1. (i) Compute $\langle \phi | \Psi \rangle$

↳ In 1st quantization: $|\Psi\rangle$ is anti-symm. state of orbitals $|\psi_1\rangle, \dots, |\psi_p\rangle$

$|\phi\rangle$ " " " $|\phi_1\rangle, \dots, |\phi_p\rangle$

$$\rightsquigarrow \langle \phi | \Psi \rangle = \frac{1}{N!} \sum_{P, P'} (-1)^{|P| + |P'|} \langle \phi_1, \dots, \phi_p | P^\dagger P' | \psi_1, \dots \psi_p \rangle =$$

$$= \sum_{\tilde{P}} (-1)^{|\tilde{P}|} \langle \phi_1, \dots, \phi_p | \tilde{P} | \psi_1, \dots, \psi_p \rangle = \sum_{\tilde{P}} (-1)^{|\tilde{P}|} \prod_{m=1}^{p} \langle \phi_m | \psi_{\tilde{P}(m)} \rangle =$$

$$\overset{\text{def. Det.}}{=} \det \begin{pmatrix} \langle \phi_1 | \psi_1 \rangle & \cdots & \langle \phi_1 | \psi_p \rangle \\ \vdots & \ddots & \vdots \\ \langle \phi_p | \psi_1 \rangle & \cdots & \langle \phi_p | \psi_p \rangle \end{pmatrix} .$$

↳ Using the algebra of field-operators in 2nd quantization:

$$|\Psi\rangle = \left(\prod_{m=1}^{p} f_m^\dagger \right) |0\rangle \quad \text{with} \quad f_m^\dagger = \sum_{j=1}^{N} \psi_m(j) c_j^\dagger \quad , \quad \psi_m(j) = \langle j | \psi_m \rangle$$

Analogous: $|\phi\rangle = \left(\prod_{m=1}^{p} d_m^+\right)|0\rangle$, $d_m^+ = \sum_{j=1}^{N} \phi_m(j)\, c_j^+$.

Then, $\langle\phi|\psi\rangle = \langle 0| d_p \cdots d_1 f_1^+ \cdots f_p^+ |0\rangle = \sum_{j_1,\dots,j_p} \sum_{k_1,\dots,k_p} \phi_p^*(j_p)\cdots\phi_1^*(j_1)\,\psi_1(k_1)\cdots\psi_p(k_p)$

$$\times \underbrace{\langle 0| c_{j_p}\cdots c_{j_1} c_{k_1}^+ \cdots c_{k_p}^+ |0\rangle}_{\neq 0 \text{ only if } k_1,\dots,k_p \text{ is permutation of } j_1,\dots,j_p.} = \sum_{j_1,\dots,j_p} \sum_{s\in S_p} (-1)^{|s|}\, \phi_p^*(j_p)\cdots\phi_1^*(j_1)\,\psi_1(j_{s(1)})\cdots\psi_p(j_{s(p)})$$

$$= \sum_{s\in S_p} (-1)^{|s|} \prod_{l=1}^{p} \Big(\underbrace{\sum_{j_l} \phi_l^*(j_l)\, \psi_{s^{-1}(l)}(j_l)}_{\langle\phi_l|\psi_{s^{-1}(l)}\rangle} \Big) \overset{\text{def. Det.}}{=} \det\begin{pmatrix} \langle\phi_1|\psi_1\rangle & \cdots & \langle\phi_1|\psi_p\rangle \\ \vdots & & \\ \langle\phi_p|\psi_1\rangle & \cdots & \langle\phi_p|\psi_p\rangle \end{pmatrix}$$

(ii) Compute $\langle\psi| n_i n_j |\psi\rangle$.

Def: $G^0(i,j) = \langle\psi| c_i^+ c_j |\psi\rangle \overset{\text{1st Q.}}{=} \sum_{m=1}^{p} \langle\psi_m|i\rangle\langle j|\psi_m\rangle = \sum_{m=1}^{p} \psi_m^*(i)\,\psi_m(j)$

$$n_i n_j = c_i^\dagger c_i \, c_j^\dagger c_j = (1 - c_i c_i^\dagger)(1 - c_j c_j^\dagger) = \underbrace{c_i c_i^\dagger c_j c_j^\dagger}_{} + 1$$

$$\boxed{= \delta_{ij}\, c_j c_j^\dagger + c_i c_j c_j^\dagger c_i^\dagger}$$

$$- c_i c_i^\dagger - c_j c_j^\dagger = c_i c_j c_j^\dagger c_i^\dagger + \dots$$

$$\langle \Psi | c_i c_j c_j^\dagger c_i^\dagger | \Psi \rangle \underset{(i)}{=} \det \left(\begin{array}{c|cc} \mathbb{1}_p & \langle \psi_1 | i \rangle & \langle \psi_1 | j \rangle \\ & \vdots & \\ & \langle \psi_p | i \rangle & \langle \psi_p | j \rangle \\ \hline & \langle i | i \rangle & \langle i | j \rangle \\ (\quad)^T & \langle j | i \rangle & \langle j | j \rangle \end{array} \right)$$

For regular A, we generally have $\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} =$

$\det(A) \det(D - C A^{-1} B)$, i.e. in our case

$$\langle \Psi | c_i c_j c_j^\dagger c_i^\dagger | \Psi \rangle = \det \left(\begin{pmatrix} 1 & \delta_{ij} \\ \delta_{ij} & 1 \end{pmatrix} - \begin{pmatrix} \sum_m \psi_m^*(i) \psi_m(i) & \sum_m \psi_m^*(i) \psi_m(j) \\ \sum_m \psi_m^*(j) \psi_m(i) & \sum_m \psi_m^*(j) \psi_m(j) \end{pmatrix} \right) =$$

def. $G^0(i,j)$

$$= \det \begin{pmatrix} 1 - G^0(i,i) & \delta_{ij} - G^0(i,j) \\ \delta_{ij} - G^0(j,i) & 1 - G^0(j,j) \end{pmatrix} =$$

$$= 1 - G^0(j,j) - G^0(i,i) + G^0(i,i)\,G^0(j,j) - G^0(i,j)\,G^0(j,i)$$

$$- \delta_{ij} - \delta_{ij}\, G^0(i,j) + \delta_{ij}\, G^0(j,i) \,.$$

Putting all terms together, we get

$$\langle \Psi | n_i n_j | \Psi \rangle = \delta_{ij}\, G^0(i,j) + G^0(i,i)\,G^0(j,j) - G^0(i,j)\,G^0(j,i) \,.$$

$\checkmark$ Wick

(iii) Thermal state $\rho = \frac{1}{Z} e^{-\beta H}$, $Z = \mathrm{Tr}\left(e^{-\beta H}\right)$, H quadratic;

Compute $\langle n_i n_j \rangle_\beta = \frac{1}{Z} \sum_n e^{-\beta E_n} \langle E_n | n_i n_j | E_n \rangle$.

With $H = \sum_{i,j} c_i^\dagger h_{ij} c_j$, $h = V D V^\dagger$, $\underset{\begin{pmatrix} \varepsilon_1 & & \\ & \ddots & \\ & & \varepsilon_N \end{pmatrix}}{D}$, $f_e^\dagger = \sum_j V_{je} c_j^\dagger$

$\leadsto H = \sum_{e=1}^{N} \varepsilon_e f_e^\dagger f_e$ and $n_i = c_i^\dagger c_i = \sum_{e,e'} V_{ie}^* V_{ie'} f_e^\dagger f_{e'}$

$\left[c_j^\dagger = \sum_e V_{je}^* f_e^\dagger \right]$

$$\langle n_i n_j \rangle_\beta = \sum_{\substack{l,l' \\ m,m'}} V_{il}^* V_{il'} V_{jm}^* V_{jm'} \underbrace{\mathrm{tr}\left(\rho f_l^\dagger f_{l'} f_m^\dagger f_{m'}\right)}_{(\mathrm{I})}$$

$$(\mathrm{I}): \quad \mathrm{tr}\left(\rho f_l^\dagger f_{l'} f_m^\dagger f_{m'}\right) \underset{\uparrow}{=}$$

$$\left[\text{use: } \begin{aligned} \rho f_l^\dagger &= e^{-\beta \varepsilon_l} f_l^\dagger \rho \\ \rho f_l &= e^{\beta \varepsilon_l} f_l \rho \end{aligned}\right]$$

$$= e^{-\beta \varepsilon_l} \mathrm{tr}\left(f_l^\dagger \rho f_{l'} f_m^\dagger f_{m'}\right) \underset{\uparrow}{=} e^{-\beta \varepsilon_l} \mathrm{tr}\left(\rho f_{l'} f_m^\dagger f_{m'} f_l^\dagger\right)$$

[cyclic property of tr]

reshuffle using algebra of f_l's

⋮

$$= e^{-\beta \varepsilon_l} \Big[\delta_{m'l} \, \mathrm{tr}(\rho f_{l'} f_m^\dagger) + \delta_{l'l} \, \mathrm{tr}(\rho f_m^\dagger f_{m'}) - \underbrace{\mathrm{tr}(\rho f_l^\dagger f_{l'} f_m^\dagger f_{m'})}_{=(\mathrm{I})} \Big]$$

solve for (I)

$$\Rightarrow \quad \mathrm{tr}(\rho f_l^\dagger f_{l'} f_m^\dagger f_{m'}) = \frac{1}{1+e^{\beta \varepsilon_l}} \Big[\delta_{m'l} \, \mathrm{tr}(\rho f_{l'} f_m^\dagger) + \delta_{ll'} \, \mathrm{tr}(\rho f_m^\dagger f_{m'}) \Big]$$

Use that $\mathrm{tr}(\rho f_m^\dagger f_n) = \delta_{m,n} \mathrm{tr}(\rho f_m^\dagger f_m) = \delta_{m,n} \langle n_m \rangle_\beta =$

$$= \delta_{m,n} n_F(\varepsilon_m) \quad \text{with} \quad n_F(\varepsilon) = \frac{1}{e^{\beta\varepsilon}+1}.$$

We then have:

$$\langle n_i n_j \rangle_\beta = \sum_{l,m} \Big\{ V_{im} V_{jm}^* V_{jl} V_{il}^* n_F(\varepsilon_l) - V_{im} V_{jm}^* n_F(\varepsilon_m) V_{jl} V_{il}^* n_F(\varepsilon_l)$$

$$+ V_{il} V_{il}^* n_F(\varepsilon_l) V_{jm} V_{jm}^* n_F(\varepsilon_m) \Big\} =$$

$$= \underbrace{\sum_m V_{im} \left(V^\dagger\right)_{mj}}_{\delta_{ij}} \sum_l V_{jl}\, n_F(\varepsilon_l) \left(V^\dagger\right)_{li}$$

$$- \left(\sum_m V_{im}\, n_F(\varepsilon_m) \left(V^\dagger\right)_{mj}\right) \left(\sum_l V_{jl}\, n_F(\varepsilon_l) \left(V^\dagger\right)_{li}\right)$$

$$+ \sum_l V_{il}\, n_F(\varepsilon_l) \left(V^\dagger\right)_{li} \sum_m V_{jm}\, n_F(\varepsilon_m) \left(V^\dagger\right)_{mj}$$

$$= \delta_{ij} \left(V N_F V^\dagger\right)_{ji} - \left(V N_F V^\dagger\right)_{ij} \left(V N_F V^\dagger\right)_{ji} + \left(V N_F V^\dagger\right)_{ii} \left(V N_F V^\dagger\right)_{jj}$$

$$\boxed{\text{with } N_F = \begin{pmatrix} n_F(\varepsilon_1) & & \\ & \ddots & \\ & & n_F(\varepsilon_N) \end{pmatrix}}$$

Since $(V N_F V^\dagger)_{ji} = \langle c_i^\dagger c_j \rangle_\beta$, we have ✓

$$\langle n_i n_j \rangle_\beta = \delta_{ij} \langle n_i \rangle_\beta - \langle c_i^\dagger c_j \rangle_\beta \langle c_j^\dagger c_i \rangle_\beta + \langle n_i \rangle_\beta \langle n_j \rangle_\beta .$$

2. GF and linear response

↳ Unperturbed SGL: $(i\partial_t - H_0) |\psi_0(t)\rangle = 0$

$G_0^r(t,t') = -i\theta(t-t') e^{-iH_0(t-t')}$, check: $(i\partial_t - H_0) G_0^r(t,t') =$

$$= \underbrace{\left(i\partial_t(-i\theta(t-t'))\right)}_{=\delta(t-t')} e^{-iH_0(t-t')} - i\theta(t-t') \underbrace{(i\partial_t - H_0) e^{-iH_0(t-t')}}_{=0 \text{ (Free SGL)}} =$$

$$= \delta(t-t') \underbrace{e^{-iH_0(t-t')}}_{=\mathbb{1} \text{ for } t=t'} = \delta(t-t') \mathbb{1} \checkmark .$$

↳ Add perturbation $V(t)$: $(i\partial_t - H_0) |\psi(t)\rangle = \underbrace{V(t) |\psi(t)\rangle}_{\text{Interpret as inhomogeneity } |\phi(t)\rangle}$

def. GF in math

$$\Rightarrow |\psi(t)\rangle = \underbrace{|\psi_0(t)\rangle}_{\substack{\text{homogeneous}\\ \text{solution}}} + \int_{-\infty}^{+\infty} dt'\, G_0^r(t,t')\, \underbrace{|\phi(t')\rangle}_{\text{"inhomogeneity"}} =$$

def. $|\phi(t)\rangle$

$$= |\psi_0(t)\rangle + \int_{-\infty}^{+\infty} dt'\, G_0^r(t,t')\, V(t')\, \underbrace{|\psi(t')\rangle}_{=|\psi_0(t')\rangle + \mathcal{O}(V)} \overset{+\mathcal{O}(V^2)}{\approx}$$

$$\approx |\psi_0(t)\rangle + \int_{-\infty}^{+\infty} dt'\, G_0^r(t,t')\, V(t')\, |\psi_0(t')\rangle \quad \text{(i)} \checkmark.$$

↳ Now assume $V(t) = F(t)\, B(t)$, $\left[\text{e.g. } V(t) = \vec{A}(t)\cdot\vec{j}\,\right]$

B: operator; $\vec{A}$: vector potential; $\vec{j}$: current op.

$$\delta\langle A\rangle(t) = \langle\psi(t)|A|\psi(t)\rangle - \langle\psi_0(t)|A|\psi_0(t)\rangle \underset{\text{(i)}}{\overset{+\mathcal{O}(F^2)}{\approx}}$$

$$\approx \int_{-\infty}^{+\infty} dt'\, F(t') \left[\langle\psi_0(t)|\, A\, G_0^r(t,t')\, B\, |\psi_0(t')\rangle + \langle\psi_0(t')|\, B\, G_0^{r\dagger}(t,t')\, A\, |\psi_0(t)\rangle\right]$$

$$= \int_{-\infty}^{+\infty} dt' F(t') \left(-i\theta(t-t')\right) \left[\langle \Psi_0(t') | U_0^+(t,t') A U_0(t,t') B - B U_0^+(t,t') A U_0(t,t') | \Psi_0(t') \rangle \right]$$

$$\left[G_0^{r+}(t,t') = -\left(-i\theta(t-t') e^{-iH_0(t'-t)}\right) \right]$$

[Use $\lim_{t_0 \to -\infty} |\Psi_0(t_0)\rangle = |\Psi_0\rangle$, initial free state]

$$= \int_{-\infty}^{+\infty} dt' F(t') \left(-i\theta(t-t')\right) \left[\langle \Psi_0 | \underbrace{U_0^+(t,t_0) A U_0(t,t_0)}_{A_D(t)} \underbrace{U_0^+(t',t_0) B U_0(t',t_0)}_{B_D(t')} - B_D(t') A_D(t) | \Psi_0 \rangle \right] \Big|_{t_0 \to -\infty}$$

$$= \int_{-\infty}^{+\infty} dt' F(t') \underbrace{\left[-i\theta(t-t') \langle \Psi_0 | [A_D(t), B_D(t')] | \Psi_0 \rangle \right]}_{\equiv G^r_{AB}(t,t')} = \int_{-\infty}^{+\infty} dt' F(t') G^r_{AB}(t,t') \quad \checkmark$$