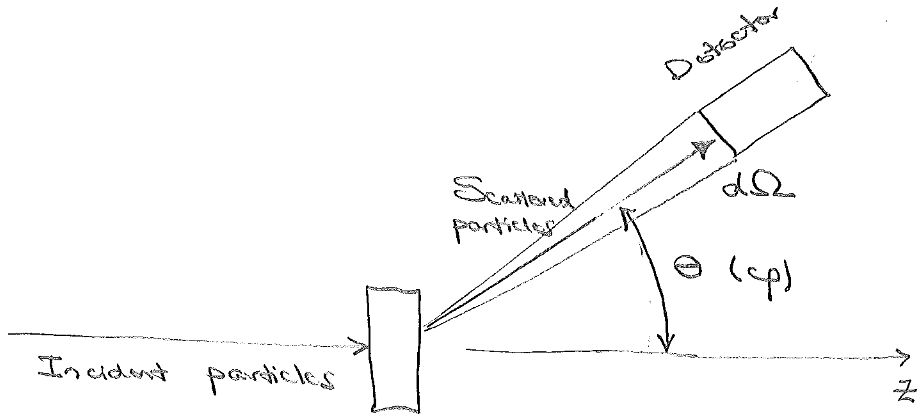
Phys 522

Scattering theory

Lectures 22-26

What's the problem?



Target - actually many targets

$$dN = \begin{pmatrix}\text{\# of particles per unit}\\ \text{time counted by detector}\end{pmatrix} = F_i \underbrace{\sigma(\theta,\varphi)}_{\text{differential cross section}} d\Omega$$

F_i: incident flux - particles per unit time per unit area

Total cross section $\sigma \equiv \int d\Omega\, \underbrace{\sigma(\theta,\varphi)}_{?} = \begin{pmatrix}\text{area scattered}\\ \text{from incident}\\ \text{beam}\end{pmatrix}$

Classical description - uniform incident flux - probs come from not knowing impact parameter

Use of probabilities:

$$dN = N_i \underbrace{dp(\theta,\varphi)}_{} = F_i\, \sigma(\theta,\varphi)\, d\Omega \Rightarrow \sigma(\theta,\varphi)\, d\Omega = \frac{N_i}{F_i} dp(\theta,\varphi)$$

probability that individual particle is scattered into detector

Classical - probs come from averaging over impact parameter

QM - probs are intrinsic

We will make following assumptions

(1) Nonrelativistic

(2) No internal structure — point particles w/ no spin

Elastic scattering

(3) No multiple scattering

(4) No coherence between targets

(5) Potential scattering : $V(\vec{r})$ Fixed target or CM w/ $\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$

Basic QM formulation:

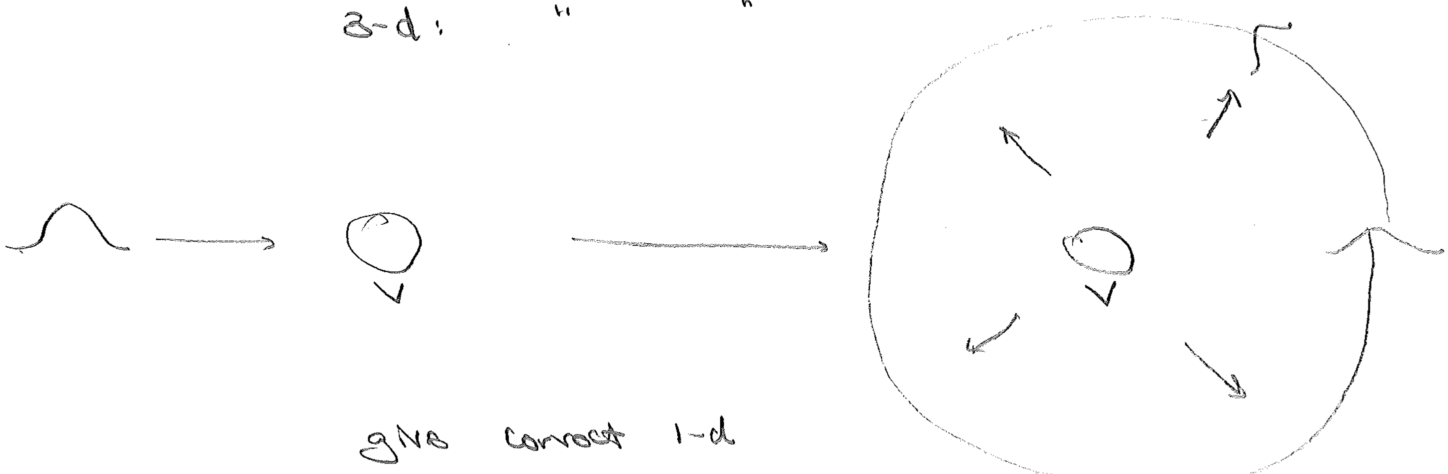
$$H = H_0 + V(\vec{r}) \quad , \quad H_0 = \vec{P}^2 / 2\mu$$

$\llcorner\!\!\rightarrow$ more localized than Coulomb (in sphere of radius a)

Wave packet description

1-d : wave packets and energy eigenstates

3-d : " " " " "



give correct 1-d analogue

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(\vec{r})\right)\varphi(\vec{r}) = E\varphi(\vec{r}) \iff \left(\nabla^2 + k^2 - U(\vec{r})\right)\varphi(\vec{r}) = 0$$

$$E = \frac{\hbar^2 k^2}{2\mu} \quad , \quad V(\vec{r}) = \frac{\hbar^2}{2\mu} U(\vec{r})$$

Energy eigenstates:

$$E_k = \frac{\hbar^2 k^2}{2m}: \quad \varphi^{(+)}_{\vec k}(\vec r) \underset{r\to\infty}{\sim} \frac{1}{(2\pi)^{3/2}}\Big(\underbrace{e^{i\vec k\cdot\vec r}}_{\text{incoming wave – one for each } \vec k} + \overbrace{f_{\vec k}(\hat r)}^{\text{scattering amplitude}} \underbrace{\frac{e^{ikr}}{r}}_{\text{outgoing spherical wave}} \Big)$$

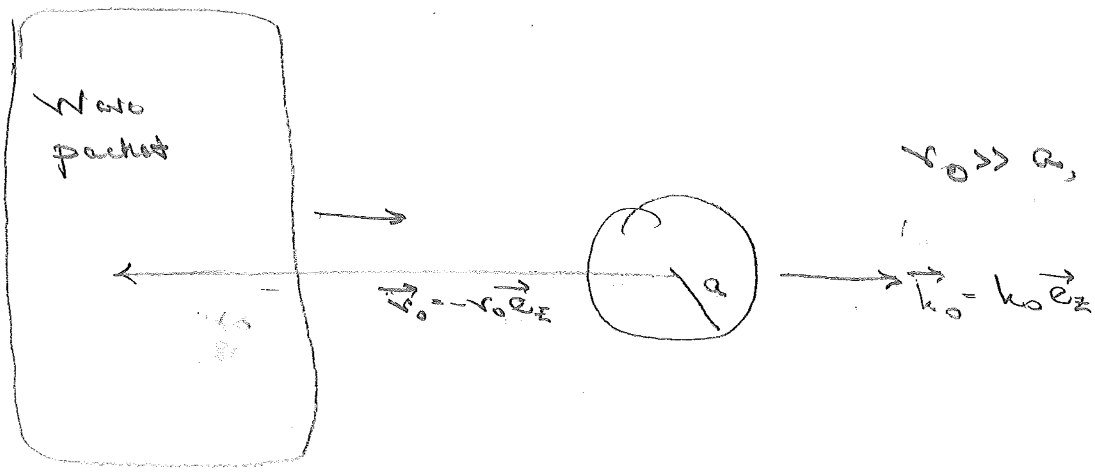
C-T: v_k^{diff}, $\vec k = k\vec e_z$

Wave packets (C-T uses probability currents instead; wave packets are more physical)

$$\psi_0(\vec r) = \int \frac{d^3k}{(2\pi)^{3/2}}\, g(\vec k)\, e^{i\vec k\cdot\vec r}$$

peaked at $\vec r_0$ with widths $\Delta x \sim \frac{1}{\Delta k_x}$, $\Delta y \sim \frac{1}{\Delta k_y}$, $\Delta z \sim \frac{1}{\Delta k_z}$

$g(\vec k)$: peaked at $\vec k = \vec k_0 = k_0\vec e_z$ with widths $\Delta k_x, \Delta k_y, \Delta k_z$



$r_0 \gg a, \Delta x, \Delta y, \Delta z$

$$\psi(\vec r, t) = \int d^3k\; g(\vec k)\, e^{-i\vec k\cdot\vec r_0}\, \varphi^{(+)}_{\vec k}(\vec r)\, e^{-i\omega_k t} \qquad \omega_k = \frac{E_k}{\hbar} = \frac{\hbar k^2}{2m}$$

$$\underset{r\to\infty}{\sim} \underbrace{\int \frac{d^3k}{(2\pi)^{3/2}}\, g(\vec k)\, e^{i\vec k\cdot(\vec r-\vec r_0)}\, e^{-i\omega_k t}}_{\psi_{\text{no scatt}}(\vec r,t)}$$

$$+ \underbrace{\int \frac{d^3k}{(2\pi)^{3/2}}\, g(\vec k)\, e^{-i\vec k\cdot\vec r_0}\, f_{\vec k}(\hat r)\, \frac{e^{ikr}}{r}\, e^{-i\omega_k t}}_{\psi_{\text{scatt}}(\vec r,t)}$$

Unscattered wave packet:

$$\psi_{\text{no scatt}}(\vec{r},0) = \psi_0(\vec{r}-\vec{r}_0)$$

① moves with velocity $\vec{v}_0 = \hbar\vec{k}_0/\mu$

② spreads at rate $\frac{\Delta p}{\mu}t \sim \frac{\hbar\Delta k}{\mu}t$

Require $\frac{\hbar\Delta k}{\mu} T \ll \Delta r \sim \frac{1}{\Delta k} \iff \boxed{\frac{(\Delta k)^2 r_0}{k_0} \ll 1}$

$$T \leftarrow \frac{2r_0}{v_0} = \frac{2r_0\mu}{\hbar k_0}$$

Small-spreading condition

$$\iff \frac{\lambda_0}{\Delta r} \ll \frac{\Delta r}{r_0} \ll 1$$

$\lambda_0 r_0 \ll (\Delta r)^2$

stays far away

Can always do this for fixed λ: keep $(\Delta r)/r_0$ fixed & let $\Delta r \to \infty$

$$\omega_k = \frac{\hbar \vec{k}^2}{2\mu} = \frac{\hbar}{2\mu}\underbrace{\left(\vec{k}_0 + \Delta\vec{k}\right)^2}_{k_0^2 + 2\vec{k}_0\cdot\Delta\vec{k} + (\Delta\vec{k})^2 = -k_0^2 + 2\vec{k}\cdot\vec{k}_0 + (\Delta\vec{k})^2} = -\omega_0 + \vec{k}\cdot\vec{v}_0 + \frac{\hbar}{2\mu}(\Delta\vec{k})^2$$

$$\omega_k t = -\omega_0 t + \vec{k}\cdot\vec{v}_0 t + \underbrace{\frac{\hbar}{2\mu}(\Delta\vec{k})^2 t}_{\ll 1}$$

$$\boxed{\begin{aligned}\psi_{\text{no scatt}}(\vec{r},t) &\simeq e^{i\omega_0 t}\int \frac{d^3k}{(2\pi)^{3/2}}\, g(\vec{k})\, e^{i\vec{k}\cdot(\vec{r}-\vec{r}_0-\vec{v}_0 t)} \\ &= e^{i\omega_0 t}\psi_0(\vec{r}-\vec{r}_0-\vec{v}_0 t)\end{aligned}}$$

Scattered wave:

$$\psi_{\text{scatt}}(\vec{r},t) = \frac{f_{\vec{k}_0}(\hat{r})}{r}\int \frac{d^3k}{(2\pi)^{3/2}}\, g(\vec{k})\, e^{-i\vec{k}\cdot\vec{r}_0}\, e^{-i\omega_k t}\, e^{ikr}$$

Scattering amplitude varies slowly over Δk

$$kr = (\vec{k}\cdot\vec{k})^{1/2} r = \left((\vec{k}_0 + \Delta\vec{k})\cdot(\vec{k}_0+\Delta\vec{k})\right)^{1/2} r$$

$$= \left(k_0^2 + 2\vec{k}_0\cdot\Delta\vec{k} + (\Delta\vec{k})^2\right)^{1/2} r$$

$$= k_0 r\left(1 + 2\hat{k}_0\cdot\frac{\Delta\vec{k}}{k_0} + \left(\frac{\Delta\vec{k}}{k_0}\right)^2\right)^{1/2}$$

$$\simeq k_0 r\left(1 + \hat{k}_0\cdot\frac{\Delta\vec{k}}{k_0} + O\left(\frac{\Delta\vec{k}}{k_0}\right)^2\right)$$

$$= k_0 r\left(1 + \frac{\hat{k}_0\cdot\vec{k}}{k_0} - 1 + O\left(\frac{\Delta\vec{k}}{k_0}\right)^2\right)$$

$$= \vec{k}\cdot r\hat{k}_0 + \underbrace{O\left(\frac{(\Delta\vec{k})^2 r}{k_0}\right)}_{\text{neglect}}$$

$$\psi_{scatt}(\vec{r},t) \simeq e^{i\omega t}\frac{f_{\vec{k}_0}(\hat{r})}{r}\int\frac{d^3k}{(2\pi)^{3/2}}\, g(\vec{k})\, e^{i\vec{k}\cdot(r\hat{k}_0 - \vec{r}_0 - \vec{v}_0 t)}$$

wave packet that has same value at $\vec{r} = r\hat{r}$ as $\psi_{no\ scatt}$ has at $r\hat{k}_0 = r\vec{e}_z$

$$= e^{i\omega t}\frac{f_{\vec{k}_0}(\hat{r})}{r}\,\psi_0(r\hat{k}_0 - \vec{r}_0 - \vec{v}_0 t)$$

Spherical wave packet centered at

$r\hat{k}_0 = \vec{r}_0 + \vec{v}_0 t$

(negative r at $t=0$)

Summarize:

$$\psi(\vec{r},t) \underset{r\to\infty}{\sim} e^{i\omega t}\left(\psi_0(\vec{r}-\vec{r}_0-\vec{v}_0 t) + \frac{f_{\vec{k}_0}(\hat{r})}{r}\psi_0(r\hat{k}_0 - \vec{r}_0 - \vec{v}_0 t)\right)$$

Cross section:

$$\sigma(\hat{r})\, d\Omega = \frac{N_i}{F_i}\, d\Omega\int_0^\infty r^2 dr\, \left|\psi(\vec{r},t)\right|^2$$

$\quad$ late times

$$\sigma(\hat{r}) = \frac{N_i}{F_i}\int_{-\infty}^{\infty}\cancel{r^2}\, dr\, \frac{|f_{\vec{k}_0}(\hat{r})|^2}{\cancel{r^2}}\left|\psi_0(r\hat{k}_0 - \vec{r}_0 - \vec{v}_0 t)\right|^2 = |f_{\vec{k}_0}(\hat{r})|^2$$

$$\int_{-\infty}^{\infty} dz\,\left|\psi_0(z\hat{k}_0 - \vec{r}_0 - \vec{v}_0 t)\right|^2 = \int_{-\infty}^{\infty} dz\,\left|\psi_0((z - r_0 - v_0 t)\vec{e}_z)\right|^2 = \frac{F_i(x{=}0,y{=}0)}{N_i}$$

$$\boxed{\sigma(\hat{r}) = \left| f_{\vec{k}_0}(\hat{r}) \right|^2}$$

Integral scattering equation and Green's functions

$$(\nabla^2 + k^2)\varphi(\vec{r}) = U(\vec{r})\,\varphi(\vec{r})$$

Green function : Why? Linear equation

$$(\nabla^2 + k^2)\, G(\vec{r},\vec{r}\,') = \delta(\vec{r}-\vec{r}\,')$$

$$\varphi_{\vec{k}}(\vec{r}) = \underbrace{\frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}}}_{\substack{\text{homogeneous} \\ \text{solution}}} + \underbrace{\int d^3r'\, G(\vec{r},\vec{r}\,')\, U(\vec{r}\,')\, \varphi_{\vec{k}}(\vec{r}\,')}_{\substack{\text{inhomogeneous (particular)} \\ \text{solution — want outgoing waves}}}$$

Why does it work? Physics / Math

Integral equation — ① can iterate to get approx solutions (Born expansion)

② can get asymptotic form

Solve: Clear that $G(\vec{r},\vec{r}\,') = G(\vec{r}-\vec{r}\,')$

FT: $G(\vec{r}-\vec{r}\,') = \int \frac{d^3q}{(2\pi)^3}\, G(\vec{q})\, e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}$

$$G(\vec{q}) = \int d^3r\, G(\vec{r}-\vec{r}\,')\, e^{-i\vec{q}\cdot(\vec{r}-\vec{r}\,')}$$

$$(k^2 - q^2)\, G(\vec{q}) = 1 \implies G(\vec{q}) = \frac{1}{k^2 - q^2} = -\frac{1}{(q-k)(q+k)}$$

$$G(\vec{r}) = -\int \frac{d^3q}{(2\pi)^3} \frac{e^{i\vec{q}\cdot\vec{r}}}{q^2 - k^2} = -\frac{1}{(2\pi)^3}\int_0^\infty q^2\,dq\, \frac{1}{q^2-k^2} \int d\Omega_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}}$$

Choose coordinate axes so that $\vec{r} = r\vec{e}_z$

$$\int d\Omega_q e^{\pm i\vec{q}\cdot\vec{r}} = 2\pi\int_0^\pi \sin\theta\, d\theta\, e^{\pm iqr\cos\theta}$$

$u = \cos\theta$
$du = -\sin\theta\, d\theta$

$$= 2\pi\int_{-1}^{+1} du\, e^{iqru}$$

$$= 2\pi\,\frac{e^{iqr} - e^{-iqr}}{iqr}$$

$$= 4\pi\,\frac{\sin qr}{qr}$$

$$G(\vec{r}) = +\frac{1}{(2\pi)^2}\frac{1}{r}\int_0^\infty dq\,\frac{iq}{q^2-k^2}\left(e^{iqr} - e^{-iqr}\right)$$

$$= \frac{1}{4\pi^2 r}\int_{-\infty}^\infty dq\,\frac{iq\,e^{iqr}}{q^2-k^2}$$

$$= \frac{1}{4\pi^2 r}\frac{d}{dr}\int_{-\infty}^\infty dq\,\frac{e^{iqr}}{(q-k)(q+k)}$$

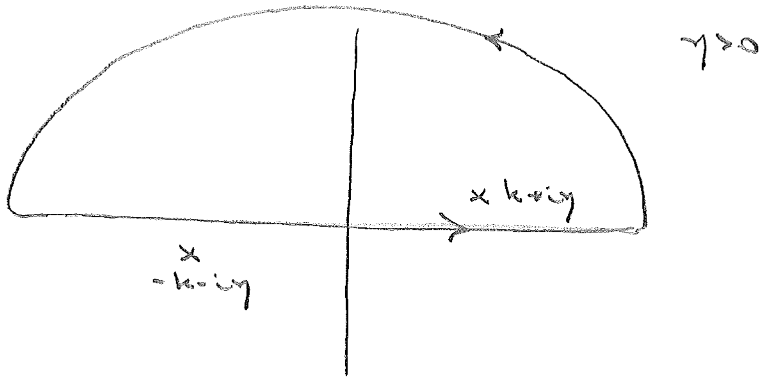
Integral doesn't converge
$\nabla^2 + k^2$ has no inverse
because there are
homogeneous solutions

$$E_k = \frac{\hbar^2(k\pm i\eta)^2}{2\mu} = \frac{\hbar^2 k^2}{2\mu} \pm i\underbrace{\frac{\hbar^2 k}{\mu}\eta}_{\epsilon} \qquad \eta > 0$$

$$\underbrace{\left(\nabla^2 + (k\pm i\eta)^2\right)}_{\text{does have an inverse}} G_\pm(\vec{r}) = \delta(\vec{r}) \Rightarrow G_\pm(\vec{q}) = -\frac{1}{(q-k\mp i\eta)(q+k\pm i\eta)}$$

convergence factors
move poles
BC's

$$G_\pm(\vec{r}) = \frac{1}{4\pi^2 r}\frac{d}{dr}\int_{-\infty}^\infty dq\,\frac{e^{iqr}}{(q-k\mp i\eta)(q+k\pm i\eta)}$$



$$\int_{-\infty}^{\infty} dq \frac{e^{iqr}}{(q-k-i\gamma)(q+k+i\gamma)} = 2\pi i \frac{e^{i(k+i\gamma)r}}{2(k+i\gamma)} = i\pi \frac{e^{i(k+i\gamma)r}}{k+i\gamma}$$

$$G_+(\vec{r}) = \frac{1}{4\pi^2 r}\left(-\pi\, e^{i(k+i\gamma)r}\right) = -\frac{1}{4\pi}\frac{e^{ikr}}{r}\, e^{-\gamma r}$$

convergence factor

outgoing spherical wave

$$G_-(\vec{r}) = -\frac{1}{4\pi}\frac{e^{-ikr}}{r}\, e^{-\gamma r}$$

incoming spherical wave

$$G_0(\vec{r}) = -\frac{1}{4\pi}\frac{\cos kr}{r}\, e^{-\gamma r}$$

Other solutions: move poles half and half — Principal value

<u>**Check:**</u>

$$\nabla^2 G_\pm = -\frac{1}{4\pi}\Big(\underbrace{e^{\pm ikr}\nabla^2\left(\frac{1}{r}\right)}_{-4\pi\,\delta(\vec{r})} + \underbrace{2\nabla\left(\frac{1}{r}\right)\cdot\nabla\left(e^{\pm ikr}\right)}_{\mp\frac{2ik}{r^2}e^{\pm ikr}}$$

$$+\frac{1}{r}\underbrace{\nabla^2\left(e^{\pm ikr}\right)}\Big)$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}e^{\pm ikr}\right) = \frac{2}{r}\frac{\partial}{\partial r}\left(e^{\pm ikr}\right) + \frac{\partial^2}{\partial r^2}\left(e^{\pm ikr}\right)$$

$$= \left(\pm\frac{2ik}{r} - k^2\right)e^{\pm ikr}$$

$$= \delta(\vec{r}) - \frac{1}{4\pi}\left(\cancel{\mp\frac{2ik}{r^2}} \cancel{\pm\frac{2ik}{r^2}} - \frac{k^2}{r}\right)e^{\pm ikr}$$

$$(\nabla^2 + k^2)\, G_\pm = \delta(\vec{r})$$

Summarize:
$$\boxed{G_\pm(\vec r,\vec r') = -\frac{1}{4\pi}\frac{e^{\pm ik|\vec r-\vec r'|}}{|\vec r-\vec r'|}}$$

Asymptotic form of eigenfunctions:

$$\varphi^{(\pm)}_{\vec k}(\vec r) = \frac{1}{(2\pi)^{3/2}} e^{i\vec k\cdot\vec r} - \frac{1}{4\pi}\int d^3r' \,\frac{e^{\pm ik|\vec r-\vec r'|}}{|\vec r-\vec r'|}\, U(\vec r')\,\varphi^{(\pm)}_{\vec k}(\vec r')$$

Notice that

$$\varphi^{(+)*}_{\vec k}(\vec r) = \frac{1}{(2\pi)^{3/2}} e^{-i\vec k\cdot\vec r} - \frac{1}{4\pi}\int d^3r' \,\frac{e^{-ik|\vec r-\vec r'|}}{|\vec r-\vec r'|}\, U(\vec r')\,\varphi^{(+)*}_{\vec k}(\vec r')$$

$$\varphi^{(-)}_{-\vec k}(\vec r) = \frac{1}{(2\pi)^{3/2}} e^{-i\vec k\cdot\vec r} - \frac{1}{4\pi}\int d^3r' \,\frac{e^{-ik|\vec r-\vec r'|}}{|\vec r-\vec r'|}\, U(\vec r')\,\varphi^{(-)}_{-\vec k}(\vec r')$$

$$\Longrightarrow \boxed{\varphi^{(-)}_{-\vec k}(\vec r) = \varphi^{(+)*}_{\vec k}(\vec r)}$$ Time-reversal invariance

$r\to\infty$
$$\frac{e^{\pm ik|\vec r-\vec r'|}}{|\vec r-\vec r'|} \underset{r\to\infty}{\sim} \frac{e^{\pm ikr}\, e^{\mp ik\hat r\cdot\vec r'}}{r}$$

$$|\vec r-\vec r'| = \sqrt{r^2+r'^2-2\vec r\cdot\vec r'} = r\left(1-2\hat r\cdot\frac{\vec r'}{r}+\frac{r'^2}{r^2}\right)^{1/2} \cong r - \hat r\cdot\vec r' + O\left(\frac{r'^2}{r}\right)$$

$$k|\vec r-\vec r'| = kr - k\hat r\cdot\vec r' + \underbrace{O\left(\frac{ka^2}{r_0}\right)}_{\frac{a^2}{\lambda_0 r_0}\ll 1}$$

make this small

$a^2 \ll \lambda_0 r_0 \ll (\Delta r)^2 \longleftarrow$ can always do this

$$\therefore\ \varphi^{(\pm)}_{\vec k}(\vec r) \underset{r\to\infty}{\sim} \frac{1}{(2\pi)^{3/2}} e^{i\vec k\cdot\vec r} + \frac{e^{ikr}}{r}\left(-\frac{1}{4\pi}\int d^3r'\, e^{\mp i\underbrace{k\hat r}_{\vec k'}\cdot\vec r'}\, U(\vec r')\,\varphi^{(\pm)}_{\vec k}(\vec r')\right)$$

$$\boxed{f_{\vec k}(\hat r) = -\frac{(2\pi)^{3/2}}{4\pi}\int d^3r'\, e^{-i\underbrace{k\hat r}_{\vec k'}\cdot\vec r'}\, U(\vec r')\,\varphi^{(+)}_{\vec k}(\vec r')}$$

Born approximation: 1st-order perturbation theory

$$f_{\vec k}(\hat r) \simeq -\frac{1}{4\pi}\int d^3r'\, e^{-i\vec k'\cdot\vec r'}\, U(\vec r')\, e^{i\vec k\cdot\vec r'}$$

1st iteration of integral equation (Born expansion)

$$= -\frac{1}{4\pi}\int d^3r'\, U(\vec r')\, e^{-i\underbrace{(\vec k'-\vec k)}_{\text{change in momentum}}\cdot\vec r'}$$

$$= -2\pi^2\langle\vec k'|U|\vec k\rangle$$

Estimate scattered wave at $\vec r\to 0$ for local central potential:

$$-\frac{1}{4\pi}\int d^3r'\,\frac{e^{ikr'}}{r'}\,U(r')\,\frac{1}{(2\pi)^{3/2}}e^{i\vec k\cdot\vec r'}$$

$$=\frac{1}{(2\pi)^{3/2}}\left(-\frac{1}{4\pi}\int r'dr'\,e^{ikr'}\,U(r')\underbrace{\int d\Omega'\,e^{i\vec k\cdot\vec r'}}_{4\pi\sin kr'/kr'}\right)$$

$$=\frac{1}{(2\pi)^{3/2}}\left(-\frac{1}{k}\int_0^\infty dr'\,e^{ikr'}\sin kr'\,U(r')\right)$$

Requires $\left|\frac{2\mu}{\hbar^2 k}\int_0^\infty dr\,e^{ikr}\sin kr\,V(r)\right| \ll 1$

Weak potential
High energy
(Interference of multiple scatterings)

Validity:

Example: Yukawa

$$V(\vec r) = V_0\,\frac{e^{-\alpha r}}{r}$$

$a \approx 1/\alpha$

$$f^{(B)}_{\vec k}(\hat r) = -\frac{1}{4\pi}\underbrace{\int d^3r'\,U(\vec r')\,e^{-i(\vec k'-\vec k)\cdot\vec r'}}$$

$$= -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int_0^\infty r'^2\,dr'\,V(r')\underbrace{\int d\Omega\, e^{-i(\vec k'-\vec k)\cdot\vec r'}}_{4\pi\frac{\sin|\vec k'-\vec k|r'}{|\vec k'-\vec k|r'}}$$

any central potential

$$= -\frac{2\mu}{\hbar^2}\frac{1}{|\vec k'-\vec k|}\int_0^\infty dr'\,r'\sin\underbrace{|\vec k'-\vec k|}_{q}r'\,V(r')$$

Yukawa $\int_0^\infty dr\, r \sin qr\, V(r) = V_0 \int_0^\infty dr\, e^{-\alpha r} \sin qr$

$$= \frac{V_0}{2i} \int_0^\infty dr\, e^{-\alpha r}\left(e^{iqr} - e^{-iqr}\right)$$

$$= \frac{V_0}{2i}\left(-\frac{1}{iq-\alpha} - \frac{1}{iq+\alpha}\right)$$

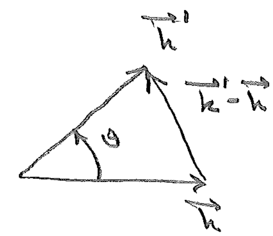
$$= \frac{V_0}{\cancel{2i}}\left(\frac{-\cancel{2i}q}{q^2+\alpha^2}\right)$$

$$= -V_0 \frac{q}{q^2+\alpha^2}$$

$$f^{(B)}_{\vec{k}}(\hat{r}) = \frac{2\mu V_0}{\hbar^2} \frac{1}{|\vec{k}'-\vec{k}| + \alpha^2}$$

right for Coulomb ($\alpha = 0$)

$$= \frac{2\mu V_0}{\hbar^2} \frac{1}{4k^2 \sin^2(\theta/2) + \alpha^2}$$



$|\vec{k}'-\vec{k}| = 2k \sin(\theta/2)$

$$\sigma^{(B)}(\hat{r}) = \left|f^{(B)}_{\vec{k}}(\hat{r})\right|^2$$

$$\sigma = \int d\Omega\, \sigma^{(B)}(\hat{r}) = \frac{4\mu^2 V_0^2}{\hbar^4} \frac{4\pi}{\alpha^2(\alpha^2+4k^2)} \xrightarrow[\alpha\to 0]{} \infty$$

Formal theory of scattering

$$H = H_0 + V$$

Unscattered plane waves: $H_0|\vec k\rangle = E_k|\vec k\rangle$

$E_k = \hbar^2 k^2/2\mu$

$\langle \vec k|\vec k'\rangle = \delta(\vec r - \vec r')$

$\mathbb{1} = \int d^3k\, |\vec k\rangle\langle \vec k|$

complete set

Scattering states:

$$H|\varphi_{\vec k}\rangle = E_k|\varphi_{\vec k}\rangle \longleftarrow$$

assumes a scattering state for each $\vec k$ with energy E_k

$$\Updownarrow$$

$$(E_k - H_0)|\varphi_{\vec k}\rangle = V|\varphi_{\vec k}\rangle$$

$(A = A^\dagger)$ Solve $A|u\rangle = |v\rangle$

① No zero eigenvalues $\Rightarrow |u\rangle = A^{-1}|v\rangle$

② Zero eigenvalues in subspace P_0. Must have $P_0|v\rangle = 0$. Then general solution is
$|u\rangle = |u_0\rangle + \frac{1-P_0}{A}|v\rangle$, $A|u_0\rangle = 0$

$P_0 A = P_0 \sum_i A_i P_i = 0$

$\therefore 0 = P_0 A|u\rangle = P_0|v\rangle$

Nothing maps into null space.

Can we write $|\varphi_{\vec k}\rangle = (E_k - H_0)^{-1}V|\varphi_{\vec k}\rangle$?
No, because $E_k - H_0$ does not have an inverse.
Instead we have
$|\varphi_{\vec k}\rangle = |\vec k\rangle + \frac{1-P_k}{E_k - H_0}V|\varphi_{\vec k}\rangle$,
but P_k can be omitted because it projects onto a set of measure zero, so we must also make $E_k - H_0$ invertible by letting $E_k - H_0 \longrightarrow E_k - H_0 \pm i\epsilon$. $\therefore$

Lippmann-Schwinger equation	$\lvert\varphi^{(\pm)}_{\vec k}\rangle = \lvert\vec k\rangle + (E_k - H_0 \pm i\epsilon)^{-1}V\lvert\varphi^{(\pm)}_{\vec k}\rangle$

$(E_k - H_0 \pm i\epsilon)^{-1}$ does have an inverse! has no zero eigenvalues for functions in Hilbert space

$$\Longrightarrow (E_k - H_0 \pm i\epsilon)|\varphi^{(\pm)}_{\vec k}\rangle = (E_k - H_0 \pm i\epsilon)|\vec k\rangle + V|\varphi^{(\pm)}_{\vec k}\rangle$$

Equation satisfied by $|\varphi^{(\pm)}_{\vec k}\rangle$ $\longrightarrow$

$$(E_k - H \pm i\epsilon)|\varphi^{(\pm)}_{\vec k}\rangle = (E_k - H_0 \pm i\epsilon)|\vec k\rangle = \pm i\epsilon|\vec k\rangle$$

Eigenstate of H in limit $\epsilon \to 0$

$|\varphi^{(\pm)}_{\vec k}\rangle = \pm i\epsilon(E_k - H \pm i\epsilon)^{-1}|\vec k\rangle$
$= (E_k - H \pm i\epsilon)^{-1}(E_k - H \pm i\epsilon)|\vec k\rangle$
$+ (E_k - H \pm i\epsilon)^{-1}\underbrace{(H - E_k)|\vec k\rangle}_{(H_0 - E_k)|\vec k\rangle + V|\vec k\rangle = V|\vec k\rangle}$
$|\varphi^{(\pm)}_{\vec k}\rangle = |\vec k\rangle + (E_k - H \pm i\epsilon)^{-1}V|\vec k\rangle$

$$(E_k - H \pm i\epsilon)|\varphi^{(\pm)}_{\vec k}\rangle = (E_k - H \pm i\epsilon)|\vec k\rangle + V|\vec k\rangle$$

$$\boxed{|\varphi^{(\pm)}_{\vec k}\rangle = |\vec k\rangle + (E_k - H \pm i\epsilon)^{-1}V|\vec k\rangle}$$

Formal solution

H not H_0

Relation to coordinate representation:

$$(E_k - H_0 \pm i\epsilon)(E_k - H_0 \pm i\epsilon)^{-1} = 1$$

$$\delta(\vec{r}-\vec{r}\,') = \int d^3r'' \underbrace{\langle \vec{r}|(E_k - H_0 \pm i\epsilon)|\vec{r}\,''\rangle}_{\left(\frac{\hbar^2}{2\mu}\nabla^2 + E_k \pm i\epsilon\right)\delta(\vec{r}-\vec{r}\,'')} \langle \vec{r}\,''|(E_k - H_0 \pm i\epsilon)^{-1}|\vec{r}\,'\rangle$$

$$= \left(\frac{\hbar^2}{2\mu}\nabla^2 + E_k \pm i\epsilon\right)\langle \vec{r}|(E_k - H_0 \pm i\epsilon)^{-1}|\vec{r}\,'\rangle$$

$$= \left(\nabla^2 + k^2 \pm i\frac{2\mu\epsilon}{\hbar^2}\right)\underbrace{\frac{\hbar^2}{2\mu}\langle \vec{r}|(E_k - H_0 \pm i\epsilon)^{-1}|\vec{r}\,'\rangle}_{G_\pm(\vec{r},\vec{r}\,')}$$

$$\epsilon = \frac{\hbar^2 k}{\mu}\gamma$$

$$\boxed{G_\pm(\vec{r},\vec{r}\,') = \frac{\hbar^2}{2\mu}\langle \vec{r}|(E_k - H_0 \pm i\epsilon)^{-1}|\vec{r}\,'\rangle} \quad \boxed{G_\pm(E_k) \equiv \frac{\hbar^2}{2\mu}(E_k - H_0 \pm i\epsilon)^{-1}}$$

$$\longrightarrow \langle \vec{r}|\varphi_{\vec{k}}^{(\pm)}\rangle = \underbrace{\langle \vec{r}|\vec{k}\rangle}_{\frac{1}{(2\pi)^{3/2}}e^{i\vec{k}\cdot\vec{r}}} + \int d^3r' \langle \vec{r}|(E_k - H_0 \pm i\epsilon)|\vec{r}\,'\rangle \underbrace{\langle \vec{r}\,'|V|\varphi_{\vec{k}}^{(\pm)}\rangle}_{V(\vec{r}\,')\langle \vec{r}\,'|\varphi_{\vec{k}}^{(\pm)}\rangle}$$

$$= \frac{1}{(2\pi)^{3/2}}e^{i\vec{k}\cdot\vec{r}} + \int d^3r'\, G_\pm(\vec{r},\vec{r}\,')\, U(\vec{r}\,')\langle \vec{r}\,'|\varphi_{\vec{k}}^{(\pm)}\rangle$$

Transition matrix: $T_{\vec{k}'\vec{k}} = \langle \vec{k}'|V|\varphi_{\vec{k}}^{(+)}\rangle$ defined when $k' \neq k$

$$f_{\vec{k}}(\hat{k}') = -\frac{(2\pi)^3}{4\pi}\langle \vec{k}'|U|\varphi_{\vec{k}}^{(+)}\rangle = -\frac{4\pi^2\mu}{\hbar^2}\langle \vec{k}'|V|\varphi_{\vec{k}}^{(+)}\rangle$$

$$\boxed{f_{\vec{k}}(\hat{k}') = -\frac{4\pi^2\mu}{\hbar^2}T_{\vec{k}'\vec{k}}} \quad \boxed{\vec{k}' = k\hat{k}'}$$

Orthonormality:

$$\langle\varphi^{(\pm)}_{\vec{k}'}|\varphi^{(\pm)}_{\vec{k}}\rangle = \langle\vec{k}'|\varphi^{(\pm)}_{\vec{k}}\rangle + \langle\vec{k}'|V\underbrace{(E_{k'}-H\mp i\epsilon)^{-1}|\varphi^{(\pm)}_{\vec{k}}\rangle}_{(E_{k'}-E_k\mp i\epsilon)^{-1}|\varphi^{(\pm)}_{\vec{k}}\rangle}$$

in limit $\epsilon\to 0$

$$= \langle\vec{k}'|(E_{k'}-E_k\mp i\epsilon)^{-1}V|\varphi^{(\pm)}_{\vec{k}}\rangle$$

$$= \langle\vec{k}'|(H_0-E_k\mp i\epsilon)^{-1}V|\varphi^{(\pm)}_{\vec{k}}\rangle$$

$$= \langle\vec{k}'|\underbrace{\left(|\varphi^{(\pm)}_{\vec{k}}\rangle - (E_k-H_0\pm i\epsilon)^{-1}V|\varphi^{(\pm)}_{\vec{k}}\rangle\right)}_{|\vec{k}\rangle}$$

$$\boxed{\langle\varphi^{(\pm)}_{\vec{k}'}|\varphi^{(\pm)}_{\vec{k}}\rangle = \langle\vec{k}'|\vec{k}\rangle = \delta(\vec{k}'-\vec{k})}$$

$|\varphi^{(\pm)}_{\vec{k}}\rangle$, together with bound states, are complete

Born expansion:

$$\left(1-(E_k-H_0\pm i\epsilon)^{-1}V\right)|\varphi^{(\pm)}_{\vec{k}}\rangle = |\vec{k}\rangle$$

$$\boxed{|\varphi^{(\pm)}_{\vec{k}}\rangle = \frac{1}{1-(E_k-H_0\pm i\epsilon)^{-1}V}|\vec{k}\rangle}$$

Expand to get the Born approximation

$$T_{\vec{k}'\vec{k}} = \langle\vec{k}'|V|\varphi^{(+)}_{\vec{k}}\rangle$$

$$= \langle\vec{k}'|V\frac{1}{1-(E_k-H_0\pm i\epsilon)^{-1}V}|\vec{k}\rangle$$

$$= \underbrace{\langle\vec{k}'|V|\vec{k}\rangle}_{\text{Born approximation}} - \langle\vec{k}'|V(E_k-H_0\pm i\epsilon)^{-1}V|\vec{k}\rangle + \dots$$

Time-reversal invariance:

$$S_{\vec{k}'\vec{k}} = \int d^3x\,\varphi^{(-)*}_{\vec{k}'}(\vec{x})\,\varphi^{(+)}_{\vec{k}}(\vec{x})$$

$$= \int d^3x\,\varphi^{(+)}_{-\vec{k}'}(\vec{x})\,\varphi^{(-)*}_{-\vec{k}}(\vec{x})$$

$$= \langle\varphi^{(-)}_{-\vec{k}}|\varphi^{(+)}_{-\vec{k}'}\rangle$$

$$\boxed{S_{\vec{k}'\vec{k}} = S_{-\vec{k},-\vec{k}'}}$$

Completeness: Bound states $|\varphi_n\rangle$ of H are $\perp$ to $|\varphi^{(\pm)}_{\vec{k}}\rangle$.

$$1 = \sum_n |\varphi_n\rangle\langle\varphi_n| + \int d^3k\, |\varphi^{(\pm)}_{\vec{k}}\rangle\langle\varphi^{(\pm)}_{\vec{k}}| = \int d^3k\, |\vec{k}\rangle\langle\vec{k}|$$

Bound states can be written in terms of plane waves

S-matrix:

$$|\varphi^{(\mp)}_{\vec{k}}\rangle = \sum_n |\varphi_n\rangle\cancel{\langle\varphi_n|\varphi^{(\mp)}_{\vec{k}}\rangle}^{\,0} + \int d^3k'\, |\varphi^{(\pm)}_{\vec{k}'}\rangle\langle\varphi^{(\pm)}_{\vec{k}'}|\varphi^{(\mp)}_{\vec{k}}\rangle$$

$$|\varphi^{(\pm)}_{\vec{k}}\rangle = \int d^3k'\, |\varphi^{(\mp)}_{\vec{k}'}\rangle\langle\varphi^{(\mp)}_{\vec{k}'}|\varphi^{(\pm)}_{\vec{k}}\rangle$$

total amplitude to end in $\vec{k}'$, starting in $\vec{k}$

$$S_{\vec{k}'\vec{k}} \equiv \langle\varphi^{(-)}_{\vec{k}'}|\varphi^{(+)}_{\vec{k}}\rangle = \langle\vec{k}'|S|\vec{k}\rangle$$

unitary matrix — unitary operator

$$|\varphi^{(+)}_{\vec{k}}\rangle = \int d^3k'\, |\varphi^{(-)}_{\vec{k}'}\rangle S_{\vec{k}'\vec{k}}$$

$$|\varphi^{(-)}_{\vec{k}}\rangle = \int d^3k'\, |\varphi^{(+)}_{\vec{k}'}\rangle S^*_{\vec{k}\vec{k}'}$$

The S-matrix is unitary because $|\varphi^{(\pm)}_{\vec{k}}\rangle$ are complete and orthonormal in the space of free states

Time-reversal invariance:

$$S_{\vec{k}'\vec{k}} = S_{-\vec{k},-\vec{k}'}$$

$$S_{\vec{k}'\vec{k}} = \langle\varphi^{(-)}_{\vec{k}'}|\varphi^{(+)}_{\vec{k}}\rangle$$

$$= \langle\vec{k}'|\varphi^{(+)}_{\vec{k}}\rangle + \langle\vec{k}'|V\underbrace{(E_{k'}-H+i\epsilon)^{-1}|\varphi^{(+)}_{\vec{k}}\rangle}_{}$$

$$= (E_{k'}-E_k+i\epsilon)^{-1}|\varphi^{(+)}_{\vec{k}}\rangle$$

$$= \underbrace{\left((E_{k'}-E_k-i\epsilon)^{-1} - 2\pi i\,\delta(E_{k'}-E_k)\right)}_{}|\varphi^{(+)}_{\vec{k}}\rangle \quad \text{in limit } \epsilon\to 0$$

$$= \langle\vec{k}'|(E_{k'}-E_k-i\epsilon)^{-1}V|\varphi^{(+)}_{\vec{k}}\rangle - 2\pi i\,\delta(E_{k'}-E_k)\langle\vec{k}'|V|\varphi^{(+)}_{\vec{k}}\rangle$$

$$= \langle \vec{k}'|(H_0 - E_k - i\epsilon)^{-1} V|\varphi_{\vec{k}}^{(+)}\rangle - 2\pi i\,\delta(E_{k'} - E_k)\, T_{\vec{k}'\vec{k}}$$

$$S_{\vec{k}'\vec{k}} = \langle \vec{k}'|\underbrace{\Big(|\varphi_{\vec{k}}^{(+)}\rangle - (E_k - H_0 + i\epsilon)^{-1} V|\varphi_{\vec{k}}^{(+)}\rangle\Big)}_{|\vec{k}\rangle} - 2\pi i\,\delta(E_{k'} - E_k)\, T_{\vec{k}'\vec{k}}$$

$$\boxed{\begin{aligned} S_{\vec{k}'\vec{k}} &= \delta(\vec{k}' - \vec{k}) - 2\pi i \underbrace{\delta(E_{k'} - E_k)}_{\frac{\mu}{\hbar^2 k}\delta(k'-k)} T_{\vec{k}'\vec{k}} \\ &= \delta(\vec{k}' - \vec{k}) + \frac{i}{2\pi k}\,\delta(k' - k)\, f_{\vec{k}}(\vec{k}') \end{aligned}}$$

Momentum representation:

$$\langle \vec{q}'|G_\pm(E_k)|\vec{q}\rangle = \underbrace{\frac{\hbar^2}{2\mu}(E_k - E_q \pm i\epsilon)^{-1}}_{\left(k^2 - q^2 \pm i\frac{2\mu\epsilon}{\hbar^2}\right)^{-1} = (k^2 - q^2 \pm 2ik\eta)^{-1} = ((k\pm i\eta)^2 - q^2)^{-1}} \delta(\vec{q}' - \vec{q})$$

$$= \underbrace{\frac{1}{((k \pm i\eta)^2 - q^2)}}_{G_\pm(\vec{q})} \delta(\vec{q}' - \vec{q})$$

$$\langle \vec{q}|\varphi_{\vec{k}}^{(\pm)}\rangle = \delta(\vec{q} - \vec{k}) + \underbrace{\langle \vec{q}|(E_k - H_0 \pm i\epsilon)^{-1} V|\varphi_{\vec{k}}^{(\pm)}\rangle}_{\frac{1}{E_k - E_q \pm i\epsilon}\underbrace{\langle \vec{q}|V|\varphi_{\vec{k}}^{(\pm)}\rangle}_{T_{\vec{q}\vec{k}} = \int d^3q' \langle \vec{q}|V|\vec{q}'\rangle\langle \vec{q}'|\varphi_{\vec{k}}^{(\pm)}\rangle}}$$

$$\boxed{\begin{aligned} \langle \vec{q}|\varphi_{\vec{k}}^{(\pm)}\rangle &= \delta(\vec{q} - \vec{k}) + \frac{T_{\vec{q}\vec{k}}}{E_k - E_q \pm i\epsilon} \\ &= \delta(\vec{q} - \vec{k}) + \frac{1}{E_k - E_q \pm i\epsilon}\int d^3q' \langle \vec{q}|V|\vec{q}'\rangle\langle \vec{q}'|\varphi_{\vec{k}}^{(\pm)}\rangle \end{aligned}}$$

Parity: $V(\vec{r}) = V(-\vec{r})$

$$\varphi^{(\pm)}_{\vec{k}}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi}\int d^3r' \frac{e^{\pm ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \mathcal{U}(\vec{r}')\,\varphi^{(\pm)}_{\vec{k}}(\vec{r}')$$

$$\varphi^{(\pm)}_{\vec{k}}(-\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{-i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi}\int d^3r' \frac{e^{\pm ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \underbrace{\mathcal{U}(-\vec{r}')}_{\mathcal{U}(\vec{r}')}\,\varphi^{(\pm)}_{\vec{k}}(-\vec{r}')$$

$$\Rightarrow \quad \varphi^{(\pm)}_{\vec{k}}(-\vec{r}) = \varphi^{(\pm)}_{-\vec{k}}(\vec{r}) = \varphi^{(\mp)*}_{\vec{k}}(\vec{r})$$

$\uparrow$ parity $\qquad \uparrow$ time-reversal

$$S_{\vec{k}'\vec{k}} = \langle \varphi^{(-)}_{\vec{k}'} | \varphi^{(+)}_{\vec{k}} \rangle = \int d^3r\, \varphi^{(-)*}_{\vec{k}'}(\vec{r})\,\varphi^{(+)}_{\vec{k}}(\vec{r})$$

$$= \int d^3r\, \varphi^{(-)*}_{\vec{k}'}(-\vec{r})\,\varphi^{(+)}_{\vec{k}}(-\vec{r})$$

$$= \int d^3r\, \varphi^{(-)*}_{-\vec{k}'}(\vec{r})\,\varphi^{(+)}_{-\vec{k}}(\vec{r})$$

$$= \langle \varphi^{(-)}_{-\vec{k}'} | \varphi^{(+)}_{-\vec{k}} \rangle$$

$$= S_{-\vec{k}',-\vec{k}}$$

Parity: $\boxed{S_{\vec{k}'\vec{k}} = S_{-\vec{k}',-\vec{k}} \implies f_{\vec{k}}(\hat{k}') = f_{-\vec{k}}(-\hat{k}')}$

Note $T_{\vec{k}'\vec{k}} = \langle \vec{k}' | V | \varphi^{(+)}_{\vec{k}} \rangle = \int d^3r\, e^{-i\vec{k}'\cdot\vec{r}}\, V(\vec{r})\,\varphi^{(+)}_{\vec{k}}(\vec{r})$

$$= \int d^3r\, e^{i\vec{k}'\cdot\vec{r}}\, V(\vec{r})\,\varphi^{(+)}_{-\vec{k}}(\vec{r})$$

$$= T_{-\vec{k}',-\vec{k}}$$

$$\boxed{T_{\vec{k}'\vec{k}} = T_{-\vec{k}',-\vec{k}}}$$

Time-reversal invariance:

$$\varphi^{(-)}_{-\vec{k}}(\vec{r}) = \varphi^{(+)*}_{\vec{k}}(\vec{r})$$

$$\Longrightarrow \boxed{S_{\vec{k}'\vec{k}} = S_{-\vec{k},-\vec{k}'} \Rightarrow f_{\vec{k}}(\hat{k}') = f_{-\vec{k}'}(-\hat{k})}$$

Parity plus time reversal: $\boxed{S_{\vec{k}'\vec{k}} = S_{\vec{k}\vec{k}'}}$

Optical theorem:

<u>Unitarity</u> $$\delta(\vec{k}'-\vec{k}) = \int d^3q\, S^*_{\vec{q}\vec{k}'} S_{\vec{q}\vec{k}}$$

$$= \int d^3q \left[\delta(\vec{q}-\vec{k}') - \frac{i}{2\pi k'}\delta(q-k') f^*_{\vec{k}'}(\hat{q})\right] \times \left[\delta(\vec{q}-\vec{k}) + \frac{i}{2\pi k}\delta(q-k) f_{\vec{k}}(\hat{q})\right]$$

$$= \delta(\vec{k}'-\vec{k}) + \frac{i}{2\pi k}\delta(k'-k) f_{\vec{k}}(\hat{k}') - \frac{i}{2\pi k'}\delta(k-k') f^*_{\vec{k}'}(\hat{k})$$

$$+ \underbrace{\int \cancel{q^2}\, dq\, d\Omega_{\hat{q}} \frac{1}{4\pi^2}\frac{1}{\cancel{q^2}}\delta(q-k')\delta(q-k) f^*_{\vec{k}'}(\hat{q}) f_{\vec{k}}(\hat{q})}_{\frac{1}{4\pi^2}\delta(k'-k)\int d\Omega_{\hat{q}} f^*_{\vec{k}'}(\hat{q}) f_{\vec{k}}(\hat{q})}$$

$$0 = \frac{i}{2\pi k}\left(f_{\vec{k}}(\hat{k}') - f^*_{\vec{k}'}(\hat{k})\right) + \frac{1}{4\pi^2}\int d\Omega_{\hat{q}} f^*_{\vec{k}'}(\hat{q}) f_{\vec{k}}(\hat{q})$$

$$\int d\Omega_{\hat{q}} f^*_{\vec{k}'}(\hat{q}) f_{\vec{k}}(\hat{q}) = -\frac{2\pi i}{k}\left(f_{\vec{k}}(\hat{k}') - f^*_{\vec{k}'}(\hat{k})\right)$$

$\vec{k}' = \vec{k}$: $$\sigma = -\frac{2\pi i}{k}\left(f_{\vec{k}}(\hat{k}) - f^*_{\vec{k}}(\hat{k})\right) = +\frac{4\pi}{k}\,\mathrm{Im}\left(f_{\vec{k}}(\hat{k})\right)$$

$$\delta(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \, e^{ikx} e^{-|k|\eta}$$

$$= \frac{1}{2\pi} \Bigg(\underbrace{\int_{-\infty}^{0} dk \, e^{ikx} e^{k\eta}}_{\frac{1}{ix+\eta}} + \underbrace{\int_{0}^{\infty} dk \, e^{ikx} e^{-k\eta}}_{-\frac{1}{ix-\eta}} \Bigg)$$

$$\delta(x) = \frac{1}{2\pi i} \left(\frac{1}{x-i\eta} - \frac{1}{x+i\eta} \right)$$

$$P\left(\frac{1}{x}\right) = \frac{1}{2} \left(\frac{1}{x-i\eta} + \frac{1}{x+i\eta} \right)$$

$$\frac{1}{x-i\eta} = P\left(\frac{1}{x}\right) + i\pi\,\delta(x)$$

$$\frac{1}{x+i\eta} = P\left(\frac{1}{x}\right) - i\pi\,\delta(x)$$

Partial-wave analysis of scattering

Free particle $(V=0)$: $(\nabla^2 + k^2)\varphi(\vec{r}) = 0$, $E_k = \hbar^2 k^2/2\mu$

CSCO H_0, P_x, P_y, P_z : $|\vec{k}\rangle$, $\langle \vec{r}|\vec{k}\rangle = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}}$

Orthonormality and completeness

CSCO: $H_0, \vec{L}^2, L_z$: $|\varphi^{(0)}_{klm}\rangle$, $\langle \vec{r}|\varphi^{(0)}_{klm}\rangle = R_{kl}(r) Y_l^m(\theta,\varphi)$

$= \frac{1}{r} u_{kl}(r) Y_l^m(\theta,\varphi)$

$$\Big(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \underbrace{\cancel{V(r)}^{\,0} + \frac{l(l+1)\hbar^2}{2\mu r^2}}_{V_{eff}(r)}\Big) u_{kl}(r) = E_k u_{kl}(r)$$

$$\Big(\frac{d^2}{dr^2} + k^2\Big) u_{kl}(r) = \frac{l(l+1)}{r^2} u_{kl}(r)$$

B.C.: $u_{kl}(0) = 0$

Asymptotics: ① $r\to\infty$: $u_{kl}(r) \sim A e^{ikr} + B e^{-ikr}$

$R_{kl}(r)$ regular singular

② r near 0: $u_{kl}(r) \sim C r^{l+1} + D r^{-l}$
$(l\neq 0)$

Note right for $l=0$

$R_{kl}(r)$

Spherical Bessel functions solve radial equation for $R(r)$:

<u>real</u> $j_l(z) = (-1)^l z^l \left(\frac{1}{z}\frac{d}{dz}\right)^l \frac{\sin z}{z} = \sqrt{\frac{\pi}{2z}}\, J_{l+1/2}(z)$

$|z| \ll 1$: $j_l(z) \sim \frac{2^l\, l!}{(2l+1)!} z^l$ ⟵ regular

$\rho \gg 1, l$: $j_l(\rho) \sim \frac{\cos(\rho - (l+1)\pi/2)}{\rho} = \frac{\sin(\rho - l\pi/2)}{\rho}$

<u>real</u> $n_l(z)$: $|z| \ll 1$: $n_l(z) \sim \frac{(2l)!}{2^l\, l!}\frac{1}{z^{l+1}}$ ⟵ singular

spherical Neumann

$\omega_l(\rho) = \sqrt{\frac{\pi}{2\rho}}\, \Omega_{l+\frac{1}{2}}(\rho)$ $\omega = j, n, h^{(1)}, h^{(2)}$ 20

$\Omega = J, N, H^{(1)}, H^{(2)}$

The explicit forms of the spherical Bessel, Hankel, and Neumann functions for $l = 0$, 1, and 2, are given below

$$\begin{aligned} j_0(z) &= \frac{\sin z}{z} \\ j_1(z) &= \frac{\sin z}{z^2} - \frac{\cos z}{z} \\ j_2(z) &= \left(\frac{3}{z^3} - \frac{1}{z}\right)\sin z - \frac{3}{z^2}\cos z \end{aligned} \tag{10.36}$$

$$\begin{aligned} n_0(z) &= -\frac{\cos z}{z} \\ n_1(z) &= -\frac{\cos z}{z^2} - \frac{\sin z}{z} \\ n_2(z) &= -\left(\frac{3}{z^3} - \frac{1}{z}\right)\cos z - \frac{3}{z^2}\sin z \end{aligned} \tag{10.37}$$

$$\begin{aligned} h_0^{(1)}(z) &= -i\,\frac{e^{iz}}{z} \\ h_1^{(1)}(z) &= \left(-\frac{i}{z^2} - \frac{1}{z}\right)e^{iz} \\ h_2^{(1)}(z) &= \left(-\frac{3i}{z^3} - \frac{3}{z^2} + \frac{i}{z}\right)e^{iz} \end{aligned} \tag{10.38}$$

$$\begin{aligned} h_0^{(2)}(z) &= i\,\frac{e^{-iz}}{z} \\ h_1^{(2)}(z) &= \left(\frac{i}{z^2} - \frac{1}{z}\right)e^{-iz} \\ h_2^{(2)}(z) &= \left(\frac{3i}{z^3} - \frac{3}{z^2} - \frac{i}{z}\right)e^{-iz} \end{aligned} \tag{10.39}$$

3. ***Spherical Harmonic Expansion of Plane Waves.*** The regular radial eigenfunctions of the Schrödinger equation for $V = 0$ constitute a complete set, as a consequence of a fundamental theorem concerning Sturm-Liouville differential equations[4] of which (10.19) is an example. Hence, we have before us two alternative complete sets of eigenfunctions of the free particle

[4] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics*, McGraw-Hill Book Company, New York, 1953, p. 738.

$$\rho \gg 1, l: \quad n_l(\rho) \sim \frac{\sin(\rho - (l+1)\pi/2)}{\rho} = -\frac{\cos(\rho - l\pi/2)}{\rho}$$

spherical Hankel

$$h_l^{(1,2)}(z) = j_l(z) \pm i n_l(z) \longleftarrow \text{singular at } z=0$$

$j_l = \frac{1}{2}(h_l^{(1)} + h_l^{(2)})$

$n_l = -\frac{i}{2}(h_l^{(1)} - h_l^{(2)})$

$$\rho \gg 1, l: \quad h_l^{(1,2)}(\rho) \sim \frac{e^{\pm i(\rho - (l+1)\pi/2)}}{\rho} = \mp i \frac{e^{i(\rho - l\pi/2)}}{\rho}$$

$$R_{kl}(r) = A j_l(kr) + \cancel{B n_l(kr)}^{\,0} = A j_l(kr) = \sqrt{\frac{2k^2}{\pi}}\, j_l(kr)$$

$$\boxed{\langle \vec{r} | \varphi^{(0)}_{klm} \rangle = \sqrt{\frac{2k^2}{\pi}}\, j_l(kr)\, Y_l^m(\theta,\varphi)}$$

Orthonormality $\longrightarrow \delta(k-k')$
and completeness

hard to show but can be done using 1-d theory

$$r \to \infty: \quad \langle \vec{r} | \varphi^{(0)}_{klm} \rangle \sim \sqrt{\frac{2}{\pi}}\, Y_l^m(\theta,\varphi) \underbrace{\frac{\sin(kr - l\pi/2)}{r}}_{\frac{1}{2i}\frac{e^{ikr}e^{-il\pi/2} - e^{-ikr}e^{il\pi/2}}{r}}$$

incoming and outgoing spherical waves with phase shift $(l+1)\pi$ between them (note sign change)

$$r \sim 0: \quad \langle \vec{r} | \varphi^{(0)}_{klm} \rangle \sim \sqrt{\frac{2k^2}{\pi}}\, Y_l^m(\theta,\varphi) \frac{2^l l!}{(2l+1)!} (kr)^l$$

$\downarrow$

Remains near 0 for $kr \lesssim \sqrt{l(l+1)}$

$$r \lesssim \frac{\hbar l}{\hbar k} \approx \frac{L}{p}$$

$\uparrow$
impact parameter

Wave-packet behavior

Relation between two bases:

$$\boxed{\begin{aligned} e^{ikz} = e^{ikr\cos\theta} &= \sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)}\, j_l(kr)\, \underbrace{Y_l^0(\theta)}_{\sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta)} \\ &= \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(kr)\, P_l(\cos\theta) \end{aligned}}$$

$$(2\pi)^{3/2} \langle \vec{r} \,|\, k_x=0, k_y=0, k_z=k \rangle = \sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)} \sqrt{\frac{\pi}{2k^2}} \langle \vec{r} \,|\, \varphi^{(0)}_{kl0} \rangle$$

$$|k_x=0, k_y=0, k_z=k\rangle = \frac{1}{k} \sum_{l=0}^{\infty} i^l \sqrt{\frac{2l+1}{4\pi}}\, |\varphi^{(0)}_{kl0}\rangle \quad \leftarrow \; L_z = 0 \text{ eigenstate}$$

same k $\qquad m=0$

Addition theorem gives

$$e^{i\vec{k}\cdot\vec{r}} = e^{ikr\cos\alpha} = \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(kr)\, \underbrace{P_l(\cos\alpha)}$$

α: angle between $\vec{k}$ and $\vec{r}$

$$P_l(\cos\alpha) = \frac{4\pi}{2l+1} \sum_m Y_l^{m*}(\hat{k})\, Y_l^m(\theta,\varphi)$$

$$\boxed{\underbrace{e^{i\vec{k}\cdot\vec{r}}}_{(2\pi)^{3/2}\langle \vec{r}|\vec{k}\rangle} = 4\pi \sum_{l,m} i^l\, Y_l^{m*}(\hat{k})\, \underbrace{j_l(kr)\, Y_l^m(\theta,\varphi)}_{=\sqrt{\frac{\pi}{2k^2}}\,\langle \vec{r}|\varphi^{(0)}_{klm}\rangle}}$$

$$\Rightarrow \boxed{|\vec{k}\rangle = \frac{1}{k} \sum_{l,m} i^l\, Y_l^{m*}(\hat{k})\, |\varphi^{(0)}_{klm}\rangle}$$

$$\boxed{\langle \varphi^{(0)}_{k'lm} | \vec{k} \rangle = \frac{1}{k}\, \delta(k-k')\, i^l\, Y_l^{m*}(\hat{k})}$$

$$\begin{aligned} |\varphi^{(0)}_{klm}\rangle &= \int d^3k'\, |\vec{k}'\rangle \langle \vec{k}' | \varphi^{(0)}_{klm} \rangle \\ &= \int k'^2 dk'\, d\Omega_{\hat{k}}\, |k'\hat{k}\rangle \frac{1}{k}\, \delta(k-k')\, (-i)^l\, Y_l^m(\hat{k}) \\ &= (-i)^l\, k \int d\Omega_{\hat{k}}\, |\vec{k}\rangle\, Y_l^m(\hat{k}) \end{aligned}$$

$$\boxed{|\varphi^{(0)}_{klm}\rangle = (-i)^l k \int d\Omega_{\hat{k}}\, |\vec{k}\rangle\, Y_l^m(\hat{k})}$$

$$\sqrt{\frac{2k^2}{\pi}}\, j_l(kr)\, Y_l^m(\theta,\varphi) = (-i)^l k \int d\Omega_{\hat{k}} \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}}\, Y_l^m(\hat{k})$$

$$\boxed{j_l(kr)\, Y_l^m(\theta,\varphi) = \frac{(-i)^l}{4\pi} \int d\Omega_{\hat{k}}\, Y_l^m(\hat{k})\, e^{i\vec{k}\cdot\vec{r}}}$$

Partial waves in potential $V(r)$ ← Specialize to central potential

Free eigenstates of H: $|\varphi_{klm}\rangle$ CSCO $H, \vec{L}^2, L_z$

$$\langle\vec{r}|\varphi_{klm}\rangle = R_{kl}(r)\, Y_l^m(\theta,\varphi) = \frac{u_{kl}(r)}{r} Y_l^m(\theta,\varphi)$$

$$\left(\frac{d^2}{dr^2} + k^2\right) u_{kl}(r) = \underbrace{\left(U(r) + \frac{l(l+1)}{r^2}\right)}_{U_{eff}(r)} u_{kl}(r)$$

BC: $u_{kl}(0) = 0$

1-d problem w/ infinite barrier at $r=0$

Asymptotic behaviour: $r \to \infty$

$$u_{kl}(r) \sim A\cos kr + B\sin kr$$

$$= C \sin(kr - l\pi/2 + \delta_l) \quad \leftarrow u \text{ is real}$$

$C = \sqrt{\frac{2}{\pi}}$ ↑ gives δ-fcn. normalization and same asymptotic constant as free states

$-l\pi/2$ ↑ $V=0$ phase shift

δ_l ↑ scattering phase shift — only difference from free wave asymptotically — $\boxed{\text{determined by BC at } r=0}$ → discuss

$$= \sqrt{\frac{2}{\pi}} \sin(kr - l\pi/2 + \delta_l)$$

$$\langle \vec{r} | \varphi_{k\ell m}\rangle \underset{r\to\infty}{\sim} \sqrt{\frac{2}{\pi}}\, Y_\ell^m(\theta,\varphi)\, \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{r}$$

$$= \sqrt{\frac{2}{\pi}}\, Y_\ell^m(\theta,\varphi)\, \frac{1}{2i}\, \frac{e^{ikr} e^{-i\ell\pi/2} e^{i\delta_\ell} - e^{-ikr} e^{i\ell\pi/2} e^{-i\delta_\ell}}{r}$$

Wave-packet behavior

Let's put the whole phase shift ($2\delta_\ell$) into the outgoing wave:

$$|\tilde{\varphi}_{k\ell m}\rangle = e^{i\delta_\ell} |\varphi_{k\ell m}\rangle$$

$\boxed{\text{As } k\to 0, \text{ only } \ell=0 \text{ counts}}$

Phase shifts vanish for $\underset{\substack{\uparrow\\ \text{impact parameter}\\ \uparrow \\ \text{turning point w/th respect to centrifugal barrier}}}{\ell/k} \gtrsim \underset{\substack{\uparrow \\ \text{range of potential}}}{a}$

$$\frac{\ell(\ell+1)\hbar^2}{2\mu r_{min}^2} = \frac{\hbar^2 k^2}{2\mu}$$

$$r_{min} = \frac{\sqrt{\ell(\ell+1)}}{k}$$

Express $|\varphi_{\vec{k}}^{(+)}\rangle$ in terms of $|\tilde{\varphi}_{k\ell m}\rangle$ ⟵ both complete in the continuum

Show $\langle \tilde{\varphi}_{k'\ell m} | \varphi_{\vec{k}}^{(+)}\rangle = \langle \varphi_{k'\ell m}^{(0)} | \vec{k}\rangle = \frac{i^\ell}{k} \underbrace{\delta(k'-k)}_{\text{know this is present because both sets are energy eigenstates}} Y_\ell^{m*}(\hat{k})$

1 Wave-packet analysis:

$$|\psi(t)\rangle = \int d^3k\, g(\vec{k})\, e^{-i\vec{k}\cdot\vec{r}_0}\, |\varphi_{\vec{k}}^{(+)}\rangle\, e^{-i\omega_k t}$$

$$|\psi(0)\rangle = \int d^3k\, g(\vec{k})\, e^{-i\vec{k}\cdot\vec{r}_0}\, |\varphi_{\vec{k}}^{(+)}\rangle$$

$$= \int d^3k\, g(\vec{k})\, e^{-i\vec{k}\cdot\vec{r}_0}\, |\vec{k}\rangle$$

(Why? Initial wave packet only uses plane-wave part of $|\varphi_{\vec{k}}^{(+)}\rangle$)

$$= \sum_{l,m} \int_0^\infty dk' \, |\varphi^{(0)}_{k'lm}\rangle \int d^3k \, g(\vec{k}) \, e^{-i\vec{k}\cdot\vec{r}_0} \langle \varphi^{(0)}_{k'lm} | \vec{k} \rangle$$

(Why? Initial wave packet only uses incoming spherical waves — same in $|\varphi^{(0)}\rangle$ + $|\tilde{\varphi}\rangle$)

$$= \sum_{l,m} \int_0^\infty dk' \, |\tilde{\varphi}_{k'lm}\rangle \int d^3k \, g(\vec{k}) \, e^{-i\vec{k}\cdot\vec{r}_0} \langle \varphi^{(0)}_{k'lm} | \vec{k} \rangle$$

$$|\psi(t)\rangle = \sum_{l,m} \int dk' \, e^{-i\omega_{k'} t} \, |\tilde{\varphi}_{k'lm}\rangle \int d^3k \, g(\vec{k}) \, e^{-i\vec{k}\cdot\vec{r}_0} \underbrace{\langle \varphi^{(0)}_{k'lm} | \vec{k} \rangle}_{\shortparallel}$$

$$= \sum_{l,m} \int dk' \, e^{-i\omega t} \, |\tilde{\varphi}_{k'lm}\rangle \int d^3k \, g(\vec{k}) \, e^{-i\vec{k}\cdot\vec{r}_0} \langle \tilde{\varphi}_{k'lm} | \varphi^{(+)}_{\vec{k}} \rangle$$

narrow

$\Rightarrow$ true for all initial states

② Know $|\varphi^{(+)}_{\vec{k}}\rangle = \sum_{l,m} a_{lm}(k) \, |\tilde{\varphi}_{klm}\rangle$

determine these by matching two sides asymptotically

$r \to \infty$:

$$\varphi^{(+)}_{\vec{k}}(\vec{r}) \sim \frac{1}{(2\pi)^{3/2}} \left(e^{i\vec{k}\cdot\vec{r}} + f_{\vec{k}}(\hat{r}) \frac{e^{ikr}}{r} \right)$$

$$= \frac{4\pi}{(2\pi)^{3/2}} \sum_{l,m} i^l \, Y_l^{m*}(\hat{k}) \, Y_l^m(\theta,\varphi) \left(\frac{e^{ikr} e^{-il\pi/2} - e^{-ikr} e^{+il\pi/2}}{2ikr} \right)$$

$$\sqrt{\frac{2}{\pi}} \qquad + \frac{1}{(2\pi)^{3/2}} f_{\vec{k}}(\hat{r}) \frac{e^{ikr}}{r}$$

$$\sum_{l,m} a_{lm}(k) \, \tilde{\varphi}_{klm}(r) \sim \sqrt{\frac{2}{\pi}} \sum_{l,m} a_{lm}(k) \, Y_l^m(\theta,\varphi) \frac{e^{ikr} e^{-il\pi/2} e^{2i\delta_l} - e^{-ikr} e^{il\pi/2}}{2ir}$$

Get $a_{lm}(k)$ by comparing coefficients of incoming wave $Y_l^m \frac{e^{-ikr}}{r}$

$$a_{lm}(k) = i^l \, Y_l^{m*}(\hat{k}) / k$$

$$\therefore\ \boxed{\begin{aligned} |\varphi^{(+)}_{\vec k}\rangle &= \frac{1}{k}\sum_{l,m} i^l\, Y_l^{m*}(\hat k)\,|\tilde\varphi_{klm}\rangle \\ \langle\tilde\varphi_{k'lm}|\varphi^{(+)}_{\vec k}\rangle &= \frac{1}{k}\,\delta(k'-k)\, i^l\, Y_l^{m*}(\hat k) \end{aligned}}$$

Get scattering amplitude by comparing coefficients of outgoing wave e^{ikr}/r:

$$\sum_{l,m}\frac{4\pi}{(2\pi)^{3/2}}\,\underbrace{i^l\, Y_l^{m*}(\hat k)\, Y_l^m(\hat r)\,\frac{e^{-il\pi/2}}{2ik}}_{1} + \frac{1}{(2\pi)^{3/2}}\, f_{\vec k}(\hat r)$$

$$= \sum_{l,m}\frac{4\pi}{(2\pi)^{3/2}}\, a_{lm}(k)\, Y_l^m(\hat r)\,\frac{e^{-il\pi/2}\,e^{2i\delta_l}}{2i}$$

$$= \sum_{l,m}\frac{4\pi}{(2\pi)^{3/2}}\,\underbrace{i^l\, Y_l^{m*}(\hat k)\, Y_l^m(\hat r)\,\frac{e^{-il\pi/2}}{2ik}}_{1}\,e^{2i\delta_l}$$

$$f_{\vec k}(\hat r) = \frac{4\pi}{k}\sum_{l,m} Y_l^{m*}(\hat k)\, Y_l^m(\hat r)\,\underbrace{\frac{e^{2i\delta_l}-1}{2i}}_{e^{i\delta_l}\sin\delta_l}$$

$$= \frac{4\pi}{k}\sum_{l,m} Y_l^{m*}(\hat k)\, e^{i\delta_l}\sin\delta_l\, Y_l^m(\hat r)$$

$$f_{\vec k}(\hat r) = \frac{4\pi}{k}\sum_{l,m} Y_l^{m*}(\hat k)\, e^{i\delta_l}\sin\delta_l\, Y_l^m(\hat r)$$

Spherical harmonic expansion of scattering amplitude

$$\vec k = k\vec e_z \rightarrow\ = \frac{1}{k}\sum_{l,m}(2l+1)\, e^{i\delta_l}\sin\delta_l\, P_l(\cos\theta)$$

$$Y_l^m(\vec e_z) = \delta_{m0}\sqrt{\frac{2l+1}{4\pi}}$$

$$Y_l^0(\hat r) = \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta)$$

$$\sigma = \frac{16\pi^2}{k^2}\sum_{l,m}|Y_l^m(\hat k)|^2\sin^2\delta_l$$

$$= \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l$$

$$\sigma \approx \frac{4\pi}{k^2}\int_0^\infty dl\,(2l+1)\sin^2\delta_l$$

$$b = (\text{impact parameter}) = \frac{l}{k}$$

$$\sigma \approx 4\int_0^\infty db\; 2\pi b\,\sin^2\delta_l$$

wave nature of matter

Hard sphere as an example

Sign of phase shifts: $\delta_l > 0$ for attractive

$\delta_l < 0$ for repulsive

(A)

1-d Scattering

$$H = H_0 + V$$

$\langle k|k'\rangle = \delta(k-k')$

Unscattered plane waves: $H_0|k\rangle = E_k|k\rangle$ $\quad 1 = \int dk\, |k\rangle\langle k|$

$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx}$

Scattering states:

$$H|\varphi_k\rangle = E_k|\varphi_k\rangle$$

$$(E_k - H_0)|\varphi_k\rangle = V|\varphi_k\rangle$$

$$|\varphi_k^{(\pm)}\rangle = |k\rangle + (E_k - H_0 \pm i\epsilon)^{-1} V |\varphi_k^{(\pm)}\rangle$$

$$\Rightarrow |\varphi_k^{(\pm)}\rangle = |k\rangle + (E_k - H \pm i\epsilon)^{-1} V|k\rangle$$

Relation to coördinate representation:

$$\Big(\frac{d^2}{dx^2} + k^2 \pm i \underbrace{\frac{2\mu\epsilon}{\hbar^2}}_{2|k|\eta}\Big) \underbrace{\frac{\hbar^2}{2\mu}\langle x|(E_k - H_0 \pm i\epsilon)^{-1}|x'\rangle}_{G_\pm(x,x')} = \delta(x-x')$$

$\epsilon = \frac{\hbar^2 |k|}{\mu}\eta$

$$\Big(\frac{d^2}{dx^2} + (|k| \pm i\eta)^2\Big) G_\pm(x,x') = \delta(x-x')$$

$$\boxed{G_\pm^*(x,x') = G_\mp(x',x)}$$

Solution: $G_\pm(x,x') = G_\pm(x-x')$

Can also solve in the Fourier domain (see homework solution)

$$\Big(\frac{d^2}{dx^2} + (|k| \pm i\eta)^2\Big) G_\pm(x) = \delta(x)$$

$$G_\pm(x) = \begin{cases} A e^{\pm i(|k| \pm i\eta)x} = A e^{\pm i|k|x} e^{-\eta x}, & x > 0 \\ A e^{\mp i(|k| \pm i\eta)x} = A e^{\mp i|k|x} e^{+\eta x}, & x < 0 \end{cases}$$

$$= A e^{\pm i|k||x|} e^{-\eta|x|}$$

BC at $x=0$: $\left.\frac{dG_\pm}{dx}\right|_{x=0^-}^{x=0^+} = 1 \Rightarrow \pm i(|k| \pm i\eta)A \pm i(|k| \pm i\eta)A = 1$

$\pm 2i|k| A = 1$

$A = \pm \frac{1}{2i|k|} = \mp \frac{i}{2|k|}$

$$G_\pm(x;x') = \mp \frac{i}{2|k|} e^{\pm i|k||x-x'|} e^{-\eta|x-x'|}$$

$$\langle x|\varphi_k^{(\pm)}\rangle = \langle x|k\rangle + \int dx' \langle x|(E_k - H_0 \pm i\epsilon)^{-1}|x'\rangle V(x')\langle x'|\varphi_k^{(\pm)}\rangle$$

$$= \frac{1}{\sqrt{2\pi}} e^{ikx} + \int dx'\, G_\pm(x,x')\, \underbrace{U(x')}_{\frac{2\mu}{\hbar^2}V(x')} \langle x'|\varphi_k^{(\pm)}\rangle$$

Time-reversal invariance:
$$\varphi_{-k}^{(-)}(x) = \varphi_k^{(+)*}(x)$$

$$\langle x|\varphi_k^{(\pm)}\rangle = \frac{1}{\sqrt{2\pi}} e^{ikx} \mp \frac{i}{2|k|}\int_{-\infty}^{\infty} dx'\, e^{\pm i|k||x-x'|} U(x')\langle x'|\varphi_k^{(\pm)}\rangle$$

$$\langle x|\varphi_k^{(+)}\rangle \underset{x\to\infty}{\sim} \frac{1}{\sqrt{2\pi}} e^{ikx} - \frac{i}{2|k|} e^{i|k|x} \underbrace{\int dx'\, e^{-i|k|x'} U(x')\langle x'|\varphi_k^{(+)}\rangle}$$

$k' = |k|$

$$\sqrt{2\pi}\int dx' \langle k'|x'\rangle\langle x'|U|\varphi_k^{(+)}\rangle$$

$$= \sqrt{2\pi}\langle k'|U|\varphi_k^{(+)}\rangle$$

$$\boxed{\langle x|\varphi_k^{(+)}\rangle \underset{x\to\infty}{\sim} \frac{1}{\sqrt{2\pi}}\left(e^{ikx} - i\frac{\pi}{|k|} e^{ik'x} \underbrace{\langle k'|U|\varphi_k^{(+)}\rangle}_{\frac{2\mu}{\hbar^2}T_{k'k}}\right)} \quad \boxed{k' = |k|}$$

$$\langle x|\varphi_k^{(+)}\rangle \underset{x\to-\infty}{\sim} \frac{1}{\sqrt{2\pi}}\left(e^{ikx} - \frac{i}{2|k|} e^{-i|k|x} \underbrace{\int dx'\, e^{+i|k|x'} U(x')\langle x'|\varphi_k^{(+)}\rangle}\right.$$

$k' = -|k|$

$$= \int dx'\, e^{-ik'x'} U(x')\langle x'|\varphi_k^{(+)}\rangle$$

$$= \sqrt{2\pi}\langle k'|U|\varphi_k^{(+)}\rangle$$

$$\boxed{\langle x|\varphi_k^{(+)}\rangle \underset{x\to-\infty}{\sim} \frac{1}{\sqrt{2\pi}}\left(e^{ikx} - i\frac{\pi}{|k|} e^{ik'x} \underbrace{\langle k'|U|\varphi_k^{(+)}\rangle}_{\frac{2\mu}{\hbar^2}T_{k'k}}\right)} \quad \boxed{k' = -|k|}$$

c

Transition matrix: $T_{k'k} = \langle k' | V | \varphi_k^{(+)} \rangle$

Scattering amplitude: $f_k(+) = -i\frac{\pi}{|k|}\langle k' | U | \varphi_k^{(+)} \rangle \qquad k' = |k|$

$$= -i\frac{2\pi\mu}{\hbar^2 |k|} T_{k'k}$$

$f_k(-) = -i\frac{\pi}{|k|}\langle k' | U | \varphi_k^{(+)} \rangle \qquad k' = -|k|$

$\hat{k}' = \frac{k'}{|k'|} = \mathrm{sign}(k')$

$$= -i\frac{2\pi\mu}{\hbar^2 |k|} T_{k'k}$$

$$\boxed{f_k(\hat{k}') = -i\frac{2\pi\mu}{\hbar^2 |k|} T_{k'k}, \quad k' = |k|\hat{k}'}$$

Orthonormality: $\langle \varphi_{k'}^{(\pm)} | \varphi_k^{(\pm)} \rangle = \langle k' | k \rangle = \delta(k'-k)$ (Same proof as 3-d)

Born expansion: same as 3-d

Completeness: add bound states to $|\varphi_k^{(\pm)}\rangle$

S-matrix:

$S_{k'k} \equiv \langle \varphi_{k'}^{(-)} | \varphi_k^{(+)} \rangle \longleftarrow$ unitary (Same proof as 3-d)

$$= \delta(k'-k) - 2\pi i \underbrace{\delta(E_{k'} - E_k)}_{\frac{\mu}{\hbar^2|k|}\delta(|k'|-|k|)} T_{k'k}$$

$$= \delta(k'-k) - i\frac{2\pi\mu}{\hbar^2 |k|}\delta(|k'|-|k|) T_{k'k}$$

$$= \delta(k'-k) + \delta(|k'|-|k|) f_k(\hat{k}')$$

Time-reversal invariance: $S_{k'k} = S_{-k,-k'}$

$k>0, k'>0$: $S_{k'k} = \delta(|k'|-|k|)\left(1 + f_k(+)\right)$

$k>0, k'<0$: $S_{k'k} = \delta(|k'|-|k|) f_k(-)$

$k<0, k'>0$: $S_{k'k} = \delta(|k'|-|k|) f_k(+)$

$k<0, k'<0$: $S_{k'k} = \delta(|k'|-|k|)\left(1 + f_k(-)\right)$

D

Time-reversal invariance:

$$\varphi^{(-)}_{-k}(x) = \varphi^{(+)*}_{k}(x)$$

$$\Longrightarrow \quad S_{k'k} = S_{-k,-k'} \quad \Longrightarrow \quad f_k(\hat{k}') = f_{-k'}(-\hat{k})$$

k positive: $f_k(+) = f_{-k}(-)$, $\cancel{f_k(-) = f_k(-)}$

k negative: $\cancel{f_k(+) = f_k(+)}$, $f_k(-) = f_{-k}(+)$

$$\boxed{k>0: \quad f_k(+) = f_{-k}(-)}$$

Parity: $V(x) = V(-x)$

$$\varphi^{(\pm)}_k(-x) = \frac{1}{\sqrt{2\pi}} e^{-ikx} \mp \frac{i}{2|k|} \underbrace{\int_{-\infty}^{\infty} dx'\, e^{\pm i|k||-x-x'|}\, U(x')\, \varphi^{(\pm)}_k(x')}_{\int_{-\infty}^{\infty} dx'\, e^{\pm i|k||-x+x'|}\, \underbrace{U(-x')}_{U(x')}\, \varphi^{(\pm)}_k(-x')}$$

$$= \frac{1}{\sqrt{2\pi}} e^{-ikx} \mp \frac{i}{2|k|} \int_{-\infty}^{\infty} dx'\, e^{\pm i|k||x-x'|}\, U(x')\, \varphi^{(\pm)}_k(-x')$$

$$\varphi^{(\pm)}_{-k}(x) = \frac{1}{\sqrt{2\pi}} e^{-ikx} \mp \frac{i}{2|k|} \int_{-\infty}^{\infty} dx'\, e^{\pm i|k||x-x'|}\, U(x')\, \varphi^{(\pm)}_{-k}(x')$$

$$\Longrightarrow \quad \boxed{\underbrace{\varphi^{(\pm)}_k(-x) = \varphi^{(\pm)}_{-k}(x)}_{\text{parity}} = \underbrace{\varphi^{(\mp)*}_k(x)}_{\text{time-reversal}}}$$

$$\Longrightarrow \quad S_{k'k} = S_{-k',-k} \quad \Longrightarrow \quad f_k(\hat{k}') = f_{-k}(-\hat{k}')$$

$$\boxed{f_k(\pm) = f_{-k}(\mp)}$$

$$\boxed{\begin{array}{l} k>0: \\ f_k(+) = f_{-k}(-) \\ f_k(-) = f_{-k}(+) \end{array}}$$ ← new

E

Unitarity

$$\delta(k'-k) = \int dq\, S^*_{qk'} S_{qk}$$

$$= \int dq \left[\delta(q-k') + \delta(|q|-|k'|)\, f^*_{k'}(\hat{q})\right] \times \left[\delta(q-k) + \delta(|q|-|k|)\, f_k(\hat{q})\right]$$

$$= \delta(k'-k) + \delta(|k'|-|k|)\, f_k(\hat{k}') + \delta(|k|-|k'|)\, f^*_{k'}(\hat{k}) + \underbrace{\int_{-\infty}^{\infty} dq\, \delta(|q|-|k'|)\, \delta(|q|-|k|)\, f^*_{k'}(\hat{q}) f_k(\hat{q})}$$

$$= \int_{-\infty}^{0} dq\, \delta(|q|-|k'|)\, \delta(|q|-|k|)\, f^*_{k'}(\hat{q})\, f_k(\hat{q}) + \int_{0}^{\infty} dq\, \delta(|q|-|k'|)\, \delta(|q|-|k|)\, f^*_{k'}(\hat{q})\, f_k(\hat{q})$$

$$= \delta(|k'|-|k|)\left(f^*_{k'}(-) f_k(-) + f^*_{k'}(+) f_k(+)\right)$$

$$\boxed{\begin{aligned}
&\Longrightarrow \quad 0 = f_k(\hat{k}') + f^*_{k'}(\hat{k}) + f^*_{k'}(-) f_k(-) + f^*_{k'}(+) f_k(+) \\
&k=k': \quad 0 = 2\,\mathrm{Re}\left(f_k(\hat{k})\right) + |f_k(-)|^2 + |f_k(+)|^2 \qquad \text{Optical theorem} \\
&k=-k': \quad 0 = f_k(-\hat{k}) + f^*_{-k}(\hat{k}) + f^*_{-k}(-) f_k(-) + f^*_{-k}(+) f_k(+)
\end{aligned}}$$

Since $|\varphi_k^{(+)}\rangle$ and $|\varphi_{-k}^{(+)}\rangle$ are degenerate, we can always define a new set of δ-normalized basis vectors by

$$k>0: \quad |\varphi_k^{(e)}\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_{-k}^{(+)}\rangle + |\varphi_k^{(+)}\rangle\right),$$

$$|\varphi_k^{(o)}\rangle = \frac{1}{\sqrt{2}}\left(|\varphi_{-k}^{(+)}\rangle - |\varphi_k^{(+)}\rangle\right).$$

We want to investigate these solutions when $\underline{\underline{V(x) = V(-x)}}$, in which case they are even and odd eigenstates, because $\varphi_k^{(+)}(-x) = \varphi_{-k}^{(+)}(x)$.

Asymptotics:

$$\varphi_k^{(e,o)}(x) \underset{x\to\infty}{\sim} \frac{1}{2\sqrt{\pi}}\Bigg(e^{-ikx} \overbrace{- i\frac{2\pi\mu}{\hbar^2|k|}T_{k,-k}}^{f_{-k}(+)}\, e^{ikx} \pm \Big(e^{ikx} \underbrace{- i\frac{2\pi\mu}{\hbar^2|k|}T_{kk}}_{f_k(+)}\, e^{ikx}\Big)\Bigg)$$

$$= \frac{1}{2\sqrt{\pi}}\Big(e^{-ikx} + e^{ikx}\underbrace{\left(\pm 1 + f_{-k}(+) \pm f_k(+)\right)}\Big)$$

$$|\pm 1 \pm f_k(+) + f_{-k}(+)|^2 = |1 + f_k(+) \pm f_{-k}(+)|^2$$

$$= 1 + 2\,\mathrm{Re}\left(f_k(+) \pm f_{-k}(+)\right)$$

$$+ |f_k(+)|^2 + \underbrace{|f_{-k}(+)|^2}_{|f_k(-)|^2 \text{ parity}} \pm 2\,\mathrm{Re}\left(f_k(+)\, f_{-k}^*(+)\right)$$

$$= 1 + \underbrace{2\mathrm{Re}(f_k(+)) + |f_k(+)|^2 + |f_k(-)|^2}_{0 \text{ by unitarity}} \quad \text{optical theorem}$$

$$\pm 2 \underbrace{\left(\mathrm{Re}(f_{-k}(+)) + \mathrm{Re}(f_k(+) f_{-k}^*(+))\right)}_{0 \text{ by unitarity}}$$

Second part of unitary becomes

$$0 = \underbrace{f_k(-)}_{f_{-k}(+)} + f_{-k}^*(+) + \underbrace{f_{-k}^*(-)}_{f_k^*(+)} \underbrace{f_k(-)}_{f_{-k}(+)} + f_{-k}^*(+) f_k(+) \quad \leftarrow \text{parity}$$

$$= 2\mathrm{Re}(f_{-k}(+)) + 2\mathrm{Re}(f_k(+) f_{-k}^*(+))$$

$$\therefore \left|\pm 1 \pm f_k(+) + f_{-k}(+)\right|^2 = 1$$

$$\Longrightarrow \pm 1 \pm f_k(+) + f_{-k}(+) = -e^{2i\delta}$$

$$\varphi_k^{(S,0)}(x) \underset{x\to\infty}{\sim} \frac{1}{2\sqrt{\pi}}\left(e^{-ikx} - e^{2i\delta} e^{ikx}\right)$$

$$= -\frac{e^{i\delta}}{2\sqrt{\pi}}\left(e^{i(kx+\delta)} - e^{-i(kx+\delta)}\right)$$

$$= -ie^{i\delta}\frac{1}{\sqrt{\pi}}\sin(kx+\delta)$$

The odd states vanish at the origin and thus are eigenstates of $V(x)$, but with an infinite barrier for negative x.

Normalization: $\delta(k'-k) = \langle \varphi_{k'}^{(S,0)} | \varphi_k^{(S,0)} \rangle$

$$= \int_{-\infty}^{\infty} dx \, \varphi_{k'}^{(S,0)*}(x) \, \varphi_k^{(S,0)}(x)$$

$$\delta(k'-k) = 2\int_0^\infty dx\, \varphi_{k'}^{(g_0)}(x)\, \varphi_k^{(g_0)}(x)$$

Thus the δ-normalized eigenstates on positive x are $\sqrt{2}\,|\varphi_k^{(g_0)}\rangle$, with asymptotic form

$$\sqrt{2}\,\varphi_k^{(g_0)}(x) \underset{x\to\infty}{\sim} -i e^{i\delta}\sqrt{\frac{2}{\pi}}\,\sin(kx+\delta)$$