Solution to problem set 3

1. $SU(N)$ **Anderson Impurity model**

We consider impurity electrons on a single site hybridizing with a bath of conduction electrons. The electrons carry $SU(N)$ spin. We consider the limiting case where the on-site Coulomb repulsion (U) at the impurity site is infinitely large. Thus, at most a single electron can occupy the impurity site (multiple occupancy is not allowed). In this limit, the allowed states of the impurity site are $|0\rangle$ (i.e., no electron), and $|m\rangle$, where $m = (1, \cdots, N)$ (i.e., a single electron with $SU(N)$ spin m). The Hubbard operators are defined as $X_{pq} = |p\rangle\langle q|$, where $p, q = (0, 1, \cdots, N)$. In this restricted subspace creation operator for an impurity electron $f_n^\dagger \equiv |n\rangle\langle 0| = X_{n0}$. Similarly, $f_n \equiv X_{0n}$. The completeness relation in this subspace (of the impurity level) is given by $X_{00} + \sum_n X_{nn} = 1$. Note, that the Hubbard operators satisfy the relation $[X_{pq}, X_{rs}]_\pm = \delta_{qr} X_{ps} \pm \delta_{ps} X_{rq}$. This is unlike standard commutation or anticommutation of bosons and fermions. The Hamiltonian for the system is given by

$$\mathcal{H} = \mathcal{H}_b + \mathcal{H}_f + \mathcal{H}_I,$$

where $\mathcal{H}_b = \sum_{\mathbf{k},n} \epsilon_k c^\dagger_{\mathbf{k}n} c_{\mathbf{k}n}$ describes the bath of conduction electrons, $\mathcal{H}_f = \epsilon_f \sum_m f^\dagger_m f_m = \epsilon_f \sum_m X_{mm}$ describes the impurity electrons, and $\mathcal{H}_I = \sum_{\mathbf{k}m} (V_\mathbf{k} c^\dagger_{\mathbf{k}m} X_{0m} + V^*_\mathbf{k} X_{m0} c_{\mathbf{k}m})$ is the hybridization between the impurity electrons and the conduction electrons.

We consider the retarded Green's function $\langle\langle f_n f_n^\dagger \rangle\rangle(\omega) = \langle\langle X_{0n} X_{n0} \rangle\rangle(\omega)$. The corresponding spectral function is given by

$$\rho_{ff^\dagger}(\omega) = -\frac{\mathrm{Im}}{\pi} G_{ff^\dagger}(\omega + i\delta).$$

The first moment is given by $\langle \{X_{0n}, X_{n0}\} \rangle = \langle X_{00} + X_{nn} \rangle$. We can write $\langle X_{00} \rangle = 1 - \langle n_f \rangle$, where $\langle n_f \rangle = \sum_n \langle X_{nn} \rangle$ is the expectation of electron occupancy at the impurity site. Also, $\langle X_{nn} \rangle = \langle n_f \rangle / N$. Thus,

$$\langle \{X_{0n}, X_{n0}\} \rangle = 1 - \left(\frac{N-1}{N} \right) \langle n_f \rangle. \tag{1}$$

Since,

$$\int_{-\infty}^{\infty} d\omega \rho_{ff^\dagger}(\omega) = \langle \{X_{0n}, X_{n0}\} \rangle,$$

the first moment gives the total spectral weight of the f-band.

For the calculation of the second moment we get

$$[\mathcal{H}, X_{0n}] = -\epsilon_f X_{0n} - \sum_{\mathbf{k}} V^*_\mathbf{k} c_{\mathbf{k}n} X_{00} - \sum_{\mathbf{k}m} V^*_\mathbf{k} c_{\mathbf{k}m} X_{mn}.$$

Then,

$$\langle \{[\mathcal{H}, X_{0n}], X_{n0}\} \rangle = -\epsilon_f \langle \{X_{0n}, X_{n0}\} \rangle - \sum_{\mathbf{k}, m \neq n} V^*_\mathbf{k} \langle c_{\mathbf{k}m} X_{m0} \rangle. \tag{2}$$

Since,

$$\int_{-\infty}^{\infty} \omega \rho_{ff^\dagger}(\omega) d\omega = -\langle\{[\mathcal{H}, X_{0n}], X_{n0}\}\rangle, \tag{3}$$

the centre of the f-band is given by

$$\frac{\int_{-\infty}^{\infty} \omega \rho_{ff^\dagger}(\omega) d\omega}{\int_{-\infty}^{\infty} d\omega \rho_{ff^\dagger}(\omega)} = \epsilon_f + \frac{1}{\langle\{X_{0n}, X_{n0}\}\rangle} \sum_{\mathbf{k}, m \neq n} V_{\mathbf{k}}^* \langle c_{\mathbf{k}m} X_{m0}\rangle.$$

Presumably (since we cannot conclusively say anything about the line shape) the spectral function is peaked at this energy. The second term is the shift in the energy of the f-level due to hybridization.

For the third moment we get

$$\begin{aligned}
\langle\{[\mathcal{H}, X_{0n}], [\mathcal{H}, X_{n0}]\}\rangle &= \langle\{-\epsilon_f X_{0n} - \sum_{vk} V_{\mathbf{k}}^* c_{\mathbf{k}n} X_{00} - \sum_{\mathbf{k}m} V_{\mathbf{k}}^* c_{\mathbf{k}m} X_{mn}\ ,\ \epsilon_f X_{n0} \\
&\quad + \sum_{\mathbf{k}} V_{\mathbf{k}} c_{\mathbf{k}n}^\dagger X_{00} + \sum_{\mathbf{k}m} V_{\mathbf{k}} c_{\mathbf{k}m}^\dagger X_{nm}\}\rangle \\
&= -\epsilon_f^2 \langle\{X_{0n}, X_{n0}\}\rangle - \epsilon_f \sum_{\mathbf{k}, m\neq n} V_{\mathbf{k}}^* \langle c_{\mathbf{k}m} X_{m0}\rangle + \epsilon_f \sum_{\mathbf{k}, m\neq n} V_{\mathbf{k}} \langle c_{\mathbf{k}m}^\dagger X_{0m}\rangle \\
&\quad - \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 + \sum_{\mathbf{k}_1\mathbf{k}_2, m_1 m_2} V_{\mathbf{k}_1}^* V_{\mathbf{k}_2} \langle c_{\mathbf{k}_2 m_2}^\dagger c_{\mathbf{k}_1 m_1} X_{m_1 m_2}\rangle \\
&\quad - \sum_{\mathbf{k}_1\mathbf{k}_2, m} V_{\mathbf{k}_1}^* V_{\mathbf{k}_2} \langle c_{\mathbf{k}_2 m}^\dagger c_{\mathbf{k}_1 m} X_{nn}\rangle.
\end{aligned} \tag{4}$$

We can show that

$$\begin{aligned}
\langle\{[\mathcal{H}, X_{0n}], X_{n0}\}\rangle &= \frac{1}{Z} \sum_{nm} \left(e^{-\beta E_n} + e^{-\beta E_m}\right) (E_n - E_m) \langle n|X_{0n}|m\rangle \langle m|X_{n0}|n\rangle \\
&= -\langle\{X_{0n}, [\mathcal{H}, X_{n0}]\}\rangle.
\end{aligned} \tag{5}$$

This is due to time translation invariance of the correlation function in equilibrium. Using this result we get,

$$-\sum_{\mathbf{k}, m\neq n} V_{\mathbf{k}}^* \langle c_{\mathbf{k}m} X_{m0}\rangle = \sum_{\mathbf{k}, m\neq n} V_{\mathbf{k}} \langle c_{\mathbf{k}m}^\dagger X_{0m}\rangle. \tag{6}$$

The $SU(N)$ spin at the impurity site can be written as $\mathbf{S} = \sum_{m_1 m_2} \Gamma_{m_1 m_2}^M X_{m_1 m_2}$, where Γ^M are the generators of $SU(N)$ group, with $M = (1, \cdots, (N^2-1))$. The spin of the conduction electrons in the momentum basis is similarly given by $\mathbf{s}_{\mathbf{k}_2\mathbf{k}_1} = \sum_{m_1 m_2} c_{\mathbf{k}_2 m_1}^\dagger \Gamma_{m_1 m_2}^M c_{\mathbf{k}_1 m_2}$. The generators of the group satisfy the completeness relation $\sum_M \Gamma_{m_1 m_2}^M \Gamma_{m_3 m_4}^M = \delta_{m_1 m_4}\delta_{m_2 m_3} - \frac{1}{N}\delta_{m_1 m_2}\delta_{m_3 m_4}$. Using this we can show that

$$\sum_{\mathbf{k}_1\mathbf{k}_2} V_{\mathbf{k}_1}^* V_{\mathbf{k}_2} \langle \mathbf{s}_{\mathbf{k}_2\mathbf{k}_1} \cdot \mathbf{S}\rangle = \sum_{\mathbf{k}_1\mathbf{k}_2, m_1 m_2} V_{\mathbf{k}_1}^* V_{\mathbf{k}_2} \langle c_{\mathbf{k}_2 m_1}^\dagger c_{\mathbf{k}_1 m_2} X_{m_2 m_1}\rangle - \frac{1}{N} \sum_{\mathbf{k}_1\mathbf{k}_2, mm'} V_{\mathbf{k}_1}^* V_{\mathbf{k}_2} \langle c_{\mathbf{k}_2 m}^\dagger c_{\mathbf{k}_1 m} X_{m'm'}\rangle. \tag{7}$$

Thus, we can write

$$\begin{aligned}
\langle\{[\mathcal{H}, X_{0n}], [\mathcal{H}, X_{n0}]\}\rangle &= -\epsilon_f^2 \langle\{X_{0n}, X_{n0}\}\rangle - 2\epsilon_f \sum_{\mathbf{k}, m\neq n} V_{\mathbf{k}}^* \langle c_{\mathbf{k}m} X_{m0}\rangle - \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 \\
&\quad + \sum_{\mathbf{k}_1\mathbf{k}_2} V_{\mathbf{k}_1}^* V_{\mathbf{k}_2} \langle \mathbf{s}_{\mathbf{k}_2\mathbf{k}_1} \cdot \mathbf{S}\rangle.
\end{aligned} \tag{8}$$

We identify the last term in the above equation as a spin-spin correlation function. The sum rule for the third moment is given by

$$\int_{-\infty}^{\infty} \omega^2 \rho_{ff^\dagger}(\omega) d\omega = \langle \{ [\mathcal{H}, [\mathcal{H}, X_{0n}]], X_{n0} \} \rangle = -\langle \{ [\mathcal{H}, X_{0n}], [\mathcal{H}, X_{n0}] \} \rangle. \tag{9}$$

The width of the impurity band (standard deviation of a distribution, in general) is given by

$$\begin{aligned} &\frac{\int_{-\infty}^{\infty} \omega^2 \rho_{ff^\dagger}(\omega) d\omega}{\int_{-\infty}^{\infty} d\omega \rho_{ff^\dagger}(\omega)} - \left(\frac{\int_{-\infty}^{\infty} \omega \rho_{ff^\dagger}(\omega) d\omega}{\int_{-\infty}^{\infty} d\omega \rho_{ff^\dagger}(\omega)} \right)^2 = \\ &\quad -\frac{1}{\langle \{ X_{0n}, X_{n0} \} \rangle} \sum_{\mathbf{k}_1 \mathbf{k}_2} V_{\mathbf{k}_1}^* V_{\mathbf{k}_2} \langle \mathbf{s}_{\mathbf{k}_2 \mathbf{k}_1} \cdot \mathbf{S} \rangle - \left(\frac{1}{\langle \{ X_{0n}, X_{n0} \} \rangle} \sum_{\mathbf{k}, m \neq n} V_{\mathbf{k}}^* \langle c_{\mathbf{k}m} X_{m0} \rangle \right)^2 \end{aligned} \tag{10}$$

Originally the f-level was a delta function peak at ϵ_f. Due to hybridization there is a shift in the energy level, and also a broadening of the band.

2. **f-sum rule**

The retarded current-current correlation function is defined by

$$\Pi_{jj}^R(\omega) = \langle \langle j, j \rangle \rangle(\omega) = \frac{1}{Z} \sum_{nm} \left(e^{-\beta E_n} - e^{-\beta E_m} \right) |\langle n|j|m \rangle|^2 \frac{1}{\omega + E_n - E_m + i\eta}. \tag{11}$$

The corresponding spectral function is

$$\begin{aligned} \rho_{jj}(\omega) &= -\frac{1}{\pi} \mathrm{Im} \Pi_{jj}^R(\omega) \\ &= \frac{1}{Z} \sum_{nm} \left(e^{-\beta E_n} - e^{-\beta E_m} \right) |\langle n|j|m \rangle|^2 \delta(\omega + E_n - E_m) \\ &= \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t} \langle [j(t), j] \rangle. \end{aligned} \tag{12}$$

In terms of the spectral function, the real part of the conductivity (which is what enters the f-sum rule) is given by,

$$\sigma(\omega) = -\frac{1}{V} \frac{1}{\omega} \mathrm{Im} \Pi_{jj}^R(\omega) = \frac{\pi}{V} \rho_{jj}(\omega). \tag{13}$$

We define the polarization operator P such that $\frac{\partial P}{\partial t} = j$. Then,

$$\begin{aligned} \rho_{jj}(\omega) &= \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t} \langle [\frac{\partial P}{\partial t}, j] \rangle \\ &= -i\omega \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t} \langle [P(t), j] \rangle \\ &= -i\omega \rho_{Pj}(\omega), \end{aligned} \tag{14}$$

where

$$\rho_{Pj}(\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{i\omega t} \langle [P(t), j] \rangle. \tag{15}$$

Then,

$$
\begin{aligned}
\int_{-\infty}^{\infty} d\omega \sigma(\omega) &= -\frac{\pi i}{V} \int_{-\infty}^{\infty} d\omega \rho_{Pj}(\omega) \\
&= -\frac{\pi i}{V} \langle [P(0), j] \rangle.
\end{aligned} \tag{16}
$$

The current operator is given by $j = \sum_{i=1}^{N} (ep_i)/m$, where p_i is the momentum of the i-th particle. The polarization operator is given by $P = \sum_{i=1}^{N} er_i$, where r_i is the position of the i-th particle. Since,

$$
[P, j] = \frac{e^2}{m} \sum_{ij} [r_i, p_j] = \frac{Ne^2 i}{m},
$$

(in units where $\hbar = 1$), we finally get the f-sum rule as

$$
\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \sigma(\omega) = \frac{ne^2}{m}, \tag{17}
$$

where $n = N/V$ is the density of particles.