Lecture 14 Perturbation Theory

Let's remind ourselves of the scattering problem in a time-dependent, regular quantum mechanics context.

Presume a potential which is non-zero for a finite time, τ, which is small compared to the time in which the projectile is in V.

$$H = H_0 + H_I \quad \text{where} \quad H_I = W \quad 0 \le t \le \tau$$
$$\qquad\qquad\qquad\qquad\qquad = 0 \quad \text{otherwise}$$

Our states satisfy

$$(H_0 + H_I)|\psi\rangle = i\frac{\partial}{\partial t}|\psi\rangle$$

For the unperturbed H, $H_0|m\rangle = |n\rangle E_m$

and we assume that the perturbed states can be expanded in terms of the unperturbed states, which ~~the~~ themselves evolve

$$e^{-iE_m t}|m\rangle$$

So, $|\psi\rangle = \sum_m a_m(t)\, e^{-iE_m t}|m\rangle$

When $t<0$, we presume plane wave propagation — a single frequency, so

$$|\psi_{in}\rangle = e^{-iE_j t}|j\rangle$$

which can be forced by $a_m(t) = \delta_{mj}$ for $t < 0$.

For long times $t > \tau$, the state will stay in whatever state it was in at $t = \tau$.

$$|\psi_{final}\rangle = \sum_m a_m(\tau)\, e^{-iE_m t}|m\rangle$$

Setting things up:

$$\sum_m (H_0 + H_I)\, a_m(t)\, e^{-iE_m t}|m\rangle = i\frac{\partial}{\partial t}\left(\sum_m a_m(t)\, e^{-iE_m t}|m\rangle\right)$$

$$\sum_m \left(a_m(t)\, e^{-iE_m t} H_0|m\rangle + a_m(t)\, e^{-iE_m t} H_I|m\rangle\right)$$

$$= i\sum_m \frac{da_m(t)}{dt}\, e^{-iE_m t}|m\rangle$$

$$+ \sum_m a_m(t)\, E_m\, e^{-iE_m t}|m\rangle$$

$$\sum_m a_m(t)\, e^{-iE_m t} E_m|m\rangle + \sum_m a_m(t)\, e^{-iE_m t} H_I|m\rangle$$

$$= i\sum_m \dot{a}_m(t)\, e^{-iE_m t}$$

$$+ \sum_m a_m(t)\, E_m\, e^{-iE_m t}|m\rangle$$

cancelling and multiplying by $\langle n|e^{iE_n t} \longrightarrow$

$$\sum_m a_m(t)\, \langle n|H_I|m\rangle\, e^{i(E_n - E_m)t} = i\sum_m \dot{a}_m(t)\, \langle n|m\rangle\, e^{i(E_n - E_m)t}$$

since the states form a complete set, $\langle n|m\rangle = \delta_{nm}$.

so,

$$\sum_m a_m(t) \langle n|H_I|m\rangle e^{i(E_n-E_m)t} = i\frac{da_n}{dt} \quad \text{exact eq.}$$

This can't be solved exactly, however. for

$$\omega_{nm} \equiv E_n - E_m \ll H_0, \text{ then } \frac{da}{dt} \text{ is not large}$$

and successive approximations can be used. In particular let $H_I \to \lambda H_I$, where λ is some measure of 'smallness'

Expand $\quad a_m = a_m^{(0)} + \lambda a_m^{(1)} + \lambda^2 a_m^{(2)} + \ldots$

so, $\quad a_m(0) = a_m^{(0)} = \delta_{mj}$ the state $t<0$.

Substituting in 1st order.

$$i\frac{d}{dt}\left(a_m^{(0)} + \lambda a_m^{(1)}\right) = \sum_m \left(a_m^{(0)} + \lambda a_m^{(1)}\right)\langle n|\lambda H_I|m\rangle e^{i(E_n-E_m)t}$$

& equate powers of λ

$$i\frac{d}{dt} a_m^{(1)} = \sum_m \delta_{mj} \langle n|W|m\rangle e^{i\omega_{nm}t}$$

$$= \langle n|W|j\rangle e^{i\omega_{nj}t}$$

$$a_m^{(1)}(t) = -i\int_0^t dt' \langle n|W|j\rangle e^{i\omega_{nj}t'}$$

We could do it again, throwing away terms > 2nd order using this result..

$$a_n^{(2)}(t) = -i\sum_\ell \int_0^t dt'' \langle n|W|\ell\rangle e^{i\omega_{n\ell}t''} a_\ell^{(1)}(t'')$$

$$= -i\sum_\ell \int_0^t dt'' \int_0^{t''} dt' \langle n|W|\ell\rangle\langle \ell|W|j\rangle e^{i\omega_{n\ell}t''} e^{i\omega_{\ell j}t'}$$

Under circumstances in which 1st order is sufficient,

$$P_{nj} = |a_n^{(1)}(t)|^2$$

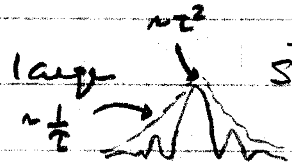
$$= \left| \int_0^\tau \langle n|W|j\rangle e^{i\omega_{nj}t} dt \right|^2$$

Sometimes the potential can be deemed to be slowly varying..

$$P_{nj}(\tau) \simeq |\langle n|W|j\rangle|^2 \underbrace{\underbrace{\underbrace{\left|\int_0^\tau dt\, e^{i\omega_{nj}t}\right|^2}_{\left|\frac{e^{i\omega_{nj}\tau}-1}{i\omega_{nj}}\right|^2}}_{2\left(\frac{1-\cos\omega\tau}{\omega^2}\right)}}_{\frac{4\sin^2(\omega\tau/2)}{\omega^2}}$$

so, $P_{nj}(\tau) = 4\,|\langle n|W|j\rangle|^2 \dfrac{\sin^2(\omega\tau/2)}{\omega^2}$

when τ is large



$\dfrac{\sin^2(\omega\tau/2)}{\omega^2} \xrightarrow[\text{as function of } \omega]{} \dfrac{\pi\tau}{2}\,\delta(\omega)$

so,

$$P_{nj}(\tau) = 2\pi\,|\langle n|W|j\rangle|^2\,\tau\,\delta(E_n - E_j)$$

If we had had a radiation problem, then the time dependence of W would have been $e^{\pm i\omega t/\hbar}$ and result would be $\delta(E_n - E_j \pm \hbar\omega)$ --

The probability rate

$$\hat{P}_{nj}(\tau) = \frac{P_{nj}(\tau)}{\tau} = 2\pi\,|\langle n|W|j\rangle|^2\,\delta(E_n - E_j)$$

Because these are transitions between continuum (not bound) states, we can't speak of the probability to a particular state of $\vec{p} = \hbar\vec{k}$, rather to a set of states centered around $E_k = \dfrac{\hbar^2 k^2}{2m}$. The

number of states ~~in this~~ interval is the density of states $\rho(E)\,dE$

density of states

$$\mathcal{P}_{nj}(\tau) = \int \hat{P}_{nj}(\tau)\,\rho(E)\,dE$$

$$\mathcal{P}_{nj}(\tau) = 2\pi\,|\langle n|W|j\rangle|^2\,\rho(E_n)\Big|_{E_n=E_j}$$

This is Fermi's Golden Rule #2.

→ the time must be long enough so that $\Delta E \gg 2\pi\hbar/t$ and short enough to justify 1st order perturbation theory.

If the potential is weak enough to not distort the incident wave, then we can put

$$\langle \vec{r}\,|j\rangle = e^{i\vec{k}_j\cdot\vec{r}} \qquad \text{(normalized 1 to a volume)}$$

and $\quad \langle \vec{r}\,|n\rangle = e^{i\vec{k}_n\cdot\vec{r}}$

The density of states (1 to volume for now).

$$d\rho_n = \frac{\#\text{ states}}{\text{energy interval}} = \frac{V\,d^3k_n}{(2\pi)^3 dE_n} = \frac{V\,k_n^2 dk_n d\Omega_n}{(2\pi)^3 dE_n}$$

nonrelativistically, $\quad E = \frac{k^2}{2m}$ so $\quad dE = \frac{2k\,dk}{2m}$

$$= \frac{k\,dk}{m}$$

$$= v\,dk$$

so $$d\rho_n = \frac{V m^2 v_n^2 dk_n d\Omega_n}{(2\pi)^3 v_n dk_n}$$

$$= \frac{V m^2 v_n d\Omega_n}{(2\pi)^3}$$

I've shown you that volume don't appear, so

$$d\rho_n = \frac{m^2 v_n d\Omega_n}{(2\pi)^3}$$

and

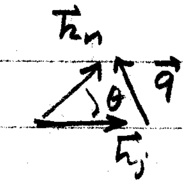
$$d\sigma = \frac{dp}{flux} \qquad flux = v_j$$ for stationary target. $N = 1$ from before.

$$= \frac{v_n}{v_j} \frac{m^2}{(2\pi)^3} 2\pi \, |\langle n|W|j\rangle|^2 d\Omega_n$$

For elastic scattering, $v_n = v_j$ plus now use the plane wave approximation.

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{(2\pi)^2} \left[\int e^{i(\vec{k}_j - \vec{k}_n)\cdot\vec{r}} W(\vec{r}) d^3r \right]^2$$

Notice



where $|\vec{q}| = 2k \sin\theta/2$ for $|\vec{k}_j| = |\vec{k}_n|$

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{(2\pi)^2} \left[\int W(\vec{r}) e^{iqr\cos\theta} \sin\theta \, d\theta \, r^2 dr \, d\varphi \right]^2$$

Assume the potential is independent of angles.

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{(2\pi)^2}\left[\int_0^\infty W(r)\,\frac{4\pi}{q}\,r\sin(qr)\,dr\right]^2$$

$$= \frac{4m^2}{q^2}\left[\int_0^\infty W(r)\,r\sin(qr)\,dr\right]^2$$

these approximations define the Born Approximation — done in the probability paper that he got the Nobel for —

Consider a shielded Coulomb potential

$$W(r) = Z_j Z_t e^2 \frac{e^{-r/r_0}}{r}$$

then

$$\int dr \longrightarrow Z_j Z_t e^2 \int_0^\infty \sin(qr)\, e^{-r/r_0}\, dr$$

$$= \frac{Z_j Z_t e^2}{q}\left[1 - \left(\frac{1}{1+(qr_0)^2}\right)\right]$$

$$\frac{d\sigma}{d\Omega} = \frac{4m^2}{q^4} Z_j^2 Z_t^2 e^4 \qquad \text{for large shielding radius}$$

$$\frac{d\sigma}{d\Omega} = \frac{m^2 Z_j^2 Z_t^2 e^4}{4h^4 \sin^4\theta/2} \qquad \text{Rutherford Cross Section}$$

Finally, let me remind you of a technique for solving inhomogeneous partial differential equations.

The solution to $(\nabla^2 + k^2)\psi(\vec{r}) = -4\pi\rho(\vec{r})$ is found by "adding up" – superimposing solutions to the point source problem → pt. sources of unit strength: $\rho(\vec{r}')$

$$\rho(\vec{r}) = \int \delta(\vec{r}-\vec{r}')\rho(\vec{r}')\,d\vec{r}'$$

These solutions are Green's Functions. Suppose a solution can be found for:

$$(\nabla^2 + k^2)\,G(\vec{r},\vec{r}') = -4\pi\,\delta(\vec{r}-\vec{r}')$$

The construction for the general solution is

$$\psi(\vec{r}) = \int G(\vec{r},\vec{r}')\rho(\vec{r}')\,d\vec{r}'$$

(check:

$$(\nabla^2+k^2)\int G(r\,r')\rho(r')\,dr' = \int(\nabla^2+k^2)G(r\,r')\rho(r')\,dr'$$
$$= \int -4\pi\,\delta(\vec{r}-\vec{r}')\rho(\vec{r}')\,d\vec{r}' = -4\pi\rho(r) \checkmark \;)$$

Our problem is similar: in

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + W(r)\right)\psi(r) = E\psi(r)$$

for free particles, $E = \frac{\hbar^2 k^2}{2m}$

so, $\hbar = 1$ $\qquad (\nabla^2 + k^2)\psi(r) = 2mW(r)\psi(r)$

and one can put the classical interpretation on the RHS as the driver, or source, $\psi(r)$ is the output.

Then, $\qquad \psi(r) = -2m \int G(rr')W(r')\psi(r')dr' + \varphi_0(r)$

where $\qquad (\nabla^2 + k^2)G(rr') = -\delta(r - r')$ $\qquad$ NEXT PAGE $\qquad$ solution to ~~homogeneous~~ equation.

The Green's function is

$$G(rr') = \frac{1}{4\pi}\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}$$

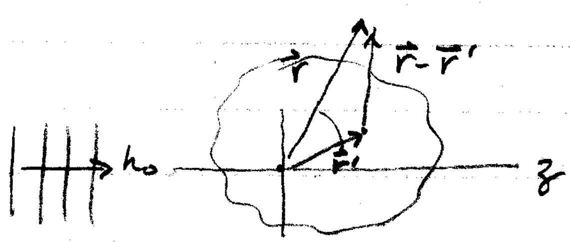
like that for Poisson's Eq, but w/ oscillating term.

Then,

$$\psi(r) = -\frac{2m}{4\pi}\int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} W(\vec{r}')\psi(r')dr' + \varphi_0(r)$$

The homogeneous solution is just our plane waves,

$\varphi(r) = e^{ikz}$ $\quad$ and $\quad \psi(r)$ is our $\psi_{out}(r)$ solution from the ~~earlier~~ discussion.



where $\vec{k}$ is along $\vec{r}'$

actually the solution to $\quad (\nabla^2 + k^2) G(r) = -\delta(r)$

is $\quad G(r) = -\frac{1}{(2\pi)^3} \int \frac{e^{i\vec{k}'\cdot\vec{r}}}{k^2 - k'^2} d^3k'$

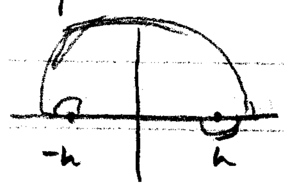
$e^{i\vec{k}'\cdot\vec{r}} = e^{ik'r\cos\theta} \qquad d^3k' = k'^2 \cos\theta \, dk \, d\theta \, d\phi$

$$G(r) = \frac{1}{4\pi^2} \frac{1}{r} \int_{-\infty}^{\infty} \frac{k' \sin k'r}{k^2 - k'^2} dk'$$

$$= \frac{1}{4\pi^2 i} \frac{1}{r} \int_{-\infty}^{\infty} \frac{k' e^{ik'r}}{\underbrace{k^2 - k'^2}_{}} dk'$$

poles at $k' = \pm k$

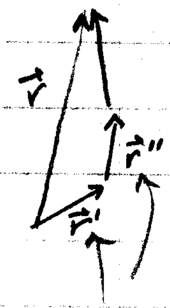
go to complex k' plane



$2\pi i \sum$ residues

so that $\quad G(r) = \frac{1}{4\pi} \frac{e^{ikr}}{r}$

Notice that if this is thought of as a perturbation series, we could substitute and iteratively solve for ψ



(Feynman)

Green's Function for each scatter →

G.F. are "propagators" carrying the wave from one sc. to the next...

Let's go far from the source $r >> r'$

$$k|\vec{r}-\vec{r}'| = k\left(r^2 - r'^2 - 2\vec{r}\,r'\cos\theta\right)^{\frac{1}{2}} \simeq k\left(1 - 2r'/r\,\cos\theta\right)^{1/2}$$
$$= k(r - r'\cos\theta)$$
$$= k(r - \vec{r}\cdot\vec{r}'/r)$$

likewise $|\vec{r}-\vec{r}'| \longrightarrow r - \dfrac{\vec{r}\cdot\vec{r}'}{r}$ $\vec{k}$ becomes along $\vec{r}$

so
$$\frac{1}{|\vec{r}-\vec{r}'|} \sim \frac{1}{r} + \frac{\vec{r}\cdot\vec{r}'}{r^3} \sim \frac{1}{r}$$

and

$$\psi(r) = e^{ik_0z} - \frac{m}{2\pi}\int \frac{e^{ik(r - \vec{r}\cdot\vec{r}'/r)}}{r} W(r')\psi(r')\,d\vec{r}'$$

in the Born approximation $\psi(r') \sim e^{ik_0z}$ $(= \varphi_0(r))$

$$\psi(r) = e^{ik_0 z} - \frac{m}{2\pi}\frac{e^{ikr}}{r}\int e^{-ik\hat{r}\cdot\vec{r}\,'} W(r')\, e^{ik_0 z'}\, d\vec{r}\,'$$

$$k_0 z' = \vec{k}_0 \cdot \vec{r}\,'$$

$$\vec{k}\cdot\vec{r}\,' = k r' \cos\theta_{rr'} = k_f r' \hat{r}\cdot\hat{r}' = k\,\hat{r}\cdot\vec{r}\,'$$

so,
$$-ik\hat{r}\cdot\vec{r}\,' + ik_0 z' = -i\vec{k}\cdot\vec{r}\,' + i\vec{k}_0\cdot\vec{r}\,'$$
$$= i\underbrace{(\vec{k}_0 - \vec{k})}_{\vec{q}}\cdot\vec{r}\,'$$
$$= i\vec{q}\cdot\vec{r}\,'$$

and

$$\psi(r) = e^{ik_0 z} - \frac{m}{2\pi}\frac{e^{ikr}}{r}\int W(r')\, e^{i\vec{q}\cdot\vec{r}\,'}\, d\vec{r}\,'$$

from which we can identify the scattering amplitude, now in terms of the potential,

$$f(\theta) = -\frac{m}{2\pi}\int W(\vec{r}\,')\, e^{i\vec{q}\cdot\vec{r}\,'}\, d\vec{r}\,'$$

notice that another way to recover the Born approximation is by iterative solution. Replacing $\psi(r')$ by the first term in $\psi(r)$ is $e^{ik_0 z}$.