

$$A(\omega) = \frac{1}{2} \sum_{m,n} \bar{e}^{-\beta E_n} \langle n | \hat{c} | m \rangle \langle m | \hat{c}^\dagger | n \rangle \delta(\omega - E_m + E_n)$$

$$B(\omega) = \frac{1}{2} \sum_{m,n} \bar{e}^{-\beta E_n} \langle n | \hat{c}^\dagger | m \rangle \langle m | \hat{c} | n \rangle \delta(\omega + E_m - E_n)$$

$$C(\omega) = A(\omega) + B(\omega)$$

① $\int d\omega C(\omega) = 1$

$$\begin{aligned} \int d\omega A(\omega) &= \frac{1}{2} \sum_{m,n} \bar{e}^{-\beta E_n} \langle n | \hat{c} | m \rangle \langle m | \hat{c}^\dagger | n \rangle = \\ &= \frac{1}{2} \sum_n \bar{e}^{-\beta E_n} \langle n | \hat{c} \hat{c}^\dagger | n \rangle \end{aligned}$$

$$\int d\omega B(\omega) = \frac{1}{2} \sum_n \bar{e}^{-\beta E_n} \langle n | \hat{c}^\dagger \hat{c} | n \rangle$$

$$\int d\omega C(\omega) = \frac{1}{2} \sum_n \bar{e}^{-\beta E_n} = 1$$

Fermi function

② $\langle \hat{n} \rangle = \int d\omega C(\omega) f(\omega)$

side remark

$\int d\omega B(\omega) = \langle \hat{n} \rangle$, but usually we know $C(\omega)$
not $A(\omega)$ and $B(\omega)$ separately

$$\int d\omega A(\omega) f(\omega) = \frac{1}{2} \sum_{n,m} \bar{e}^{-\beta E_n} \langle n | \hat{c} | m \rangle \langle m | \hat{c}^\dagger | n \rangle \frac{1}{1 + e^{\beta(E_m - E_n)}} \quad \textcircled{\pi}$$

$\delta(\omega \neq E_m + E_n) \Rightarrow \omega = E_m - E_n$

$$= \frac{1}{2} \sum_{n,m} \bar{e}^{-\beta E_m} \langle n | \hat{c}^\dagger | m \rangle \langle m | \hat{c} | n \rangle \frac{1}{1 + e^{\beta(E_n - E_m)}}$$

$$\int d\omega B(\omega) f(\omega) = \frac{1}{2} \sum_{n,m} \bar{e}^{-\beta E_n} \langle n | \hat{c}^\dagger | m \rangle \langle m | \hat{c} | n \rangle \frac{1}{1 + e^{\beta(E_n - E_m)}}$$

$$\begin{aligned} \int d\omega (A(\omega) + B(\omega)) f(\omega) &= \frac{1}{2} \sum_{n,m} \langle n | \hat{c}^\dagger | m \rangle \langle m | \hat{c} | n \rangle \frac{\bar{e}^{-\beta E_n} + \bar{e}^{-\beta E_m}}{1 + e^{\beta(E_n - E_m)}} = \\ &= \frac{1}{2} \sum_{n,m} \langle n | \hat{c}^\dagger | m \rangle \langle m | \hat{c} | n \rangle \bar{e}^{-\beta E_n} \frac{1 + e^{\beta(E_n - E_m)}}{1 + e^{\beta(E_n - E_m)}} = \\ &= \frac{1}{2} \sum_n \langle n | \hat{c}^\dagger \hat{c} | n \rangle \bar{e}^{-\beta E_n} \\ &= \langle \hat{n} \rangle \end{aligned}$$

③ $C(\omega)$ in a non-interacting system

$$H = \sum_{\alpha} \epsilon_{\alpha} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha} \quad \hat{c}_i = \sum_{\alpha} \hat{a}_{i\alpha}$$

$$\begin{aligned}
 A_{ij}(\omega) &= \frac{1}{2} \sum_{n,m} \bar{e}^{\beta E_n} \langle n | \hat{c}_i | m \rangle \langle m | \hat{c}_j^{\dagger} | n \rangle \delta(\omega - E_m + E_n) \\
 &= \frac{1}{2} \sum_{n,m} \sum_{\gamma,\beta} \bar{e}^{\beta E_n} \sum_{i\alpha} \sum_{j\beta} \langle n | \hat{a}_{i\alpha} | m \rangle \langle m | \hat{a}_{j\beta}^{\dagger} | n \rangle \delta(\omega - E_m + E_n) \\
 &= \frac{1}{2} \sum_{n,m,\alpha} \bar{e}^{\beta E_n} |\sum_{i\alpha}|^2 \langle n | \hat{a}_{i\alpha} | m \rangle \langle m | \hat{a}_{i\alpha}^{\dagger} | n \rangle \delta(\omega - E_m + E_n) \\
 &= \frac{1}{2} \sum_{n,\alpha} \bar{e}^{\beta E_n} |\sum_{i\alpha}|^2 \delta(\omega - \epsilon_{\alpha}) \\
 &\quad \uparrow \text{orbital } \alpha \text{ is empty}
 \end{aligned}$$

$$\begin{aligned}
 B_{ij}(\omega) &= \frac{1}{2} \sum_{n,m,\alpha} \bar{e}^{\beta E_n} |\sum_{i\alpha}|^2 \langle n | \hat{a}_{i\alpha}^{\dagger} | m \rangle \langle m | \hat{a}_{i\alpha} | n \rangle \delta(\omega + E_m - E_n) \\
 &= \frac{1}{2} \sum_{n,m,\alpha} \bar{e}^{\beta E_m} |\sum_{i\alpha}|^2 \langle n | \hat{a}_{i\alpha} | m \rangle \langle m | \hat{a}_{i\alpha}^{\dagger} | n \rangle \delta(\omega - E_m + E_n) \\
 &= \frac{1}{2} \sum_{n,\alpha} \bar{e}^{\beta E_m} |\sum_{i\alpha}|^2 \delta(\omega - \epsilon_{\alpha}) \\
 &\quad \uparrow \text{orbital } \alpha \text{ is full}
 \end{aligned}$$

$$\begin{aligned}
 A_{ij}(\omega) + B_{ij}(\omega) &= \left(\frac{1}{2} \sum_n \bar{e}^{\beta E_n} \right) \sum_{\alpha} |\sum_{i\alpha}|^2 \delta(\omega - \epsilon_{\alpha}) = \\
 &\quad \uparrow \text{all states} \\
 &= \sum_{\alpha} |\sum_{i\alpha}|^2 \delta(\omega - \epsilon_{\alpha})
 \end{aligned}$$