**Physics 514 Computational Physics, Fall 2020**

**Final Project Report : H-Kr Scattering Problem and Beyond**

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# 1 Background

For my final project, I will discuss the quantum elastic scattering problem with a spherically symmetric potential. Broadly speaking, the scattering experiments are powerful tools to understand how particles interact with each others. In most of the experimental set-ups, a beam of particles hits the target which also consists of many particles, then the measurements including the distribution of the particles will give more insights of the physical process.

If we have a good estimation of what the potential involved in the process might look like, we could parameterise the potential to meet the actual experimental data. The parameterisation of the potential is to write the analytical expression with several constants. In this case, I will reproduce the results from a 1979 paper [1] and feel the how good the parameterisation is.

# 2 Problems

## 2.1 Differential Equation

The quantum scattering problem could be described by the solutions of the single-particle Schrödinger equation with the reduced mass $m = m_1 m_2/(m_1 + m_2)$, and relative position $\vec{r}$:

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

This equation is a 3 dimensional partial differential equation at the first sight. If the problem is under the assumption that the potential is spherically symmetric, the solution of the 1 can always be written as

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

where $u_l(r)$ satisfies the radial Schrödinger equation:

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

Therefore, the 3-D Schrödinger equation becomes a relatively easy 1-D problem.

### 2.2 Potential

Now, the next question is what the spherically symmetric potential may look like in this case. In the molecular dynamics project, the Lennard-Jones potential is used for the potential between molecules. Here it is still acting a important role. In this problem, it has the form:

$$V_{LJ}(r) = \epsilon[(\frac{\rho}{r})^{12} - 2(\frac{\rho}{r})^{6}] \tag{4}$$

And the $\epsilon$ and $\rho$ in the equation are the parameters in the paper[1].

### 2.3 Physical Quantity

After setting up and solving the equation step by step, the comparison between the calculation and experimental data is the next goal. Although the wave function is not directly measurable, the intensity of the outgoing beam for various direction could still provide detailed information of the process[2]. The differential cross section, $d\sigma(\Omega)/d\Omega$ describes how these intensities distributes over the various direction, and the integration of it, $\Omega_{\text{tot}}$, would be the final quantity to compare. The expression of the integrated cross section is,

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2}\Sigma_{l=0}^{\infty}(2l+1)\sin^2\delta_l \tag{5}$$

where $\delta_l$ is the function of energy and $l$. And it is obtained from the asymptotic shift in the location of the radial wave function calculated for the given potential with respect to a wave function calculated without a potential[1].

Up to this point, the mission is more than clear right now. We use the parameterised potential to solve the simplified 1-D Schrödinger equation. The phase shift could be obtained from the radial wave equation and acts as an intermediate quantity between the wave function and the total cross section.

## 3 Techniques and Practical Considerations

The numerov algorithm will be used to solve the 1-D radial wave equation after re-organizing the equation in the following form:

$$F(l,r,E) = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} - E \tag{6}$$

$$\frac{d^2}{dr^2}u(r) = \frac{2m}{\hbar^2}F(l,r,E)u(r) \tag{7}$$

$$V_{LJ}(r) = \epsilon[(\frac{\rho}{r})^{12} - 2(\frac{\rho}{r})^{6}] \tag{8}$$

At here, the $m$ will the effective mass and the $r$ will be the relative difference. For krypton, $\epsilon = 5.9$meV and $\rho = 3.57\mathring{A}$[1],[3]. And for xeon, $\epsilon = 7.08$meV and $\rho = 3.82\mathring{A}$. In order to reduce the numerical error, I will covert the $\hbar^2/2m$ from SI units into the meV $\cdot\, \rho^2$ and the value of it is 1/6.12[2]. This will change with different particle-pairs because of different effective masses and $\rho$.

For the numerov algorithm, the two initial points are quite important. And in this case, they cannot be naively assigned due to the symmetric property of the effective potential. Instead, the analytical approximated solution will be use for calculating the two initial points. As $r \to 0$, $1/r^{12}$ diverges quickly than other terms, so the original equation could be written to:

$$\frac{d^2}{dr^2}u(r) = \epsilon\alpha\frac{1}{r^{12}}u(r) \tag{9}$$

And the solution of it is:

$$u(r) = \exp(-Cr^{-5}), C = \sqrt{\frac{\epsilon\alpha}{25}} \tag{10}$$

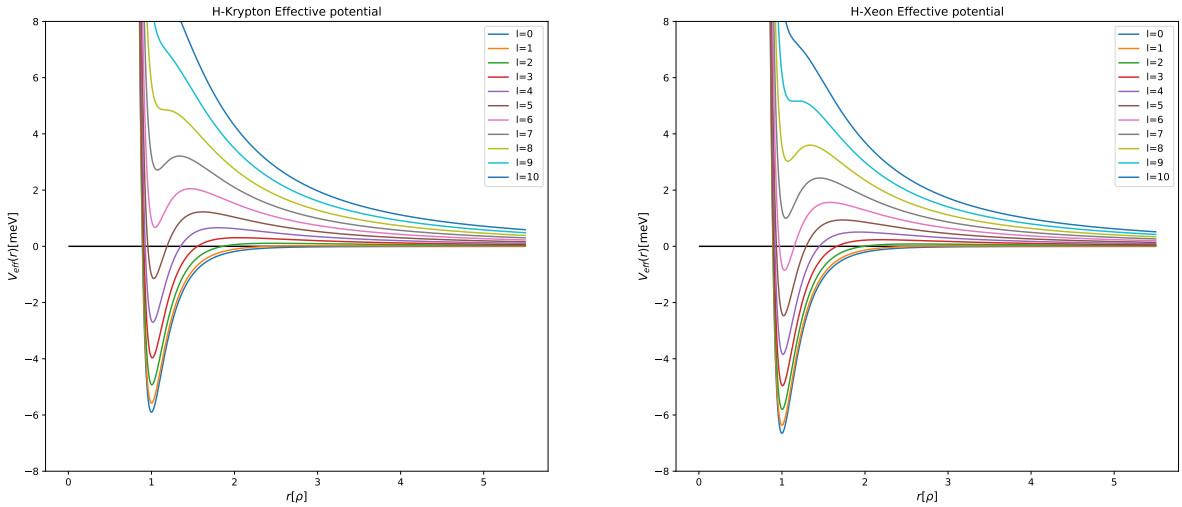
As for the ending point, the $r_{\max}$ is the point where the potential is roughly 0. For the krypton case, the value would be 5.5 $\rho$.

# 4 Result

First, let us look at the effective potential plots for Krypton and Xeon.

$$V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \tag{11}$$

For relatively higher $l$, the potential consists of three part, which are a hard core, a well and a barrier. And in such potential, the quasi-bound states are possible. The particle will resonate in the well at certain injected energy, and give a peak in the total cross section. Those are unstable bound states and eventually decay.

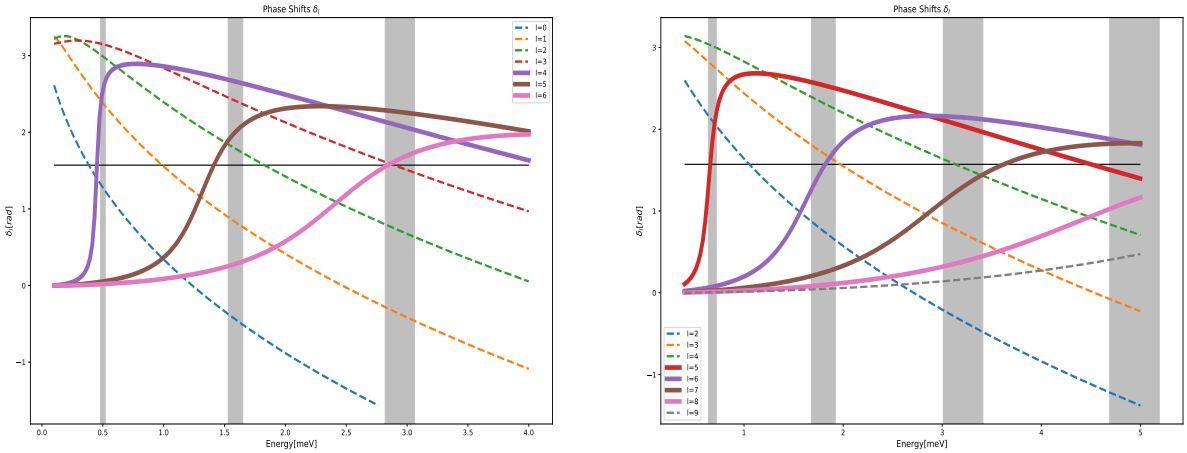



(a) Krypton (b) Xeon

Figure 1: Effective Potential for Krypton and Xeon

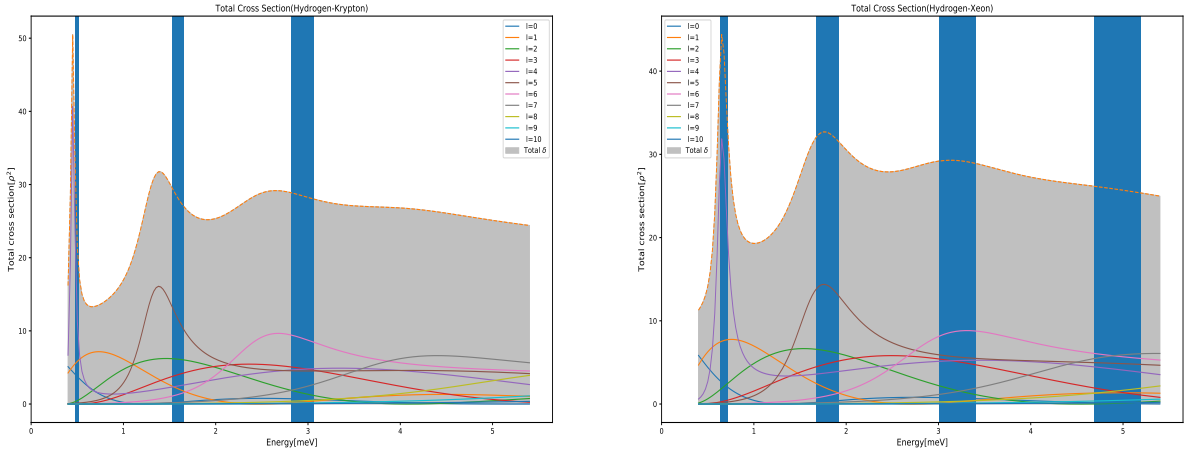
The radial wave function will also show the peak at the so-called resonance energy. The peaks are obvious for krypton in $l = 4, 5, 6$ cases and for Xeon in $l = 5, 6, 7, 8$ cases. I will include the animation for both Krypton and Xeon radial wave function in the final submission for the project.

Before examining the total cross section plot, let us look at the the relation between the phase shift and total cross section. In order to have a sharp peak in the total spectrum, the $\sin \delta_l$ needs to be maximized, which means $\delta_l \approx \frac{\pi}{2}$. So, in the phase shift diagram, we will see $\delta_l \approx \frac{\pi}{2}$ around the resonance energies.




(a) Krypton (b) Xeon

Figure 2: Phase Shifts for Krypton and Xeon




(a) Krypton (b) Xeon

Figure 3: Total cross section for Krypton and Xeon

More and more evidences show that we are going to see the nice sharp peaks at the resonance energies in the total cross section with no surprise. When comparing with the experimental data, the phase shifts show the similar trends for the same $l$ and the cross section plots show the peaks at the similar energy and the relative height of the peaks are pretty much the same.

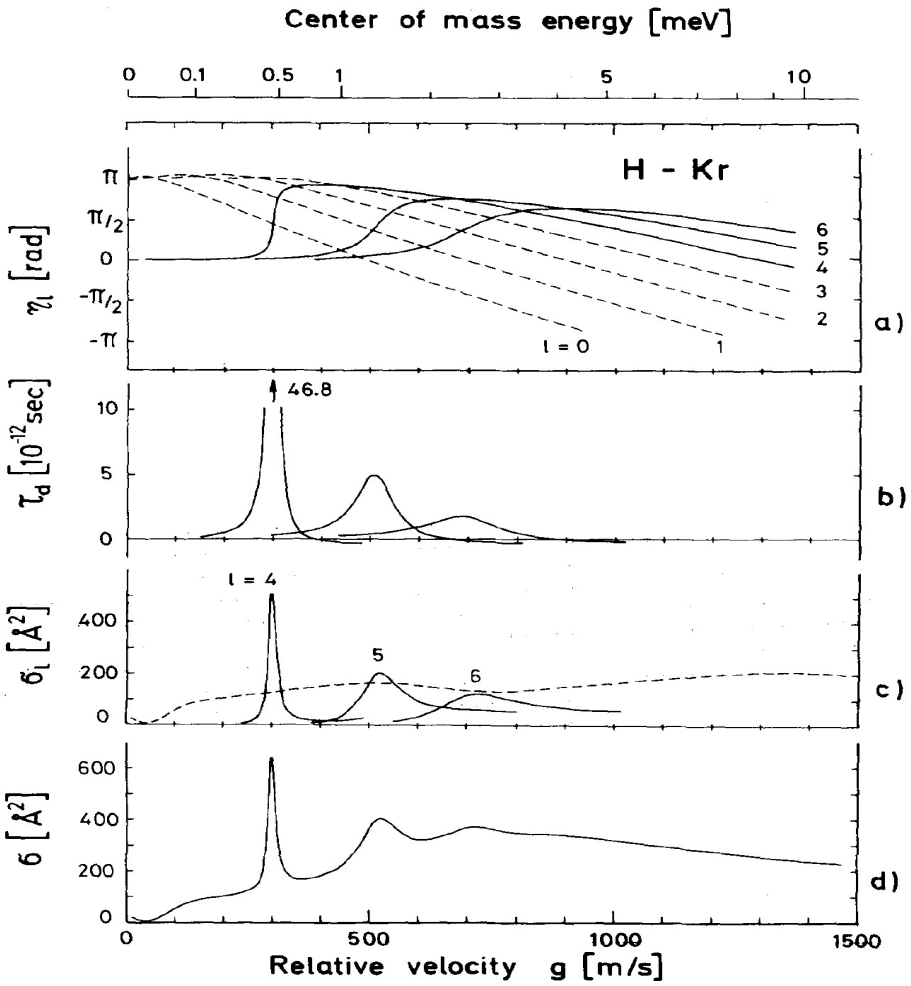



Figure 4: Result from the paper [1]

# References


[1] J. Peter Toennies, Wolfgang Welz, and Günther Wolf. Molecular beam scattering studies of orbiting resonances and the determination of van der Waals potentials for H–Ne, Ar, Kr, and Xe and for $H_2$–Ar, Kr, and Xe. *J. Chem. Phys.*, 71(614):614–642, 1979.

[2] J. Thijssen. *Computational Physics (2nd ed.)*. Cambridge University Press., Cambridge, 2007.

[3] V.Aquilanti, G.Liuti, F.Vecchio-Cattivi, and G.G.Volpi. Absolute total cross sections for scattering of hydrogen atoms by argon, krypton and xenon. *Chemical Physics Letters*, 15(2):305–308, 1972.