Exercises

2.4 **Perfume walk.**[1] [2] (Computation) ②

The trajectory of a perfume molecule in still air, or more generally any molecule in a dilute gas, is a chaotic path of nearly straight segments followed by collisions—a random walk. You may download our molecular dynamics software [10] from the text web site [129].

Run a simulation of an interacting dilute gas, setting the average velocity of the atoms to zero.[3] Watch the motion of a single 'perfume' atom. Notice that as it passes the edge of the container, it reappears at the opposite face; this simulation uses *periodic boundary conditions*[4] Your software should have options to 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.*

[1] From *Statistical Mechanics: Entropy, Order Parameters, and Complexity* by James P. Sethna, copyright Oxford University Press, 2007, page 27. A pdf of the text is available at pages.physics.cornell.edu/sethna/StatMech/ (select the picture of the text). Hyperlinks from this exercise into the text will work if the latter PDF is downloaded into the same directory/folder as this PDF.

[2] This exercise and the associated software were developed in collaboration with Christopher Myers.

[3] The atoms interact via a Lennard–Jones pair potential, which is a good approximation for the forces between noble gas molecules like argon.

[4] Periodic boundary conditions are an artificial method which allows a small simulation to mimic infinite space, by mathematically identifying the opposite faces of a square region; $(x, y, z) \equiv (x \pm L, y, z) \equiv (x, y \pm L, z) \equiv (x, y, z \pm L)$.