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Computational Quantum Physics Exercise 3

FS 10
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Problem 3.1 $H - Kr$ scattering

Introduction In this exercise, we will solve the quantum $3d$ elastic scattering problem of hydrogen atoms scattering on (much heavier) krypton atoms. The most relevant quantity for scattering experiments is the differential cross section, $\frac{d\sigma}{d\Omega}(\Omega)$, which describes scattering intensities as a function of the angle Ω. We will however first restrict ourselves to calculating the total cross section σ_{tot}.

To this end, we have to solve the Schrodinger equation in three dimensions,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\Psi(\vec{r}) = E\Psi(\vec{r}). \tag{1}$$

From basic quantum mechanics, we know that all eigenfunctions of a spherically symmetric Hamiltonian are also eigenfunctions of the angular momentum operators. Therefore, they decompose into linear combinations of the spherical harmonics:

$$\Psi(\vec{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} A_{lm}\frac{u_l(r)}{r}Y_l^m(\theta,\phi). \tag{2}$$

Using this ansatz, we can perform separation of variables and only have to solve the radial Schrodinger equation,

$$\left[\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \left(E - V(r) - \frac{\hbar l(l+1)}{2mr^2}\right)\right]u_l(r) = 0. \tag{3}$$

We have therefore reduced the $3d$ problem to a one-dimensional problem, to which we can apply the techniques learned in the last two exercises.

As will be demonstrated in class, the central quantity for quantum scattering is the phase shift. We can calculate the phase shift from the asymptotic behaviour of the numerically integrated wave function at two points $r_1, r_2 > r_{max}$:

$$\tan\delta_l = \frac{Kj_l(kr_1) - j_l(kr_2)}{Kn_l(kr_1) - n_l(kr_2)} \tag{4}$$

$$K = \frac{r_1 u_2}{r_2 u_1}, \tag{5}$$

where j_l, n_l are spherical Bessel functions which you can find implemented in libraries. Then, the total scattering cross section is given by

$$\sigma_{tot} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \tag{6}$$

The potential that we will use to describe the $H - Kr$ interaction is the Lennard-Jones potential,

$$V_{LJ}(r) = \epsilon\left[\left(\frac{\sigma}{r}\right)^1 2 - 2\left(\frac{\sigma}{r}\right)^6\right], \tag{7}$$

with $\epsilon = 5.9$ meV and $\sigma = 3.57$ A.

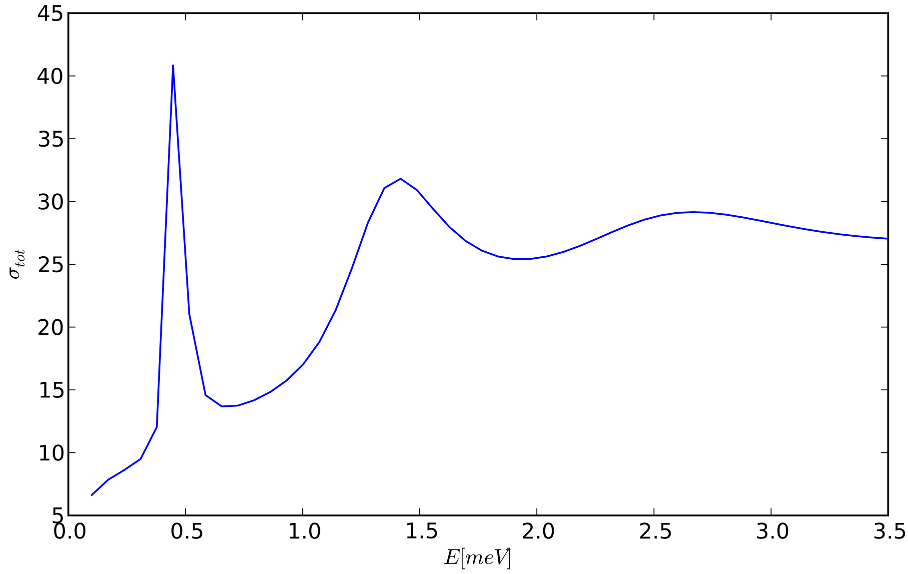

Figure 1: Total scattering cross section σ_{tot} for $r_0 = 0.5\sigma, r_{max} = 5\sigma, l_{max} = 10$.

Hints

- Be careful to work in correct units. It is useful to work in units of σ for all length scales. With that choice, $\frac{2m}{\hbar^2} = 6.12\ \text{meV}^{-1}\sigma^{-2}$.
- Since the potential diverges for $r \to 0$, we need to be careful with the choice of initial values. Since the $1/r^{12}$ term dominates for small r, we can drop the other term and arrive at an asymptotic solution,

$$u(r) = \exp(-Cr^{-5}) \tag{8}$$

  with $C = \sqrt{6.12\epsilon/25}$ (in units of σ). Start your Numerov integration from some $r_0 \sim 0.5\sigma$ and use (8) to set up the boundary conditions.
- A reasonable upper bound for the integration is $r_{\text{max}} = 5\sigma$.
- In (3), values of l range from 0 to ∞. Of course we cannot perform this summation to infinity. Instead, truncate at some l_{max} (see below).
- You can use these values to check whether you're using the correct Bessel functions:

$$j_5(1.5) = 6.69620596 \cdot 10^{-4} \tag{9}$$

$$n_5(1.5) = -94.2361101 \tag{10}$$

Exercise

1. Reproduce the example shown in Fig. 1.
2. Change the truncation of l in (3). Observe how the scattering cross section changes. How do you interpret this change, and can you deduce a physical motivation for truncating l?