EOM

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Aqui, tentarei justificar a equação (11) do paper "Quantitative comparison of Anderson impurity solvers applied to transport in quantum dots" de acordo com a aproximação que descobri que dá o resultado correto: $[n_{\overline{\sigma}}, H] \approx 0$.

1 Fatos

- Equação de movimento:

$$\omega^+ \langle\langle A : B \rangle\rangle = \langle \{A, B\} \rangle + \langle\langle [A, H] : B \rangle\rangle .$$

- Básicos:

$$[a, bc] = [a, b]c + b[a, c] \quad \text{e} \quad [a, bc] = \{a, b\}c - b\{a, c\}.$$

2 Modelo

Nosso modelo é

$$H = H_{\text{imp}} + H_{\text{C}} + H_{\text{B}},$$

onde

$$H_{\text{imp}} = \sum_{\sigma} \epsilon_\sigma f_\sigma^\dagger f_\sigma + U n_\uparrow n_\downarrow,$$

$$H_{\text{B}} = \sum_{\alpha,\mathbf{k},\sigma} \epsilon_{\alpha\mathbf{k}\sigma} c_{\alpha\mathbf{k}\sigma}^\dagger c_{\alpha\mathbf{k}\sigma},$$

$$H_{\text{C}} = \sum_{\alpha,\mathbf{k},\sigma} \Big(V_{\alpha\mathbf{k}\sigma} c_{\alpha\mathbf{k}\sigma}^\dagger f_\sigma + V_{\alpha\mathbf{k}\sigma}^* f_\sigma^\dagger c_{\alpha\mathbf{k}\sigma} \Big).$$

Temos que $\alpha \in \{L, R\}$ e assumimos que $\epsilon_{\alpha\mathbf{k}\sigma}$ e $V_{\alpha\mathbf{k}\sigma}$ não dependem de σ. A equação de movimento exata para $G_\sigma(\omega^+) = \left\langle\left\langle f_\sigma : f_\sigma^\dagger \right\rangle\right\rangle$ é a mesma que calculamos em nossos estudos anteriores:

$$\Big(\omega^+ - \epsilon_\sigma - \Sigma_0(\omega^+)\Big) G_\sigma(\omega^+) = 1 + U \left\langle\left\langle n_{\overline{\sigma}} f_\sigma : f_\sigma^\dagger \right\rangle\right\rangle ,$$

onde $\Sigma_0(\omega^+) = \sum_{\alpha\mathbf{k}} \frac{|V_{\alpha\mathbf{k}}^2|}{\omega - \epsilon_{\alpha\mathbf{k}}}$. Lembremos que, para chegar na equação acima, tínhamos calculado os comutadores

$$[f_\sigma, H] = \epsilon_0 f_\sigma + U n_{\overline{\sigma}} f_\sigma + \sum_{\alpha\mathbf{k}} V_{\alpha\mathbf{k}}^* c_{\alpha\mathbf{k}\sigma},$$

$$[c_{\alpha\mathbf{k}\sigma}, H] = \epsilon_{\alpha\mathbf{k}} c_{\alpha\mathbf{k}\sigma} + V_{\alpha\mathbf{k}} f_\sigma.$$

Vamos mais fundo e calculemos agora a equação de movimento para $\langle\langle n_{\overline{\sigma}} f_\sigma : f_\sigma^\dagger \rangle\rangle$:

$$\omega^+ \langle\langle n_{\overline{\sigma}} f_\sigma : f_\sigma^\dagger \rangle\rangle = \langle \{ n_{\overline{\sigma}} f_\sigma, f_\sigma^\dagger \} \rangle + \langle\langle [n_{\overline{\sigma}} f_\sigma, H] : f_\sigma^\dagger \rangle\rangle .$$

Temos que

$$\{ n_{\overline{\sigma}} f_\sigma, f_\sigma^\dagger \} = n_{\overline{\sigma}} \{ f_\sigma, f_\sigma^\dagger \} = n_{\overline{\sigma}},$$

$$[n_{\overline{\sigma}} f_\sigma, H] = \overset{\approx 0}{\cancel{[n_{\overline{\sigma}}, H]}} f_\sigma + n_{\overline{\sigma}} [f_\sigma, H] = \epsilon_0 n_{\overline{\sigma}} f_\sigma + U n_{\overline{\sigma}}^2 f_\sigma + \sum_{\alpha \mathbf{k}} V_{\alpha \mathbf{k}}^* n_{\overline{\sigma}} c_{\alpha \mathbf{k} \sigma} =$$

$$= \epsilon_0 n_{\overline{\sigma}} f_\sigma + U n_{\overline{\sigma}} f_\sigma + \sum_{\alpha \mathbf{k}} V_{\alpha \mathbf{k}}^* n_{\overline{\sigma}} c_{\alpha \mathbf{k} \sigma}.$$

Acima, estamos fazendo a aproximação $[n_{\overline{\sigma}}, H] = [n_{\overline{\sigma}}, H_{\mathrm{C}}] \approx 0$. Usamos também que $n_{\overline{\sigma}}^2 = n_{\overline{\sigma}}$. Temos então

$$\Big(\omega^+ - \epsilon_0 - U \Big) \langle\langle n_{\overline{\sigma}} f_\sigma : f_\sigma^\dagger \rangle\rangle = \langle n_{\overline{\sigma}} \rangle + \sum_{\alpha \mathbf{k}} V_{\alpha \mathbf{k}}^* \langle\langle n_{\overline{\sigma}} c_{\alpha \mathbf{k} \sigma} : f_\sigma^\dagger \rangle\rangle$$

Vamos mais fundo de novo, e calculemos a equação de movimento para $\langle\langle n_{\overline{\sigma}} c_{\alpha \mathbf{k} \sigma} : f_\sigma^\dagger \rangle\rangle$:

$$\omega^+ \langle\langle n_{\overline{\sigma}} c_{\alpha \mathbf{k} \sigma} : f_\sigma^\dagger \rangle\rangle = \langle \{ n_{\overline{\sigma}} c_{\alpha \mathbf{k} \sigma}, f_\sigma^\dagger \} \rangle + \langle\langle [n_{\overline{\sigma}} c_{\alpha \mathbf{k} \sigma}, H] : f_\sigma^\dagger \rangle\rangle .$$

Os comutadores dão

$$\{ n_{\overline{\sigma}} c_{\alpha \mathbf{k} \sigma}, f_\sigma^\dagger \} = n_{\overline{\sigma}} \{ c_{\alpha \mathbf{k} \sigma}, f_\sigma^\dagger \} = 0,$$

$$[n_{\overline{\sigma}} c_{\alpha \mathbf{k} \sigma}, H] = \overset{\approx 0}{\cancel{[n_{\overline{\sigma}}, H]}} c_{\alpha \mathbf{k} \sigma} + n_{\overline{\sigma}} [c_{\alpha \mathbf{k} \sigma}, H] = \epsilon_{\alpha \mathbf{k}} n_{\overline{\sigma}} c_{\alpha \mathbf{k} \sigma} + V_{\alpha \mathbf{k}} n_{\overline{\sigma}} f_\sigma.$$

Substituindo na EOM, temos

$$\langle\langle n_{\overline{\sigma}} c_{\alpha \mathbf{k} \sigma} : f_\sigma^\dagger \rangle\rangle = \frac{V_{\alpha \mathbf{k}}}{\omega^+ - \epsilon_{\alpha \mathbf{k}}} \langle\langle n_{\overline{\sigma}} f_\sigma : f_\sigma^\dagger \rangle\rangle .$$

Agora substituiremos esse resultado na EOM para $\langle\langle n_{\overline{\sigma}} f_\sigma : f_\sigma^\dagger \rangle\rangle$:

$$\Big(\omega^+ - \epsilon_0 - U \Big) \langle\langle n_{\overline{\sigma}} f_\sigma : f_\sigma^\dagger \rangle\rangle = \langle n_{\overline{\sigma}} \rangle + \sum_{\alpha \mathbf{k}} \frac{|V_{\alpha \mathbf{k}}|^2}{\omega^+ - \epsilon_{\alpha \mathbf{k}}} \langle\langle n_{\overline{\sigma}} f_\sigma : f_\sigma^\dagger \rangle\rangle \Rightarrow$$

$$\langle\langle n_{\overline{\sigma}} f_\sigma : f_\sigma^\dagger \rangle\rangle = \frac{\langle n_{\overline{\sigma}} \rangle}{\omega^+ - \epsilon_0 - U - \Sigma_0(\omega^+)}.$$

Finalmente, podemos voltar na EOM para G_σ:

$$\Big(\omega^+ - \epsilon_\sigma - \Sigma_0(\omega^+) \Big) G_\sigma(\omega^+) = 1 + \frac{U \langle n_{\overline{\sigma}} \rangle}{\omega^+ - \epsilon_0 - \Sigma_0(\omega^+) - U} \Rightarrow$$

$$G_\sigma(\omega^+) = \frac{\omega^+ - \epsilon_0 - \Sigma_0(\omega^+) - U(1 - \langle n_{\overline{\sigma}} \rangle)}{\Big(\omega^+ - \epsilon_\sigma - \Sigma_0(\omega^+) \Big) \Big(\omega^+ - \epsilon_0 - \Sigma_0(\omega^+) - U \Big)}.$$

Agora, chame $x = \omega^+ - \epsilon_\sigma - \Sigma_0(\omega^+)$. Temos que (somando e subtraindo $x \cdot \langle n_{\overline{\sigma}} \rangle$):

$$G_\sigma(\omega^+) = \frac{x - U(1 - \langle n_{\overline{\sigma}} \rangle)}{x \Big(x - U \Big)} = \frac{x \langle n_{\overline{\sigma}} \rangle}{x \Big(x - U \Big)} + \frac{x - x \langle n_{\overline{\sigma}} \rangle - U(1 - \langle n_{\overline{\sigma}} \rangle)}{x \Big(x - U \Big)} =$$

$$= \frac{\langle n_{\overline{\sigma}} \rangle}{x - U} + \frac{1 - \langle n_{\overline{\sigma}} \rangle}{x}.$$

Assim, chegamos finalmente à equação (11) do paper.

$$\boxed{G_\sigma(\omega^+) = \frac{1 - \langle n_{\overline{\sigma}} \rangle}{\omega^+ - \epsilon_\sigma - \Sigma_0(\omega^+)} + \frac{\langle n_{\overline{\sigma}} \rangle}{\omega^+ - \epsilon_\sigma - U - \Sigma_0(\omega^+)}.}$$