plot and analyze the trajectory $\mathbf{r}_u = (x_u, y_u, z_u)$ of a given atom unfolded into a continuous path which ignores the periodic boundary conditions.

(a) *Does the trajectory of the perfume atom appear qualitatively like a random walk? Plot $x_u(t)$ versus t, and $x_u(t)$ versus $y_u(t)$.* The time it takes the atom to completely change direction (lose memory of its original velocity) is the collision time, and the distance it takes is the collision length. *Crudely estimate these.*

(b) *Plot $\mathbf{r}_u^2(t)$ versus t, for several individual particles (making sure the average velocity is zero). Do they individually grow with time in a regular fashion? Plot $\langle \mathbf{r}_u^2 \rangle$ versus t, averaged over all particles in your simulation. Does it grow linearly with time? Estimate the diffusion constant D.*

(2.5) **Generating random walks.**[35] (Computation) ③

One can efficiently generate and analyze random walks on the computer.

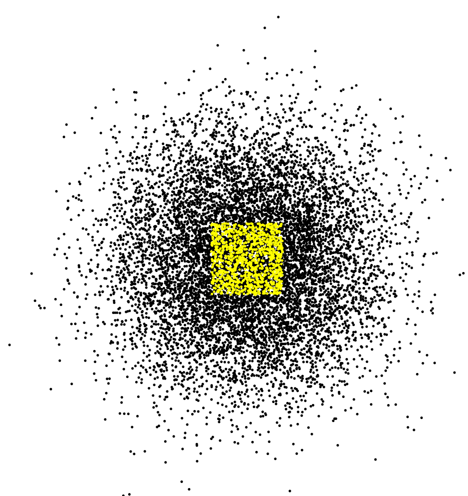

Fig. 2.10 Emergent rotational symmetry. Endpoints of many random walks, with one step (central square of bright dots) and ten steps (surrounding pattern). Even though the individual steps in a random walk break rotational symmetry (the steps are longer along the diagonals), multistep random walks are spherically symmetric. The rotational symmetry emerges as the number of steps grows.

(a) *Write a routine to generate an N-step random walk in d dimensions, with each step uniformly distributed in the range $(-1/2,\ 1/2)$ in each dimension. (Generate the steps first as an $N \times d$ array, then do a cumulative sum.) Plot x_t versus t for a few 10,000-step random walks. Plot x versus y for a few two-dimensional random walks, with N = 10, 1,000, and 100,000. (Try to keep the aspect ratio of the XY plot equal to one.) Does multiplying the number of steps by one hundred roughly increase the net distance by ten?*

Each random walk is different and unpredictable, but the *ensemble* of random walks has elegant, predictable properties.

(b) *Write a routine to calculate the endpoints of W random walks with N steps each in d dimensions. Do a scatter plot of the endpoints of 10,000 random walks with N = 1 and 10, superimposed on the same plot. Notice that the longer random walks are distributed in a circularly symmetric pattern, even though the single step random walk $N = 1$ has a square probability distribution (Fig. 2.10).*

This is an *emergent symmetry*; even though the walker steps longer distances along the diagonals of a square, a random walk several steps long has nearly perfect rotational symmetry.[36]

The most useful property of random walks is the *central limit theorem*. The endpoints of an ensemble of N step one-dimensional random walks with RMS step-size a has a Gaussian or normal probability distribution as $N \to \infty$,

$$\rho(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-x^2/2\sigma^2), \tag{2.35}$$

with $\sigma = \sqrt{N}a$.

(c) *Calculate the RMS step-size a for one-dimensional steps uniformly distributed in $(-1/2,\ 1/2)$. Write a routine that plots a histogram of the endpoints of W one-dimensional random walks with N steps and 50 bins, along with the prediction of eqn 2.35, for x in $(-3\sigma, 3\sigma)$. Do a histogram with $W = 10{,}000$ and N = 1, 2, 3, and 5. How quickly does the Gaussian distribution become a good approximation to the random walk?*

[35] This exercise and the associated software were developed in collaboration with Christopher Myers. Hints for the computations can be found at the book website [181].

[36] The square asymmetry is an *irrelevant perturbation* on long length and time scales (Chapter 12). Had we kept terms up to fourth order in gradients in the diffusion equation $\partial\rho/\partial t = D\nabla^2\rho + E\nabla^2(\nabla^2\rho) + F(\partial^4\rho/\partial x^4 + \partial^4\rho/\partial y^4)$, then F is square symmetric but not isotropic. It will have a typical size $\Delta t/a^4$, so is tiny on scales large compared to a.