2 Exercises Lectures 3 and 4 (due 12th of February)

2.1 Lyapunov exponents of the Lorentz gas

Consider the two-dimensional random Lorentz gas. This is a set of randomly placed, hard, circular scatterers with a single point particle bouncing around between them. When the point particle bounces elastically off the scatterer, its velocity is reflected.

a) How many degrees of freedom does this system have? How many dimensions does the phase space have?

b) In this exercise, the aim is to calculate all the Lyapunov exponents of the system. These are the possible rates at which infinitessimal perturbations in phase space can blow up or shrink after long time. There are as many Lyapunov exponents as the phase space has dimensions. Show that for any Hamiltonian system, including this one, the sum of all Lyapunov exponents is 0.

c) Show that there are two Lyapunov exponents in the two-dimensional Lorentz gas that are 0. The easiest way to do this is to come up with two examples of perturbations that will not grow or shrink exponentially. Then use this and the result from b) to obtain a relation between the largest and smallest Lyapunov exponents.

The largest positive Lyapunov exponent can be calculated by considering the growth of an arbitrary infinitessimal pertubation that is not one of the two perturbations you have found in c). After long time, the growth of this perturbation will be dominated by the largest Lyapunov exponent. Consider two nearby paths with the same absolute velocity, but slightly different direction. The difference between the two trajectories can be described by the relative difference in angle $\delta\theta$. The largest Lyapunov exponent can then be written as

$$\lambda^+ = \lim_{t\to\infty} \frac{1}{t} \log(\delta\theta(t)/\delta\theta(0)) \ . \tag{1}$$

One could obtain the Lyapunov exponents numerically by simulating a trajectory and calculating this expresssion. At low densities, however, it is not necessary to resort to numerics.

d) During a free flight between collisions, the relative angle of the velocities does not change. Consider the growth of the difference in position between the two trajectories during a free flight, and calculates how this affects the collision normal for the next collision. Show that the difference in angles after a collision, $\delta\theta'$, can be written as

$$\delta\theta' = (1 + 2l/(a\cos\phi))\,\delta\theta \ , \tag{2}$$

where ϕ is the angle between the velocity and the collision normal, a is the radius of a scatterer, and l is the length of the free flight. Low density, i.e. $\rho a^2 \ll 1$, means that for the mean free path l, $l/a \gg 1$. Thus, in the term between parentheses, the 1 can be neglected.

e) Explain that this Lyapunov exponent can be calculated as

$$\lambda^+ = \nu\langle\log(2l/(a\cos\phi)\rangle \ , \tag{3}$$

with ν the average collision frequency and $\langle\rangle$ the averaging over the distribution of l and ϕ.

f) In a Monte-Carlo simulation of this system, you would also need to know these distributions. You would have to draw collision parameters for the next collision with a scatterer from these distributions. Show that the probability densities are given by

$$P(l) = \frac{1}{l}_{mf} \exp(-l/l_{mf}) \ , \tag{4}$$

$$P(\phi) = \frac{1}{2}\cos(\phi), \text{with} -\frac{\pi}{2} < \phi < \frac{\pi}{2} \ . \tag{5}$$

Here, l_{mf} is the mean free path between two successive collisions. Show also that $l_{mf} = 1/(2\rho a)$ and $\nu = v/l_{mf} = 2\rho v a$.

To get the final result, you will have to integrate over these distributions. If you were doing a Monte-Carlo simulation using the above distributions, instead of an analytical calculation, you would have used a Monte-Carlo method to calculate that integral. Monte-Carlo methods are often used to numerically calculate integrals. If you had done this particular integral manually, you would have found that

$$\lambda^+ = 2\rho a v \left(\ln(1/\rho a^2) + 1 - \ln 2 - C\right) \ , \tag{6}$$

with C Euler's constant, $C = 0.577215\ldots$

2.2 Integrating equations of motion

a) Show that the RK2 algorithm is not symplectic, by calculating the jacobian for a general Hamiltonian system and demonstrating that, in general, phase-space volume is not conserved.

b) RK2 and RK4 are shown in the book and explained using midpoints. That is to say, the second order version uses two mid points, k_1 and k_2, and the fourth order one uses k_1, k_2, k_3, and k_4. Choose some similar k_1, k_2, k_3 that you find convenient. Derive a third-order RK3 algorithm, by Taylor expanding and finding the constants c_1, c_2, and c_3 such that $x(h) = x(0) + c_1 k_1 + c_2 k_2 + c_3 k_3 + O(h^4)$.

c) When you use a time-step size that is much too large, for example when you simulate the Argon fluid in the programming exercise, there will be a drift in the energy. Explain why, on average, the energy will increase.

d) Why is it not recommended to integrate Hamiltonian equations of motion with a Runge-Kutta method? If you end up doing this anyway, for whatever reason (probably lazyness), what should you do to make sure that your simulations produce valid results?