S4.A.1. One Dimensional Lattice

If the length a of each step is fixed, the path of a random walker forms a lattice of spacing a. Some aspects of the problem was already discussed in §4.E.4.

Many interesting results of the random walk problem are obtained by computer simulations. For a *d*-D lattice with N points in each dimension, recording the time development of any function defined on the lattice requires one to deal with an array of N^d elements. For example, the data shown in Fig.4.4 was obtained for $N = 120$. Those who have used the accompanying *Mathematica* code to generate the results should also notice that the walker often wander off range so that the result must be discarded. Now, the 3-D version of the code must deal with an array of $120^3 \approx 10^6$ elements, which, by itself, may already put a strain on the computer resources. Yet the results will be unsatisfactory owing to the missing scenarios.

Since the change in each time step is spatially localized, the data array is effectively a sparse matrix for which numerous techniques exist to minimize the actual data storage. Here, we shall discuss a technique that is valid even for dense matrices, namely, the imposing of the periodic boundary condition so that the walker never wanders off range. An additional benefit of doing so is that the problem can now be analyzed using Fourier series.

Fig.4.6.

Fig.4.6. shows a 1-D lattice with $2N+1$ sites. Imposing the periodic boundary condition means that

$$g\left[l + k(2N+1)\right] = g(l) \qquad \forall\, k = 0, \pm 1, \ldots \quad \& \quad l = -N, \ldots, N \tag{4.82a}$$

for all functions g defined on the lattice.

Consider a random walk on the periodic lattice. Let

$P_s(l)$ = probability of finding the walker at site l at time step s.

$$= P_s\left[l \pm (2N+1)\right] \qquad [\,(4.82a)\text{ used.}\,] \tag{4.82b}$$

Let D be the stochastic variable for the displacement of the walker at each time step, and Δ its realization (in units of a). Owing to the periodic boundary condition, there are only $2N+1$ inequivalent displacements, which can be chosen as $\Delta = \{-N, \ldots, N\}$.

In the following, we shall assume that, at each time step, the walker can only go one step either to the left ($\Delta = -1$) with probability $q = \frac{1}{2}$, or to the right ($\Delta = +1$) with probability $p = \frac{1}{2}$. The displacement probability density for the i^{th} step is therefore

$$p_D(\Delta_i) = q\,\delta_{\Delta_i,-1} + p\,\delta_{\Delta_i,1} = \frac{1}{2}\left(\delta_{\Delta_i,-1} + \delta_{\Delta_i,1}\right) \tag{4.82}$$

Note: Since l is the label of a lattice site, we have decided against using l_i to denote the displacement at time step i, as was done in Reichl's text.

Assuming the walker starts at site $l = 0$ at time step $s = 0$, his position at time s (after s steps) is given by the (accumulative) stochastic variable

$$D^{(s)} = D_1 + \ldots + D_s = \sum_{i=1}^{s} D_i \quad \text{with realization} \quad \Delta^{(s)} = \Delta_1 + \ldots + \Delta_s = \sum_{i=1}^{s} \Delta_i \quad \& \quad \Delta^{(0)} = 0 \qquad (4.82c)$$

Since each step is statistically independent of the others, the discrete version of (4.40) gives the probability of finding the walker at site l at time s as

$$P_s(l) \equiv P_{D^{(s)}}\left(\Delta^{(s)}\right) = \sum_{\Delta_1=-N}^{N} \ldots \sum_{\Delta_s=-N}^{N} \delta_{\Delta^{(s)},\, \Delta_1+\ldots+\Delta_s}\, p_D(\Delta_1) \ldots p_D(\Delta_s) \qquad [\; l = \Delta^{(s)} \text{ since } \Delta^{(0)} = 0\,.\,] \quad (4.83)$$

$$= \frac{1}{2N+1} \sum_{n=-N}^{N} f_s(k_n)\, e^{-i k_n l} \qquad [\text{ c.f. (4.82b). }] \qquad (4.84)$$

where $f_s(k_n)$ is the Fourier amplitude of the periodic function $P_s(l)$ and

$$k_n = \frac{2\pi n}{2N+1} \qquad (4.84a)$$

Note: We have used $e^{-i k_n l}$ instead of the usual $e^{i k_n l}$ in (4.84) because we wish to identify $f_s(k_n)$ with the characteristic function [see (4.85b) below]. Else, we could have defined the characteristic function (4.15) as $\langle e^{-i k x} \rangle$.

Using the identity

$$\sum_{l=-N}^{N} e^{\pm i k_n l} = \begin{cases} 2N+1 & \text{if } n = 0 \\ \dfrac{e^{\mp i k_n N} - e^{\pm i k_n (N+1)}}{1 - e^{\pm i k_n}} & \text{if } n \neq 0 \end{cases}$$

$$= \begin{cases} 2N+1 & \text{if } n = 0 \\ \dfrac{e^{\mp i k_n N}\left(1 - e^{\pm i k_n (2N+1)}\right)}{1 - e^{\pm i k_n}} = 0 & \text{if } n \neq 0 \end{cases} \qquad [\; e^{\pm i k_n (2N+1)} = e^{\pm 2\pi i n} = 1 \text{ used. }]$$

$$= (2N+1)\, \delta_{n0} \qquad (4.85a)$$

we can invert the Fourier series (4.84) by $\sum_{l=-N}^{N} e^{i k_m l}$ both sides of the equation to get

$$\sum_{l=-N}^{N} P_s(l)\, e^{i k_m l} = \frac{1}{2N+1} \sum_{l=-N}^{N} \sum_{n=-N}^{N} f_s(k_n)\, e^{-i k_n l}\, e^{i k_m l}$$

$$= \sum_{n=-N}^{N} f_s(k_n)\, \delta_{nm} \qquad [\text{ (4.85a) used. }]$$

$$= f_s(k_m)$$

Hence,

$$f_s(k_n) = \sum_{l=-N}^{N} P_s(l)\, e^{i k_n l} \qquad (4.85)$$

$$= \sum_{l=-N}^{N} P_{D^{(s)}}\left(\Delta^{(s)}\right) e^{i k_n \Delta^{(s)}} \qquad [\text{ (4.83-4) used. }]$$

$$= f_{D^{(s)}}(k_n) \qquad (4.85b)$$

where $f_{D^{(s)}}(k_n)$ is the characteristic function of $D^{(s)}$ [discrete version of (4.15) used.].

The Fourier components for (4.82) is

$$f_D(k_n) = \sum_{\Delta=-N}^{N} p_D(\Delta)\, e^{i k_n \Delta} = \frac{1}{2}\left(e^{-i k_n} + e^{i k_n}\right) = \cos k_n \tag{4.86}$$

which is also the characteristic function of D.

Putting (4.83) into (4.85) gives

$$\begin{aligned} f_s(k_n) &= \sum_{\Delta_1=-N}^{N} \ldots \sum_{\Delta_s=-N}^{N} \delta_{l,\,\Delta_1+\ldots+\Delta_s}\, p(\Delta_1) \ldots p(\Delta_s)\, e^{i k_n l} \\ &= \sum_{\Delta_1=-N}^{N} \ldots \sum_{\Delta_s=-N}^{N} p(\Delta_1) \ldots p(\Delta_s)\, e^{i k_n (\Delta_1+\ldots+\Delta_s)} \\ &= \overbrace{f_D(k_n) \ldots f_D(k_n)}^{s \text{ terms}} \qquad [\text{ (4.86) used. }] \\ &= (\cos k_n)^s \end{aligned} \tag{4.87}$$

From (4.84a), we have

$$\delta k_n = \frac{2\pi}{2N+1}\delta n = \frac{2\pi}{2N+1} = \text{spacing of } k_n \text{ since spacing of } n \text{ is } \delta n = 1$$

$$\xrightarrow[N\to\infty]{} 0$$

which means k_n becomes a continuous variable as $N \to \infty$. Hence, for any function g, we have

$$\begin{aligned} \sum_{n=-N}^{N} g(k_n) &= \sum_{n=-N}^{N} g(k_n)\,\delta n = \frac{2N+1}{2\pi} \sum_{n=-N}^{N} g(k_n)\,\delta k_n \\ &\approx \frac{L}{2\pi}\int_{-\pi/a}^{\pi/a} g(k)\, dk \qquad \text{for} \quad N >> 1 \end{aligned} \tag{4.88a}$$

where

$$k = \frac{k_n}{a} = \text{wave vector} \qquad \& \qquad L = (2N+1)\,a = \text{length of inequivalent sites.}$$

The interval $\left(-\frac{\pi}{a}, \frac{\pi}{a}\right)$ is called the Brillouin zone of the lattice.

(4.84) thus becomes, for $N \to \infty$,

$$P_s(l) = \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} dk\, f_s(k a)\, e^{-i k a l} \qquad [\text{ (4.88a) used. }] \tag{4.88}$$

while (4.85) turns into

$$f_s(k a) = \sum_{l=-N}^{N} P_s(l)\, e^{i k a l} \tag{4.89}$$

Similarly, the displacement probability density (4.82) can be written as the inverse transform of (4.86), so that as $N \to \infty$,

$$\begin{aligned} p_D(\Delta) &= \frac{1}{2N+1}\sum_{n=-N}^{N} f_D(k_n)\, e^{-i k_n \Delta} \\ &= \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} dk\, f_D(k a)\, e^{-i k a \Delta} \end{aligned} \tag{4.90}$$

while (4.87) becomes

$$f_s(k a) = f_D(k a) \ldots f_D(k a) = (\cos k a)^s \tag{4.91}$$

$$\to \quad f_0(k a) = 1 \tag{4.91a}$$

Putting (4.91) into (4.88) gives

$$P_s(l) = \frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} dk\,(\cos k a)^s\, e^{-i k a l}$$

$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi (\cos\phi)^s e^{-i\phi l} \qquad [\,\phi = k a\,]$$
$$= \frac{1}{2^{s+1}\pi} \int_{-\pi}^{\pi} d\phi \left(e^{i\phi} + e^{-i\phi} \right)^s e^{-i\phi l}$$
$$= \frac{1}{2^{s+1}\pi} \sum_{n=0}^{s} \frac{s!}{(s-n)!\,n!} \int_{-\pi}^{\pi} d\phi\, e^{i(s-2n)\phi} e^{-i\phi l} \qquad [\text{ Binomial expansion. }]$$
$$= \frac{1}{2^{s+1}\pi} \sum_{n=0}^{s} \frac{s!}{(s-n)!\,n!} \frac{1}{(s-2n-l)\,i} \left(e^{i(s-2n-l)\pi} - e^{-i(s-2n-l)\pi} \right)$$
$$= \frac{1}{2^s} \sum_{n=0}^{s} \frac{s!}{(s-n)!\,n!} \frac{\sin(s-2n-l)\pi}{(s-2n-l)\pi}$$
$$= \frac{1}{2^s} \sum_{n=0}^{s} \frac{s!}{(s-n)!\,n!} \delta_{n,(s-l)/2} \qquad \left[\frac{\sin n\pi}{n\pi} = \delta_{n0} \text{ used. } \right]$$

Since $n \geq 0$,

$$n = \frac{1}{2}(s-l) \quad \text{can be satisfied only if } s-l \text{ is even and } s-l \geq 0.$$

Therefore,

$$P_s(l) = \begin{cases} \dfrac{1}{2^s} \displaystyle\sum_{n=0}^{s} \frac{s!}{\left(\frac{s+l}{2}\right)!\left(\frac{s-l}{2}\right)!} & \text{for } s-l \geq 0 \text{ is even} \\ 0 & \text{otherwise} \end{cases} \qquad (4.92)$$

We now proceed to find the probability P_{escape} that the walker escapes from the site where he started.

Let

$Q_s(l)$ = probability that the walker arrives at site l at time s for the first time.

→ $\sum_{s=1}^{\infty} Q_s(l) =$ probability for the walker to reach site l at least once, after he started ($s \neq 0$).

$$\therefore \quad P_{\text{escape}} = 1 - \sum_{s=1}^{\infty} Q_s(0) \qquad (4.101a)$$

= probability for the walker to never reach starting site 0 again after $s = 0$ (he escapes).

In order to evaluate (4.101a), we introduce the generating function

$$V(z, l) = \sum_{s=1}^{\infty} z^s Q_s(l) \qquad (4.95)$$

from which $Q_s(l)$ can be “generated” as [c.f. (4.17) of §4.D.3]

$$Q_s(l) = \frac{1}{s!} \frac{\partial^s V(z, l)}{\partial z^s} \bigg|_{z=0} \qquad (4.94a)$$

Normally, a generating function should be able to generate all possible members in its family. The member $s = 0$ is excluded from (4.95) to make it easier to use in (4.101a).

Comparing (4.95) with (4.101a) gives

$$P_{\text{escape}} = 1 - V(1, 0) \qquad (4.101b)$$

Our task is to express $V(z, l)$ in terms of $P_s(l)$. However, it is easier to work with the generating function

$$U(z, l) = \sum_{s=0}^{\infty} z^s P_s(l) \qquad (4.93a)$$

where the sum starts at $s = 0$ so that $U(z, l)$ generates all possible $P_s(l)$.

Putting (4.88) into (4.93a), we get

$$U(z, l) = \frac{a}{2\pi} \sum_{s=0}^{\infty} z^s \int_{-\pi/a}^{\pi/a} dk\, f_s(ka)\, e^{-ikal}$$

$$= \frac{a}{2\pi} \sum_{s=0}^{\infty} \int_{-\pi/a}^{\pi/a} dk\, (z \cos ka)^s\, e^{-ikal} \qquad \text{[(4.91) used.]}$$

$$= \frac{a}{2\pi} \lim_{s\to\infty} \int_{-\pi/a}^{\pi/a} dk\, \frac{1-(z\cos ka)^{s+1}}{1 - z\cos ka}\, e^{-ikal}$$

$$= \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} dk\, \frac{1}{1 - z\cos ka}\, e^{-ikal} \qquad \text{for } |z \cos ka| < 1 \tag{4.93b}$$

$$= \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi\, \frac{1}{1 - z\cos\phi}\, e^{-i\phi l} \qquad \phi = ka \tag{4.93c}$$

Now,

$$P_0(0) = 1 \qquad \to \qquad P_0(l) = \delta_{l,0} \tag{4.96}$$

Furthermore, for $s \geq 1$, we can write

$P_s(l)$ = sum of probabilities that walker starts at time $s - j$ at site 0 (for $j = 1, \ldots, s$)
and then arrives at l at time s for the 1st time.

$$= \sum_{j=1}^{s} P_{s-j}(0)\, Q_j(l) \qquad \text{for } s \geq 1 \tag{4.97}$$

(4.93a) thus becomes

$$U(z, l) = \delta_{l,0} + \sum_{s=1}^{\infty} z^s P_s(l)$$

$$= \delta_{l,0} + \sum_{s=1}^{\infty} z^s \sum_{j=1}^{s} P_{s-j}(0)\, Q_j(l) \tag{4.98}$$

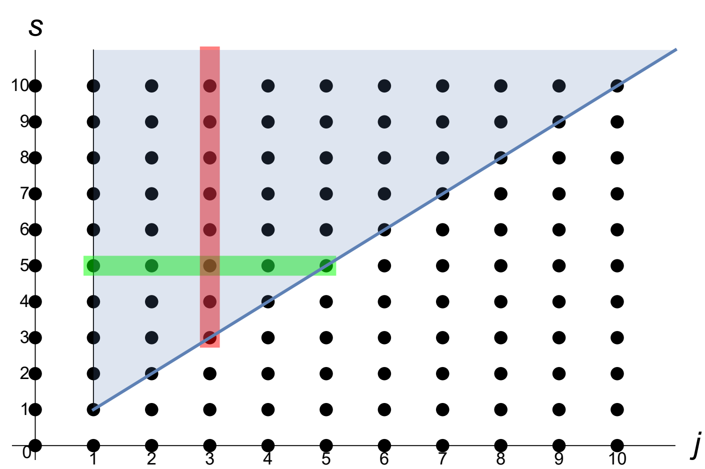

Fig.4.6a.

The double sum in (4.98) is the sum over the points in the triangular area above the diagonal line in the j-s plane, with the lowest vertex at $(1, 1)$ and one leg parallel to the positive s-axis [see shaded area in Fig.4.6a]. (4.98) does it by summing line by horizontal (s = const) lines. Obviously, the same area can be summed line by vertical (j = const) lines, giving

$$U(z,l) = \delta_{l,0} + \sum_{j=1}^{\infty}\sum_{s=j}^{\infty} z^s P_{s-j}(0)\, Q_j(l)$$

$$= \delta_{l,0} + \sum_{j=1}^{\infty}\sum_{n=0}^{\infty} z^{j+n} P_n(0)\, Q_j(l) \qquad n = s - j$$

$$= \delta_{l,0} + U(z,0)\, V(z,l) \qquad \text{[(4.93a) \& (4.95) used.]} \qquad (4.98a)$$

$$\rightarrow \quad V(z,l) = \frac{U(z,l) - \delta_{l,0}}{U(z,0)} \qquad (4.99)$$

$$\therefore \quad V(1,0) = 1 - \frac{1}{U(1,0)} \qquad (4.100)$$

and (4.101a) becomes

$$P_{\text{escape}} = \frac{1}{U(1,0)} \qquad (4.101)$$

From (4.93), we have

$$U(1,0) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi\, \frac{1}{1-\cos\phi}$$

$$= \frac{1}{\pi}\int_{0}^{\pi} d\phi\, \frac{1}{1-\cos\phi}$$

$$= -\frac{1}{\pi}\cot\frac{\phi}{2}\Big|_0^{\pi}$$

$$= \infty$$

Hence

$$P_{\text{escape}} = 0$$

and the 1-D random walker never escapes.

Ex.4.12.

Compute $U(z,0)$, which generates the probability for the walker to visit site 0 at any time s.

Answer

(4.93c) gives

$$U(z,0) = \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi\, \frac{1}{1 - z\cos\phi}$$

$$= \frac{1}{\pi}\int_{0}^{\pi} d\phi\, \frac{1}{1 - z\cos\phi}$$

$$= \frac{2}{\pi\sqrt{1-z^2}} \tan^{-1}\left(\frac{(1+z)}{\sqrt{1-z^2}}\tan\frac{\phi}{2}\right)\Bigg|_0^{\pi}$$

$$= \frac{1}{\sqrt{1-z^2}}$$

$$\rightarrow \quad U(1,0) = \sum_{s=0}^{\infty} P_s(l) = \infty$$

Code

In[ ]:= $\int \frac{1}{1 - \text{Cos}[\phi]} \, d\phi$

Out[ ]= $-\text{Cot}\left[\frac{\phi}{2}\right]$

In[ ]:= $\int \frac{1}{1 - z\,\text{Cos}[\phi]} \, d\phi$

Out[ ]= $-\frac{2\,\text{ArcTanh}\left[\frac{(1+z)\,\text{Tan}\left[\frac{\phi}{2}\right]}{\sqrt{-1+z^2}}\right]}{\sqrt{-1+z^2}}$

In[ ]:= ArcTanh[ⅈ a]

Out[ ]= ⅈ ArcTan[a]

In[76]:=
```
(* Fig.4.6a *)
n = 10; m = 5; k = 3;
pts = Table[{x, y}, {x, 0, n}, {y, 0, n}] // Flatten[#, 1] &;
tic = {Table[i, {i, 0, n}], Table[i, {i, 0, n}]};
Plot[x, {x, 1, n + 1},
     PlotRange → {{-.4, n + 1}, {-.4, n + 1}},
     AxesLabel → {"j", "S"},
     Ticks → tic,
     Filling → Top,
     Prolog → {PointSize[.02], Point[pts],
       Line[{{1, 1}, {1, n + 1}}], Text["0", -.2 {.7, 1}],
       Opacity[.5], Thickness[.03],
       Green, Line[{{1, m}, {m, m}}],
       Red, Line[{{k, k}, {k, n + 1}}]
       }
]
```