Basic scattering theory

This exercise intends to teach a few basics on scattering theory. At various instances you are asked to complete calculations or to add physical interpretation.

6.1. General setting of scattering scenario

6.1.A Consider two particles of mass m interacting via the collision potential $V(\vec{r}_1 - \vec{r}_2)$ and the trapping potential $V_{trap}(\vec{r}_1,\vec{r}_2) = \frac{m\Omega^2}{2}\left(\vec{r}_1^{\,2} + \vec{r}_1^{\,2}\right)$ subject to the Schrödinger-equation $\left[-\frac{\hbar^2}{2m}\Delta_1 - \frac{\hbar^2}{2m}\Delta_2 + V(\vec{r}_1-\vec{r}_2) + V_{trap}(\vec{r}_1,\vec{r}_2)\right]\phi(\vec{r}_1,\vec{r}_2) = E\,\phi(\vec{r}_1,\vec{r}_2)$.

Employ centre of mass coordinates $\vec{r} \equiv \vec{r}_1 - \vec{r}_2,\ \vec{R} \equiv \frac{\vec{r}_1+\vec{r}_2}{2}$, $\mu \equiv \frac{m}{2},\ M = 2m$ and introduce the separation Ansatz $\phi(\vec{r},\vec{R}) = \phi_k(\vec{r})\,\chi_K(\vec{R})$ to show that

$$\left[-\frac{\hbar^2}{2\mu}\Delta_r + V(\vec{r}) + \frac{\mu\Omega^2}{2}\vec{r}^{\,2}\right]\phi_k(\vec{r}) = \frac{\hbar^2 k^2}{2\mu}\,\phi_k(\vec{r})$$
$$\left[-\frac{\hbar^2}{2M}\Delta_R + \frac{M\Omega^2}{2}\vec{R}^2\right]\chi_K(\vec{R}) = \frac{\hbar^2 K^2}{2M}\,\chi_K(\vec{R})$$

6.1.B Verify that for $\Omega = 0$ and $V(\vec{r}) = \frac{\hbar^2}{2\mu}U(\vec{r})$ the relative coordinate Schrödinger equation simplifies to $\left[\Delta + k^2 - U(\vec{r})\right]\phi_k(\vec{r}) = 0$ (1)

Show that a wave function $\phi_k(\vec{r})$ is solution to eq.(1) if the *integral scattering equation* holds

$$\phi_k(\vec{r}) = \phi_{0,k}(\vec{r}) + \int d^3r'\,G(\vec{r}-\vec{r}\,')\,U(\vec{r}\,')\,\phi_k(\vec{r}\,') \qquad (2)$$

with $\left[\Delta + k^2\right]G(\vec{r}) = \delta(\vec{r})$ and $\left[\Delta + k^2\right]\phi_{0,k}(\vec{r}) = 0$.

6.1.C Using the relations $\Delta\frac{1}{r} = -4\pi\,\delta(\vec{r})$, verify that the solutions to $\left[\Delta + k^2\right]G(\vec{r}) = \delta(\vec{r})$ are the (outgoing and incoming) Green's functions

$$G_\pm(\vec{r}) = -\frac{1}{4\pi}\frac{e^{\pm ikr}}{r} \quad .$$

6.1.D Now choose an incoming wave $\phi_{0,k}(\vec{r}) = e^{ik\hat{k}_{in}\vec{r}}$ propagating along the unit vector $\hat{k}_{in}$ with wavenumber k. Upon insertion of $G_+(\vec{r})$ into eq. (2) one obtains

$$\phi_k(\vec{r}) \;=\; e^{ik\hat{k}_{in}\vec{r}} \;-\; \frac{1}{4\pi} \int d^3r' \, \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \, U(\vec{r}') \, \phi_k(\vec{r}') \qquad (3)$$

i.e., the scattering wave function is a superposition of an incoming plane wave propagating along the direction $\hat{k}_{in}$ and a scattered wave given by the integral.

Now consider the asymptotic behavior of $\phi_k(\vec{r})$ i.e., its behavior far away from where the scattering potential acts. Assume that the scattering potential $U(\vec{r}')$ is centered closely around $\vec{r}' \approx 0$ and consider large $|\vec{r}|$ such that the relevant values of $\vec{r}'$ in the integral in eq. (3) satisfy $|\vec{r}'| \ll |\vec{r}|$. Convince yourself that then you may approximate $|\vec{r}-\vec{r}'| \approx r - \hat{r}\,\vec{r}'$ and replace $\dfrac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}$ by $\dfrac{e^{ik|\vec{r}|}e^{-ik\,\hat{r}\,\vec{r}'}}{|\vec{r}|}$ in eq. (3). Verify that then

$$\phi_k(\vec{r}) \;\approx\; e^{i\,k\hat{k}_{in}\vec{r}} \;+\; f_k(k,\hat{k}_{in},\hat{r}) \, \frac{e^{ikr}}{r} \qquad (4)$$

with the *scattering amplitude* $\quad f_k(k,\hat{k}_{in},\hat{r}) \;=\; -\dfrac{1}{4\pi} \displaystyle\int d^3r' \;\, e^{-ik\,\hat{r}\,\vec{r}'} \, U(\vec{r}') \, \phi_k(\vec{r}') \qquad$ (4b)

and the *differential scattering cross section* $\quad \sigma(k,\hat{k}_{in},\hat{r}) = \left|f_k(k,\hat{k}_{in},\hat{r})\right|^2$. $\qquad$ (5)

6.2. Expansion in terms of spherical harmonics

We now refer to what we now about central potentials from studying the hydrogen atom. For central potentials $U(\vec{r}) = U(r)$ the eigensolutions of the stationary Schrödinger equation have the form

$$\phi_{k,\ell,m}(\vec{r}) \;=\; \frac{1}{r}\, Y_\ell^m(\phi,\theta) \;\; u_{k,\ell}(r) \qquad (6)$$

$$\left[\frac{\partial^2}{\partial r^2} - \frac{\ell(\ell+1)}{r^2} - U(\vec{r}) + k^2\right] u_{k,\ell}(r) = 0 \qquad (7)$$

where for $r \to \infty$ eq.(7) becomes $\left[\dfrac{\partial^2}{\partial r^2} + k^2\right] u_{k,\ell}(r) \approx 0 \qquad$ (8)

(if $U(\vec{r})$ was the Coulomb potential, eq.(7) would be the radial equation of the hydrogen atom)

The regular solutions of eq.(7) with $U = 0$ are $r\;J_\ell(kr)$ with the spherical Bessel functions (first kind) $J_\ell(kr)$ of order ℓ. Other solutions (von Neuman & Hankel functions) have a pole at $r = 0$.

Our goal is to construct scattering solutions with an asymptotic behavior of the form given in eq.(4) superposing the basis states in eq.(6). Begin with noting that the general solution for eq. (8) is $u_{k,\ell}(r) \approx A\, e^{ikr} + B\, e^{-ikr}$ with complex amplitudes A, B. Assuming that the potential satisfies $U(r<0) = \infty$, i.e., no wave is transmitted into the region $r<0$, we have $|A| = |B|$. Setting $A = -e^{i2\delta_\ell(k)} B$ (which defines $\delta_\ell(k)$ in terms of A and B) and $B = \frac{-e^{i\ell\pi/2}}{i2kr}$ and making use of eq.(6), we thus find solutions of the stationary Schrödinger equation with an asymptotic behavior

$$\phi_{k,\ell,m}(\vec{r}) \xrightarrow[r\to\infty]{} Y_\ell^m(\phi,\theta)\, \frac{-1}{i2kr} \left[e^{i\ell\pi/2} e^{-ikr} - e^{-i\ell\pi/2} e^{i2\delta_\ell(k)} e^{ikr} \right] \tag{9}$$

The most general solution of the Schrödinger equation $\phi(\vec{r}) \equiv \sum_{\ell,m} C_{k,\ell,m}\, \phi_{k,\ell,m}(\vec{r})$ then has the asymptotic form

$$\phi(\vec{r}) \xrightarrow[r\to\infty]{} \sum_{\ell,m} C_{k,\ell,m}\, Y_\ell^m(\phi,\theta)\, \frac{-1}{i2kr} \left[e^{i\ell\pi/2} e^{-ikr} - e^{-i\ell\pi/2} e^{i2\delta_\ell(k)} e^{ikr} \right]. \tag{10}$$

$$= \sum_{\ell,m} C_{k,\ell,m}\, Y_\ell^m(\phi,\theta)\, \frac{-1}{i2kr} \left[e^{i\ell\pi/2} e^{-ikr} - e^{-i\ell\pi/2} e^{ikr} \right] + \sum_{\ell,m} C_{k,\ell,m}\, Y_\ell^m(\phi,\theta)\, \frac{1}{i2kr}\, e^{-i\ell\pi/2} (e^{i2\delta_\ell(k)} - 1)\, e^{ikr}$$

$$= \sum_{\ell,m} C_{k,\ell,m}\, Y_\ell^m(\phi,\theta)\, \frac{1}{kr} \sin(kr - \ell\pi/2) + i^{-\ell} \sum_{\ell,m} C_{k,\ell,m}\, Y_\ell^m(\phi,\theta)\, \frac{1}{i2kr} (e^{i2\delta_\ell(k)} - 1)\, e^{ikr}$$

Using $e^{i2\delta_\ell(k)} - 1 = 2i\, e^{i\delta_\ell(k)} \sin(\delta_\ell(k))$ one obtains

$$\phi(\vec{r}) \xrightarrow[r\to\infty]{}$$
$$\sum_{\ell,m} C_{k,\ell,m}\, Y_\ell^m(\phi,\theta)\, \frac{1}{kr} \sin(kr - \ell\pi/2) + i^{-\ell} \sum_{\ell,m} C_{k,\ell,m}\, Y_\ell^m(\phi,\theta)\, \frac{1}{kr}\, e^{i\delta_\ell(k)} \sin(\delta_\ell(k))\, e^{ikr} \tag{11}$$

Assume that $\hat{k}_{in}$ points into the z-direction in order to write

$$e^{ik\hat{k}_{in}\vec{r}} = e^{ikz} = \sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)}\; Y_\ell^0(\theta) J_\ell(kr) \tag{12}$$

with the spherical Bessel function $J_\ell(kr)$ of order ℓ. The asymptotic behavior of $J_\ell(kr)$ is

$$J_\ell(kr) = \xrightarrow[r\to\infty]{} \frac{1}{kr} \sin(kr - \ell\pi/2) \tag{13}$$

and thus asymptotically

$$e^{ik\hat{k}_{in}\vec{r}} \xrightarrow[r\to\infty]{} \sum_{\ell=0}^{\infty} i^\ell \sqrt{4\pi(2\ell+1)}\; Y_\ell^0(\theta)\, \frac{1}{kr} \sin(kr - \ell\pi/2) \tag{14}$$

Upon choosing $C_{k,\ell,m} = i^{\ell}\ \sqrt{4\pi(2\ell+1)}\ \delta_{m,0}$ in eq.(11) we obtain a solution of the stationary Schrödinger equation, which satisfies the asymptotic condition

$$\phi(\vec{r}) \xrightarrow[r\to\infty]{} e^{i\ k\hat{k}_{in}\vec{r}} + f_k(k,\hat{k}_{in},\hat{r})\ \frac{e^{ikr}}{r} \tag{15}$$

with $$f_k(k,\hat{k}_{in},\hat{r}) = \frac{1}{k}\sum_{\ell} \sqrt{4\pi(2\ell+1)}\ Y_{\ell}^{0}(\theta)\ \ e^{i\delta_{\ell}(k)}\sin(\delta_{\ell}(k))$$

Define the ℓ-wave *scattering length* $$a_{\ell} \equiv -\lim_{k\to 0}\left[\frac{1}{k}e^{i\delta_{\ell}(k)}\sin(\delta_{\ell}(k))\right] \tag{16}$$

The *total cross section* is

$$\begin{aligned}
\sigma(k) &= \int d\Omega\ \frac{d}{d\Omega}\sigma(\phi,\theta) = \int d\Omega\ \left|f_k(k,\hat{k}_{in},\hat{r})\right|^2 \\
&= \frac{4\pi}{k^2}\sum_{\ell,\ell'} \sqrt{(2\ell+1)}\ \sqrt{(2\ell'+1)}\ e^{i[\delta_{\ell}(k)-\delta_{\ell'}(k)]}\sin(\delta_{\ell}(k))\sin(\delta_{\ell'}(k))\ \int d\Omega\ Y_{\ell}^{0}(\theta)\ Y_{\ell'}^{0}(\theta) \\
&= \frac{4\pi}{k^2}\sum_{\ell,} (2\ell+1)\sin^2(\delta_{\ell}(k)) = \sum_{\ell,} \sigma_{\ell}(k)
\end{aligned}$$

with the total scattering cross section for ℓ-wave scattering length

$$\sigma_{\ell}(k) = \frac{4\pi}{k^2}\ (2\ell+1)\sin^2(\delta_{\ell}(k)) \tag{17}$$

Note1: The maximal possible value of $\sigma_{\ell}(k)$ is $\sigma_{\ell}(k) = \frac{4\pi}{k^2}\ (2\ell+1)$, which is called the unitarity limit.

Note2: $$\sigma_{\ell}(0) = 4\pi\ a_{\ell}^2$$

Note3: (Optical theorem) $$\sigma = \frac{4\pi}{k}\ \mathrm{Im}\left(f_k(k,\hat{k}_{in},\hat{k}_{in})\right)$$

follows directly with $Y_{\ell}^{0}(0) = \sqrt{(2\ell+1)/4\pi}$ and hence

$$\mathrm{Im}\left[f_k(k,\hat{k}_{in},\hat{k}_{in})\right] = \frac{1}{k}\sum_{\ell} \sqrt{4\pi(2\ell+1)}\ Y_{\ell}^{0}(0)\ \sin^2(\delta_{\ell}(k)) = \frac{1}{k}\sum_{\ell} (2\ell+1)\sin^2(\delta_{\ell}(k))$$

Bosons and Fermions

The above considerations concerned distinguishable particles. What about bosons and fermions? The scattering wave function must satisfy $\phi(\vec{r}) = \varepsilon\ \phi(-\vec{r})$ with $\varepsilon = \pm 1$ for bosons and fermions, respectively. We thus have to consider the asymptotic behavior

$$\phi(\vec{r}) \xrightarrow[r\to\infty]{} \frac{1}{\sqrt{2}}\left(e^{ik\hat{k}_{in}\vec{r}} + \varepsilon\ e^{-ik\hat{k}_{in}\vec{r}}\right) + \frac{1}{\sqrt{2}}\left[f_k(k,\theta,\phi) + \varepsilon\ f_k(k,\pi-\theta,\pi+\phi)\right]\frac{e^{ikr}}{r}$$

$$= \frac{1}{\sqrt{2}}\left(e^{ik\hat{k}_{in}\vec{r}} + e^{-ik\hat{k}_{in}\vec{r}}\right) + \bar{f}_k(k,\theta,\phi)\frac{e^{ikr}}{r}\ ,\quad \bar{f}_k(k,\theta,\phi) = \frac{1}{\sqrt{2}}\left[f_k(k,\theta,\phi) + \varepsilon\ f_k(k,\pi-\theta,\pi+\phi)\right]$$

With eq.(15) we get

$$\bar{f}_k(k,\theta,\phi) = \frac{1}{\sqrt{2}k}\sum_{\ell}\sqrt{4\pi(2\ell+1)}\ \left(Y_\ell^0(\theta)+\varepsilon\ Y_\ell^0(\pi-\theta)\right)\ e^{i\delta_\ell(k)}\sin(\delta_\ell(k))$$

$$= \frac{1}{\sqrt{2}k}\sum_{\ell}\left(1+\varepsilon\ (-1)^\ell\ \right)\sqrt{4\pi(2\ell+1)}\ Y_\ell^0(\theta)\ e^{i\delta_\ell(k)}\sin(\delta_\ell(k))$$

and thus $$\bar{\sigma}_\ell = \frac{4\pi\ (1+(-1)^\ell\varepsilon)}{k^2}\ (2\ell+1)\ \sin^2(\delta_\ell(k))$$

Note: for bosons (fermions) only partial waves with even (odd) angular momentum contribute.

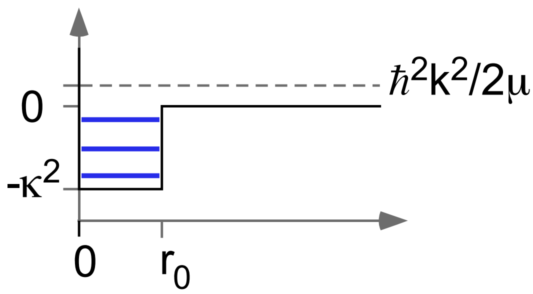
6.3. S-wave scattering from a square well potential

As the simplest possible approximation of a real molecular potential, we consider a square well with respect to the radial relative coordinate.

Consider the $\ell = 0$ radial equation $\left[\frac{\partial^2}{\partial r^2} - U(\vec{r}) + k^2\right] u_{k,\ell}(r) = 0$

and the square well

potential $U(r) = \begin{cases} -\kappa^2 & \text{if } r < r_0 \\ 0 & \text{if } r > r_0 \end{cases}$



6.3.A First consider a scattering state, i.e., $k > 0$:

For $r > r_0$ the general solution is $u_{k,0}(r) = A\ \sin(kr + \delta_0)$. With $u_{k,0}(0) = 0$ the solution for $r < r_0$ is $u_{k,0}(r) = B\ \sin(\sqrt{\kappa^2 + k^2}\ r)$. Show that the requirement of continuous differentiability at $r = r_0$ leads to

$$\tan\left(\delta_0 + kr_0\right) = \frac{k}{\sqrt{\kappa^2+k^2}} \tan\left[\sqrt{\kappa^2+k^2}\ r_0\right] \tag{17}$$

$$\left(\frac{B}{A}\right)^2 = \frac{1}{1+\dfrac{\kappa^2}{k^2}\cos^2\left[\sqrt{\kappa^2+k^2}\ r_0\right]} \tag{18}$$

and thus $\delta_0 = -kr_0 + \arctan\left[\frac{k}{\sqrt{\kappa^2+k^2}} \tan\left[\sqrt{\kappa^2+k^2}\ r_0\right]\right] + \pi\ n(\kappa,k)$ with (19)

$$n(\kappa,k) \equiv \text{IntegerPart}\left[\frac{\sqrt{\kappa^2+k^2}\ r_0}{\pi} + \frac{1}{2}\right]$$

Show also that the s-wave scattering length $a_0 \equiv -\lim_{k\to 0}\left[\frac{1}{k} e^{i\delta_0(k)} \sin(\delta_0(k))\right]$ reads

$$a_0 = r_0 - \left[\frac{1}{\kappa}\tan\left[\kappa\ r_0\right]\right] \tag{20}$$

and the s-wave scattering cross section is

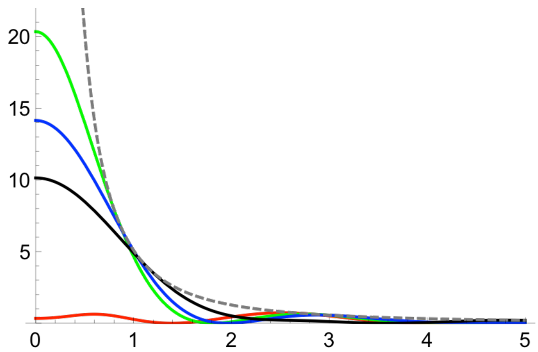
$$\sigma_0(k) = \frac{4\pi}{k^2}\sin^2(\delta_0(k)) = \frac{4\pi}{k^2}\sin^2\left(kr_0 - \arctan\left[\frac{k}{\sqrt{\kappa^2+k^2}}\tan\left[\sqrt{\kappa^2+k^2}\ r_0\right]\right]\right) \tag{21}$$

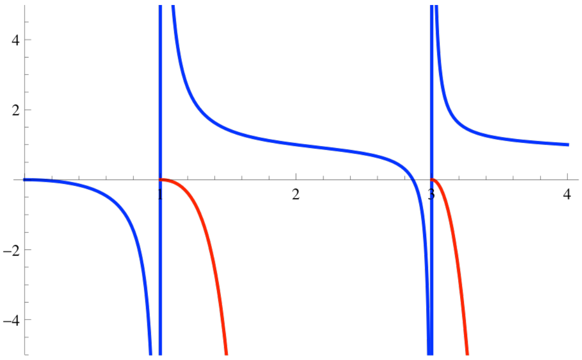
6.3.B Now consider a bound state with an energy $\varepsilon < 0$ below the dissociation limit: With $u_{k,0}(0) = 0$ the solution for $r < r_0$ is $u_{k,0}(r) = B\sin(\sqrt{\kappa^2+\varepsilon}\ r)$, while for $r > r_0$ the general solution is $u_{k,0}(r) = A\exp(-\sqrt{-\varepsilon}\ r)$. The boundary conditions for $r = r_0$ impose

$$\frac{\tan\left[\sqrt{\kappa^2+\varepsilon}\ r_0\right]}{\sqrt{\kappa^2+\varepsilon}} = \frac{-1}{\sqrt{-\varepsilon}}$$

For small ε one gets $-\frac{\tan\left[\kappa\ r_0\right]}{\kappa} = \frac{1}{\sqrt{-\varepsilon}}$ which can be expressed in terms of the scattering length

$$a_0 - r_0 = -\frac{\tan\left[\kappa\ r_0\right]}{\kappa} \approx \frac{1}{\sqrt{-\varepsilon}} \tag{22}$$





Left: σ_0 / r_0^2 versus $\frac{\kappa r_0}{\pi / 2}$ for $\frac{\kappa r_0}{\pi / 2} = (2 n_{bound} - 1) + \delta n$ with a number of bound states $n_{bound} = 4$ and $\delta n = -0.05$ (red), 0.2 (green), 0.6 (blue), 1.6 (black). The grey dashed line indicates the s-wave unitarity limit.

Right: scattering length a_0 / r_0 versus $\kappa r_0 / (\pi / 2)$ (blue) and binding energy of bound state εr_0^2 versus $\kappa r_0 / (\pi / 2)$ (red).

What can be learned from these graphs with respect to a possible tuning of the scattering length? Can you imagine a way to actually implement tuning of the scattering length experimentally?