Physics 270: Introduction to Computational Physics

Problem 13: Atom scattering

1. Introduction

This problem builds on the previous one. In this problem, we will simulate one of the most important techniques that is used in physics to study materials. This is the technique of "scattering", which is used to indirectly measure the atomic potentials of a sample.

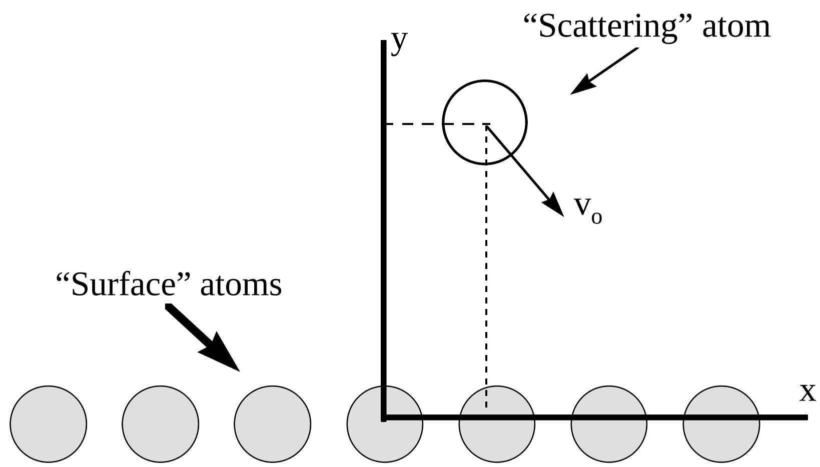

Figure 1.

We will use the methods developed over the past few problems. In the Kepler problem, we learned how to model the trajectory of two particles interacting by a gravitational field. In the first "molecular dynamics" problem, we learned how to calculate the interaction of an atom with a large ensemble of neighboring atoms.

In this problem, we will use the potential of interaction of atoms, the Lennard-Jones potential, and the equation of motion techniques from the Kepler problem, to determine the trajectory of an atom that is incident on a model "surface".

2. Approach

The problem is confined to two-dimensions, the "x-y" plane. We will use a classical interaction.

There is a "scattering atom", which is directed towards a line of atoms that form the "surface" of our sample (see Figure 1.). All of the atoms in the surface are fixed in position (an extreme and unrealistic assumption made for simplicity). The scattering atom interacts with the target surface through the L-J potential. We need to turn the potential into a force.

The Lennard-Jones potential is given by

$$V(r) = 4E\left[\left(\frac{s}{r}\right)^{12} - \left(\frac{s}{r}\right)^{6}\right], \qquad [1]$$

where r is the distance between any two atoms, E is the energy scaling factor E=0.012 eV, and *s* is the length scaling factor, *s*=0.34 nanometers. These parameters are appropriate for an Argon atom.

The force between any two atoms can be calculated from the potential. Remember that there are two forces, which are equal and opposite in direction, acting between any two pairs of atoms. In our simplified problem, we are only interested in the force on the "scattering" atom.

Make a "surface" of atoms that lie along the "x" axis. The spacing between atoms should be equal to *s* (0.34 nanometers).

Use the following modified algorithm to calculate the equation of motion of the scattering atom. It is of better accuracy than the Euler method, and is just as simple. It is called the Verlet algorithm.

$$x_{n+1} = x_n + vx_n \Delta t + \frac{1}{2} ax_n (\Delta t)^2$$
$$vx_{n+1} = vx_n + \frac{1}{2}\left(ax_{n+1} + ax_n\right)\Delta t \qquad [2]$$

where "vx" is the x-component of the velocity, "ax" is the x-component of the acceleration. Note that there are two more formulas needed for the "y" direction.

The only tricky part of this problem is choosing a set of units so as to make the problem easy to set up. A suggestion is to use a set of units in which energy, length and mass are given in terms of E, *s*, and the mass of the argon atom m. In these units the velocity is given in units of $(E/m)^{1/2}$, and the time is in units of $(ms^2E)^{1/2}$. You simply set E, *s* and m equal to one, and make your measurements in terms of these parameters. To get back to MKS, if needed, you put back in the values of mass (6.7 x 10^{-23} gm) and the time unit (1.8 x 10^{-12} sec).

We also need the force on the scattering atom. The total force is the sum of the forces between the scattering atom and each of the surface atoms. We need an expression for the force acting on the scattering atom from some particular surface atom. This is derived by differentiating the L-J potential.

$$F_x = -E \cdot \Delta x \cdot \left[48 \frac{s^{12}}{r^{14}} - 24 \frac{s^6}{r^8} \right], \qquad [3]$$
$$r = \sqrt{\Delta x^2 + \Delta y^2}$$

There is a similar equation for the force in the y direction. You must be *very careful* to choose a convention on your definition of Δx so that the force is attractive for large r, and repulsive for small r. Just test it by hand. Now you can see why we want to have *s*=1, and m=1! The acceleration is just the force divided by the mass (which is set to unity).

3. Tasks

a. For initial conditions of x=0, y=10*s* (i.e. y=10), and KE=+E (=1), calculate and plot the trajectory of the scattering atom for an initial velocity that is directed straight "down".

b. For the same initial position, change the velocity to point "off axis" towards an atom to the side, and calculate the trajectory of the scattering atom.

c. Repeat the calculations in (a) and (b), for an initial position "x" that lies half-way between two surface atoms.

d. Plot all of your trajectories.