Non-perturbative calculation of transition amplitudes

A: Evolution operator and resolvent

1. Issue with perturbation series: energy denominators

We saw in a simple model (API C1) how this can be fixed

$$\frac{1}{E-E_b+i\eta} \longrightarrow \frac{1}{E-E_b+i\frac{\hbar\Gamma}{2}+i\eta} = \sum_{n=0}^{\infty}(-1)^n\frac{\left(i\frac{\hbar\Gamma}{2}\right)^n}{(E-E_b)^{n+1}}$$

Let's introce now a general formalism to calculate transition amplitudes non-perturbatively.

Start with $i\hbar\frac{d}{dt}U(t,t') = (H_0+V)U(t,t')$

with $U(t',t') = 1$

$$(*) \quad U(t,t') = U_0(t,t') + \frac{1}{i\hbar}\int_{t'}^{t} dt_1\, U_0(t,t_1)VU(t_1,t')$$

with $U_0(t,t') = \exp(-iH_0(t-t')/\hbar)$

$(*)$ contains "almost" a convolution product, but the limits of integration would need to be $\pm\infty$.

2. To fix this (and then be able to go to Fourier space, which turns a convolution into a simple product):

$$K_+(t,t') = U(t,t')\theta(t-t')$$
$$K_{0+}(t,t') = U_0(t,t')\theta(t-t')$$

Multiply $(*)$ by $\theta(t-t')$ and replace

$$\int_{t'}^{t} dt_1 \longrightarrow \int_{-\infty}^{\infty} dt_1\, \theta(t-t_1)\theta(t_1-t') \ldots$$

① $K_+(t,t') = K_{0+}(t,t') + \frac{1}{i\hbar}\int_{-\infty}^{\infty} dt_1\, K_{0+}(t,t_1) V K_+(t_1,t')$

K_+ obeys $\left(i\hbar \frac{d}{dt} - H\right) K_+(t,t') = \hbar\,\delta(t-t')$

$\Rightarrow K_+$ is the retarded Green's function.

Advanced Green's function:

$$K_-(t,t') = -U(t,t')\,\theta(t'-t)$$

K_- also obeys $\left(i\hbar \frac{d}{dt} - H\right) K_-(t,t') = \hbar\,\delta(t-t')$

Fourier: $$K_+(\tau) = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} dE\, e^{-iE\tau/\hbar}\, G_+(E)$$

$$G_+(E) = \frac{1}{i\hbar}\int_{-\infty}^{\infty} d\tau\, e^{iE\tau/\hbar}\, K_+(\tau)$$

Since $K_+(\tau) = e^{-iH\tau/\hbar}\,\theta(\tau)$, we get

$$G_+(E) = \frac{1}{i\hbar}\int_{0}^{\infty} d\tau\, e^{i(E-H)\tau/\hbar}$$

$$= \lim_{\eta\to 0_+} \frac{1}{i\hbar}\int_{0}^{\infty} d\tau\, e^{i(E-H+i\eta)\tau/\hbar}$$

$$= \lim_{\eta\to 0_+} \frac{1}{E-H+i\eta}$$

Same way $G_-(E) = \lim_{\eta\to 0^+} \frac{1}{E-H-i\eta}$

① becomes $$\boxed{G_+(E) = G_{0+}(E) + G_{0+}(E)\, V\, G_+(E)}$$

3. Resolvent of H:

$$G(z) = \frac{1}{z - H} \qquad z \text{ complex}$$

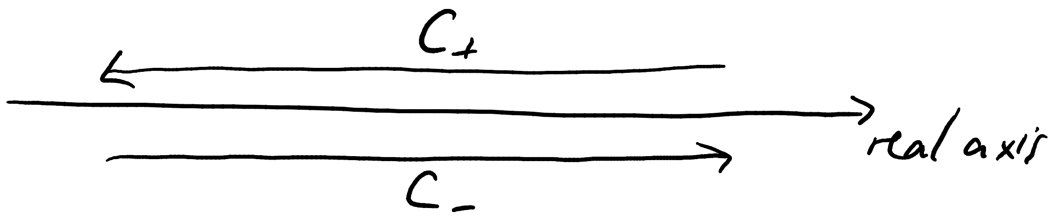
$$\Rightarrow \quad G_\pm(E) = \lim_{\eta \to 0^+} G(E \pm i\eta)$$

Back out evolution operator:

$$U(\tau) = K_+(\tau) - K_-(\tau)$$

$$= \frac{1}{2\pi i} \int_{-\infty}^{\infty} dE \, e^{-iE\tau/\hbar} \left[G_-(E) - G_+(E) \right]$$

$$U(\tau) = \frac{1}{2\pi i} \int_{C_+ + C_-} dz \, e^{-iz\tau/\hbar} \, G(z)$$



Singularities of $G(z)$ are all on the real axis.
Consist of poles at discrete Eigenvalues of H,
and cuts extending over the continuous spectrum of H.

Use $\frac{1}{A} = \frac{1}{B} + \frac{1}{B}(B-A)\frac{1}{A}$ with $A = z - H$, $B = z - H_0$:

$$G(z) = G_0(z) + G_0(z) V G(z)$$

Series expansion:

$$G(z) = G_0(z) + G_0(z) V G_0(z) + G_0(z) V G_0(z) V G_0(z) + \dots$$

$G_{kl}(z) = \langle \varphi_k | G(z) | \varphi_l \rangle$, $\quad V_{ij} = \langle \varphi_i | V | \varphi_j \rangle \quad |\varphi_j\rangle$ - e.s. of H_0

$$G_{kl}(z) = \frac{1}{z-E_k}\delta_{kl} + \frac{1}{z-E_k} V_{kl} \frac{1}{z-E_l} +$$

$$+ \sum_i \frac{1}{z-E_k} V_{ki} \frac{1}{z-E_i} V_{il} \frac{1}{z-E_l} + \dots$$

B. Formal resummation of the perturbation series

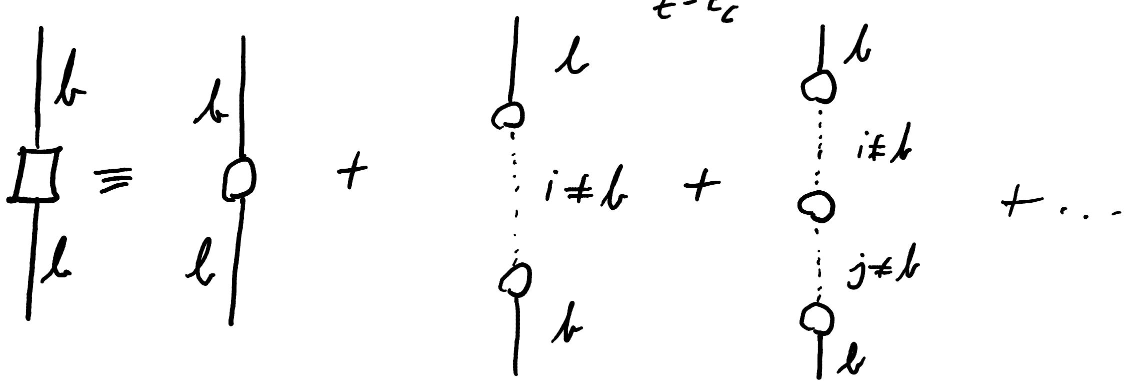
1. Diagrammatic Method, simple case.

Say $|\varphi_b\rangle$ is discrete state of H_0 with energy E_b.

$G_{0b}(z) = \langle \varphi_b | G_0(z) | \varphi_b \rangle = \dfrac{1}{z-E_b}$ varies rapidly near $z = E_b$.

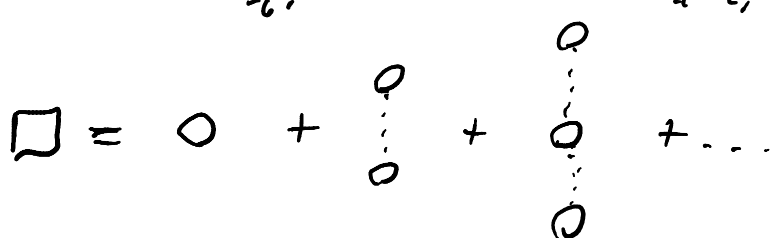
$\rightarrow$ regroup terms of expansion:

All terms that include $\dfrac{1}{z-E_b}$ twice:



solid line $\frac{1}{z-E_b}$, dotted line $\frac{1}{z-E_i}$ with $i \neq b$, 

$= V_{ib}$



$$R_b(z) = V_{bb} + \sum_{i\neq b} V_{bi}\frac{1}{z-E_i}V_{ib} + \sum_{i\neq b}\sum_{j\neq b} V_{bi}\frac{1}{z-E_i}V_{ij}\frac{1}{z-E_j}V_{jb} + \dots$$

3 denominators $\frac{1}{z-E_b}$:

 $$= \frac{1}{(z-E_b)^3}\left[R_b(z)\right]^2$$

$$\Rightarrow \quad G_b(z) = \sum_{n=1}^{\infty} \frac{\left[R_b(z)\right]^{n-1}}{(z-E_b)^n} = \frac{1}{z-E_b}\sum_{n=0}^{\infty}\left(\frac{R_b(z)}{z-E_b}\right)^n$$

$$\circledast \qquad = \frac{1}{z-E_b-R_b(z)} \qquad \underline{\text{exact}}$$

Can be generalized for more than one state $|\varphi_b\rangle$ singled out.

2. Algebraic method using projection operators

$\mathcal{E}_0$ subspace containing eigenstates of H_0 important to the physical process and to be singled out.

$P = |\varphi_a\rangle\langle\varphi_a| + \ldots + |\varphi_k\rangle\langle\varphi_k|$ projector on $\mathcal{E}_0$

$\mathcal{F}_0$ supplementary subspace of $\mathcal{E}_0$

$Q = \mathbb{1} - P$

Then (API pp. 175): $$R(z) = V + V\frac{Q}{z - QH_0H - QVQ}V$$

and $$P\,G(z)\,P = \frac{P}{z - PH_0P - PR(z)P}$$

generalizes $\circledast$.

Analyze $R(z)$ close to the real axis:

$$R_{bc}(E \pm i\eta) = V_{bc} + \langle \varphi_b | V Q \frac{}{E - QHQ \pm i\eta} QV | \varphi_c \rangle$$

Use $\frac{1}{x \pm i\eta} = \frac{x}{x^2+\eta^2} \mp \frac{i\eta}{x^2+\eta^2} = \mathcal{P}\left(\frac{1}{x}\right) \mp i\pi\delta(x)$

$$R_{bc}(E \pm i\eta) = V_{bc} + \hbar\left(\Delta_{bc}(E) \mp i\,\frac{\Gamma_{bc}(E)}{2}\right)$$

where $\Delta_{bc}(E) = \frac{1}{\hbar}\mathcal{P}\langle \varphi_b | V \frac{Q}{E - QHQ} V | \varphi_c \rangle$

$$\Gamma_{bc}(E) = \frac{2\pi}{\hbar}\langle \varphi_b | V Q\, \delta(E - QHQ) QV | \varphi_c \rangle$$

3. Approximations

a) Near $z = E_b$, all other energy denominators are large if $|\varphi_b\rangle$ is well isolated. Also, V might be small. Then we can approximate

$$R_b(z) = V_{bb} + \sum_{i \neq b} V_{bi} \frac{1}{z - E_i} V_{ib}$$

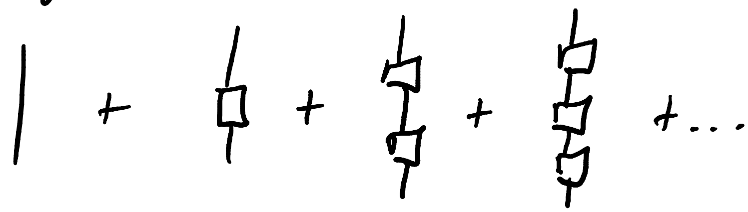
or $\Delta = O +$ 

This does not correspond to a perturbative approx. for G. In fact

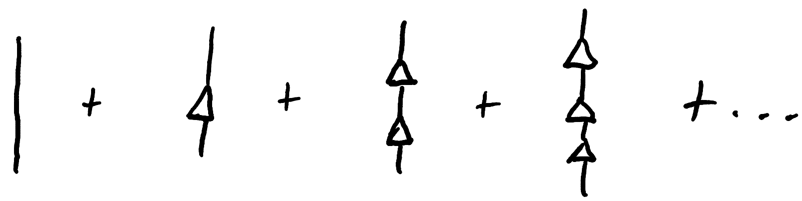
$$G(z) \simeq \frac{1}{z - E_b - R_b(z)} = \sum_{n=0}^{\infty} \frac{[R_b(z)]^n}{(z - E_b)^{n+1}}$$

contains arbitrarily high powers of V.

The infinite sum



is replaced by another infinite sum



b) Can approximate neglecting energy dependence of $R_\ell(E)$:

$$G_\ell(E \pm i\eta) = \frac{1}{E \pm i\eta - E_\ell - R_\ell(E \pm i\eta)}$$

$R_\ell(E \pm i\eta)$ varies slowly around $E \approx E_\ell$.

$\Rightarrow R_\ell(E \pm i\eta) \approx R_\ell(E_\ell \pm i\eta)$.

Real part: level shift

Imag part: broadening

Example: Evolution of excited atomic state

$$|\psi_0\rangle = |b;0\rangle$$

Find $G_b(z) = \langle b;0|G(z)|b;0\rangle$

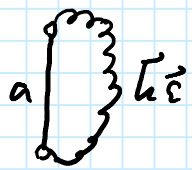
to deduce $U_b(\tau) = \langle b,0|U(\tau)|b;0\rangle$

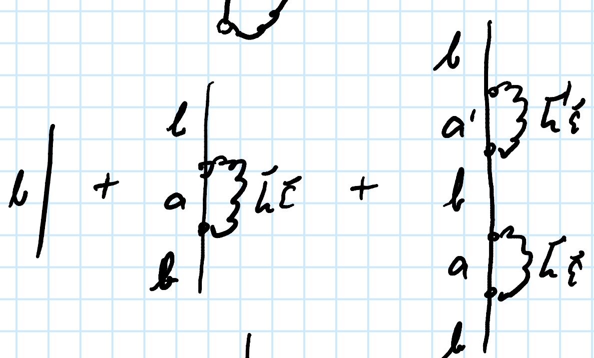
$$G_b(z) = \frac{1}{z - E_b - R_b(z)}$$

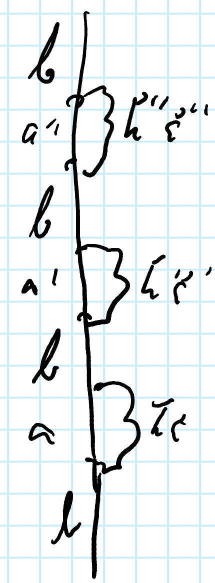
$$R_b(z) = \langle b;0|H_{I_2}|b;0\rangle + \sum_a \sum_{\vec{k}\vec{\varepsilon}} \frac{\langle b,0|H_{I_1}|a;\vec{k}\vec{\varepsilon}\rangle\langle a,\vec{k}\vec{\varepsilon}|H_{I_1}|b;0\rangle}{z - E_a - \hbar\omega}$$

incorporate into H_0.

to 2nd order

$=$ 

$G_b(z) \approx$  $+ \dots$



ignore  . . .

$$R_b(E \pm i\eta) = \sum_a \sum_{k\varepsilon} \frac{|\langle a, k\varepsilon | H_{I,n} | b, 0\rangle|^2}{E \pm i\eta - E_a - \hbar\omega}$$

$$= \hbar\, \Delta_b(E) \mp i\hbar \frac{\Gamma_b(E)}{2}$$

$$\Delta_b(E) = \frac{1}{\hbar}\, \mathcal{P} \sum_a \sum_{k\varepsilon} \frac{|\langle a, k\varepsilon | H_{I,n} | b; 0\rangle|^2}{E - E_a - \hbar\omega}$$

$$\Gamma_b(E) = \frac{2\pi}{\hbar} \sum_a \sum_{k\varepsilon} |\langle a, k\varepsilon | H_{I,n} | b; 0\rangle|^2\, \delta(E - E_a - \hbar\omega)$$

$$\Rightarrow \quad G_b(E \pm i\eta) = \frac{}{E \pm i\eta - E_b - \hbar\Delta_b(E) \pm i\frac{\hbar}{2}\Gamma_b(E)}$$

Note: $\Delta_b(E) = \frac{1}{2\pi}\, \mathcal{P} \int dE' \frac{\Gamma_b(E')}{E - E'}$

Approximate $E \simeq E_b$ in $\Delta_b(E)$ and $\Gamma_b(E)$:

$$\Delta_b = \Delta_b(E_b) = \frac{1}{\hbar}\, \mathcal{P} \sum_a \sum_{k\varepsilon} \frac{|\langle a, k\varepsilon | H_{I,n} | b; 0\rangle|^2}{E_b - E_a - \hbar\omega}$$

$$\Gamma_b = \Gamma_b(E_b) = \frac{2\pi}{\hbar} \sum_a \sum_{k\varepsilon} |\langle a, k\varepsilon | H_{I,n} | b; 0\rangle|^2\, \delta(E_b - E_a - \hbar\omega)$$

Δ_b: <u>shift</u> ($\rightarrow$ Lamb shift)

Γ_b: broadening due to spont. emission

$$\Rightarrow \quad U_b(\tau) = e^{-i(E_b + \hbar\Delta_b)\tau/\hbar}\, e^{-\Gamma_b|\tau|/2}$$

Similarly:

$$\langle a, \hbar\xi | U(\tau) | b, 0\rangle = \frac{1}{\hbar} \frac{\langle a, \hbar\xi | H_{I} | b, 0\rangle}{\omega - \tilde{\omega}_{ba} + i\Gamma_b/2} e^{-i(\tilde{E}_a + \hbar\omega)\tau/\hbar}$$

$$\tilde{\omega}_{ba} = (\tilde{E}_b - \tilde{E}_a)/\hbar$$

frequency distribution: $\frac{1}{(\omega - \tilde{\omega}_{ba})^2 + \left(\frac{\Gamma_b}{2}\right)^2} \rightarrow$ Lorentzian