Quantum Theory of Many-Body systems in Condensed Matter (4302112) 2020

Prof. Luis Gregório Dias
luisdias@if.usp.br

Today's class: *Time-ordered Green's functions and Wick's theorem*

- Time-ordered Green's functions.
- Gell-Mann and Low theorem.
- Perturbation theory (e.g. the interaction).
- Wick's theorem.

Time-ordered Green's functions (T=0)

$$\mathcal{G}(\vec{r},t;\vec{r}\,',t') = -i\left\langle \mathcal{T}\left[\hat{\psi}(\vec{r},t)\hat{\psi}^{\dagger}(\vec{r}\,',t')\right]\right\rangle_0$$

$$\hat{\psi}(\vec{r},t) = e^{+i\hat{H}t}\hat{\psi}(\vec{r})e^{-i\hat{H}t}$$

Heisenberg

- Time ordering operator: $\mathcal{T}\left[\hat{a}_k(t)\hat{a}^{\dagger}_{k'}(t')\right] = \begin{cases} \hat{a}_k(t)\hat{a}^{\dagger}_{k'}(t') \text{ if } t > t' \\ \pm\hat{a}^{\dagger}_{k'}(t')\hat{a}_k(t) \text{ if } t' > t \end{cases}$

+: Bosons -: Fermions

Connection with other Green's functions.

$$\begin{cases} \mathcal{G}(\vec{r},\vec{r}\,';t>t') = -i\left\langle \hat{\psi}(\vec{r},t)\hat{\psi}^{\dagger}(\vec{r}\,',t')\right\rangle_0 = G^{>}(\vec{r},t;\vec{r}\,',t') \\ \mathcal{G}(\vec{r},\vec{r}\,';t<t') = -i(\pm 1)\left\langle \hat{\psi}^{\dagger}(\vec{r}\,',t')\hat{\psi}(\vec{r},t)\right\rangle_0 = G^{<}(\vec{r},t;\vec{r}\,',t') \end{cases}$$

"Greater":

"Lesser":

Lehmann Representation (T=0)

Many-particle spectrum:

$$\hat{H}|\alpha\rangle = E_\alpha|\alpha\rangle$$
$$E_0 = 0$$

Matrix elements:

$$\langle\alpha'|\hat{a}_k^\dagger|\alpha\rangle = \left(\langle\alpha|\hat{a}_k|\alpha'\rangle\right)^\dagger$$

We can write a GF as:

$$G_{km}^{>}(t,t') = \frac{-i}{Z}\sum_\alpha \langle 0|\hat{a}_k|\alpha\rangle\langle\alpha|\hat{a}_m^\dagger|0\rangle e^{-iE_\alpha(t-t')}$$

In frequency:

$$G_{km}^{>}(\omega) = -i\frac{2\pi}{Z}\sum_\alpha \langle 0|\hat{a}_k|\alpha\rangle\langle\alpha|\hat{a}_m^\dagger|0\rangle\delta\left(\omega - E_\alpha\right)$$

Lehmann Representation (T=0)

Lehmman Representation for the retarded/advanced GF:

$$\begin{cases} G^R_{km}(t,t') = \theta(t-t')\left(G^>_{km}(t,t') - G^<_{km}(t,t')\right) \\ G^A_{kk'}(t,t') = \theta(t'-t)\left(G^<_{kk'}(t,t') - G^>_{kk'}(t,t')\right) \end{cases}$$

In frequency:

$$G^{R,A}_{km}(\omega^+) = \frac{1}{Z}\sum_\alpha \left[\frac{\langle 0|\hat{a}_k|\alpha\rangle\langle\alpha|\hat{a}^\dagger_m|0\rangle}{\omega \pm i\eta - E_\alpha} + \frac{\langle 0|\hat{a}^\dagger_m|\alpha\rangle\langle\alpha|\hat{a}_k|0\rangle}{\omega \pm i\eta + E_\alpha}\right]$$

Assignment: show that

$$\mathcal{G}_{km}(\omega^+) = \frac{1}{Z}\sum_\alpha \left[\frac{\langle 0|\hat{a}_k|\alpha\rangle\langle\alpha|\hat{a}^\dagger_m|0\rangle}{\omega + i\eta - E_\alpha} + \frac{\langle 0|\hat{a}^\dagger_m|\alpha\rangle\langle\alpha|\hat{a}_k|0\rangle}{\omega - i\eta + E_\alpha}\right]$$

Why use the time-ordered GF?

It is very appropriate for perturbation theory :

$$\begin{cases} \hat{H} = \hat{H}_0 + \hat{H}_1 \\ \hat{H}_0|\Phi_0\rangle = E_0|\Phi_0\rangle \end{cases}$$

$$i\mathcal{G}_{km}(t,t') = \frac{\langle\Phi_0|\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{+\infty}dt_1\ldots dt_n\mathcal{T}\left[\hat{H}_1(t_1)\ \ldots\hat{H}_1(t_n)(\hat{a}_k)_I(t)(\hat{a}_m^{\dagger})_I(t')\right]|\Phi_0\rangle}{\langle\Phi_0|\hat{U}(+\infty,-\infty)|\Phi_0\rangle}$$

which relates expected values of operators in Heisenberg and interaction pictures.

$$\hat{\mathcal{O}}_H(t) \equiv e^{+i\hat{H}t}\hat{\mathcal{O}}_S e^{-i\hat{H}t} \qquad \hat{\mathcal{O}}_I(t) \equiv e^{+i\hat{H}_0 t}\hat{\mathcal{O}}_S e^{-i\hat{H}_0 t}$$

$$\hat{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t}\hat{H}_1(t_1)\,dt_1 + \left(\frac{-i}{\hbar}\right)^2\frac{1}{2}\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\mathcal{T}\left[\hat{H}_1(t_1)\,\hat{H}_1(t_2)\right] + \ldots$$

Adiabatic “switching on”

Perturbation “turned on” at t = -∞: $\hat{H}_{\eta t} = \hat{H}_0 + e^{-\eta|t|}\hat{H}_1$

Interaction picture:

$$|\psi_I(t)\rangle = \hat{U}_\eta(t,t_0)|\psi_I(t_0)\rangle \qquad |\psi_I(t)\rangle \equiv e^{+i\hat{H}_0 t/\hbar}|\psi_S(t)\rangle$$

$$\hat{U}_\eta(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t} e^{-\eta|t_1|}\hat{H}_1(t_1)\,dt_1 + \left(\frac{-i}{\hbar}\right)^2 \frac{1}{2}\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 e^{-\eta(|t_1|+|t_2|)}\mathcal{T}\left[\hat{H}_1(t_1)\,\hat{H}_1(t_2)\right] + \ldots$$

At t=0:

$$|\psi_I(0)\rangle = |\psi_S(0)\rangle = \hat{U}_\eta(0,-\infty)|\Phi_0\rangle$$

$$\hat{H}_0|\Phi_0\rangle = E_0|\Phi_0\rangle$$

Gell-Mann and Low theorem

If we can define the quantity:

$$\lim_{\eta\to 0} \frac{\hat{U}_\eta(0,-\infty)|\Phi_0\rangle}{\langle\Phi_0|\hat{U}_\eta(0,-\infty)|\Phi_0\rangle} \equiv \frac{|\Psi\rangle}{\langle\Phi_0|\Psi\rangle}$$

in all orders of perturbation theory,

then:

$$\hat{H}\frac{|\Psi\rangle}{\langle\Phi_0|\Psi\rangle} = E\frac{|\Psi\rangle}{\langle\Phi_0|\Psi\rangle}$$

with $\hat{H} = \hat{H}_0 + \hat{H}_1$

i.e., it's an *eigenstate* of H (but not necessarily the GS!)

M. Gell-Mann and F. Low, *Phys. Rev.* **84** 350 (1951).
(for a full proof: Fetter & Walecka, Cap 3 Sec 6)

Important corolary

From the G&L theorem, one can show the following property:

$$\frac{\langle\Psi|\mathcal{T}\left[\hat{\mathcal{O}}_H(t)\hat{\mathcal{O}}_H(t')\right]|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Phi_0|\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{+\infty}dt_1\ldots dt_n\mathcal{T}\left[\hat{H}_1(t_1)\;\ldots\hat{H}_1(t_n)\hat{\mathcal{O}}_I(t)\hat{\mathcal{O}}_I(t')\right]|\Phi_0\rangle}{\langle\Phi_0|\hat{U}(+\infty,-\infty)|\Phi_0\rangle}$$

which relates expected values of operators in Heisenberg and interaction pictures.

$$\hat{\mathcal{O}}_H(t) \equiv e^{+i\hat{H}t}\hat{\mathcal{O}}_S e^{-i\hat{H}t} \qquad \hat{\mathcal{O}}_I(t) \equiv e^{+i\hat{H}_0 t}\hat{\mathcal{O}}_S e^{-i\hat{H}_0 t}$$

$$\hat{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t}\hat{H}_1(t_1)\,dt_1 + \left(\frac{-i}{\hbar}\right)^2\frac{1}{2}\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\mathcal{T}\left[\hat{H}_1(t_1)\,\hat{H}_1(t_2)\right] + \ldots$$

(for a full proof: Fetter & Walecka, Cap 3 Sec 8)

Example: quartic terms

Perturbation theory in the interaction:

$$i\mathcal{G}_{km}(t,t') = \frac{\langle\Phi_0|\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{+\infty}dt_1\ldots dt_n\mathcal{T}\left[\hat{H}_1(t_1)\ \ldots\hat{H}_1(t_n)(\hat{a}_k)_I(t)(\hat{a}_m^{\dagger})_I(t')\right]|\Phi_0\rangle}{\langle\Phi_0|\hat{U}(+\infty,-\infty)|\Phi_0\rangle}$$

[redacted]

$$\begin{cases} \hat{H}_0 = \sum_{k} \epsilon_k \hat{a}_k^{\dagger}\hat{a}_k \\ \hat{H}_1 = \sum_{\substack{km \\ k'm'}} U_{\substack{km \\ k'm'}} \hat{a}_k^{\dagger}\hat{a}_m^{\dagger}\hat{a}_{m'}\hat{a}_{k'} \end{cases}$$

$$\hat{H}_0|\Phi_0\rangle = E_0|\Phi_0\rangle$$

$$\hat{U}(t,t_0) = \mathbb{1} - \frac{i}{\hbar}\int_{t_0}^{t}\hat{H}_1(t_1)\,dt_1 + \left(\frac{-i}{\hbar}\right)^2\frac{1}{2}\int_{t_0}^{t}dt_1\int_{t_0}^{t}dt_2\mathcal{T}\left[\hat{H}_1(t_1)\ \hat{H}_1(t_2)\right] + \ldots$$