Green's function formalism

"Zoo" of methods.

[van Leeuwen, Stefanucci, non-equilibrium many body theory of quantum systems]

(Chap 4, "the contour idea")

1) zero temperature. adiabatic. (Gellmann-Low)

2) zero temperature limit. ($\beta \to \infty$).

3) finite temperature, real time (β finite)

4) finite temperature, imag time (β finite, Matsubara)

5) Non-equilibrium. (Keldysh).

pick 4). Simplicity. 2nd quantization.

Partition function.

$$Z = \mathrm{Tr}\left[e^{-\beta(\hat{H} - \mu \hat{N})} \right]$$

$$N = \mathrm{Tr}\left[\hat{N} e^{-\beta(\hat{H} - \mu \hat{N})} \right] / Z \rightarrow \text{fix } \mu$$

$$\hat{H} = \hat{H}_0 + \frac{1}{2} \hat{V}$$

Interaction picture

$$\hat{V}_I(\tau) = e^{\tau(\hat{H}_0 - \mu\hat{N})}\,\hat{V}\,e^{-\tau(\hat{H}_0 - \mu\hat{N})}$$

$$\mathcal{T}\left[\hat{V}_I(\tau_1)\,\hat{V}_I(\tau_2)\right] = \begin{cases} \hat{V}_I(\tau_1)\,\hat{V}_I(\tau_2), & \tau_1 \geq \tau_2 \\ +\,\hat{V}_I(\tau_2)\,\hat{V}_I(\tau_1), & \tau_1 < \tau_2 \end{cases}$$

$$Z = \mathrm{Tr}\left[e^{-\beta(\hat{H}_0 + \frac{1}{2}\hat{V} - \mu\hat{N})}\right]$$

$$\overset{\text{exer}}{=} \mathrm{Tr}\left[e^{-\beta(\hat{H}_0 - \mu\hat{N})}\,\mathcal{T}\left[e^{-\frac{1}{2}\int_0^\beta \hat{V}_I(\tau)\,d\tau}\right]\right]$$

$$= \sum_{n=0}^{\infty} \frac{1}{2^n n!} \mathrm{Tr}\left[e^{-\beta(\hat{H}_0 - \mu \hat{N})} \mathcal{T} \int_0^{\beta} \cdots \int_0^{\beta} (-V_I(\tau_1)) \cdots (-V_I(\tau_n)) \, d\tau_1 \cdots d\tau_n \right]$$

How to compute

$$\mathrm{Tr}\left[e^{-\beta \underbrace{(\hat{H}_0 - \mu \hat{N})}_{\text{quadratic}}} \underbrace{\hat{V}_I(\tau_1) \cdots \hat{V}_I(\tau_n)}_{\sim 4n \text{ order polynomial.}} \right] ?$$

Creation/annihilation operators in the interaction picture

$$c_p^+(\tau) = e^{\tau(\hat{H}_0 - \mu\hat{N})} c_p^+ e^{-\tau(\hat{H}_0 - \mu\hat{N})}$$

$$c_p(\tau) = e^{\tau(\hat{H}_0 - \mu\hat{N})} c_p e^{-\tau(\hat{H}_0 - \mu\hat{N})}$$

$$c_p^+(\tau) \neq [c_p(\tau)]^+ \; !$$

Green's Function

$$G^0(p,\tau;p',\tau') := -\frac{1}{Z}\mathrm{Tr}\left[e^{-\beta(\hat{H}_0-\mu\hat{N})}\mathcal{T}\left[c_p(\tau)c^{\dagger}_{p'}(\tau')\right]\right]$$

$$:= -\left\langle \mathcal{T}\left[c_p(\tau)c^{\dagger}_{p'}(\tau')\right]\right\rangle_0$$

$$\mathcal{T}\left[A(\tau_1)A(\tau_2)\right] = \begin{cases} A(\tau_1)A(\tau_2), & \tau_1 > \tau_2 \\ -A(\tau_2)A(\tau_1), & \tau_1 < \tau_2 \end{cases}$$

$A(\tau) = c^{\dagger}_p(\tau)$ or $c_p(\tau)$

$$T\left[c_p(\tau)\, c_q^\dagger(\tau)\right] = -\, c_q^\dagger(\tau)\, c_p(\tau)$$

$$= -\, T\left[c_q^\dagger(\tau)\, c_p(\tau)\right]$$

exer : Def of T agree w. def of T

for $\hat{V}_I(\tau)$

$$G^0(p,\tau\,;\,p',\tau') := G^0_{pp'}(\tau-\tau')$$

$$\hat{V} = \sum_{pqrs} V_{pqrs}\, c_p^\dagger c_q^\dagger c_s c_r$$

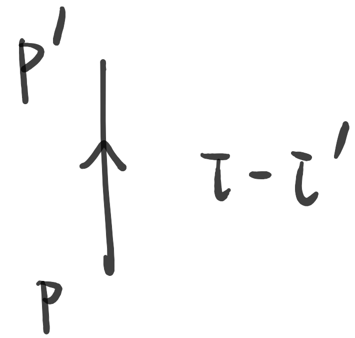
exer. $\hat{V}_I(\tau) = \sum_{pqrs} V_{pqrs}\, c_p^\dagger(\tau)\, c_q^\dagger(\tau)\, c_s(\tau)\, c_r(\tau)$

Remark: to remove ambiguity for $\tau_1 = \tau_2$.

often written as

$$\hat{V}_I(\tau) = \sum_{pqrs} V_{pqrs}\, c_p^\dagger(\tau_+)\, c_q^\dagger(\tau_+)\, c_s(\tau)\, c_r(\tau)$$

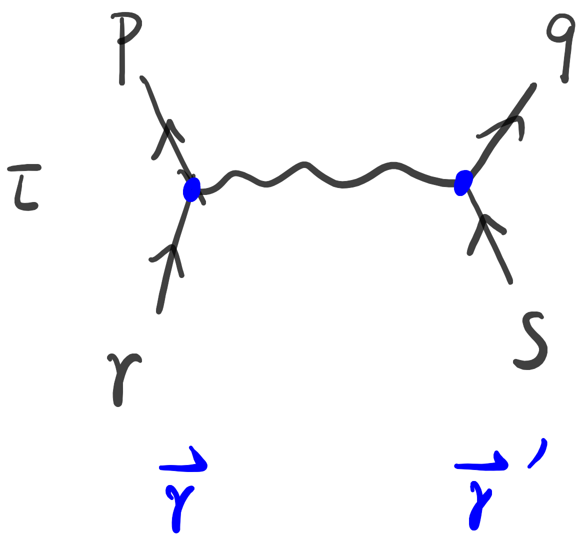
Graphical representation.



$$G^{0}_{pp'}(\tau-\tau')$$

in: annihilation

out: creation



$$\hat{V}_I(\tau)$$

Wick theorem

$$\langle T[\, c_{p_1}(\tau_1)\cdots c_{p_n}(\tau_n)\, c^{\dagger}_{p'_n}(\tau'_n)\cdots c^{\dagger}_{p'_1}(\tau'_1)]\rangle_0$$

$$= \sum_{\pi \in \mathrm{Sym}(n)} (-1)^{\pi} \prod_i \langle T[\, c_{p_i}(\tau_i)\, c^{\dagger}_{p'_{\sigma(i)}}(\tau'_{\sigma(i)})]\rangle$$

$$= (-1)^{m} \begin{vmatrix} G^{0}_{p_1 p'_1}(\tau_1-\tau'_1) & \cdots & G^{0}_{p_1 p'_n}(\tau_1-\tau'_n) \\ \vdots & & \vdots \\ G^{0}_{p_n p_1}(\tau_n-\tau'_1) & \cdots & G^{0}_{p_n p'_n}(\tau_n-\tau'_n) \end{vmatrix}$$

First order to Z

$$-\frac{1}{2}\int_0^\beta \sum_{pqrs} V_{pqrs} \langle c_p^\dagger(\tau) c_q^\dagger(\tau) c_s(\tau) c_r(\tau) \rangle_0 \, d\tau$$

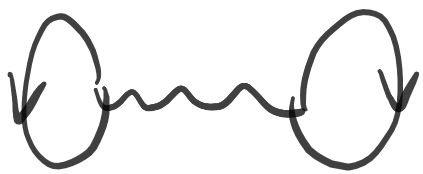
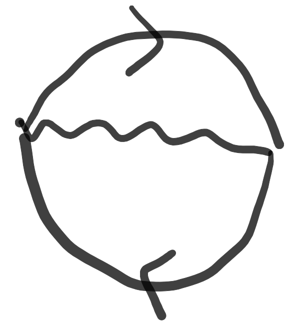
$$= -\frac{1}{2}\int_0^\beta \sum_{pqrs} V_{pqrs} \Big[\langle c_p^\dagger(\tau) c_r(\tau) \rangle_0 \langle c_q^\dagger(\tau) c_s(\tau) \rangle_0$$

$$- \langle c_p^\dagger(\tau) c_s(\tau) \rangle_0 \langle c_q^\dagger(\tau) c_r(\tau) \rangle_0 \Big]$$

$$= \frac{\beta}{2} \sum_{pqrs} (-V_{pqrs}) \Big(G^0_{pr}(0_-) G^0_{qs}(0_-)$$

$$- G^0_{ps}(0_-) G^0_{qr}(0_-) \Big)$$

graphical.

 − 

Hartree "Dumbbell".

Fock "Oyster"

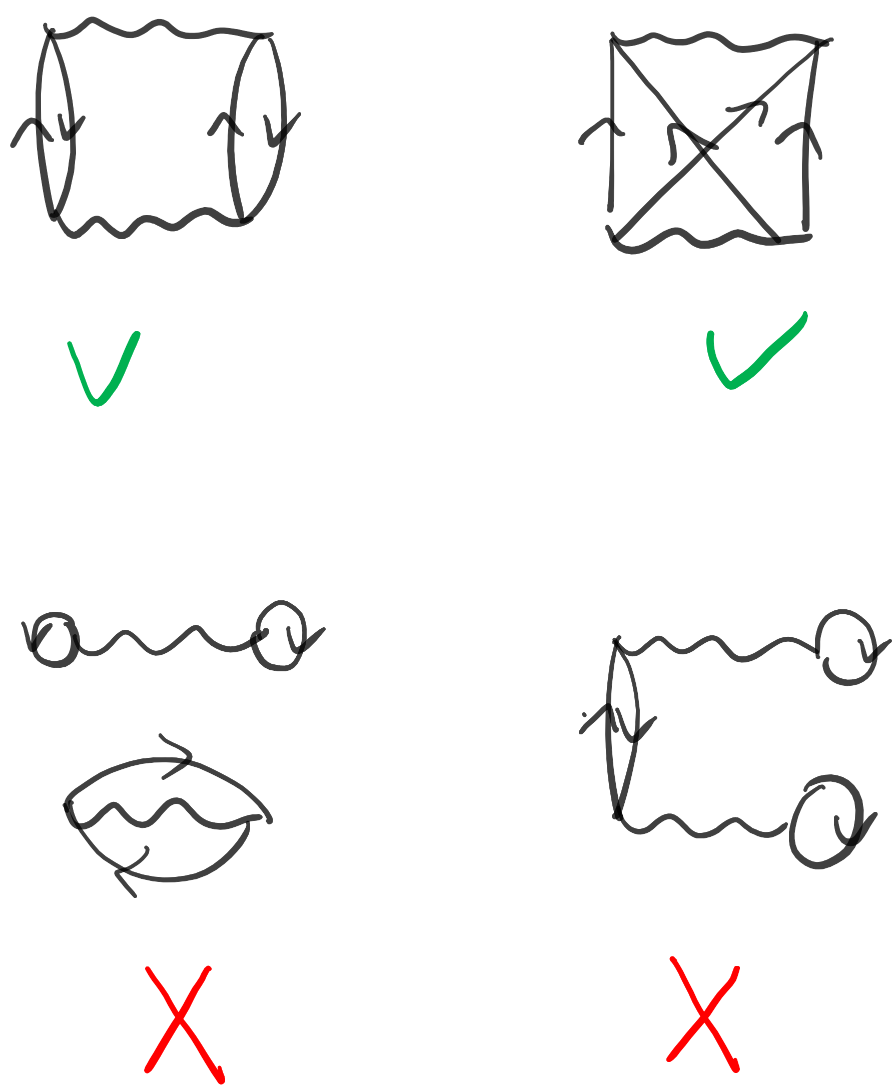
2nd order

$$\frac{1}{2^2 2!} \int_0^\beta \int_0^\beta \sum_{\substack{p_1 q_1 r_1 s_1 \\ p_2 q_2 r_2 s_2}} V_{p_1 q_1 r_1 s_1} V_{p_2 q_2 r_2 s_2}$$

$$\langle T [c^\dagger_{p_1}(\tau_1) c^\dagger_{q_1}(\tau_1) c_{s_1}(\tau_1) c_r(\tau_1) c^\dagger_{p_2}(\tau_2) c^\dagger_{q_2}(\tau_2)$$

$$c_{s_2}(\tau_2) \; c_{r_2}(\tau_2)] \rangle_0$$

Some diagrams.



"trivial" information

Green's function formulation (Feynman diagrams)

1) Z. partition function

2) $\Omega = -\log Z$. free energy

3) G. Green's function

4) Σ. self energy

5) Bold diagram. renormalize G.

6) renormalize interaction. GW etc.

7) 2-particle Green's function. BSE etc.

8) zero temperature. non-equilibrium etc.

Gibbs measure setting

(Euclidean lattice field theory)

$$Z = \int_{\mathbb{R}^d} e^{-\frac{1}{2}x^T A x - U(x)} dx$$

$A \in \mathbb{R}^{d\times d}$. $A = A^T$.

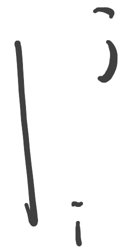
$$U(x) = \frac{1}{2^2 2!} \sum_{ij} v_{ij} x_i^2 x_j^2$$

Feynman diagram.

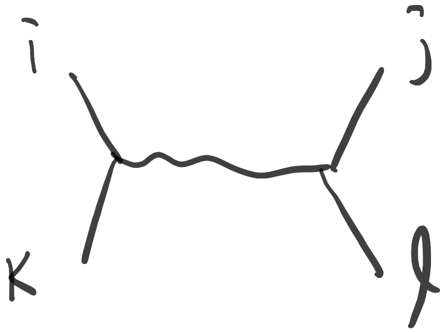
$$Z^0 = \int_{\mathbb{R}^d} e^{-\frac{1}{2}x^T A x}\, dx. \qquad \text{require } A \text{ P.D.}$$

$$G^0_{ij} = \frac{1}{Z^0} \int_{\mathbb{R}^d} x_i x_j e^{-\frac{1}{2}x^T A x}\, dx = (A^{-1})_{ij}$$

$$G_{ij} = \frac{1}{Z} \int_{\mathbb{R}^d} x_i\, x_j\, e^{-\frac{1}{2}x^T A x - U(x)}\, dx$$



G^{0}_{ij}



$-V_{ij}\,\delta_{ik}\,\delta_{jl}.$

reproduce structural information of Feynman diagrams in electronic structure.

[Lin, Lindsey. 1809.02900]