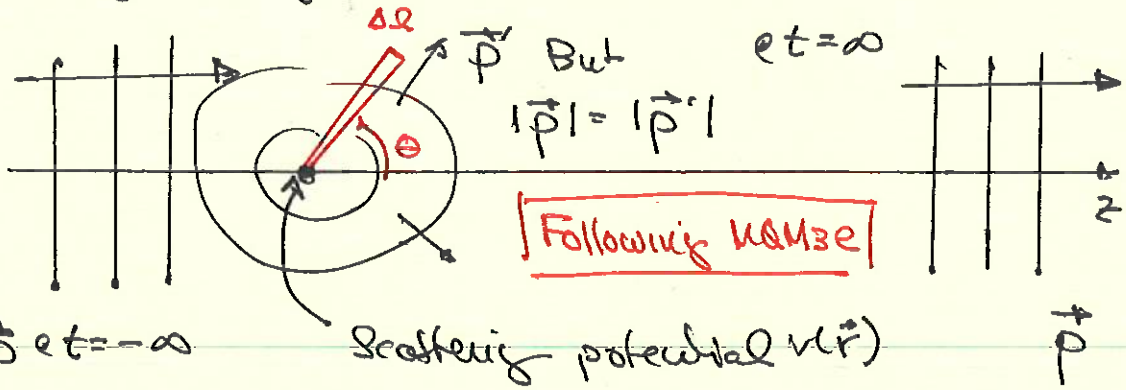
Phys 4702 Intro QM II Fall 2024 5 Nov 2024

* Status: HW #11
* Syllabus: I mis-remembered!
  Next 4 weeks: Individual topics
  (But not much depth)

Quantum Mechanical Scattering

No longer trying to solve $H|n\rangle = E|n\rangle$. Instead...



"Elastic Scattering from a massive target"

Want to find flux scattered into $\Delta\Omega$

Procedure: Time-Dependent Perturbation Theory

$$H = H_0 + V \qquad V = V(\vec{r}) \text{ time independent}$$

$$H_0 = \frac{1}{2m}\vec{p}^{\,2} \Rightarrow \text{Use Interaction Picture!}$$

- write $U^{(I)}(t,t_0)$ for time translation $t_0 \to t$
- will take $t_0 \to -\infty$ for $|i\rangle$ = incident particle wave
- will have to be careful with the $t_0 \to -\infty$ limit!

~~Starting Point:~~ $\cancel{i\hbar\frac{d}{dt}U^{(I)}(t,t_0) = V^{(I)}U \Rightarrow U^{(I)}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} V^{(I)}(t')U^{(I)}(t')\,dt'}$

"Start from the Beginning"

$$i\hbar \frac{d}{dt} U^{(I)}(t,t_0) = V^{(I)}(t)\, U^{(I)}(t,t_0)$$

<u>Integrate</u>: $$U^{(I)}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} V^{(I)}(t')\, U^{(I)}(t',t_0)\, dt'$$

<u>Transition amplitude</u>: Do $\langle n|$ ... $|i\rangle$

$$1 = \sum_m |m\rangle\langle m|$$

$$\langle n|U^{(I)}(t,t_0)|i\rangle = \delta_{ni} - \frac{i}{\hbar}\int_{t_0}^{t} \langle n|\underline{V^{(I)}}(t')\, U^{(I)}(t',t_0)|i\rangle\, dt'$$

$$= e^{iH_0 t/\hbar}\, V\, e^{-iH_0 t/\hbar}$$

$$= \delta_{ni} - \frac{i}{\hbar}\sum_m \int_{t_0}^{t} e^{i\omega_{nm} t'}\, V_{nm}\, \langle m|U^{(I)}(t',t_0)|i\rangle\, dt'$$

Must devise a way to work with this as $t_0 \to -\infty$.
[This is where we have our initial state defined.]

Introduce the <u>T-matrix T_{ni}</u>

Makes $\to 0$ as $t_0 \to -\infty$

$$\langle n|U^{(I)}(t,t_0)|i\rangle = \delta_{ni} - \frac{i}{\hbar} T_{ni}\int_{t_0}^{t} e^{i\omega_{ni} t'}\, \underline{e^{\varepsilon t'}}\, dt'$$

<u>Definition</u>! We will have to find a way to use it!

<u>Note</u>: Must take $\varepsilon \to 0$ before we take $t \to \infty$!!

$$\Rightarrow S_{ni} \equiv \lim_{t\to\infty}\left[\lim_{\varepsilon\to 0} \langle n|U^{(I)}(t,-\infty)|i\rangle\right]$$

$$= \delta_{ni} - \frac{i}{\hbar} T_{ni}\int_{-\infty}^{\infty} e^{i\omega_{ni} t'}\, dt'$$

$$= \delta_{ni} - \frac{i}{\hbar}\, 2\pi\, \delta(\omega_{ni})$$

Concepts (5.22)

$$= \delta_{ni} - 2\pi i\, \delta(E_n - E_i)\, T_{ni}$$

"Nothing happens" "Something happens"

Transition Rate and Cross Section

Define $w(i \to n) = \frac{d}{dt} \left| \langle n | U^{(\varepsilon)}(t,-\infty) | i \rangle \right|^2$

For $i \neq n$, $\langle n | U^{(\varepsilon)}(t,-\infty) | i \rangle = -\frac{i}{\hbar} T_{ni} \int_{-\infty}^{t} e^{i\omega_{ni}t' + \varepsilon t'} dt'$

$$= -\frac{i}{\hbar} T_{ni} \frac{e^{i\omega_{ni}t + \varepsilon t}}{i\omega_{ni} + \varepsilon}$$

See how the $e^{\varepsilon t}$ helped us out!

$$\Rightarrow w(i \to n) = \frac{1}{\hbar^2} |T_{ni}|^2 \frac{d}{dt} \left[\frac{e^{2\varepsilon t}}{\omega_{ni}^2 + \varepsilon^2} \right] = \frac{|T_{ni}|^2}{\hbar^2} \frac{2\varepsilon e^{2\varepsilon t}}{\omega_{ni}^2 + \varepsilon^2}$$

Now take $\varepsilon \to 0$ and then $t \to \infty$

But $w \to 0$ as $\varepsilon \to 0$ unless $\omega_{ni} = 0$! $w \to \infty$ if $\omega_{ni} = 0$!

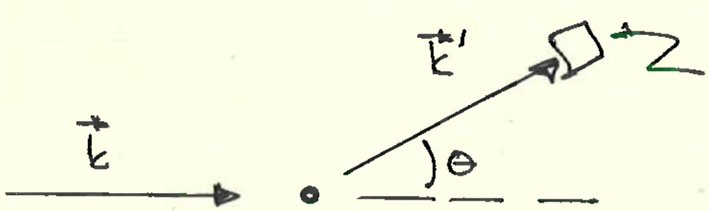
and $\int_{-\infty}^{\infty} \frac{1}{\omega^2 + \varepsilon^2} d\omega = \frac{\pi}{\varepsilon}$ Homework!

$$\Rightarrow w(i \to n) = \frac{2\pi}{\hbar} |T_{ni}|^2 \delta(E_n - E_i)$$

- Independent of $t \Rightarrow \lim t \to \infty$ is trivial!
- Looks like Fermi's Golden Rule
- Still need to figure out how to find T_{ni}!!

But first, let's make a connection to reality:

"Fermi's Golden Rule" $\Rightarrow$ "Integrate over density of states"



"Detector" covers solid angle $d\Omega$

Use "Big Box" again!

$$E = \frac{\hbar^2 \vec{k}^2}{2m} = \frac{\hbar^2 \vec{k}'^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{2\pi}{L}\right)^2 |\vec{n}|^2 \Rightarrow dE = \frac{\hbar^2}{m}\left(\frac{2\pi}{L}\right)^2 \underset{\checkmark}{|\vec{n}|}\, \underset{\times}{d|\vec{n}|}$$

$$dN = 4\pi \underset{\checkmark}{|\vec{n}|^2}\, \underset{\times}{d|\vec{n}|} \times \frac{\Delta\Omega}{4\pi}$$

Fraction that scatter into detector.

$$\therefore \rho(E) = \frac{dN}{dE} = |\vec{n}|\,\Delta\Omega\, \frac{m}{\hbar^2}\left(\frac{L}{2\pi}\right)^2$$

But $\vec{k}' = \frac{2\pi}{L}\vec{n} \Rightarrow |\vec{n}| = \frac{L}{2\pi}|\vec{k}'| = \frac{L}{2\pi}k$

$$\therefore \rho(E) = \frac{mk}{\hbar^2}\left(\frac{L}{2\pi}\right)^3 d\Omega \quad \underline{\underline{\text{and}}} \quad w = \underline{\frac{mkL^3}{(2\pi)^2\hbar^3}\,|T_{ni}|^2\, d\Omega}$$

<u>Cross Section</u> $\quad d\sigma = \dfrac{\text{"Transition Scattering Rate"}}{\text{"Incident Flux"}}$

Incident wave function $u_E(\vec{r}) = N e^{i\vec{k}\cdot\vec{r}}$

"Big Box" $\Rightarrow 1 = \int_{Box} u_E^* u_E \, d^3r = N^2 L^3 \Rightarrow N = \frac{1}{L^{3/2}}$

Incident Flux: (See Feb. 13 last semester)

$$\vec{j} = \frac{\hbar}{2im}\left[u_E^* \vec{\nabla} u_E - (\vec{\nabla} u_E^*) u_E\right] = \frac{\hbar}{2im}\left[\frac{1}{L^3}(i\vec{k}) - \frac{1}{L^3}(-i\vec{k})\right]$$

$$= \frac{\hbar \vec{k}}{mL^3} \quad \left(= \frac{1}{L^3} \times \frac{1}{(L/v)}\right)$$

So, "finally"...

$$d\sigma = \frac{mkL^3}{2\pi^2\hbar^3}|T_{ni}|^2 d\Omega \times \frac{mL^3}{\hbar k} \Rightarrow \frac{d\sigma}{d\Omega} = \frac{(mL^3)^2}{(2\pi\hbar)^2}|T_{ni}|^2$$

Finding the T-Matrix

We have two expressions for $\langle n|U^{(I)}(t,-\infty)|i\rangle$:

(1) $\langle n|U^{(I)}(t,-\infty)|i\rangle = \delta_{ni} - \frac{i}{\hbar} T_{ni} \frac{e^{i\omega_{ni}t+\varepsilon t}}{i\omega_{ni}+\varepsilon}$ $\times\frac{i}{i}$

put back in

$$= \delta_{ni} + \frac{1}{\hbar} T_{ni} \frac{e^{i\omega_{ni}t+\varepsilon t}}{-\omega_{ni}+i\varepsilon}$$

[This is from the Definition of T_{ni}]

We also have our original expression:

(2) $\langle n|U^{(I)}(t,-\infty)|i\rangle =$

Need this for $t_0 \to -\infty$

$$\delta_{ni} - \frac{i}{\hbar}\sum_m V_{nm}\int_{-\infty}^{t} e^{i\omega_{nm}t'+\varepsilon t'} \langle \underline{\underline{m}}|U^{(I)}(t',-\infty)|i\rangle\, dt'$$

Now insert (1) into right side of (2)

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i.e. write (1) = (2) w/ (1) inserted; Drop the δ_{ni}, so...

$$\frac{1}{\hbar}T_{ni}\frac{e^{i\omega_{ni}t+\varepsilon t}}{-\omega_{ni}+i\varepsilon} = -\frac{i}{\hbar}\sum_m V_{nm} \times \ldots$$

$$\ldots\int_{-\infty}^{t} e^{i\omega_{nm}t'+\varepsilon t'}\left[\delta_{\underline{\underline{m}}i} + \frac{1}{\hbar}T_{\underline{\underline{m}}i}\frac{e^{i\omega_{\underline{\underline{m}}i}t'+\varepsilon t'}}{-\omega_{\underline{\underline{m}}i}+i\varepsilon}\right]dt'$$

$$= -\frac{i}{\hbar}V_{ni}\frac{e^{i\omega_{ni}t+\varepsilon t}}{i\omega_{ni}+\varepsilon}$$

$$= \frac{E_n-E_m}{\hbar} + \frac{E_m-E_i}{\hbar} = \omega_{ni}$$

$$-\frac{i}{\hbar}\sum_m \frac{V_{nm}\frac{1}{\hbar}T_{mi}}{-\omega_{mi}+i\varepsilon}\int_{-\infty}^{t} e^{i\underline{\underline{(\omega_{nm}+\omega_{mi})}}t'+2\varepsilon t'}\,dt'$$

Now multiply through by $\hbar$:

$$T_{ni}\frac{e^{i\omega_{ni}t+\varepsilon t}}{-\omega_{ni}+\varepsilon} = V_{ni}\frac{e^{i\omega_{ni}t+\varepsilon t}}{-\omega_{ni}+\varepsilon} {}^{*}$$

* these three factors are all the same since $\varepsilon \to 0$, so...

$$^{*}\;-\frac{i}{\hbar}\sum_m V_{nm}\frac{T_{mi}}{-\omega_{mi}+i\varepsilon}\;\frac{e^{i\omega_{ni}t+2\varepsilon t}}{i\omega_{ni}+2\varepsilon}{}^{*}$$

$$T_{ni} = V_{ni} + \sum_m V_{nm}\frac{T_{mi}}{\hbar(-\omega_{mi}+i\varepsilon)}$$

"System of Linear Algebraic Eqs for T_{ni}"

$$= V_{ni} + \sum_m V_{nm}\frac{T_{mi}}{E_i-E_m+i\varepsilon}$$

Redefine $\hbar\varepsilon \to \varepsilon$ (Still positive!)

Whew! Big Deal! You can see the emergence of a perturbation expansion! i.e. Put left into right, etc...

Formalize: Define a state $|\psi\rangle$ via $T_{ni} = \langle n|V|\psi\rangle$

$$\text{so}\quad \langle n|V|\psi\rangle = \langle n|V|i\rangle + \sum_m \langle n|V|m\rangle\frac{\langle m|V|\psi\rangle}{E_i-E_m+i\varepsilon}$$

$$|\psi\rangle = |i\rangle + \sum_m |m\rangle\frac{\langle m|V|\psi\rangle}{E_i-E_m+i\varepsilon}$$

$$= |i\rangle + \sum_m \frac{1}{E_i-H_0+i\varepsilon}|m\rangle\langle m|V|\psi\rangle$$

$$\text{i.e.}\quad |\psi\rangle = |i\rangle + \frac{1}{E_i-H_0+i\varepsilon}V|\psi\rangle$$

"Lippman-Schwinger Eq"

Cheap way!! $(E_i - H_0)|\psi\rangle = V|\psi\rangle$ i.e. $H|\psi\rangle = E_i|\psi\rangle$