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Computational Physics I
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10.1 Scattering angle

The angle of deflection (or scattering angle) for a particle with asymptotic kinetic energy E scattered of a spherically symmetric potential $V(r)$ is given by

$$\chi(b) = \pi - 2\int_{r_+}^{\infty} \frac{bdr}{r^2\sqrt{1 - b^2/r^2 - V(r)/E}} \tag{1}$$

Verify that for $V = 0$ the scattering angle vanishes.
Determine the scattering angle for a repulsive potential $V(r) = 1/r^2$ and verify that it drops monotonically from π for $b = 0$ to 0 for very large b.
Determine the scattering angle for an attractive potential $V(r) = -\exp(-r)$: what are the differences to the repulsive case?
Determine the scattering angle for a 6-12 Lennard-Jones potential $V(r) = r^{-12} - 2r^{-6}$.
Hint: it is useful to plot the function in the denominator for different impact parameters and energies in order to determine the boundaries of integration and to find hints for critical values where special care is required.

10.2 Scattering trajectories

Calculate trajectories for the unbounded motion in a radially symmetric potential

$$V(r) = \frac{1}{r^{12}} - 2\frac{1}{r^6} \tag{2}$$

at positive energies for different impact parameters. Because of the symmetry, you may integrate the equations in the x-y-plane. Pick initial conditions typical for scattering experiments: x negative and sufficiently far out so that the potential can be neglected, $y = b$ equal to the impact parameter, $\dot{y} = 0$ and $\dot{x}$ determined from the initial energy. The aim is to study trajectories for different b until they leave the interaction region and to then determine the scattering angle $\varphi(b)$.
How does the integration step size vary along the trajectory?
How well are energy and angular momentum conserved?
Extract the scattering angle as a function of impact parameter from the trajectories, and compare with the results from the previous problem.

10.3 Morseoscillator

Calculate trajectories for the bounded motion in a 1-d potential

$$V(x) = \exp(-2x) - 2\exp(-x) \tag{3}$$

Try different energies and monitor energy conservation and the step size used in the integrators.