To do the integral on the right-hand side of (7.70), we multiply both sides of (7.68) by x and formally integrate over x:

$$\int_{-\infty}^{\infty} x\frac{\partial P(x,t)}{\partial t}\,dx = D\int_{-\infty}^{\infty} x\frac{\partial^2 P(x,t)}{\partial x^2}\,dx. \tag{7.71}$$

The left-hand side can be expressed as

$$\int_{-\infty}^{\infty} x\frac{\partial P(x,t)}{\partial t}\,dx = \frac{\partial}{\partial t}\int_{-\infty}^{\infty} xP(x,t)\,dx = \frac{d}{dt}\langle x\rangle. \tag{7.72}$$

The right-hand side of (7.71) can be written in the desired form by doing an integration by parts:

$$D\int_{-\infty}^{\infty} x\frac{\partial^2 P(x,t)}{\partial x^2}\,dx = Dx\frac{\partial P(x,t)}{\partial x}\Big|_{x=-\infty}^{x=\infty} - D\int_{-\infty}^{\infty}\frac{\partial P(x,t)}{\partial x}\,dx. \tag{7.73}$$

The first term on the right-hand side of (7.73) is zero because $P(x=\pm\infty,t)=0$ and all the spatial derivatives of P at $x=\pm\infty$ are zero. The second term is also zero because it integrates to $D[P(x=\infty,t)-P(x=-\infty,t)]$. Hence, we find that

$$\frac{d\langle x\rangle}{dt} = 0, \tag{7.74}$$

or $\langle x\rangle$ is a constant, independent of time. Because $x=0$ at $t=0$, we conclude that $\langle x\rangle=0$ for all t.

To calculate $\langle x^2(t)\rangle$, we can use a similar procedure and perform two integrations by parts. The result is

$$\frac{d}{dt}\langle x^2(t)\rangle = 2D, \tag{7.75}$$

or

$$\langle x^2(t)\rangle = 2Dt. \tag{7.76}$$

We see that the random walk and the diffusion equation have the same time dependence. In d-dimensional space, $2D$ is replaced by $2dD$.

The solution of the diffusion equation shows that the time dependence of $\langle x^2(t)\rangle$ is equivalent to the long time behavior of a simple random walk on a lattice. In the following, we show directly that the continuum limit of the one-dimensional random walk model is a diffusion equation.

If there is an equal probability of taking a step to the right or left, the random walk can be written in terms of the simple master equation

$$P(i,N) = \frac{1}{2}[P(i+1,N-1)+P(i-1,N-1)], \tag{7.77}$$

where $P(i,N)$ is the probability that the walker is at site i after N steps. To obtain a differential equation for the probability density $P(x,t)$, we identify $t=N\tau$, $x=ia$, and

$P(i,N)=aP(x,t)$, where τ is the time between steps and a is the lattice spacing. This association allows us to rewrite (7.77) in the equivalent form

$$P(x,t) = \frac{1}{2}[P(x+a,t-\tau)+P(x-a,t-\tau)]. \tag{7.78}$$

We rewrite (7.78) by subtracting $P(x,t-\tau)$ from both sides of (7.78) and dividing by τ:

$$\frac{1}{\tau}[P(x,t)-P(x,t-\tau)]$$
$$= \frac{a^2}{2\tau}[P(x+a,t-\tau)-2P(x,t-\tau)+P(x-a,t-\tau)]a^{-2}. \tag{7.79}$$

If we expand $P(x,t-\tau)$ and $P(x\pm a,t-\tau)$ in a Taylor series and take the limit $a\to 0$ and $\tau\to 0$ with the ratio $D\equiv a^2/2\tau$ finite, we obtain the diffusion equation

$$\frac{\partial P(x,t)}{\partial t} = D\frac{\partial^2 P(x,t)}{\partial x^2}. \tag{7.80a}$$

The generalization of (7.80a) to three dimensions is

$$\frac{\partial P(x,y,z,t)}{\partial t} = D\nabla^2 P(x,y,z,t), \tag{7.80b}$$

where $\nabla^2 = \partial^2/\partial x^2+\partial^2/\partial y^2+\partial^2/\partial x^2$ is the Laplacian operator. Equation (7.80) is known as the *diffusion* equation and is frequently used to describe the dynamics of fluid molecules.

The direct numerical solution of the prototypical *parabolic* partial differential equation (7.80) is a nontrivial problem in numerical analysis (cf. Press et al. or Koonin and Meredith). An indirect method of solving (7.80) numerically is to use a Monte Carlo method; that is, replace the partial differential equation (7.80) by a corresponding random walk on a lattice with discrete time steps. Because the asymptotic behavior of the partial differential equation and the random walk model are equivalent, this approach uses the Monte Carlo technique as a method of *numerical analysis*. In contrast, if our goal is to understand a random walk lattice model directly, the Monte Carlo technique is a *simulation* method. The difference between simulation and numerical analysis is sometimes in the eyes of the beholder.

Problem 7.43 Biased random walk

Show that the form of the differential equation satisfied by $P(x,t)$ corresponding to a random walk with a drift, that is, a walk for $p\neq q$, is

$$\frac{\partial P(x,t)}{\partial t} = D\nabla^2 P(x,y,z,t) - v\frac{\partial P(x,t)}{\partial x}. \tag{7.81}$$

How is v related to p and q? ■