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

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Today’s class: *Time-ordered Green’s functions*

- Single-particle Green’s functions.
- Retarded and advanced Green’s functions.
- Many-particle Green’s functions
- Lehmann representation.

Single-particle GFs: time-independent

- Great intro to Green's functions : https://arxiv.org/abs/1604.02499

Time-independent Schrödinger's equation:

$$\begin{cases} \left(E - \hat{H}\right)\psi_E(\vec{r}) = 0 \\ \left(E - \hat{H}_0\right)\psi_E^{(0)}(\vec{r}) = 0 \end{cases}$$

$$\hat{H} = \hat{H}_0 + \hat{V}$$

Associated GFs:

$$\begin{cases} \left(E - \hat{H}\right) G(\vec{r}, \vec{r}\,'; E) = \delta(\vec{r} - \vec{r}\,') \\ \left(E - \hat{H}_0\right) G_0(\vec{r}, \vec{r}\,'; E) = \delta(\vec{r} - \vec{r}\,') \end{cases}$$

Formally:

$$\begin{cases} G^{-1}(\vec{r}; E) = \left(E - \hat{H}\right) \\ (G_0)^{-1}(\vec{r}; E) = \left(E - \hat{H}_0\right) \end{cases} \Rightarrow \begin{cases} G^{-1}(\vec{r}; E)\psi_E(\vec{r}) = 0 \\ (G_0)^{-1}(\vec{r}; E)\psi_E^{(0)}(\vec{r}) = 0 \end{cases}$$

Single-particle GFs: time-independent

Integral equation (if we know G_0) (Lippmann-Schwinger):

$$\psi_E(\vec{r}) = \psi_E^{(0)}(\vec{r}) + \int d\vec{r}\,'\; G_0(\vec{r}, \vec{r}\,'; E) V(\vec{r}\,') \psi_E(\vec{r}\,')$$

Also (formally):

$$\psi_E(\vec{r}) = \psi_E^{(0)}(\vec{r}) + \int d\vec{r}\,'\; G(\vec{r}, \vec{r}\,'; E) V(\vec{r}\,') \psi_E^{(0)}(\vec{r}\,')$$

Integral equation for G (if we know G_0) (Dyson's equation):

$$G(\vec{r}, \vec{r}\,'; E) = G_0(\vec{r}, \vec{r}\,'; E) + \int d\vec{r}_1\; G_0(\vec{r}, \vec{r}_1; E) V(\vec{r}_1) G(\vec{r}_1, \vec{r}\,'; E)$$

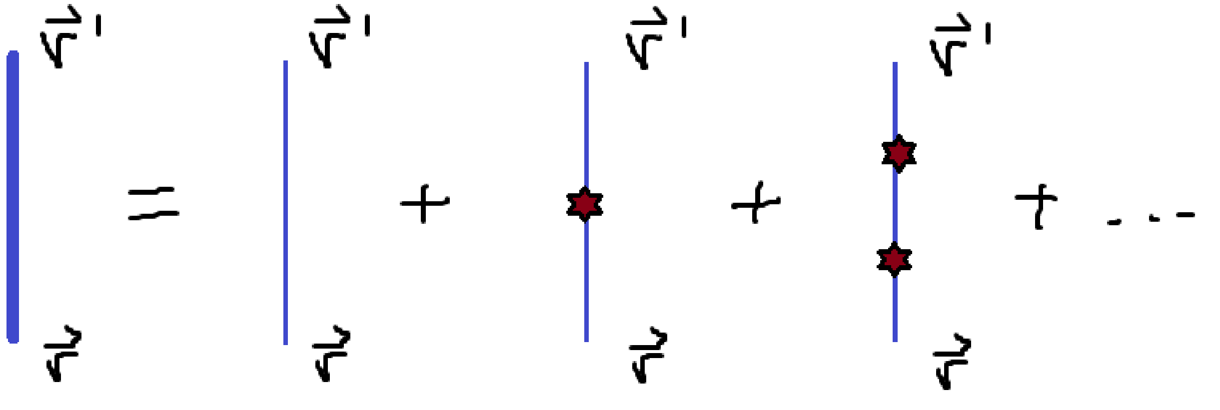
"Pictoric view" :Diagrams!

Single-particle GFs: time-independent

$$G(\vec{r},\vec{r}\,';E) = G_0(\vec{r},\vec{r}\,';E) + \int d\vec{r}_1\; G_0(\vec{r},\vec{r}_1;E)V(\vec{r}_1)G(\vec{r}_1,\vec{r}\,';E)$$

$$G = G_0 + G_0\,VG$$

$$G = G_0 + G_0\,VG_0 + G_0\,VG_0\,VG_0 + \ldots$$



"Pictoric view" :Diagrams!

Single-particle GFs: time-dependent

Time-dependent Schrödinger's equation:

$$\begin{cases} \left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) \psi(\vec{r}, t) = 0 \\ \left(i\hbar \frac{\partial}{\partial t} - \hat{H}_0 \right) \psi^{(0)}(\vec{r}, t) = 0 \end{cases}$$

$$\hat{H} = \hat{H}_0 + \hat{V}$$

Associated GFs:

$$\begin{cases} \left(i\hbar \frac{\partial}{\partial t} - \hat{H} \right) G(\vec{r}, t; \vec{r}\,', t') = \delta(\vec{r} - \vec{r}\,')\delta(t - t') \\ \left(i\hbar \frac{\partial}{\partial t} - \hat{H}_0 \right) G_0(\vec{r}, t; \vec{r}\,', t') = \delta(\vec{r} - \vec{r}\,')\delta(t - t') \end{cases}$$

Integral equations:

$$\psi(\vec{r}, t) = \psi^{(0)}(\vec{r}, t) + \int d\vec{r}\,' \int dt' \; G_0(\vec{r}, t; \vec{r}\,', t') V(\vec{r}\,') \psi(\vec{r}\,', t')$$

$$\psi(\vec{r}, t) = \psi^{(0)}(\vec{r}, t) + \int d\vec{r}\,' \int dt' \; G(\vec{r}, t; \vec{r}\,', t') V(\vec{r}\,') \psi^{(0)}(\vec{r}\,', t')$$

Retarded GF: propagator

t $\neq$ t'

Notice that: $$\psi(\vec{r},t) = \int d\vec{r}\,'\; G(\vec{r},t;\vec{r}\,',t')\psi(\vec{r}\,',t')$$ [redacted]

satisfies $$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)\psi(\vec{r},t) = 0$$

"Propagator":
(Retarded)

$$G^R(\vec{r},t;\vec{r}\,',t') = \theta(t-t')G(\vec{r},t;\vec{r}\,',t')$$

t > t'

also: $$G^R(\vec{r},t;\vec{r}\,',t') = -i\theta(t-t')\langle\vec{r}|e^{-i\hat{H}(t-t')}|\vec{r}\,'\rangle \qquad \hbar \equiv 1$$

satisfies
: $$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)G^R(\vec{r},t;\vec{r}\,',t') = \delta(\vec{r}-\vec{r}\,')\delta(t-t')$$ (Show!)

In general: $$G^R(n,t;n',t') = -i\theta(t-t')\langle n|e^{-i\hat{H}(t-t')}|n'\rangle$$

Many-particle GFs: time-ordered

Many-particle propagator:

$$G^R(\vec{r},t;\vec{r}\,',t') = -i\theta(t-t')\left\langle\left[\hat{\psi}(\vec{r},t),\hat{\psi}^\dagger(\vec{r}\,',t')\right]_{\mp}\right\rangle$$

$$\langle\ldots\rangle = \frac{1}{Z}\mathrm{Tr}\ (\hat{\rho}\ldots)$$

field operators

-: Bosons

+: Fermions

Other definitions:

Advanced:

$$G^A(\vec{r},t;\vec{r}\,',t') = +i\theta(t'-t)\left\langle\left[\hat{\psi}(\vec{r},t),\hat{\psi}^\dagger(\vec{r}\,',t')\right]_{\mp}\right\rangle$$

“Greater”:

$$G^>(\vec{r},t;\vec{r}\,',t') = -i\left\langle\hat{\psi}(\vec{r},t)\hat{\psi}^\dagger(\vec{r}\,',t')\right\rangle$$

“Lesser”:

$$G^<(\vec{r},t;\vec{r}\,',t') = -i(\pm 1)\left\langle\hat{\psi}^\dagger(\vec{r}\,',t')\hat{\psi}(\vec{r},t)\right\rangle$$

+: Bosons

-: Fermions

Change of basis

$$\hat{a}_k^\dagger|0\rangle = |k\rangle \qquad \hat{\psi}^\dagger(\vec{r}) = \sum_k \left(\langle\vec{r}|k\rangle\right)^* \hat{a}_k^\dagger \qquad \hat{\psi}(\vec{r}) = \sum_k \langle\vec{r}|k\rangle \hat{a}_k$$

$$\Rightarrow \quad G^R(\vec{r},t;\vec{r}\,',t') = \sum_{kk'} \langle\vec{r}|k\rangle G^R_{kk'}(t,t') \left(\langle\vec{r}\,'|k'\rangle\right)^*$$

In general:

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

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

$$G^<_{kk'}(t,t') = -i(\pm 1)\left\langle \hat{a}^\dagger_{k'}(t')\hat{a}_k(t)\right\rangle$$

+: Bosons

-: Fermions

$$G^>_{kk'}(t,t') = -i\left\langle \hat{a}_k(t)\hat{a}^\dagger_{k'}(t')\right\rangle$$

Lehmann Representation

Many-particle spectrum: $\hat{H}|\alpha\rangle = E_\alpha|\alpha\rangle$

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: [redacted]

$$G^{>}_{km}(t,t') = \frac{-i}{Z}\sum_{\alpha\alpha'} e^{-\beta E_\alpha}\langle\alpha|\hat{a}_k|\alpha'\rangle\langle\alpha'|\hat{a}_m^\dagger|\alpha\rangle e^{+i(E_\alpha - E_{\alpha'})(t-t')}$$

In frequency:

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

Lehmman Representation:

Spectral function

Lehmman Representation for the retarded GF: [redacted]

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

Spectral function (diagonal): $A_k(\omega^+) \equiv \frac{-\mathrm{Im}}{\pi} G^R_{kk}(\omega^+)$

[redacted]

$$A_k(\omega^+) = \frac{1}{Z}\sum_{\alpha\alpha'}\left(e^{-\beta E_\alpha} + e^{-\beta E_{\alpha'}}\right)|\langle\alpha'|\hat{a}^\dagger_k|\alpha\rangle|^2\delta\left(\omega^+ - (E_{\alpha'} - E_\alpha)\right)$$

At T=0 (transitions to the GS):

$$A^{T=0}_k(\omega^+) = \frac{1}{Z}\sum_{\alpha'}|\langle\alpha'|\hat{a}^\dagger_k|0\rangle|^2\delta\left(\omega^+ - E_{\alpha'}\right)$$