Green's functions

(intro) QM: Recall the propagator : $\langle \bar{r} | e^{-i\hat{H}t} | \bar{r}' \rangle$ $(\hbar = 1)$ $\hat{H}$ - time independent.

(Retarded - particle can propagate only forward in time)

One-particle Green's function: $G^R(\bar{r},\bar{r}',t) := -i\theta(t)\langle \bar{r} | e^{-i\hat{H}t} | \bar{r}' \rangle = -i\theta(t)\sum_n e^{-i\epsilon_n t}\varphi_n(\bar{r})\varphi_n^*(\bar{r}')$

satisfies $G^R(\bar{r},\bar{r}',0^+) = -i\delta(\bar{r}-\bar{r}')$

(retarded prop) (spin ignored)

Fourier transform: $\tilde{G}^R(\bar{r},\bar{r}',\omega) = \int_{-\infty}^{\infty} dt\, e^{i(\omega+i\eta)t} G^R(\bar{r},\bar{r}',t) = \sum_n \frac{\varphi_n(\bar{r})\varphi_n^*(\bar{r}')}{\omega + i\eta - \epsilon_n}$ $(\eta = 0^+)$

ASSURES CONVERGENCE, ALSO SEE LATER

$\parallel$ notation

$G^R(\bar{r},\bar{r}',\omega)$

{Recall the calculation: $\theta(t) = \frac{i}{2\pi}\int_{-\infty}^{\infty} dx \frac{e^{-ixt}}{x + i0^+}$ }

Eigenenergies $(\epsilon_n) \longleftrightarrow$ Poles of $G^R(\bar{r},\bar{r}',\omega)$

Residues $\longleftrightarrow$ Information about wavefunctions $\varphi_n(\bar{r}) = \langle \bar{r} | n \rangle$

Many-body systems

$$G^R(\bar{r},\bar{r}',t) = -i\theta(t)\langle 0 | [\hat{\Psi}(\bar{r},t)\hat{\Psi}^+(\bar{r}',0)]_{-\zeta} | 0 \rangle \qquad (T=0)$$

Heisenberg op. (position representation)

$$G^R(\bar{r},\bar{r}',0) = -i\delta(\bar{r}-\bar{r}')$$

{ $A(t) = e^{iHt}Ae^{-iHt}$ $(\hbar=1)$ }

$$G^R(\alpha,\alpha',t) = -i\Theta(t)\langle [a_\alpha(t), a^+_{\alpha'}(0)]_{-\zeta} \rangle = -i\theta(t)\frac{1}{Z}\mathrm{Tr}\, e^{-\beta\hat{H}}[a_\alpha(t), a_{\alpha'}^+(0)]_{-\zeta}$$

$\rightarrow$ retarded one-particle Green's function at any T, for any 1 particle basis $\{|\alpha\rangle\}$.

$\hat{H} \longleftrightarrow \hat{H} - \mu\hat{N}$ (GCE).

Non-interacting systems: $\hat{H} = \sum_\alpha (\epsilon_\alpha - \mu) a^+_\alpha a_\alpha$ (diagonal basis)

Solving the e.o.m $\longrightarrow$ $G_0^R(\alpha,t) = -i\theta(t)e^{-i(\epsilon_\alpha - \mu)t}$ $(\times\delta_{\alpha\alpha'})$

{Another point of view - see later today}

$$G_0^R(\alpha,\omega)=\int_{-\infty}^{\infty}dt\, e^{i(\omega+i\eta)t}G_0^R(\alpha,t)=\frac{1}{\omega-(\epsilon_\alpha-\mu)+i\eta} \qquad (\eta=0^+)$$ ②

[Poles $\longleftrightarrow$ single-particle excitation energies]

{in what follows, we will be mostly interested in imaginary-time G functions, which appear in finite-T perturbation theory}

Matsubara Green's function (1-particle) ("imaginary time", "thermal" G.f.)

sign conventional (absent in Negele-Orland)

(G) $G(\alpha,\alpha',\tau)=-\langle T_\tau\, a_\alpha(\tau)\, a_{\alpha'}^+\rangle=-\theta(\tau)\langle a_\alpha(\tau)a_{\alpha'}^+\rangle-\zeta\theta(-\tau)\langle a_{\alpha'}^+a_\alpha(\tau)\rangle$

(or $G(\alpha\tau,\alpha'\tau')$) $\tau'=0$

OR EQUIVALENTLY $-\langle T\, a_\alpha(\tau)a_{\alpha'}^+(\tau')\rangle$

defined by this

T_τ – time-ordering operator.
$$\begin{cases} a_\alpha(\tau):=e^{\tau\hat H}a_\alpha e^{-\tau\hat H}\\ a_\alpha^+(\tau):=e^{\tau\hat H}a_\alpha^+e^{-\tau\hat H}\end{cases}\qquad \{a_\alpha^+(\tau)\neq[a_\alpha(\tau)]^+\}$$

the operators are evolved in imaginary time.

For $\tau=it$ recover the standard Heisenberg op.

{No specification of the meaning of $G(\alpha,\alpha',0)$ for now.}

{
- often easier calculable
- recall the connection between real-time dynamics and stat. phys.
}

Consider only $\tau\in[-\beta,\beta]$ • $G(\alpha,\alpha',\tau)$ is (anti)periodic with period β.

- Demonstrate for $\tau\in]-\beta,0[$: $G(\alpha,\alpha',\tau)=-\zeta\langle a_{\alpha'}^+a_\alpha(\tau)\rangle=-\frac{\zeta}{Z}\mathrm{Tr}\left(e^{-\beta\hat H}a_{\alpha'}^+e^{\tau\hat H}a_\alpha e^{-\tau\hat H}\right)$

$$=-\frac{\zeta}{Z}\mathrm{Tr}\left(e^{\tau\hat H}a_\alpha\, e^{-(\tau+\beta)\hat H}a_{\alpha'}^+\right)=$$

$$=-\frac{\zeta}{Z}\mathrm{Tr}\Big(\underbrace{e^{-\beta\hat H}e^{\beta\hat H}}_{1}\underbrace{e^{\beta\hat H}e^{\tau\hat H}a_\alpha e^{-(\tau+\beta)\hat H}}_{a_\alpha(\tau+\beta)}a_{\alpha'}^+\Big)=-\frac{\zeta}{Z}\mathrm{Tr}\left(e^{-\beta\hat H}a_\alpha(\underbrace{\tau+\beta}_{>0})a_{\alpha'}^+\right)=$$

$$=-\zeta\langle a_\alpha(\tau+\beta)a_{\alpha'}^+\rangle=\zeta G(\alpha,\alpha',\tau+\beta)$$

- Analogous calculation for $\tau\in]0,\beta[$ $\longrightarrow$ $G(\alpha,\alpha',\tau)=\zeta G(\alpha,\alpha',\tau-\beta)$ (•)

Expansion in Fourier series:
$$\begin{cases} G(\alpha,\alpha',\tau)=\frac{1}{\beta}\sum_{\omega_n}e^{-i\omega_n\tau}G(\alpha,\alpha',i\omega_n)\\ G(\alpha,\alpha',i\omega_n)=\int_0^\beta d\tau\, e^{i\omega_n\tau}G(\alpha,\alpha',\tau)\end{cases}$$ (•)

with $\omega_n=\begin{cases}\frac{2\pi}{\beta}n & \text{(bosons)}\\ \frac{2\pi}{\beta}(n+\frac{1}{2}) & \text{(fermions)}\end{cases}$ – Matsubara frequencies

$$\left(\sum_{\omega_n}=\sum_{n=-\infty}^{\infty}\right)\qquad \left(\sum_{\omega_n}\xrightarrow{T\to 0^+}\int\frac{d\omega}{2\pi}\right)$$

{COMPARE TO $\vec k$ IN FINITE VOLUME}

Non-interacting systems: $\hat{\mathcal{H}} = \sum_\alpha (\epsilon_\alpha - \mu) a_\alpha^\dagger a_\alpha$, evolution of $a_\alpha, a_\alpha^\dagger$ calculated before: $a_\alpha(\tau) = e^{-(\epsilon_\alpha-\mu)\tau} a_\alpha$

$a_\alpha^\dagger(\tau) = e^{-(\epsilon_\alpha-\mu)\tau} a_\alpha^\dagger$

(from def, or solving the e.o.m.)

$$G_0(\alpha,\tau) = -e^{-(\epsilon_\alpha-\mu)\tau}\left[\theta(\tau)(1+\zeta n_\alpha) + \theta(-\tau)\zeta n_\alpha\right] \; ; \quad n_\alpha = \langle a_\alpha^\dagger a_\alpha \rangle$$

$$G_0(\alpha, i\omega_n) = \frac{1}{i\omega_n - (\epsilon_\alpha - \mu)}$$

{another approach – later today}

$$G_0(\alpha,\omega) = G_0(\alpha, i\omega_n \longrightarrow \omega + i\eta)$$

(true also for interacting systems)

Not of high relevance for the time being

Many-particle Green's functions:

- $G^{(2n)}(\alpha_1\tau_1 \ldots \alpha_n\tau_n ; \alpha_n'\tau_n' \ldots \alpha_1'\tau_1') = (-1)^n \langle T_\tau\, a_{\alpha_1}(\tau_1) \ldots a_{\alpha_n}(\tau_n)\, a_{\alpha_n'}^\dagger(\tau_n') \ldots a_{\alpha_1'}^\dagger(\tau_1') \rangle$

  (imaginary time) $\qquad T_\tau \hat{A}_{\alpha_1}(\tau_1) \ldots \hat{A}_{\alpha_n}(\tau_n) = \zeta^P A_{\alpha P(1)}(\tau_{P(1)}) \ldots \hat{A}_{\alpha P(n)}(\tau_{P(n)})$

  such that $\tau_{P(1)} > \tau_{P(2)} > \ldots > \tau_{P(n)}$

- $G^{(2n)}(\alpha_1 t_1 \ldots \alpha_n t_n ; \alpha_n' t_n' \ldots \alpha_1' t_1') = (-i)^n \langle T_t\, a_{\alpha_1}(t_1) \ldots a_{\alpha_n}(t_n)\, a_{\alpha_n'}^\dagger(t_n') \ldots a_{\alpha_1'}^\dagger(t_1') \rangle$

One-body Green's function – path integral

Consider $\quad G(\alpha\tau, \alpha'\tau') = -\langle T_\tau\, a_\alpha(\tau)\, a_{\alpha'}^\dagger(\tau') \rangle$

Take $\tau > \tau'$

$$\hookrightarrow G(\alpha\tau, \alpha'\tau') = -\frac{1}{Z}\mathrm{Tr}\left\{ e^{-(\beta-\tau)\hat{\mathcal{H}}}\, a_\alpha\, e^{-(\tau-\tau')\hat{\mathcal{H}}}\, a_{\alpha'}^\dagger\, e^{-\tau'\hat{\mathcal{H}}} \right\} \qquad (\hat{\mathcal{H}} = \hat{H} - \mu\hat{N})$$

Split the time intervals into M steps. Take $\tau = k_1\epsilon$, $\tau' = k_2\epsilon$. $\epsilon = \frac{\beta}{M}$

Alike for the partition function → use the coherent-state representation of the trace
→ plug the coherent-state unity between each two neighboring time slices.

$$G(\alpha\tau, \alpha'\tau') = -\frac{1}{Z}\int \prod_{k=1}^{M} d\mu_k(\xi_k)\, e^{-\sum_{k=1}^{M}\sum_\alpha \xi_{k\alpha}^* \xi_{k\alpha}} \langle \xi_M | e^{-\epsilon\hat{\mathcal{H}}} | \xi_{M-1}\rangle \langle \xi_{M-1} | e^{-\epsilon\hat{\mathcal{H}}} | \xi_{M-2}\rangle \ldots \langle \xi_{k_1+1} | e^{-\epsilon\hat{\mathcal{H}}} a_\alpha | \xi_{k_1}\rangle$$

$$\cdot \langle \xi_{k_1} | e^{-\epsilon\hat{\mathcal{H}}} | \xi_{k_1-1}\rangle \ldots \langle \xi_{k_2} | a_{\alpha'}^\dagger\, e^{-\epsilon\hat{\mathcal{H}}} | \xi_{k_2-1}\rangle \langle \xi_{k_2-1} | \ldots \langle \xi_1 | e^{-\epsilon\hat{\mathcal{H}}} | \xi_0 \rangle$$

With the b.c. $\xi_M = \zeta \xi_0$, $\xi^*_M = \zeta \xi_0$ $\quad \left(\begin{smallmatrix} M \to \infty \\ \epsilon \to 0 \end{smallmatrix}\right)$

$$G(\alpha\tau, \alpha'\tau') = -\frac{1}{Z} \int \mathcal{D}[\xi^* \xi]\, \xi_\alpha(\tau) \xi^*_{\alpha'}(\tau')\, e^{-S[\xi^*, \xi]}$$

- Take $\tau < \tau'$

$$\hookrightarrow \quad G(\alpha\tau, \alpha'\tau') = -\frac{\zeta}{Z} \operatorname{Tr}\left[e^{-(\beta-\tau')\hat{H}} a^+_{\alpha'} e^{-(\tau'-\tau)\hat{H}} a_\alpha e^{-\tau \hat{H}} \right] = \dots \text{(the same steps)}$$

$$= -\frac{\zeta}{Z} \int \mathcal{D}[\xi^* \xi]\, \xi^*_{\alpha'}(\tau') \xi_\alpha(\tau) e^{-S[\xi^* \xi]} =$$

$$= -\frac{1}{Z} \int \mathcal{D}[\xi^* \xi]\, \xi_\alpha(\tau) \xi^*_{\alpha'}(\tau')\, e^{-S[\xi^* \xi]}$$

$\tau = \tau' \to$ chronological ordering equivalent to normal ordering
$\to$ creation op. evaluated one step (ϵ_M) later
$\to$ use the expression for $\tau < \tau'$.

$$G(\alpha\tau, \alpha'\tau') = -\frac{1}{Z} \int \mathcal{D}[\xi^* \xi]\, \xi_\alpha(\tau) \xi^*_{\alpha'}(\tau')\, e^{-S[\xi^*, \xi]}$$

(no $\mathcal{T}$ operator!).

This generalizes to statistical averages of time-ordered products of arbitrary operators, n-particle Green's functions in particular.

$$\left\langle \mathcal{T}_\tau\, \mathcal{O}_1(a^+_\alpha(\tau_1), a_\alpha(\tau_1)) \dots \mathcal{O}_n(a^+_\alpha(\tau_n), a_\alpha(\tau_n)) \right\rangle = (\cdot)$$

Chronological ordering taken care of automatically!

$$= \frac{1}{Z} \int \mathcal{D}[\xi^* \xi]\, \mathcal{O}_1(\xi^*_\alpha(\tau_1), \xi_\alpha(\tau_1)) \dots \mathcal{O}_n(\xi^*_\alpha(\tau_n), \xi_\alpha(\tau_n))\, e^{-S[\xi^* \xi]}$$

Example:

Non-interacting particles

- $G_0(\alpha\tau, \alpha'\tau') = 0$ for $\alpha \neq \alpha'$

Take $\alpha = \alpha'$.

$$\hat{H} = \sum_\alpha (\epsilon_\alpha - \mu) a^+_\alpha a_\alpha \qquad \xi \Longleftrightarrow \phi$$

$$Z_0 = \lim_{M\to\infty} \int \prod_{k=1}^{M} \prod_\alpha \frac{1}{N} d\phi^*_{\alpha k} d\phi_{\alpha k} \exp\left\{ -\epsilon \sum_{k=2}^{M} \left[\sum_\alpha \phi^*_{\alpha k} \frac{\phi_{\alpha k} - \phi_{\alpha, k-1}}{\epsilon} + \sum_\alpha (\epsilon_\alpha - \mu) \phi^*_{\alpha k} \phi_{\alpha k-1} \right] + \right.$$
$$\left. - \epsilon \sum_\alpha \phi^*_{\alpha 1} \frac{\phi_{\alpha 1} - \zeta \phi_{\alpha M}}{\epsilon} + \sum_\alpha (\epsilon_\alpha - \mu) \phi^*_{\alpha 1} \phi_{\alpha M} \right\} =$$

$$\left\{ \epsilon = \frac{\beta}{M} \qquad a := 1 - \frac{\beta}{M}(\epsilon_\alpha - \mu) \right\}$$

$$Z_0 = \lim_{M\to\infty} \int \prod_{k=1}^{M} \prod_\alpha \frac{1}{N} d\phi^*_{\alpha k} d\phi_{\alpha k} \exp\left\{ -\sum_\alpha \left[\phi^*_{\alpha 1} \dots \phi^*_{\alpha M} \right] \underbrace{\begin{bmatrix} 1 & 0 & \dots & -\zeta a \\ -a & 1 & & \vdots \\ 0 & -a & \ddots & \vdots \\ \vdots & \vdots & \ddots & \\ 0 & & -a & 1 \end{bmatrix}}_{S^{(\alpha)}} \begin{bmatrix} \phi_{\alpha 1} \\ \vdots \\ \vdots \\ \phi_{\alpha M} \end{bmatrix} \right.$$

$$\boxed{\begin{array}{c}\text{Notation} \\ \phi \longleftrightarrow \xi\end{array}}$$ below $\xi \to \phi$

$$G_0(\alpha, \tau_{k_1} - \tau_{k_2}) = -\lim_{M\to\infty} \frac{1}{Z_0} \int \prod_{k=1}^{M} \left(\prod_{\alpha'} \frac{1}{N} d\phi^*_{\alpha' k} d\phi_{\alpha' k} \right) \phi_{k_1 \alpha} \phi^*_{k_2 \alpha}\, e^{-\sum_{kk'=1}^{M} \sum_\alpha \phi^*_{k\alpha} S^{(\alpha)}_{kk'} \phi_{k'\alpha}} =$$

$\to$ Moments of the Gaussian distribution (see the exercise class)

$$= -\lim_{M\to\infty} \left[\left[S^{(\alpha)} \right]^{-1} \right]_{k_1 k_2}$$

Inversion of $S^{(\alpha)}$ $\longrightarrow$

$$\left[S^{(\alpha)}\right]^{-1} = \begin{pmatrix} 1 & \zeta a^{M-1} & \zeta a^{M-2} & \cdots & \zeta a \\ a & 1 & \zeta a^{M-1} & & \vdots \\ a^2 & a & 1 & \ddots & \vdots \\ \vdots & \ddots & a & \ddots & \zeta^{M-1} \\ a^{M-1} & & \cdots & a & 1 \end{pmatrix} \frac{1}{1-\zeta a^M}$$

$$G_0(\alpha, \tau_{k_1}-\tau_{k_2}) = -\lim_{M\to\infty} \begin{cases} \dfrac{1}{1-\zeta a^M}\, \zeta a^{M+k_1-k_2} & \tau_{k_1}-\tau_{k_2} \le 0 \quad (\text{row} \,\# < \text{column} \,\#) \\ \dfrac{1}{1-\zeta a^M}\, a^{k_1-k_2} & \tau_{k_1}-\tau_{k_2} > 0 \end{cases}$$

$\tau_1-\tau_2 = (k_1-k_2)\epsilon$

$\epsilon = \frac{\beta}{M}$

$k_1-k_2 = M\frac{\tau_1-\tau_2}{\beta}$

Remember to use the expression valid for $\tau_{k_1}-\tau_{k_2} \le 0$ in the case $k_1 = k_2$! (see p. (4))

- $a^M = \left[1-\frac{\beta}{M}(\epsilon_\alpha-\mu)\right]^M \xrightarrow{M\to\infty} e^{-\beta(\epsilon_\alpha-\mu)}$
- $a^{k_1-k_2} = \left[1-\frac{\beta}{M}(\epsilon_\alpha-\mu)\right]^{\frac{M}{\beta}(\tau_1-\tau_2)} \xrightarrow{M\to\infty} e^{-(\epsilon_\alpha-\mu)(\tau_1-\tau_2)}$
- $\dfrac{1}{1-\zeta a^M} = \dfrac{1}{1-\zeta e^{-\beta(\epsilon_\alpha-\mu)}} = \dfrac{e^{\beta(\epsilon_\alpha-\mu)}}{e^{\beta(\epsilon_\alpha-\mu)}-\zeta} = n_\alpha e^{\beta(\epsilon_\alpha-\mu)}$

  $\hookrightarrow$ F-D or B-E distribution
- $\dfrac{1}{1-\zeta a^M}\zeta a^M a^{k_1-k_2} \Rightarrow n_\alpha \cancel{e^{\beta(\epsilon_\alpha-\mu)}} \zeta \cancel{e^{-\beta(\epsilon_\alpha-\mu)}} e^{-(\epsilon_\alpha-\mu)(\tau_1-\tau_2)} = n_\alpha \zeta e^{-(\epsilon_\alpha-\mu)(\tau_1-\tau_2)}$
- $\dfrac{1}{1-\zeta a^M} a^{k_1-k_2} \longrightarrow n_\alpha e^{\beta(\epsilon_\alpha-\mu)} e^{-(\epsilon_\alpha-\mu)(\tau_1-\tau_2)} = \dfrac{e^{\beta(\,)}-\zeta+\zeta}{e^{\beta(\,)}-\zeta} e^{-(\,)(\,)} = (1+\zeta n_\alpha)e^{-(\epsilon_\alpha-\mu)(\tau_1-\tau_2)}$

$$G_0(\alpha, \tau_1-\tau_2) = \begin{cases} -\zeta n_\alpha e^{-(\tau_1-\tau_2)(\epsilon_\alpha-\mu)} & \tau_1 \le \tau_2 \\ -(1+\zeta n_\alpha) e^{-(\tau_1-\tau_2)(\epsilon_\alpha-\mu)} & \tau_1 > \tau_2 \end{cases}$$

(in agreement with the result from solving the e.o.m.)

Another way (simpler) to calculate the path integral for G_0 (and $\mathcal{G}_0$ alike)

$$G(\alpha\tau, \alpha'\tau') = -\frac{1}{Z}\int \mathcal{D}[\zeta^*\zeta]\, \zeta_\alpha(\tau)\zeta^*_{\alpha'}(\tau')\, e^{-S[\zeta^*\zeta]} \longrightarrow \text{diagonalize } S \text{ by Fourier transform.}$$

$$\longrightarrow G_0(\alpha, \tau_1-\tau_2) = -\langle T a_\alpha(\tau_1) a^\dagger_{\alpha'}(\tau_2)\rangle_0 = -\delta_{\alpha\alpha'} e^{-(\epsilon_\alpha-\mu)(\tau_1-\tau_2)} \left\{ \Theta(\tau_1-\tau_2-\eta)(1+\zeta n_\alpha) + \zeta n_\alpha \Theta(\tau_2-\tau_1+\eta) \right\} =$$

$$= -\delta_{\alpha\alpha'}\, g_\alpha(\tau_1-\tau_2-\eta) \qquad \eta = 0^+$$

$\longrightarrow$ Key quantity for perturbation theory.