Lecture 19: The Partial Wave Expansion

• Overview

As with our studies of bound state problems, we can exploit the symmetries of the Hamiltonian to find solutions. The same is true for the scattering problem. Of utmost importance is the case of a central force between the ~~the~~ target and scatterer so that the potential seen by the latter is spherically symmetric $V(|\vec{x}|) = V(r)$.

Under these conditions the Hamiltonian is rotationally invariant. The same is true for the scattering operator

$$\hat{S} = \lim_{\substack{t_i \to -\infty \\ t_f \to +\infty}} \hat{U}_0^\dagger(t_f)\, \hat{U}(t_f, t_i)\, \hat{U}_0(t_i)$$

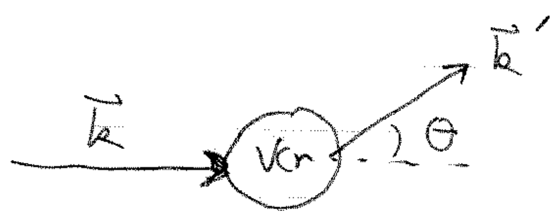
Since both the free particle evolution U_0
and the interacting " U
are rotational invariant. This has clear implication for the scattering amplitude.

$$f(\vec{k}' \leftarrow \vec{k}) = \langle \vec{k}' | (\hat{S} - \mathbb{1}) | \vec{k} \rangle \text{ (constants)}$$

since $\hat{\mathbb{D}}^\dagger \hat{S} \hat{D} = \hat{S}$ for any rotation $\hat{D}$

$\Rightarrow f(\vec{k}' \leftarrow \vec{k}) = f(\vec{k}_R' \leftarrow \vec{k}_R)$ where $\hat{D}|\vec{k}\rangle = |\vec{k}_R\rangle$

$\Rightarrow$ the scattering amplitude depends only on the angle between $\vec{k}$ and $\vec{k}'$ and the magnitude of $|\vec{k}| = |\vec{k}'| = \sqrt{\frac{2mE}{\hbar^2}}$ (Next Page)



$$f(\vec{k} \leftarrow \vec{k}') = f(E, \theta)$$

Since f has azimuthal symmetry about the $\vec{k}$ axis we know that it can be expanded in term of the complete set of Legendre Polynomials:

$$\boxed{f(\vec{k} \leftarrow \vec{k}') = \sum_{l=0}^{\infty} (2l+1)\, f_l(E)\, P_l(\cos\theta)}$$

where $f_l(E) = \int d(\cos\theta)\, f(E, \theta)\, P_l(\cos\theta)$

are known as the <u>partial-wave amplitudes</u>

The goal of this lecture is to express $f_l(E)$ in terms of properties of the S-matrix.

- <u>Free particle states with spherical symmetry</u>

We have generally taken free particle eigenstates as <u>plane waves</u> $|\vec{k}\rangle = |k_x\rangle |k_y\rangle |k_z\rangle$ $\quad \langle \vec{x} | \vec{k} \rangle = \dfrac{e^{i\vec{k}\cdot\vec{x}}}{(2\pi)^{3/2}}$

This follows since the Hamiltonian

$$\hat{H}_0 = \frac{\hat{\vec{P}}^2}{2m} = \frac{\hat{P}_x^2}{2m} + \frac{\hat{P}_y^2}{2m} + \frac{\hat{P}_z^2}{2m}$$

is translationally invariant in all 3D and the set $\{\hat{P}_x, \hat{P}_y, \hat{P}_z\}$ form a C.S.C.O.

We can, however, make a different choice based on the fact that the free particle Hamiltonian is rotationally invariant and thus commutes with $\hat{L}$ and $\hat{L}_z$ (or any one component)

$\Rightarrow$ C.S.C.O $\{\hat{H}_0, \hat{L}^2, \hat{L}_z\}$

$$\hat{H}_0 = \frac{\hat{P}_r^2}{2m} + \frac{\hat{L}^2}{2mr^2}$$

Eigenkets $|E, l, m\rangle = \underbrace{|E l\rangle}_{\text{radial}} \otimes \underbrace{|l m\rangle}_{\text{angular}}$

where $\langle \vec{x} | E, l, m\rangle = \underbrace{\langle r | E l\rangle}_{R_{E,l}(r)} \otimes \underbrace{\langle \vec{e}_r | l, m\rangle}_{Y^l_m(\vec{e}_r)}$

The reduced radial wave function satisfies

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

General solution: $u_{El}(r) = a_l j_l(kr) + b_l n_l(kr)$

where $j_l(kr)$ (and $n_l(kr)$) are spherical Bessel (Neumann) functions. The boundary condition at $r=0$ $\Rightarrow$ Only $j_l(kr)$ solutions for free particle

For future reference define spherical Hankel

$$h_l^{(1,2)}(z) = j_l(z) \pm i\, n_l(z)$$

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Examples of spherical Bessel etc.

$$j_0(z) = \frac{\sin z}{z}, \quad n_0(z) = \frac{-\cos z}{z}, \quad h_0^{(1,2)}(z) = \mp i \frac{e^{\pm iz}}{z}$$

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}, \quad n_1(z) = -\frac{\cos z}{z^2} - \frac{\sin z}{z}, \quad h_1^{(1,2)}(z) = \left(\mp\frac{i}{z} - \frac{1}{z}\right)e^{\pm i}$$

Thus the functions $\langle \vec{x} | E, l, m\rangle$ represent <u>spherical waves</u>, with a particular angular dependence dictating the angular momentum; j_l and n_l are like sine and cosine <u>standing waves</u>; $h_l^{(1,2)}$ are out going and in coming <u>travelling waves</u>

Thus we have two bases of complete sets for the free particle problem $\{|\vec{k}\rangle\}$, $\{|E,l,m\rangle\}$

$$\Rightarrow \quad \mathbb{1} = \int d^3\vec{k}\, |\vec{k}\rangle\langle\vec{k}| = \int_0^\infty dE \sum_{l=0}^{\infty}\sum_{m=-l}^{l} |Elm\rangle\langle Elm|$$

A change of basis is achieved ~~thus~~ by expressing one representation in terms of the other:

$$\langle \vec{k} | E, l, m\rangle = \left(\langle k| \otimes \langle \vec{e}_k|\right)\left(|E,l\rangle \otimes |l,m\rangle\right)$$

$$= \underbrace{\langle k | E, l\rangle}_{g_l(E,k)} \underbrace{\langle \vec{e}_k | l m\rangle}_{Y^l_m(\vec{e}_k)}$$

Since these are both eigenstates of H_0 with $E = \frac{\hbar^2 k^2}{2m} \equiv E_k$

$$\Rightarrow g_l(E,k) = N\delta(E - E_k) \qquad N = \frac{\hbar}{\sqrt{mk}} \quad \text{(normalization)}$$

$$\Rightarrow \boxed{\langle \vec{k} | E, l, m\rangle = \frac{\hbar}{\sqrt{mk}}\,\delta(E-E_k)\, Y^l_m(\vec{e}_k)}$$

Scattering phase and partial-wave amplitudes

The $\hat{S}$ operator map "in" states to "out" states. these are free particle states with the exact solution asymptotes to at $\pm\infty \Rightarrow [\hat{S}, \hat{H}_0] = 0$

Since $\hat{S}$ commutes with $\hat{H}_0$ $\hat{L}^2$ and $\hat{L}_z$ the partial wave basis $\{|E\,l\,m\rangle\}$ are <u>also</u> <u>eigenstates of</u> $\hat{S}$

$$\Rightarrow \langle E'l'm|\hat{S}|E\,l\,m\rangle = S_l(E)\,\delta(E'-E)\,\delta_{l'l}\,\delta_{m'm}$$

$S_l(E)$ ← eigenvalue (indep of m)

Since $\hat{S}$ is unitary the eigenvalue is just a <u>phase</u>

By convention we write $S_l(E) = e^{2i\delta_l(E)}$

$\delta_l(E) \equiv$ Scattering phase shift

Now $\langle \vec{k}'|(\hat{S}-1)|\vec{k}\rangle = \dfrac{i\hbar^2}{2\pi m}\,\delta(E_k - E_{k'})\,f(\vec{k}' \leftarrow \vec{k})$

$$= \int_0^\infty dE \sum_{l,m} \langle \vec{k}'|(\hat{S}-1)|E\,l\,m\rangle\langle E\,l\,m|\vec{k}\rangle$$

$$= \frac{\hbar^2}{mk}\,\delta(E_k - E_{k'}) \sum_{l,m} Y^l_m(\vec{e}_k{}')\,(S_l(E)-1)\,Y^{l\,*}_m(\vec{e}_k)$$

$$\Rightarrow f(\vec{k}' \leftarrow \vec{k}) = \frac{2\pi}{ik}\sum_l [S_l(E)-1]\, \underbrace{\sum_m Y^l_m(\vec{e}_k{}')\,Y^{l\,*}_m(\vec{e}_k)}_{= \frac{4\pi}{2l+1} P_l(\vec{e}_k \cdot \vec{e}_{k'})}$$

Thus

$$\boxed{\begin{aligned} f(\vec{k}' \leftarrow \vec{k}) &= \sum_{\ell=0}^{\infty} (2\ell+1)\, f_\ell(E)\, P_\ell(\cos\theta) \\ \text{where} \quad \cos\theta &= \vec{e}_k \cdot \vec{e}_{k'} \\ f_\ell(E) &= \frac{S_\ell(E) - 1}{2ik} = \frac{e^{2i\delta_\ell(E)} - 1}{2ik} = \frac{e^{i\delta_\ell(E)} \sin\delta_\ell(E)}{k} \end{aligned}}$$

This is the basic result. Note: the partial wave amplitudes depend only on the scattering phase-shift (for a given energy). Thus the problem of finding the phase-shifts for a given potential as a function of E.

The total cross-section decomposes in terms of partial waves

$$\sigma_{total} = \int d\Omega\, |f(E,\theta)|^2 = \sum_{\ell=0}^{\infty} \underbrace{4\pi\,(2\ell+1)\,|f_\ell(E)|^2}_{\equiv\, \sigma_\ell}$$

(using orthogonality of Legendre)

$\Rightarrow$ Partial cross section $\boxed{\sigma_\ell = 4\pi(2\ell+1)\,\frac{\sin^2\delta_\ell(E)}{k^2}}$

Because δ_ℓ is real ($\hat{S}$ is unitary) $\quad \sigma_\ell \leq 4\pi\lambda\!\!\!^{-2}(2\ell+1)$

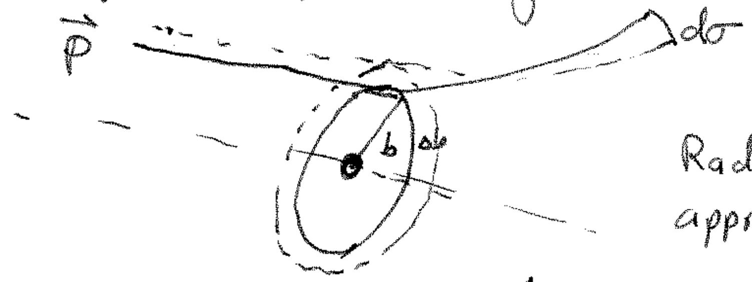
Note: Optical theorem is satisfied

$$\mathrm{Im}\left[f(\theta=0)\right] = \sum_\ell \frac{(2\ell+1)}{k}\,\mathrm{Im}\left[e^{i\delta_\ell}\sin\delta_\ell\right] \underbrace{P_\ell(1)}_{=1} = \sum_\ell \frac{(2\ell+1)}{k}\sin^2\delta_\ell$$

$$= \frac{k}{4\pi}\,\sigma_{total}$$

Physical picture of the partial cross-section

- Classical picture of scattering in central force potential



Radius of closest approach b

Angular momentum $\vec{L} = \vec{r} \times \vec{p}$
$= (bp)\,\hat{z}$

Cross-section in range of angular momenta $L \to L + \Delta L$

$$\sigma_L = 2\pi b\,\Delta b = \frac{2\pi\, L\,\Delta L}{p^2}$$

- Quantum picture

Particle wave $|E, l, m\rangle$ $\Rightarrow$ Impact parameter

$$b \cong \frac{\hbar l}{p} = \frac{l}{k}$$

(Note: This is rough. Quantum mechanically we cannot specify $\vec{L}$ and $\vec{p}$ simutaneouly)

$\Rightarrow$ Cross section in range $\hbar l \to \hbar(l+1)$ $\quad \Delta L = \hbar$

Semi Class picture $\Rightarrow$ $$\sigma_l^{semi} \cong \frac{2\pi(\hbar l)(\hbar)}{p^2} = \frac{2\pi}{k^2}\, l$$

Quantum: $$(\sigma_l)_{max} = \frac{4\pi}{k^2}(2l+1) \gtrsim 4\left(\frac{2\pi}{k^2}\, l\right)$$

Factor of 4 $\Rightarrow$ Wave property

Frenel Zone