Ex 1: Partial Wave Expansion

1. $\vec{k}\cdot\vec{r} = kr\cos(\theta) = \rho\cos(\theta)$

Addition theorem for spherical harmonics:

$$\sum_{m=-l}^{l} \frac{4\pi}{2l+1} Y^*_{lm}(\theta_k, \phi_k) Y_{lm}(\theta_r, \phi_r) = P_l(\hat{k}\cdot\hat{r}) = P_l(\cos(\theta))$$

$$\Rightarrow 4\pi \sum_{m=-l}^{l} Y^*_{lm}(\theta_k, \phi_k) Y_{lm}(\theta_r, \phi_r) = (2l+1) P_l(\cos(\theta))$$

2. $$\int_{-1}^{1} d\cos(\theta)\, P_{l'}(\cos(\theta)) \sum_{l=0}^{\infty} (2l+1)\, i^l j_l(\rho) P_l(\cos(\theta)) =$$

$$= \sum_{l=0}^{\infty} (2l+1)\, i^l j_l(\rho) \underbrace{\int_{-1}^{1} d\cos(\theta)\, P_{l'}(\cos(\theta)) P_l(\cos(\theta))}_{= \frac{2\delta_{ll'}}{2l+1}} = 2 i^{l'} j_{l'}(\rho)$$

For the other side of the equation, we have

$$\int_{-1}^{1} d\cos(\theta)\, P_{l'}(\cos(\theta))\, e^{i\rho\cos(\theta)}$$

$$\xRightarrow{s=\cos(\theta)} j_l(\rho) = \frac{(-i)^l}{2} \int_{-1}^{1} ds\, P_l(s)\, e^{i\rho s}$$

3. $$\frac{1}{2}\int_{-1}^{1} ds\, e^{i\rho s} = \frac{1}{2i\rho}\left(e^{i\rho} - e^{-i\rho}\right) = \frac{\sin(\rho)}{\rho}$$

To show eq. (7), we perform a proof by induction.

$l=1$: $$(-\rho)\cdot\left(\frac{1}{\rho}\frac{d}{d\rho}\right)\frac{1}{2}\int_{-1}^{1} ds\, e^{i\rho s} =$$

$$= -\frac{i}{2}\int_{-1}^{1} ds\, s\, e^{i\rho s} = -\frac{i}{4}\left\{\underbrace{\left[(s^2-1)e^{i\rho s}\right]_{-1}^{1}}_{=0} - \int_{-1}^{1} ds\,(s^2-1)\, i\rho e^{i\rho s}\right\}$$

$$= \frac{(-\rho)^1}{2^{1+1}1!}\int_{-1}^{1} ds\,(s^2-1)^1 e^{i\rho s}$$

$l \to l+1$:

$$j_{l+1}(\rho) = (-\rho)^{l+1}\left(\frac{1}{\rho}\frac{d}{d\rho}\right)^{l+1}\frac{\sin(\rho)}{\rho} =$$

$$= (-\rho)^{l+1}\left(\frac{1}{\rho}\frac{d}{d\rho}\right)\left(\frac{j_l(\rho)}{(-\rho)^l}\right) =$$

$$\underset{\text{induction hypothesis}}{=} \frac{(-\rho)^{l+1}}{2^{l+1}l!}\frac{1}{\rho}\frac{d}{d\rho}\int_{-1}^{1} ds\,(s^2-1)^l e^{i\rho s} =$$

$$= \frac{(-\rho)^{l+1}}{2^{l+1}l!}\frac{i}{\rho}\int_{-1}^{1} ds\,(s^2-1)^l\, s\, e^{i\rho s} =$$

$$= \frac{(-p)^{\ell+1}}{2^{\ell+1}\ell!}\frac{i}{p}\cdot\left\{\underbrace{\left[\frac{(s^2-1)^{\ell+1}}{2(\ell+1)}e^{ips}\right]_{-1}^{1}}_{=0}-\int_{-1}^{1}ds\,\frac{(s^2-1)^{\ell+1}}{2(\ell+1)}ip\,e^{ips}\right\}=$$

$$= \frac{(-p)^{\ell+1}}{2^{\ell+2}(\ell+1)!}\int_{-1}^{1}ds\,(s^2-1)^{2\ell+1}e^{ips}$$

4.

$$j_\ell(p)=\frac{(-p)^\ell}{2^{\ell+1}\ell!}\int_{-1}^{1}ds\,(s^2-1)^\ell e^{ips}=$$

$$=\frac{i^\ell}{2^{\ell+1}\ell!}\int_{-1}^{1}ds\,(s^2-1)^\ell\left(\frac{d^\ell}{ds^\ell}e^{ips}\right)=$$

$$=\frac{i^\ell}{2^{\ell+1}\ell!}\left\{\left[(s^2-1)^\ell\frac{d^{\ell-1}}{ds^{\ell-1}}e^{ips}\right]_{-1}^{1}-\int_{-1}^{1}ds\left(\frac{d}{ds}(s^2-1)^\ell\right)\left(\frac{d^{\ell-1}}{ds^{\ell-1}}e^{ips}\right)\right\}=$$

$$=\frac{i^\ell}{2^{\ell+1}\ell!}(-1)\int_{-1}^{1}ds\left(\frac{d}{ds}(s^2-1)^\ell\right)\left(\frac{d^{\ell-1}}{ds^{\ell-1}}e^{ips}\right)=$$

$$=\frac{i^\ell}{2^{\ell+1}\ell!}(-1)^\ell\int_{-1}^{1}ds\left(\frac{d^\ell}{ds^\ell}(s^2-1)^\ell\right)e^{ips}=$$

repeat $\ell-1$ more times: the boundary term always takes the form

$$\left[\left(\frac{d^{n-1}}{ds^{n-1}}(s^2-1)^\ell\right)\cdot\left(\frac{d^{\ell-n}}{ds^{\ell-n}}e^{ips}\right)\right]_{-1}^{1}=0\quad\forall\, n\le\ell$$

$$=\frac{(-i)^\ell}{2}\int_{-1}^{1}ds\,P_\ell(s)\,e^{ips}$$

Exercise 2: Phase Shifts for the potential well

1. For $r > R$, the Schrödinger equation for the particle is the one for a free particle with

angular wavefunctions: $Y_{\ell m}(\theta,\varphi)$ (spherical harmonics)

radial wavefunctions: $\underset{\substack{\uparrow\\ \rho = k\cdot r}}{j_\ell(\rho)}$, $y_\ell(\rho)$ (spherical Bessel functions)

So the most general form of the wave function for $r > R$ is

$$\Psi(r,\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell}\left(a_{\ell m}\, j_\ell(k\cdot r)\, Y_{\ell m}(\theta,\phi) + b_{\ell m}\, y_\ell(k\cdot r)\, Y_{\ell m}(\theta,\phi)\right)$$

some coefficients

However, we also know that the wave function of a free particle can be written as

$$\Psi(r,\theta,\phi) = A\, e^{i\vec{k}\cdot\vec{r}} + B\, e^{-i\vec{k}\cdot\vec{r}} = A\, e^{ik\cdot r\cos(\theta)} + B e^{-ik\cdot r\cos(\theta)}$$

which is independent of ϕ. This can only be true for the above expansion if

$$a_{\ell m}, b_{\ell m} \sim \delta_{m0}$$

We define $a_\ell \equiv a_{\ell 0}$, $b_\ell \equiv b_{\ell 0}$ and find

$$\Psi(r,\theta,\phi) = \sum_{\ell=0}^{\infty}\left(a_\ell\, j_\ell(k\cdot r)\, Y_{\ell 0}(\theta,\phi) + b_\ell\, y_\ell(k\cdot r)\, Y_{\ell 0}(\theta,\phi)\right)$$

for $r > R$.

For $r < R$ the potential is a constant. Hence the solution to the Schrödinger equation is still the one for a free particle, but there are two differences

- as the Schrödinger equation is modified by the potential to

$$\nabla^2 \Psi(\vec{r}) = -\underbrace{\frac{2m(E - V_0)}{\hbar^2}}_{= k^2 - \frac{2mV_0}{\hbar^2} \equiv k'^2}\Psi(\vec{r})$$

$\Rightarrow$ we have to replace $k \to k'$ in the formula for the wave function

- the solution should be regular at $r = 0$, but $y_\ell(x)$ diverges as $x \to 0$

$\Rightarrow$ all the coefficients for the y_ℓ vanish

To conclude, we have for $r < R$

$$\Psi(r,\theta,\phi) = \sum_{\ell=0}^{\infty} c_\ell\, j_\ell(k'\cdot r)\, Y_{\ell 0}(\theta,\phi)$$

2. As spherical harmonics are linearly independent functions, we can impose continuity and differentiability term by term at $r=R$, so for all ℓ, we have

$$c_\ell\, j_\ell(k'R) = a_\ell\, j_\ell(kR) + b_\ell\, y_\ell(kR) \qquad \text{(cont.)}$$

$$c_\ell\, k'\, j_\ell'(k'R) = a_\ell\, k\, j_\ell'(kR) + b_\ell\, k\, y_\ell'(kR) \qquad \text{(diff.)}$$

$$\Rightarrow \frac{a_\ell j_\ell(kR) + b_\ell y_\ell(kR)}{j_\ell(k'R)} = \frac{a_\ell k\, j_\ell'(kR) + b_\ell k\, y_\ell'(kR)}{k'\, j_\ell'(k'R)}$$

$$\Rightarrow \frac{b_\ell}{a_\ell} = \frac{k\, j_\ell'(kR)\, j_\ell(k'R) - k'\, j_\ell'(k'R)\, j_\ell(kR)}{k'\, j_\ell'(k'R)\, y_\ell(kR) - k\, y_\ell'(kR)\, j_\ell(k'R)}$$

3. $$\Psi(r,\theta,\phi) \xrightarrow{r\to\infty} \sum_{\ell=0}^{\infty} \frac{1}{kr}\left[a_\ell \cos\left(kr - \frac{(\ell+1)\pi}{2}\right) + b_\ell \sin\left(kr - \frac{(\ell+1)\pi}{2}\right)\right] Y_{\ell m}(\theta,\phi)$$

$$= \sum_{\ell=0}^{\infty} \frac{1}{2kr}\left[(a_\ell - i b_\ell)\, e^{ikr - i(\ell+1)\frac{\pi}{2}} + (a_\ell + i b_\ell)\, e^{-ikr + i(\ell+1)\frac{\pi}{2}}\right] Y_{\ell m}(\theta,\phi)$$

$$\Rightarrow a_\ell - i b_\ell = e^{i\delta_\ell} \quad \text{and} \quad a_\ell + i b_\ell = e^{-i\delta_\ell} \quad \text{(consistent)}$$

Dividing the two, we have

$$e^{2i\delta_\ell} = \frac{a_\ell - i b_\ell}{a_\ell + i b_\ell} = \frac{1 - i\alpha_\ell}{1 + i\alpha_\ell}$$

4. $$j_0(\rho) = \frac{\sin(\rho)}{\rho}, \quad j_0'(\rho) = \frac{\rho\cos(\rho) - \sin(\rho)}{\rho^2}$$

$$y_0(\rho) = -\frac{\cos(\rho)}{\rho}, \quad y_0'(\rho) = \frac{\rho\sin(\rho) + \cos(\rho)}{\rho^2}$$

$$\Rightarrow \alpha_0 = \frac{(kR\cos(kR) - \sin(kR))\sin(k'R) - (k'R\cos(k'R) - \sin(k'R))\sin(kR)}{(k'R\cos(k'R) - \sin(k'R))(-\cos(kR)) - (kR\sin(kR) + \cos(kR))\sin(k'R)} =$$

$$= \frac{k'\cos(k'R)\sin(kR) - k\cos(kR)\sin(k'R)}{k'\cos(k'R)\cos(kR) + k\sin(kR)\sin(k'R)}$$

We expand for small potential $V_0 \ll \frac{\hbar^2 k^2}{2m}$:

$$k' = \sqrt{k^2\left(1 - \frac{2mV_0}{\hbar^2 k^2}\right)} \simeq k - \frac{mV_0}{\hbar^2 k} + \mathcal{O}(V_0^2)$$

$$\cos(k'R) \approx \cos(kR) + \frac{mV_0}{\hbar^2 k} R \sin(kR) + \mathcal{O}(V_0^2)$$

$$\sin(k'R) \approx \sin(kR) - \frac{mV_0}{\hbar^2 k} R\cos(kR) + \mathcal{O}(V_0^2)$$

$$\Rightarrow \alpha_0 \simeq \underbrace{\frac{kR - \cos(kR)\sin(kR)}{\cos^2(kR) + \sin^2(kR)}}_{= kR - \cos(kR)\sin(kR)} \cdot \frac{mV_0}{\hbar^2 k^2} + \mathcal{O}(V_0^2)$$

5. The scattering amplitude is given by

$$f_k(\theta,\phi) = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1)\, e^{i\delta_l} \sin(\delta_l)\, P_l(\cos(\theta)) =$$

$$= \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \frac{1}{2i} \left(e^{2i\delta_l} - 1\right) P_l(\cos(\theta)) =$$

$$= \frac{1}{k} \frac{1}{2i} \left(e^{2i\delta_0} - 1\right) + \frac{1}{k} \sum_{l=1}^{\infty} (2l+1) e^{i\delta_l} \sin(\delta_l) P_l(\cos(\theta))$$

$$\frac{1}{2i}\left(e^{2i\delta_0} - 1\right) = \frac{1}{2i}\left(\frac{1-i\alpha_0}{1+i\alpha_0} - 1\right) = -\frac{\alpha_0}{1-i\alpha_0} =$$

$$= -\alpha_0 + \sigma(V_0^2) = \left(kR - \cos(kR)\sin(kR)\right)\frac{mV_0}{\hbar^2 k^2} + \sigma(V_0^2)$$

$$\uparrow$$

$$\alpha_0 = \sigma(V_0)$$

So we have

$$f_k(\theta,\phi) = -\frac{\alpha_0}{k} + (\text{partial waves } l \geq 1) =$$

$$= -\frac{mV_0}{\hbar^2} \frac{kR - \cos(kR)\sin(kR)}{k^3} + O(V_0^2) + (\text{p. w. } l \geq 1)$$

6. The contribution of only the $l=0$ partial wave to the cross section is

$$\sigma_{l=0} = \int d\Omega \left| -\frac{mV_0}{\hbar^2} \cdot \frac{kR - \cos(kR)\sin(kR)}{k^3}\right|^2 =$$

$$= 4\pi \frac{m^2 V_0^2}{\hbar^4} \cdot \frac{(kR - \cos(kR)\sin(kR))^2}{k^6} =$$

$$= \frac{\pi m^2 V_0^2}{\hbar^4} \frac{(2kR - \sin(2kR))^2}{k^6} =$$

$$= \frac{\pi m^2 V_0^2}{\hbar^4} \frac{\left(\frac{(2kR)^3}{6}\right)^2 + O((kR)^8)}{k^6} =$$

$$= \frac{16\pi m^2 V_0^2}{9\hbar^4} R^6 + \sigma((kR)^2)$$

This is exactly the same as the full cross section, so in the low energy limit, the contribution of the $l=0$ partial wave to the cross section dominates.

Exercise 3: Sommerfeld enhancement

1. Define $u_{k,l}(r) \equiv r\, R_{k,l}(r)$.

For a potential blowing up no faster than $\frac{1}{r}$ at the origin, the asymptotic behaviour is governed by the dominant angular term,

$$\frac{\hbar^2}{2m}\frac{d^2 u_{k,l}(r)}{dr^2} = \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}u_{k,l}(r) \quad , \quad l \neq 0$$

The general solution is

$$u_{k,l}(r) = c_1\, r^{l+1} + c_2\, r^{-l}$$

but demanding regularity at $r=0$, we have $c_2 = 0$.

So $u_{k,l}(r) \overset{r\to 0}{\sim} r^{l+1}$, which implies $R_{k,l}(r) \overset{r\to 0}{\sim} r^{l}$.

Note: for $l=0$, the asymptotic behavior depends on the potential!

2. We have

$$\Psi_k(\vec{r}) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\, i^l\, e^{i\delta_l}P_l(\cos(\theta))\, R_{k,l}(r) =$$

$$= \frac{1}{k}e^{i\delta_0}R_{k,0}(\vec{r}) + \underbrace{\frac{1}{k}\sum_{l=1}^{\infty}(2l+1)\, i^l e^{i\delta_l}P_l(\cos(\theta))\, R_{k,l}(r)}_{\text{goes to zero as } r\to 0 \text{ as } R_{k,l}(r)\overset{r\to 0}{\sim} r^{l}}$$

$$\Rightarrow \Psi_k(0) = \frac{1}{k}e^{i\delta_0}R_{k,0}(0)$$

So the Sommerfeld enhancement factor reads

$$S_k = |\Psi_k(0)|^2 = \left|\frac{R_{k,0}(0)}{k}\right|^2 .$$

3. For the Coulomb potential, we have

$$S_k = \left|\frac{\eta}{e^{\eta}-1}\right| = \frac{\eta}{e^{\eta}-1}$$

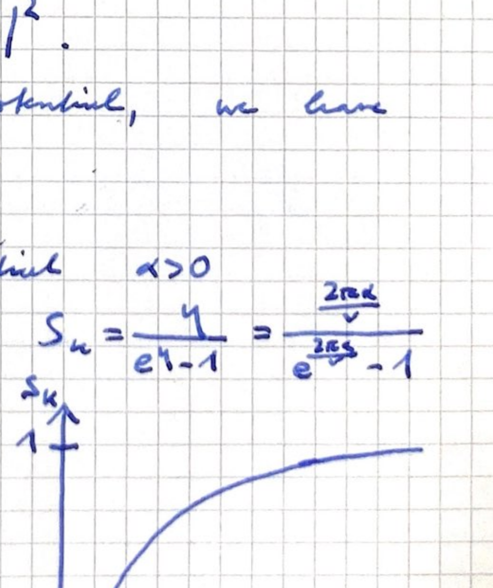
Case 1: repulsive potential $\alpha > 0$

$$\Rightarrow \eta = \frac{2\pi\alpha}{v} > 0 \quad \Rightarrow S_k = \frac{\eta}{e^{\eta}-1} = \frac{\frac{2\pi\alpha}{v}}{e^{\frac{2\pi\alpha}{v}}-1}$$

qualitative behaviour:

$$S_k \xrightarrow{v\to 0} 0$$

$$S_k \xrightarrow{v\to \infty} 1$$



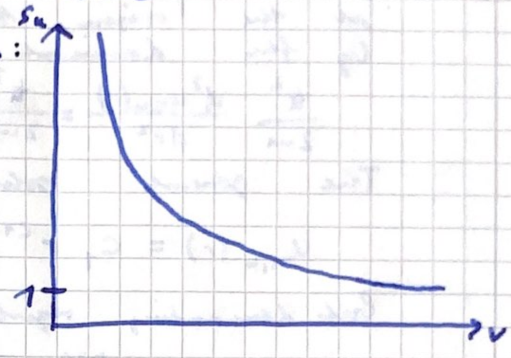
Case 2: attractive potential $\alpha < 0$

$$\Rightarrow \eta < 0 \quad \Rightarrow S_u = \frac{-\frac{2\pi\alpha}{v}}{1 - e^{\frac{2\pi\alpha}{v}}}$$

qualitative behaviour:

$$S_u \xrightarrow{v \to 0} \infty$$

$$S_u \xrightarrow{v \to \infty} 1$$



Discussion:

- for a high velocity particle, $v \to c$, the impact of the potential becomes small and $S_u \sim 1$ in both the attractive and repulsive case (a proper treatment requires a relativistic framework, however)
- for a low velocity particle, the potential has large effects on the interaction probability
  - in the repulsive case: $S_u \to 0$ as $v \to 0$, i.e. the repulsion makes it unlikely for the particles to interact
  - in the attractive case: $S_u \to \infty$ as $v \to 0$, i.e. the attraction enhances the interaction probability drastically