ by substituting these results in (2.24) and obtain

$$\mathcal{D}(\vec{q};z) = \frac{1}{4}(g_L+\frac{2}{L^2})(1-\frac{g_L^2}{4})\,q^2+(L^2-1)(1+\frac{g_L}{2})^2(g_L+\frac{2}{L^2})(1-z)+\ldots \tag{2.79}$$

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

$$q^2 \ll 1, \qquad 1-z \ll \frac{1}{L^2 a_0(L)}, \quad \text{and } L \text{ fixed}\ . \tag{2.80}$$

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

$$q^2 \sim L^2(1-z), \qquad L \text{ fixed}, \tag{2.81}$$

instead of (2.53). We now argue as in the case of the infinite lattice that for large t the important term in $\widehat{U}_{\vec{\beta}}$ is the one quadratic in the q_i. From this we find

$$\widehat{U}_{\vec{\beta}}(\vec{q};z) \simeq -\frac{1}{4}(g_L+\frac{2}{L^2})(1-\frac{g_L^2}{4})\,q^2, \tag{2.82}$$

valid under condition (2.80). Since, just as happened in equation (2.54), this result is to lowest order independent of $\vec{\beta}$, the third quantity in equation (2.26) which we have to expand is

$$\begin{aligned}
\sum_{\vec{\beta}} \widehat{W}(\vec{\beta},\vec{x}_0;z) &= 1-\mathcal{G}(\vec{x}_0;z)/G_L(z)\\
&= 1-L^2(1-z)\,\mathcal{G}(\vec{x}_0;1)+\mathcal{O}(\,(1-z)^2), \qquad z\to 1,
\end{aligned} \tag{2.83}$$

where we used successively equations (2.9), (2.32), (2.33), and (2.73). Upon using for $\mathcal{G}(\vec{x};1)$ the large-x expression (2.34), we see that we can replace expression (2.83) by unity if

$$1 - z \ll \frac{1}{L^2 \ln x_0}, \tag{2.84}$$

an inequality which in view of (2.80) and (2.75) is certainly satisfied. Hence the results that we shall obtain will be independent of the starting position $\vec{x}_0$ of the hole. Substituting the relations (2.79), (2.82), and (2.83) in equation (2.26) for $\hat{P}^*(\vec{q}; z)$, we find

$$\hat{P}^*(\vec{q}; z) \simeq \frac{1}{(1-z) + D_L q^2}, \tag{2.85}$$

which is valid under condition (2.80) and where we have defined

$$D_L \equiv \frac{1}{4\,(L^2-1)} \, \frac{2 - g_L}{2 + g_L} \,. \tag{2.86}$$

Equation (2.85) is the finite-lattice analogue of equation (2.57).

2.4.2 Results for $P_t(\vec{y})$

Expression (2.85) for $\hat{P}^*(\vec{q}; z)$ has to be substituted in (2.40) 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 (2.75) leads to

$$D_L q^2 \ll \begin{cases} 1/L^2 a_0(L), & L \text{ fixed, arbitrary,} \\ 1/L^2 \ln L, & L \text{ fixed, large .} \end{cases} \tag{2.87}$$

After performing the z integration we obtain

$$P_t(\vec{y}) \simeq \frac{1}{L^2} \sum_{\vec{q}} \frac{\exp(-i\vec{q}\cdot\vec{y})}{(1 + D_L q^2)^{t+1}} \,. \tag{2.88}$$

For $t = \infty$ only the term with $\vec{q} = \vec{0}$ contributes, so that $P_\infty(\vec{y}) = 1/L^2$, as it should be. Since the denominator of the summand in (2.88) has been derived in a small-q expansion, we can relate the scales of t and q as

$$t \sim \frac{1}{D_L q^2} \,. \tag{2.89}$$

In view of condition (2.87), this means that the times to be considered are

$$t \gg \begin{cases} L^2 a_0(L), & L \text{ fixed, arbitrary,} \\ L^2 \ln L, & L \text{ fixed, large .} \end{cases} \tag{2.90}$$

Hence, for large t we have

$$P_t(\vec{y}) \simeq \frac{1}{L^2} \sum_{\vec{q}} \exp(-i\vec{q} \cdot \vec{y} - D_L q^2 t) \tag{2.91}$$

subject to the conditions in equations (2.89) and (2.90). This expression shows that the time and space scales are connected by

$$y^2 \sim D_L t \ . \tag{2.92}$$

Equation (2.91) is precisely the probability distribution for a simple random walker which diffuses on a square lattice with diffusion constant D_L. Using (2.86) and (2.77), we find

$$D_L = \frac{1}{4\,(\pi-1)\,L^2}\left[1 + \frac{\pi^2 + 2\pi - 2}{2\,(\pi-1)\,L^2} + \ldots\right] \quad \text{as } L \to \infty, \tag{2.93}$$

of which the first term is the result (2.2).

In the large-L limit we obtain from (2.91) the Gaussian distribution

$$P_t(\vec{y}) \simeq \frac{(\pi-1)\,L^2}{\pi t} \exp[-\,(\pi-1)\,L^2 y^2/t], \tag{2.94}$$

which, if we combine the conditions (2.90) and (2.92), is valid for

$$\begin{aligned} &t \gg L^2 \ln L, \\ &y^2 \gg \ln L, \\ &L^2 y^2/t \ \text{ finite}, \end{aligned} \tag{2.95}$$

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.

2.4.3 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 $\vec{y}$, 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 Δy^2, which, on the basis of the infinite lattice calculation, is given by

$$\Delta y^2 \sim \ln \tau_1 \sim \ln L \ . \tag{2.96}$$

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 τ_2 needed, after crossing, to return for its next visit to the tagged particle is

$$\tau_2 \sim L^2 \ln L \ . \tag{2.97}$$

(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 [20, 21]; and this number should equal L^2 if the tagged particle is to have a reasonable probability of having 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

$$y^2 \sim \left(\frac{t}{\tau_2}\right)\Delta y^2 \sim L^{-2}\, t\ . \tag{2.98}$$

Not only is this in full agreement with the exact result (2.94), but it also explains the conditions of validity (2.95).

2.4.4 Correlation factor

If one is just interested by the result (2.86) 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, 23, 24] as the diffusion constant of a corresponding walk with the same jump frequency but uncorrelated jumps, times a correction factor f_{corr}. For the latter one can derive [23, 24]

$$f_{corr} = \frac{1+\langle\cos\theta\rangle}{1-\langle\cos\theta\rangle}, \tag{2.99}$$

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

In our specific case we therefore have

$$D_L = D_L^0\, f_{corr}, \tag{2.100}$$

where D_L^0 refers to the corresponding uncorrelated walk. Both f_{corr} and D_L^0 are easily calculated. Firstly, from the definition of $\widehat{A}(z)$, $\widehat{B}(z)$, $\widehat{C}(z)$, and the small-$(1-z)$ expansion (2.78) we find that

$$\begin{aligned}\langle\cos\theta\rangle &= \widehat{B}(1)-\widehat{A}(1)\\ &= -\tfrac{1}{2}g_L\ .\end{aligned} \tag{2.101}$$

For $L\to\infty$ the result for f_{corr} for the infinite square lattice, as was evaluated by Schoen and Lowen [25], is recovered. Secondly, $4\,D_L^0$ 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 $\frac{1}{4}$, a jump across the tracer particle, so that in the original coordinate frame the tracer jump frequency, and hence $4\,D_L^0$, is given by

$$4\, D_L^0 = \frac{1}{L^2 - 1} \tag{2.102}$$

Upon combining equations (2.99) – (2.102), one arrives directly at the expression (2.86) for D_L.

2.4.5 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 responsable 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 behaviour in the main decay regime. For the Manhattan distance $|y_1| + |y_2|$ considered in ref. [6] we find, however (indicating the average with respect to the distribution (2.94) by angular brackets)

$$\langle |y_1| + |y_2| \rangle_t^2 \simeq \frac{4t}{\pi\,(\pi - 1)\,L^2} = 0.5945\ldots \left(\frac{t}{L^2}\right), \tag{2.103}$$

valid in the regime (2.95), for large L, and as long as $t \ll L^4$. Hence, this purely diffusive behaviour (albeit on a time scale L^2) excludes the appearance of stretched exponentials. Simulations recently performed by Ajay and Palmer [27] indeed confirm equation (2.103).

2.5 Strip of width L

In this section we study the $t \to \infty$ limit of the probability distribution $P_t(\vec{y})$ 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 (2.26) for $\hat{P}^*(\vec{q}; z)$ for small q_1, q_2, and $1 - z$. In this section we shall denote the function $\hat{G}(\vec{x}; z)$ of equation (2.29) as $\hat{G}_L(\vec{x}; z)$, so that

$$\hat{G}_L(\vec{x}; z) = \frac{1}{L} \sum_{k=0}^{L-1} \frac{1}{2\pi} \int_{-\pi}^{\pi} dq_1\, \frac{\exp(-iq_1 x_1 - 2\pi i k x_2/L)}{1 - \frac{z}{2}(\cos q_1 + \cos \frac{2\pi k}{L})}\,. \tag{2.104}$$

From the general expressions (2.37) for $\widehat{A}(z)$, $\widehat{A'}(z)$, $\widehat{B}(z)$, $\widehat{B'}(z)$, and $\widehat{C}(z)$ we see that we need $\widehat{G}_L(\vec{x}; z)$ for $\vec{x} = \vec{0}$, $\vec{e}_1$, $\vec{e}_2$, $2\vec{e}_1$, $2\vec{e}_2$, $\vec{e}_1 + \vec{e}_2$. We can, for all these cases, perform the q_1 integration in (2.104) and find, for $L \geq 2$,

$$\widehat{G}_L(\vec{0}; z) = C_{L,0}(z),$$

$$\widehat{G}_L(\vec{e}_1; z) = \frac{2}{z}\left(C_{L,0}(z) - 1\right) - C_{L,1}(z),$$

$$\widehat{G}_L(\vec{e}_2; z) = C_{L,1}(z),$$

$$\widehat{G}_L(2\vec{e}_1; z) = -\frac{8}{z^2} + \left(\frac{8}{z^2} - 1\right) C_{L,0}(z) - \frac{8}{z} C_{L,1}(z) + 2\, C_{L,2}(z),$$

$$\widehat{G}_L(2\vec{e}_2; z) = 2\, C_{L,2}(z) - C_{L,0}(z),$$

$$\widehat{G}_L(\vec{e}_1 + \vec{e}_2; z) = \frac{2}{z} C_{L,1}(z) - C_{L,2}(z), \tag{2.105}$$

where we have used the abbreviation

$$C_{L,n}(z) \equiv \frac{1}{L} \sum_{k=0}^{L-1} \frac{\cos^n \frac{2\pi k}{L}}{\sqrt{(1 - \frac{z}{2}\cos\frac{2\pi k}{L})^2 - \frac{z^2}{4}}}, \qquad n = 0,\ 1,\ 2\ . \tag{2.106}$$

As a check, one may verify that the expressions (2.105) satisfy equation (2.30) for $\vec{x} = \vec{0}$, $\vec{e}_1$, $\vec{e}_2$.

2.5.1 Expansion of $\widehat{P}^*(\vec{q}; z)$ for small q and $1 - z$

Expanding the expressions (2.105) in powers of $1 - z$ is straightforward, and we obtain

$$\widehat{G}_L(\vec{0}; z) = \frac{1}{L\sqrt{1-z}} + S_{L,-1} + \mathcal{O}(1-z),$$

$$\widehat{G}_L(\vec{e}_1; z) = \frac{1}{L\sqrt{1-z}} + S_{L,-1} + 2S_{L,1} - 2 + \frac{2}{L}\sqrt{1-z} + \mathcal{O}(1-z),$$

$$\widehat{G}_L(\vec{e}_2; z) = \frac{1}{L\sqrt{1-z}} + S_{L,-1} - 2S_{L,1} + \mathcal{O}(1-z),$$

$$\widehat{G}_L(2\vec{e}_1; z) = \frac{1}{L\sqrt{1-z}} + S_{L,-1} + 8S_{L,1} + 8S_{L,3} - 8 + \frac{8}{L}\sqrt{1-z} + \mathcal{O}(1-z),$$

$$\widehat{G}_L(2\vec{e}_2; z) = \frac{1}{L\sqrt{1-z}} + S_{L,-1} - 8S_{L,1} + 8S_{L,3} + \mathcal{O}(1-z),$$

$$\hat{G}_L(\vec{e}_1 + \vec{e}_2; z) = \frac{1}{L\sqrt{1-z}} + S_{L,-1} - 4S_{L,3} + \frac{2}{L}\sqrt{1-z} + \mathcal{O}(1-z), \tag{2.107}$$

where we introduced the sums

$$S_{L,n} \equiv \frac{1}{L}\sum_{k=1}^{L-1} \frac{\sin^n \frac{\pi k}{L}}{\sqrt{1+\sin^2 \frac{\pi k}{L}}}, \qquad n = -1,\ 1,\ 3, \tag{2.108}$$

for which a large-L expansion gives

$$\begin{aligned} S_{L,-1} &= \frac{2}{\pi}\ln L + \mathcal{O}(L^0), \\ S_{L,1} &= \frac{1}{2} + \mathcal{O}(L^{-2}), \\ S_{L,3} &= \frac{1}{\pi} + \mathcal{O}(L^{-4})\ . \end{aligned} \tag{2.109}$$

By substituting (2.107) in (2.37), we find the small-$(1-z)$ expansions

$$\hat{A}(z) = 1 - S_{L,1} - (\ (1-S_{L,1})^2 + \frac{1}{L^2}\ )\, L\sqrt{1-z} + \mathcal{O}(1-z),$$

$$\widehat{A'}(z) = S_{L,1} - S_{L,1}^2\, L\sqrt{1-z} + \mathcal{O}(1-z),$$

$$\hat{B}(z) = S_{L,1} + 2\,S_{L,3} - 1 - (\ (1-S_{L,1})^2 - \frac{1}{L^2}\ )\, L\sqrt{1-z} + \mathcal{O}(1-z),$$

$$\widehat{B'}(z) = -S_{L,1} + 2\,S_{L,3} - S_{L,1}^2\, L\sqrt{1-z} + \mathcal{O}(1-z),$$

$$\hat{C}(z) = \frac{1}{2} - S_{L,3} - S_{L,1}\,(1-S_{L,1})\, L\sqrt{1-z} + \mathcal{O}(1-z)\ . \tag{2.110}$$

The quantities $\hat{A}(1), \ldots, \hat{C}(1)$ represent again the correlations between two successive step directions; horizontal and vertical steps are clearly inequivalent now. Substituting the expansions (2.110) in formula (2.24) for $\mathcal{D}(\vec{q}; z)$, one finds

$$\begin{aligned} \mathcal{D}(\vec{q}; z) \ \simeq\ & 2\,(1-2S_{L,3})(3-2S_{L,1}-2S_{L,3})(1+2S_{L,1}-2S_{L,3})\, L\sqrt{1-z} \\ & + (1+2S_{L,1}-2S_{L,3})(1-2S_{L,3})(S_{L,1}+S_{L,3}-\tfrac{1}{2})\, q_1^2 \\ & + (3-2S_{L,1}-2S_{L,3})(1-2S_{L,3})(S_{L,3}-S_{L,1}+\tfrac{1}{2})\, q_2^2 \\ & \text{as } q \to 0, \quad z \to 1\ . \end{aligned} \tag{2.111}$$

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

$$q_i^2 \sim L\sqrt{1-z}, \qquad L \ \text{ fixed}\ . \tag{2.112}$$

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

$$\begin{aligned}\widehat{U}_{\vec{\beta}}(\vec{q};z) \;\simeq\; & -(1-2S_{L,3})(1+2S_{L,1}-2S_{L,3})(S_{L,1}+S_{L,3}-\frac{1}{2})\,q_1^2 \\ & -(1-2S_{L,3})(3-2S_{L,1}-2S_{L,3})(-S_{L,1}+S_{L,3}+\frac{1}{2})\,q_2^2, \end{aligned} \tag{2.113}$$

for $q \to 0$ and $z \to 1$, which is independent of the index $\vec{\beta}$. Furthermore, one can check that

$$\sum_{\vec{\beta}} \widehat{W}(\vec{\beta},\vec{x}_0;z) = 1 + \mathcal{O}(h(\vec{x}_0)\sqrt{1-z}), \qquad z \to 1, \tag{2.114}$$

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

$$|x_{0,1}|\sqrt{1-z} \ll 1\ . \tag{2.115}$$

Upon substituting the results (2.111), (2.113), and (2.114) in equation (2.26) we find after some algebra that

$$\begin{aligned}\widehat{P}^{*}(\vec{q};z) \;\simeq\; & \left[\sqrt{1-z} + \frac{S_{L,1}+S_{L,3}-\frac{1}{2}}{2(3-2S_{L,1}-2S_{L,3})}\,\frac{q_1^2}{L} + \frac{\frac{1}{2}-S_{L,1}+S_{L,3}}{2(1+2S_{L,1}-2S_{L,3})}\,\frac{q_2^2}{L}\right]^{-1} \\ & \times \frac{1}{\sqrt{1-z}}\,, \qquad \text{for} \quad q \to 0, \quad z \to 1\ . \end{aligned} \tag{2.116}$$

2.5.2 Results for $P_t(\vec{y})$

The inverse Fourier and Laplace transform (2.40) reads in this case

$$P_t(\vec{y}) = \frac{1}{L}\sum_{q_2}\frac{1}{2\pi}\int_{-\pi}^{\pi} dq_1\, e^{-i\vec{q}\cdot\vec{y}}\,\frac{1}{2\pi i}\oint \frac{dz}{z^{t+1}}\,\widehat{P}^{*}(\vec{q};z)\ . \tag{2.117}$$

The main contribution to this integral will once again come from the region $(\vec{q},z) \approx (\vec{0},1)$. Since q_2 takes discrete values separated by $2\pi/L$, equations (2.111) and (2.112) now show that when $\sqrt{1-z} \ll L^{-3}$, the expression for $\mathcal{D}$ can become $\ll L^{-3}$ only for $q_2 = 0$. We shall abbreviate

$$\gamma_L \equiv \sqrt{\frac{S_{L,1}+S_{L,3}-\frac{1}{2}}{3-2S_{L,1}-2S_{L,3}}}, \tag{2.118}$$

which for large L becomes

$$\gamma_L \simeq \frac{1}{\sqrt{2(\pi-1)}}\ . \tag{2.119}$$

Using $\hat{P}^{*}(\vec{q}; z)$ from equation (2.116) in (2.117), 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

$$P_t(\vec{y}) \simeq \frac{1}{L}\frac{1}{2\pi^2}\int_{-\pi}^{\pi} dq_1\, e^{-iq_1 y_1} \int_1^{\infty} \frac{dz}{z^{t+1}} \frac{2\,L\,\gamma_L^2\, q_1^2}{4\,L^2\,(z-1)^{\frac{3}{2}} + \gamma_L^4\, q_1^4\,(z-1)^{\frac{1}{2}}}, \tag{2.120}$$

for $t \to \infty$. After scaling

$$z \equiv 1 + \frac{x^2}{t}, \tag{2.121a}$$

$$q_1 \equiv \frac{\kappa}{t^{\frac{1}{4}}}, \tag{2.121b}$$

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

$$P_t(\vec{y}) \simeq \frac{\gamma_L^2}{2\pi^2 L^2 t^{\frac{1}{4}}} \int_{-\infty}^{\infty} d\kappa\, \kappa^2\, e^{-i\kappa\xi} \int_0^{\infty} dx \frac{e^{-x^2}}{x^2 + \gamma_L^4 \kappa^4/4L^2} \tag{2.122a}$$

$$= \frac{\gamma_L^2}{2\pi^2 L^2 t^{\frac{1}{4}}} \int_{-\infty}^{\infty} d\kappa\, \kappa^2 e^{-i\kappa\xi} \int_0^{\infty} d\lambda\, e^{-\lambda\gamma_L^4\kappa^4/4L^2} \int_0^{\infty} dx\, e^{-(1+\lambda)x^2}\,. \tag{2.122b}$$

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

$$P_t(\vec{y}) \simeq \frac{1}{\pi^{\frac{3}{2}} L t^{\frac{1}{4}}} \int_{-\infty}^{\infty} d\kappa\, \exp(-i\kappa\xi) \int_0^{\infty} d\mu\, \exp\left(-\mu^2 - \mu\frac{\gamma_L^2\,\kappa^2}{L}\right)$$

$$= \frac{2}{\pi L^{\frac{1}{2}} t^{\frac{1}{4}} \gamma_L} \int_0^{\infty} du\, \exp\left(-u^4 - \frac{\xi^2 L}{4\gamma_L^2}\frac{1}{u^2}\right), \tag{2.123}$$

where in the last step we have performed the integration on κ and set $\mu = u^2$. Instead, we could have done the κ integration in (2.122a) first to find [28, p. 409]

$$P_t(\vec{y}) \simeq \frac{2\sqrt{2}}{\pi L^{\frac{1}{2}} t^{\frac{1}{4}} \gamma_L} \int_0^{\infty} du\, \exp\left(-u^4 - u\frac{|\xi|\sqrt{L}}{\gamma_L}\right) \cos\left(\frac{\pi}{4} + u\frac{|\xi|\sqrt{L}}{\gamma_L}\right), \tag{2.124}$$

where we have put $x = u^2$. Neither of the integral representations (2.123) or (2.124) of $P_t(\vec{y})$ can, to our knowledge, be evaluated analytically. However, both show that $P_t(\vec{y})$ has the scaling form

$$P_t(\vec{y}) \simeq \frac{2}{\pi L^{\frac{1}{2}} t^{\frac{1}{4}} \gamma_L} \mathcal{F}\left(\frac{|y_1|\, L^{\frac{1}{2}}}{\gamma_L t^{\frac{1}{4}}}\right), \quad |y_1|,\ t \to \infty,\ \frac{y_1}{t^{\frac{1}{4}}}\ \text{fixed},\ \ L\ \text{fixed}\ . \tag{2.125}$$

It is again easy to verify, especially via (2.123), that $P_t(\vec{y})$ is properly normalized and that its variance in the y_1-direction is given by

$$\langle y_1^2 \rangle_t \simeq \frac{2}{\sqrt{\pi}} \frac{\gamma_L^2}{L} t^{\frac{1}{2}} \simeq \frac{t^{\frac{1}{2}}}{\sqrt{\pi}\,(\pi - 1)\,L}, \qquad L \to \infty\,. \tag{2.126}$$

Both (2.123) and (2.124) are useful for making asymptotic expansions. With $s \equiv |\xi|\sqrt{L}/\gamma_L$ one easily finds from (2.123)

$$\mathcal{F}(s) = \int_0^\infty du \, \exp\left(-u^4 - \frac{s^2}{4\,u^2}\right) \simeq \sqrt{\frac{\pi}{6}}\, s^{-1/3} \exp(-\frac{3}{4}\, s^{4/3}), \qquad s \to \infty, \tag{2.127}$$

and from (2.124)

$$\begin{aligned} \mathcal{F}(s) &= \sqrt{2} \int_0^\infty du \, \exp(-u^4 - su)\cos(\frac{\pi}{4} + su) \\ &\simeq \Gamma(\frac{5}{4}) - \frac{1}{2} s\sqrt{\pi} + \frac{1}{4} s^2\,\Gamma(\frac{3}{4}), \qquad s \downarrow 0\,. \end{aligned} \tag{2.128}$$

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

$$P_t(\vec{y}) \simeq \frac{2}{\pi L^{\frac{1}{2}} t^{\frac{1}{4}} \gamma_L} \Gamma(\frac{5}{4}), \qquad \vec{y} \text{ fixed and } t \to \infty\,. \tag{2.129}$$

2.5.3 Discussion

Root-mean-square displacements increasing with time as $t^{\frac{1}{4}}$ are known to occur in several one-dimensional systems. An example is the reptation model introduced by De Gennes [29] 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 Brownian 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 [30] that in such a system the root mean square displacement of a tagged particle increases as $t^{\frac{1}{4}}$, and, moreover, that its distribution function approaches a *Gaussian* for long times. For these $t^{\frac{1}{4}}$ dependences several heuristic explanations are known (see, e.g., Alexander and Pincus [31]). In our case the heuristic argument runs as follows. With respect to the hole, the tagged particle position $\vec{y}$ 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 $L \geq 2$, 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 $t^{\frac{1}{4}}$ 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 (2.123).

References

[1] C.A. Sholl, J. Phys. C **14** (1981) 2723.

[2] S. Ishioka and M. Koiwa, Phil. Mag. A **41** (1980) 385.

[3] K.W. Kehr, R. Kutner, and K. Binder, Phys. Rev. B **23** (1981) 4931.

[4] H. van Beijeren, K.W. Kehr, and R. Kutner, Phys. Rev. B **28** (1983) 5711.

[5] H. van Beijeren and K.W. Kehr, J. Phys. C **19** (1986) 1319.

[6] R.G. Palmer in: *Heidelberg Colloquium on Glassy Dynamics,* eds. J.L. van Hemmen and I. Morgenstern, Lecture Notes in Physics 275 (Springer, Berlin, 1987), p. 275.

[7] K.W. Kehr and R. Kutner, Physica **110A** (1982) 535.

[8] F. Spitzer, *Principles of Random Walk* (Van Nostrand, Princeton, 1964).

[9] E.W. Montroll and G.H. Weiss, J. Math. Phys. **6** (1965) 167.

[10] M.N. Barber and B.W. Ninham, *Random and Restricted Walks* (Gordon and Breach, New York, 1970).

[11] G.H. Weiss and R.J. Rubin in: *Advances in Chemical Physics, Vol. 52*, eds. I. Prigogine and S.A. Rice (Wiley, New York, 1983), p. 363.

[12] J.W. Haus and K.W. Kehr, Phys. Rep. **150** (1987) 263.

[13] O. Benoist, J.L. Bocquet, and P. Lafore, Acta Metall. **25** (1977) 165.

[14] G. Zumofen and A. Blumen, J. Chem. Phys. **76** (1982) 3713.

[15] W. McCrea and F. Whipple, Proc. R. Soc. Edinb. **60** (1940) 281.

[16] G.N. Watson, *Theory of Bessel Functions* (Cambridge University Press, 1958).

[17] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).

[18] E.W. Montroll, J. Math. Phys. **10** (1969) 753.

[19] W.Th.F. den Hollander and P.W. Kasteleyn, Physica **112A** (1982) 523.

[20] E.W. Montroll, Proc. Symp. Appl. Math. **16** (1964) 193.

[21] F.S. Henyey and V. Seshadri, J. Chem. Phys. **76** (1982) 5530.

[22] J. Bardeen and C. Herring in: *Imperfections in Nearly Perfect Crystals*, ed. W. Shockley (Wiley, New York, 1952), p. 261.

[23] K. Compaan and Y. Haven, Trans. Faraday Soc. **52** (1956) 786.

[24] A.D. Le Claire in: *Physical Chemistry, Vol. 10*, eds. H. Eyring, D. Henderson, and W. Jost (Academic Press, New York, 1970), p. 261.

[25] A. Schoen and R. Lowen, Bull. Am. Phys. Soc. **5** (1960) 280.

[26] R.G. Palmer, D.L. Stein, E. Abrahams, and P.W. Anderson, Phys. Rev. Lett. **53** (1984) 958.

[27] Ajay and R.G. Palmer, J. Phys. A **23** (1990) 2139.

[28] I.S. Gradshteyn and I.M. Ryzhik, *Table of integrals, series and products* (Academic Press, London, 1980).

[29] P.G. de Gennes, J. Chem. Phys. **55** (1971) 572.

[30] T.E. Harris, J. Appl. Prob. **2** (1965) 323.

[31] S. Alexander and P. Pincus, Phys. Rev. B **18** (1978) 2011.

Chapter 3

Tracer particle motion in a two-dimensional lattice gas with low vacancy density

3.1 Introduction

In this chapter we consider a lattice gas on a two-dimensional square lattice with a very small density ρ of vacancies. A time evolution is assumed whereby lattice gas atoms move randomly to unoccupied neighbour sites. We arbitrarily select and "tag" one lattice gas particle, to be called the "tracer particle", and want to study its motion. It is usually assumed implicitly that for sufficiently large times and distances this motion is diffusive and fully characterizable by a coefficient of self-diffusion, D. Once this is taken for granted, there are several ways (see [1, 2, 3, 4, 5, 6]) to find an expression for D in the low-density limit. The result for a two-dimensional square lattice is

$$D = \frac{\rho}{4\,(\pi - 1)}, \quad \rho \ll 1 \,. \tag{3.1}$$

The steps of a tracer particle are due to its encounters (or "interactions") with the vacancies: a tracer particle can move only by exchanging its position with that of a vacancy. The vacancies themselves, to lowest order in their density ρ, perform independent simple random walks.

In *three* dimensions it is not hard to argue that the tracer particle should perform ordinary diffusive motion: new vacancies meet with it at a constant rate, stay in its neighbourhood for an effectively finite time [7, 8], after which, with probability one, they disappear to infinity. The tracer particle's total displacement therefore is the sum of finite, identically distributed, random contributions whose number increases linearly with time. Hence the distribution of the total displacement asymptotically becomes Gaussian.

In *two* dimensions, the case of interest here, the situation is much more subtle. Since a two-dimensional simple random walk is recurrent, a vacancy which meets the tracer particle once, will meet it an infinity of times thereafter (with probability one). In chapter 2 of this thesis we investigated the interaction between a tracer particle and a *single* vacancy initially near to each other (say neighbours). It was found that the displacement vector $\vec{y}$ of the tracer particle after a time t has a *non-Gaussian* distribution $P_t^{SV}(\vec{y})$ which, for the case of an infinite lattice, is given by

$$P_t^{SV}(\vec{y}) \simeq \frac{2(\pi-1)}{\ln t} K_0\left(\sqrt{\frac{4\pi(\pi-1)}{\ln t}}\, y\right), \quad y,t \to \infty, \ \vec{y}/\sqrt{\ln t} \text{ fixed} \tag{3.2}$$

(where K_0 is the modified Bessel function of order zero). The variance of this distribution is

$$\langle y^2 \rangle_t^{SV} \simeq \frac{\ln t}{\pi(\pi-1)}, \quad t \to \infty . \tag{3.3}$$

In the light of these results it is clearly nontrivial to explain how, for a finite (nonzero) *density* of vacancies, their combined effect can lead to ordinary diffusion of the tracer particle. This is the subject of this chapter.

In section 3.2 we consider the probability distribution $\overline{\mathcal{P}}_t(\vec{y})$ of the total displacement $\vec{y}$ of the tracer particle at time t. Since $\rho \ll 1$ we can reduce this quantity to an expression involving only the solution (3.2) of the single-vacancy problem. In section 3.3 we show that $\overline{\mathcal{P}}_t(\vec{y})$, for the case of an infinite square lattice and in the limit of low vacancy density, large times, and large distances, takes the scaling form

$$\overline{\mathcal{P}}_t(\vec{y}) \simeq \frac{1}{f \ln t} F\left(\frac{y^2}{f \ln t}, \frac{\rho\pi t}{\ln t}\right), \tag{3.4}$$

where f is a numerical constant. We study the crossover of F between the two limits $\rho\pi t/\ln t \ll 1$, which makes contact with the known single-vacancy problem, and $\rho\pi t/\ln t \gg 1$, where we show that Gaussian behaviour is obtained. We argue that the tagged particle performs diffusive motion only when considered at time intervals $\Delta t \sim \rho^{-1}\ln\rho^{-1}$, corresponding to mean square displacements $\Delta y^2 \sim \ln\rho^{-1}$. In section 3.4 we show how analogous results hold for an infinite strip of finite width.

Section 3.5 is a general conclusion.

3.2 An expression for the probability distribution $\overline{\mathcal{P}}_t(\vec{y})$

3.2.1 Reduction to a one-vacancy problem

We consider a square lattice of $L_1 \times L_2$ sites $\vec{x} \equiv (x_1, x_2)$ with integer valued components, and impose periodic boundary conditions. In this way any given site becomes equivalent to all others. This holds in particular for the origin of the lattice, which we choose as the initial position of the tagged particle. The initial positions of the vacancies are denoted by $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_V$, and are all different from each other and from $\vec{0}$. All other lattice sites are filled with untagged particles. In what follows we shall use a discrete time $t = 0, 1, \ldots$ and restrict ourselves to (dimensionless) vacancy densities ρ such that

$$\rho \equiv \frac{V}{L_1 L_2} \ll 1 . \tag{3.5}$$

We adopt the rule that at each instant of time all vacancies make a step. Each vacancy does this by exchanging its position with a particle chosen at random from among its four neighbours. Hence an isolated vacancy (i.e., a vacancy as long as it is surrounded only by lattice gas particles) performs a simple random walk. In a complete description of the lattice gas dynamics, this rule would have to be supplemented for cases where two vacancies are adjacent or have common neighbours; however, these cases contribute only to $\mathcal{O}(\rho^2)$, and we can leave the rules for them unstated. The total displacement $\vec{y}$ of the tracer particle from its initial site is the sum of displacements $\vec{y}_j$ ($j = 1, 2, \ldots, V$) induced only by its interaction with the vacancy initially at $\vec{x}_j$.

Now, let $\mathcal{P}_t(\vec{y}; \vec{x}_1, \ldots, \vec{x}_V)$ denote the probability of finding the tagged particle at lattice site $\vec{y}$ at time t as a result of its interaction with *all vacancies* collectively. The dependence of $\mathcal{P}_t$ on the initial vacancy configuration has been indicated explicitly. Let furthermore $P_t(\vec{y}_j; \vec{x}_j)$ denote the solution of a problem with *only a single* vacancy, viz. the probability of finding the tagged particle at site $\vec{y}_j$ at time t as a consequence of its interaction with a vacancy initially at $\vec{x}_j$. In the low density limit (3.5) the vacancies contribute independently to the total tagged particle displacement so that one has

$$\mathcal{P}_t(\vec{y}; \vec{x}_1, \ldots, \vec{x}_V) \simeq \sum_{\vec{y}_1} \ldots \sum_{\vec{y}_V} \delta_{\vec{y}, \vec{y}_1 + \cdots + \vec{y}_V} P_t(\vec{y}_1; \vec{x}_1) \ldots P_t(\vec{y}_V; \vec{x}_V) . \tag{3.6}$$

Upon averaging over all initial vacancy configurations, and denoting this average by an overbar, one finds

$$\overline{\mathcal{P}_t(\vec{y}; \vec{x}_1, \ldots, \vec{x}_V)} \simeq \sum_{\vec{y}_1} \ldots \sum_{\vec{y}_V} \delta_{\vec{y}, \vec{y}_1 + \cdots + \vec{y}_V} \overline{P_t(\vec{y}_1; \vec{x}_1) \ldots P_t(\vec{y}_V; \vec{x}_V)} . \tag{3.7}$$

In the limit of low vacancy density (3.5) we may replace the average over all allowed $t = 0$ configurations of the vacancies on the right-hand side of equation (3.7) by independent averages over the initial vacancy positions $\vec{x}_1, \ldots, \vec{x}_V$ separately, still however excluding the origin from being an allowed site. That is, we use

$$\overline{P_t(\vec{y}_1; \vec{x}_1) \ldots P_t(\vec{y}_V; \vec{x}_V)} \simeq \overline{P_t(\vec{y}_1; \vec{x}_1)} \cdots \overline{P_t(\vec{y}_V; \vec{x}_V)}, \tag{3.8}$$

valid for $\rho \ll 1$, and where we defined

$$\overline{P_t(\vec{y};\vec{x})} = \frac{1}{L_1L_2 - 1}\sum_{\vec{x}\neq\vec{0}} P_t(\vec{y};\vec{x}) \ . \tag{3.9}$$

We introduce the abbreviations

$$\overline{\mathcal{P}}_t(\vec{y}) = \overline{\mathcal{P}_t(\vec{y};\vec{x}_1,\ \dots,\ \vec{x}_V)}, \tag{3.10}$$

$$\overline{P}_t(\vec{y}) = \overline{P_t(\vec{y};\vec{x})}, \tag{3.11}$$

and, for any space-dependent quantity $X(\vec{y})$ define a Fourier transform, $X^*(\vec{q})$, by

$$X^*(\vec{q}) = \sum_{\vec{y}} \exp(i\vec{q}\cdot\vec{y})\, X(\vec{y}), \tag{3.12}$$

where the sum runs through all lattice sites and $\vec{q}$ takes the values

$$q_i = 2\pi\frac{k_i}{L_i}, \quad k_i = 0,\ 1,\ \dots,\ L_i - 1, \quad i = 1,\ 2\ . \tag{3.13}$$

With these definitions we find from (3.7) and (3.8)

$$\overline{\mathcal{P}}_t^*(\vec{q}) \simeq \left(\overline{P}_t^*(\vec{q})\right)^V, \tag{3.14}$$

valid for $\rho \ll 1$. This equation expresses in a concise form the reduction of the quantity of interest, $\overline{\mathcal{P}}_t$, to the single-vacancy quantity $\overline{P}_t$.

3.2.2 A recursion relation for $P_t(\vec{y};\vec{x})$

The function $P_t(\vec{y};\vec{x})$ gives the probability that a tagged particle initially at the origin has undergone a displacement $\vec{y}$ at time t due to its interaction with a vacancy initially at $\vec{x}$. When at a fixed time t the lattice size L_1L_2 tends to infinity, the average $\overline{P}_t(\vec{y})$ will be dominated by initial vacancy sites $\vec{x}$ far away from the origin, and hence $\overline{P}_t(\vec{y})$ will differ from its initial value $\overline{P}_0(\vec{y}) = \delta_{\vec{y},\vec{0}}$ only by a vanishing amount. In order to isolate this amount we shall, for each vacancy, divide the time axis into an initial time interval *preceding* the time τ at which it first arrives at the origin, and a subsequent time interval, of length $t-\tau$, during which it may interact many times with the tagged particle. For the description of what happens during this latter interval we shall then be able to profit from the results of chapter 2.

Let $W_\tau(\vec{\nu},\vec{x})$, for $\vec{x}\neq\vec{0}$, $\tau = 1,\ 2,\ \dots$ and $\vec{\nu}$ one of the unit vectors $\pm\vec{e}_1$, $\pm\vec{e}_2$, where

$$\vec{e}_1 = (1,0) \quad \text{and} \quad \vec{e}_2 = (0,1), \tag{3.15}$$

denote the probability that a simple random walker initially at $\vec{x}$

(*i*) hits the origin for the first time at time τ, *and* that

(*ii*) its position at $\tau - 1$ was $\vec{\nu}$.

Furthermore define $W_0(\vec{\nu},\vec{x}) \equiv 0$ for $\vec{x}\neq\vec{0}$. Then, evidently, the *first passage time distribution*

$$F_\tau(\vec{x}) \equiv \sum_{\vec{\nu}} W_\tau(\vec{\nu}, \vec{x}), \quad \tau = 0, 1, \ldots \tag{3.16}$$

is the probability that the simple random walker (initially at $\vec{x} \neq \vec{0}$) will hit the origin for the first time at time τ, regardless of the direction it comes from.

We now apply these definitions to the case where one has a tagged particle, initially at the origin, and a single vacancy, initially at $\vec{x} \neq \vec{0}$, which performs a simple random walk. Then clearly $W_\tau(\vec{\nu}, \vec{x})$ is the probability that at time τ the tagged particle will make its first step, and that this step is in the direction $\vec{\nu}$, and consequently $F_\tau(\vec{x})$ is the probability that at time τ the tagged particle will make its first step, irrespective of the direction in which it leaves. Therefore $1 - \sum_{\tau=0}^{t} F_\tau(\vec{x})$ is the probability that at time t the particle has not stepped yet. Now, since at time t the tagged particle either has made no move at all, in which case it is still at the origin, or has made at least one step, its first step taking place at time τ $(0 \leq \tau \leq t)$ and being in the direction $\vec{\nu}$ (so that at time τ the position of the vacancy with respect to the tagged particle is given by $-\vec{\nu}$), the displacement distribution function $P_t(\vec{y}; \vec{x})$ satisfies the recursion relation

$$\begin{aligned} P_t(\vec{y}; \vec{x}) &= [1 - \sum_{\tau=0}^{t} F_\tau(\vec{x})]\, \delta_{\vec{y},\vec{0}} \\ &+ \sum_{\tau=0}^{t} \sum_{\vec{\nu}} P_{t-\tau}(\vec{y} - \vec{\nu}; -\vec{\nu})\, W_\tau(\vec{\nu}, \vec{x}), \quad \vec{x} \neq \vec{0}\,. \end{aligned} \tag{3.17}$$

The function P in the right-hand member has as its second argument only nearest neighbour vectors and is the quantity to which the results of chapter 2 apply. Averaging over all $\vec{x}$ $(\neq \vec{0})$ and Fourier transforming, one finds from (3.17), using definitions (3.10), (3.11), and (3.16):

$$\overline{P}_t^*(\vec{q}) = 1 - \frac{1}{L_1 L_2 - 1} \sum_{\tau=0}^{t} \sum_{\vec{\nu}} [1 - P_{t-\tau}^*(\vec{q}; -\vec{\nu})\, e^{i\vec{q}\cdot\vec{\nu}}] \sum_{\vec{x}\neq\vec{0}} W_\tau(\vec{\nu}, \vec{x})\,. \tag{3.18}$$

Here the second term is the desired correction expressing the effect of a vacancy hitting the origin before or at the time t; on a large lattice this correction is small. Substituting this result in equation (3.14) and using that $W_\tau(-\vec{\nu}, \vec{x}) = W_\tau(\vec{\nu}, -\vec{x})$ so that $\sum_{\vec{x}\neq\vec{0}} W_\tau(\vec{\nu}, \vec{x}) = \sum_{\vec{x}\neq\vec{0}} W_\tau(-\vec{\nu}, \vec{x})$ one gets

$$\overline{\mathcal{P}}_t^*(\vec{q}) \simeq \left(1 - \frac{1}{L_1 L_2 - 1} \sum_{\tau=0}^{t} \sum_{\vec{\nu}=\vec{e}_1,\vec{e}_2} \Delta_{t-\tau}(\vec{q}; \vec{\nu}) \sum_{\vec{x}\neq\vec{0}} W_\tau(\vec{\nu}, \vec{x})\right)^{\rho L_1 L_2}, \tag{3.19}$$

where we introduced the abbreviation

$$\Delta_t(\vec{q}; \vec{\nu}) \equiv 2 - P_t^*(\vec{q}; -\vec{\nu})\, e^{i\vec{q}\cdot\vec{\nu}} - P_t^*(\vec{q}; \vec{\nu})\, e^{-i\vec{q}\cdot\vec{\nu}}, \tag{3.20}$$

and where the result is valid for $\rho \ll 1$ and $t = 0, 1, \ldots$. Now, if we let the number of lattice sites go to infinity while keeping the vacancy density ρ fixed, the expression for $\overline{\mathcal{P}}_t^*(\vec{q})$ becomes

$$\overline{\mathcal{P}}_t^*(\vec{q}) \simeq \exp\left(-\rho \sum_{\tau=0}^{t} \sum_{\vec{\nu}=\vec{e}_1,\vec{e}_2} \Delta_{t-\tau}(\vec{q};\vec{\nu}) \sum_{\vec{x}\neq\vec{0}} W_\tau(\vec{\nu},\vec{x})\right) \equiv \exp\left(-\rho\Omega_t(\vec{q})\right) . \quad (3.21)$$

3.2.3 An expression for $\ln \overline{\mathcal{P}}_t^*(\vec{q})$

For any time-dependent quantity X_t we define as in chapter 2 its (discrete) Laplace transform (or: generating function), $\widehat{X}(z)$, by

$$\widehat{X}(z) \equiv \sum_{t=0}^{\infty} z^t X_t . \quad (3.22)$$

Applying this definition to $\Omega_t(\vec{q})$ one finds that $\widehat{\Omega}(\vec{q};z)$ is given by

$$\widehat{\Omega}(\vec{q};z) = \sum_{\vec{\nu}=\vec{e}_1,\vec{e}_2} \widehat{\Delta}(\vec{q};\vec{\nu};z) \sum_{\vec{x}\neq\vec{0}} \widehat{W}(\vec{\nu},\vec{x};z) . \quad (3.23)$$

Now let $G_t(\vec{x})$, for $t = 0, 1, \ldots$ and $\vec{x}$ arbitrary, denote the probability of finding a random walker at time t on lattice site $\vec{x}$, given that at $t = 0$ it started at $\vec{x} = \vec{0}$. Then, see e.g. [9, 10, 11, 12], the random walk generating function is given by

$$\widehat{G}(\vec{x};z) = \frac{1}{L_1 L_2} \sum_{\vec{p}} \frac{\exp(-i\vec{p}\cdot\vec{x})}{1-(z/2)(\cos p_1 + \cos p_2)}, \quad (3.24)$$

where the wavevector $\vec{p} = (p_1, p_2)$ runs through the same values as $\vec{q}$ in equation (3.13). The relation between the generating functions $\widehat{W}(\vec{\nu},\vec{x};z)$, needed in (3.23) and $\widehat{G}(\vec{x};z)$, for $\vec{x} \neq \vec{0}$, is easily found to be (see section 2.2.4 for a derivation)

$$\widehat{W}(\vec{\nu},\vec{x};z) = \frac{z}{4}\left[\widehat{G}(\vec{\nu}-\vec{x};z) - \frac{\widehat{G}(\vec{\nu};z)\widehat{G}(\vec{x};z)}{\widehat{G}(\vec{0};z)}\right] . \quad (3.25)$$

Since $\sum_{\vec{x}} G_t(\vec{x}) = 1$, we have

$$\sum_{\vec{x}} \widehat{G}(\vec{x};z) = \frac{1}{1-z} . \quad (3.26)$$

Therefore, also using the well-known relation [10, 11, 12]

$$\widehat{F}(\vec{x};z) = \frac{\widehat{G}(\vec{x};z)}{\widehat{G}(\vec{0};z)}, \ \vec{x} \neq \vec{0}, \quad (3.27)$$

between the generating function for the first passage time distribution, $\widehat{F}$, and the random walk generating function $\widehat{G}$ we find from (3.25)

$$\sum_{\vec{x} \neq \vec{0}} \widehat{W}(\vec{\nu}, \vec{x}; z) = \frac{z}{4\,(1-z)} \left(1 - \widehat{F}(\vec{\nu}; z)\right) . \tag{3.28}$$

Substituting this result in (3.23) we obtain

$$\widehat{\Omega}(\vec{q}; z) = \frac{z}{4\,(1-z)} \sum_{\vec{\nu}=\vec{e}_1,\vec{e}_2} \widehat{\Delta}(\vec{q}; \vec{\nu}; z)(1 - \widehat{F}(\vec{\nu}; z)) . \tag{3.29}$$

For the remaining development it will be convenient to recall the abbreviations

$$\begin{aligned} A_\tau &\equiv W_\tau(\vec{e}_1, \vec{e}_1), \\ A'_\tau &\equiv W_\tau(\vec{e}_2, \vec{e}_2), \\ B_\tau &\equiv W_\tau(-\vec{e}_1, \vec{e}_1), \\ B'_\tau &\equiv W_\tau(-\vec{e}_2, \vec{e}_2), \\ C_\tau &\equiv W_\tau(\vec{e}_2, \vec{e}_1), \end{aligned} \tag{3.30}$$

introduced in chapter 2. The quantities A_τ and A'_τ, B_τ and B'_τ, and C_τ describe the probability for two successive moves of the tagged particle, separated by a time τ, to be in opposite, equal, and perpendicular directions, respectively. In a square geometry (an $L \times L$ or an $\infty \times \infty$ lattice) the additional invariance of the lattice under rotations over $\pi/2$ reduces the number of independent quantities in (3.30) to three, since then $A'_\tau = A_\tau$ and $B'_\tau = B_\tau$. We remark that from (3.16), (3.22), and (3.30) one has

$$\begin{aligned} \widehat{F}(\vec{e}_1; z) &= \widehat{A}(z) + \widehat{B}(z) + 2\widehat{C}(z) \\ \widehat{F}(\vec{e}_2; z) &= \widehat{A'}(z) + \widehat{B'}(z) + 2\widehat{C}(z) . \end{aligned} \tag{3.31}$$

By letting $z \to 1$, and using (3.24) and (3.27), one obtains the equalities

$$\begin{aligned} \widehat{A}(1) + \widehat{B}(1) + 2\widehat{C}(1) &= 1, \\ \widehat{A'}(1) + \widehat{B'}(1) + 2\widehat{C}(1) &= 1, \end{aligned} \tag{3.32}$$

which express the fact that a two-dimensional simple random walk is recurrent.

Using formulas (3.20), (3.22), (3.30), as well as formulas (2.24) – (2.28), we find

$$\widehat{\Delta}(\vec{q}; \vec{\nu}; z) = \frac{\mathcal{N}(\vec{q}; \vec{\nu}; z)}{(1-z)\,\mathcal{D}(\vec{q}; z)}, \quad \vec{\nu} = \vec{e}_1, \vec{e}_2, \tag{3.33}$$

where

$$\begin{aligned} \mathcal{N}(\vec{q}; \vec{e}_1; z) \equiv\ & 4\{\widehat{C}\,(1 - \widehat{A'} + \widehat{B'}) - \widehat{B'}\,(1 - \widehat{A} + \widehat{B})\}(1 - \cos q_1)(1 - \cos q_2) \\ & - 2\,(1 - \widehat{A'} - \widehat{B'})(1 + \widehat{A'} - \widehat{B'})(1 - \widehat{A} + \widehat{B})(1 - \cos q_1) \\ & - \quad 4\,\widehat{C} \quad (1 + \widehat{A} - \widehat{B})(1 - \widehat{A'} + \widehat{B'})(1 - \cos q_2), \end{aligned} \tag{3.34}$$

and

$$\begin{aligned}\mathcal{D}(\vec{q};z) \equiv\ & (1-2\widehat{B}\cos q_1+\widehat{B}^2-\widehat{A}^2)(1-2\widehat{B'}\cos q_2+\widehat{B'}^2-\widehat{A'}^2)\\ & -4\widehat{C}^2\,(\widehat{B}-\widehat{A}-\cos q_1)(\widehat{B'}-\widehat{A'}-\cos q_2),\end{aligned} \tag{3.35}$$

and where the z-dependence of $\widehat{A}(z)$, ..., $\widehat{C}(z)$ has been indicated only implicitly by the hat. An expression for $\mathcal{N}(\vec{q};\vec{e}_2;z)$ can be found from (3.34) by interchanging the roles of q_1 and q_2, of $\widehat{A}$ and $\widehat{A'}$, and of $\widehat{B}$ and $\widehat{B'}$. Note that $\mathcal{D}$ is invariant under this operation. Using formulas (3.31) and (3.33) – (3.35) we can express the sum on $\vec{\nu}$ in (3.29) fully in terms of $\widehat{A}(z)$, ..., $\widehat{C}(z)$, which in turn, via (3.25), can be expressed in terms of the simple random walk generating function $\widehat{G}(\vec{x};z)$. Therefore, $\widehat{\Omega}(\vec{q};z)$ can now be regarded to be a known quantity.

To find $\Omega_t(\vec{q})$ we have to perform the inverse Laplace transformation

$$\Omega_t(\vec{q})=\frac{1}{2\pi i}\oint\frac{dz}{z^{t+1}}\widehat{\Omega}(\vec{q};z), \tag{3.36}$$

where the integral is around the origin of the complex z plane. Hence our task is to determine the analytic structure of $\widehat{\Omega}(\vec{q};z)$. It is not possible to determine the zeros of the denominator $\mathcal{D}$ in (3.35) exactly. However, since we are interested in a long-time expansion, the only knowledge required is the behaviour of the integrand around its singular point nearest to $z=0$. With the aid of equations (3.29) and (3.31) – (3.35) one can verify that this is the point $(\vec{q};z)=(\vec{0};1)$:

$$\mathcal{D}(\vec{0};1)=0\ . \tag{3.37}$$

Therefore, we have to perform a double expansion, for small $1-z$ and for small q. In sections 3.3 and 3.4 we shall perform such an expansion of $\widehat{\Omega}(\vec{q};z)$, for the cases of an infinite lattice and of a strip of width L, respectively, and determine the asymptotic form of $\overline{\mathcal{P}}_t(\vec{y})$ for $y,t\to\infty$.

3.3 Infinite lattice

3.3.1 Long-time limit of the distribution function $\overline{\mathcal{P}}_t(\vec{y})$

We begin by considering $\widehat{A}(z)$, $\widehat{B}(z)$, and $\widehat{C}(z)$ in the limit L_1, $L_2\to\infty$ and expanding them around $z=1$. Using equations (3.24), (3.25), and (3.30) one derives

$$\begin{aligned}\widehat{A}(z) &= \frac{1}{2}-\frac{\pi}{4\ln(\frac{8}{1-z})}+\frac{1}{2\pi}(1-z)\ln(1-z)+\mathcal{O}(1-z),\\ \widehat{B}(z) &= (\frac{2}{\pi}-\frac{1}{2})-\frac{\pi}{4\ln(\frac{8}{1-z})}-\frac{1}{2\pi}(1-z)\ln(1-z)+\mathcal{O}(1-z),\\ \widehat{C}(z) &= (\frac{1}{2}-\frac{1}{\pi})-\frac{\pi}{4\ln(\frac{8}{1-z})}+\mathcal{O}(1-z)\ .\end{aligned} \tag{3.38}$$

Because of symmetry $\widehat{A'}(z) = \hat{A}(z)$ and $\widehat{B'}(z) = \hat{B}(z)$. If we substitute the expansions (3.38) in (3.29) and (3.33) - (3.35), then the expansion of $\hat{\Omega}(\vec{q}; z)$, to leading order in the q_i and in $1 - z$, is found to be given by

$$\hat{\Omega}(\vec{q}; z) \simeq \frac{\pi f q^2}{(1-z)^2 \left\{1 + f q^2 \ln\left(\frac{8}{1-z}\right)\right\}}, \tag{3.39}$$

where

$$f \equiv \frac{1}{4\pi(\pi - 1)}. \tag{3.40}$$

In the Appendix to this chapter we show explicitly how to perform the inverse Laplace transformation (3.36) for the case at hand. The result for $q \ll 1$ and $t \gg 1$ is

$$\Omega_t(\vec{q}) \simeq \frac{\pi f q^2 t}{1 + f q^2 \ln t}. \tag{3.41}$$

It remains to evaluate $\overline{\mathcal{P}}_t(\vec{y})$ as the inverse Fourier transform of $\overline{\mathcal{P}}_t^*(\vec{q})$. For an infinite lattice and for asymptotically large times, and if we use equation (3.21) and the large-t, small-q, expansion (3.41) of $\Omega_t(\vec{q})$, this function takes the form

$$\overline{\mathcal{P}}_t(\vec{y}) \simeq \frac{1}{(2\pi)^2} \iint_{-\pi}^{\pi} d\vec{q} \exp\left(-i\vec{q} \cdot \vec{y} - \frac{\rho \pi f q^2 t}{1 + f q^2 \ln t}\right). \tag{3.42}$$

Now, one may show that [12, eq. (2.20)]

$$\langle y^2 \rangle_t \equiv \sum_{\vec{y}} y^2 \overline{\mathcal{P}}_t(\vec{y}) = -\Delta \overline{\mathcal{P}}_t^*(\vec{0}), \tag{3.43}$$

provided $\langle y^2 \rangle_t$ exists, and where Δ is the Laplacian with respect to $\vec{q}$. Using (3.42) we therefore find

$$\langle y^2 \rangle_t \simeq \frac{\rho t}{\pi - 1}, \tag{3.44}$$

valid for $t \gg 1$ and $\rho \ll 1$. This result is compatible with numerical simulations by Ajay and Palmer [13], who study the Manhattan distance covered by a tagged particle on a square $L \times L$-lattice in the presence of one or more vacancies, as a function of t. *If* $\langle y^2 \rangle_t$ is due to a diffusion process (i.e., if it results from the addition of a large number of independent displacements), then the diffusion constant D is as given in (3.1). However, (3.44) *does not imply* that diffusion is the underlying process, nor even that $\overline{\mathcal{P}}_t(\vec{y})$ *is a Gaussian.* In fact we shall show that only for asymptotically long times does $\overline{\mathcal{P}}_t(\vec{y})$ become Gaussian.

3.3.2 The scaling limit

The function $\overline{\mathcal{P}}_t(\vec{y})$ depends on the variables t and $\vec{y}$, as well as on the parameter ρ. We define a *scaling limit*

$$\begin{cases} t \to \infty, \quad \rho \to 0^+, \quad y \to \infty \\ \rho\pi t/\ln t \equiv \sigma \text{ fixed}, \quad \vec{y}/\sqrt{f \ln t} \equiv \vec{\eta} \text{ fixed}, \end{cases} \tag{3.45}$$

and shall show that in this limit $\overline{\mathcal{P}}_t(\vec{y})$ takes the form (3.4), i.e., depends only on the two fixed combinations in (3.45). Starting from equation (3.42), introducing the variable of integration $\vec{\kappa} = \vec{q}\sqrt{f \ln t}$, and extending the integration limits to infinity we find

$$\begin{aligned} \overline{\mathcal{P}}_t(\vec{y}) &\simeq \frac{1}{(2\pi)^2} \iint_{-\infty}^{\infty} \frac{d\vec{\kappa}}{f \ln t} \exp[-i\vec{\kappa} \cdot \frac{\vec{y}}{\sqrt{f \ln t}} - \left(\frac{\rho\pi t}{\ln t}\right) \frac{\kappa^2}{1+\kappa^2}] & \text{(3.46a)} \\ &= \delta(\vec{y}) \exp\left(-\frac{\rho\pi t}{\ln t}\right) \\ &\quad + \frac{\exp\left(-\frac{\rho\pi t}{\ln t}\right)}{f \ln t} \frac{1}{(2\pi)^2} \iint_{-\infty}^{\infty} d\vec{\kappa}\, e^{-i\vec{\kappa}\cdot\frac{\vec{y}}{\sqrt{f\ln t}}} [\exp\left(\frac{\rho\pi t}{\ln t} \frac{1}{1+\kappa^2}\right) - 1] & \text{(3.46b)} \\ &\equiv \frac{1}{f \ln t} F(\eta^2, \sigma) \,. & \text{(3.46c)} \end{aligned}$$

This establishes the validity of the scaling form (3.4) and gives an explicit expression for the scaling function $F(\eta^2, \sigma)$. Consistent with extending the integration limits to infinity we have also instead of a Kronecker delta written a Dirac delta function, $\delta(\vec{y})$, thus regarding $\vec{y}$ as a continuous variable. The coefficient of this delta function, $\exp(-\rho\pi t/\ln t)$, gives the probability that at time t the tagged particle has not stepped yet. The function $F(\eta^2, \sigma)$ in (3.46c) can be written as a power series in σ. By Taylor expanding the exponent in the integrand in (3.46b), and using formulas (9.1.18) and (11.4.44) from [14], one finds

$$F(\eta^2, \sigma) = \delta(\vec{\eta}) e^{-\sigma} + \frac{\exp(-\sigma)}{2\pi} \sum_{n=1}^{\infty} \frac{\sigma^n}{n!\,(n-1)!} \left(\frac{\eta}{2}\right)^{n-1} K_{n-1}(\eta) \tag{3.47}$$

where K_m is the modified Bessel function of order m. The series converges for all σ when $\eta \neq 0$. Furthermore, using [15, p. 388]

$$\int_0^{\infty} dx\, K_\nu(x)\, x^{\mu-1} = 2^{\mu-2} \Gamma\left(\frac{\mu-\nu}{2}\right) \Gamma\left(\frac{\mu+\nu}{2}\right), \tag{3.48}$$

one may verify that $\overline{\mathcal{P}}_t(\vec{y})$ as given by (3.46) and (3.47) is properly normalized, and also reobtain equation (3.44).

3.3.3 Initial time regime and crossover

In equation (3.47) there is no restriction on the value of the combination $\sigma = \rho\pi t/\ln t$. However, although describing the *full crossover* between small and large values of this parameter, equation (3.47) is really useful only for values of $\rho\pi t/\ln t$ which are not too large, since then the series on the right-hand side of this equation is rapidly converging. In fact, for $\rho\pi t/\ln t \ll 1$ (that is, times t such that $1 \ll t \ll \rho^{-1}\ln\rho^{-1}$) one finds from (3.47)

$$\overline{\mathcal{P}}_t(\vec{y}) \simeq \left(1 - \frac{\rho\pi t}{\ln t}\right)\delta(\vec{y}) + \frac{2\pi(\pi-1)\rho t}{\ln^2 t}K_0\left(\sqrt{\frac{4\pi(\pi-1)}{\ln t}}\,y\right). \tag{3.49}$$

This expression makes contact with the single-vacancy case studied in chapter 2, where, for the infinite lattice, we found the result (3.2). As we will show in section 3.3.7, $\rho\pi t/\ln t$ is, to leading order in t, precisely the mean number of different vacancies which have met the tagged particle at time t. Hence, when much smaller than one, it is just the probability that at time t the tagged particle has been met by one single vacancy, the probability for interacting with more than one vacancy being negligibly small. Therefore, equation (3.49) can be interpreted as saying that for ρ very small, and for a typical initial vacancy configuration, we can find a time regime in which the tagged particle has either interacted with a single vacancy, thereby producing the distribution (3.2), or has seen no vacancy at all, in which case it is still at the origin.

3.3.4 Long-time regime

Although equation (3.47) is also valid in this limit, it is no longer a very useful expansion, the series being no longer rapidly converging. Therefore, to obtain an (asymptotic) expansion for large values of $\rho\pi t/\ln t$, we shall now return to equation (3.46a). Introducing again an appropriate variable of integration, $\vec{p} \equiv \sqrt{\rho\pi t/\ln t}\,\vec{\kappa}$, and expanding the integrand, we find

$$\begin{aligned}\overline{\mathcal{P}}_t(\vec{y}) &= \frac{1}{4\pi^3 f\rho t}\iint_{-\infty}^{\infty} d\vec{p}\exp\left(-i\vec{p}\cdot\frac{\vec{y}}{\sqrt{\pi f\rho t}} - p^2\right)\\ &\times\left[1 + \left(\frac{\ln t}{\rho\pi t}\right)p^4 + \frac{1}{2}\left(\frac{\ln t}{\rho\pi t}\right)^2(p^8 - 2p^6) + \ldots\right].\end{aligned} \tag{3.50}$$

We remark that in the scaling limit (3.45) the quantity $\vec{y}/\sqrt{\pi f\rho t} = \vec{\eta}/\sqrt{\sigma}$ also remains fixed. Hence (3.50) is easily seen to be of the scaling form (3.46c) (as had to be the case). Upon carrying out the $\vec{p}$ integrals in (3.50) we now find a large-σ expansion for the function F, viz.

$$F(\eta^2,\sigma) = \frac{\exp(-\eta^2/4\sigma)}{4\pi\sigma} \sum_{n=0}^{\infty} f_n\left(\frac{\eta^2}{4\sigma}\right)\frac{1}{\sigma^n}, \tag{3.51a}$$

with

$$f_0(x) = 1, \quad f_1(x) = 2 - 4x + x^2, \ \dots \tag{3.51b}$$

Retaining only the first term in (3.51a) we obtain, using (3.46c) and (3.40),

$$\overline{\mathcal{P}}_t(\vec{y}) \simeq \frac{\pi - 1}{\pi \rho t} \exp\left(-\frac{(\pi-1)y^2}{\rho t}\right), \tag{3.52}$$

valid in the limit $t \gg \rho^{-1}\ln\rho^{-1}$ and $\rho \ll 1$. It is not difficult to verify that $\overline{\mathcal{P}}_t(\vec{y})$ is indeed properly normalized, and that its variance is given by (3.44).

We note, incidentally, that the Gaussian distribution (3.52) and the conditions under which it is valid coincide with an analogous expression for a single vacancy on a finite, but large, $L \times L$ lattice with periodic boundary conditions if one replaces ρ by $1/L^2$ (cf. section 2.4).

The result (3.52) shows explicitly that in the presence of a finite density of vacancies and for asymptotically long times, the tagged particle position has a Gaussian probability distribution.

3.3.5 Scale of tracer particle diffusion: heuristic argument

Equation (3.52), together with its conditions of validity, is a strong indication that the tagged particle performs diffusive motion on a coarse grained scale with time intervals of size

$$\Delta t \sim \rho^{-1}\ln\rho^{-1} \tag{3.53a}$$

and a corresponding spatial resolution

$$\Delta y^2 \sim \ln\rho^{-1}\ . \tag{3.53b}$$

We do not prove this mathematically but present a heuristic argument analogous to one used in chapter 2.

One may imagine the tagged particle surrounded by a circle of radius $\rho^{-\frac{1}{2}}$. We consider processes of the following type: a vacancy (i) enters the circle, (ii) displaces the particle at least once, and (iii) leaves the circle again. One process will take a typical time $\Delta t = \tau_1 + \tau_2 \sim \rho^{-1}\ln\rho^{-1}$, as may be seen as follows. A time $\tau_1 \sim \rho^{-1}\ln\rho^{-1}$ is needed for the vacancy to reach the tagged particle from a site at the edge of the circle; a time $\tau_2 \sim \rho^{-1}$ is needed for it to leave the circle again after its first encounter with the tagged particle. During the time interval τ_2 more encounters with the tagged particle will take place, so that, by (3.3), during one process the latter acquires a mean square displacement $\Delta y^2 \sim \ln\rho^{-1}$. Since there is, on average, ~ 1

vacancy outside the circle ready to start a process, processes of the above type take place at a constant average rate $\sim 1/\Delta t$. It remains to be shown that displacements due to different processes are independent. This is certainly true for displacements due to different vacancies. In the case that two processes are due to the same vacancy, there is a finite (nonzero) probability for the vacancy to approach the tagged particle the second time from a direction differing from the one of the first time. Therefore, displacements due to different processes by the same vacancy become decorrelated at least exponentially fast with their number. This then establishes that the tracer particle diffuses on a scale set by equation (3.53).

3.3.6 The usual argument to obtain the diffusion constant

In previous work the motion of the tagged particle has always been assumed implicitly to be diffusive. The expression (3.1) for the diffusion constant is then arrived at as follows. For diffusion in two dimensions one can write quite generally (cf. [12])

$$D = \frac{1}{4}\Gamma f_{corr} . \tag{3.54}$$

Here Γ is the average jump frequency of the diffusing particle, i.e., the fraction of all time steps for which the particle is displaced, and f_{corr}, called the *correlation factor*, was introduced by Bardeen and Herring [1] to take into account any correlations between successive steps of the diffusing particle.

In the present case the tagged particle jumps with probability $\frac{1}{4}$ when one of its four neighbouring sites is vacant; since a site is vacant with probability ρ we have

$$\Gamma = \rho . \tag{3.55}$$

Furthermore, f_{corr} clearly differs from unity. This is because the particle's next step is more likely to be opposite to its previous step than in any other direction, so that its motion becomes strongly anti-correlated. For a tracer particle interacting with a *single* vacancy it is not hard to derive an explicit expression [2, 3] for f_{corr} involving only $\langle \cos\theta \rangle$, the average of the cosine being taken over all pairs of successive jumps of the tagged particle, and where θ is the angle between two successive jump vectors. For an infinite square lattice one finds [4]

$$f_{corr} = \frac{1}{\pi - 1}, \tag{3.56}$$

a result also derived in chapter 2. Van Beijeren and Kehr [5] argue why the expression (3.56) can, to lowest order in the density, also be used in the case of a small, but *finite*, vacancy density. Combining (3.54), (3.55), and (3.56) one then immediately finds the correct result (3.1). Yet this argument fails to establish that in order to be able to speak of diffusion one has to consider the tagged particle on the scale (3.53).

3.3.7 A shortcut calculation of the mean square displacement

If we are just interested in the total mean square displacement $\langle y^2 \rangle_t$ of the tagged particle but not in the full displacement distribution (3.42), then we can just add the mean square displacements due to the various vacancies individually. However, we have to take into account that the interaction of a given vacancy with the particle does not start until this vacancy reaches the particle for the first time. Therefore, we have to know the mean number of new vacancies which meet the tracer particle at a time τ. In our calculation we average over all initial configurations of the vacancies so that any site has a probability ρ of being vacant. Then the mean number of new vacancies which meet the particle at time τ is equal to ρ times the mean number of new sites visited at time τ by a random walker which has started its random walk at time zero. Montroll and Weiss [10] showed that for a square lattice, S_τ, the average number of distinct sites visited in a τ-step random walk, is asymptotically given by

$$S_\tau \simeq \frac{\pi \tau}{\ln \tau}, \quad \tau \to \infty \, . \tag{3.57}$$

Therefore, the mean number of new lattice sites visited by the random walker at time τ is in this limit, to leading order, given by

$$S_\tau - S_{\tau-1} \simeq \frac{\pi}{\ln \tau}, \quad \tau \to \infty \, . \tag{3.58}$$

From the foregoing we conclude that the mean square displacement of the tagged particle is given by

$$\langle y^2 \rangle_t \simeq \rho \sum_{\tau=1}^{t} (S_\tau - S_{\tau-1}) \langle y^2 \rangle_{t-\tau}^{SV}, \quad t \gg 1 \, . \tag{3.59}$$

The quantity that multiplies ρ on the right-hand side of this equation is a function only of time. Using equations (3.3) and (3.58) we now find

$$\begin{aligned} \langle y^2 \rangle_t &\simeq \frac{\rho}{\pi - 1} \sum_{\tau=m}^{t-M} \frac{\ln(t-\tau)}{\ln \tau} \\ &\simeq \frac{\rho}{\pi - 1} \int_m^{t-M} d\tau \frac{\ln(t-\tau)}{\ln \tau} \\ &\simeq \frac{\rho t}{\pi - 1}, \quad t \gg 1, \end{aligned} \tag{3.60}$$

where m and M are cutoffs introduced so that we may use the asymptotic expressions (3.3) and (3.58), and where one can derive the last line from the second by introducing the scaling $\tau = tx$, extracting a factor t from the integral, and letting $t \to \infty$ in the remainder. The result is independent of the cutoffs m and M. It is, once more, equation (3.44).

3.4 Strip of width L

3.4.1 Long-time limit of the distribution $\overline{\mathcal{P}}_t(\vec{y})$

The equations (3.24), (3.25), and (3.30) are again our starting point. In the case of a strip of finite width L we have, for $z \to 1$, the expansions (cf. section 2.5)

$$
\begin{aligned}
\widehat{A}(z) &= 1 - S_{L,1} - (\,(1-S_{L,1})^2 + \frac{1}{L^2}\,)\, L\sqrt{1-z} + \mathcal{O}(1-z), \\
\widehat{A'}(z) &= S_{L,1} - S_{L,1}^2\, L\sqrt{1-z} + \mathcal{O}(1-z), \\
\widehat{B}(z) &= S_{L,1} + 2\,S_{L,3} - 1 - (\,(1-S_{L,1})^2 - \frac{1}{L^2}\,)\, L\sqrt{1-z} + \mathcal{O}(1-z), \\
\widehat{B'}(z) &= -S_{L,1} + 2\,S_{L,3} - S_{L,1}^2\, L\sqrt{1-z} + \mathcal{O}(1-z), \\
\widehat{C}(z) &= \frac{1}{2} - S_{L,3} - S_{L,1}\,(1-S_{L,1})\, L\sqrt{1-z} + \mathcal{O}(1-z)\;. \qquad (3.61)
\end{aligned}
$$

Here we have introduced the sums

$$S_{L,n} \equiv \frac{1}{L}\sum_{k=1}^{L-1} \frac{\sin^n \frac{\pi k}{L}}{\sqrt{1+\sin^2\frac{\pi k}{L}}}, \quad n = 1,\ 3, \qquad (3.62)$$

which have the large-L expansions

$$
\begin{aligned}
S_{L,1} &= \frac{1}{2} + \mathcal{O}(L^{-2}) \\
S_{L,3} &= \frac{1}{\pi} + \mathcal{O}(L^{-4})\;. \qquad (3.63)
\end{aligned}
$$

Therefore, using (3.61) in (3.29) and (3.33) - (3.35) we find to leading order in the q_i and in $1-z$,

$$\widehat{\Omega}(\vec{q};z) \simeq \frac{Q^2}{(1-z)^2\left\{1+\frac{Q^2}{L\sqrt{1-z}}\right\}}, \qquad (3.64)$$

where

$$Q^2 \equiv \frac{2\,S_{L,1}+2\,S_{L,3}-1}{3-2\,S_{L,1}-2\,S_{L,3}}\,\frac{q_1^2}{4} + \frac{1-2\,S_{L,1}+2\,S_{L,3}}{1+2\,S_{L,1}-2\,S_{L,3}}\,\frac{q_2^2}{4}\;. \qquad (3.65)$$

Note that

$$Q^2 \to \frac{1}{4\,(\pi-1)}\,q^2 \quad \text{for} \quad L\to\infty\;. \qquad (3.66)$$

The inverse Laplace transformation (3.36) cannot be performed explicitly. However, as for the infinite lattice we *can* shift the path of integration, folding it around the branchcut of the square root, which starts at $z = 1$ and which we choose to run along the positive real axis. Then integrating the discontinuity of the integrand one finds for $t \gg 1$ and $Q \ll 1$

$$\Omega_t(\vec{q}) \simeq \frac{Q^2}{\pi} \int_1^\infty \frac{dz}{\sqrt{z-1}} \frac{1-z^{-t}}{z-1} \frac{Q^2 L^{-1}}{z-1+Q^4 L^{-2}} \; . \tag{3.67}$$

For the strip $\overline{\mathcal{P}}_t(\vec{y})$ is recovered from $\overline{\mathcal{P}}_t^*(\vec{q})$ through

$$\overline{\mathcal{P}}_t(\vec{y}) = \frac{1}{L} \sum_{q_2} \frac{1}{2\pi} \int_{-\pi}^{\pi} dq_1 e^{-i\vec{q}\cdot\vec{y}}\, \overline{\mathcal{P}}_t^*(\vec{q}) \; . \tag{3.68}$$

Since q_2 takes discrete values separated by $2\pi/L$ (cf. (3.13)) equation (3.37) shows that for $t \to \infty$ and L finite (which corresponds to $z \to 1$ and $q \to 0$ in Laplace-Fourier space) only the term with $q_2 = 0$ contributes. The time needed for $\overline{\mathcal{P}}_t(\vec{y})$ to become independent of y_2 is $\mathcal{O}(L^2/\rho)$. If we wanted to calculate the transient behaviour of $\overline{\mathcal{P}}_t(\vec{y})$ in the y_2 direction, more values of q_2 near 0 would have to be taken into account. However, we shall instead completely eliminate the y_2-dependence of $\overline{\mathcal{P}}_t(\vec{y})$ by summing on y_2. In this way we find from (3.68), (3.21), (3.67), and (3.65)

$$\begin{aligned} \overline{\mathcal{P}}_t'(y_1) &\equiv \sum_{y_2} \overline{\mathcal{P}}_t(\vec{y}) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dq_1 e^{-iq_1 y_1}\, \overline{\mathcal{P}}_t^*(q_1, 0) \\ &\simeq \frac{1}{2\pi} \int_{-\pi}^{\pi} dq_1\, e^{-iq_1 y_1} \exp\left(-\frac{\rho f_L q_1^2}{\pi} \int_1^\infty \frac{dz}{\sqrt{z-1}} \frac{1-z^{-t}}{z-1} \frac{f_L q_1^2 L^{-1}}{z-1+f_L^2 q_1^4 L^{-2}} \right) \end{aligned} \tag{3.69}$$

valid for $\rho \ll 1$, $t \gg 1$, and with

$$f_L \equiv \frac{2\,S_{L,1} + 2\,S_{L,3} - 1}{4\,(3 - 2\,S_{L,1} - 2\,S_{L,3})} \; . \tag{3.70}$$

For $L \to \infty$ this constant tends to πf of equation (3.40). Just as for the infinite lattice we shall discuss two limiting cases.

3.4.2 The scaling limit

For the case at hand we define a *scaling limit*

$$\begin{cases} t \to \infty, \;\; \rho \to 0^+, \;\; |y_1| \to \infty \\ \rho L \sqrt{t} \text{ fixed}, \;\; y_1 \sqrt[4]{L^2/f_L^2 t} \equiv \xi \text{ fixed} \; . \end{cases} \tag{3.71}$$

Then, from equation (3.69), introducing new variables of integration κ and u according to $q_1 = \kappa\sqrt[4]{L^2/f_L^2 t}$ and $z = 1 + u^2/t$, extending the integration limits of the κ integration to infinity, and using that for fixed u we have that $\left(1+\frac{u^2}{t}\right)^t \to \exp(u^2)$ as $t \to \infty$, we find

$$\overline{\mathcal{P}}'_t(y_1) \simeq \frac{1}{2\pi}\sqrt[4]{\frac{L^2}{f_L^2 t}}\int_{-\infty}^{\infty} d\kappa \exp\left(-i\kappa\xi - \frac{2\rho L\sqrt{t}}{\pi}\int_0^{\infty} du \frac{1-e^{-u^2}}{u^2}\frac{\kappa^4}{u^2+\kappa^4}\right) \quad (3.72a)$$

$$= \exp\left(-2\rho L\sqrt{\frac{t}{\pi}}\right)\delta(y_1)$$

$$+\frac{\exp\left(-2\rho L\sqrt{\frac{t}{\pi}}\right)}{2\pi\sqrt[4]{f_L^2 t/L^2}}\int_{-\infty}^{\infty} d\kappa\, e^{-i\kappa\xi}\left[\exp\left(\frac{2\rho L\sqrt{t}}{\pi}\int_0^{\infty} du \frac{1-e^{-u^2}}{u^2+\kappa^4}\right)-1\right] \quad (3.72b)$$

$$\equiv \sqrt[4]{\frac{L^2}{f_L^2 t}}\, F_1(\xi, 2\rho L\sqrt{\frac{t}{\pi}}), \quad (3.72c)$$

where F_1 is a scaling function. This expression is easily shown to be properly normalized. It is valid for all values of $2\rho L\sqrt{t/\pi}$, and therefore describes the full crossover from very small to very large values of this variable.

3.4.3 Initial time regime and crossover

For $2\rho L\sqrt{t/\pi} \ll 1$ (that is, times t such that $1 \ll t \ll \rho^{-2}L^{-2}$) we find from (3.72b)

$$\overline{\mathcal{P}}'_t(y_1) \simeq (1 - 2\rho L\sqrt{\frac{t}{\pi}})\delta(y_1) + \frac{\rho L}{\pi^2}\sqrt[4]{\frac{L^2 t}{f_L^2}}\int_{-\infty}^{\infty} d\kappa\, e^{-i\kappa\xi}\int_0^{\infty} du \frac{1-e^{-u^2}}{u^2+\kappa^4}. \quad (3.73)$$

Now a difference appears between this expression and its two-dimensional analogue, equation (3.49). We first remark that $2\rho L\sqrt{t/\pi}$ is the leading order term of a large-t expansion of the expected number of different vacancies having met the tagged particle up until time t (see below). Since in (3.73) this parameter is much smaller than one, it is just the probability that for a typical initial vacancy configuration the particle has seen exactly one vacancy until time t. Therefore (cf. (3.49)), one would expect the second term on the right-hand side of (3.73) to be closely related to the probability distribution for the single vacancy case on the strip, which we studied in chapter 2. There we established the asymptotic result

$$P_t^{SV}(y_1) \simeq \frac{1}{\pi^2}\sqrt[4]{\frac{L^2}{f_L^2 t}}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega\xi}\int_0^{\infty} dv \frac{\omega^2 e^{-v^2}}{v^2+\omega^4}, \quad (3.74)$$

which is independent of the initial position of the single vacancy. However, whereas for the infinite lattice the link between the single-vacancy case and the initial time regime of the finite density case seems to be obvious (cf. (3.49)), here we must work a little harder to show that the results (3.73) and (3.74) are compatible. In fact, we shall now show that the second term in (3.73) can be derived from the single vacancy result (3.74) if the *distribution* of the first encounter times between the tagged particle and a single vacancy is taken into account. To this end we shall follow a reasoning similar to the one in section 3.3.7.

For a strip of width L, the average number of distinct sites visited in a t-step random walk, S_t, is asymptotically given by

$$S_t \simeq 2L\sqrt{\frac{t}{\pi}}, \quad t \to \infty \tag{3.75}$$

(this slightly generalizes equation (III.15a) of [10]). Therefore, the mean number of new lattice sites visited by this random walker at time t is, to leading order in t, given by

$$S_t - S_{t-1} \simeq \frac{L}{\sqrt{\pi t}}, \quad t \to \infty \, . \tag{3.76}$$

For the tagged particle problem this implies that the probability that the particle meets a vacancy at time t is, to leading order in t, given by $L\rho/\sqrt{\pi t}$. Since furthermore $2\rho L\sqrt{t/\pi} \ll 1$, one has that $L\rho/\sqrt{\pi t}$ is also, to leading order, the probability that the tagged particle encounters its *first* vacancy at time t. Now consider a (not normalized) distribution $\mathcal{A}_t(y_1)$, defined as the contribution to $\overline{\mathcal{P}}_t'(y_1)$ of all situations in which up until time t the tracer particle has interacted with precisely one vacancy (the possibility of having interacted with more than one vacancy will contribute only to order ρ^2). Taking into account the distribution of first encounter times we can then express $\mathcal{A}_t(y_1)$ with the aid of the single vacancy result as

$$\mathcal{A}_t(y_1) \simeq \rho \sum_{\tau=1}^{t} (S_\tau - S_{\tau-1}) P_{t-\tau}^{SV}(y_1), \; t \gg 1 \, . \tag{3.77}$$

To evaluate $\mathcal{A}_t(y_1)$ asymptotically we replace the sum on τ by an integral running from 0 to t, use the asymptotic results (3.74) and (3.76), and put $\omega = \kappa\sqrt[4]{1-x^2}, v = w\sqrt{1-x^2}$, and $\tau = tx^2$. In this way we find

$$\mathcal{A}_t(y_1) \simeq \frac{2\rho L}{\pi^2} \sqrt[4]{\frac{L^2 t}{\pi^2 f_L^2}} \int_{-\infty}^{\infty} d\kappa \, e^{-i\kappa\xi} \int_0^{\infty} dw \, \frac{\kappa^2 e^{-w^2}}{w^2+\kappa^4} \int_0^1 dx \, e^{w^2 x^2} \, . \tag{3.78}$$

If one uses the integral representation

$$\frac{1}{w^2+\kappa^4} = \int_0^{\infty} d\lambda \, \exp[-\lambda\,(w^2+\kappa^4)], \tag{3.79}$$

the integrals on w and x can be carried out, which gives

$$\begin{aligned} \mathcal{A}_t(y_1) &\simeq \frac{\rho L}{\pi^2}\sqrt[4]{\frac{L^2 t}{f_L^2}}\int_{-\infty}^{\infty} d\kappa\, e^{-i\kappa\xi}\int_0^{\infty} d\lambda\, \kappa^2 e^{-\lambda\kappa^4}\arcsin\left(\frac{1}{\sqrt{\lambda+1}}\right) \\ &= \frac{\rho L}{\pi^2}\sqrt[4]{\frac{L^2 t}{f_L^2}}\int_{-\infty}^{\infty} d\kappa\, e^{-i\kappa\xi}\int_0^{\infty} du\, \frac{1-e^{-u^2}}{u^2+\kappa^4}, \quad \xi = y_1\sqrt[4]{L^2/f_L^2 t}, \end{aligned} \tag{3.80}$$

where in the second line we rewrote the λ-integration by first performing an integration by parts and then substituting $u = \kappa^2\sqrt{\lambda}$. Finally we see that the resulting distribution is precisely given by the second term on the right-hand side of (3.73), so that we have indeed shown that this term is nothing more than the single vacancy result obtained in chapter 2 but then convoluted with the distribution of first encounter times.

For the infinite lattice one can verify that the distribution for the single vacancy case (3.2) and the one obtained by applying the convolution (3.77) to (3.2) are asymptotically equal. This is due to the slowly varying character of the logarithm, and explains the appearance of the single vacancy result itself in (3.49).

3.4.4 Long-time regime

We return to equation (3.72a). Introducing new variables of integration p and x according to $\kappa = p/\sqrt[4]{\rho^2 L^2 t}$ and $u = p^2 x/\rho L\sqrt{t}$ we find

$$\begin{aligned} \overline{\mathcal{P}}'_t(y_1) \simeq \int_{-\infty}^{\infty} \frac{dp}{2\pi\sqrt{\rho f_L t}} \exp\Bigg[&-ip\frac{y_1}{\sqrt{\rho f_L t}} \\ &-\frac{2}{\pi}\int_0^{\infty}\frac{dx}{1+x^2}\frac{\rho^2 L^2 t}{p^2 x^2}\left(1-\exp(-\frac{p^4 x^2}{\rho^2 L^2 t})\right)\Bigg] . \end{aligned} \tag{3.81}$$

Now, since in the scaling limit (3.71) both $\rho L\sqrt{t}$ and $y_1\sqrt[4]{L^2/f_L^2 t}$ are kept fixed, so that $y_1/\sqrt{\rho f_L t}$ is a fixed quantity, we have that for $\rho^2 L^2 t \gg 1$

$$\overline{\mathcal{P}}'_t(y_1) \simeq \int_{-\infty}^{\infty} \frac{dp}{2\pi\sqrt{\rho f_L t}} \exp\left(-ip\frac{y_1}{\sqrt{\rho f_L t}} - p^2\right) = \frac{1}{2\sqrt{\pi\rho f_L t}}\exp\left(-\frac{y_1^2}{4\rho f_L t}\right) \tag{3.82}$$

which is again a properly normalized Gaussian distribution. For $L \to \infty$ it coincides with equation (3.52) integrated over y_2.

3.5 Conclusion

We have shown that a tracer particle in a two-dimensional lattice gas with a low vacancy density ρ performs diffusive motion only when considered at time intervals of size $\Delta t \sim \rho^{-1} \ln \rho^{-1}$. The mean square displacement in such a time interval is $\Delta y^2 \sim \ln \rho^{-1}$. As a consequence, for a given tracer particle starting at an arbitrary position at $t = 0$, there is an initial time regime $t \ll \rho^{-1} \ln \rho^{-1}$ in which the distribution function of its displacement, $\overline{\mathcal{P}}_t(\vec{y})$, is not a Gaussian but a modified Bessel function K_0. Nevertheless for all $t \gg 1$ the mean square displacement increases linearly with time. We have considered the scaling limit $t \to \infty$, $y \to \infty$, and $\rho \to 0^+$ at fixed $\rho t / \ln t$ and $\vec{y}/\sqrt{\ln t}$, and calculated the scaling function describing the crossover between the initial time regime and true diffusive behaviour. We have also considered the same problem on an infinite strip of width L, where the initial time regime is given by $t \ll \rho^{-2} L^{-2}$.

Finally, we remark that if there is a finite density of tracer particles (in addition to the finite vacancy density), then the same initial time effect will appear in the self-contribution to the dynamic structure factor, which is nothing but $\overline{\mathcal{P}}_t^*(\vec{q})$. Hence, this effect is, in principle, experimentally observable. It is interesting to point out that just recently Van Veluwen and Lekkerkerker [16] have been able to observe non-Gaussian displacement distributions in dynamic light scattering experiments on concentrated dispersions of colloidal particles. In this (three-dimensional) system the non-Gaussian statistics arise from slowly decaying correlations, introduced by the interactions of the colloidal particles among themselves.

Appendix

We calculate the inverse Laplace transform $\Omega_t(\vec{q})$ of $\hat{\Omega}(\vec{q}; z)$ for the infinite lattice. Consider a function $h(z)$ of the complex (Laplace) variable z, which is regular on the unit disk. Then

$$\oint \frac{dz}{z^t} \frac{h(z)}{1-z} = \oint \frac{dz}{z^t} \frac{z^t - 1}{z-1} h(z), \quad t = 1, 2, \ldots, \tag{3.A1}$$

where the integral is around the origin. The validity of this equation is readily established by expanding $(1-z)^{-1}$ on the left-hand side in powers of z, thereby finding $\sum_{k=0}^{\infty} \oint dz\, z^{k-t} h(z)$, then remarking that, because $h(z)$ is regular on the unit disk, $\oint dz\, z^{k-t} h(z) = 0$ for $k \geq t$, and using that $\sum_{k=0}^{t-1} z^k = \frac{z^t - 1}{z - 1}$. From (3.36) and (3.39), also using (3.A1), we now find that for $t \gg 1$

$$\begin{aligned}
\Omega_t(\vec{q}) &\simeq \frac{1}{2\pi i} \oint \frac{dz}{z^t} \frac{\pi f q^2}{(1-z)^2 \left(1 + f q^2 \ln\left(\frac{8}{1-z}\right)\right)} \\
&= \frac{1}{2\pi i} \oint \frac{dz}{z^t} \frac{z^t - 1}{z-1} \frac{\pi f q^2}{(1-z)\left(1 + f q^2 \ln\left(\frac{8}{1-z}\right)\right)} \\
&= \pi f q^2 \int_1^{\infty} \frac{dz}{z^t} \frac{z^t - 1}{z-1} \frac{1}{z-1} \frac{f q^2}{\left(1 + f q^2 \ln\left(\frac{8}{z-1}\right)\right)^2 + \pi^2 f^2 q^4},
\end{aligned} \tag{3.A2}$$

where, in the last line, we have taken the branchcut of the logarithm, which starts at $z = 1$, along the positive real axis, folded the contour around it, and integrated the discontinuity of the integrand. By introducing $z = 1 + 8t^{-w}$ and extracting a factor t from the integrand, we can rewrite (3.A2) as

$$\Omega_t(\vec{q}) \simeq \pi f q^2 t \int_{-\infty}^{\infty} dw \, \frac{1-(1+8t^{-w})^{-t}}{8t^{1-w}} \, \frac{fq^2 \ln t}{(1+fq^2 w \ln t)^2 + \pi^2 f^2 q^4} \, . \tag{3.A3}$$

Since, for $w \neq 1$,

$$\lim_{t\to\infty} \frac{1-(1+8t^{-w})^{-t}}{8t^{1-w}} = \Theta(w-1), \tag{3.A4}$$

where Θ is the Heaviside step function, and also taking $q \ll 1$ so that for $w > 0$ we may neglect $\pi^2 f^2 q^4$ compared to $(1 + fq^2 w \ln t)^2$, we find from (3.A3)

$$\Omega_t(\vec{q}) \simeq \pi f q^2 t \int_{1}^{\infty} dw \frac{fq^2 \ln t}{(1+fq^2 w \ln t)^2} = \frac{\pi f q^2 t}{1 + fq^2 \ln t}, \tag{3.A5}$$

the result being valid for $q \ll 1$ and $t \gg 1$.

References

[1] J. Bardeen and C. Herring in: *Imperfections in Nearly Perfect Crystals*, ed. W. Shockley (Wiley, New York, 1952), p. 261.

[2] K. Compaan and Y. Haven, Trans. Faraday Soc. **52** (1956) 786.

[3] A.D. Le Claire in: *Physical Chemistry, Vol. 10*, eds. H. Eyring, D.Henderson, and W. Jost (Academic Press, New York, 1970), p. 261.

[4] A. Schoen and R. Lowen, Bull. Am. Phys. Soc. **5** (1960) 280.

[5] H. van Beijeren and K.W. Kehr, J. Phys. C **19** (1986) 1319.

[6] K.W. Kehr and K. Binder in: *Applications of the Monte Carlo Method in Statistical Physics* (Topics in Current Physics 36), ed. K. Binder (Springer-Verlag, Berlin Heidelberg, 1984), p. 181.

[7] S. Ishioka and M. Koiwa, Phil. Mag. A **41** (1980) 385.

[8] C.A. Sholl, J. Phys. C **14** (1981) 2723.

[9] F. Spitzer, *Principles of Random Walk* (Van Nostrand, Princeton, 1964).

[10] E.W. Montroll and G.H. Weiss, J. Math. Phys. **6** (1965) 167.

[11] G.H. Weiss and R.J. Rubin in : *Advances in Chemical Physics, Vol. 52*, eds. I. Prigogine and S.A. Rice (Wiley, New York, 1983), p. 363.

[12] J.W. Haus and K.W. Kehr, Phys. Rep. **150** (1987) 263.

[13] Ajay and R.G. Palmer, J. Phys. A **23** (1990) 2139.

[14] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).

[15] G.N. Watson, *Theory of Bessel Functions* (Cambridge University Press, 1958).

[16] A. van Veluwen and H.N.W. Lekkerkerker, Phys. Rev. A **38** (1988) 3758.

Chapter 4

The number of distinct sites visited by a tracer particle

We first briefly recall the tracer particle problem. Consider an infinite d-dimensional hypercubic lattice with a fraction $1-\rho$ of its sites occupied by identical particles. The remaining sites are empty. *All* particles on the lattice perform Brownian motion, but subject to a "no double occupancy" condition. Alternatively, one may think of the vacancies (empty sites) as performing simple random walks, which in the limit $\rho \downarrow 0$ become independent. One of the particles is selected at random and is called the *tracer particle*. The object now is to investigate its motion, for example by calculating its diffusion constant.

When studying this problem, the general observation usually made is that many of the properties of the motion of the tracer particle can be found by first considering the corresponding property for a simple random walk on the same lattice and then afterwards applying a "renormalization of time" in the obtained result. As an example, consider the mean square displacement of a simple random walk on a d-dimensional hypercubic lattice and in a discrete time $t = 0, 1, \ldots$. It is given by

$$\langle \vec{r}^2 \rangle_t = t \; . \tag{4.1}$$

For the corresponding tracer particle problem (see e.g. the review article by Kehr and Binder [1]) one finds for the mean square displacement of the tracer particle, if the step frequency of an isolated vacancy is taken as the unit of time,

$$\langle \vec{r}_{tr}^{\,2} \rangle_t \simeq \rho f(\rho)\, t, \quad \rho t \gg 1 \; . \tag{4.2}$$

Obviously, (4.2) may be obtained from (4.1) by replacing t by $\rho f(\rho)\, t$. The factor ρ comes in since the tracer particle can move only when it is reached by a vacancy, which, on average, happens every ρ^{-1} time units. The factor $f(\rho)$ is called the correlation factor and takes into account the characteristic backward correlation effects in the motion of the tracer particle (to see that these effects are there just consider two successive moves of the tracer particle due to the same vacancy). Only for $\rho = 0$ and $\rho = 1$ can its value be calculated exactly, but for general ρ a rather accurate approximation exists [2].

As Czech [3] showed, however, in three and higher dimensions, the "renormalization procedure" sketched above does *not* work for the calculation of S_t, the average number of distinct sites visited by the tracer particle at time t. In fact, he found that S_t could, asymptotically, be described remarkably well by modelling the tracer particle motion as a special *correlated random walk*, called the Backward Jump (BJ) model, with appropriately chosen, ρ-dependent, step probabilities, see [3]. The reason for this good agreement was not fully clear. We shall show now that, arguing along the same lines as Czech, one can find the exact answer for S_t in the limit $\rho \downarrow 0$ and $\rho t \gg 1$. We shall indeed describe the tracer particle motion as a correlated random walk, with afterwards t replaced by ρt for the reasons given above, but, instead of the BJ model Czech used, we shall use a more general correlated random walk model.

To be specific, we consider a correlated random walk with a one-step memory on a d-dimensional hypercubic lattice in discrete time t. At any instant of time the walker steps to one of its nearest-neighbour sites. Let A denote the probability that two consecutive steps of the walker are in opposite directions, B the probability that they are in the same direction, and C the probability for them to be in any of the other, right-angled, configurations. Then obviously

$$A + B + 2(d-1)C = 1 \,. \tag{4.3}$$

The BJ model employed by Czech corresponds to taking $B = C$. Ernst [4] has studied this ABC model and finds

$$\sum_{t=0}^{\infty} P_t(\vec{0}\,) = \frac{1}{(2\pi)^d} \int_{-\pi}^{\pi} d^d\vec{q}\, \frac{\frac{1}{d}\sum_{i=1}^{d} \frac{1+(A-B)\cos q_i}{1-2(B-C)\cos q_i+(B-A)(B+A-2C)}}{1-2C\sum_{i=1}^{d} \frac{\cos q_i + A - B}{1-2(B-C)\cos q_i+(B-A)(B+A-2C)}}, \tag{4.4}$$

where $P_t(\vec{0}\,)$ denotes the probability for the walk to be at its starting point at time t. Formula (4.4) was in fact first derived by Gillis [5], albeit in a rather complicated way involving a lengthy manipulation of determinants. The average number of distinct sites S_t visited by a random walk (whether correlated or not) in three and higher dimensions is asymptotically given by [6]

$$S_t \simeq \frac{t}{\sum_{t=0}^{\infty} P_t(\vec{0}\,)}, \quad t \gg 1 \,. \tag{4.5}$$

Hence, using (4.4), S_t is known for the ABC model.

We shall now explicitly treat the three-dimensional tracer particle problem, in order to be able to compare with Czech's results. The procedure is easily generalized to higher dimensions. We first consider a tracer particle and a *single* vacancy on the infinite three-dimensional lattice. The probability B_0 that after a first step the tracer particle will *ever* make a second step in the same direction, as well as the corresponding probabilities A_0 for reversal and C_0 for stepping sideways are known. Sholl [7] states them as

$$\begin{aligned} A_0 &= 0.223423\ldots \\ B_0 &= 0.013581\ldots \\ C_0 &= 0.025883\ldots . \end{aligned} \tag{4.6}$$

Since $A_0+B_0+4C_0<1$ it is not certain that there will be a second step. However, if we now introduce a finite density ρ of vacancies, then the tracer particle will make an infinite number of steps, since vacancies will keep arriving at the site of the particle at a constant rate ρ. In the limit $\rho \downarrow 0$ moves of the tracer particle due to different vacancies are uncorrelated. If a given vacancy, after having caused a step of the tracer particle, does not come back to it, then a different vacancy will come in and cause a step in an independent direction. This shows that the ABC model applies *exactly* to the tracer particle motion if one chooses the probabilities A, B, and C according to

$$X = X_0 + \frac{1}{6}(1 - A_0 - B_0 - 4C_0), \quad X = A,\ B,\ C, \text{ also in } X_0\ . \tag{4.7}$$

It is possible to show that with this prescription the low density limit of the correlation factor $f(\rho)$ has the correct value [7, 8]. Also one may show that

$$A = \frac{1}{3} \tag{4.8a}$$

(and that in d dimensions $A = 1/d$). For B and C we find from (4.6) and (4.7)

$$B = 0.12349\ldots, \qquad C = 0.13579\ldots . \tag{4.8b}$$

But then it is clear, B and C being rather close to one another, why the BJ model works so well. In the low density limit Czech uses the values $A = 0.34153\ldots$, $B = C = 0.13169\ldots$, very close to the values in (4.8a) and (4.8b), respectively. Evaluating (4.4) numerically for the three-dimensional case with the values A, B, C of (4.8a) and (4.8b), we find

$$S_t \simeq 0.4907\ldots \rho t, \quad \rho \ll 1, \quad \rho t \gg 1\ . \tag{4.9}$$

This should be compared to Czech's

$$S_t \approx 0.4863\ldots \rho t\ . \tag{4.10}$$

Our result is $\approx 0.9\%$ higher than Czech's BJ approximation and is consistent with his simulation results which systematically are somewhat higher than the prediction of the BJ model but where " the deviations are less than $\approx 1.5\%$ " [3].

References

[1] K.W. Kehr and K. Binder in: *Applications of the Monte Carlo Method in Statistical Physics*, 2nd ed., ed. K. Binder (Springer, Berlin, 1987).

[2] K. Nakazato and K. Kitahara, Progr. Theor. Phys. **64** (1980) 2261.

[3] R. Czech, J. Chem. Phys. **91** (1989) 2498.

[4] M.H. Ernst, J. Stat. Phys. **53** (1988) 191.

[5] J. Gillis, Proc. Camb. Phil. Soc. **51** (1955) 639.

[6] E.W. Montroll and G.H. Weiss, J. Math. Phys. **6** (1965) 167.

[7] C.A. Sholl, J. Phys. C **14** (1981) 2723.

[8] H. van Beijeren and K.W. Kehr, J. Phys. C **19** (1986) 1319.

Chapter 5

Covering of a finite lattice by a random walk

5.1 Introduction

In a recent paper, Nemirovsky et al. [1] considered the "lattice covering-time problem". They took a finite d-dimensional hypercubic lattice consisting of $N^{1/d} \times \ldots \times N^{1/d} = N$ sites, and then by simulation calculated the mean time, τ_N, it takes a simple random walk to cover the lattice, i.e., to visit *all* sites at least once. The problem was investigated in one through four dimensions, both with periodic and reflecting boundary conditions. In dimension $d = 1$, for both types of boundary conditions, analytical expressions for the mean times τ_N could subsequently be conjectured for general N. For example, for periodic boundary conditions one found $\tau_N = \frac{1}{2}N\,(N-1)$. Yokoi et al. [2] proved these conjectures by reformulating the problem as an exactly solvable first-passage time problem. However, this method of solution seems tractable only for the case $d = 1$. For dimensions 2, 3, and 4, Nemirovsky et al. found that in the limit $N \to \infty$ a good fit to the simulation data is given by

$$\tau_N \simeq \begin{cases} A\,N \ln^2 N\,(1 + C/\ln N), & d = 2, \\ A\,N \ln N\,(1 + C/\ln N), & d = 3,\ 4, \end{cases} \tag{5.1}$$

where A and C are dimension-dependent constants for which numerical values were determined [1]. The constant A, for a given dimension d, is supposed to be independent of boundary conditions, whereas C does depend on them. Coverings by random walks have also been considered in the mathematical literature, in the much more general setting of continuous time random walks on arbitrary finite groups. Results for τ_N there were given by Aldous [3]. For related work also see [4, 5, 6].

In this chapter we do two things. First, in section 5.2, we investigate a problem closely related to the one described above. It will be called the "last-site problem". Instead of considering the *time* at which the lattice is covered by the random walk, we study the *probability* $L_N(\vec{x})$ that site $\vec{x}$ is the last site visited in the covering process, *irrespective* of the time at which this happens. Formally, for a random walk in discrete time $t = 0, 1, 2, \ldots$, introducing the probability $L_N(\vec{x};t)$ that at time t the random walk completes the lattice covering by visiting site $\vec{x}$, we can write

$$L_N(\vec{x}) = \sum_{t=0}^{\infty} L_N(\vec{x};t), \tag{5.2}$$

whereas

$$\tau_N = \sum_{\vec{x}} \sum_{t=0}^{\infty} t L_N(\vec{x};t) \ . \tag{5.3}$$

In (5.3) the sum on $\vec{x}$ runs over all sites of the lattice. We shall study the last-site problem on finite hypercubic lattices with $N^{1/d} \times \ldots \times N^{1/d} = N$ sites, applying periodic boundary conditions and using a discrete time variable.

In section 5.2.1 we find for the case $d = 1$, with the walker starting at the origin,

$$\begin{aligned} L_N(x) &= \frac{1}{N-1}, \quad x = 1, 2, \ldots, N-1, \\ L_N(0) &= 0, \end{aligned} \tag{5.4}$$

for all $N \geq 2$. In sections 5.2.2 – 5.2.4 the case $d \geq 2$ is discussed. In the limit N, $|\vec{x}| \to \infty$ with $\vec{x}/N^{1/d}$ fixed, we find in dimensions $d > 2$ that $L_N(\vec{x})$ has the scaling form

$$L_N(\vec{x}) \simeq \frac{1}{N}\left[1 - \frac{h_d\left(\frac{\vec{x}}{N^{1/d}}\right)}{N^{1-2/d}}\right], \tag{5.5}$$

where h_d is a decaying function of its argument (cf. (5.41)). Hence, $L_N(\vec{x})$ is a function which increases with distance and tends asymptotically to a constant. For the exceptional dimension $d = 2$ the scaling form

$$L_N(\vec{x}) \simeq \frac{1}{N}\left[1 - \frac{h_2\left(\frac{\vec{x}}{\sqrt{N}}\right)}{\ln cN}\right] \tag{5.6}$$

is obtained, where c is a constant (cf. (5.41)). Both expressions (5.5) and (5.6) yield $\sum_{\vec{x}} L_N(\vec{x}) = 1$ to leading order in N. In our calculations there appears a characteristic time, $\tilde{\tau}_N$, at which, on average, all sites except for a number that remains finite when $N \to \infty$ have been visited at least once. If one is willing to identify the leading order behaviour in N of $\tilde{\tau}_N$ with that of τ_N, we can confirm equation (5.1) and give values for A for the different dimensions (see (5.37)). The A values thus obtained agree with those calculated by Aldous [3] and are in reasonable agreement with the numerical values found by Nemirovsky et al. [1].

In section 5.3 we study a second problem, different from, but closely related to, the last-site problem: we there investigate the structure of the *set of sites* not yet visited by the random walk at large times t. Whereas in $d = 1$ this structure is trivial, it is quite interesting in $d = 2$, where on the time scale $\bar{\tau}_N$ it is *fractal-like with a time-dependent fractal dimension*. More precisely, we take $t \simeq \alpha\bar{\tau}_N$, thus introducing the reduced time variable α. For given α, the average number of sites which have not been visited yet at that time is shown to be $\sim N^{1-\alpha}$ as $N \to \infty$. The structure of the nonvisited set is then studied by calculating $N_{\vec{x}}(R,t)$. This quantity, by definition, denotes the number of sites not yet visited at time t within a disk of radius R around a nonvisited site $\vec{x}$. We find that

$$N_{\vec{x}}(R, \alpha\bar{\tau}_N) \sim R^{2-\alpha}, \qquad 0 < \alpha < 2, \tag{5.7}$$

which is independent of $\vec{x}$, and which is in fact valid for those R for which $\ln R/\ln cN$ is negligible. If there were no correlations between the nonvisited sites, the probability for a given site not to have been visited at given α would, in view of the average number of nonvisited sites, be of the order of $N^{-\alpha}$. One would then find $N_{\vec{x}}(R,\alpha\bar{\tau}_N) \sim R^2N^{-\alpha}$. Equation (5.7) shows, however, that the actual number of nonvisited sites around the site $\vec{x}$ is much larger. This leads to the conclusion that the nonvisited sites in $d = 2$ have a strong tendency to cluster. This conclusion is supported by a calculation of $N_{\vec{x}}(R,\alpha\bar{\tau}_N)$ for general R. Taking the finite size effects of the lattice into account, we find for $0 < \alpha < 2$ and $N \to \infty$:

$$N_{\vec{x}}(R, \alpha\bar{\tau}_N) \sim \begin{cases} R^{2-\frac{\alpha}{1-\ln R/\ln cN}}, & \frac{\ln R}{\ln cN} < 1 - \sqrt{\frac{\alpha}{2}}, \\ \sqrt{\ln cN}\, N^{(\sqrt{2}-\sqrt{\alpha})^2}, & \frac{\ln R}{\ln cN} > 1 - \sqrt{\frac{\alpha}{2}}. \end{cases} \tag{5.8}$$

Formula (5.7) is a special case of (5.8). Not only does the density of nonvisited sites around the nonvisited site $\vec{x}$ decrease with increasing R, as is clear from (5.8), but for $\frac{1}{2} < \alpha < 2$ there is in fact even a radius $R \sim N^{\beta^*}$ with $\beta^* = 1 - [\alpha/2]^{1/2}$, outside which there are no longer any contributions to the leading order behaviour of $N_{\vec{x}}(R,\alpha\bar{\tau}_N)$. This may be interpreted as saying that the typical size of the nonvisited region then is of the order of N^{β^*}. For $\alpha > 2$ a nonvisited site $\vec{x}$ (*if* there then is still one left) is essentially alone. Finally, we show that in dimensions $d > 2$ the correlations between sites not yet visited are weak.

Section 5.4 is a general conclusion.

5.2 The last-site problem

In this section we consider the problem of calculating $L_N(\vec{x})$ for general dimension d. Since the problem in $d = 1$ can be solved exactly for any N, we consider this dimension separately.

5.2.1 The one-dimensional case

Consider a ring with N sites, labelled 0, 1, ..., $N-1$, and suppose that a simple random walk on this ring starts at 0. Let $F_t(x)$ denote the probability that the walk arrives at site x for the first time at time t. Furthermore $F_t^{\{x,y\}}(\rho)$ will denote the probability that the walk enters the set of two points $\{x, y\}$ for the first time at time t by reaching its point ρ ($\rho = x$ or $\rho = y$). Then we can write

$$
\begin{aligned}
L_N(x;t) &= \sum_{t_1=0}^{\infty} \sum_{t_2=0}^{\infty} \sum_{t_3=0}^{\infty} \delta_{t,t_1+t_2+t_3} \\
&\quad \times \sum_{\rho=x\pm1} F_{t_1}^{\{x-1,x+1\}}(\rho)\, F_{t_2}^{\{1,2\}}(2)\, F_{t_3}(1), \quad x \neq 0 .
\end{aligned}
\tag{5.9}
$$

This is so because if x is the point visited last, at time t, one must first (at a time t_1) visit one of its neighbouring sites $x \pm 1$, then (in a time t_2) go all the way around the ring and visit its other neighbouring site without visiting x itself, and finally (in a time $t_3 = t - t_1 - t_2$) visit x itself. Of course $L_N(0,t) = 0$ for all t and $N \geq 2$ since the walk starts in 0. Summing (5.9) on t and using (5.2), we find for $x \neq 0$

$$
L_N(x) = \left(\sum_{t_1=0}^{\infty} \sum_{\rho=x\pm1} F_{t_1}^{\{x-1,x+1\}}(\rho) \right) \left(\sum_{t_2=0}^{\infty} F_{t_2}^{\{1,2\}}(2) \right) \left(\sum_{t_3=0}^{\infty} F_{t_3}(1) \right) . \tag{5.10}
$$

But the random walk will eventually reach any site of the lattice so that

$$
\sum_{t_1=0}^{\infty} \sum_{\rho=x\pm1} F_{t_1}^{\{x-1,x+1\}}(\rho) = \sum_{t_3=0}^{\infty} F_{t_3}(1) = 1 . \tag{5.11}
$$

This implies that $L_N(x)$, for $x \neq 0$, is a constant *independent of* x. Since obviously

$$
\sum_{x=0}^{N-1} L_N(x) = 1, \tag{5.12}
$$

we find

$$
\begin{aligned}
L_N(x) &= \frac{1}{N-1}, \quad x = 1, 2, \ldots, N-1, \\
L_N(0) &= 0,
\end{aligned}
\tag{5.13}
$$

which is (5.4). Using standard random-walk theory, one may check that indeed

$$
\sum_{t_2=0}^{\infty} F_{t_2}^{\{1,2\}}(2) = \frac{1}{N-1} . \tag{5.14}
$$

The calculation of the sum in (5.14) is a classic first exit problem on an interval, discussed in ref. [7].

This, then, concludes our investigation of the case $d = 1$, and we now want to consider the same problem in dimensions $d > 1$. There, like in $d = 1$, one can write down a formal expression for $L_N(\vec{x};t)$. It involves a sum over all paths that reach site $\vec{x}$ for the first time at time t, after having visited all other sites. However, in these dimensions, this formal expression is of no use for obtaining explicit results for $L_N(\vec{x};t)$. The problem is that the property "$\vec{x}$ is the last site visited" in dimensions $d > 1$ depends on the whole history of the walk. There exists then no simple equation, neither for $L_N(\vec{x})$ nor for $L_N(\vec{x};t)$, from which $L_N(\vec{x})$ can be solved directly. To obtain $L_N(\vec{x})$, we shall first look at a different problem and then later on make the connection with calculating $L_N(\vec{x})$.

5.2.2 Probability that site $\vec{x}$ has not been visited at time t

We consider the probability $\mathcal{L}_t(\vec{x})$ that the simple random walk starting at site $\vec{0}$ at time 0 has not yet visited site $\vec{x}$ at time t, irrespective of the number of other sites it has visited up till then. Obviously,

$$\mathcal{L}_t(\vec{x}) = 1 - \sum_{\tau=0}^{t} F_\tau(\vec{x}), \tag{5.15}$$

where $F_\tau(\vec{x})$ is the d-dimensional first-passage probability. For any time-dependent quantity X_t we introduce the discrete Laplace transform (or: generating function)

$$\widehat{X}(z) = \sum_{t=0}^{\infty} z^t X_t \ . \tag{5.16}$$

Then we find from (5.15)

$$\widehat{\mathcal{L}}(\vec{x};z) = \frac{1 - \widehat{F}(\vec{x};z)}{1 - z} \ . \tag{5.17}$$

Let $\widehat{G}(\vec{x};z)$ denote the generating function of the probability $G_t(\vec{x})$ to find the random walk at site $\vec{x}$ at time t, given that it started at site $\vec{0}$ at $t = 0$. It is well-known (see e.g. [7, 8, 9]) that

$$\widehat{F}(\vec{x};z) = \frac{\widehat{G}(\vec{x};z)}{\widehat{G}(\vec{0};z)} \ . \tag{5.18}$$

If we define $F_\tau(\vec{0}) = \delta_{\tau,0}$, then (5.18) is valid for all $\vec{x}$. Performing an inverse Laplace transformation of (5.17) we find, using (5.18),

$$\mathcal{L}_t(\vec{x}) = \frac{1}{2\pi i} \oint \frac{dz}{z^{t+1}} \frac{1}{1 - z} \left[1 - \frac{\widehat{G}(\vec{x};z)}{\widehat{G}(\vec{0};z)}\right] , \tag{5.19}$$

where the integral is around the origin of the z plane.

For a hypercubic lattice [7, 8, 9]

$$\hat{G}(\vec{x};z) = \frac{1}{N}\sum_{\vec{q}} \frac{\exp(-i\vec{q}\cdot\vec{x})}{1-(z/d)(\cos q_1 + \ldots + \cos q_d)} . \tag{5.20}$$

Here $\vec{q}$ is a d-dimensional vector with components $q_i = 2\pi k_i/L$, where $k_i = 0, 1, \ldots, L-1$, with $L = N^{1/d}$ the linear size of the lattice. In (5.20) only the $\vec{q} = \vec{0}$ term diverges as $z \to 1$. To make this divergence explicit we write

$$\hat{G}(\vec{x};z) = \frac{1}{N(1-z)} + g_N(\vec{x};z), \tag{5.21}$$

so that $g_N(\vec{x};z)$ remains finite as $z \to 1$. For later reference we record the following properties of $g_N(\vec{x}) \equiv g_N(\vec{x};1)$. For $N \to \infty$ one has [8, 10]

$$g_N(\vec{0}) \simeq \begin{cases} \frac{1}{\pi}\ln cN, & d = 2, \\ g_\infty(\vec{0}), & d > 2, \end{cases} \tag{5.22}$$

where $c = 1.8456\ldots$ [10] and where $g_\infty(\vec{0})$ is the average number of visits to the origin on the infinite lattice. By inspection of (5.20) one obtains

$$g_N(\vec{x}) \simeq \frac{f\left(\frac{\vec{x}}{N^{1/d}}\right)}{N^{1-2/d}} \quad \text{as } |\vec{x}|,\ N \to \infty \ \text{ with } \frac{\vec{x}}{N^{1/d}} \text{ fixed, } d \geq 2 \tag{5.23}$$

Here

$$f(\vec{y}) = \frac{d}{2\pi^2}\sum_{\vec{k}\neq\vec{0}} \frac{\exp(-2\pi i\vec{k}\cdot\vec{y})}{k^2} . \tag{5.24}$$

This infinite sum, which is not absolutely convergent, runs over all vectors ($\neq \vec{0}$) with integer valued components, and should be taken as $\lim_{L\to\infty}\prod_{i=1}^{d}\sum_{k_i=-L}^{L}$, i.e., over ever increasing hypercubes centered on the origin. One easily shows that for $|\vec{y}| \downarrow 0$

$$f(\vec{y}) \simeq \begin{cases} -\dfrac{2}{\pi}\ln|\vec{y}|, & d = 2, \\[2ex] \dfrac{d\Gamma(\frac{d}{2}-1)}{2\pi^{d/2}|\vec{y}|^{d-2}}, & d > 2, \end{cases} \tag{5.25}$$

which is consistent with the well-known fact that [7, 11]

$$g_\infty(\vec{x})\begin{cases} \sim |\vec{x}|^{-(d-2)}, & d > 2,\ |\vec{x}| \to \infty, \\ = \infty, & d = 2 . \end{cases} \tag{5.26}$$

The lattice Green function

$$\mathcal{G}_N(\vec{x}) \equiv g_N(\vec{0}) - g_N(\vec{x}) \tag{5.27}$$

remains finite as $N \to \infty$, also for the case $d = 2$. In fact [7]

$$\mathcal{G}_\infty(\vec{x}) = \frac{2}{\pi} \ln \frac{|\vec{x}|}{r_0} + \mathcal{O}(\frac{1}{|\vec{x}|}), \qquad d = 2, \quad |\vec{x}| \to \infty, \tag{5.28}$$

where $r_0 = \exp(-\gamma)/2\sqrt{2} = 0.19850\ldots$ with γ Euler's constant.

With (5.21) equation (5.19) becomes

$$\mathcal{L}_t(\vec{x}) = \frac{1}{2\pi i} \oint \frac{dz}{z^{t+1}} \frac{g_N(\vec{0}; z) - g_N(\vec{x}; z)}{\frac{1}{N} + (1-z)\, g_N(\vec{0}; z)} \,. \tag{5.29}$$

The long-time behaviour of $\mathcal{L}_t(\vec{x})$ is determined by the root of

$$\frac{1}{N} + (1-z)\, g_N(\vec{0}; z) = 0 \tag{5.30}$$

closest to the unit circle. This root is in absolute value larger than one. As remarked by Weiss et al. [12], for $N \gg 1$ this root is in fact close to $z = 1$. Expanding the left-hand side of (5.30) around $z = 1$ gives

$$\frac{1}{N} + (1-z)\, g_N(\vec{0}) - (1-z)^2 g_N'(\vec{0}) + \ldots = 0 \,. \tag{5.31}$$

One easily verifies that $g_N'(\vec{0}) \equiv (\partial g_N/\partial z)(\vec{0}; 1) \sim N^{4/d-1}$. The first two terms on the left-hand side of equation (5.31) are of comparable magnitude when

$$(z-1) \sim \frac{1}{N g_N(\vec{0})} \,. \tag{5.32}$$

This relation determines how to scale the time t with the lattice size N as $N \to \infty$, since eventually, due to the inverse Laplace transformation, $t \sim 1/(1-z)$. Using the scaling (5.32), one may verify that for $d \geq 2$ only the first two terms on the left-hand side of (5.31) contribute to the leading order result for $\mathcal{L}_t(\vec{x})$, the higher order terms giving rise to corrections. It is remarked that for $d = 1$ where $g_N(\vec{0}) \simeq N/6$ and $g_N'(\vec{0}) \simeq N^3/180$ [8], all higher order terms in (5.31) are of the same order as the first two and therefore (5.31) then is useless. From (5.29) we finally find that for $d \geq 2$

$$\begin{aligned} \mathcal{L}_t(\vec{x}) \;&\simeq\; \left[1 - \frac{g_N(\vec{x})}{g_N(\vec{0})}\right] \exp\left(-\frac{t}{N\, g_N(\vec{0})}\right) \\ &\times \left[1 + \mathcal{O}\left(\frac{t}{N^{3-4/d} g_N^3(\vec{0})}\right) + \mathcal{O}\left(\frac{1}{N^{2-4/d} g_N^2(\vec{0})}\right)\right] \end{aligned} \tag{5.33}$$

which is valid for $N \gg 1$ and $t \gtrsim N g_N(\vec{0})$. Obviously, since we want $t/N^{3-4/d} g_N^3(\vec{0})$ to be negligible with respect to 1 for the result (5.33) to be useful, there is also an upper bound on the allowed t values. Furthermore, using (5.22), one can see that for $d = 2$ the corrections to the leading order behaviour are at best of relative order $\ln^{-2} cN$, and thus disappear only very slowly with increasing N.

5.2.3 The characteristic time τ_N to visit the last site

Now that we have calculated $\mathcal{L}_t(\vec{x})$, we can use it to determine the average number of sites S_t visited by the random walk at time t since $S_t = \sum_{\vec{x}}(1 - \mathcal{L}_t(\vec{x}))$. The result is

$$S_t \simeq N\left[1 - \exp\left(-\frac{t}{Ng_N(\vec{0})}\right)\right] . \tag{5.34}$$

In the derivation one uses that

$$\sum_{\vec{x}} g_N(\vec{x}) = 0, \tag{5.35}$$

as may be deduced from (5.20), (5.21), and the fact that $\sum_{\vec{x}} \exp(-i\vec{q}\cdot\vec{x}) = N\delta_{\vec{q},\vec{0}}$. Formula (5.34) is valid for large N and $Ng_N(\vec{0}) \lesssim t \ll N^{3-4/d}g_N^3(\vec{0})$, and agrees with the one given by Weiss et al. [12].

Let $\bar{\tau}_N$ be the time at which, on average, almost all of the sites of the lattice have been visited, i.e., for which $S_t = N - M$ with M of order 1. From equation (5.34) we then find

$$\bar{\tau}_N \simeq g_N(\vec{0})N\ln N \simeq \begin{cases} \frac{1}{\pi}N\ln^2 N, & d=2, \\ g_\infty(\vec{0})N\ln N, & d>2, \end{cases} \tag{5.36}$$

so that, to leading order in N, $\bar{\tau}_N$ is independent of M. Although in principle τ_N, the average of the times at which the last site is visited in the lattice covering-time problem [1], is different from $\bar{\tau}_N$, one might expect that they are equal to leading order in N (which is supported by the fact that $\bar{\tau}_N$, to leading order in N, is independent of M). Since, according to (5.1) and (5.36), they are of the same order in dimensions $d \geq 2$ (this is not true for $d = 1$) we would expect (5.36) also to hold for τ_N. Under this assumption we find for the constant A in (5.1):

$$A = \begin{cases} \frac{1}{\pi} = 0.318\ldots, & d=2, \\ 1.516\ldots, & d=3, \\ 1.239\ldots, & d=4\,. \end{cases} \tag{5.37}$$

This result in fact agrees with the result found by Aldous [3] in his investigation of the covering-time problem. The value for $g_\infty(\vec{0})$ in $d = 3$ was first evaluated analytically by Watson [13]. We note that there exists an asymptotic large-d expansion of $g_\infty(\vec{0})$ in powers of $1/2d$, given by Montroll [14]. The A values in (5.37) should be compared to the numerical values found by Nemirovsky et al. [1]

$$A = \begin{cases} 0.33\ (0.30), & d=2, \\ 1.55\ (1.63), & d=3, \\ 1.30\ (1.23), & d=4\,. \end{cases} \tag{5.38}$$

Here the first set of values is found from a fit of the data to equation (5.1) for lattices with periodic boundary conditions, only taking the leading order term into account. The values in parentheses are found when assuming that A is independent of boundary conditions, so that both the data for periodic and for reflecting boundary conditions can be used; moreover, the correction terms in (5.1) have been taken into account.

5.2.4 The higher-dimensional case

Let us now return to equation (5.2) and to the original "last-site problem" in $d \geq 2$. One can write $L_N(\vec{x};t)$ as the probability that the last site is visited at time t, irrespective of which site it concerns, times the conditional probability that it concerns site $\vec{x}$, which we shall denote by $C(\vec{x}\,|t)$. Then

$$L_N(\vec{x}\,) = \sum_{t=0}^{\infty} C(\vec{x}\,|t) \sum_{\vec{y}} L_N(\vec{y};t) \ . \tag{5.39}$$

Our next step is guided by the following observation. Divide the time axis in intervals of length $t_{corr} \equiv N g_N(\vec{0}\,)$. According to (5.36) and the argument below it, the last site is visited only after $\sim \ln N$ intervals. After the first interval, when $t = t_{corr}$, a site $\vec{x}$ has not yet been visited with a probability $\mathcal{L}_{t_{corr}}(\vec{x}\,)$, whose $\vec{x}$ dependence is contained in the prefactor in brackets in equation (5.33). In view of equation (5.33), sites closer to the origin have a larger probability of having been visited. Since, however, for $t \gtrsim t_{corr}$, the probability distribution of the walker is effectively uniform over the lattice, one should expect that from $t \approx t_{corr}$ on all sites that still survive are visited with an equal probability per unit of time. This expectation is confirmed by a calculation of the probability $\mathcal{L}_t(\vec{x}\,)/\sum_{\vec{y}} \mathcal{L}_t(\vec{y}\,)$ that site $\vec{x}$ is not yet visited relative to the total number of sites still left. Indeed, with the aid of equation (5.33) one finds that for $N g_N(\vec{0}\,) \lesssim t \ll N^{3-4/d} g_N^3(\vec{0}\,)$

$$\frac{\mathcal{L}_t(\vec{x}\,)}{\sum_{\vec{y}} \mathcal{L}_t(\vec{y}\,)} \simeq \frac{1}{N}\left[1 - \frac{g_N(\vec{x}\,)}{g_N(\vec{0}\,)}\right], \tag{5.40}$$

which is independent of time. Now, since the sum on t in equation (5.39) is certainly dominated by times $\sim N g_N(\vec{0}\,) \ln N \gg t_{corr}$, we may replace the quantity $C(\vec{x}\,|t)$ by $\mathcal{L}_t(\vec{x}\,)/\sum_{\vec{y}} \mathcal{L}_t(\vec{y}\,)$, and obtain, using (5.40),

$$L_N(\vec{x}\,) \simeq \frac{1}{N}\left[1 - \frac{g_N(\vec{x}\,)}{g_N(\vec{0}\,)}\right], \tag{5.41}$$

which is valid for $N \gg 1$ ($\ln cN \gg 1$ in $d = 2$). Combined with (5.22) and (5.23) we find (5.5) for $d > 2$ and (5.6) for $d = 2$.

5.3 The set of sites not yet visited in $d \geq 2$

Having found the typical time at which the last site is visted, as well as the probability that $\vec{x}$ is the site visited last, it is natural to ask next about the structure of the set of sites not yet visited at a given time t. In particular, we shall study pair correlations between the sites of this set.

5.3.1 Probability of a nonvisited pair

In order to study pair correlations, we first consider the probability $\mathcal{L}_t(\vec{x},\vec{y})$ that the simple random walk starting at site $\vec{0}$ at time 0 has visited neither site $\vec{x}$ nor site $\vec{y}$ at time t yet. Evidently,

$$\mathcal{L}_t(\vec{x},\vec{y}) = 1 - \sum_{\vec{\rho}=\vec{x},\vec{y}} \sum_{t'=0}^{t} F_{t'}^{\{\vec{x},\vec{y}\}}(\vec{\rho}), \tag{5.42}$$

where $F_t^{\{\vec{x},\vec{y}\}}(\vec{\rho})$, as in the case $d = 1$, denotes the probability that the walk enters the set $\{\vec{x},\vec{y}\}$ for the first time at time t by reaching the point $\vec{\rho}$ ($\vec{\rho} = \vec{x}$ or $\vec{\rho} = \vec{y}$). The Laplace transform of (5.42) is

$$\widehat{\mathcal{L}}(\vec{x},\vec{y};z) = \frac{1 - \sum_{\vec{\rho}=\vec{x},\vec{y}} \widehat{F}^{\{\vec{x},\vec{y}\}}(\vec{\rho};z)}{1-z}. \tag{5.43}$$

Now

$$G_t(\vec{\omega}) = \sum_{\vec{\rho}=\vec{x},\vec{y}} \sum_{t'=0}^{t} F_{t'}^{\{\vec{x},\vec{y}\}}(\vec{\rho})\, G_{t-t'}(\vec{\omega}-\vec{\rho}), \qquad \vec{\omega} = \vec{x},\vec{y}, \tag{5.44}$$

since to be at a given time t at a specified point $\vec{\omega}$ of a given set of points, there must be some previous time t' at which one enters this set for the first time (at the point $\vec{\rho}$), after which one uses the remaining time $t - t'$ to move to the specified point. From (5.44) we get, summing on $\vec{\omega}$,

$$G_t(\vec{x}) + G_t(\vec{y}) = \sum_{t'=0}^{t} \sum_{\vec{\rho}=\vec{x},\vec{y}} F_{t'}^{\{\vec{x},\vec{y}\}}(\vec{\rho}) \left[G_{t-t'}(\vec{0}) + G_{t-t'}(\vec{x}-\vec{y})\right] \tag{5.45}$$

so that

$$\sum_{\vec{\rho}=\vec{x},\vec{y}} \widehat{F}^{\{\vec{x},\vec{y}\}}(\vec{\rho};z) = \frac{\widehat{G}(\vec{x};z) + \widehat{G}(\vec{y};z)}{\widehat{G}(\vec{0};z) + \widehat{G}(\vec{x}-\vec{y};z)}. \tag{5.46}$$

The result (5.46) is also valid for $\vec{x} = \vec{y}$, in which case it reduces to (5.18). Substituting it in (5.43), using (5.21), and performing an inverse Laplace transformation as in section 5.2.2, we get

$$\mathcal{L}_t(\vec{x},\vec{y}) \simeq \left[1 - \frac{g_N(\vec{x}) + g_N(\vec{y})}{g_N(\vec{0}) + g_N(\vec{x}-\vec{y})}\right] \exp\left(-\frac{2t}{N[g_N(\vec{0}) + g_N(\vec{x}-\vec{y})]}\right), \quad (5.47)$$

which is thus valid for $N \gg 1$ and $t \gtrsim N g_N(\vec{0})$. As in the case of $\mathcal{L}_t(\vec{x})$ there is an upper limit on the allowed times t, given by $t \ll N^{3-4/d} g_N^3(\vec{0})$, for (5.47) to be useful. Since we shall use it later on, we remark here that for the case $d = 2$, for times $t \sim N \ln^2 cN$, and for $|\vec{x}|$, $|\vec{y}| \sim \sqrt{N}$, the expression in square brackets in (5.47) should be replaced by unity. This is because in $d = 2$ for $|\vec{x}|$, $|\vec{y}| \sim \sqrt{N}$, the expression in square brackets is actually $1 + \mathcal{O}(\ln^{-1} cN)$, as may be concluded from (5.22) – (5.24), while, for $t \sim N \ln^2 cN$, there then are also other corrections to (5.47) of order $\ln^{-1} cN$, not shown here (Cf. the situation for $\mathcal{L}_t(\vec{x})$ given in (5.33)). Thus, for reasons of consistency, the $\mathcal{O}(\ln^{-1} cN)$ corrections should then be dropped.

5.3.2 Pair correlations and variances

The structure of the set of sites not yet visited is reflected in the correlation function

$$\delta\mathcal{L}_t(\vec{x},\vec{y}) \equiv \mathcal{L}_t(\vec{x},\vec{y}) - \mathcal{L}_t(\vec{x})\,\mathcal{L}_t(\vec{y})\,. \quad (5.48)$$

For $\vec{x} \neq \vec{y}$ this is just the probability that both members of the pair $(\vec{x},\vec{y})$ have not yet been visited at time t, in excess of what a purely random distribution of nonvisited sites would give. In fact, summing (5.48) on $\vec{x}$ and $\vec{y}$ one obtains the variance of the total number of nonvisited sites. For times $N g_N(\vec{0}) \lesssim t \ll N^{3-4/d} g_N^3(\vec{0})$ we may use equations (5.33) and (5.47) for $\mathcal{L}_t(\vec{x})$ and $\mathcal{L}_t(\vec{x},\vec{y})$, respectively, to find

$$\sum_{\vec{x},\vec{y}} \delta\mathcal{L}_t(\vec{x},\vec{y}) \simeq e^{-\frac{2t}{N g_N(\vec{0})}}\, N \sum_{\vec{\xi}} [\exp\left(\frac{2t}{N g_N(\vec{0})} \frac{g_N(\vec{\xi})}{g_N(\vec{0}) + g_N(\vec{\xi})}\right) - 1], \quad (5.49)$$

where we have first written $\vec{y} = \vec{x} + \vec{\xi}$ and subsequently performed the sum on $\vec{x}$, taking the sum rule (5.35) into account. The sum on $\vec{\xi}$ runs over all the sites of the lattice. Now, to leading order in N, the expression $N \exp(-t/N g_N(\vec{0}))$ is just the average value of the total number of nonvisited sites at time t, as may be seen from (5.34). Therefore we can rewrite (5.49) as

$$\Delta \simeq \frac{1}{N} \sum_{\vec{\xi}} [\exp\left(\frac{2t}{N g_N(\vec{0})} \frac{g_N(\vec{\xi})}{g_N(\vec{0}) + g_N(\vec{\xi})}\right) - 1], \quad (5.50)$$

where $\Delta \equiv N^{-2} \exp(2t/N g_N(\vec{0})) \times \sum_{\vec{x},\vec{y}} \delta\mathcal{L}_t(\vec{x},\vec{y})$ denotes the ratio of the variance to the square of the average of the total number of sites not yet visited at time t. Simulations performed by us on lattices of up to 20×20 sites in $d = 2$ and up to $10 \times 10 \times 10$ sites in $d = 3$ show that with increasing N the behaviour (5.50) is gradually approached, the convergence being faster for larger t. However, in $d = 2$

where the corrections to (5.50) decay only logarithmically with increasing N, one would probably need lattices which are orders of magnitude larger than the ones employed in our simulations to fully see the behaviour (5.50) over the whole time range $N \ln cN \lesssim t \ll N \ln^3 cN$ for which it is valid. In the following, we shall study (5.50) for $d \geq 2$. As $d = 2$ turns out to be special, we shall postpone its discussion and first concentrate on the case $d > 2$.

5.3.3 Fluctuations in the number of nonvisited sites in $d > 2$

We shall be interested in times $t \sim \bar{\tau}_N$. Therefore we introduce a reduced time variable α according to $t = \alpha N g_N(\vec{0}) \ln N \simeq \alpha \bar{\tau}_N$. Formula (5.34) shows that for these times the average number of sites which have not yet been visited by the random walk is given by $N^{1-\alpha}$. Furthermore (5.50) becomes

$$\Delta_\alpha \simeq \frac{1}{N} \sum_{\vec{\xi}} [\exp\left(2\alpha \ln N \frac{g_N(\vec{\xi})}{g_N(\vec{0}) + g_N(\vec{\xi})}\right) - 1], \tag{5.51}$$

the subscript α indicating that we are looking at times t scaled with the lattice size N according to the prescription given above. To evaluate this expression asymptotically, we divide the sum on $\vec{\xi}$ in a sum on all $\vec{\xi}$ with $|\vec{\xi}| < \lambda$ and another with $|\vec{\xi}| \geq \lambda$, where we take λ large and of order N^0. Equation (5.23) shows that in dimensions $d > 2$ the function $g_N(\vec{\xi})$ for large N and $|\vec{\xi}|$ is rapidly decaying with increasing $|\vec{\xi}|$. This suggests that in order to find an asymptotic expansion for the sum on $\vec{\xi}$ with $|\vec{\xi}| \geq \lambda$ one should expand the summand in terms of $g_N(\vec{\xi})/g_N(\vec{0})$. Doing so, we find that for α fixed and $N \to \infty$

$$\frac{1}{N} \sum_{|\vec{\xi}| \geq \lambda} I_{N,\alpha}(\vec{\xi}) \simeq 2\alpha^2 \frac{\ln^2 N}{N} \sum_{|\vec{\xi}| \geq \lambda} \frac{g_N^2(\vec{\xi})}{g_N^2(\vec{0})}, \tag{5.52}$$

where $I_{N,\alpha}(\vec{\xi})$ stands for the expression in square brackets in (5.51), and where we have once again taken into account the sum rule (5.35).

Now, with the aid of (5.23) and (5.24), replacing the sum on $|\vec{\xi}| \geq \lambda$ by an integral, one easily shows that for $d < 4$ asymptotically

$$\frac{1}{N} \sum_{|\vec{\xi}| \geq \lambda} \frac{g_N^2(\vec{\xi})}{g_N^2(\vec{0})} \simeq \left(\frac{d}{2\pi^2 g_\infty(\vec{0})}\right)^2 \left(\sum_{\vec{k} \neq \vec{0}} \frac{1}{k^4}\right) \frac{1}{N^{2-4/d}} \equiv \frac{K_d}{N^{2-4/d}}, \tag{5.53}$$

where a constant K_d has been introduced. The sum on $\vec{k}$ runs over all vectors $\vec{k} \neq \vec{0}$ having integer valued components. Note that the asymptotic expression (5.53) is independent of λ. The leading order contribution to the other sum, with $|\vec{\xi}| < \lambda$, comes from the term with $\vec{\xi} = \vec{0}$, while the leading corrections stem from the terms where $\vec{\xi}$ is a nearest-neighbour vector:

$$\frac{1}{N}\sum_{|\vec{\xi}|<\lambda} I_{N,\alpha}(\vec{\xi}) = N^{\alpha-1}[1+2dN^{-\frac{\alpha}{2g_\infty(\vec{0})-1}}+\ldots] \,. \tag{5.54}$$

In the derivation of (5.54) we used that for $\vec{\delta}$ a nearest-neighbour vector: $g_N(\vec{\delta}) = g_N(\vec{0}) - 1 + \frac{1}{N} \simeq g_\infty(\vec{0}) - 1$. So the result we obtain for $2 < d < 4$, α fixed, and $N \to \infty$ is

$$\Delta_\alpha \simeq N^{\alpha-1}[1+2dN^{-\frac{\alpha}{2g_\infty(0)-1}}+\ldots] + 2\alpha^2 K_d \frac{\ln^2 N}{N^{2-4/d}}[1+\ldots] \,. \tag{5.55}$$

At this point, remembering that the definition of $\delta\mathcal{L}_t(\vec{x},\vec{y})$ used to calculate (5.55) involves a subtraction of two quantities for which we have only used the leading order results, one might worry about the importance of the subleading order terms in (5.33) and (5.47) and thus about the validity of (5.55) itself. However, we have explicitly verified that in the scaling limit we study (α fixed, $N \to \infty$) the contributions of these terms are of lower order (namely $\mathcal{O}(\ln N/N^{2-4/d})$), so that the result (5.55) is in fact correct. From it we see that there is a crossover in time of the asymptotic behaviour of the variance of the number of nonvisited sites: for $\alpha \le \frac{4}{d} - 1$ the second part ($\sim \ln^2 N/N^{2-4/d}$) is the dominant one while for $\alpha > \frac{4}{d} - 1$ the first one takes over. This reflects that with increasing time, the structure on the scale of the lattice itself becomes more and more important. Explicitly, we find from (5.55) that for $2 < d < 4$ and $N \to \infty$, α remaining fixed,

$$\Delta_\alpha \simeq \begin{cases} 2\alpha^2 K_d \frac{\ln^2 N}{N^{2-4/d}}, & 0 < \alpha \le \frac{4}{d} - 1, \\ N^{\alpha-1} + 2\alpha^2 K_d \frac{\ln^2 N}{N^{2-4/d}}, & \frac{4}{d} - 1 < \alpha \le R_d(\frac{4}{d} - 1), \\ N^{\alpha-1}[1+2dN^{-\frac{\alpha}{2g_\infty(0)-1}}], & R_d(\frac{4}{d} - 1) < \alpha, \end{cases} \tag{5.56}$$

with $R_d \equiv 1 + [2(g_\infty(\vec{0}) - 1)]^{-1}$.

For $d > 4$ the sum $\sum_{|\vec{\xi}|>\lambda} g_N^2(\vec{\xi})$ is no longer dominated by the large-$|\vec{\xi}|$ terms. In fact, we find

$$\sum_{|\vec{\xi}|\ge\lambda} g_N^2(\vec{\xi}) = \begin{cases} \mathcal{O}(\ln N), & d = 4, \\ \mathcal{O}(N^0), & d > 4, \end{cases} \tag{5.57}$$

so that for $d \ge 4$ the term with $\vec{\xi} = \vec{0}$ in (5.51) becomes the dominant contribution for all $\alpha > 0$. Hence

$$\Delta_\alpha \simeq N^{\alpha-1}, \qquad \alpha > 0, \;\; d \ge 4, \tag{5.58}$$

is the mean-field behaviour for this problem.

5.3.4 A check for the mean-field case

One may check the result (5.58) independently for the mean-field ("$d = \infty$") version of the problem. To do so, we consider a lattice of N points, where every point is connected to the other $(N-1)$ points. At $t=0$, the random walker occupies one of the lattice points, which we shall call the origin 0. Then at every instant of time $t = 1, 2, \ldots$ it chooses randomly one from among the $(N-1)$ points differing from its then current position and subsequently goes there. Now, let $P(s,t)$ denote the probability that at time t there are s sites (among the N) which have not been visited yet. Obviously, for $s = 0, 1, \ldots, N-1$ and $t \geq 1$, we have

$$P(s,t) = \frac{N-s-1}{N-1} P(s,t-1) + \frac{s+1}{N-1} P(s+1,t-1) \ . \tag{5.59a}$$

This is so because if there are to be s sites which have not been visited yet at time t, there must either already be s of these sites at time $t-1$ with the walker subsequently moving to a site which has already been visited previously, or there are $s+1$ nonvisited sites at $t-1$, the walker arriving at any one of them at time t. The boundary condition that comes with (5.59a) reads

$$P(s,0) = \delta_{s,N-1} \ . \tag{5.59b}$$

For the average $\langle s \rangle_t \equiv \sum_{s=0}^{N-1} sP(s,t)$, using (5.59a), one obtains the recurrence relation

$$\langle s \rangle_t = \left(\frac{N-2}{N-1}\right) \langle s \rangle_{t-1}, \qquad t \geq 1, \tag{5.60}$$

which, with (5.59b), has the solution

$$\langle s \rangle_t = (N-1) \left(\frac{N-2}{N-1}\right)^t, \quad t \geq 0 \ . \tag{5.61}$$

Also, it is easy to derive that for $\langle s^2 \rangle_t \equiv \sum_{s=0}^{N-1} s^2 P(s,t)$ we have

$$\langle s^2 \rangle_t = \left(\frac{N-3}{N-1}\right) \langle s^2 \rangle_{t-1} + \frac{1}{N-1} \langle s \rangle_{t-1}, \quad t \geq 1, \tag{5.62}$$

which, using the solution (5.61) for $\langle s \rangle_t$ and the boundary condition (5.59b), gives

$$\langle s^2 \rangle_t = (N-1)^2 \left(\frac{N-3}{N-1}\right)^t + (N-1)[\left(\frac{N-2}{N-1}\right)^t - \left(\frac{N-3}{N-1}\right)^t], \quad t \geq 0 \ . \tag{5.63}$$

Now, the probability $G_t(0)$ to find the walker at the origin at time t satisfies

$$G_t(0) = \frac{1}{N-1} \sum_{x \neq 0} G_{t-1}(x) = \frac{1}{N-1}[1 - G_{t-1}(0)], \quad t \geq 1, \tag{5.64a}$$

with boundary condition

$$G_0(0) = 1, \tag{5.64b}$$

so that

$$\widehat{G}(0; z) = \frac{N - 1 + z/(1 - z)}{N - 1 + z}, \tag{5.65}$$

and hence

$$g_N(0) = \left(\frac{N-1}{N}\right)^2 . \tag{5.66}$$

Taking $t = \alpha N g_N(0) \ln N$ we find indeed that asymptotically

$$\Delta_\alpha = \frac{\langle s^2\rangle_t - \langle s\rangle_t^2}{\langle s\rangle_t^2} \simeq N^{\alpha-1}, \qquad \alpha > 0 . \tag{5.67}$$

So this takes care of all dimensions $d > 2$. We shall now study what happens in the exceptional dimension $d = 2$.

5.3.5 Fluctuations in the number of nonvisited sites in $d = 2$

The starting point will again be equation (5.50). We take $t = \alpha N g_N(\vec{0}) \ln cN$. Note that here we are using $\ln cN$, with c as in (5.22), instead of $\ln N$ as we did in the $d > 2$ case. This is in fact not essential, but proves to be aesthetically more pleasing later on; for instance in formula (5.71). From (5.50) we now obtain

$$\begin{aligned} \Delta_\alpha &\simeq \frac{4}{N} \iint_{\lambda}^{\frac{1}{2}\sqrt{N}} d\vec{\xi}\, [\exp\left(2\alpha \ln cN \frac{g_N(\vec{\xi}\,)}{g_N(\vec{0}\,) + g_N(\vec{\xi}\,)}\right) - 1] \\ &\simeq 4 \iint_0^{\frac{1}{2}} d\vec{y}\, [\exp(2\alpha\pi f(\vec{y}\,)) - 1], \end{aligned} \tag{5.68}$$

where $f(\vec{y}\,)$ is as given in (5.24). In the first line in (5.68) we introduced a cutoff λ, which is supposed to be large and of order N^0, so that we could replace the sum on $\vec{\xi}$ in (5.50) by an integral. We shall come back to this cutoff later. Furthermore, to obtain the second line, we have written $\vec{\xi} = \sqrt{N}\,\vec{y}$ and subsequently, using equations (5.22) and (5.23), taken the limit $N \to \infty$ everywhere. One may check that the final result is nonnegative (as it should be), using the inequality $e^x \geq 1 + x$ and the fact that $\iint_0^{1/2} d\vec{y} f(\vec{y}\,) = 0$. The result (5.68) does no longer depend on λ. Of course, in obtaining it we have not taken the contributions from the terms with small $|\vec{\xi}\,|$ into account. But, as we shall see in a moment, for $\alpha < 2$ these do not contribute to the leading order behaviour. As it stands, however, the result is only useful for $\alpha < \frac{1}{2}$, since the integral is divergent for $\alpha \geq \frac{1}{2}$. This may be concluded from the fact that $f(\vec{y}\,) \simeq -\frac{2}{\pi} \ln |\vec{y}\,|$ for $|\vec{y}\,| \downarrow 0$ (cf. (5.25)) so that then $\exp(2\alpha\pi f(\vec{y}\,)) \sim |\vec{y}\,|^{-4\alpha}$. To obtain an asymptotic expansion for $\alpha \geq \frac{1}{2}$ we must therefore work a little harder. The key to obtaining such an expansion lies in noting that for $\alpha > \frac{1}{2}$ the main contributions to Δ_α will very likely come from those terms for which $|\vec{\xi}\,|$ is still large, but no longer on the scale $\sqrt{N}$. This implies, namely, that one then can use that for N, $|\vec{\xi}\,| \to \infty$ with $|\vec{\xi}\,|/\sqrt{N} \to 0^+$,

$$g_N(\vec{\xi}\,) = g_N(\vec{0}\,) - \mathcal{G}_N(\vec{\xi}\,) \simeq \frac{1}{\pi}\ln cN - \mathcal{G}_\infty(\vec{\xi}\,) \simeq \frac{1}{\pi}\ln cN - \frac{2}{\pi}\ln\frac{|\vec{\xi}\,|}{r_0}, \tag{5.69}$$

as follows from equations (5.22) and (5.28). Doing so we obtain from (5.50)

$$\Delta_\alpha \simeq \frac{2\pi}{N}\int_{O(N^0)}^{O(\sqrt{N})} d\xi\,\xi\,\exp\left(\alpha\ln cN\frac{\ln cN - 2\ln(\xi/r_0)}{\ln cN - \ln(\xi/r_0)}\right). \tag{5.70}$$

Substituting $\xi = r_0(cN)^u$ we then get

$$\Delta_\alpha \simeq 2\pi c r_0^2(\ln cN)\int_{O(\ln^{-1}cN)}^{\frac{1}{2}+O(\ln^{-1}cN)} du\,\exp[(\ln cN)\,(2u - \frac{\alpha}{1-u} + 2\alpha - 1)]\,. \tag{5.71}$$

The integrand in (5.71) reaches its maximum value for $u_0 = 1 - \sqrt{\frac{\alpha}{2}}$. For $\frac{1}{2} < \alpha < 2$, this point u_0 lies within the range of integration as $N \to \infty$. Applying the method of steepest descent one then easily finds

$$\Delta_\alpha \simeq \pi c r_0^2\sqrt[4]{2\alpha\pi^2}\sqrt{\ln cN}(cN)^{(\sqrt{2\alpha}-1)^2}, \quad \frac{1}{2} < \alpha < 2\,. \tag{5.72}$$

Obviously, for $\frac{1}{2} < \alpha < 2$, the most important contributions to the sum in (5.50) come from the vicinity of $|\vec{\xi}\,| \sim N^{u_0} = N^{1-\sqrt{\alpha/2}}$, thus justifying the use of (5.69) as $N \to \infty$. Again, because of the logarithms involved, we expect the asymptotic behaviour (5.72) to be reached extremely slowly, which is consistent with the findings of simulations performed by us on lattices of up to 20×20 sites. Other evidence for this slow convergence comes from the point $\alpha = \frac{1}{2}$, separating the two regimes in which the asymptotic results (5.68) and (5.72) hold. Here, namely, we find that $\Delta_{\frac{1}{2}}$ is asymptotically given by one half of what one finds by just taking $\alpha = \frac{1}{2}$ in (5.72). On the basis of this one can actually find a scaling form for Δ_α, in the variable $w \equiv (\alpha - \frac{1}{2})\sqrt{\ln cN}$, which is valid for $\alpha \to \frac{1}{2}$, $N \to \infty$, and w fixed. However, even for $N = 400$ this scaling form differs considerably from the behaviours (5.68) and (5.72).

For $\alpha > 2$ the maximum of the integrand in (5.71) becomes a boundary maximum at $u = 0$, implying that the lattice structure becomes important, so that then the terms with small $|\vec{\xi}\,|$, which we have neglected up till now, must be taken into account. These terms are, to leading order, represented by the $\vec{\xi} = \vec{0}$ term in (5.50) which, for

$t = \alpha N g_N(\vec{0}) \ln cN$, gives a contribution $c^{-1}(cN)^{\alpha-1}$. Compared to the asymptotic behaviours (5.68) and (5.72), this contribution is indeed negligible in the time range for which $0 < \alpha < 2$. However for $\alpha > 2$ this term is dominant and represents the asymptotic behaviour as $N \to \infty$.

5.3.6 Spatial structure of the nonvisited set in $d = 2$

We want to study the *structure* of the set of sites not yet visited in $d = 2$ at times $t \sim \tau_N$. To do so, we consider the *conditional probability* $C_t(\vec{y}\,|\vec{x}\,)$ that site $\vec{y}$ has not been visited at time t, *given* that at this time site $\vec{x}$ has not yet been visited:

$$\begin{aligned} C_t(\vec{y}\,|\vec{x}\,) &= \mathcal{L}_t(\vec{x},\vec{y}\,)/\mathcal{L}_t(\vec{x}\,) \\ &\simeq \frac{\left[1 - \frac{g_N(\vec{x}\,)+g_N(\vec{y}\,)}{g_N(\vec{0}\,)+g_N(\vec{x}-\vec{y}\,)}\right]}{\left[1 - \frac{g_N(\vec{x}\,)}{g_N(\vec{0}\,)}\right]} \exp\left(-\frac{t}{N g_N(\vec{0}\,)} \frac{g_N(\vec{0}\,) - g_N(\vec{x}-\vec{y}\,)}{g_N(\vec{0}\,) + g_N(\vec{x}-\vec{y}\,)}\right) \end{aligned} \quad (5.73)$$

where we again used equations (5.33) and (5.47). This quantity, namely, allows one to study the average number of sites $N_{\vec{x}}(R,t)$ not yet visited by the random walk at time t within a radius R around a site $\vec{x}$ which itself has not been visited yet, because

$$N_{\vec{x}}(R,t) = \sum_{|\vec{\xi}\,|<R} C_t(\vec{x}+\vec{\xi}\,|\vec{x}\,)\,. \quad (5.74)$$

Since we shall want $\vec{x}$ to be an arbitrary site, we scale $\vec{x} = \sqrt{N}\vec{x}_1$ with $\vec{x}_1$ fixed as $N \to \infty$. If we now also take $R = o(\sqrt{N})$ so that $|\vec{x}+\vec{\xi}\,| \sim \sqrt{N}$ in (5.74) we may, to leading order in N, replace the expressions in square brackets in (5.73) by unity, as becomes clear when looking at (5.22) – (5.24). Hence we obtain

$$N_{\vec{x}}(R,t) \simeq \sum_{|\vec{\xi}\,|<R} \exp\left(-\frac{t}{N g_N(\vec{0}\,)} \frac{g_N(\vec{0}\,) - g_N(\vec{\xi}\,)}{g_N(\vec{0}\,) + g_N(\vec{\xi}\,)}\right), \quad (5.75)$$

which is independent of $\vec{x}$. As discussed before, we take $t = \alpha N g_N(\vec{0}\,) \ln cN$ and furthermore choose R to depend on N by taking $R = (cN)^\beta$. Here β is restricted to $0 < \beta < \frac{1}{2}$. But then, in obtaining an asymptotic expression for $N_{\vec{x}}(R,t)$, we may use (5.69) and find, once again introducing a cutoff λ,

$$N_{\vec{x}}(R,t) \simeq 2\pi \int_\lambda^{(cN)^\beta} d\xi\, \xi \exp\left(-\alpha \ln cN \frac{\ln(\xi/r_0)}{\ln cN - \ln(\xi/r_0)}\right)\,. \quad (5.76)$$

Thus we arrive at a formula which has pretty much the same structure as (5.70), the integrand here only differing from the integrand in (5.70) by a factor $(cN)^\alpha$. Following the lines of reasoning outlined after (5.70) we readily find that for $0 < \alpha < 2$ and $0 < \beta < \frac{1}{2}$:

$$N_{\vec{x}}(R,t) \simeq \begin{cases} \frac{2\pi}{2-\alpha/(1-\beta)^2}\, r_0^{\alpha/(1-\beta)^2}\,(cN)^{\beta(2-\frac{\alpha}{1-\beta})}, & \frac{\alpha}{(1-\beta)^2} < 2, \\ 2\pi r_0^2 \left(\frac{\pi}{2}\sqrt{\frac{\alpha}{2}}\right)^{\frac{1}{2}} \sqrt{\ln cN}\,(cN)^{(\sqrt{2}-\sqrt{\alpha})^2}, & \frac{\alpha}{(1-\beta)^2} > 2, \end{cases} \tag{5.77}$$

which translated back in terms of R is (5.8). For $\alpha/(1-\beta)^2 = 2$ we get just one half of what we find for $\alpha/(1-\beta)^2 > 2$. The result (5.77) is valid in the scaling limit

$$|\vec{x}\,| \sim \sqrt{N}, \quad R = (cN)^\beta, \quad t = \alpha N g_N(\vec{0}\,) \ln cN, \quad \text{with} \quad N \to \infty, \tag{5.78}$$

α and β fixed, and $c = 1.8456\ldots$. Again it does not depend on the cutoff λ used. The "critical" value $\beta^* = 1 - \sqrt{\alpha/2}$ can be interpreted as saying that, while for $\alpha < \frac{1}{2}$ the nonvisited sites are essentially distributed all over the lattice, for $\frac{1}{2} < \alpha < 2$ the typical size of the nonvisited cluster of sites is of the order of N^{β^*}. Equation (5.75) shows that the contribution of the terms with small $|\vec{\xi}\,|$ to $N_{\vec{x}}(R,t)$ is of order N^0, which is indeed dominated by the terms displayed in (5.77). It is merely remarked here that if one takes R large but of order N^0 one obtains

$$N_{\vec{x}}(R,t) \simeq \frac{2\pi}{2-\alpha} r_0^\alpha R^{2-\alpha}, \quad 0 < \alpha < 2, \tag{5.79}$$

which in fact corresponds to letting $\beta \downarrow 0$ in (5.77), taking $R = (cN)^\beta$ fixed. Obviously, the set of nonvisited sites has a fractal-like structure with a time-dependent fractal dimension $2-\alpha$. Letting $\beta \uparrow \frac{1}{2}$ in (5.77) we see that then

$$N_{\vec{x}}(\sqrt{N}, \alpha\bar{\tau}_N) \sim \begin{cases} (cN)^{1-\alpha}, & 0 < \alpha < \frac{1}{2}, \\ \sqrt{\ln cN}\,(cN)^{(\sqrt{2}-\sqrt{\alpha})^2}, & \frac{1}{2} < \alpha < 2\,. \end{cases} \tag{5.80}$$

Comparing this to the average number of nonvisited sites, $\sum_{\vec{x}} \mathcal{L}_t(\vec{x}\,)$, we get

$$\frac{N_{\vec{x}}(\sqrt{N}, \alpha\bar{\tau}_N)}{\sum_{\vec{x}} \mathcal{L}_{\alpha\bar{\tau}_N}(\vec{x}\,)} \sim \begin{cases} 1, & 0 < \alpha < \frac{1}{2}, \\ \sqrt{\ln cN}\,(cN)^{(\sqrt{2\alpha}-1)^2}, & \frac{1}{2} < \alpha < 2, \end{cases} \tag{5.81}$$

where we have used (5.33) for $t = \alpha N g_N(\vec{0}\,) \ln cN$. At first sight it might seem surprising that for $\frac{1}{2} < \alpha < 2$ this ratio can become much larger than 1. However, there is nothing strange about it, since it is a direct consequence of the fact that here one only looks at a subclass of all possible random walks on the lattice. Namely, one demands the site $\vec{x}$ not to have been visited yet at time t. What it says then, is that the nonvisited sites have a strong tendency to cluster: *If* $\vec{x}$ has not been visited yet, *then* there are many sites around it which also have not been visited yet. But, of course, the probability that $\vec{x}$ has not been visited yet is rapidly diminishing with increasing time. In the same spirit, the result for $0 < \alpha < \frac{1}{2}$ means that then there are still plenty of sites left which have not been visited yet, and demanding $\vec{x}$ to be a nonvisited site is not a severe restriction at all.

Finally, we note that from (5.73) it also follows that for $d > 2$ the correlation $C_t(\vec{y}|\vec{x})$ is rapidly decaying with increasing $|\vec{x} - \vec{y}|$, implying that the nonvisited sites no longer have a strong clustering tendency. The mean decay regime for the correlations now lies on the time scale set by $t \sim N g_N(\vec{0}) \ll \bar{\tau}_N$.

5.4 Conclusion

We have studied the covering process of a d-dimensional finite hypercubic lattice with periodic boundary conditions by a random walk, for general d. In $d = 1$ the probability that site x is the last site visited in this covering process was evaluated analytically for general lattice size N. Although in dimensions $d > 1$ this was no longer possible, we could nevertheless evaluate the analogous probability in the limit of large lattice sizes. We then found that there is a dimension-dependent characteristic time scale on which the last site is visited. In $d = 2$ the structure of the set of sites not yet visited, viewed on this characteristic time scale, is fractal-like. In dimensions $d > 2$ this is not the case, and the correlations between the sites not yet visited decay much more rapidly with distance than in the $d = 2$ case.

References

[1] A.M. Nemirovsky, H.O. Mártin, and M.D. Coutinho-Filho, Phys. Rev. A **41** (1990) 761.

[2] C.S.O. Yokoi, A. Hernández-Machado, and L. Ramírez-Piscina, Phys. Lett. A **145** (1990) 82.

[3] D.J. Aldous, Z. Wahrscheinlichkeitstheorie verw. Gebiete **62** (1983) 361.

[4] J.T. Cox, Ann. Probab. **17** (1989) 1333.

[5] J.T. Cox and D. Griffeath, Ann. Probab. **14** (1986) 347.

[6] P. Erdős and P. Révész, J. Multivariate Anal. **27** (1988) 169.

[7] F. Spitzer, *Principles of Random Walk* (Van Nostrand, Princeton, 1964).

[8] E.W. Montroll and G.H. Weiss, J. Math. Phys. **6** (1965) 617.

[9] M.N. Barber and B.W. Ninham, *Random and Restricted Walks* (Gordon and Breach, New York, 1970).

[10] W.Th.F. den Hollander and P.W. Kasteleyn, Physica **112A** (1982) 523.

[11] C. Itzykson and J.-M. Drouffe, *Statistical field theory 1* (Cambridge University Press, Cambridge, 1989).

[12] G.H. Weiss, S. Havlin, and A. Bunde, J. Stat. Phys. **40** (1985) 191.

[13] G.N. Watson, Quart. J. Math. Oxf. **10** (1939) 266.

[14] E.W. Montroll, Proc. Symp. Appl. Math. **16** (1964) 193.

Chapter 6

Correlations between two Ising chains subjected to a common thermal noise

6.1 Introduction

Not long ago a new method, which has become known as "damage spreading", was introduced to study critical phenomena of lattice systems [1, 2]. It consists of studying the time evolution of the distance ("damage") between two configurations s and s' of the same system, subjected to the same thermal noise. Typically, one uses the same sequence of random numbers to apply to each system an ordinary Monte Carlo (MC) simulation. The idea is to learn, through the study of the time evolution of the distance, about the properties of *one* system. E.g., if the system has a critical temperature, then qualitatively different time-dependences of this distance are expected above and below the critical temperature.

The method has been applied both to models of physical systems (to the ANNNI model [3], to the Ising model for different dimensions, different dynamics, different initial damages, and both with and without a magnetic field [2, 4, 5, 6, 7], similarly to spin glass models [1, 5, 8, 9, 10, 11], to the XY-model [12], ...) and to various types of cellular automata, see [13] and references therein.

For ferromagnets, employing heat bath dynamics, one has been able to establish analytically a connection between the long-time behaviour of the distance on the one hand and the equilibrium spontaneous magnetization [5, 14, 15] and two-point intrasystem equilibrium correlation function [15] on the other hand. In general, however, it has proven nontrivial to relate the observed differences in the behaviour of the distance to the properties of the single system. Both in the study of spin glasses [1] and for XY-models [12], using the damage spreading method, one has found new critical temperatures not present in the equilibrium phase diagrams of these systems. These temperatures now appear to be of a purely "dynamical" nature [16]. Therefore it is interesting to study the effects of the introduction of correlations in the dynamics of the single systems in more detail.

The damage spreading case belongs to a more general class of MC simulations, which we shall call "dynamically correlated MC simulations": Fundamentally, there is a master equation for the joint probability distribution $P^{(2)}(s,s';t)$ on the configuration pairs (s,s') (t is the time variable). Its transition probabilities determine the degree and the nature of the dynamical correlations. The damage spreading case corresponds to a specific choice for these probabilities. However, one may also consider other choices. The master equation itself must be a rather special one, since, if one disregards one of the systems, the other one should evolve according to a usual MC simulation. Mathematically, this means that the single system distributions

$$P(s;t) \equiv \sum_{s'} P^{(2)}(s,s';t), \tag{6.1a}$$

$$P(s';t) \equiv \sum_{s} P^{(2)}(s,s';t), \tag{6.1b}$$

are solutions of single system master equations having all the usual properties of detailed balancing etc., and that therefore as $t \to \infty$

$$P(s;t) \to P_{eq}(s) \propto \exp[-\beta\mathcal{H}_1(s)], \tag{6.2a}$$

$$P(s';t) \to P_{eq}(s') \propto \exp[-\beta\mathcal{H}_1(s')] \,. \tag{6.2b}$$

Here $\mathcal{H}_1$ is a prescribed single system Hamiltonian and $\beta = 1/k_BT$, with k_B Boltzmann's constant and T the absolute temperature.

Given this, it is clear that if the joint probability distribution $P^{(2)}(s,s';t)$ tends to some limiting (or: "equilibrium") distribution $P^{(2)}_{eq}(s,s') > 0$, for all s and s', as $t \to \infty$, then one can introduce a combined-system Hamiltonian $\mathcal{H}_2(s,s')$ via

$$P^{(2)}_{eq}(s,s') \propto \exp[-\beta\mathcal{H}_2(s,s')] \,. \tag{6.3}$$

Even if $\mathcal{H}_1$ is short ranged $\mathcal{H}_2$ will in general not be, and will be hard to find. Moreover, even if one knows $\mathcal{H}_2$ the master equation for $P^{(2)}$ will in general not satisfy detailed balancing with respect to $\mathcal{H}_2$. In the damage spreading work mentioned above, the transition probabilities are chosen in such a way that two configurations which at a certain time become equal will remain equal forever after, and one has (for heat bath dynamics) $P^{(2)}_{eq}(s,s') = \delta_{s,s'}\, P_{eq}(s)$. Hence in this case $\mathcal{H}_2$ must have infinite couplings.

Due to all of this it has proven extremely difficult to find any analytical results at all for models of dynamically correlated simulation, even in one dimension. In this chapter we obtain an exact result for the equilibrium state in a special case of dynamically correlated simulation of two Ising spin chains, $s \equiv (s_1, \ldots, s_N)$ and $s' \equiv (s'_1, \ldots, s'_N)$. The characteristic features of this case are

(i) the single chains have Glauber dynamics, and

(ii) the product spins $u_i \equiv s_i s'_i$ play a role completely equivalent to s_i and s'_i: the equations of motion are invariant under permutations of (s, s', u), where u denotes the configuration of the product spins.

We let $\langle \ldots \rangle_t$ denote the average with respect to $P^{(2)}(s, s'; t)$. Since the single-chain magnetizations $\langle s_i \rangle_t$ and $\langle s'_i \rangle_t$ relax to zero with time (the system has no phase transition), so does $\langle u_i \rangle_t = \langle s_i s'_i \rangle_t$. We further show that $\langle s_i s'_j \rangle_{eq} = 0$ for all i and j. Hence, there are no interchain equilibrium *pair* correlations and the distance between the chains

$$D(t) \equiv \frac{1}{2N} \langle \sum_{i=1}^{N} (1 - s_i s'_i) \rangle_t \tag{6.4}$$

relaxes to 1/2, which is also the average distance between two randomly picked configurations. Nevertheless, the correlated dynamics does cause correlations between the chains in the equilibrium state. These appear in the four-point equilibrium correlation function $g(j-i, k-j) \equiv \langle u_i s_j s'_k \rangle_{eq} = \langle s_i s_j s'_i s'_k \rangle_{eq}$, closely reflecting the "triangle-symmetry" (in (s, s', u)) of the problem. It is this function that we calculate.

If the combined-system Hamiltonian $\mathcal{H}_2$ had strictly finite-ranged interactions, then $g(p, q)$ would be the sum of a finite number of exponentials with decay constants corresponding to the spectrum of the transfer matrix. The result of our calculation, equation (6.65), shows, however, that such is not the case: $g(p, q)$ is expressed as the integral over a spectrum with both a discrete and a continuous part. Hence, $\mathcal{H}_2$ is not of strictly finite range. Our calculation does not provide, however, the precise form of this Hamiltonian. The function $g(p, q)$ is determined not by averaging over an equilibrium ensemble but as the stationary solution of the time evolution equations for the correlation functions. Just as for the single-chain Glauber dynamics, these equations constitute, for each n, a closed system at the n-site level. The time-dependence of $\langle u_i s_j s'_k \rangle_t$ can be reformulated as a problem of three interacting random walkers of which any two, when they meet, fuse. It is reminiscent of the vicious walker problem studied by Fisher [17, 18], but differs from it in that there they annihilate upon meeting.

The organization of this chapter is as follows. In section 6.2 we establish the notations and concepts we shall be using. Section 6.3 covers the derivation of the most general expression for the combined-system transition probabilities consistent with the procedure described above. In section 6.4 we derive equations obeyed by the time-dependent correlation functions, which we shall need to study the equilibrium properties of the specific dynamically correlated MC simulation studied in section 6.5. Also, in section 6.5.2, we shall explicitly find the solution for $\langle s_i s'_i s_j s'_k \rangle_{eq}$, reflecting some of the properties of $\mathcal{H}_2$. In section 6.6 the approach to equilibrium is discussed. Finally, section 6.7 is a general conclusion.

6.2 One chain

To establish the notation we use and to introduce some concepts which will be useful when considering the dynamically correlated simulation of two systems, we first briefly review the properties of the single system. To this end we consider a one-dimensional Ising chain with periodic boundary conditions, consisting of N spins s_j ($j = 1, \ldots, N$) with configuration $s \equiv \{s_j\}_{j=1}^{N}$, described by the Hamiltonian

$$\mathcal{H}_1(s) = -J \sum_{i=1}^{N} s_i s_{i+1} \ . \tag{6.5}$$

Here $s_j = \pm 1$ and $J > 0$. Let $P(s;t)$ be the probability to find the system in configuration s at time t. Then one can write down a master equation, governing the time evolution of this system, which reads

$$P(s;t+1) = \frac{1}{N} \sum_{i=1}^{N} [W_i(1|s)P(s;t) + W_i(-1|s^i)P(s^i;t)] \ , \ t = 0, \ 1, \ \ldots \ . \tag{6.6}$$

In this equation $\frac{1}{N} W_i(\sigma|s)$, where $\sigma = \pm 1$, denotes the probability per time step for the system to jump from a configuration s to a configuration in which s_i has become σs_i, all other spins remaining the same. Furthermore s^i denotes the configuration obtained from s by flipping spin i.

For $P(s;t)$ to approach the canonical equilibrium distribution, where $P_{eq}(s) \propto \exp(-\beta \mathcal{H}_1(s))$, it is sufficient that the $W_i(\sigma|s)$ obey a detailed balancing relation with respect to the Hamiltonian $\mathcal{H}_1$. However, there then are still many ways in which the $W_i(\sigma|s)$ can be chosen. We shall follow Glauber [19] and choose

$$W_i(\sigma|s) = \frac{1}{2} + 2\sigma f_i(s), \tag{6.7}$$

where

$$f_i(s) = \frac{1}{8} \gamma s_i (s_{i-1} + s_{i+1}) \tag{6.8}$$

with

$$\gamma \equiv \tanh 2\beta J \ . \tag{6.9}$$

An advantage of this choice is that the time-dependent equations for, for example, the magnetization and the two-point correlation function can be solved exactly [19].

6.3 Two chains

So the single chain dynamics is completely known. Therefore let us now consider *two copies* of the chain (6.5), with configurations s and s', respectively. We shall imagine that we are performing an MC simulation on the combined system (s, s'). More specifically, with $P^{(2)}(s, s'; t)$ denoting the probability to find at time t the first chain in configuration s and the second one in s', we shall describe the time evolution of the combined system by the master equation

$$\begin{aligned} P^{(2)}(s,s';t+1) &= \frac{1}{N}\sum_{i=1}^{N}[\, W_i^{(2)}(+1\;+1|s\;s'\,)\,P^{(2)}(s\,,s'\,;t) \\ &\quad + W_i^{(2)}(+1\;-1|s\;s'^i)\,P^{(2)}(s\,,s'^i;t) \\ &\quad + W_i^{(2)}(-1\;+1|s^i\,s'\,)\,P^{(2)}(s^i,s'\,;t) \\ &\quad + W_i^{(2)}(-1\;-1|s^i\,s'^i)\,P^{(2)}(s^i,s'^i;t)]\;. \end{aligned} \tag{6.10}$$

Here the $W_i^{(2)}(\sigma\,\sigma'|s\,s')$, with $\sigma,\sigma'=\pm1$, denote the (conditional) probabilities that, starting from the configuration (s,s') and given that we have selected to probe sites i, the pair (s_i,s'_i) will undergo a transition to its new value $(\sigma s_i,\sigma' s'_i)$.

These probabilities, as in the case of the one-chain MC simulation, directly determine *how* the spins s_i and s'_i are updated, and therefore also the equilibrium correlations. So let us see what freedom one has in choosing them.

We use the expansion

$$W_i^{(2)}(\sigma\,\sigma'|s\,s') = a_i(s,s') + \sigma b_i(s,s') + \sigma' c_i(s,s') + \sigma\sigma' g_i(s,s'), \tag{6.11}$$

where a_i, b_i, c_i, and g_i are arbitrary functions of the configurations s and s', restricted by the conditions

$$W_i^{(2)}(\sigma\,\sigma'|s\,s') \geq 0, \quad \text{for all } \sigma,\sigma',s,s', \tag{6.12}$$

$$\sum_{\sigma,\sigma'=\pm1} W_i^{(2)}(\sigma\,\sigma'|s\,s') = 1\;. \tag{6.13}$$

Furthermore, the requirement that the MC procedure for the combined system be also a valid MC procedure for each system separately implies that, with the definitions (6.1a) and (6.1b), summing the two-chain master equation (6.10) on s' should reduce it to the one-chain master equation (6.6) for $P(s;t)$. Summing on s should turn it into the one-chain master equation for $P(s';t)$. As one can easily check, for this to be the case, it is sufficient to have

$$\sum_{\sigma'=\pm1} W_i^{(2)}(\sigma\,\sigma'|s\,s') = W_i(\sigma|s), \tag{6.14}$$

$$\sum_{\sigma=\pm1} W_i^{(2)}(\sigma\,\sigma'|s\,s') = W_i(\sigma'|s')\;. \tag{6.15}$$

Here the $W_i(\sigma|s)$ are the one-chain transition probabilities appearing in (6.6). Then, using (6.13), (6.14), (6.15), and (6.7) in (6.11), we find that this expression reduces to

$$W_i^{(2)}(\sigma\,\sigma'|s\,s') = \frac{1}{4} + \sigma f_i(s) + \sigma' f_i(s') + \sigma\sigma' g_i(s,s'), \tag{6.16}$$

where $f_i(s)$ is given by (6.8). Hence the only freedom left is the function $g_i(s, s')$.

Also, the symmetry relations

$$W_i^{(2)}(\sigma\,\sigma'|s\,s') = W_i^{(2)}(\sigma'\,\sigma|s'\,s), \tag{6.17}$$

reflecting the interchangeability of the two subsystems s and s', and

$$W_i^{(2)}(\sigma\,\sigma'|s\,s') = W_i^{(2)}(\sigma\,\sigma'|-s\;-s'), \tag{6.18}$$

representing global spin flip invariance which, in the absence of a magnetic field, should certainly be present, must be obeyed. Hence, in equation (6.16) for the transition probabilities we must have

$$g_i(s, s') = g_i(-s, -s') = g_i(-s', -s) = g_i(s', s)\,. \tag{6.19}$$

However, this does not uniquely determine $g_i(s, s')$. Rather, with the restrictions (6.12) and (6.19), $g_i(s, s')$ can be chosen at will. In fact, the very choice of $g_i(s, s')$ determines how the dynamics of the separate chains are correlated.

6.4 Time-dependent correlation functions

Since for general $g_i(s, s')$ the Hamiltonian $\mathcal{H}_2(s, s')$, as defined in (6.3), is not known the only way to find expressions for the equilibrium correlation functions is to set up their equations of motion and solve for the stationary state. Therefore, we must study time-dependent correlation functions even if we would only be interested in the equilibrium situation. So let us suppose that one wants to study the correlation function

$$\langle s_{j_1} \ldots s_{j_m} s'_{k_1} \ldots s'_{k_n} \rangle_t, \tag{6.20}$$

where $\langle \ldots \rangle_t$ is the average with respect to $P^{(2)}(s, s'; t)$. Here it is understood that all the j_i ($i = 1, \ldots, m$) are different. The same rule applies to the k-indices of the s'-spins. From the two-chain master equation (6.10) one can easily derive the equations of motion for the correlation functions (6.20):

$$\begin{aligned}
&\langle s_{j_1} \ldots s_{j_m} s'_{k_1} \ldots s'_{k_n} \rangle_{t+1} = \\
&\frac{1}{N}\sum_{s,s'}\sum_{i=1}^{N}[(s_{j_1} \ldots s_{j_m})^i (s'_{k_1} \ldots s'_{k_n})^i W_i^{(2)}(-1\;-1|s\,s') \\
&\quad + (s_{j_1} \ldots s_{j_m})^i (s'_{k_1} \ldots s'_{k_n})\, W_i^{(2)}(-1\;+1|s\,s') \\
&\quad + (s_{j_1} \ldots s_{j_m})\, (s'_{k_1} \ldots s'_{k_n})^i\, W_i^{(2)}(+1\;-1|s\,s') \\
&\quad + (s_{j_1} \ldots s_{j_m})\, (s'_{k_1} \ldots s'_{k_n})\, W_i^{(2)}(+1\;+1|s\,s')]\, P^{(2)}(s, s'; t)\,.
\end{aligned} \tag{6.21}$$

Here

$$(s_{j_1}\dots s_{j_m})^i \equiv \begin{cases} -s_{j_1}\dots s_{j_m} & \text{if } i \in \{j_1, \dots, j_m\} \\ +s_{j_1}\dots s_{j_m} & \text{otherwise,} \end{cases} \tag{6.22}$$

and a similar notation applies to $(s'_{k_1}\dots s'_{k_n})^i$. We now introduce three sets $\mathcal{J}$, $\mathcal{K}$, and $\mathcal{L}$, where $\mathcal{L}$ is the set of indices common to both $\{j_1, \dots, j_m\}$ and $\{k_1, \dots, k_n\}$, $\mathcal{J}$ contains the indices belonging to $\{j_1, \dots, j_m\}$ which are not in $\mathcal{L}$, and $\mathcal{K}$ consists of the indices in $\{k_1, \dots, k_n\}$ which are not in $\mathcal{L}$. Then, using this and inserting the specific form (6.16) for the two-chain transition probabilities in equation (6.21), one ultimately finds

$$\begin{aligned} \langle s_{j_1}\dots s_{j_m} s'_{k_1}\dots s'_{k_n}\rangle_{t+1} &= (1-\frac{m+n-l}{N})\langle s_{j_1}\dots s_{j_m} s'_{k_1}\dots s'_{k_n}\rangle_t \\ &+\frac{4}{N}\sum_{i\in\mathcal{J}}\langle s_{j_1}\dots s_{j_m} s'_{k_1}\dots s'_{k_n} f_i(s)\rangle_t \\ &+\frac{4}{N}\sum_{i\in\mathcal{K}}\langle s_{j_1}\dots s_{j_m} s'_{k_1}\dots s'_{k_n} f_i(s')\rangle_t \\ &+\frac{4}{N}\sum_{i\in\mathcal{L}}\langle s_{j_1}\dots s_{j_m} s'_{k_1}\dots s'_{k_n} g_i(s,s')\rangle_t, \end{aligned} \tag{6.23}$$

where l is the number of elements in the set $\mathcal{L}$. It is understood that for $n = 0$ (which means that there are no s'-spins present, so that also $l = 0$) the sums on $i \in \mathcal{L}$ and $i \in \mathcal{K}$ are empty and one recovers the equations corresponding to the well-known one-chain Glauber dynamics [19]. An analogous observation holds for $m = 0$. Once again it is clear that only when considering interchain correlations, then the $g_i(s, s')$ come into the game, so that the expression one is using for the $g_i(s, s')$ in fact determines the interchain correlations.

6.5 Interchain correlation functions in a specific case

6.5.1 Preliminaries

In this section we shall make a specific choice for $g_i(s, s')$, consistent with the remaining constraints (6.12) and (6.19), and investigate the equilibrium properties of the combined system (s, s') when subjected to the resulting transition probabilities (6.16). More precisely, with $u_j \equiv s_j s'_j$ for all $j = 1, \dots, N$, we take (also compare equation (6.8) for $f_i(s)$)

$$g_i(s,s') = \frac{1}{8}\gamma\, u_i(u_{i-1}+u_{i+1}), \tag{6.24}$$

so that

$$
\begin{aligned}
W_i^{(2)}(\sigma\,\sigma'|s\,s') \;=\;& \frac{1}{4}+\frac{1}{8}\gamma(\sigma s_i)\,(s_{i-1}+s_{i+1})+\frac{1}{8}\gamma(\sigma' s_i')\,(s_{i-1}'+s_{i+1}') \\
&+\frac{1}{8}\gamma(\sigma s_i)\,(\sigma' s_i')\,(s_{i-1}s_{i-1}'+s_{i+1}s_{i+1}')\;. \qquad (6.25)
\end{aligned}
$$

The first thing to notice is that expression (6.25) depends only on the proposed spin values (σs_i) and $(\sigma' s_i')$ at site i and not on the current ones. Furthermore, (6.25) has a lot of symmetry in it; not only does it obey (6.17) and (6.18) as required, but we also have

$$
W_i^{(2)}(\sigma\,\sigma'|s\,s') = W_i^{(2)}(\sigma\,\sigma'|-s\,s') = W_i^{(2)}(\sigma\,\sigma'|s\;-s')\;. \qquad (6.26)
$$

However, what is still more remarkable is that in making the choice (6.24) for $g_i(s,s')$, we have introduced a threefold (or: "triangle") symmetry between s, s', and the "*product system*"

$$
u \equiv \{u_j\}_{j=1}^{N} = \{s_j s_j'\}_{j=1}^{N}, \qquad (6.27)
$$

since

$$
W_i^{(2)}(\sigma\,\sigma'|s\,s') = W_i^{(2)}(\sigma\sigma'\;\sigma'|u\,s') = W_i^{(2)}(\sigma\;\sigma\sigma'|s\,u)\;. \qquad (6.28)
$$

Note that $u_j = -1$ corresponds to a site j where s_j and s_j' are different, whereas $u_j = +1$ means that $s_j = s_j'$. Therefore, in the damage spreading language, the u_j can be thought of as indicating whether there is damage at site j (in the sense that $s_j \neq s_j'$) or not.

The equations for the equilibrium correlation functions $\langle s_{j_1}\ldots s_{j_m} s_{k_1}'\ldots s_{k_n}'\rangle_{eq}$ can be found simply by taking the limit $t \to \infty$ in (6.23) at fixed N. That this is permissable for $\gamma < 1$ is easily inferred from the two-chain master equation (6.10) linking the 2^{2N} component vector $P_{t+1}^{(2)} \equiv \{P^{(2)}(s,s';t+1)\}_{(s,s')}$ to $P_t^{(2)}$ via a time-independent $2^{2N}\times 2^{2N}$ transition matrix which, when making the choice (6.25) for the $W_i^{(2)}(\sigma\,\sigma'|s\,s')$, satisfies the Perron-Frobenius theorem [20] (all elements are non-negative and there is a path from any configuration to any other). Then namely there is a single eigenvalue 1 with a (normalized) eigenvector $P_{eq}^{(2)}$ whose elements can be chosen to be all positive. All other eigenvalues have a modulus less than one, so that $P_t^{(2)} \to P_{eq}^{(2)}$ as $t \to \infty$. Therefore, for the choice (6.24) and for any finite N, one can indeed define an effective Hamiltonian $\mathcal{H}_2(s,s')$ via (6.3). However, we note that this Hamiltonian must be rather special since all symmetry properties of the transition probabilities are directly transferred to $\mathcal{H}_2(s,s')$ itself, as we shall show for a concrete case below. (See the argument following equation (6.30).) One cannot deduce that the $W_i^{(2)}(\sigma\,\sigma'|s\,s')$ in (6.25) obey a detailed balancing relation with respect to this $\mathcal{H}_2(s,s')$, since "detailed balancing", though sufficient, is not per se necessary to reach the prescribed equilibrium. With $\langle\ldots\rangle$ denoting the equilibrium

($t = \infty$) ensemble average and substituting the choices (6.8) and (6.24) made for $f_i(s)$ and $g_i(s,s')$ we find from (6.23)

$$(m+n-l)\langle s_{j_1}\ldots s_{j_m}s'_{k_1}\ldots s'_{k_n}\rangle = \frac{1}{2}\gamma\sum_{i\in\mathcal{J}}\langle s_{j_1}\ldots s'_{k_n}s_i(s_{i-1}+s_{i+1})\rangle$$
$$+\frac{1}{2}\gamma\sum_{i\in\mathcal{K}}\langle s_{j_1}\ldots s'_{k_n}s'_i(s'_{i-1}+s'_{i+1})\rangle$$
$$+\frac{1}{2}\gamma\sum_{i\in\mathcal{L}}\langle s_{j_1}\ldots s'_{k_n}s_is'_i\,(s_{i-1}s'_{i-1}+s_{i+1}s'_{i+1})\rangle \tag{6.29}$$

Now, we are interested in the *interchain* correlations in equilibrium induced by the specific choice of the transition probabilities (6.25), since these equilibrium correlations are directly governed by the *unknown* $\mathcal{H}_2(s,s')$. The intrachain correlations can be calculated using the canonical ensemble connected with $\mathcal{H}_1$, see equations (6.1a) – (6.2b). Let us point out that the relations

$$P^{(2)}_{eq}(s,s') = P^{(2)}_{eq}(-s,s') = P^{(2)}_{eq}(s,-s'), \tag{6.30}$$

are direct consequences of the symmetry properties (6.26) of the $W^{(2)}_i(\sigma\,\sigma'|s\,s')$. For any finite N this is easy to see. For example: define $Q(s,s') \equiv P^{(2)}_{eq}(-s,s')$. Then, using (6.26) one may show that $Q(s,s')$, like $P^{(2)}_{eq}(s,s')$, is a solution of the two-chain master equation for $t = \infty$. But the Perron-Frobenius theorem certifies that the $t = \infty$ solution is unique. Therefore we must have $Q(s,s') \propto P^{(2)}_{eq}(s,s')$. Moreover since $\sum_{s,s'} Q(s,s') = \sum_{s,s'} P^{(2)}_{eq}(-s,s') = \sum_{s,s'} P^{(2)}_{eq}(s,s') = 1$ we in fact find that $Q(s,s') = P^{(2)}_{eq}(s,s')$, and so have proven the first equality in (6.30). From this equation it then follows that any correlation function of an odd number of s-spins and/or an odd number of s'-spins must, in equilibrium, necessarily be equal to zero. Therefore the first nonzero equilibrium interchain correlation function has at least two s-spins and two s'-spins in it.

6.5.2 Four-point interchain equilibrium correlation functions

6.5.2.1 Calculating $\langle s_is'_is_js'_j\rangle$

The first interchain correlation function in this category we want to study has two different indices, i and j, and is of the form $\langle s_is'_is_js'_j\rangle$. Because of the threefold symmetry of the transition probabilities as expressed in equation (6.28) we immediately find that

$$\langle s_is'_is_js'_j\rangle = \langle s_is_j\rangle = \langle s'_is'_j\rangle = z^{|i-j|}, \tag{6.31}$$

where

$$z \equiv \tanh \beta J, \tag{6.32}$$

and where, for the last equality in (6.31), we have taken $N \to \infty$ and used the known result for the two-point intrachain equilibrium correlation function in an infinite system. Note that in order to obtain the four-point equilibrium correlation function in (6.31) it has not been necessary to know an explicit form for $\mathcal{H}_2(s, s')$. On the contrary, one can use the obtained result to study $\mathcal{H}_2(s, s')$ to some extent: By comparing the result for the four-point equilibrium correlation function in (6.31) to what one finds for the same correlation function in the case of uncorrelated simulation of the two chains, this being

$$\langle s_i s_i' s_j s_j' \rangle = \langle s_i s_j \rangle \langle s_i' s_j' \rangle = z^{2|i-j|}, \tag{6.33}$$

where the last equality again applies for an infinite system, one can conclude that certainly $\mathcal{H}_2(s, s') \neq \mathcal{H}_1(s) + \mathcal{H}_1(s')$. Also, by remarking that for a "maximally correlated" (or: "damage spreading") simulation, where eventually the systems s and s' will become equal and then stay equal forever after, one has $\langle s_i s_i' s_j s_j' \rangle = 1$, we see that the simulation we are studying is indeed somewhere in between the uncorrelated and the maximally correlated ones. To define this quantitatively one could, for example, look at a correlation length ξ_c, for the infinite system defined through $\langle s_i s_i' s_j s_j' \rangle = \exp[-|i-j|/\xi_c]$, which for our case is twice as large as for the uncorrelated case but smaller than for the maximally correlated one (where it is ∞). It is interesting to see that even this simplest of nonzero interchain equilibrium correlation functions clearly shows the effects of the introduction of dynamical correlations.

6.5.2.2 Calculating $\langle s_i s_i' s_j s_k' \rangle$

To extend our picture of the effects of dynamical correlations we also look at another member of the category of four-point interchain equilibrium correlation functions, having three different indices, i, j, and k, and being of the form

$$\langle s_i s_i' s_j s_k' \rangle \, . \tag{6.34}$$

This correlation function reflects the triangle symmetry of the problem. Though one can link it to several other correlation functions employing the various symmetries of the transition probabilities, its value is not as easily found as in the previous case. We shall have to solve explicitly the complete set of equations (6.29) for this kind of correlation function. Because of the translational invariance in the system, (6.34) is a function of only two independent variables taking integer values, say

$$p \equiv j - i, \quad \text{and} \quad q \equiv k - j, \tag{6.35}$$

and we write

$$\langle s_i s_i' s_j s_k' \rangle \equiv g(p,q) \; . \tag{6.36}$$

For reasons of symmetry one may always take $0 \le q \le p$. However it turns out to be easier to consider $g(p,q)$ for all integer $p,\ q \ge 0$. For p and q both strictly positive, so that i, j, and k in (6.36) are all different, we get from (6.29)

$$\begin{aligned} 3g(p,q) &= \frac{1}{2}\gamma[\, g(p-1,q) + g(p+1,q) \\ &\quad + g(p,q-1) + g(p,q+1) \\ &\quad + g(p+1,q-1) + g(p-1,q+1)], \quad p,q \ge 1, \end{aligned} \tag{6.37}$$

whereas, for $N \to \infty$ (cf. (6.31)),

$$g(p,0) = z^p, \;\; p \ge 0, \tag{6.38}$$

and

$$g(0,q) = z^q, \;\; q \ge 0 \; . \tag{6.39}$$

Obviously this is a boundary value problem with two inhomogeneous boundary conditions. In order to solve it we first introduce

$$\begin{aligned} x &\equiv p + \frac{1}{2}q, \\ y &\equiv \frac{1}{2}q\sqrt{3} \; . \end{aligned} \tag{6.40}$$

Then, with $g(p,q) \equiv \tilde{g}(x,y)$, equations (6.37)–(6.39) become

$$\begin{aligned} 3\tilde{g}(x,y) &= \frac{1}{2}\gamma[\, \tilde{g}(x-1,y) + \tilde{g}(x+1,y) \\ &\quad + \tilde{g}(x-\frac{1}{2}, y-\frac{1}{2}\sqrt{3}) + \tilde{g}(x+\frac{1}{2}, y+\frac{1}{2}\sqrt{3}) \\ &\quad + \tilde{g}(x+\frac{1}{2}, y-\frac{1}{2}\sqrt{3}) + \tilde{g}(x-\frac{1}{2}, y+\frac{1}{2}\sqrt{3})], \end{aligned} \tag{6.41}$$

$$\tilde{g}(x,0) = z^x, \tag{6.42}$$

and

$$\tilde{g}(\frac{1}{2}x, \frac{1}{2}x\sqrt{3}) = z^x \; . \tag{6.43}$$

Here x and y can only take a discrete set of values, p and q being integer valued. Nevertheless, in the limit that the correlation functions are only slowly varying (as compared to the lattice spacing), one may go to a continuum description. Taylor expanding (6.41) around (x,y) and rearranging the resulting equation a bit gives

$$\tilde{g}(x,y) = c^2[\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\tilde{g}(x,y) + \ldots], \tag{6.44}$$

where we introduced

$$c \equiv \sqrt{\frac{\gamma}{4(1-\gamma)}} = \frac{1}{1-z}\sqrt{\frac{z}{2}}, \tag{6.45}$$

and where the dots indicate terms involving fourth and higher order derivatives. Now it is easy to see that one can neglect these terms in the limit

$$c \to \infty \text{ with } \frac{x}{c}, \frac{y}{c} \text{ remaining fixed }. \tag{6.46}$$

This corresponds to considering the problem for large distances and at low temperatures, where the correlation functions are indeed slowly varying. Actually dropping these higher order terms, introducing coordinates (r, ϕ) according to

$$\frac{x}{c} = r\cos\phi \tag{6.47a}$$

$$\frac{y}{c} = r\sin\phi, \tag{6.47b}$$

and defining $\bar{g}(x,y) \equiv G(r,\phi)$ we find the boundary value problem

$$\Delta G(r,\phi) = G(r,\phi), \quad \text{for } 0 < \phi < \frac{\pi}{3}, \quad r > 0, \tag{6.48}$$

with

$$G(r,0) = z^{cr}, \quad r > 0 \tag{6.49a}$$

and

$$G(r,\frac{\pi}{3}) = z^{cr}, \quad r > 0. \tag{6.49b}$$

Here

$$\Delta \equiv \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} \,. \tag{6.50}$$

Since the solution of a linear problem with more than one inhomogeneous boundary condition can be written as the sum of solutions of problems each of which has only one inhomogeneous condition [21], we first concentrate on finding $G_1(r,\phi)$, defined as the solution of (6.48) which does satisfy (6.49b), but instead of (6.49a) we demand that $G_1(r,0) = 0$. To this end we look for solutions $G_1^0(r,\phi)$ of (6.48), which satisfy the homogeneous boundary condition at $\phi = 0$, by making the Ansatz

$$G_1^0(r,\phi) = R(r)\,\Phi(\phi)\,. \tag{6.51}$$

Substituting this in (6.48) we find

$$r^2\frac{R''}{R} + r\frac{R'}{R} - r^2 = -\frac{\ddot{\Phi}}{\Phi}, \tag{6.52}$$

where $'$ denotes a derivative with respect to r and $\dot{}$ a derivative with respect to ϕ. As usual, since the left hand side depends only on r, whereas the right hand side is a function only of ϕ, both sides must be equal to a (real valued) constant, say $-\xi^2 \leq 0$. Then it follows that [22]

$$\begin{aligned} \Phi(\phi) &= \alpha_1 \sinh \xi\phi + \alpha_2 \cosh \xi\phi \\ R(r) &= \alpha_3 K_{i\xi}(r) + \alpha_4 I_{i\xi}(r), \end{aligned} \tag{6.53}$$

where $\alpha_1, \ldots, \alpha_4$ are arbitrary constants and $I_{i\xi}$ and $K_{i\xi}$ modified Bessel functions of purely imaginary order $i\xi$. The homogeneous boundary condition $G_1^0(r,0) = 0$ implies that $\alpha_2 = 0$. Furthermore, since we want $G_1^0(r,\phi) \to 0$ for $r \to \infty$ we must reject the $I_{i\xi}$ solution (which diverges at infinity) and thus take $\alpha_4 = 0$. We therefore find

$$G_1^0(r,\phi) \propto \sinh \xi\phi \, K_{i\xi}(r) \ . \tag{6.54}$$

One may check that if instead of $-\xi^2 \leq 0$ we had taken the separation constant $+\xi^2 \geq 0$ the reasoning above would have led to solutions of the form

$$G_1^0(r,\phi) \propto \sin \xi\phi \, K_{\xi}(r) \ . \tag{6.55}$$

However since $K_\xi(r)$, with ξ real, diverges logarithmically for $r \downarrow 0$ (when the order is purely imaginary this is not the case) we must reject this solution, implying that a positive separation constant gives no new solutions $G_1^0(r,\phi)$ to the problem.

Now $G_1(r,\phi)$ is a linear combination of the solutions $G_1^0(r,\phi)$:

$$G_1(r,\phi) = \int_0^\infty d\xi \, b(\xi) \, \sinh \xi\phi \, K_{i\xi}(r), \tag{6.56}$$

with $b(\xi)$ chosen so as to satisfy the inhomogeneous boundary condition (6.49b), that is:

$$\int_0^\infty d\xi \, b(\xi) \sinh(\frac{\pi\xi}{3}) K_{i\xi}(r) = \exp[-rc\ln(\frac{1}{z})] \ . \tag{6.57}$$

From [23, 6.795(1)] one finds

$$b(\xi) \sinh(\frac{\pi\xi}{3}) = \frac{2}{\pi} \cosh \xi\theta, \tag{6.58}$$

where

$$\theta \equiv \arccos\left(c\ln(\frac{1}{z})\right) = \arccos(-\frac{\ln z}{1-z}\sqrt{\frac{z}{2}}) \ . \tag{6.59}$$

Note that in general, since $z \in [0,1]$, we have $\theta \in [\frac{\pi}{4}, \frac{\pi}{2}]$. In the limit (6.46) where the continuum approximation is valid, one has $z \to 1$ and thus $\theta \to \frac{\pi}{4}$. Combining (6.56) with (6.58) we get

$$G_1(r,\phi) = \frac{2}{\pi} \int_0^\infty d\xi \, \cosh\theta\xi \frac{\sinh\phi\xi}{\sinh(\frac{\pi\xi}{3})} K_{i\xi}(r), \quad 0 \le \phi \le \frac{\pi}{3}, \quad r > 0, \tag{6.60}$$

with θ as defined in (6.59).

The solution $G_2(r,\phi)$ to (6.48) satisfying (6.49a) and $G_2(r,\frac{\pi}{3}) = 0$ can easily be found by realizing that this problem is just the previous problem, except for a reflection in $\phi = \frac{\pi}{6}$, so that:

$$G_2(r,\phi) = G_1(r, \frac{\pi}{3} - \phi) \,. \tag{6.61}$$

Since $G(r,\phi)$ is the sum of $G_1(r,\phi)$ and $G_2(r,\phi)$ we thus get

$$\begin{aligned} G(r,\phi) &= \frac{2}{\pi} \int_0^\infty d\xi \, \cosh\theta\xi \left(\frac{\sinh\phi\xi + \sinh(\frac{\pi}{3} - \phi)\xi}{\sinh\frac{\pi\xi}{3}} \right) K_{i\xi}(r) \\ &= \frac{2}{\pi} \int_0^\infty d\xi \, \cosh\theta\xi \frac{\cosh(\phi - \frac{\pi}{6})\xi}{\cosh\frac{\pi\xi}{6}} K_{i\xi}(r), \end{aligned} \tag{6.62}$$

for $0 \le \phi \le \frac{\pi}{3}$, $r > 0$ and with θ as defined in (6.59). By introducing the integral representation [23, 8.432(4)]

$$K_{i\xi}(r) = \frac{1}{\cosh(\frac{\pi\xi}{2})} \int_0^\infty du \, \cos(r\sinh u) \cos\xi u, \tag{6.63}$$

and subsequently interchanging the order of integration, (6.62) becomes

$$G(r,\phi) = \frac{2}{\pi} \int_0^\infty du \, \cos(r\sinh u) \int_0^\infty d\xi \, \frac{\cosh\theta\xi}{\cosh\frac{\pi\xi}{2}} \frac{\cosh(\phi - \frac{\pi}{6})\xi}{\cosh\frac{\pi\xi}{6}} \cos\xi u \,. \tag{6.64}$$

One can easily check (for example by first using [23, 3.981(10)] then introducing $\overline{u} \equiv \sinh u$ as new variable of integration and finally using [23, 3.723(2)]) that the boundary conditions (6.49a) and (6.49b) are indeed fulfilled. In the Appendix to this chapter, we explicitly evaluate the expression (6.64) for $G(r,\phi)$. From this, retracing our steps, remembering that in general $\theta \in [\frac{\pi}{4}, \frac{\pi}{2}]$ (cf. (6.59)), and only considering $\phi \in [0, \frac{\pi}{6}]$ (which for reasons of symmetry can be done without loss of generality and corresponds to taking $0 \le q \le p$ in (6.35)) we find

$$\begin{aligned} \langle s_i s_i' s_j s_k' \rangle &= e^{-r\cos(\theta-\phi)} \\ &\quad + e^{-r\cos(\theta+\phi-\frac{\pi}{3})} I_{(\frac{\pi}{3},\frac{5\pi}{6})}(\theta+\phi) \\ &\quad - e^{-r\cos(\theta-\phi-\frac{\pi}{3})} I_{(\frac{\pi}{3},\frac{5\pi}{6})}(\theta-\phi) \\ &\quad + \frac{3}{\pi} \int_{-\infty}^\infty dv \, e^{-r\cosh v} \sum_{\mu=\phi\pm\theta} \frac{\cosh 3v \, \sin 3\mu}{\cosh 6v - \cos 6\mu}, \end{aligned} \tag{6.65}$$

where

$$r = \sqrt{\frac{2(1-\gamma)}{\gamma}}\sqrt{(j-i)^2+(k-i)^2+(k-j)^2}, \quad \gamma = \tanh 2\beta J, \tag{6.66a}$$

and

$$\phi = \arctan\left[\frac{(k-j)\sqrt{3}}{k+j-2i}\right] . \tag{6.66b}$$

The result is valid in the limit of low temperatures and large distances. Note that if θ is close enough to $\frac{\pi}{4}$ (its $T = 0$ value), then the third term in (6.65) is identically zero and can be dropped. One should compare (6.65) to the result we would have found when no interchain correlations had been present, namely

$$\langle s_i s_i' s_j s_k' \rangle = \langle s_i s_j \rangle \langle s_i' s_k' \rangle = z^{2p+q} = \exp(-2r\cos\theta\cos\phi) . \tag{6.67}$$

Once again the effect of correlations is clearly visible.

Finally let us remark that, since the result (6.65) can in general not be written as the sum of finitely many exponentials, as follows from the asymptotic expansion (6.A20) and the fact that only for $\phi = 0$ the terms of the sum on μ under the integral sign in (6.65) cancel, one concludes that $\mathcal{H}_2(s, s')$ must have long-range interactions.

6.6 The approach to equilibrium

Now that we have investigated the equilibrium properties of a dynamically correlated MC simulation, one may wonder how long it takes for the interchain equilibrium correlations to build up. To answer this question we return to equation (6.23). Then, introducing the "sweep-time" variable

$$\tau \equiv \frac{t}{N}, \tag{6.68}$$

we can in the limit $N \to \infty$ at fixed τ convert this equation into a differential equation in τ which, apart from an extra term $\frac{d}{d\tau}\langle s_{j_1} \ldots s_{j_m} s'_{k_1} \ldots s'_{k_n}\rangle(\tau)$ on the left-hand side, closely resembles (6.29). Here $\langle \ldots \rangle(\tau)$ denotes the still *time-dependent* average with respect to $P^{(2)}(s, s'; N\tau)$. For $\tau \to \infty$ equilibrium is attained, $\frac{d}{d\tau}\langle \ldots \rangle(\tau) \to 0$, and we retrieve equation (6.29). Let us suppose that at $\tau = 0$, the *individual* systems are already in equilibrium. By virtue of the MC procedure used this implies that then the individual systems will be in equilibrium for all $\tau \geq 0$, and thus that

$$\langle s_j s_k \rangle(\tau) = \langle s_j' s_k' \rangle(\tau) = z^{|j-k|}, \quad \text{for all } \tau \geq 0 . \tag{6.69}$$

Now if this $\tau = 0$ situation has been reached by previously applying independent MC simulations to the individual systems we have that

$$\langle u_j u_k \rangle(0) = \langle s_j s_k \rangle(0) \langle s_j' s_k' \rangle(0) = z^{2|j-k|} . \tag{6.70}$$

For $\tau > 0$ the quantity $\langle u_j u_k \rangle(\tau)$ will, because of the triangle symmetry, evolve as a single chain pair correlation function and tend to its equilibrium value $z^{|j-k|}$. Glauber [19] shows that the time scale τ_0 for this to happen is given by

$$\tau_0 \gg \frac{1}{1-\gamma} \,. \tag{6.71}$$

If we suppose, however, that also $\langle u_j u_k \rangle(0) = z^{|j-k|}$, which therefore then holds for all $\tau \geq 0$, we can easily go one step further and solve the equations of motion for $\langle u_i s_j s'_k \rangle(\tau)$ in the limit $1-\gamma \ll 1$, where we can again neglect the discrete structure of the underlying spatial lattice. The solution involves looking for the eigenmodes $\propto \exp(-\lambda\tau)$ of the time-dependent equations for $\langle u_i s_j s'_k \rangle(\tau)$. Here λ is a constant. Obviously, the $\lambda = 0$ eigenmode is just the equilibrium solution we found previously, whereas for other λ we must solve an equation of the form

$$\Delta f(x,y) = \frac{4(1-\gamma-\lambda/3)}{\gamma} f(x,y), \tag{6.72}$$

for $f(x,y)$ in the interior of the sector bounded by $y = x\sqrt{3}$ and $y = 0$, but now with *homogeneous boundary conditions.* This is not a difficult problem. Apart from the eigenmode at $\lambda = 0$ there exist eigenmodes only for $\lambda > 3(1-\gamma)$, and they are of the form:

$$F(r,\phi)e^{-\lambda\tau} = J_{3n}\left(\sqrt{\frac{4(\lambda/3-1+\gamma)}{\gamma}}\, r\right) \sin(3n\phi)\, e^{-\lambda\tau}, \quad n = 1,\ 2,\ \ldots, \tag{6.73}$$

where J_{3n} is a Bessel function of the first kind of order $3n$. Hence also in this case equilibrium is attained on the time scale (6.71).

6.7 Conclusion

We have studied two copies s and s' of a one-dimensional Ising chain subjected to a common thermal noise. The spin flip probabilities were chosen in such a way that the product spins $u_i = s_i s'_i$ played a role completely equivalent to s_i and s'_i. With this choice we could show that the combined system tends to an equilibrium state. The Hamiltonian $\mathcal{H}_2(s,s')$ governing this equilibrium is unknown. Nevertheless, we were able to solve for the interchain equilibrium correlation function $\langle u_i s_j s'_k \rangle$. We showed that the decay in space of this quantity consists of a sum of two or three exponentials, depending on the temperature, *plus* an integral on a continuum of decay lengths. Therefore we concluded that $\mathcal{H}_2(s,s')$ is not of strictly finite range. The approach to equilibrium was also discussed.

Appendix

In this appendix we shall evaluate the expression (6.64) for $G(r,\phi)$. We begin by rewriting it in the form

$$G(r,\phi) = \sum_{\mu=\phi-\frac{\pi}{6}\pm\theta} \mathcal{I}(\mu;r), \tag{6.A1}$$

where

$$\mathcal{I}(\mu;r) \equiv \frac{1}{\pi}\sum_{\sigma=\pm1}\int_{-\infty}^{\infty} du \cos(r\sinh u)\int_0^{\infty} d\xi \frac{e^{-(\frac{2\pi}{3}+\sigma\mu+iu)\xi}}{(1+e^{-\pi\xi})(1+e^{-\pi\xi/3})} \tag{6.A2}$$

and shall now concentrate on evaluating $\mathcal{I}(\mu;r)$ for real μ. To this end we expand the denominator of the integrand, using that $[(1+e^{-\pi\xi})(1+e^{-\pi\xi/3})]^{-1} = \sum_{m,n=0}^{\infty}(-1)^{m+n}e^{-(m\pi+n\pi/3)\xi}$ for $\xi>0$, after which we can calculate the inner integral in (6.A2) with the result

$$\begin{aligned}\mathcal{I}(\mu;r) &= \frac{1}{\pi}\lim_{\epsilon\downarrow 0}\sum_{\sigma=\pm1}\sum_{m,n=0}^{\infty}(-1)^{m+n}\int_{-\infty}^{\infty} du\ \cos(r\sinh u)\frac{e^{-(\beta_{mn}^{\sigma\mu}+iu)\epsilon}}{\beta_{mn}^{\sigma\mu}+iu}\\ &= \frac{1}{2\pi}\lim_{\epsilon\downarrow 0}\sum_{\sigma=\pm1}\sum_{m,n=0}^{\infty}(-1)^{m+n}\int_{-\infty}^{\infty} du\, e^{ir\sinh u}\left[\frac{e^{-(\beta_{mn}^{\sigma\mu}+iu)\epsilon}}{\beta_{mn}^{\sigma\mu}+iu}+\frac{e^{-(\beta_{mn}^{\sigma\mu}-iu)\epsilon}}{\beta_{mn}^{\sigma\mu}-iu}\right].\end{aligned} \tag{6.A3}$$

Here we introduced the abbreviation

$$\beta_{mn}^{\sigma\mu} \equiv \frac{2\pi}{3}+\sigma\mu+m\pi+\frac{n\pi}{3}. \tag{6.A4}$$

Note that $\beta_{mn}^{\sigma\mu}>0$ since $|\mu|$ must be smaller than $\frac{2\pi}{3}$ for the inner integral in (6.A2) to converge and since $m,n\geq 0$. Furthermore it should be noted that $\lim_{\epsilon\downarrow 0}$ and $\sum_{m,n=0}^{\infty}$ do not commute! Shifting the integration contour to run parallel to the real axis from $-\infty+\frac{\pi}{2}i$ to $\infty+\frac{\pi}{2}i$, and subsequently introducing a new variable of integration $v\equiv u-\frac{\pi}{2}i$, leads to the expression

$$\begin{aligned}\mathcal{I}(\mu;r) &= \sum_{\sigma=\pm1}\sum_{m,n=0}^{\infty}(-1)^{m+n}e^{-r\sin\beta_{mn}^{\sigma\mu}}I_{(0,\frac{\pi}{2})}(\beta_{mn}^{\sigma\mu})\\ &+\frac{1}{2\pi}\lim_{\epsilon\downarrow 0}\sum_{\sigma=\pm1}\sum_{m,n=0}^{\infty}(-1)^{m+n}\int_{-\infty}^{\infty} dv\, e^{-r\cosh v}\left[\frac{e^{-(\beta_{mn}^{\sigma\mu}-\frac{\pi}{2}+iv)\epsilon}}{\beta_{mn}^{\sigma\mu}-\frac{\pi}{2}+iv}+\frac{e^{-(\beta_{mn}^{\sigma\mu}+\frac{\pi}{2}-iv)\epsilon}}{\beta_{mn}^{\sigma\mu}+\frac{\pi}{2}-iv}\right],\end{aligned} \tag{6.A5}$$

where $I_{(a,b)}$ denotes the indicator of the interval (a,b):

$$I_{(a,b)}(x) \equiv \begin{cases} 1 & \text{for } x \in (a,b) \\ 0 & \text{otherwise .} \end{cases} \tag{6.A6}$$

For $\mu = \pm\frac{\pi}{6}, \pm\frac{\pi}{2}$ there is a pole on the shifted integration contour and one has to use some kind of a limiting procedure to evaluate $\mathcal{I}(\mu;r)$, and give a proper meaning to (6.A5). However, for the moment being let's not worry about this and continue with evaluating $\mathcal{I}(\mu;r)$ for all other (real) μ-values for which (6.A2) converges. Afterwards, then, we shall return to the four special cases mentioned above. Now, using the equality $\beta^{\sigma\mu}_{mn} + \frac{\pi}{2} = \beta^{\sigma\mu}_{(m+1)n} - \frac{\pi}{2}$, writing $\overline{m}$ for $m+1$, and shifting the variable of integration $v \to -v$ it is straightforward to derive that

$$\begin{aligned} &\sum_{m,n=0}^{\infty} (-1)^{m+n} \int_{-\infty}^{\infty} dv\, e^{-r\cosh v} \frac{e^{-(\beta^{\sigma\mu}_{mn}+\frac{\pi}{2}-iv)\epsilon}}{\beta^{\sigma\mu}_{mn} + \frac{\pi}{2} - iv} \\ &\quad = -\sum_{\overline{m}=1}^{\infty} \sum_{n=0}^{\infty} (-1)^{\overline{m}+n} \int_{-\infty}^{\infty} dv\, e^{-r\cosh v} \frac{e^{-(\beta^{\sigma\mu}_{\overline{m}n}-\frac{\pi}{2}+iv)\epsilon}}{\beta^{\sigma\mu}_{\overline{m}n} - \frac{\pi}{2} + iv} . \end{aligned} \tag{6.A7}$$

Therefore (6.A5) reduces to

$$\begin{aligned} \mathcal{I}(\mu;r) &= \sum_{\sigma=\pm1} \sum_{m,n=0}^{\infty} (-1)^{m+n} e^{-r\sin\beta^{\sigma\mu}_{mn}} I_{(0,\frac{\pi}{2})}(\beta^{\sigma\mu}_{mn}) \\ &\quad + \frac{1}{2\pi} \lim_{\epsilon\downarrow 0} \sum_{\sigma=\pm1} \sum_{n=0}^{\infty} (-1)^n \int_{-\infty}^{\infty} dv\, e^{-r\cosh v} \frac{e^{-(\frac{\pi}{6}+\sigma\mu+\frac{n\pi}{3}+iv)\epsilon}}{\frac{\pi}{6} + \sigma\mu + \frac{n\pi}{3} + iv} . \end{aligned} \tag{6.A8}$$

Let us introduce the abbreviation

$$\mathcal{F}(\mu;r) \equiv \frac{1}{2\pi} \lim_{\epsilon\downarrow 0} \sum_{\sigma=\pm1} \sum_{n=0}^{\infty} (-1)^n \int_{-\infty}^{\infty} dv\, e^{-r\cosh v} \frac{e^{-(\frac{\pi}{6}+\sigma\mu+\frac{n\pi}{3}+iv)\epsilon}}{\frac{\pi}{6} + \sigma\mu + \frac{n\pi}{3} + iv} \tag{6.A9}$$

for the part of $\mathcal{I}(\mu;r)$ still to be evaluated. For the actual evaluation we first consider the case where $|\mu| < \frac{\pi}{6}$. Then, namely, $\alpha^{\sigma\mu}_n \equiv \frac{\pi}{6} + \sigma\mu + \frac{n\pi}{3} > 0$ for all σ and $n \geq 0$, so that

$$\frac{\exp[-(\alpha^{\sigma\mu}_n + iv)\epsilon]}{\alpha^{\sigma\mu}_n + iv} = \int_{\epsilon}^{\infty} dw\, \exp[-(\alpha^{\sigma\mu}_n + iv)w] . \tag{6.A10}$$

This equality now allows us to evaluate the sums on n and σ in (6.A9) and subsequently to take the limit $\epsilon \downarrow 0$. We find

$$\begin{aligned} \mathcal{F}(\mu;r) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dv\, e^{-r\cosh v} \int_{0}^{\infty} dw\, \frac{\cosh \mu w}{\cosh \frac{\pi w}{6}} \cos vw \\ &= \frac{3}{\pi} \cos 3\mu \int_{-\infty}^{\infty} dv\, e^{-r\cosh v} \frac{\cosh 3v}{\cosh 6v + \cos 6\mu}, \end{aligned} \tag{6.A11}$$

where, to establish the last equality, we used [23, 3.981(10)]. Having done this calculation for a restricted range of μ-values, we now remark that starting from the definition of $\mathcal{F}(\mu;r)$ one easily shows that for general μ

$$\mathcal{F}(\mu+\frac{\pi}{3};r) = -\mathcal{F}(\mu;r)\ . \tag{6.A12}$$

But then, defining

$$\tilde{\mu} \equiv \mu - m_\mu\frac{\pi}{3}, \tag{6.A13}$$

where m_μ is an integer chosen such that $\tilde{\mu} \in (-\frac{\pi}{6},\frac{\pi}{6})$, which is possible for $\mu \neq \pm\frac{\pi}{6},\pm\frac{\pi}{2}$, we immediately find that for this larger class of μ-values

$$\begin{aligned}\mathcal{F}(\mu;r) &= (-1)^{m_\mu}\mathcal{F}(\tilde{\mu};r)\\ &= (-1)^{m_\mu}\frac{3}{\pi}\cos 3\tilde{\mu}\int_{-\infty}^{\infty} dv\, e^{-r\cosh v}\frac{\cosh 3v}{\cosh 6v+\cos 6\tilde{\mu}}\\ &= \frac{3}{\pi}\cos 3\mu\int_{-\infty}^{\infty} dv\, e^{-r\cosh v}\frac{\cosh 3v}{\cosh 6v+\cos 6\mu}\ .\end{aligned} \tag{6.A14}$$

Therefore expression (6.A11) still holds for this more general class, and for these values of μ

$$\begin{aligned}\mathcal{I}(\mu;r) &= \sum_{\sigma=\pm1}\sum_{m,n=0}^{\infty}(-1)^{m+n}e^{-r\sin\beta_{mn}^{\sigma\mu}}I_{(0,\frac{\pi}{2})}(\beta_{mn}^{\sigma\mu})\\ &\quad+\frac{3}{\pi}\cos 3\mu\int_{-\infty}^{\infty} dv\, e^{-r\cosh v}\frac{\cosh 3v}{\cosh 6v+\cos 6\mu}\\ &= \sum_{\sigma=\pm1}\sum_{n=0}^{1}(-1)^n e^{-r\sin(\frac{2\pi}{3}+\sigma\mu+\frac{n\pi}{3})}I_{(0,\frac{\pi}{2})}(\frac{2\pi}{3}+\sigma\mu+\frac{n\pi}{3})\\ &\quad+\frac{3}{\pi}\cos 3\mu\int_{-\infty}^{\infty} dv\, e^{-r\cosh v}\frac{\cosh 3v}{\cosh 6v+\cos 6\mu}\ .\end{aligned} \tag{6.A15}$$

Note that we have used that for $m=0, n\geq 2$ and for $m\geq 1, n\geq 0$, one has $\beta_{mn}^{\sigma\mu} > \frac{\pi}{2}$ so that then $I_{(0,\frac{\pi}{2})}(\beta_{mn}^{\sigma\mu}) = 0$. Let us now return to the special values $\mu = \pm\frac{\pi}{6},\pm\frac{\pi}{2}$. Because of continuity one would expect to find $\mathcal{I}(\mu;r)$ for these values by taking the limits $\mu \to \pm\frac{\pi}{6},\pm\frac{\pi}{2}$, respectively, in (6.A15). That this is indeed the case will now be shown: First we turn to equation (6.A14). By introducing the combination $\sinh 3v/|\cos 3\mu|$ as a new variable of integration and subsequently letting $\cos 3\mu$ go to zero one finds

$$\mathcal{F}(\mu;r) \to \begin{cases} +\frac{1}{2}e^{-r} & \text{for}\quad \cos 3\mu \downarrow 0\\ -\frac{1}{2}e^{-r} & \text{for}\quad \cos 3\mu \uparrow 0\ .\end{cases} \tag{6.A16}$$

Although this implies that the limits $\lim_{\mu \to \pm\frac{\pi}{6}, \pm\frac{\pi}{2}} \mathcal{F}(\mu; r)$ are not well-defined, one may check that this is not the case for $\lim_{\mu \to \pm\frac{\pi}{6}, \pm\frac{\pi}{2}} \mathcal{I}(\mu; r)$, the reason being that for each of these four μ-values there is another term in (6.A15) with a discontinuity just compensating the discontinuity in $\mathcal{F}(\mu; r)$ indicated in (6.A16). In fact, we have

$$\lim_{\mu \to \pm\frac{\pi}{6}} \mathcal{I}(\mu; r) = \frac{1}{2} e^{-r}, \tag{6.A17}$$

$$\lim_{\mu \to \pm\frac{\pi}{2}} \mathcal{I}(\mu; r) = e^{-r/2} - \frac{1}{2} e^{-r}. \tag{6.A18}$$

On the other hand, however, one can, for these four μ-values, also evaluate $\mathcal{I}(\mu; r)$ directly from (6.A2) (for example by first performing the sum on σ, using [23, 3.981(3)] to evaluate the inner integral and then, after introducing a new variable of integration $\overline{u} \equiv \sinh u$, performing a standard contour integration) thereby finding the same result, so that indeed

$$\mathcal{I}(\pm\frac{\pi}{6}; r) = \lim_{\mu \to \pm\frac{\pi}{6}} \mathcal{I}(\mu; r) \quad \text{and} \quad \mathcal{I}(\pm\frac{\pi}{2}; r) = \lim_{\mu \to \pm\frac{\pi}{2}} \mathcal{I}(\mu; r) . \tag{6.A19}$$

In this sense we have thus proven (6.A15) to be valid for all real μ with $|\mu| < \frac{2\pi}{3}$. Combining (6.A15) with (6.A1) we have found an explicit expression for $G(r, \phi)$.

Finally we remark that for $\mu \neq \pm\frac{\pi}{6}, \pm\frac{\pi}{2}$ it is not possible to evaluate the integral in equation (6.A14) for $\mathcal{F}(\mu; r)$ explicitly so as to obtain a closed expression for all r. Fortunately the second best thing one can do, that is, to make an asymptotic expansion, turns out to be fairly easy. Concretely, starting from (6.A14), extracting a factor e^{-r}, writing $v = \frac{\kappa}{\sqrt{r}}$, subsequently expanding the integrand in powers of $\frac{1}{r}$ and performing the integrals on κ one finds

$$\mathcal{F}(\mu; r) = \frac{3e^{-r}}{\sqrt{2\pi r} \cos 3\mu} \left[1 + \mathcal{O}\left(\frac{1}{r}\right) \right], \quad r \to \infty . \tag{6.A20}$$

References

[1] B. Derrida and G. Weisbuch, Europhys. Lett. **4** (1987) 657.

[2] H.E. Stanley, D. Stauffer, J. Kertész, and H.J. Herrmann, Phys. Rev. Lett. **59** (1987) 2326.

[3] M.N. Barber and B. Derrida, J. Stat. Phys. **51** (1988) 877.

[4] U.M.S. Costa, J. Phys. A **20** (1987) L583.

[5] A.U. Neumann and B. Derrida, J. Phys. (Paris) **49** (1988) 1647.

[6] A.M. Mariz, H.J. Herrmann, and L. de Arcangelis, J. Stat. Phys. **59** (1990) 1043.

[7] A.M. Mariz and H.J. Herrmann, J. Phys. A **22** (1989) L1081.

[8] G. Le Caër, J. Phys. A **22** (1989) L647.

[9] H.R. da Cruz, U.M.S. Costa, and E.M.F. Curado, J. Phys. A **22** (1989) L651.

[10] L. de Arcangelis, A. Coniglio, and H.J. Herrmann, Europhys. Lett. **9** (1989) 749.

[11] L. de Arcangelis, H.J. Herrmann, and A. Coniglio, J. Phys. A **22** (1989) 4659.

[12] O. Golinelli and B. Derrida, J. Phys. A **22** (1989) L939.

[13] B. Derrida in: *Fundamental Problems in Statistical Mechanics VII*, Proceedings of the 1989 Altenberg Summerschool, ed. H. van Beijeren, (North-Holland, 1990).

[14] J.L. Lebowitz, 1987, unpublished.

[15] A. Coniglio, L. de Arcangelis, H.J. Herrmann, and N. Jan, Europhys. Lett. **8** (1989) 315.

[16] O. Golinelli, Ph.D.-thesis Université Paris VI, 1990.

[17] M.E. Fisher, J. Stat. Phys. **34** (1984) 667.

[18] M.E. Fisher and M.P. Gelfand, J. Stat. Phys. **53** (1988) 175.

[19] R.J. Glauber, J. Math. Phys. **4** (1963) 294.

[20] D.R. Cox and H.D. Miller, *The theory of stochastic processes* (Methuen & Co Ltd, London, 1965).

[21] R.V. Churchill, *Fourier series and boundary value problems* (McGraw-Hill, New York, 1941).

[22] M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).

[23] I.S. Gradshteyn and I.M. Ryzhik, *Table of integrals, series and products* (Academic Press, London, 1980).

[7] [illegible] and H.J. Herrmann, J. Phys. A [illegible]

[8] [illegible], J. Phys. A [illegible]

[9] [illegible], J. Phys. A [illegible]

[10] L. de Arcangelis, A. Coniglio, and H.J. Herrmann, Europhys. Lett. 9 (1989) 749.

[11] L. de Arcangelis, H.J. Herrmann, and A. Coniglio, J. Phys. A 22 (1989) [illegible].

[12] [illegible] and [illegible], J. Phys. A [illegible] (1990).

[13] B. Derrida, in: Fundamental Problems in Statistical Mechanics VII, Proceedings of the 1989 Altenberg Summer School, ed. H. van Beijeren, North Holland, 1990.

[14] [illegible], 1987, unpublished.

[15] A. Coniglio, L. de Arcangelis, H.J. Herrmann, and N. Jan, Europhys. Lett. 8 (1989)(3) [illegible].

[16] [illegible], Ph.D. thesis, Université Paris [illegible], 1990.

[17] [illegible]

[18] [illegible] and M.H. [illegible], J. Stat. Phys. [illegible]

[19] [illegible], J. Math. Phys. [illegible]

[20] [illegible]

[21] R.V. Churchill, Fourier series and boundary value problems, McGraw-Hill, New York, [illegible].

[22] M. Abramowitz and I.A. Stegun, Handbook of Mathematical Functions, Dover, New York, [illegible].

[23] I.S. Gradshteyn and I.M. Ryzhik, Table of Integrals, Series and Products, Academic Press, London, 1980.

Samenvatting

Dit proefschrift gaat over stochastische wandelingen en hun toepassingen. Een stochastische wandeling, ook wel bekend onder de naam "dronkemanswandeling", is een stapproces waarbij de individuele stappen (in het eenvoudigste geval) onafhankelijke en identiek verdeelde stochastische variabelen zijn, met een gegeven waarschijnlijkheidsverdeling. Sinds het begin van deze eeuw worden en zijn de eigenschappen van zo'n stochastische wandeling uitvoerig bestudeerd. Niet alleen gebeurt dit uit interesse voor de wandeling en haar eigenschappen zelf, maar ook omdat zij soms als hulpmiddel gebruikt wordt bij de beschrijving van andere tijdafhankelijke systemen. Hierbij valt bijvoorbeeld te denken aan een systeem met vele vrijheidsgraden. Zo'n systeem kan namelijk vaak in goede benadering beschreven worden in termen van enkele collectieve vrijheidsgraden, die dan een stochastische wandeling door hun waardenbereik uitvoeren. Beide aspecten, de bestudering van de eigenschappen van de stochastische wandeling op zich, alsook het gebruik van een stochastische wandeling als "input" bij een ander proces, komen in dit proefschrift aan de orde.

In het eerste deel van het proefschrift wordt de diffusie van een gemarkeerd deeltje in een roostergas bestudeerd. Het probleem waar het om gaat kan als volgt worden omschreven. Men begint met een oneindig rooster of een eindig rooster met periodieke randvoorwaarden in dimensie d en zet deeltjes op de roosterpunten. Niet alle roosterpunten worden bezet. De onbezette plaatsen heten de *gaten*. De gaten voeren via deeltje-gat uitwisselingsprocessen zogenaamde "eenvoudige stochastische wandelingen" uit, waarbij op regelmatige tijdstippen alleen naar naaste-buur plaatsen gestapt wordt en wel zonder enige richtingsvoorkeur. Alleen situaties waarbij de gatendichtheid zo laag is dat de gaten met een verwaarloosbare fout *onafhankelijke* wandelingen over het rooster uitvoeren, zullen worden beschouwd. Vervolgens kiest men aselect één van de deeltjes op het rooster uit en markeert het. De vraag waar nu alles om draait is de beweging van dit deeltje te beschrijven. Het is duidelijk dat dit probleem twee opmerkelijke aspecten kent. Ten eerste is er een *waarschijnlijkheidsverdeling voor de wachttijd* tussen twee opeenvolgende stappen van het gemarkeerde deeltje. Dit komt doordat het gemarkeerde deeltje alleen kan stappen als er zich een gat op een naaste-buur plaats van dit deeltje bevindt. Ten tweede is de beweging van het gemarkeerde deeltje sterk geanticorreleerd: net nadat dit deeltje en een gat van plaats zijn verwisseld zijn ze nog steeds naaste buren, maar nu in omgekeerde richting. Derhalve is er dan een aanzienlijke kans dat het gemarkeerde deeltje bij zijn volgende stap naar zijn vorige positie terug zal stappen. Het samenspel van juist deze twee effecten maakt de beweging van het gemarkeerde deeltje interessant.

In hoofdstuk 2 wordt gekeken naar de interactie tussen het gemarkeerde deeltje en *slechts één gat.* Op een eindig rooster vindt men dat de waarschijnlijkheidsverdeling voor de verplaatsing van het gemarkeerde deeltje voor grote tijden Gaussisch is. De beweging van het gemarkeerde deeltje is dan diffusief. Op het oneindige rooster blijkt dit niet meer het geval te zijn, zelfs niet voor grote tijden en afstanden. De verdeling blijft niet-Gaussisch. De oorzaak ligt in het feit dat de wachttijdsverdeling tussen twee opeenvolgende stappen van het gemarkeerde deeltje op het oneindige rooster een lange-tijdstaart kent, waardoor de *gemiddelde wachttijd* tussen twee opeenvolgende stappen oneindig is. De vorm die de waarschijnlijkheidsverdeling voor de verplaatsing voor grote tijden dan wel aanneemt wordt in hoofdstuk 2 berekend. Ook het geval van een strook met oneindige lengte en eindige breedte, waarvoor de gemiddelde wachttijd tussen twee opeenvolgende stappen eveneens oneindig is, wordt daar bekeken.

Hoofdstuk 3 bestudeert wat er gebeurt als men in het oneindige tweedimensionale systeem een kleine, maar *eindige gatendichtheid* introduceert. Er blijkt dan een "crossover" te zijn van het in hoofdstuk 2 beschreven gedrag, dat nu gevonden wordt voor tijden waarop het gemarkeerde deeltje met slechts één gat in wisselwerking is geweest, naar een diffusief gedrag, dat men vindt voor voldoend grote tijden en afstanden, als het gemarkeerde deeltje vele gaten heeft gezien. De overgang tussen deze twee gebieden wordt in dit hoofdstuk volledig beschreven. Bij de bestudering van de strook met een kleine, eindige gatendichtheid wordt een analoge crossover gevonden.

Hoofdstuk 4 houdt zich bezig met het berekenen van het gemiddelde aantal verschillende roosterplaatsen dat het gemarkeerde deeltje na een gegeven tijd bezocht heeft. Alleen het drie- en hogerdimensionale geval met een kleine, eindige gatendichtheid wordt bekeken. De moeilijkheid hier ligt hem erin de anticorrelatie van de beweging van het gemarkeerde deeltje op de juiste manier in de berekening mee te nemen. Voor lage dichtheden en grote tijden wordt een exact resultaat gevonden voor het gemiddelde aantal roosterplaatsen dat dan door dit deeltje bezocht is.

Het tweede probleem dat in dit proefschrift bestudeerd wordt is hoe een eenvoudige stochastische wandeling een eindig d-dimensionaal hypercubisch rooster met periodieke randen bedekt. Dit gebeurt in hoofdstuk 5. De door de wandeling bezochte roosterplaatsen worden gekleurd teneinde ze van de andere roosterpunten te onderscheiden. Er wordt gekeken welk punt van het rooster als laatste gekleurd wordt. In dimensie $d = 1$ blijkt het mogelijk te zijn de kansverdeling van dit punt over het rooster voor willekeurige roostergrootte exact te berekenen; in hogere dimensies worden resultaten voor grote roostergrootte afgeleid. Ook wordt in de verschillende dimensies gekeken naar de vraag hoeveel stappen de stochastische wandeling gemiddeld nodig heeft om het rooster volledig te bedekken. Verder wordt bestudeerd hoe de verzameling nog niet bezochte roosterpunten er na een groot aantal stappen van de stochastische wandeling uit ziet. Hier blijkt vooral het tweedimensionale geval interessant te zijn; de genoemde verzameling heeft dan namelijk fractale kenmerken.

Tenslotte wordt in hoofdstuk 6 een derde probleem onderzocht. Er wordt daar bestudeerd wat er gebeurt als men correlaties aanbrengt in de tijdevoluties van twee verschillende copieën van een één-dimensionale Ising keten, die ieder op zich naar een voorgeschreven evenwicht gaan. De beantwoording van dit probleem wordt aangepakt door te trachten evenwichtscorrelatiefuncties van spins in keten "1" met spins in keten "2" te berekenen. Dit is in het algemeen niet mogelijk, doordat de Hamiltoniaan die het evenwicht van het gecombineerde systeem beschrijft niet bekend is. In het bijzonder is deze Hamiltoniaan, door het aanbrengen van de correlaties in de tijdevoluties van de afzonderlijke ketens, niet langer de som van de Hamiltonianen van de individuele ketens, zoals dat voor twee ongekoppelde ketens het geval is. Toch blijkt er een speciale, niet triviale keuze van de "dynamische correlaties" tussen de twee ketens mogelijk te zijn, waarbij eerder genoemde evenwichtscorrelatiefuncties berekend kunnen worden. In hoofdstuk 6 wordt voor dit speciale geval een evenwichtscorrelatiefunctie van twee spins in de ene met twee spins in de andere keten berekend, hetgeen neerkomt op het oplossen van een stelsel vergelijkingen behorende bij een speciale stochastische wandeling op een tweedimensionaal rooster. Ook de gang naar evenwicht wordt hier besproken.

Curriculum vitae

Ik werd geboren op 29 oktober 1962 te Borne. Na in 1981 aan het Twickel College te Hengelo (Ov.) het eindexamen Atheneum te hebben behaald, begon ik aan de studie Scheikunde aan de Rijksuniversiteit Groningen. Na een jaar zwaaide ik om naar de studie Natuurkunde aan dezelfde universiteit. In april 1985 legde ik (cum laude) het kandidaatsexamen N1, Natuurkunde en Wiskunde, af. Als experimentele stage deed ik onder leiding van dr. R.J. de Meijer aan het Kernfysisch Versneller Instituut (KVI) onderzoek naar de gevolgen van het reactorongeluk te Tsjernobyl voor Nederland. Mijn theoretische afstudeerscriptie behelsde een onderzoek naar de beschrijving van eindige kernen met behulp van relativistische veldentheorieën. Dit onderzoek werd eveneens gedaan aan het KVI, onder leiding van dr. A.E.L. Dieperink. Het doctoraalexamen Natuurkunde met bijvak Hoofdstukken uit de Wiskunde werd (cum laude) in augustus 1987 afgelegd. Per 1 september 1987 trad ik in dienst van de Rijksuniversiteit te Leiden om bij prof. dr. H.J. Hilhorst aan een promotieonderzoek te beginnen. Het resultaat daarvan ligt nu voor u.

Tijdens mijn promotieperiode bezocht ik verscheidene congressen. Het betrof hier het "Special Seminar on Fractals", dat in 1988 te Erice, Sicilië gehouden werd, de "International Conference on Thermodynamics and Statistical Mechanics, Statphys 17" die in 1989 te Rio de Janeiro, Brazilië plaatsvond, alsmede drie bezoeken aan de jaarlijks gehouden "Rencontre de Physique Statistique" te Parijs, in de jaren 1989, 1990 en 1991. Tevens nam ik deel aan de "1989 International Summer School on Fundamental Problems in Statistical Mechanics VII" te Altenberg, West-Duitsland en aan de "Ecole de physique de la matière condensée: Systèmes et matériaux désordonnés" te Beg-Rohu, Quiberon, Frankrijk. Tenslotte bracht ik verscheidene werkbezoeken aan het "Laboratoire de Physique Théorique et Hautes Energies" van de Université de Paris-Sud te Orsay, die met steun van de Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO) mogelijk werden gemaakt.

List of publications

1. M.J.A.M. Brummelhuis and H.J. Hilhorst, *Single-vacancy induced motion of a tracer particle in a two-dimensional lattice gas*, J. Stat. Phys. **53** (1988) 249.

2. M.J.A.M. Brummelhuis and H.J. Hilhorst, *Tracer particle motion in a two-dimensional lattice gas with low vacancy density*, Physica A **156** (1989) 575.

3. M.J.A.M. Brummelhuis and H.J. Hilhorst, *Correlations between two Ising chains subjected to a common thermal noise*, Physica A **166** (1990) 75.

4. M.J.A.M. Brummelhuis and H.J. Hilhorst, *The number of distinct sites visited by a tracer particle*, J. Phys. A **23** (1990) L827.

5. R.J. de Meijer, F.J. Aldenkamp, M.J.A.M. Brummelhuis, J.F.W. Jansen, and L.W. Put, *Radionuclide concentrations in the northern part of the Netherlands after the Chernobyl reactor accident*, Health Physics **58** (1990) 441.

6. M.J.A.M. Brummelhuis and H. Kuijf, *Enumeration of externally labelled trees*, J. Phys. A, in press.

7. M.J.A.M. Brummelhuis and H.J. Hilhorst, *Covering of a finite lattice by a random walk*, Physica A, submitted.

Publications 1 – 4 and 7 formed the basis for the different chapters of this thesis.

Stellingen

1. Beschouw een stochastische wandeling op een ééndimensionaal rooster, waarbij alleen naar naaste-buur plaatsen gestapt kan worden. Zij ϵ de kans om bij een stap terug te gaan naar de voorgaande positie, $c\epsilon$ de kans dat de wandeling afgelopen is en bijgevolg $1-(1+c)\epsilon$ de kans op een stap in dezelfde richting als de vorige. Laat verder de eerste stap met kans één naar één van de buurplaatsen van de beginpositie zijn. Dan kan worden afgeleid dat het gemiddelde aantal keren $N_c(\epsilon)$ dat de wandelaar op zijn beginpositie is voordat de wandeling beëindigd wordt voldoet aan:

$$\lim_{\epsilon \downarrow 0} N_c(\epsilon) = \frac{1}{2} + \frac{1}{2}\sqrt{\frac{c+2}{c}} > 1 = N_c(0) \; .$$

   Door $c = 2(d-1)$ te nemen kan dit resultaat direct worden toegepast op het d-dimensionale "Forward Stepping" model op een hyperkubisch rooster.

2. Bij de door Kehr en Argyrakis gedane simulaties aan het driedimensionale "Forward Stepping" model wordt voor de beschouwde tijden onvoldoende rekening gehouden met de eindigheid van het door hen gebruikte periodieke rooster. Hierdoor wordt het gemiddelde aantal verschillende plaatsen dat de wandeling op het oneindige rooster in de gegeven tijd zou aandoen significant onderschat. De correctie kan worden berekend – is een functie van de fractie reeds bezochte roosterplaatsen – en bedraagt voor de beschouwde tijden zo'n 2%.

   K.W. Kehr en P. Argyrakis, J. Chem. Phys. 84 *(1986) 5816.*

3. Hoe vervelend het gebruik van periodieke randvoorwaarden kan zijn, wordt goed duidelijk bij het beluisteren van Erik Satie's muziekstuk Vexations.

   DECCA NL 425 221-2 (Alan Marks, piano).

4. Gegeven is een eenvoudige stochastische wandeling op de eenheidskubus, beginnend in $(0,0,0)$. Zij $L(\vec{x})$ de kans dat hoekpunt $\vec{x}$ bij het bedekkingsproces, zoals beschreven in hoofdstuk 5 van dit proefschrift, als laatste wordt bezocht. Dan is per definitie $L(0,0,0)=0$, terwijl

$$L(1,0,0) = L(0,1,0) = L(0,0,1) = \frac{1}{7}\left[1 - \frac{922}{9405}\right] = 0,1288\ldots$$
$$L(1,1,0) = L(1,0,1) = L(0,1,1) = \frac{1}{7}\left[1 + \frac{492}{9405}\right] = 0,1503\ldots$$
$$L(1,1,1) = \frac{1}{7}\left[1 + \frac{1290}{9405}\right] = 0,1624\ldots \; .$$

5. In tegenstelling tot wat Reichl beweert, is de thermodynamische gelijkheid

$$dU = TdS + YdX + \sum_i \mu_i dN_i$$

ook geldig voor niet-reversibele processen.

L.E. Reichl, A Modern Course in Statistical Physics (University of Texas Press, 1980).

6. Bij de behandeling van de klassieke mechanica zou een uitstapje naar een pretpark als Efteling tot de verplichte nummers moeten behoren.

7. Zij $D_n^{(m)}$ het aantal verschillende Feynman boomdiagrammen met n externe genummerde lijnen dat bestaat in een theorie met één soort deeltjes met zelfinteractie, als de interactie via 3-, 4-, ..., m-punts vertices kan plaatsvinden en als ervan uitgegaan wordt dat het verwisselen van externe lijnen deel uitmakend van dezelfde vertex geen nieuw diagram oplevert. Dan geldt voor grote n:

$$\frac{D_n^{(m)}}{nD_{n-1}^{(m)}} \simeq \Xi^{(m)} \left[1 - \frac{5}{2n}\right] .$$

Hierin is de groeifactor $\Xi^{(m)}$ monotoon stijgend met m en begrensd. In het bijzonder is:

$$\begin{aligned} \Xi^{(3)} &= 2, \\ \Xi^{(4)} &= \frac{3}{11}(4 + 3\sqrt{3}) = 2,508\ldots, \\ \Xi^{(\infty)} &= [2\ln 2 - 1]^{-1} = 2,588\ldots . \end{aligned}$$

M.J.A.M. Brummelhuis en H. Kuijf, te verschijnen in J. Phys. A.

8. Voor $J_0 \in [-1, 1]$ en $L \geq 1$ geldt:

$$\int_{-J_0}^{1} dJ_1 \int_{-J_1}^{1} dJ_2 \ldots \int_{-J_{L-1}}^{1} dJ_L = \left(\frac{4}{\pi}\right)^{L+1} \sum_{k=-\infty}^{\infty} (-1)^k \frac{\sin[kJ_0\pi + \pi(J_0 + 1)/4]}{(4k + 1)^{L+1}}$$

9. Eu's reactie op Banach's artikel is diep bedroevend.

B.C. Eu, Physica A **171** *(1991) 313,*
Z. Banach, Physica A **159** *(1989) 343.*

10. De psychologische afstand tussen de Randstad en Noord Nederland is aanzienlijk groter dan de geografische.

M.J.A.M. Brummelhuis, april 1991.