Now, since this is true for all three of $q = 0, \pm 1$,

$$\underbrace{\langle \alpha', j, m' | \vec{V} | \alpha, j, m \rangle = \frac{\langle \alpha', j, m | \vec{J} \cdot \vec{V} | \alpha, j, m \rangle}{\hbar^2 j(j+1)} \langle j, m' | \vec{J} | j m \rangle}_{\text{in Cartesian } x, y, z \text{ basis, if you want.}}$$

We've already used this sub-case of the Wigner-Eckhart theorem, to derive $\Delta E_{\text{spin-orbit}}$ for the fine structure. (See page 15 of notes, where it was called the Lande formula.)

Another important use for Wigner-Eckhart: multipole radiation. We won't cover this. (Not in Sakurai, covered in Baym p. 376-379.)

One more comment about Wigner-Eckhart: how do you compute reduced matrix elements in general?

Answer:

$$\langle \alpha', j' \| T^{(k)} \| \alpha, j \rangle = \sqrt{2j+1} \; \underbrace{\frac{\langle \alpha', j', m' | T_q^{(k)} | \alpha, j, m \rangle}{\langle j k; m q | j k; j' m' \rangle}}$$

Evaluate this for some convenient, particular choice of m, m', q.

Restriction: no fair choosing m, m', q so that denominator vanishes!

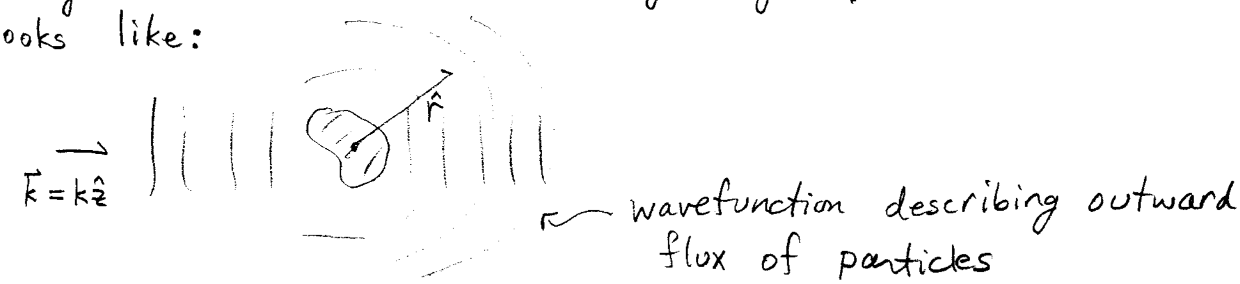
Scattering Theory

The typical problem: send free particles with momentum $\vec{k}$ towards a scattering region:

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} = \langle \vec{r} | \vec{k} \rangle = \text{solution } \underline{\text{without}}\ V(\vec{r}).$$

(Normalization fixed so that $\langle \vec{k}' | \vec{k} \rangle = \int d^3\vec{r}\, \langle \vec{k}' | \vec{r} \rangle \langle \vec{r} | \vec{k} \rangle = \delta^{(3)}(\vec{k} - \vec{k}')$.)

Taking into account the scattering region, the solution looks like:



To give you an idea where we're going, lets write down the answer in advance:

$$\psi(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \Big[\underset{\substack{\uparrow \\ \text{incoming} \\ \text{plane} \\ \text{wave}}}{e^{i\vec{k}\cdot\vec{r}}} + \underbrace{\frac{e^{ikr}}{r} f(\vec{k}', \vec{k})}_{\text{outgoing spherical wave}} \Big] \qquad \underline{\text{for large } r}.$$

where $f(\vec{k}', \vec{k}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \int d^3\vec{r}\,' \, \frac{e^{-i\vec{k}'\cdot\vec{r}\,'}}{(2\pi)^{3/2}} V(\vec{r}\,') \psi(\vec{r}\,')$.

Where $\vec{k}' = k\hat{r}$.

Our tasks remaining:
1) Prove this (and develop useful machinery).
2) Find solutions (note $\psi(\vec{r})$ appears on both sides).
3) Interpret result in terms of observable quantities (differential cross-section, etc.)

Start with Hamiltonian: $H = H_0 + V$, where

$H_0 = \frac{P^2}{2m}$, and for now, imagine $V(\vec{R})$ only non-zero within a localized region. (Not true of Coulomb potential!)

Suppose $|\phi\rangle$ is an energy eigenket of H_0.

(For example, $|\phi\rangle = |\vec{k}\rangle$ would work.)

So $H_0|\phi\rangle = E|\phi\rangle$.

Now look for solutions to full Schrodinger equation with the same E:

$$(H_0 + V)|\psi\rangle = E|\psi\rangle. \qquad (\text{As } V \to 0, \text{ expect } |\psi\rangle \to |\phi\rangle.)$$

Formally, $|\psi\rangle = \frac{1}{E - H_0} V|\psi\rangle + |\phi\rangle$.

But, need to worry that this can blow up!

To avoid the blow-up problem, try instead:

$$|\psi^{\pm}\rangle = |\phi\rangle + \frac{1}{E - H_0 \pm i\epsilon} V|\psi^{\pm}\rangle \qquad \text{(Lippmann-Schwinger)}$$

where ϵ = real infinitesimal (take to 0 later).

The + sign will turn out to be what we want.

But keep both for now.

Think of $|\phi\rangle$ as known; the L-S equation can be solved for the full ket $|\psi^{\pm}\rangle$.

In the position representation,

$$\langle\vec{r}|\psi^{\pm}\rangle = \langle\vec{r}|\phi\rangle + \int d^3\vec{r}\,' \underbrace{\langle\vec{r}|\frac{1}{E - H_0 \pm i\epsilon}|\vec{r}\,'\rangle}_{\text{Call this } G_{\pm}(\vec{r},\vec{r}\,')\left(\frac{2m}{\hbar^2}\right)} \langle\vec{r}\,'|V|\psi^{\pm}\rangle$$

$G_{\pm}(\vec{r},\vec{r}\,')$ is a Green function; independent of V or $|\phi\rangle$ or $|\psi^{\pm}\rangle$.

Evaluate the Green function:

$$G_\pm(\vec{r},\vec{r}\,') = \frac{\hbar^2}{2m}\langle\vec{r}|\frac{1}{E-H_0\pm i\epsilon}|\vec{r}\,'\rangle = \frac{\hbar^2}{2m}\int d^3\vec{p}\int d^3\vec{p}\,'\ \langle\vec{r}|\vec{p}\,'\rangle\langle\vec{p}\,'|\frac{1}{E-\frac{p'^2}{2m}\pm i\epsilon}|\vec{p}\,''\rangle\langle\vec{p}\,''|\vec{r}\,'\rangle$$

(Used $1 = \int d^3\vec{p}\,'\ |\vec{p}\,'\rangle\langle\vec{p}\,'|$ and $\langle\vec{p}\,'|H_0 = \langle\vec{p}\,'|\frac{p'^2}{2m}$.)

Now $\langle\vec{p}\,'|\frac{1}{E-\frac{p'^2}{2m}\pm i\epsilon}|\vec{p}\,''\rangle = \frac{1}{E-\frac{p'^2}{2m}\pm i\epsilon}\langle\vec{p}\,'|\vec{p}\,''\rangle = \frac{\delta^{(3)}(\vec{p}-\vec{p}\,'')}{E-\frac{p'^2}{2m}\pm i\epsilon}$

Also use $\langle\vec{r}|\vec{p}\,'\rangle = \frac{1}{(2\pi\hbar)^{3/2}}e^{i\vec{p}\,'\cdot\vec{r}/\hbar}$ and

$\langle\vec{p}\,''|\vec{r}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}e^{-i\vec{p}\,''\cdot\vec{r}/\hbar}$.

So $G_\pm(\vec{r},\vec{r}\,') = \frac{\hbar^2}{2m}\int\frac{d^3\vec{p}\,'}{(2\pi\hbar)^3}\frac{e^{i\vec{p}\,'\cdot(\vec{r}-\vec{r}\,')/\hbar}}{E-\frac{p'^2}{2m}\pm i\epsilon}$ (did the $\int d^3\vec{p}\,''$ using the δ-fn.)

Now let $\vec{q} = \vec{p}\,'/\hbar$ and $E = \frac{\hbar^2k^2}{2m}$. Then:

$$G_\pm(\vec{r},\vec{r}\,') = \int\frac{d^3\vec{q}}{(2\pi)^3}\frac{e^{i\vec{q}\cdot(\vec{r}-\vec{r}\,')}}{k^2-q^2\pm i\epsilon}.$$

Act with ∇^2 on this:

$$\nabla^2 G_\pm(\vec{r},\vec{r}\,') = \int\frac{d^3\vec{q}}{(2\pi)^3}\frac{\nabla^2\left(e^{iq\cdot(\vec{r}-\vec{r}\,')}\right)}{k^2-q^2\pm i\epsilon} = i^2q^2\int\frac{d^3\vec{q}}{(2\pi)^3}\frac{e^{iq\cdot(\vec{r}-\vec{r}\,')}}{k^2-q^2\pm i\epsilon}$$

So $(\nabla^2+k^2)G_\pm(\vec{r},\vec{r}\,') = \int\frac{d^3\vec{q}}{(2\pi)^3}e^{iq\cdot(\vec{r}-\vec{r}\,')} = \delta^{(3)}(\vec{r}-\vec{r}\,')$

So $G_\pm$ is the Green function for the Helmholtz equation $(\nabla^2+k^2)f(\vec{r})=0$.

To evaluate it, do the integral:

$$G_\pm(\vec{r},\vec{r}\,') = \frac{1}{(2\pi)^3}\int_0^\infty q^2\,dq\int_0^{2\pi}d\phi\int_{-1}^{1}d(\cos\theta)\ \frac{e^{iq|\vec{r}-\vec{r}\,'|\cos\theta}}{k^2-q^2\pm i\epsilon}$$

Where ϕ,θ are measured from the direction $\vec{r}-\vec{r}\,'$.

Now do the $d\phi$ and $d(\cos\theta)$ integrals...

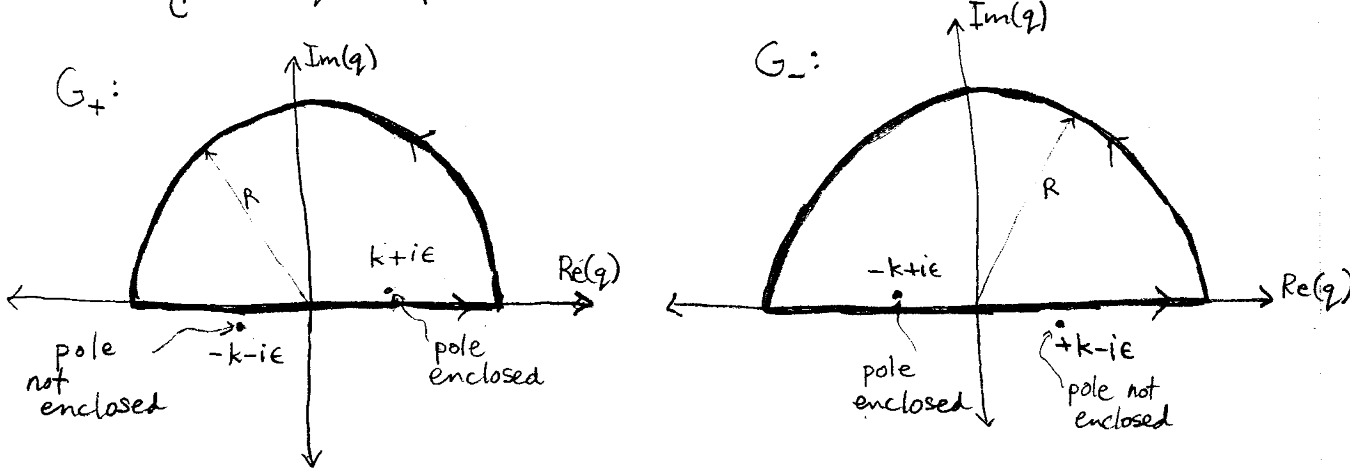
$$G_{\pm}(\vec{r},\vec{r}\,') = \frac{i}{4\pi^2|\vec{r}-\vec{r}\,'|} \underbrace{\int_0^{\infty} dq \, \frac{q}{q^2-k^2 \mp i\epsilon}\left(e^{iq|\vec{r}-\vec{r}\,'|} - e^{-iq|\vec{r}-\vec{r}\,'|}\right)}_{\text{Let } x \equiv |\vec{r}-\vec{r}\,'|, \text{ call this } I(x,k)}$$

$$I(x,k) = \int_{-\infty}^{\infty} dq \, \frac{q}{q^2-k^2 \mp i\epsilon}\, e^{iqx}$$

Use the method of residues, treating q as complex variable. The integrand has poles at $q^2 = k^2 \pm i\epsilon$, or $q = \begin{cases} k \pm i\epsilon \\ -k \mp i\epsilon . \end{cases}$

Since $e^{iqx} \to 0$ for $q \to i\infty$,

$$I(x,k) = \oint_C dq \, \frac{q\, e^{iqx}}{q^2-k^2 \mp i\epsilon} \quad \text{along the contour (with } R \to \infty)$$



Using the theory of integration of complex variables:

$$I(x,k) = 2\pi i\,(\text{residue of pole}) = \begin{cases} 2\pi i \left(\dfrac{q\, e^{iqx}}{q+k}\right)\Bigg|_{q=k} & \text{for } G_+ \\[2em] 2\pi i \left(\dfrac{q\, e^{iqx}}{q-k}\right)\Bigg|_{q=-k} & \text{for } G_- \end{cases}$$

$$= \begin{cases} i\pi\, e^{ikx} & \text{for } G_- \\ -i\pi\, e^{-ikx} & \text{for } G_- \end{cases}$$

(Here, the $i\epsilon$ just tells us which way the contour avoids the pole.)

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

Now plug this into Lippmann–Schwinger:

$$\underbrace{\langle \vec{r}\,|\psi^{\pm}\rangle}_{\text{total wavefunction}} = \underbrace{\langle \vec{r}\,|\phi\rangle}_{\text{incident wavefunction}} \underbrace{- \frac{2m}{\hbar^2}\int d^3\vec{r}\,' \, \frac{e^{\pm ik|\vec{r}-\vec{r}\,'|}}{4\pi|\vec{r}-\vec{r}\,'|}\langle \vec{r}\,'|V|\psi^{\pm}\rangle}_{\text{effect of scattering}}$$

If $V(\vec{r})$ is a <u>local</u> potential: diagonal in the position rep, so

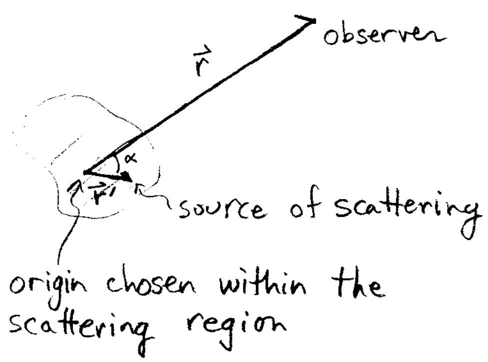
$$\langle \vec{r}\,'|V|\vec{r}\,''\rangle = V(\vec{r}\,')\,\delta^{(3)}(\vec{r}\,'-\vec{r}\,''),$$ then

$$\langle \vec{r}\,'|V|\psi^{\pm}\rangle = \int d^3\vec{r}\,'' \, \langle \vec{r}\,'|V|\vec{r}\,''\rangle\langle \vec{r}\,''|\psi^{\pm}\rangle = V(\vec{r}\,')\,\langle \vec{r}\,'|\psi^{\pm}\rangle.$$

Then:

$$\psi^{\pm}(\vec{r}) = \phi(\vec{r}) - \frac{2m}{\hbar^2}\int d^3\vec{r}\,' \, \frac{e^{\pm ik|\vec{r}-\vec{r}\,'|}}{4\pi|\vec{r}-\vec{r}\,'|}V(\vec{r}\,')\,\psi^{\pm}(\vec{r}\,').$$

Now, specialize to points very far from the scattering region:



<u>With $r \gg r'$:</u>

$$\begin{aligned}|\vec{r}-\vec{r}\,'| &= \sqrt{r^2 - 2rr'\cos\alpha + r'^2}\\ &= r\sqrt{1 - \frac{2r'}{r}\cos\alpha + \dots}\\ &= r - r'\cos\alpha + \dots\\ &= r - \hat{r}\cdot\vec{r}\,'.\end{aligned}$$

Recall that $E = \frac{\hbar^2k^2}{2m}$, so we can take the incident wavefunction to be:

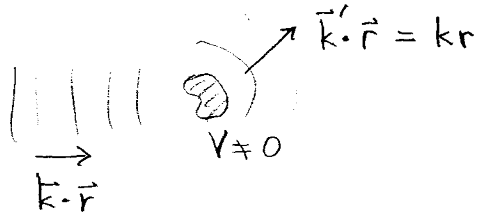
$$\phi(\vec{r}) = \langle \vec{r}\,|\phi\rangle = \langle \vec{r}\,|\vec{k}\rangle = \frac{e^{i\vec{k}\cdot\vec{r}}}{(2\pi)^{3/2}}.$$

Also define $\vec{k}\,' = k\hat{r}$ (same magnitude wavevector as incoming, but directed away from scattering region).

Then $e^{\pm ik|\vec{r}-\vec{r}\,'|} \sim e^{\pm ikr}\,e^{\mp i\vec{k}\,'\cdot\vec{r}\,'}$, and...

$$\psi^{\pm}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi}\frac{2m}{\hbar^2}\, \underbrace{e^{\pm ikr}}_{\text{outgoing for } +,\ \text{ingoing for } -.} \frac{1}{r}\int d^3\vec{r}\,' e^{-i\vec{k}'\cdot\vec{r}\,'}\, V(\vec{r}\,')\, \psi^{\pm}(\vec{r}\,')$$

So choose + sign; scattered waves move <u>away</u> from target



So the relevant solution physically is:

$$\psi^{+}(\vec{r}) = \frac{1}{(2\pi)^{3/2}}\left[e^{i\vec{k}\cdot\vec{r}} + \frac{e^{ikr}}{r} f(\vec{k},\vec{k}')\right], \qquad \text{where}$$

$$f(\vec{k},\vec{k}') = -\frac{1}{4\pi}\left(\frac{2m}{\hbar^2}\right)(2\pi)^3 \int d^3\vec{r}\,' \frac{e^{-i\vec{k}'\cdot\vec{r}\,'}}{(2\pi)^{3/2}}\, V(\vec{r}\,')\, \psi^{+}(\vec{r}\,')$$

$$\underset{\substack{\text{go to momentum}\\ \text{representation}}}{=} -\frac{1}{4\pi}(2\pi)^3 \frac{2m}{\hbar^2} \langle \vec{k}' | V | \psi^{+} \rangle$$

Note that momentum eigenstates $|\vec{k}'\rangle$ are normalized like $\langle \vec{k}' | \vec{k} \rangle = \delta^{(3)}(\vec{k}-\vec{k}')$.

In this formalism, $f(\vec{k},\vec{k}')$ encodes the amplitude of the scattered particle wavefunction (which also falls off like $\frac{1}{r}$, and oscillates in space with wavenumber k).

To interpret this physically, need to define the differential cross-section and relate it to $f(\vec{k},\vec{k}')$.