

Quantum Scattering from Spherically Symmetric Potential

- Scattering is one of the best method to obtain the structure of matter.
- Scattering can be used to measure the interaction (Inverse problem).

Scattering:

X-ray

Neutron

Electron

Elastic scattering \iff Energy conserved.

Inelastic scattering \iff Energy dissipated.

Measured quantity in an scattering experiment: The cross section.

$\frac{d\sigma}{d\Omega}$ differential cross section

$\sigma_{tot} = \int \frac{d\sigma}{d\Omega} d\Omega$ total cross section

We consider the simplest case, the potential scattering from a spherical symmetric potential here.

The theory:

Starting point:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \Psi(\mathbf{r}) = E\Psi(\mathbf{r}).$$

In a scattering experiment, one have incident wave and scattered wave. We measure the scattering wave far from the scattering center. The wave function $\Psi(\mathbf{r})$ under scattering experiment can be written as in the most general case as:

$$\Psi(\mathbf{r}) = \Psi_i(\mathbf{r}) + \Psi_s(\mathbf{r}).$$

The incident wave is a plane wave and can be written

$$\Psi_i(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}},$$

and scattering wave is spherical wave at large distance from the scattering center,

$$\Psi_s(\mathbf{r}) = f(\theta) \frac{e^{ikr}}{r}.$$

So that

$$\Psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \mathbf{f}(\theta) \frac{e^{ikr}}{r}.$$

From here the differential cross section is

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2,$$

and the total cross section

$$\sigma_{tot} = \int |f(\theta)|^2 d\Omega.$$

Solution of the Schödinger Equation

For a spherical symmetric potential, the solution of the Schödinger equation can always be written as

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

Where $u_l(r)$ satisfies the radial Schödinger equation

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

when $r \rightarrow 0$, if $V(r) \sim \frac{1}{r^\alpha}$, $\alpha > 2$, we have

$$\left(\frac{d^2}{dr^2} - \frac{C}{r^\alpha} \right) u = 0,$$

set $u = e^f$, we get

$$f'' + f'^2 - \frac{C}{r^\alpha} = 0,$$

let $f = ar^s$,

$$s(s-1)ar^{s-2} + s^2a^2r^{2(s-1)} - Cr^{-\alpha} = 0,$$

if $s-2 = -\alpha$, $s = 2 - \alpha$, $2(s-1) = 2 - 2\alpha < s-2$, inconsistent.

if $2(s-1) = -\alpha$, $s = 1 - \alpha/2$, $s-2 = -1 - \alpha/2 > 2(s-1)$.

remember: $\alpha > 2$.

$$s^2a^2 = C, \quad a^2 = \frac{C}{s^2}.$$

There is no real solution if $C < 0$, i.e. the attractive potential.

In the case of $C > 0$,

$$u \sim \exp\left(-\frac{a}{r^{1-\alpha/2}}\right).$$

For attractive potential we must have $\alpha \leq 2$.

The physics:

Landau collapse

When $r > r_{\max}$, we assume that $V(r) \equiv 0$. The Schödinger equation can be written as

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

define $k^2 = \frac{2mE}{\hbar^2}$, The solution of the above equation are

$$u_l(r) = \begin{pmatrix} r j_l(kr) \\ r n_l(kr) \end{pmatrix}.$$

$j_l(kr)$ and $n_l(kr)$ are spherical Bessel functions of the first and second kind. We write the solution as

$$u_l(r) \sim r (\cos \delta_l j_l(kr) - \sin \delta_l n_l(kr)).$$

When $kr \rightarrow \infty$, we have

$$\begin{aligned} j_l(kr) &\simeq \frac{\sin\left(kr - \frac{l\pi}{2}\right)}{kr} \\ n_l(kr) &\simeq -\frac{\cos\left(kr - \frac{l\pi}{2}\right)}{kr} \end{aligned}$$

which leads to

$$u_l(r) \sim \sin\left(kr - \frac{l\pi}{2} + \delta_l\right),$$

δ_l is called *phase shift*.

Since

$$\begin{aligned} \Psi(\mathbf{r}) &= \sum_{l=0}^{\infty} A_l \frac{u_l(r)}{r} P_l(\cos \theta) \\ &= e^{ikr \cos \theta} + f(\theta) \frac{e^{ikr}}{r}, \end{aligned}$$

when $r \rightarrow \infty$. Using the expansion

$$e^{ikr \cos \theta} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta),$$

suppose that:

$$f(\theta) = \sum_{l=0}^{\infty} f_l P_l(\cos \theta).$$

We have

$$\begin{aligned} & \sum_{l=0}^{\infty} A_l \frac{\sin(kr - \frac{l\pi}{2} + \delta_l)}{kr} P_l(\cos \theta) \\ &= \sum_{l=0}^{\infty} \left(f_l \frac{e^{ikr}}{r} + (2l+1)i^l \frac{\sin(kr - \frac{l\pi}{2})}{kr} \right) P_l(\cos \theta), \end{aligned}$$

considering that $P_l(\cos \theta)$ are linear independent (actually orthogonal) for different l , the coefficients have to be equal.

$$\begin{aligned} & \frac{A_l}{2ikr} \left(e^{ikr} e^{i\delta_l} (-i)^l - e^{-ikr} e^{-i\delta_l} (i)^l \right) \\ &= f_l \frac{e^{ikr}}{r} + (2l+1)i^l \frac{1}{2ikr} \left(e^{ikr} (-i)^l - e^{-ikr} (i)^l \right), \end{aligned}$$

here we used

$$e^{i\frac{l\pi}{2}} = i^l \quad e^{-i\frac{l\pi}{2}} = (-i)^l.$$

The coefficients of e^{ikr} and e^{-ikr} should be equal respectively,

$$\begin{aligned} A_l (-i)^l e^{i\delta_l} &= 2ikf_l + (2l+1) \\ A_l i^l e^{-i\delta_l} &= (2l+1)(-1)^l \end{aligned}$$

Solve for A_l and f_l we have

$$\begin{aligned} A_l &= (2l+1)i^l e^{i\delta_l} \\ f_l &= \frac{2l+1}{k} e^{i\delta_l} \sin \delta_l \end{aligned}$$

The differential cross section thus given by

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{1}{k^2} \left| \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l} \sin \delta_l P_l(\cos \theta) \right|^2,$$

and the total cross section is

$$\sigma_{tot} = \int |f(\theta)|^2 d\Omega = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l,$$

here we used the relation

$$\int P_l(\cos \theta) P_{l'}(\cos \theta) d\Omega = \frac{4\pi}{2l+1} \delta_{ll'}.$$

Calculation of the phase shifts

In order to calculate the phase shifts, we have to solve the Schödinger equation numerically. The procedure is as the following:

- 1, Integration the Schödinger equation to some points beyond r_{\max} .
- 2, Compare the solution with the asymptotic expressions.

In real calculations we integration the Schödinger equation to two points both beyond the r_{\max} , say to r_1 and r_2 , and determine the phase shifts from these two points.

At large distance we have

$$u_l(r) \sim r (\cos \delta_l j_l(kr) - \sin \delta_l n_l(kr))$$

Integration to r_1 and r_2 , we should have

$$\begin{aligned} u_l(r_1) &\sim r_1 (\cos \delta_l j_l(kr_1) - \sin \delta_l n_l(kr_1)) \\ u_l(r_2) &\sim r_2 (\cos \delta_l j_l(kr_2) - \sin \delta_l n_l(kr_2)) \end{aligned}$$

where $u_l(r_1)$ and $u_l(r_2)$ are two numbers, from the above equation we get

$$\frac{r_1 u_l(r_2)}{r_2 u_l(r_1)} = \frac{j_l(kr_2) - \tan \delta_l n_l(kr_2)}{j_l(kr_1) - \tan \delta_l n_l(kr_1)},$$

solve for phase shift we have

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

here

$$K = \frac{r_1 u_l(r_2)}{r_2 u_l(r_1)}.$$

Integration, start point and method:

Start point

We have to integration the Schödinger equation from $r = 0$, that means we need to know two values at the starting point since the equation is second order, if the potential tends to infinity slower than $\frac{1}{r^2}$, the form of u_l near the origin is

$$u_l(r) \sim r^{l+1}$$

The algorithm: Numerov method

Consider a more general equation

$$y''(x) = f(x)y(x) + g(x)$$

Expand $y(x+h)$:

$$\begin{aligned}
y(x+h) &= y(x) + y'(x)h + \frac{1}{2}y''(x)h^2 + \frac{1}{3!}y^{(3)}(x)h^3 \\
&\quad + \frac{1}{4!}y^{(4)}(x)h^4 + \frac{1}{5!}y^{(5)}(x)h^5 + O(h^6) \\
y(x-h) &= y(x) - y'(x)h + \frac{1}{2}y''(x)h^2 - \frac{1}{3!}y^{(3)}(x)h^3 \\
&\quad + \frac{1}{4!}y^{(4)}(x)h^4 - \frac{1}{5!}y^{(5)}(x)h^5 + O(h^6)
\end{aligned}$$

add the two to get

$$y(x+h) + y(x-h) = 2y(x) + y''(x)h^2 + \frac{1}{12}y^{(4)}h^4 + O(h^6).$$

Similarly we have

$$y''(x+h)h^2 + y''(x-h)h^2 = 2y''(x)h^2 + y^{(4)}(x)h^4 + O(h^6).$$

Combined these two

$$\begin{aligned}
y(x+h) + y(x-h) &= 2y(x) + \left(1 - \frac{1}{6}\right) [f(x)y(x) + g(x)] h^2 \\
&\quad - \frac{h^2}{12} [f(x+h)y(x+h) + g(x+h)] \\
&\quad - \frac{h^2}{12} [f(x-h)y(x-h) + g(x-h)] + O(h^6).
\end{aligned}$$

Define

$$W(x) = \left(1 - \frac{h^2}{12}f(x)\right) y(x),$$

then

$$\begin{aligned}
W(x+h) &= 2W(x) - W(x-h) + h^2(f(x)y(x) + g(x)) \\
&\quad + h^2 \delta^{(2)}g(x) + O(h^6),
\end{aligned}$$

here

$$\delta^{(2)}g(x) = g(x+h) + g(x-h) - 2g(x).$$

Back to our problem

Define

$$\begin{aligned}
F(l, E, r) &= V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} - E, \\
W(l, r) &= \left(1 - \frac{h^2}{12}F(l, E, r)\right) u_l(r)
\end{aligned}$$

the Schödinger equation can be discretized as

$$W(l, r+h) = 2W(l, r) - W(l, r-h) + h^2F(l, E, r)u_l(r).$$

For regular potential, we may choose

$$\begin{aligned} u_l(0) &= 0 \\ u_l(h) &= h^{l+1} \end{aligned}$$

and starting calculations. For irregular potentials. the start point will be studied case by case.

A Real Problem

Calculation of the cross section of low energy scattering of Hydrogen atom by Krypton.

The Interaction:

$$V(r) = \varepsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right],$$

where

$$\varepsilon = 5.9 \text{meV}, \quad \sigma = 3.57 \text{\AA}.$$

When $r \rightarrow 0$, the potential is irregular, lets study the solution close to origin. At extreme small r , the dominate contribution comes from the part proportional to $\frac{1}{r^{12}}$, so the Schödinger equation reduced to

$$\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} - \varepsilon \left(\frac{\sigma}{r} \right)^{12} u = 0,$$

which can be simplified to

$$\frac{d^2 u}{dr^2} - \frac{\varepsilon \alpha}{r^{12}} u = 0,$$

where

$$\alpha = \frac{2m}{\hbar^2} \sigma^{12}.$$

Let

$$u = e^f,$$

as before we get

$$u = e^{-\frac{C}{r^5}},$$

here $C^2 = \frac{\varepsilon \alpha}{25}$.

Now we are in the position of practical implementation

1, Set up units, in this problem, we use meV as unit of energy and σ as unit of length. We may also use ε as unit of energy. In the first place

$$\begin{aligned} \alpha &= \frac{2m_H}{\hbar^2} \frac{1}{1 + \frac{m_H}{m_{Kr}}} = \frac{2 \times 1.67 \times 10^{-24} \text{g}}{(1.05 \times 10^{-27})^2 \text{erg}^2 \text{s}^2} \frac{1}{1 + \frac{1}{83.8}} \\ &= \frac{2 \times 1.67 \times 10^{-24}}{(1.05 \times 10^{-27})^2} \frac{1}{1 + \frac{1.01}{83.8}} \frac{1.602 \times 10^{-15} \times 3.57^2}{10^{16}} \frac{1}{\text{meV} \sigma^2} \\ &= 6.11 (\text{meV})^{-1} \sigma^{-2}. \end{aligned}$$

In the second place

$$\begin{aligned}
 \alpha &= \frac{2m_H}{\hbar^2} \frac{1}{1 + \frac{m_H}{m_{Kr}}} = \frac{2 \times 1.67 \times 10^{-24} g}{(1.05 \times 10^{-27})^2 erg^2 s^2} \frac{1}{1 + \frac{1}{83.8}} \\
 &= \frac{2 \times 1.67 \times 10^{-24}}{(1.05 \times 10^{-27})^2} \frac{1}{1 + \frac{1.01}{83.8}} \frac{1.602 \times 10^{-15} \times 3.57^2 \times 5.9}{10^{16}} \frac{1}{\varepsilon \sigma^2} \\
 &= 36.1 \varepsilon^{-1} \sigma^{-2}.
 \end{aligned}$$

2, Instead of energy E , we use wave vector k , defined as $k = \frac{\sqrt{2mE}}{\hbar}$.

3, Cut the LJ potential at some point, say $r_{\max} = 5\sigma$; The error due to this cut off can be corrected by the Born approximation(tail correction).

$$\Delta\delta_l = -\frac{2m}{\hbar^2} k \int_{r_{\max}}^{\infty} j_l(kr)^2 V(r) r^2 dr.$$

4, Integration at a point start from r_{\min} , where the analytic asymptotic solution is valid when $r < r_{\min}$, try to find an appropriate r_{\min} , try $r_{\min} = 0.5\sigma$.

5, We need routines to calculate values of spherical Bessel functions; If we want to obtain the differential cross section we also need routines to calculate values of Legendra polynomials; Try to find routines yourselves, in NMS, in my computational physics lecture notes or in any commercial packages or write one yourselves.

6, The sum over l should converge at some values of l_{\max} , classically determined by

$$\hbar l_{\max} = \hbar k r_{\max}.$$

Homework:

- 1, Write code for Numerov method, test it with some analytically solved problems;
- 2, Find or write routines for spherical Bessel functions and Legendra polynomials;
- 3, Calculate total cross section of H-Kr scattering as function of energy;
- 4, Calculate differential cross sections for 5-10 θ values as functions of energy.