Advanced Computational Physics - Exercise 1

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08/03/2019

Scattering of H atoms on a Kr atom

In this exercise we will try to model and reproduce the total cross section of H-Kr (elastic) scattering, as measured in the paper by J.P. Toennies, W. Welz, and G. Wolf, J. Chem. Phys. **71**, 614 (1979). We will start assuming a simple form of the interaction:

$$v(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^1 2 - \left(\frac{\sigma}{r}\right)^6 \right],$$

where $\epsilon = 5.9\text{meV}$, $\sigma = 3.18\text{Å}$, and r is the interatomic H-Kr distance. Notice that in general the parameters in the potential should be *fitted* against the experiment.

In order write a code that computes the desired cross section you will have to go through the following steps:[1]

1. Start writing a code solving the Schrödinger's equation for a simple one dimensional harmonic oscillator using the Numerov algorithm illustrated in class.

   Use a dimensionless Hamiltonian:

   $$-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2$$

   and plot the first 5 solutions (eigenvalues and eigenfunctions) in order to check the correctness of your code. Try in particular to check the dependence of your solution on the number of points in the mesh. [20 points]

[1]In the exercise report you will have to separately comment on each of the items in the list.

2. Repeat the same check for a 3-dimensional harmonic oscillator (use spherical coordinates) for values of the angular momentum $\ell = 0, 1, 2$ and for 3 values of the principal quantum number for each ℓ. [10 points]

3. Build a small program (that you will later transform into a function) to compute the Bessel functions j_ℓ and n_ℓ using the recursion formulae given in class:

$$j_{-1}(x) = \frac{\cos(x)}{x} \quad j_0(x) = \frac{\sin(x)}{x}$$

$$n_{-1}(x) = \frac{\sin(x)}{x} \quad n_0(x) = -\frac{\cos(x)}{x}$$

$$s_{\ell+1}(x) = \frac{2\ell+1}{x} s_\ell(x) - s_{\ell-1}(x).$$

Check the results against the exact values. [5 points]

4. Compute the constant $\hbar^2/2m$ in "natural" units of the problem, *i.e.* lengths in σ and energies in ϵ. [5 points]

5. Prove that the function $u(r) = A \exp\left[-\left(\frac{b}{r}\right)^5\right]$ is a solution for the Schrödinger equation including the interaction in the limit $r \to 0$. [5 points]

6. Modify your Numerov code in order to compute the solution of the SE inclusive of the interatomic potential. Use as boundary conditions the solution defined in the previous item (what about ℓ?) at some point $0 < r_{low} < \sigma$ and compute the phase shift δ_ℓ for $\ell = 0, 1, ..., 6$ and for an energy $E/\epsilon = 0.3$ from two points larger than $r_{max} = 5\sigma$. Discuss the variation of the results against small variations of r_{low} and r_{max}. [35 points]

7. Compute σ_{tot} in the interval $0 < E < 3.5 meV$ and for $\ell \leq 6$. Give a physical argument for truncating the sum over the angular momentum states, and compute the total cross section. Compare with the experimental results of the reference above, and discuss your findings. [20 points]