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Computational Quantum Physics
Exercise Sheet 3

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Exercise 1. H–Kr **scattering**

In this exercise, we consider the scattering of hydrogen atoms 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. In this exercise we will however restrict ourselves to calculating the total cross section $\sigma_{\text{tot}} = \oint d\Omega \, \frac{d\omega}{d\Omega}$.
To this end, we have to solve the Schrödinger equation in three dimensions,

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

where $V(r)$ is a spherically symmetric potential. From basic quantum mechanics, we know that in this case all eigenfunctions are also eigenfunctions of the angular momentum operators. In particular, they can be decomposed into a linear combination of spherical harmonics of the form

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

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

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

We have thus reduced the three-dimensional problem to a one-dimensional problem, to which we can apply the techniques learned in the last exercise.

The central quantity for quantum scattering is the phase shift δ_l. It can be computed from the asymptotic behaviour of the numerically integrated wave function at two points $r_1, r_2 \approx r_{\max}$ by using the formula

$$\tan\delta_l = \frac{K j_l(k_0 r_1) - j_l(k_0 r_2)}{K n_l(k_0 r_1) - n_l(k_0 r_2)}, \tag{1}$$

where $k_0 = \sqrt{2mE/\hbar^2}$, $K = r_1 u_2 / r_2 u_1$ and $u_{1,2} = u_l(r_{1,2})$, and where j_l and n_l are the spherical Bessel functions which you can find implemented in libraries. Then, the total scattering cross section is given by

$$\sigma_{\text{tot}} = \frac{4\pi}{k_0^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l. \tag{2}$$

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

$$V_{\text{LJ}}(r) = \epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - 2\left(\frac{\sigma}{r}\right)^{6}\right], \tag{3}$$

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

1. Reproduce the example shown in Fig. 1.
2. Observe how the scattering cross section changes with the cutoff $l_{\max}$. How do you interpret this change, and can you deduce a physical motivation for the truncation?

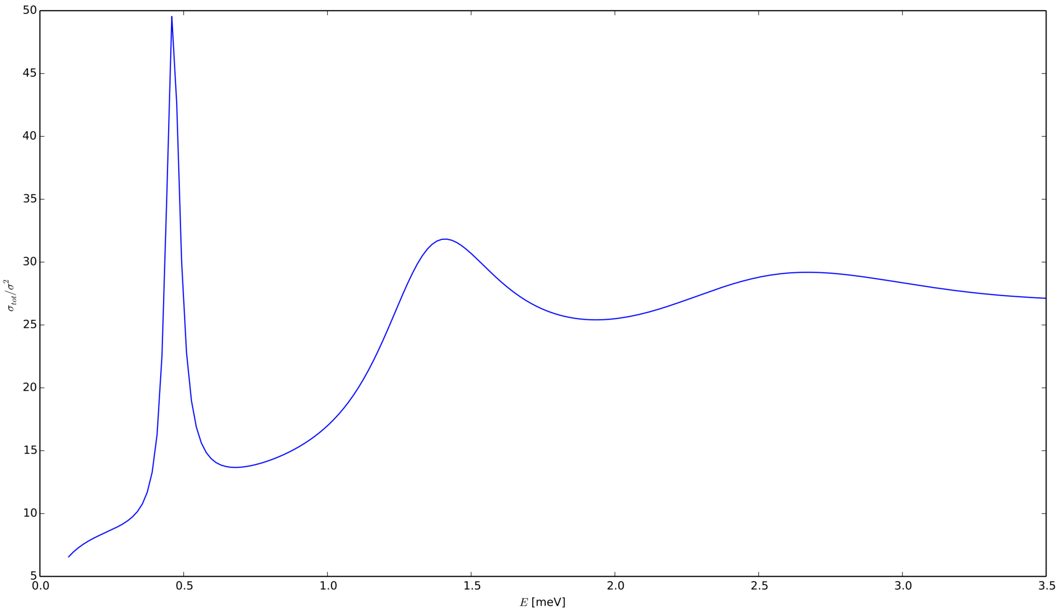

Figure 1: Total scattering cross section σ_{tot} for $r_{\text{min}} = 0.5\sigma$, $r_{\text{max}} = 5\sigma$, $l_{\text{max}} = 10$.

Practical Considerations

- 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,
$$u(r) = \exp(-Cr^{-5}) \tag{4}$$
with $C = \sqrt{6.12\epsilon/25}$ (in units of σ). Start your Numerov integration from some $r_{\text{min}} \sim 0.5\sigma$ and use (4) to set up the boundary conditions.
- A reasonable upper bound for the integration is $r_{\text{max}} = 5\sigma$.
- In (2), l ranges from 0 to ∞. Of course we cannot perform this summation to infinity. Instead, truncate at some l_{max}.
- You can use these values to check whether you're using the correct Bessel functions:
$$\begin{aligned} j_5(1.5) &= 6.69620596 \cdot 10^{-4} \\ n_5(1.5) &= -94.2361101 \end{aligned}$$

Exercise 2. Transverse field Ising model - Part I

In this exercise we will get familiar with the symmetries of the transverse field Ising model. The transverse field Ising chain with open boundary conditions is defined by the following Hamiltonian

$$\hat{H} = \hat{H}_{\text{Ising}} + \hat{H}_{\text{transv}} = J \sum_{i=1}^{N-1} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - h^x \sum_{i=1}^{N} \hat{\sigma}_i^x, \tag{5}$$

where we replaced the spin operators $\hat{S}_i^\mu = \frac{\hbar}{2}\hat{\sigma}_i^\mu, \mu = x, y, z$ with the Pauli matrices $\hat{\sigma}^\mu$ and set $\hbar = 1$. As the dimension of the Hilbert space grows exponentially in the number of sites on the chain we will only be able to tackle small problems. The symmetries of the Hamiltonian however allow us to simplify the problem: By organizing the basis states so that elements corresponding to the same symmetry sector are grouped together, the Hamiltonian becomes block diagonal. We can then solve the eigenvalue problem for the blocks independent of each other.

1. In the transverse field Ising model, the parity symmetry is defined as $\hat{P} = \prod_i \sigma_i^x$. Show that it commutes with the Hamiltonian.

For a system with periodic boundary conditions we can also exploit translational symmetries. Such a translation is represented by the operator T or a multiple of it. T is thereby defined as

$$T|s_1, s_2, ..., s_N\rangle = |s_N, s_1, ..., s_{N-1}\rangle.$$

The eigenvalues of the translation operator are the N-th roots of unity $z_k = \exp\left(i\frac{2\pi k}{N}\right)$ with $k = 0, ..., N-1$. The shift operator commutes with the Hamiltonian. It can therefore be decomposed into different $p_k = 2\pi k/N$ momentum subspaces. This means constructing cycles of states which are connected by T:

$$|\psi_n\rangle = T^n|\phi\rangle \qquad n \in \{1, 2, ..., N-1\}.$$

This cycle is spanned by the eigenstates of T with momentum p_k:

$$|\chi_k\rangle = \frac{1}{\sqrt{N_\phi}} \sum_{\nu=0}^{N-1} \left(e^{-ip_k}\ T\right)^\nu |\phi\rangle \qquad k = 0, 1, ..., N-1. \tag{6}$$

If the dimension of the cycle does not equal the number of lattice sites N, k is changed according to $k = 0, N/D, ..., (D-1)N/D$ with D being the dimension of the cycle.

2. Consider a system with N = 4 lattice sites. Find the momentum states $|\chi_k\rangle$ with momenta $p_k \in \{0, \pi/2, \pi, 3\pi/2, 2\pi\}$, by constructing the translation cycles for each basis state.

3. How should we choose the normalization constant N_ϕ of the states $|\chi_k\rangle$? If it helps, consider explicitly the case of N = 4 lattice sites.

4. Express the Hamiltonian of the transverse field Ising model in this new basis, i.e. calculate

$$\langle\chi'_{k'}|H_{\text{Ising}}|\chi_k\rangle,$$

$$\langle\chi'_{k'}|H_{\text{transv}}|\chi_k\rangle.$$