**Problem 1.** ***Time evolution of the transverse field Ising chain***

The goal of the exercise is to perform time evolution using on-the-fly matrix-vector multiplication.

The transverse field Ising chain with open boundary conditions is defined by the following Hamiltonian

$$\widehat{H} = \widehat{H}_{\text{Ising}} + \widehat{H}_{\text{transv}} = J \sum_{i=1}^{N-1} \widehat{\sigma}_i^z \widehat{\sigma}_{i+1}^z - h^x \sum_{i=1}^{N} \widehat{\sigma}_i^x.$$

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. To ensure optimal memory usage represent the wave function in a real space basis, using integers as basis states, e.g.

$$|\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow\uparrow\rangle = \text{bit}(10001011) = 139.$$

As a first step we split the time evolution operator into 2 non-commuting factors, the diagonal part given by $H_{\text{Ising}}$ and the nondiagonal part given by $H_{\text{transv}}$. The error involved in doing this can be kept small by choosing a small time step $\tau$ (see section 4.3.1 and 4.3.2):

$$\widehat{U} = \exp(-i\tau\,\widehat{H}) \approx \exp(-i\frac{\tau}{2}\,\widehat{H}_{\text{Ising}}) \exp(-i\tau\,\widehat{H}_{\text{transv}}) \exp(-i\frac{\tau}{2}\,\widehat{H}_{\text{Ising}}) + O(\tau^3)$$

The diagonal part $\exp(-i\frac{\tau}{2}\,\widehat{H}_{\text{Ising}})$ multiplies each basis state with a phase factor. The nondiagonal part can be further simplified into a product of single site operators

$$\exp(-i\tau\,\widehat{H}_{\text{transv}}) = \prod_{i=1}^{N} \exp(i\tau h^x\,\widehat{\sigma}_i^x).$$

1. Work out the time evolution operator $\exp(i\tau h^x\,\widehat{\sigma}_i^x)$ on a single site.
2. Implement the code that performs time evolution of the transverse field Ising chain with open boundary conditions.
3. Use your code to calculate the time evolution of a single basis state. Plot the magnetisation per site as a function of time. Start with an all-down configuration using only a transverse field $h^x$. You should see oscillations. Can you relate the period of the oscillations to the magnitude of $h^x$?
4. Now set the Ising coupling $J = 1$ and use a transverse field of $h^x = 0.4$. The starting configuration is again all-down except of a single spin flipped in the middle. What do you observe? How does the behaviour change with $h^x$.

**Problem 2.** 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 $\Omega$. In this exercise we will however restrict ourselves to calculating the *total cross section* $\sigma_{tot} = \oint d\Omega \, \frac{d\omega}{d\Omega}$.

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

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

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

The central quantity for quantum scattering is the *phase shift* $\delta_l$. 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

$$\tan \delta_l = \frac{K j_l(kr_1) - j_l(kr_2)}{K n_l(kr_1) - n_l(kr_2)},$$

where $k = \sqrt{2mE/\hbar^2}$, $K = r_1 u_2 / r_2 u_1$ 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

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

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

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

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?

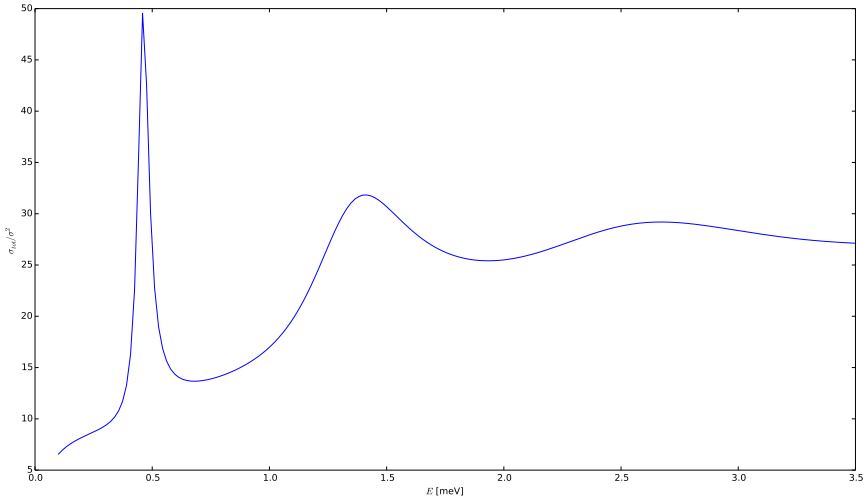


Figure 1: Total scattering cross section $\sigma_{\text{tot}}$ for $r_{\text{min}} = 0.5\sigma$, $r_{\text{max}} = 5\sigma$, $l_{\text{max}} = 10$.

## Practical Considerations

- Be careful to work in correct units. It is useful to work in units of $\sigma$ 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,
$$u(r) = \exp(-Cr^{-5}) \tag{2}$$
with $C = \sqrt{6.12\epsilon/25}$ (in units of $\sigma$). Start your Numerov integration from some $r_{\text{min}} \sim 0.5\sigma$ and use (2) to set up the boundary conditions.
- A reasonable upper bound for the integration is $r_{\text{max}} = 5\sigma$.
- In (1), $l$ ranges from 0 to $\infty$. Of course we cannot perform this summation to infinity. Instead, truncate at some $l_{\text{max}}$.
- You can use these values to check whether you're using the correct Bessel functions:
$$\begin{aligned} j_5(1.5) &= 6.69620596 \cdot 10^{-4} \\ n_5(1.5) &= -94.2361101 \end{aligned}$$