Lecture Fys4480, November 24, 2023

$$\Delta E = \lim_{\alpha \to 0} \frac{\langle \Phi_0 | H_1 U_\alpha(0, -\infty) | \Phi_0 \rangle}{\langle \Phi_0 | U_\alpha(0, -\infty) | \Phi_0 \rangle}$$

$$= \lim_{\alpha \to 0} i \left[\frac{\partial}{\partial t} \log \langle \Phi_0 | U_\alpha(t, -\infty) | \Phi_0 \rangle \right]_{t=0}$$

$$\langle \Phi_0 | U_\alpha(0, -\infty) | \Phi_0 \rangle =$$

$$\langle \Phi_0 | 1 + \sum_{n=1}^{\infty} U_n | \Phi_0 \rangle =$$

$$1 + \sum_{n=1}^{\infty} A_n \quad \wedge \quad A_n = \langle \Phi_0 | U_n | \Phi_0 \rangle$$

$$\log \langle \Phi_0 | U_\alpha(t, -\infty) | \Phi_0 \rangle$$

$$= \sum A_n - \frac{1}{2}\left(\sum A_n\right)^2 + \frac{1}{3}\left(\sum A_n\right)^3 + \cdots$$

$$= A_1 + A_2 + A_3 + \cdots - \frac{1}{2}A_1^2 - A_1 A_2$$

$$\cdots + \frac{1}{3}A_1^3 + \cdots$$

$$\Delta E = \underbrace{\Delta E^{(1)}}_{\langle \Phi_0 | H_1 | \Phi_0 \rangle} + \Delta E^{(2)} + \cdots$$

$$\Delta E^{(1)} = \lim_{\alpha \to 0} i \left[\frac{\partial A_1}{\partial t}\right]_{t=0}$$

$$\Delta E^{(2)} = \lim_{\alpha \to 0} i \left[\frac{\partial}{\partial t}\left[A_2 - \frac{1}{2}A_1^2\right]\right]$$

$$A_1 = \langle \Phi_0 | U_1 | \Phi_0 \rangle$$

$$= \langle \Phi_0 | (-i) \int_{-\infty}^{t} H_1(t_1)\, dt_1 | \Phi_0 \rangle$$

$H_1 e^{\alpha t}$

$$\frac{\partial A_1}{\partial t} = -i \langle \Phi_0 | H_1(t) | \Phi_0 \rangle$$

$$\left[\frac{\partial A_1}{\partial t}\right]_{t=0} = -i \langle \Phi_0 | H_1(0) | \Phi_0 \rangle$$

$$= -i \langle \Phi_0 | H_1 | \Phi_0 \rangle \Rightarrow$$

$$\Delta E^{(1)} = \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

Single-particle Green's function

$$\underbrace{H}_{\text{one body } H} |\psi_\alpha(t_0)\rangle = H|\alpha; t_0\rangle = \varepsilon_\alpha |\alpha; t_0\rangle$$

one body state

$$i\hbar \frac{\partial}{\partial t} |\alpha; t\rangle = H|\alpha; t\rangle$$

$$\psi_\alpha(\vec{r}; t) = \langle \vec{r} | \alpha; t\rangle$$

$$= \langle \vec{r} | e^{-iH/\hbar (t-t_0)} | \alpha; t_0\rangle$$

insert complete basis

$$\psi_\alpha(\vec{r};t) = \int d\vec{r}\,' \langle \vec{r} | e^{-i/\hbar\, H(t-t_0)} | \vec{r}\,' \rangle$$

$$\times \underbrace{\langle \vec{r}\,' | \alpha; t_0 \rangle}_{\psi_\alpha(\vec{r}\,'; t_0)}$$

$$= i\hbar \int d\vec{r}\,' \, G(\vec{r}, \vec{r}\,'; t-t_0)\, \psi_\alpha(\vec{r}\,'; t_0)$$

$$G = G(\vec{r}, \vec{r}\,'; t-t_0) = -\frac{i}{\hbar} \langle \vec{r} | e^{-i/\hbar\, H(t-t_0)} | \vec{r}\,' \rangle$$

Alternative to this derivation

$$H|n\rangle = E_n|n\rangle \quad \text{(exact solutions)}$$

$$G(\vec{r},\vec{r}\,';t-t_0) = -\frac{i}{\hbar}\langle 0|a_{\vec{r}}\, e^{-i/\hbar\, H(t-t_0)}\, a^{\dagger}_{\vec{r}\,'}|0\rangle$$

$$= -\frac{i}{\hbar}\sum_n \overbrace{\langle 0|a_{\vec{r}}|n\rangle}^{u_n(\vec{r})}\langle n|a^{\dagger}_{\vec{r}\,'}|0\rangle \times e^{-i/\hbar\, E_n(t-t_0)}$$

$$= -\frac{i}{\hbar}\sum_n u_n(\vec{r})\, u_n^{*}(\vec{r}\,')\, e^{-i/\hbar\, E_n(t-t_0)}$$

To obey causality, we need $t \geq t_0$

To include causality, we introduce $\Theta(t-t_0)$, and to perform a Fourier Transform (FT), we need

$$G(t-t_0) = -\frac{1}{2\pi i}\int dE' \frac{e^{-i/\hbar\, E'(t-t_0)}}{E'+i\eta}$$

$\eta \to 0^+$

$t > t_0$, integration closing the lower half plane the contrib. from the enclosed pole gives

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For $t < t_0$, upper half plane gives zero contribution,

$t > t_0$, the step function jumps from zero to one,

$$\frac{d}{dt} G(t-t_0) = \delta(t-t_0)$$

The FT of $G(\vec{r},\vec{r}\,';t-t_0)$

$$G(\vec{r},\vec{r}\,';E) = \sum_n \frac{u_n(\vec{r})\,u_n^*(\vec{r}\,')}{E-E_n+i\eta}$$

$$= \sum_n \frac{\langle 0 | a_{\vec{r}} | n \rangle \langle n | a^\dagger_{\vec{r}'} | 0 \rangle}{E - E_n + i\eta}$$

$\uparrow$ exact energies

$$= \langle 0 | a_{\vec{r}} \frac{1}{E - H + i\eta} a^\dagger_{\vec{r}'} | 0 \rangle$$

$$= \langle \vec{r} | \frac{1}{E - H + i\eta} | \vec{r}' \rangle$$

$$A = E - H_0 + i\eta \qquad B = H_I$$

$$[H_0, H_I] \neq 0 \qquad [A, B] \neq 0$$

Example: $H_0 = T$ (kinetic energy)

$H_1 = V$

$$\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A} B \frac{1}{A-B}$$

$$G = \frac{1}{E - \underbrace{H_0 - H_1}_{H} + i\eta} = \frac{1}{A-B}$$

$$G^{(0)} = \frac{1}{A} = \frac{1}{E - H_0 + i\eta}$$

$$G = \frac{1}{A - B} = \frac{1}{A} + \frac{1}{A} B \frac{1}{A - B}$$

$$= G^{(0)} + G^{(0)} H_I G$$

$$= G^{(0)} + G^{(0)} H_1 G^{(0)} +$$

$$G^{(0)} H_1 G^{(0)} H_1 G^{(0)} + \cdots$$

$$G^{(0)} = \langle 0 | a_\alpha \frac{1}{E - H_0 + i\eta} a_\beta^\dagger | 0 \rangle$$

$$= G^{(0)}(\alpha, \beta; E)$$

$$G^{(0)} = \langle \alpha | \frac{1}{E - H_0 + i\eta} | \beta \rangle$$

$$H_0 |\beta\rangle$$

$$\varepsilon_\beta |\beta\rangle$$

$$G = \langle \alpha | \frac{1}{E - H + i\eta} | \beta \rangle$$

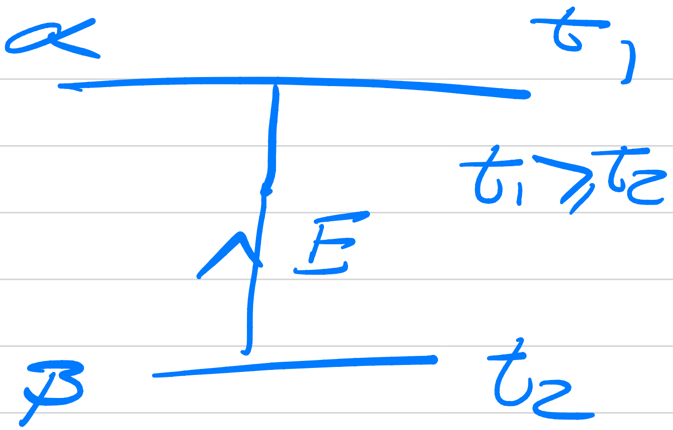
$$= \langle \alpha | \frac{1}{E - H_0 + i\eta} | \beta \rangle$$

$$+ \sum_{\gamma\delta} \langle \alpha | \frac{1}{E - H_0 + i\eta} | \gamma \rangle \langle \gamma | H_1 | \delta \rangle$$

$$\times \langle \delta | \frac{1}{E - H + i\eta} | \beta \rangle$$

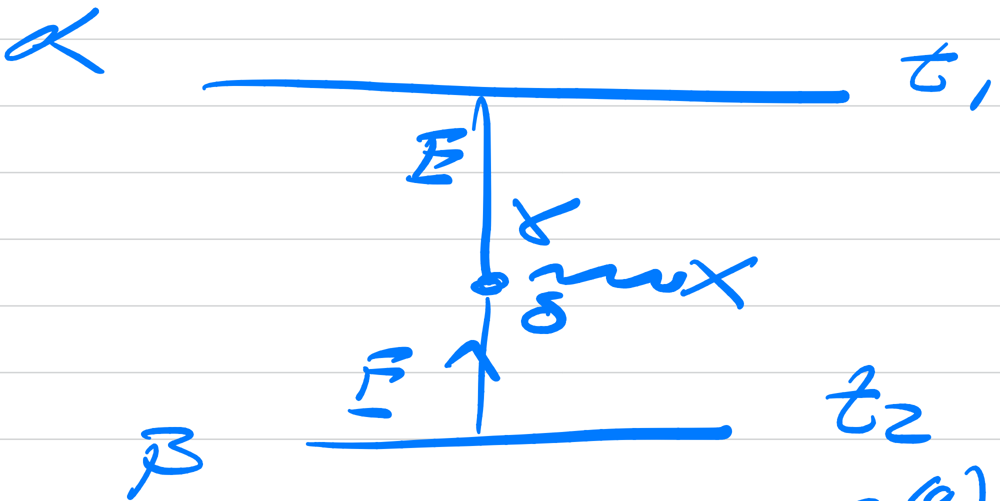
$$G^{(0)} = \frac{\delta_{\alpha\beta}}{E - \varepsilon_\alpha + i\eta}$$

$G^{(0)}$ graphically



$G^{(0)}(\alpha,\beta;E)$

A 2nd order term



$$\sum_{\gamma\delta} G^{(0)}(\alpha,\gamma;E)\langle\gamma|H_1|\delta\rangle \times G^{(0)}(\delta,\beta;E)$$

$$G = G^{(0)} + G^{(0)} H_1 G^{(0)} + G^{(0)} H_1 G^{(0)} H_1 G^{(0)} + \cdots$$

$$= G^{(0)} + G^{(0)} H_1 \left(G^{(0)} + G^{(0)} H_1 G^{(0)} + \cdots \right)$$

$$= G^{(0)} + G H_1 G^{(0)}$$

$$= G^{(0)} + \left\{ G^{(0)} + G^{(0)} H_1 G^{(0)} + \cdots \right\} H_1 G^{(0)}$$

$$= G^{(0)} + G H_1 G^{(0)}$$

$$= G^{(0)} + G^{(0)} \left\{ H_1 + H_1 G^{(0)} H_1 + \cdots \right\} \times G^{(0)}$$

Define T-matrix (effective interaction $\tilde{H}_1$)

$$T = H_1 + H_1 G^{(0)} H_1 + \cdots$$

$$G = G^{(0)} + G^{(0)} T(E) G^{(0)}$$

$$T = H_1 + H_1 G^{(0)} \{ H_1 + H_1 G^{(0)} H_1 + \cdots \}$$

$$= H_1 + H_1 G^{(0)} T =$$

$$H_1 + H_1 G H_1$$

Example : $H_0 = K$

$$K|k\rangle = \frac{k^2}{2m}|k\rangle$$

$$\hbar = c = \underline{1}$$

$H_1 = V$ (no E-dep)

$$\langle k_1|T(E)|k_2\rangle = \langle k_1|V|k_2\rangle$$

$$+ \int dk \; \frac{\langle k_1|V|k\rangle\langle k|T|k_2\rangle}{E - \frac{k^2}{2m} + i\eta}$$

$$G^{(c)}$$

numerical digression

$$k \in [0, \infty) \longrightarrow k = \{k_0, k_1, k_2 \ldots k_n\}$$

$$\langle k_i | T | k_j \rangle = T_{ij}$$

$$\langle k_i | V | k_j \rangle = V_{ij}$$

$$\frac{|k\rangle\langle k| \, dk}{E - \frac{k^2}{2m} + i\eta} \Longrightarrow D_{jj} = \frac{w_j}{E - \frac{k_j^2}{2m} + i\eta}$$

$$T_{ij} = V_{ij} + \sum_k V_{ik} D_{kk} T_{kj}$$

$$T = V + V \cdot D \cdot T \Longrightarrow$$

$$T = \frac{1}{1 - VD} V$$

Step towards Dyson's equation

Heisenberg picture

$$a_\alpha(t) = e^{i/\hbar H t} a_\alpha e^{-i/\hbar H t}$$

Schrödinger picture

$$a_\alpha^+(t) = e^{i/\hbar H t} a_\alpha^+ e^{-i/\hbar H t}$$

$$H|\Psi_0\rangle = E_0 |\Psi_0\rangle$$

$$H|\Psi_i\rangle = E_i |\Psi_0\rangle$$

$|\Psi_0\rangle$ can be a single-particle or many-body state.

Time-ordered product

$$T\left[a_\alpha(t)\, a_\beta^\dagger(t')\right] =$$

$$\Theta(t-t')\, a_\alpha(t)\, a_\beta^\dagger(t')$$

$$- \Theta(t'-t)\, a_\beta^\dagger(t')\, a_\alpha(t)$$

$$G(\alpha, \beta; t, t') =$$

$$-\frac{i}{\hbar} \langle \Psi_0 | T\left[a_\alpha(t)\, a_\beta^\dagger(t')\right] | \Psi_0 \rangle$$