PHY 456 : "Lecture 3" Spherical Potentials, Partial Waves

Generally:

$$\varphi^{SCATT}(\vec{r})\Big|_{r\to\infty} = e^{ikz} + f_k(\theta,\varphi)\,\frac{e^{ikr}}{r}.$$

- If we expect $V(r)$ to be symmetric, no φ-dependence (see Yukawa example in Lec 2) so for $V(\vec{r}) = V(|\vec{r}|) = V(r)$,

$f_k(\theta,\varphi) \to f_k(\theta)$:

$$\varphi^{SCATT}(\vec{r})\Big|_{r\to\infty} = e^{ikz} + f_k(\theta)\,\frac{e^{ikr}}{r}.$$

MATH BACKGROUND: a function of θ, φ can be expanded into eigenfunctions of $\hat{L}^2$, $\hat{L}_z$, the $Y_\ell^m(\theta,\varphi)$ spherical harmonics (just functions with $P_\ell(x)$ as a basis) which are the coordinate-basis eigenfunctions

$$\hat{L}^2\,|\ell,m\rangle = \ell(\ell+1)\hbar^2\,|\ell,m\rangle$$

$$L_z\,|\ell,m\rangle = m\hbar\,|\ell,m\rangle$$

(Angular momentum)

For φ-independence, $m=0$ $\left(L_z \equiv -i\hbar \frac{\partial}{\partial\varphi}\right)$ and we use

$$Y_\ell^0(\theta) = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta)$$

Legendre Polynomial

$$\int_{-1}^{1} dx\, P_\ell(x) P_{\ell'}(x) = \frac{2\delta_{\ell\ell'}}{2\ell+1}$$

$$P_\ell(x) \equiv \frac{1}{2^\ell \ell!} \frac{d^\ell}{dx^\ell} (x^2-1)^\ell$$

So we can expand $f_k(\theta)$ as a change of basis into the P_ℓ basis (like a Fourier series)

$$f_k(\theta) = \sum_{\ell=0}^{\infty} \underbrace{(2\ell+1)}_{\text{Convention}}\, \underbrace{a_\ell(k)}_{\text{if } f_k(\theta) \text{ depends on } k \text{, all } k\text{-dependence is represented by functions } a(k)}\, \underbrace{P_\ell(\cos\theta)}_{\text{Legendre Polynomial}}$$

In this expansion, our incoming plane waves $e^{ikz} = e^{ikr\cos\theta}$ go into

$$e^{ikz} = \sum_{\ell=0}^{\infty} i^\ell (2\ell+1)\, \underbrace{j_\ell(kr)}_{\text{Spherical Bessel Function of first kind}}\, \underbrace{P_\ell(\cos\theta)}_{\text{Legendre polynomial (again)}}$$

For a plane wave in the $\vec{k}$-direction,

$$\boxed{e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} i^\ell\, Y_\ell^{m*}(\theta_k, \varphi_k)\, j(kr)\, Y_\ell^m(\theta,\varphi)}$$

"Proof": $Y_\ell^m(\theta,\varphi)$ constitute an orthonormalized basis,

that is,

$$Y_\ell^m(\theta,\varphi) = \frac{(-1)^{\ell+m}}{2^\ell \ell!}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, e^{im\varphi}(\sin\theta)^m \frac{d^{\ell+m}}{d(\cos\theta)^{\ell+m}}(\sin\theta)^{2\ell}$$

or

$$Y_\ell^m(\theta,\varphi) = N e^{im\varphi} P_\ell^m(\cos\theta)$$

$$= N e^{im\varphi}\left\{(-1)^m (1-x^2)^{m/2}\frac{d^m}{dx^m}(P_\ell(x))\right\}$$

Associated Legendre Polynomials

and

$$\int_0^{2\pi} d\varphi \int_0^\pi \sin\theta\, d\theta\; Y_\ell^{m*}(\theta,\varphi)\, Y_{\ell'}^{m'}(\theta,\varphi) = \delta_{\ell\ell'}\delta_{mm'}\,.$$

Any square-integrable function $f(\theta,\varphi)$ can be expanded in one and only way via these spherical harmonics:

$$f(\theta,\varphi) = \sum_\ell \sum_m c_{\ell,m} Y_\ell^m(\theta,\varphi)$$

$$\text{with} \quad c_{\ell,m} = \int_0^{2\pi} d\varphi \int_0^\pi \sin\theta\, d\theta\; Y_\ell^{m*}(\theta,\varphi)\, f(\theta,\varphi)\,.$$

Similarly, with the closure relation

$$\sum_\ell \sum_m Y_\ell^m(\theta,\varphi)\, Y_\ell^{m*}(\theta',\varphi') = \delta(\cos\theta - \cos\theta')\,\delta(\varphi-\varphi').$$

For $f(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} = e^{ikr\cos\theta} = \sum c_n Y_\ell^0$, φ-independence $\Rightarrow m=0$

by orthogonality $\quad c_n = 2\pi \int_0^\pi \sin\theta\, d\theta\; Y_n\, e^{ikr\cos\theta}$.

The spherical Bessel function of the first kind is

$$j(kr) = \frac{(-i)^n}{2}\int_0^\pi \sin\theta\, d\theta\; e^{ikr\cos\theta} P_n(\cos\theta),$$

So making this substitution with $Y_n^o = \sqrt{\frac{2n+1}{4\pi}}\, P_n(\cos\theta)$

we obtain

$$j(kr) \cdot \frac{(-i)^{-n}}{2^{-1}} = \int_0^\pi \sin\theta d\theta\, e^{ikr\cos\theta} \left(\frac{2n+1}{4\pi}\right)^{-\frac{1}{2}} Y_n^o$$

$$= \left(\frac{2n+1}{4\pi}\right)^{-\frac{1}{2}} C_n \cdot \frac{1}{2\pi}$$

$$\Rightarrow C_n = j(kr) \cdot 2 \cdot 2\pi \cdot (-i)^{-n} \sqrt{\frac{2n+1}{4\pi}}$$

$$= j(kr) \cdot 4\pi\, (i)^n \sqrt{\frac{2n+1}{4\pi}}$$

$$= j(kr) \cdot i^n \cdot [4\pi(2n+1)]^{\frac{1}{2}}$$

thus $$e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_\ell \underbrace{i^\ell [4\pi(2\ell+1)]^{1/2} j_\ell(kr)}_{C_n} Y_\ell^o \qquad (*)$$

for $\vec{k} = \hat{z}$, $$e^{i\overset{kr\cos\theta\ldots}{kz}} = 4\pi \sum_\ell i^\ell [4\pi(2\ell+1)]^{\frac{1}{2}} j_\ell(kr) \left[\frac{2\ell+1}{4\pi}\right] P_\ell(\cos\theta)$$

$$= \boxed{4\pi \sum_\ell i^\ell (2\ell+1) j_\ell(kr) P_\ell(\cos\theta)}$$

as required.

You can use the addition theorem to write $(*)$ in an arbitrary coordinate frame:

$$e^{i\vec{k}\cdot\vec{r}} = 4\pi \sum_\ell \sum_m i^\ell j_\ell(kr) Y_\ell^m(\hat{k}) Y_\ell^{m*}(\hat{r}).$$

"■"

Back to notes...

Logic: free particle uses eigenstates of $\hat{P}$,

$E = \frac{\hbar^2 k^2}{2\mu}$ and $\vec{P} = (0, 0, P_z = \hbar k)$.

Label these eigenstates $|k, \vec{p}\rangle$.

For angular momentum operators $\hat{L}^2$, $\hat{L}_z$ and $E = \frac{\hbar^2 k^2}{2\mu}$,

label these eigenstates $|k, \ell, m\rangle$.

We need the change of basis between these two states,

$$|k, \vec{p}\rangle = \sum_{\ell, m} \underbrace{|k, \ell, m\rangle\langle k, \ell, m|}_{= 1 \text{ in } E = \frac{\hbar^2 k^2}{2\mu} \text{ Space}} k, \vec{p}\rangle$$

and

$$\langle \vec{r} | k, \ell, m\rangle = \varphi^{(0)}_{k,\ell,m}(\vec{r}) \quad \text{"free"}$$

$$= \sqrt{\frac{2k^2}{\pi}}\, j_\ell(kr)\, Y_\ell^m(\theta, \varphi)$$

with $j_\ell(x) = (-1)^\ell x^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\sin x}{x}$ (Spherical Bessel Function of First Kind)

Accepting the above expansions, we have $\varphi^{(0)}(\vec{r})\big|_{r\to\infty}$ in $V=0$ (Free) potential,

$$\varphi^{SCATT\,(0)}(\vec{r})\Big|_{r\to\infty} = \sum_{\ell=0}^{\infty} \underbrace{i^\ell}_{e^{i\frac{\pi}{2}\ell}} (2\ell+1)\, \underbrace{j_\ell(kr)}_{\xrightarrow{r\to\infty} \frac{\sin(kr - \ell\frac{\pi}{2})}{kr}}\, P_\ell(\cos\theta)$$

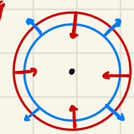
$$\frac{\sin(kr - \ell\frac{\pi}{2})}{kr} = \frac{e^{i(kr - \frac{\ell\pi}{2})}}{2ikr} - \frac{e^{-i(kr - \frac{\ell\pi}{2})}}{2ikr}$$

(outgoing spherical) (incoming waves)

which superimposes a phase shift $\ell\pi$:

$$= \sum_{\ell=0}^{\infty} (2\ell+1)\, e^{i\frac{\pi}{2}\ell} \left(\frac{e^{i(kr-\frac{\ell\pi}{2})}}{2ikr} - \frac{e^{-i(kr-\frac{\ell\pi}{2})}}{2ikr} \right) P_\ell(\cos\theta)$$

$$= \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{2ik} \left(\underbrace{\frac{e^{ikr}}{r}}_{\text{outgoing}} - \underbrace{\frac{e^{-i(kr-\ell\pi)}}{r}}_{\text{incoming}} \right) P_\ell(\cos\theta) \qquad (*)$$



What's happening here?

Since ℓ is conserved, for each value of ℓ we must also have probability conserved.

So, at ∞, where the solution is a spherical wave, we have an incoming and outgoing wave with the same amplitude, but different phases.

For free wave, the phase shift is $\ell\pi$ (none if $\ell=0$!)

Eventually, we shall argue that when a potential is present, the same must occur - except that the phase shift is not $\ell\pi$ but is something different which can depend on ℓ and k.

Generally, k-dependence contains all information about $V(r)$!

Back to initial problem - what about the scattering function

$$f_k(\theta) = \sum_{\ell=0}^{\infty} (2\ell+1)\, a_\ell(k)\, P_\ell(\cos\theta) \quad ?$$

The only possible choice for $a_\ell(k)$ is

$$a_\ell(k) = \frac{e^{2i\delta_\ell} - 1}{2ik}.$$

How?

Accept and interpret:

$$\varphi^{SCATT}(r)\Big|_{r\to\infty} = e^{ikz} + f_\ell(\theta)\, \frac{e^{ikr}}{r}$$

$$= \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{2ik} \left(\frac{e^{ikr}}{r} - \frac{e^{-i(kr-\ell\pi)}}{r} \right) P_\ell(\cos\theta)$$ ← incoming wave (free particle)

$$+ \sum_{\ell=0}^{\infty} (2\ell+1)\, \frac{e^{2i\delta_\ell}-1}{2ik}\, \frac{e^{ikr}}{r}\, P_\ell(\cos\theta)$$ ← form of scattered wave; with $\delta_\ell(k)$ as a phase shift.

$$= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2ik} \left(-\frac{e^{-i(kr-\ell\pi)}}{r} + \frac{e^{i(kr+2\delta_\ell)}}{r} \right) P_\ell(\cos\theta)$$

↑ incoming wave (same as in free case $V=0$)

↑ outgoing wave has phase shift $\delta_\ell(k)$ due to interaction

May look "cooked up" but is very sensible - due to angular momentum conservation and probability conservation.

Again, any stationary solution at (ℓ, k)

Should have the property : wave in $\left(\sim \frac{e^{-ikr}}{r}\right)$,

wave out $\left(\frac{e^{ikr}}{r}\right)$

with phase shift $\underline{l\pi}$ for free,

$\underline{l\pi + 2\delta_l(k)}$ for non-free

We can use this partial-wave expansion to find $\sigma(\delta_l)$.

What about the differential cross-section $\frac{d\sigma(\theta)}{d\Omega} = |f_k(\theta)|^2$?

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

function of θ with infinitely many δ_l's ...
only a limited number of δ_l's are important.

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

$$\Rightarrow \quad \sigma = \frac{2\pi}{4k^2} \sum_{l,l'}^{\infty} (2l+1)(2l'+1)\left(e^{2i\delta_l} - 1\right)\left(e^{-2i\delta_{l'}} - 1\right) \cdot \underbrace{\int_{-1}^{1} dx \, P_l(x) P_{l'}(x)}_{\frac{2}{2l+1}\delta_{ll'}}$$

$$= \frac{\pi}{k^2} \sum_{l=1}^{\infty} (2 - 2\cos(2\delta_l))(2l+1)$$

$$= \frac{2\pi}{k^2} \sum_{l=1}^{\infty} (2l+1) \cdot 2\sin^2(\delta_l)$$

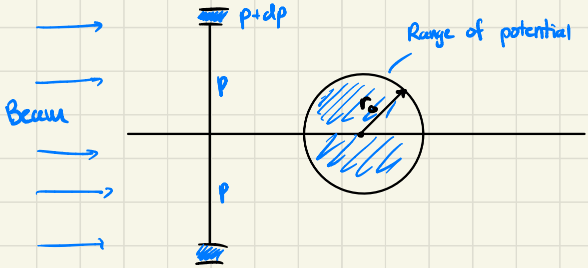
$$= \frac{4\pi}{k^2} \sum_{l=1}^{\infty} \sin^2(\delta_l) \cdot (2l+1)$$

Thus $\sigma = \sum_l \sigma_l$

where $\sigma_l = \frac{4\pi}{k^2} (2l+1) \sin^2(\delta_l)$

COMMENTS:

1) Number of partial waves contributing



Angular momentum of particles with p is $\mu p v_\infty$ (and $\mu v_\infty = \hbar k$; $E = \frac{\hbar^2 k^2}{2\mu}$)

so $\hbar \ell \sim \hbar k p \Rightarrow \ell \sim kp$

but if $r_0 << p$, particles miss target

($\ell >> kr_0 \Rightarrow$ no scattering)

Therefore for a given k, only a small number of ℓ-modes (partial waves) will contribute : $\ell \leq \ell_{max} = kr_0$; therin lies the usefulness of σ_ℓ.

2) Uniterity bound :

Clearly, since $\sin^2(\delta_\ell) \leq 1$,

$$\sigma_\ell \leq \sigma_{\ell, max} = \frac{4\pi}{k^2}(2\ell+1)$$

3) Optical theorem:

$$f_k(\theta) = \sum_{\ell=0}^{\infty} (2\ell+1) \frac{e^{2i\delta_\ell}-1}{2ik} P_\ell(\cos\theta)$$

so $f_k(0) =$ forward scattering amplitude ($\forall \ell$, $P_\ell(1) = 1$)

$$= \sum_{\ell=0}^{\infty} (2\ell+1) \frac{e^{i\delta_\ell}}{k} \sin\delta_\ell$$

hence $\operatorname{Im}\{f_k(0)\} = \sum_{\ell=0}^{\infty} (2\ell+1) \frac{\sin^2\delta_\ell}{k}$

But we also had that $\sigma = \frac{4\pi}{k^2} \sum_\ell \sin^2(\delta_\ell)(2\ell+1)$

therefore

$$\boxed{\sigma = \frac{4\pi}{k} \cdot \mathrm{Im}\{f_k(0)\}}$$

is the total scattering cross-section.

↑ ~ forward scattering amplitude

Example: a calculation using partial waves. Let $V(r) = \begin{cases} \infty & r \leq r_0 \\ 0 & r > r_0 \end{cases}$

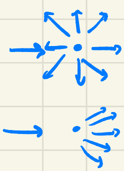
be the 'impenetrable ball' potential.

To simplify, consider low energies and only study $\ell=0$ partial wave:

$$f_k(\theta) = \frac{1}{k} e^{i\delta_0(k)} \sin(\delta_0(k))$$

This will be leading order in cross-section if $k \ll \frac{1}{r_0}$;

Clearly $\ell=0$ means isotropic scattering



(isotropic)

(anisotropic)

Find $\delta_0(k)$ by solving Schrödinger equation with $\ell=0$:

$$\varphi_{k\ell m} = R_{k\ell}(r)\, Y_\ell^m(\theta,\varphi)$$

$$= \frac{1}{r} u_{k\ell}(r)\, Y_\ell^m(\theta,\varphi)$$

with

$$\left(-\frac{\hbar^2}{2M}\nabla^2 + V(r)\right)\varphi_{k\ell m} = \underbrace{\frac{\hbar^2 k^2}{2\mu}}_{E(k)} \varphi_{k\ell m}$$

So since V is spherically symmetric,

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu r^2} + V(r)\right) u_{k\ell} = E(k)\, u_{k\ell}$$

$$\xRightarrow[r > r_0]{\ell=0} \left(\frac{d^2}{dr^2} + k^2\right) u_{k0}(r) = 0 \qquad [V(r > r_0) = 0]$$

with the boundary condition $u_{k0}(r \le r_0) = 0$.

We have

$$u_{k,0}(r) = \begin{cases} 0 & , \ r \le r_0 \\ C\sin(k(r-r_0)) & , \ r > r_0 \end{cases} .$$

Recall that the phase shift was determined by the $r \to \infty$ limit

$$u_{k0}(r) \sim \sin(kr + \delta_0(k)) = \sin(kr - kr_0).$$

Thus $\delta_0(k) = -kr_0$ and $\sigma \simeq \underbrace{\sigma_0 = \frac{4\pi}{k^2}\sin^2(kr_0) \simeq}_{kr_0 \ll 1} 4\pi r_0^2$

x4 cross sectional area of spherical potential...

For simple potentials, s-wave ($\ell=0$) and/or p-wave ($\ell=1$) dominate at low energies.