TIME-DEPENDENT PERTURBATION THEORY

often called $V(t)$;

setup: $\boxed{\mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}'(t)}$

often, perturbat$^{\underline{n}}$ is temporary

t-indep, e-solvable: $\{|n^{(0)}\rangle, E_n^{(0)}\}$ will serve as our basis

goal: find transition $P_{if} = |i^{(0)}\rangle \longrightarrow |f^{(0)}\rangle$ of unperturbed $\mathcal{H}_0$

solution form: $|\psi(t)\rangle = \sum_n |n^{(0)}\rangle \cdot \text{blah}(t)$

... we KNOW t-evolution of $|n^{(0)}\rangle$ under $\mathcal{H}_0$ $\because$ t-indep

$$|n^{(0)}(t)\rangle = |n^{(0)}\rangle e^{-i\omega_n t}$$

$$\boxed{\omega_n \equiv \frac{E_n^{(0)}}{\hbar}}$$

... remove this t-dep from blah(t)

FORM: $$\boxed{|\psi(t)\rangle = \sum_n \underbrace{|n^{(0)}\rangle e^{-i\omega_n t}}_{|n^{(0)}(t)\rangle \text{ under } \mathcal{H}_0} \underbrace{c_n(t)}_{t\text{-evolution due to } \mathcal{H}'(t)}}$$

PLUG: into SE $\left(\hat{\mathcal{H}} - i\hbar\frac{\partial}{\partial t}\right)\Psi(t) = 0$

$$0 = \left(\hat{\mathcal{H}}_0 + \hat{\mathcal{H}}'(t) - i\hbar\partial_t\right)\sum_n \underbrace{c_n(t)}_{\text{WANT!}} e^{-i\omega_n t}|n^{(0)}\rangle$$

e-states of $\hat{\mathcal{H}}_0$, t-indep

$$= \sum_n \left[\cancel{E_n^{(0)}} c_n + \hat{\mathcal{H}}' c_n - i\hbar\left(\dot{c}_n - \cancel{i\omega_n} c_n\right)\right] \times e^{-i\omega_n t}|n^{(0)}\rangle$$

Project onto some $|f^{(0)}\rangle$ ("f" = final state of interest) via taking inner product $\langle f^{(0)}|$. EQUATION

$$0 = \langle f^{(0)}| \sum_n \left[\hat{\mathcal{H}}' c_n - i\hbar\dot{c}_n\right] e^{-i\omega_n t}|n^{(0)}\rangle$$

$$= \sum_n \langle f^{(0)}|\hat{\mathcal{H}}'|n^{(0)}\rangle c_n e^{-i\omega_n t}$$

matrix elem $\boxed{\mathcal{H}'_{fn} \equiv \langle f^{(0)}|\mathcal{H}'|n^{(0)}\rangle}$

$$- \sum_n i\hbar\dot{c}_n e^{-i\omega_n t} \cancel{\langle f^{(0)}|n^{(0)}\rangle} \to \delta_{fn}$$

↳ only $n=f$ survives ∴

$$\boxed{i\hbar\,\dot{c}_f = \sum_n c_n \hat{\mathcal{H}}'_{fn} e^{i\omega_{fn}t}}$$

$$\boxed{\omega_{fn} \equiv \omega_f - \omega_n} = \frac{(E_f^{(0)} - E_n^{(0)})}{\hbar}$$

EXACT {ODEs} for $\underbrace{\{c_n(t)\}}_{\text{coefficients}}$

⊕ NO APPROX's made @ this point!

∃ a few exactly solvable systems, e.g. some 2-state systems

⊕ "Transition frequency ω_{fn}" & "Transition matrix elem. $\mathcal{H}'_{fn}$"

Perturbation Theory, t-dep: useful when $\mathcal{H}' \ll \mathcal{H}_0$

Introduce ⊕ parameter of explicit smallness ε:

$$\mathcal{H}(t) = \mathcal{H}_0 + \varepsilon \mathcal{H}'$$

$$c_n(t) = c_n^{(0)}(t) + \varepsilon c_n^{(1)}(t) + \varepsilon^2 c_n^{(2)}(t) + \ldots$$

Plug expansions into {exact ODEs}:

$$\left[\dot{C}_f^{(0)} + \varepsilon \dot{C}_f^{(1)} + \varepsilon^2 \dot{C}_f^{(2)} + \cdots\right]$$

$$= \sum_n \left[C_n^{(0)} + \varepsilon C_n^{(1)} + \cdots\right] \frac{\varepsilon \mathcal{H}'_{fn} e^{i\omega_{fn}t}}{i\hbar}$$

Now, SUPPOSE that the system starts in $|i^{(0)}\rangle$ INITIAL STATE

@ time $t=0$

Match orders of ε:

$\boxed{\varepsilon^0}$ $\dot{C}_f^{(0)} = 0 \longrightarrow C_f^{(0)}(t) = \text{CONSTANT}$

$= \emptyset$ except when $f=i$, ie. NO TRANSITION possible when $\varepsilon=0$

↳ ie. set $\varepsilon=0$

ie. NO PERTURBATION!

$$\boxed{C_f^{(0)}(t) = \delta_{fi}}$$

$\boxed{\varepsilon^1}$ $$\dot{C}_f^{(1)} = \sum_n C_n^{(0)} \frac{\mathcal{H}'_{fn} e^{i\omega_{fn}t}}{i\hbar}$$

⊕ Recursive technique: plug PREVIOUS-ORDER solution into equ. for NEXT ORDER, then solve for NEXT ORDER here: $\dot{c}_f^{(1)} = \sum_n \delta_{ni} \frac{\mathcal{H}'_{fn} e^{i\omega_{fn} t}}{i\hbar} = \frac{\mathcal{H}'_{fi}}{i\hbar} e^{i\omega_{fi} t}$

only $n = i$ survives

$$\boxed{c_f^{(1)}(t) = \int_0^t dt' e^{i\omega_{fi} t'} \frac{\mathcal{H}'_{fi}(t')}{i\hbar}}$$

So: Given that system's $|\psi\rangle = |i^{(0)}\rangle$ @ $t=0$,

INITIAL

$$|\psi(t)\rangle = \sum_f |f^{(0)}\rangle e^{-i\omega_f t} c_f(t)$$

where to order $\Sigma^0 + \Sigma^1$,

$$c_f^{(0)+(1)}(t) = \delta_{if} - \frac{i}{\hbar} \int_0^t dt' e^{i\omega_{fi} t'} \mathcal{H}'_{fi}(t')$$

and what we are usually seeking is:

$c_f(t)$: "transition amplitude"

transition probability $\boxed{P_{i \to f} = |c_f(t)|^2}$ where "i" & "f" refer to e-states of $\mathcal{H}_0$

ALL ORDERS of t-dep PT

Given $\mathcal{H}(t) = \mathcal{H}_0 + V(t)$

★ switching notation from $\mathcal{H}' \longrightarrow V$, very common

& form $|\psi(t)\rangle = \sum_n c_n(t)\, |n^{(0)}\rangle e^{i\omega_n t}$

then EXACT ODEs:

$$\boxed{\dot{c}_f(t) = \frac{1}{i\hbar} \sum_n V_{fn}\, e^{i\omega_{fn} t}\, c_n(t)}$$

Ingredients:

- Perturb. expansion for $V \ll \mathcal{H}_0$

$$\mathcal{H}(t) = \mathcal{H}_0 + \varepsilon V(t)$$

$$c_n(t) = c_n^{(0)}(t) + \varepsilon c_n^{(1)}(t) + \varepsilon^2 c_n^{(2)}(t) + \cdots$$

- starting state $|\psi(t_0)\rangle = |i^{(0)}\rangle$

Plug into exact {ODEs}:

$$\sum_n \varepsilon V_{fn}\, e^{i\omega_{fn} t} \left[c_n^{(0)} + \varepsilon c_n^{(1)} + \cdots \right]$$

$$= \dot{c}_f^{(0)} + \varepsilon \dot{c}_f^{(1)} + \varepsilon^2 \dot{c}_f^{(2)} + \cdots$$

RESULTING EQU'S @ each order:

$\boxed{\varepsilon^0}$ $\dot{c}_f^{(0)}(t) = 0$

idea = 0^{th} order solution goes here

$\boxed{\varepsilon^1}$ $\dot{c}_f^{(1)}(t) = \frac{1}{i\hbar} \sum_n V_{fn}(t)\, e^{i\omega_{fn} t}\, c_n^{(0)}(t)$

⋮

$\boxed{\varepsilon^j}$ $\underline{j \geq 1}$ $$\boxed{\dot{c}_f^{(j)}(t) = \frac{1}{i\hbar} \sum_n V_{fn}(t)\, e^{i\omega_{fn} t}\, c_n^{(j-1)}(t)}$$

then solve for next higher order

order j RECURSIVE RELATION! order $j-1$ ∴ RECURSIVE SOLUTION!

SOLUTIONS:

$\boxed{\varepsilon^0}$ $c_f^{(0)}(t) = \text{CONST} = \delta_{fi}$ ∵ starting in unperturbed $|i^{(0)}\rangle$ @ $t=0$

$\boxed{\varepsilon^1}$ $c_f^{(1)}(t) = \int_0^t dt' \sum_n \frac{V_{fn}(t')}{i\hbar} e^{i\omega_{fn} t'} \underline{\underline{c_n^{(0)}(t)}}$ plug in δ_{ni}

$$= \int_0^t dt' \frac{V_{fi}(t')}{i\hbar} e^{i\omega_{fi} t'}$$

$$\boxed{\varepsilon^2} \quad C_f^{(2)}(t) = \int_0^t dt' \sum_n \frac{V_{fn}(t')}{i\hbar} e^{i\omega_{fn}t'} \underline{\underline{C_n^{(1)}(t')}}$$

Plug in

$$= \int_0^t dt' \sum_n \frac{V_{fn}(t')}{i\hbar} e^{i\omega_{fn}t'} \int_0^{t'} dt'' \frac{V_{ni}(t'')}{i\hbar} e^{i\omega_{ni}t''}$$

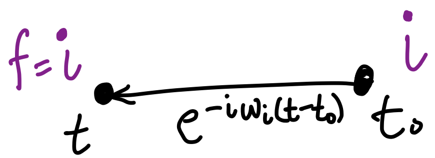
$$\& \quad \omega_{fn} \equiv \omega_f - \omega_n \equiv \left[E_f^{(0)} - E_n^{(0)}\right]/\hbar$$

$$= \frac{1}{(i\hbar)^2} \sum_n \int_0^t dt' \int_0^{t'} dt'' \underbrace{e^{i\omega_f t'}}_{\text{t-dep of } \langle f^{(0)}|} \underbrace{V_{fn}(t')}_{\text{ME } n\to f} \underbrace{e^{-i\omega_n(t'-t'')}}_{\text{t-dep of } |n^{(0)}\rangle} \underbrace{V_{ni}(t'')}_{\text{ME } i\to n} \underbrace{e^{-i\omega_i t''}}_{\text{t-dep of } |i^{(0)}\rangle}$$

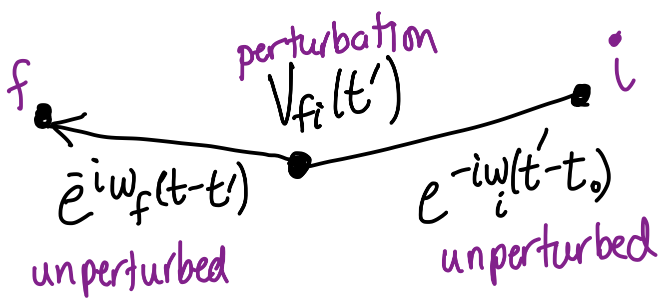
Graphical Representation of nested integrals:

define $t_0 \equiv 0$

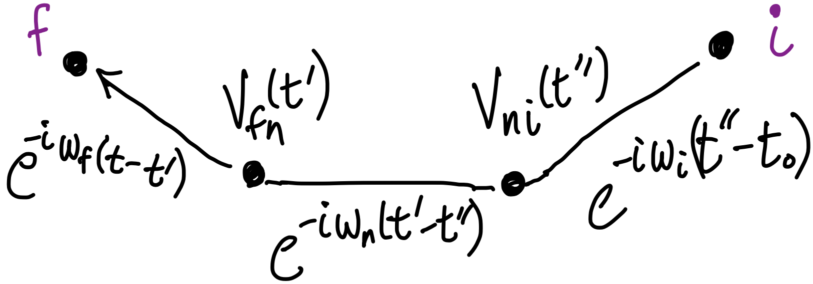
$C_f^{(0)}(t) =$



$c_f^{(1)}(t) =$

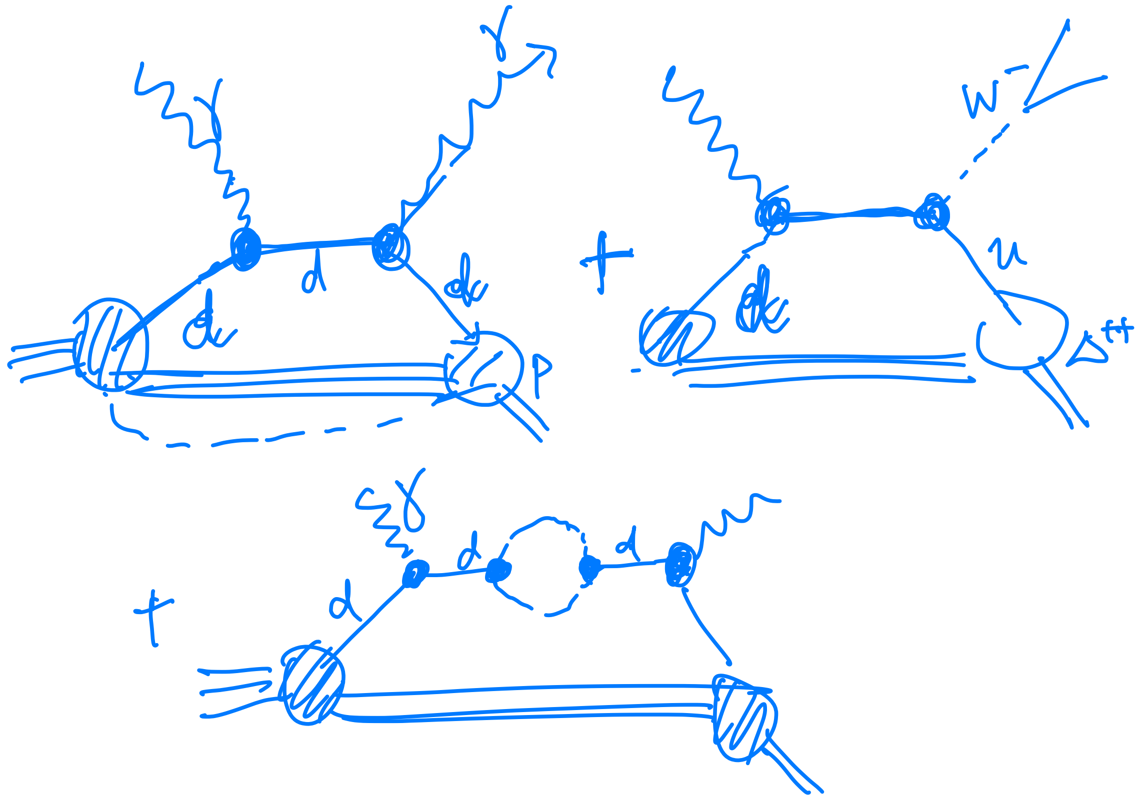


$C_f^{(2)}(t) =$



implicit $\int dt', \int dt''$ $\sum_n$

Non-relativistic pre-cursor of Feynman Diagrams



PT w sinusoidal $\mathcal{H}'(t)$ just to 1st order in $\mathcal{H}' \ll \mathcal{H}_0$

$$\mathcal{H}'(t) = \left[V(\vec{r})\, e^{i\omega t} + \underbrace{V^*(\vec{r})\, e^{-i\omega t}}\right]/2$$

$$= V(\vec{r}) \cos \omega t$$

$\mathcal{H}'$ must be **HERMITIAN**

to match Griffiths

FIND $P_{i\to f}(t) = |c_f^{(1)}(t)|^2$

1st order = lowest order causing a TRANSITION w $i \neq f$

$$c_f^{(1)}(t) = \int_0^t \frac{\mathcal{H}'_{fi}(t')}{i\hbar} e^{i\omega_{fi} t'} dt'$$

where $\mathcal{H}'_{fi}(t) = \frac{1}{2}\left[V_{fi}\, e^{i\omega t} + V_{fi}^*\, e^{-i\omega t}\right]$

$\omega_{fi} \equiv \dfrac{E_f^{(0)} - E_i^{(0)}}{\hbar}$ TRANSITION FREQUENCY

vs

$\omega \equiv$ DRIVING FREQUENCY

$$\therefore c_f^{(1)}(t) = \frac{1}{2i\hbar} \int_0^t dt' \left[V_{fi}\, e^{i(\omega_{fi}+\omega)t'} + V_{fi}^*\, e^{i(\omega_{fi}-\omega)t'}\right]$$

define $\boxed{\Omega_\pm \equiv \omega_{fi} \pm \omega} = \dfrac{E_f^{(0)} - E_i^{(0)}}{\hbar} \pm \omega$

integrate:

$$c_f^{(1)}(t) = -\frac{1}{2\hbar}\left[\frac{V_{fi}\, e^{i\Omega_+ t'}}{\Omega_+} + \frac{V_{fi}^*\, e^{i\Omega_- t'}}{\Omega_-}\right]_0^t$$

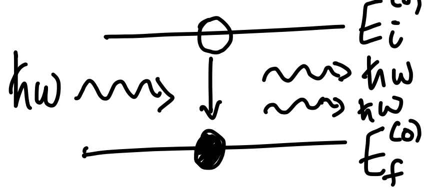
2 resonances! (when denom = 0)

$$\begin{cases} \Omega_+ = 0: & \hbar\omega = E_i^{(0)} - E_f^{(0)} \\ \Omega_- = 0: & \hbar\omega = E_f^{(0)} - E_i^{(0)} \end{cases}$$

OR

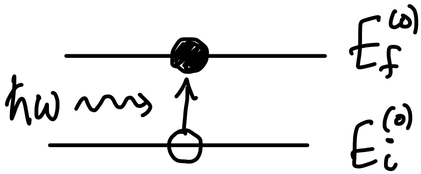
set $\omega > 0$ w.l.o.g. :

$E_i^{(0)} - E_f^{(0)} > 0$



STIMULATED EMISSION ★

$E_f^{(0)} - E_i^{(0)} > 0$



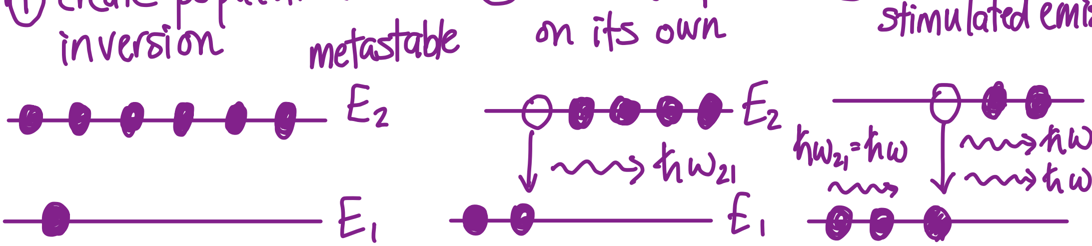
ABSORPT$^{\underline{n}}$ of energy from osc. perturbation

★ STIMULATED EMISSION → lasers! $\hbar\omega = E_i - E_f$

① create population inversion

② one e^- drops on its own

③ avalanche of stimulated emission



Features of stimulated emission:

- stimulating photons have same energy as those they cause to be emitted $\Rightarrow$ light = MONOCHROMATIC!

(proven already)

- incoming & outgoing photons are also IN PHASE & PARALLEL (momenta) $\Rightarrow$ light = COHERENT!

Consider cases where ONE of $\Omega_\pm = \omega_{fi} \pm \omega \simeq \emptyset$

(+ OR −) ie. NEAR a RESONANCE

$\Rightarrow$ one term of $c_f^{(1)}(t)$ dominates:

or *

$$c_f^{(1)}(t) \approx \frac{-1}{2\hbar}\left[\frac{V_{fi}}{\Omega_\pm}\left(e^{i\Omega_\pm t}-1\right)\right]$$

$$\therefore P_{i\to f} \approx \frac{1}{4\hbar^2}\frac{|V_{fi}|^2}{\Omega_\pm^2}\underbrace{\left(e^{i\Omega_\pm t}-1\right)\left(e^{-i\Omega_\pm t}-1\right)}_{2-2\cos\Omega_\pm t}$$

$$= 4\sin^2\frac{\Omega_\pm t}{2}$$

rearrange a bit: $\times\left(\frac{t/2}{t/2}\right)^2 \dots$

$$P_{i\to f} \approx \frac{|V_{fi}|^2}{\hbar^2}\left[\frac{\sin \Omega_\pm t/2}{\Omega_\pm t/2}\right]^2 \left(\frac{t}{2}\right)^2$$

NEAR a RESONANCE ($\Omega_+ \approx \emptyset$ OR Ω_-)

CANCEL

$$\left[\frac{\sin x}{x}\right]^2 \xrightarrow[x\to 0]{} 1 \text{ @ resonance } \Omega_\pm = 0 \quad \left(\text{with } x = \frac{\Omega_\pm t}{2}\right)$$

$$\therefore P_{i\to f} \approx \frac{|V_{fi}|^2}{\hbar^2}\left(\frac{t}{2}\right)^2$$

@ PEAK

$\left[\frac{\sin x}{x}\right]^2 \approx \frac{1}{2}$ when $x \approx \pm 1.4$

$\left(\frac{\Omega t}{2} \approx \pm 1.4\right.$

$\Delta\Omega \approx 2\left[\frac{2\times 1.4}{t}\right] \approx \frac{6}{t}$

@ $\frac{1}{2}$ max

$\Delta\Omega_\pm \approx \frac{6}{t}$ $\xrightarrow{t\to 0} \infty$, $\xrightarrow{t\to\infty} 0$

WIDTH of resonance

$$\boxed{\text{FREQUENCY DEPENDENCE}}$$

@ fixed, finite t

observations:

- as t grows, PEAK in frequency response of $P_{i\to f}$ gets higher ($\sim t^2$) & narrower ($\sim \frac{6}{t}$)

- cf. @ $t=\emptyset$, $P_{i\to f}$ is FLAT $\approx \emptyset$ @ all $\Omega_\pm$ $\approx$ no resonance

$\Rightarrow$ Resonance becomes sharper with time, as if the system NEEDS TIME to FOURIER ANALYZE the perturbation & "learn" that it is oscillating @ ω !! ☺

- $P_{i\to f} \sim t^2$ suggests that $P_{i\to f}$ will become > 1 ! ⊙⊙

- Problem arises when $P_{i\to f}$ is NOT $\ll 1$, then 1st order PT is not appropriate!

- Recall HW 3 NMR spin-flip calculation: that was EXACT, & $P_{\text{spin}\uparrow\to\downarrow}$ never exceeded 1.

$$\boxed{\text{Limit } t\to\infty}$$

- DISC 11: math result $\quad \dfrac{\sin^2(ax)}{ax^2} \xrightarrow[a\to\infty]{} \pi\,\delta(x) \Rightarrow$ Take $a = \dfrac{t}{2} \to \infty$ & $x = \Omega_\pm$ in ★ near-reson. formula

$$P_{i\to f} \approx \frac{|V_{fi}|^2}{\hbar^2}\underbrace{\left[\frac{\sin^2(t/2\,\Omega_\pm)}{t/2\,\Omega_\pm^{\,2}}\right]}_{\text{as } t\to\infty,\ \text{becomes } \pi\,\delta(\Omega_\pm)}\frac{t}{2}$$

near resonance

(Infinitely sharp resonant peak in frequency!)

$$\xrightarrow[t\to\infty]{} \frac{|V_{fi}|^2}{\hbar^2}\pi\,\delta(\Omega_\pm)\,\frac{t}{2}$$ ← <u>linear</u> with time!

near resonance, in limit $t\to\infty$

Define

$$\boxed{\text{TRANSITION RATE} \equiv \frac{P_{i\to f}}{t} \equiv R_{i\to f} = \frac{|V_{fi}|^2}{2\hbar^2}\pi\,\delta(\Omega_\pm)}$$

Also on DISC II: $\delta(ax) = \delta(x)/a$

$$\therefore \delta(\hbar\Omega_\pm) = \frac{\delta(\Omega_\pm)}{\hbar} = \delta(E_f - E_i \pm \hbar\omega)$$

$$\Rightarrow R_{i\to f} = \frac{\pi}{2\hbar}|V_{fi}|^2\,\delta(E_f - E_i \pm \hbar\omega)$$

Finally, consider transitions from/to a CONTINUUM

- USUAL: E_f can be in a CONTINUUM of final states if
  e.g. ionizing an atom: $E_f > 0 \Rightarrow$ SCATTERING
  OR final states with $n_f \gg 1$: states are CLOSELY PACKED
  ≈ approx. continuum
- GRIFF. §9: $E_{perturb.} = \hbar\omega$ from perturbation can be part of a continuum e.g. photon spectrum produced by a light bulb → BBody spectrum

In such cases, integrate over continuum & the $\tilde{\delta}$-function peak:

replace $\delta(E_f - E_i \pm \hbar\omega)$ with $n(E_f - E_i \pm \hbar\omega)$

<u>number density</u> of states

$$n(E)\,dE = \begin{bmatrix} \#\text{ states in range} \\ E - \frac{dE}{2} \to E + \frac{dE}{2} \end{bmatrix} dE$$

The point? Unlike $\delta(E\cdots)$, $n(E)$ is FINITE everywhere ☺

$$\Rightarrow R_{i\to\int E_f} = \int \frac{\pi}{2\hbar} |V_{fi}|^2 \underbrace{dE_f\, n(E_f)}_{\substack{\text{OR} \\ dE_{perturbation}\, n(E_{perturb} = \hbar\omega)}} \times \delta(E_{fi} - \hbar\omega)$$

FERMI'S GOLDEN RULE

$$\boxed{R_{i\to\int E_f} = W_{i\to f} = \frac{\pi}{2\hbar} |V_{fi}|^2\, n(E_f)\Big|_{E_i \pm \hbar\omega}} = \frac{\text{USUAL F.G.R.}}{4}$$

- neighbourhood of resonance
- 1st order PT
- $t \to \infty$
- sinusoidal perturbation @ freq. ω

<u>OR</u> DISC II: constant perturbation, as if you change factor of 2 problem

GR. CHOICE $\mathcal{H}' = \frac{[Ve^{i\omega t} + V^* e^{-i\omega t}]}{2}$

GR.-ONLY

USUAL F.G.R. → formula sheet

$$W_{i\to f} = \frac{2\pi}{\hbar} \left| \bar{V}_{fi} \right|^2 n\left(E_f \middle| \begin{array}{ll} E_i \pm \hbar\omega & \text{for } \overset{\text{osc.}}{\mathcal{H}'} = V e^{i\omega t} + V^* e^{-i\omega t} \\ E_i & \text{for constant } \mathcal{H}' \end{array} \right)$$

OR

⇒ same result for both cases