Homework 2 - Advanced Computational Physics

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Problem: A program for calculating cross sections [100 points]

Construct a program for calculating cross sections for a particular scattering problem: hydrogen atoms scattered off (much heavier) krypton atoms. *Note:* Both atoms are considered as single particles and their structure (nucleus and electrons) is not explicitly considered. *Hint:* Follow the procedure outlined in Chapter 2.2 of the textbook.

Desired output: Total cross section as a function of energy.

Compare the output with experimentally reported values (Ref [1] or similar).

[1] J. P. Toennies, W. Welz, and G. Wolf, 'Molecular beam scattering studies of orbiting resonances and the determination of Van der Waals potentials for H–He, Ar, Kr, and Xe and for H2–Ar, Kr and Xe", J. Chem. Phys., 71, 614–42 (1979)

Background

In this problem, we examine the scattering of hydrogen atoms on significantly heavier krypton atoms. The primary quantity of interest in scattering experiments is the differential cross-section $\frac{d\sigma}{d\Omega}(\Omega)$, which describes the scattering intensity as a function of the angle Ω. However, in this problem, we will focus on computing the total cross-section, given by:

$$\sigma_{tot} = \int d\Omega \frac{d\sigma}{d\Omega}. \tag{1}$$

To achieve this, we need to solve the three-dimensional Schrödinger equation:

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

Where $V(r)$ is a spherically symmetric potential. From fundamental quantum mechanics, we know that in such a case, all eigenfunctions are also eigenfunctions of the angular momentum operators. These eigenfunctions can be expressed as a linear combination of spherical harmonics:

$$\Psi(\vec{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} A_{lm}\frac{u_l(r)}{r}Y_l^m(\theta,\phi). \tag{3}$$

By applying the separation of variables, this reduces the problem to the radial Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \left(V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} - E\right)\right]u_l(r) = 0 \tag{4}$$

A crucial quantity in quantum scattering is the phase shift δ_l. It can be determined from the asymptotic behavior of the numerically integrated wave function at two points $r_1, r_2 \approx r_{\max}$, using the formula:

$$\tan\delta_l = \frac{Kj_l(kr_1) - j_l(kr_2)}{Kn_l(kr_1) - n_l(kr_2)}, \tag{5}$$

where $k = \sqrt{2mE/\hbar^2}$, $K = r_1u_2/r_2u_1$, and $u_{1,2} = u_l(r_{1,2})$. Here, j_l and n_l are the first and second kind of spherical Bessel functions.

The total scattering cross-section is then given by:

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

To describe the H-Kr interaction, we use the Lennard-Jones potential, given by:

$$V_{LJ}(r) = \epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - 2\left(\frac{\sigma}{r}\right)^{6}\right], \tag{7}$$

Where the parameters are $\epsilon = 5.9$ meV and $\sigma = 3.57$ Å.

Solving the Radial Schrödinger Equation

In this problem, we will use Numerov's method to solve the differential equation numerically as suggested in the "Computational Physics" book by Thijssen. First, we will write equation (4) to the following form:

$$\frac{d^2}{dr^2}u_l(r) = -\alpha\Big(E - V(r) - \frac{l(l+1)}{\alpha r^2}\Big)u_l(r), \tag{8}$$

Where $\alpha = \frac{2m}{\hbar^2}$.

Starting from two initial values, y_1, y_2, and a step size $h := x_n - x_{n-1}$, Numerov's method lets us find the next values using auxiliary variables w defined as:

$$w_n = \left(1 - \frac{h^2}{12}F_n\right)y_n \tag{9}$$

whereupon we have:

$$w_{n+1} = 2w_n - w_{n-1} + h^2F_ny_n. \tag{10}$$

In our case, we have $y_n = u_l(r)$ and:

$$Fn = F(l, r, E) = \alpha\Big(V(r) + \frac{l(l+1)}{\alpha r^2} - E\Big) \tag{11}$$

Next, we would like to identify our initial condition. For the Lennard–Jones potential, We avoid integrating in the region of small r and start at a nonzero radius rmin where we use the analytic approximation of the solution for small r to find the starting values of the numerical solution that we use as our initial value u(0) as below:

$$u(r) = exp(-Cr^-5) \tag{12}$$

With $C = \sqrt{\epsilon\alpha/25}$ and $\alpha = 6.12$.

For the next value u(h), we will use the Numerov's formula as below:

$$u(h) = \frac{\left[2 + \frac{5h^2}{6}F(l, r_{min}, E)\right]\left[1 - \frac{h^2}{12}F(l, r_{min} - h, E)\right]u(0) + 2h\dot{u}(0)\left[1 - \frac{h^2}{6}F(l, r_{min} - h, E)\right]}{\left[1 - \frac{h^2}{12}F(l, r_{min} + h, E)\right]\left[1 - \frac{h^2}{6}F(l, r_{min} - h, E)\right] + \left[1 - \frac{h^2}{12}F(l, r_{min} - h, E)\right]\left[1 - \frac{h^2}{6}F(l, r_{min} + h, E)\right]} \tag{13}$$

Starting with u(0) and u(h), the Numerov algorithm can be applied straightforwardly.

Calculating the Phase Shift and Cross Section

To calculate the phase shift, we can use formula from equation (5) as below:

$$\delta_l = \tan^{-1}\left(\frac{Kj_l(kr_1) - j_l(kr_2)}{Kn_l(kr_1) - n_l(kr_2)}\right), \tag{14}$$

Where $k = \sqrt{\alpha E}$, $K = r_1 u_2 / r_2 u_1$, and $u_{1,2} = u_l(r_{1,2})$. Here, j_l and n_l are the first and second kind of spherical Bessel functions.

For the total cross section we first need the correction for the cutoff error. It can be shown that the error from cutting off at finite is given by:

$$\Delta\delta_l = -\frac{2m}{\hbar^2} k \int_{r_{max}}^{\infty} j_l^2(kr) V_{LJ}(r) r^2 \, dr \tag{15}$$

As before, $k = \sqrt{\alpha E}$ and j_l the regular spherical Bessel function.We cannot integrate out to infinity, but we can choose a large cutoff radius of $10r_{max}$.

Finally, we can sum the contributions to the cross section as per equation no. (6).

Computation result and discussion

Putting all the pieces together, we can run the program with the input parameter as below:

$$l_{max} = 50, h = 0.001, \epsilon = 5.9, \rho = 3.57, \alpha = 6.12/(\rho)^2, r_{min} = 0.5\rho, r_{max} = 5\rho$$

We divide the α with the factor of ρ^2 to have the dimension of $meV/\mathring{A}$ while we put $l_{max} = 50$ and $h = 0.001$ for accuracy purpose. However, this cost us the computation time which take almost an hour with Python, we can lower down this parameter to be $l_{max} = 10$ and $h = 0.01$ which should give enough accuracy. The rest of the parameters are suggested by the "Computational Physics" book by Thijssen. Below is the total cross section result compared as the function of energy:

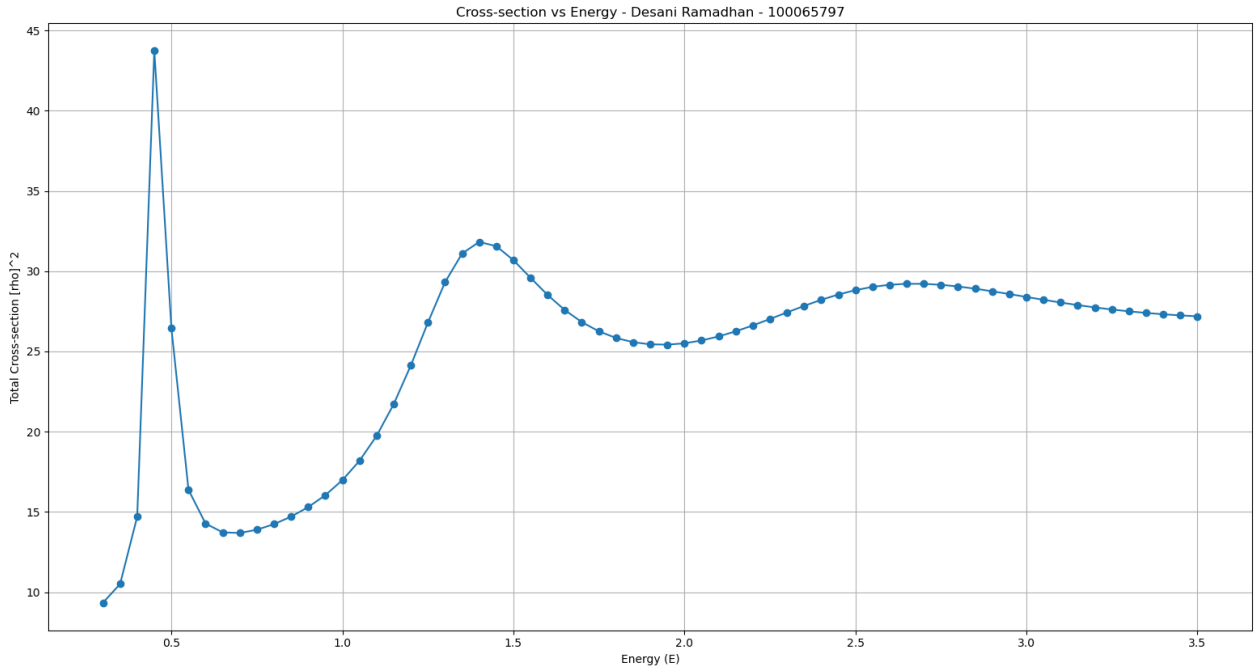

Figure 1. The total cross section shown as function of the energy for a Lennard– Jones potential modelling the H–Kr system calculated by 100065797

We can see, that the result from the program is similar to the experimental result as below:

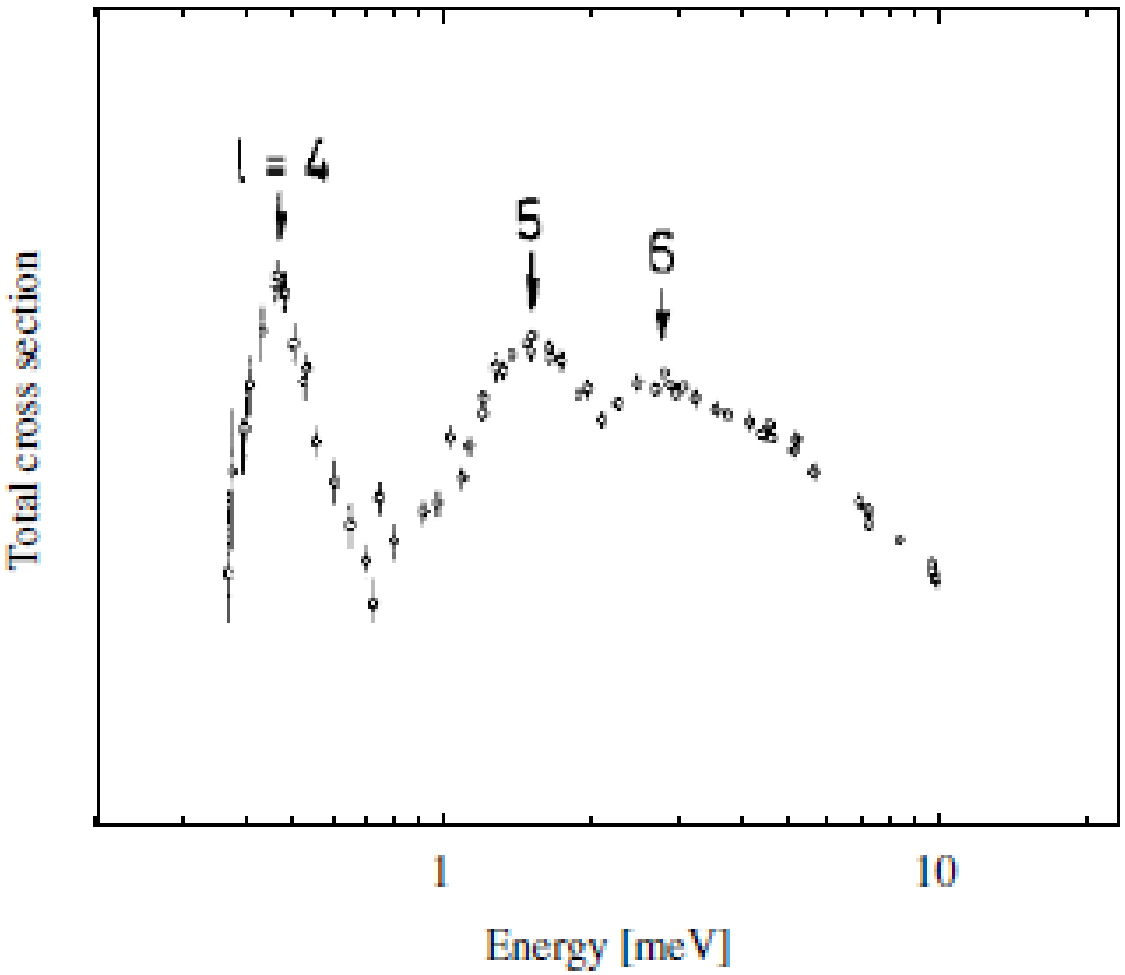

Figure 2. Experimental results as obtained by Toennies et al. [1] for the total cross section (arbitrary units) of the scattering of hydrogen atoms by krypton atoms as function of centre of mass energy.

Reference

[1] J. P. Toennies, W. Welz, and G. Wolf, 'Molecular beam scattering studies of orbiting resonances and the determination of Van der Waals potentials for H–He, Ar, Kr, and Xe and for H2–Ar, Kr and Xe", J. Chem. Phys., 71, 614–42 (1979)