

Anderson

Mateus Marques

31 de agosto de 2022

1 Modelo

Nós tínhamos exatamente

$$[\omega^+ - \epsilon_0 - \Sigma^{(0)}(\omega^+)] G_{d\sigma}(\omega^+) = 1 + U \cdot D_{d\sigma}(\omega^+),$$

onde, pela aproximação de *mean-field*

$$\Sigma^{(0)}(\omega^+) = \sum_{\mathbf{k}} \frac{|t_{\mathbf{k}}|^2}{\omega^+ - \epsilon_{\mathbf{k}}} \quad \text{e} \quad D_{d\sigma}(\omega^+) = \left\langle \left\langle \hat{n}_{d\bar{\sigma}} \hat{c}_{d\sigma} : \hat{c}_{d\sigma}^\dagger \right\rangle \right\rangle \approx \langle \hat{n}_{d\bar{\sigma}} \rangle G_{d\sigma}(\omega^+).$$

Portanto

$$G_{d\sigma}(\omega^+) = \frac{1}{\omega^+ - \epsilon_0 - \Sigma^{(0)}(\omega^+) - U \langle \hat{n}_{d\bar{\sigma}} \rangle} = \frac{1}{(\omega - \epsilon_0 - U \langle \hat{n}_{d\bar{\sigma}} \rangle - \text{Re}\{\Sigma^{(0)}(\omega^+)\}) + i(\eta - \text{Im}\{\Sigma^{(0)}(\omega^+)\})}.$$

e

$$\text{Im}\{G_{d\sigma}(\omega^+)\} = \frac{-[\eta - \text{Im}\{\Sigma^{(0)}(\omega^+)\}]}{(\omega - \epsilon_0 - U \langle \hat{n}_{d\bar{\sigma}} \rangle - \text{Re}\{\Sigma^{(0)}(\omega^+)\})^2 + (\eta - \text{Im}\{\Sigma^{(0)}(\omega^+)\})^2}.$$

Podemos então calcular $\Sigma^{(0)}(\omega^+)$ por

$$\Sigma^{(0)}(\omega^+) = \sum_{\mathbf{k}} \frac{|t_{\mathbf{k}}|^2}{\omega^+ - \epsilon_{\mathbf{k}}} = \text{Vol} \cdot \int \frac{d^d \mathbf{k}}{(2\pi)^d} \frac{|t(\mathbf{k})|^2}{\omega^+ - \epsilon(\mathbf{k})}.$$

Supondo que $t(k)$ e $\epsilon(k)$ só dependem do módulo $k = |\mathbf{k}|$, temos

$$\Sigma^{(0)}(\omega^+) = \frac{\text{Vol}}{(2\pi)^d} \int d\Omega \int \frac{|t(k)|^2 dk}{\omega^+ - \epsilon(k)}.$$

Sendo então que $dk = d(\epsilon) d\epsilon$ e $\omega^+ = \omega + i\eta$, temos

$$\begin{aligned} \Sigma^{(0)}(\omega^+) &= \frac{\Omega \cdot \text{Vol}}{(2\pi)^d} \int \frac{|t(\epsilon)|^2}{\omega - \epsilon + i\eta} d(\epsilon) d\epsilon \\ &= \frac{\Omega \cdot \text{Vol}}{(2\pi)^d} \left\{ P.V. \int \frac{|t(\epsilon)|^2}{\omega - \epsilon} d(\epsilon) d\epsilon - i\pi \int \delta(\omega - \epsilon) |t(\epsilon)|^2 d(\epsilon) d\epsilon \right\} \end{aligned}$$

Definindo então $\Delta(\epsilon) = \pi \frac{\Omega \cdot \text{Vol}}{(2\pi)^d} |t(\epsilon)|^2 d(\epsilon)$, temos que

$$\Sigma^{(0)}(\omega^+) = P.V. \int \frac{\Delta(\epsilon)}{\omega - \epsilon} d\epsilon - i\Delta(\omega).$$

Chamando $\Lambda(\omega) = \text{Re}\{\Sigma^{(0)}(\omega^+)\} = P.V. \int \frac{\Delta(\epsilon)}{\omega - \epsilon} d\epsilon$ e tomando $\eta \rightarrow 0^+$, temos

$$A_{d\sigma}(\omega) = -\frac{1}{\pi} \text{Im}\{G_{d\sigma}(\omega^+)\} \Rightarrow$$

$$A_{d\sigma}(\omega) = \frac{\Delta(\omega)/\pi}{\left[\omega - \epsilon_0 - U \langle \hat{n}_{d\bar{\sigma}} \rangle - \Lambda(\omega)\right]^2 + \left[\Delta(\omega)\right]^2}.$$

Para temperatura $T = 1/(k_B\beta)$, temos $n_F(\omega) = (e^{\beta\omega} + 1)^{-1}$ e então

$$\langle \hat{n}_{d\sigma} \rangle = \int_{-\infty}^{\infty} \frac{A_{d\sigma}(\omega)}{e^{\beta\omega} + 1} d\omega.$$

No caso especial onde $T = 0$ ($\beta = \infty$), temos que $e^{\beta\omega} = +\infty \cdot \theta(\omega)$, o que nos dá

$$\langle \hat{n}_{d\sigma} \rangle = \int_{-\infty}^0 A_{d\sigma}(\omega) d\omega, \quad T = 0.$$

Como $A_{d\sigma}$ depende de $\langle \hat{n}_{d\bar{\sigma}} \rangle$, as equações acima são de **ponto fixo**

$$\langle \hat{n}_{d\sigma} \rangle = \mathcal{F}\{\langle \hat{n}_{d\bar{\sigma}} \rangle\}, \text{ onde } \mathcal{F}\{\langle \hat{n}_{d\sigma} \rangle\} = \int_{-\infty}^{\infty} \frac{A_{d\sigma}(\omega, \langle \hat{n}_{d\bar{\sigma}} \rangle)}{e^{\beta\omega} + 1} d\omega.$$

Por enquanto escolheremos

$$\Delta(\omega) = \Delta_0 \left[1 - \left(\frac{\omega}{D} \right)^2 \right].$$