

# Computational Physics 1

Recitation class, March 10, 2021

## Classical scattering

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## 1 Deflection angle

A classical particle of mass  $m$  and kinetic energy  $E$  is deflected by a Lennard-Jones potential. Compute and plot the deflection angle as a function of the impact parameter  $b$  for energies  $E^* = E/\varepsilon \in (0.1, 0.5, 1, 2, 3, 5)$ . Check your answers by comparing the results obtained using the explicit formula for  $\theta(E, b)$  with those obtained by integration of the Newton equations of motion in 2D.

### 1.1 No deflection

Compute the value of  $b$  for which  $\theta(E, b) = 0$  as a function of the same energies considered previously, and plot the corresponding trajectories.

### 1.2 Orbiting

For some specific values of  $E$  the function  $\theta(E, b)$  diverges for a certain value of the impact parameter  $b$ . This corresponds to the fact that impinging particles perform some orbits before being scattered. Assuming  $E^* = 0.1$ , find the value of  $b$  for which  $|\theta(E, b)| = 4\pi$ ; that is, the particle makes *two* orbits before being scattered.

## 2 Cross section of the Lennard-Jones potential

Compute and plot the “reduced” differential cross section  $\bar{\sigma}(E^*)$  in the case of the Lennard-Jones potential at energies  $E^* \in (0.1, 0.5, 1, 2, 3, 5)$ . Choose the binning-slot size  $\delta\theta$  in order to have a resolution of  $1^\circ$ .

## 2.1 Rainbow scattering

For sufficiently high energies, the function  $\theta(E, b)$  has a *minimum* in the variable  $b$ , hence the differential cross section – which is proportional to  $\left| \frac{db}{d\theta} \right|$  – diverges. Compute the value of  $b$  for which  $\theta(E, b)$  has a minimum in the case of  $E^* \in (2, 3, 5)$ , and verify that the differential cross section has an asymptote at the corresponding deflection angle.

## 2.2 Small-angle scattering

Analyze the behavior of the reduced scattering cross section  $\bar{\sigma}(E, \theta)$  as  $\theta \rightarrow 0$  in the case of the Lennard-Jones potential. Verify the validity of the asymptotic regime

$$\bar{\sigma}(E, \theta) \underset{\theta \rightarrow 0}{\propto} \frac{\theta^{-4/3}}{E^{1/3}}. \quad (1)$$

Notice that  $\bar{\sigma}(E, \theta)$  has a non-integrable divergence for  $\theta \rightarrow 0$  hence the *total* classical scattering cross section for the Lennard-Jones potential is infinite.