Quantum dynamics computer assignment 3: He+Xe elastic scattering

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(Dated: May 24, 2024)

Energy grid

Compute and plot the integral elastic cross sections for He+Xe scattering on a grid of 100 collision energies from 10^{-4} cm−1 to 10 cm−1 (use a log scale). Energy unit conversion: 1 E_h = 219 474.631 370 98 cm^{-1}.

Morse potential

The interaction between He and Xe is given by a Morse potential,

$$V(r) = D_e(1 - e^{-\beta(r-r_e)})^2 - D_e, \tag{1}$$

with dissociation energy $D_e = 20.41$ cm^{-1}, equilibrium distance $r_e = 7.52\ a_0$, and exponent $\beta = 0.8931385\ a_0^{-1}$.

Masses

The atomic masses are $m_{\mathrm{He}} = 4.002\,603\,2497$ amu and $m_{\mathrm{Xe}} = 131.293$ amu. Conversion of atomic mass units (amu) to atomic units of mass (m_e): 1 amu = 1822.8885 m_e.

Grid

Calculate the de Broglie wave length λ at the equilibrium distance r_e for the highest collision energy $E_{\max} = 10$ cm^{-1}. Take a grid spacing of $\Delta = \lambda/20$. Setup a grid $R_i = R_0 + i\Delta$, $i = 1, \ldots, n$, with $R_0 = 4\ a_0$ and $R_n = 15\ a_0$.

Upper limit for l

In the partial wave expansion, choose the upper limit of the rotational quantum number l such that it corresponds to an impact parameter of $b = R_n$ at a collision energy $E_{\max}$.

Spherical Bessel functions

Spherical Bessel functions of the first kind, $j_l(z)$, can be computed using this relation

$$j_l(z) = \sqrt{\frac{\pi}{2z}} J_{l+1/2}(z), \tag{2}$$

where the Bessel functions of the first kind, $J_{l+1/2}(z)$, are available in Scilab as `besselj(l+0.5, z)`.

Spherical Bessel functions of the second kind, $y_l(z)$, can be computed from

$$y_l(z) = \sqrt{\frac{\pi}{2z}} Y_{l+1/2}(z), \tag{3}$$

and the Bessel functions of the second kind, $Y_{l+1/2}(z)$, are available in Scilab as `bessely(l+0.5, z)`.

The relation between spherical Hankel functions and spherical Bessel functions are given in section 7.5 of the lecture notes. Note that you will actually need $zh_l^{(2)}(z)$ and $zh_l^{(1)}(z)$ for matching.

Spherical Bessel functions in Python

In Python some libraries have to be imported. The spherical Hankel functions, times the factor z can be computed with:

```
import numpy as np
import matplotlib.pyplot as plt
import math
from scipy.special import spherical_jn, spherical_yn

def SphericalHankelPlus(z,l):
    return spherical_jn(l,z)+1j*spherical_yn(l,z)
def SphericalHankelMin(z,l):
    return spherical_jn(l,z)-1j*spherical_yn(l,z)
```