UNIVERSITY OF TRENTO

Computational Physics (M.Sc.) - Homework 1

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INTRODUCTION

One of the most useful applications of solving the radial Schrödinger's Equation (SE) for a 3D problem with spherical symmetry is the determination of the cross section for a scattering experiment. In this homework you will study the case of H atoms scattering on a target of Kr atoms. The interaction between Kr and H is reasonably well described by a Lennard-Jones potential:

$$V_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right],$$

where $\epsilon = 5.99$ meV and σ is a parameter that will be computed based on the experimental data found in J.P. Toennis et al., J. Chem. Phys. **71**, 614 (1979) (available on Moodle). The variable r is the relative coordinate between the H and Kr atoms. Therefore the parameter σ provides a way to give a (very) rough estimate of the dimension of the Kr atom. In the following you will find the steps that are needed to solve the problem. State in the report all the procedures and the results for each of them. Codes can be developed in C, C++ or Python. Please attach a final version of the code inclusive of comments, or use a notebook (e.g., Jupyter notebook).

1 STEP 1 - VERIFY THE SOLUTIONS OF THE SE

- In the potential assume $\sigma = 2$Å up to Step 4.
- Compute $\hbar^2/2m_r$, where m_r is the reduced mass of the system in such a way that energies are expressed in meV and lengths in Å.

- Start from the code that was provided in class (available on Moodle) that solves the radial SE, and modify its structure to compute a set of solutions depending on l (the angular momentum) for a fixed value of the energy of the atoms in the center of mass frame of reference (take for instance $E = 1.5meV$)
- The numerical solution of the SE requires two initial points. From the condition:

$$\lim_{r\to 0} \frac{H\Psi(r)}{\Psi(r)} \neq \infty,$$

where $\Psi(r)$ is the solution of the SE:

$$\frac{\hbar^2}{2m_r}\nabla_r^2\Psi(r) + V_{LJ}(r) = E(r),$$

it is possible to see that for $r \to 0$ the radial wavefunction must be of the form:

$$\Psi(r) = \alpha \exp[-(b/r)^5].$$

Use this information to initialize the numerical solution of the SE. Start the mesh not from $r = 0$ but rather from some point $r_0 < \sigma$ (for example $r_0 = \sigma/2$ should work pretty well).

- Produce a series of curves for different values of l (for example in the range $l = 0 \ldots 6$ and verify that for $r >> \sigma$ the solution is oscillatory with a phase that depends on l.

2 Step 2 - Compute the phase shifts

- Implement a routine that computes the Bessel functions j_l and n_l with the iterative formula explained in class (and that can be found on the lecture notes available on Moodle). Compare your results to those available from library implementations.
- Use the curves that you have generated in the previous step to compute the phase shifts δ_l for the same value of energy that was used in step 1 choosing a few pairs of values of the distance $(r_1, r_2) >> \sigma$ and verifying that the result is independent on the specific choice

3 Step 3 - Compute the cross section

- Generalize the code in such a way that it computes the phase shifts for a whole range of values of E. Choose for example a range $E = 0 \ldots 3.5$ meV.
- Construct the total cross section for the H-Kr scattering process from the formula:

$$\sigma_{tot}(E) = \frac{4\pi\hbar^2}{2m_r E}\sum_{l=0}^{l_{max}}(2l+1)\sin^2(\delta_l(E)).$$

- Verify and discuss how the structure of $\sigma_{tot}(E)$ changes changing l_{max} from $l_{max} = 6$ to $l_{max} = 8$. Pay special attention to the position and shape of the peaks.

4 Step 4 - Fit the parameter σ of the LJ potential

- Use the values reported in Table I of Toennis' paper to fit the best value of the σ parameter in the potential. In particular, given the position in energy of the three peaks $E_1^{exp}, E_2^{exp}, E_3^{exp}$ visible in the H-Kr scattering,and the corresponding positions $E_i^{th}(\sigma)$ from your calculation minimize the quantity:

  $$\Delta^2(\sigma) = \sum_{i=1}^{3} (E_i^{th}(\sigma) - E_i^{exp})^2,$$

  and report the optimal value of σ, with an estimate of the error.

- (Optional) Use the values of σ_{tot}^{exp} available in literature to plot the computed and experimental cross sections, and comment the results. Pay attention to the definition of velocities (and the consequent values of the energies), and apply the necessary conversions.