Lehmann representation for a non-interacting system

Consider a generic non-interacting system of fermions, whose Hamiltonian is quadratic, i.e.,

$$\hat{H} = \sum_{ij} [\boldsymbol{h}]_{ij} \hat{c}_i^\dagger \hat{c}_j, \tag{1}$$

where $\hat{c}_i^\dagger$ creates a fermionic particle in the i-th spin-orbital, and the spin-orbitals form the orthonormal basis. The single-particle Hamiltonian $\boldsymbol{h}$, which is Hermitian, can be diagonalized as

$$\boldsymbol{h} = \boldsymbol{V}\boldsymbol{\epsilon}\boldsymbol{V}^\dagger, \tag{2}$$

where $[\boldsymbol{\epsilon}]_{ij} = \epsilon_i \delta_{ij}$ is the diagonal matrix containing the single-particle energy eigenvalues ϵ_i, and $\boldsymbol{V} = (\vec{v}_1 \vec{v}_2 \cdots)$ is the unitary matrix whose column vectors are the eigenvectors of $\boldsymbol{h}$.

Since the (many-body) Hamiltonian $\hat{H}$ is quadratic, the retarded Green's function,

$$G[\hat{c}_i, \hat{c}_j^\dagger](t) = -i\theta(t) \operatorname{Tr}\Big(\hat{\rho} \, [\hat{c}_i(t), \hat{c}_j^\dagger]_\pm] \Big), \tag{3}$$

and its spectral function,

$$A[\hat{c}_i, \hat{c}_j^\dagger](\omega) = \frac{-1}{\pi} \mathrm{Im} \int_{-\infty}^{+\infty} \mathrm{d}t \, e^{\mathrm{i}\omega t} \, G[\hat{c}_i, \hat{c}_j^\dagger](t), \tag{4}$$

can be computed exactly.

(a) Evaluate the spectral function $A[\hat{c}_i, \hat{c}_j^\dagger](\omega)$ by using the Lehmann representation.

[Solution] The diagonalized form of the Hamiltonian is

$$\hat{H} = \sum_k \epsilon_k \hat{d}_k^\dagger \hat{d}_k = \sum_k \epsilon_k \hat{n}_k, \tag{5}$$

where $\hat{d}_k^\dagger = \sum_i \hat{c}_i^\dagger [\boldsymbol{V}]_{ik}$ creates a particle in the eigenmode of energy ϵ_k and $\hat{n}_k = \hat{d}_k^\dagger \hat{d}_k$ counts the particle number in the eigenmode. (Here we call the single-particle energy eigenstates as eigenmodes, to distinguish from many-body energy eigenstates.) The number operators $\hat{n}_k$ commute each other, and they also commute with the Hamiltonian. Therefore, the eigenvalues of the number operators are good quantum numbers. Indeed, we can represent the eigenstates as

$$|\boldsymbol{n}\rangle = \cdots |n_{k+1}\rangle |n_k\rangle |n_{k-1}\rangle \cdots, \tag{6}$$

where $[\boldsymbol{n}]_k = n_k = 0, 1$ is the eigenvalue of $\hat{n}_k$. The energy eigenvalue corresponding to $|\boldsymbol{n}\rangle$ is $E_{\boldsymbol{n}} = \sum_k \epsilon_k n_k$.

Then, the Lehmann representation of $A[\hat{d}_k, \hat{d}_l^\dagger](\omega)$ is given as follows:

$$\sum_{\boldsymbol{n},\boldsymbol{n'}} \left(\langle \boldsymbol{n}|\hat{\rho}|\boldsymbol{n}\rangle \langle \boldsymbol{n}|\hat{d}_k|\boldsymbol{n'}\rangle \langle \boldsymbol{n'}|\hat{d}_l^\dagger|\boldsymbol{n}\rangle + \langle \boldsymbol{n}|\hat{d}_k|\boldsymbol{n'}\rangle \langle \boldsymbol{n'}|\hat{\rho}|\boldsymbol{n'}\rangle \langle \boldsymbol{n'}|\hat{d}_l^\dagger|\boldsymbol{n}\rangle \right) \delta(\omega - (E_{\boldsymbol{n'}} - E_{\boldsymbol{n}})). \tag{7}$$

We see that $\langle \boldsymbol{n}|\hat{d}_k|\boldsymbol{n'}\rangle$ is finite only when $n'_k = 1$, $n_k = 0$, and $n'_m = n_m$ for $m \neq k$. Similarly, $\langle \boldsymbol{n'}|\hat{d}_l^\dagger|\boldsymbol{n}\rangle$ is finite only when $n'_l = 1$, $n_l = 0$, and $n'_m = n_m$ for $m \neq l$. Therefore, it should hold that $k = l$; otherwise $A[\hat{d}_k, \hat{d}_l^\dagger](\omega) = 0$.

So we get

$$A[\hat{d}_k, \hat{d}_l^\dagger](\omega) = \delta_{kl} \sum_{\boldsymbol{n},\boldsymbol{n'}} \left(\langle \boldsymbol{n}|\hat{\rho}|\boldsymbol{n}\rangle + \langle \boldsymbol{n'}|\hat{\rho}|\boldsymbol{n'}\rangle \right) \underbrace{|\langle \boldsymbol{n}|\hat{d}_k|\boldsymbol{n'}\rangle|^2}_{=1} \; \delta(\omega - \underbrace{(E_{\boldsymbol{n'}} - E_{\boldsymbol{n}})}_{=\epsilon_k}). \tag{8}$$

The underbraced terms are independent from $\boldsymbol{n}$ and $\boldsymbol{n}'$ as long as they are finite. So they can be pulled out of the summation $\sum_{\boldsymbol{n},\boldsymbol{n}'}$,

$$A[\hat{d}_k, \hat{d}_l^\dagger](\omega) = \delta_{kl}\delta(\omega - \epsilon_k) \underbrace{\sum_{\boldsymbol{n},\boldsymbol{n}'} (\langle \boldsymbol{n}|\hat{\rho}|\boldsymbol{n}\rangle + \langle \boldsymbol{n}'|\hat{\rho}|\boldsymbol{n}'\rangle)}_{=\sum_{\boldsymbol{n}''}\langle \boldsymbol{n}''|\hat{\rho}|\boldsymbol{n}''\rangle = 1} . \tag{9}$$

The equality in this underbrace holds because the sets $\{|\boldsymbol{n}\rangle\}$ and $\{|\boldsymbol{n}'\rangle\}$ are exclusive, since $n_k \neq n'_k$, and their union equals to the set of all the eigenstates, since there is no further constraint other than $n_m = n'_m$ for $m \neq k$.

Therefore, we obtain the spectral function defined by $\hat{c}$ operators by applying the unitary transformation $\hat{c}_i^\dagger = \sum_k \hat{d}_k^\dagger [\boldsymbol{V}^{-1}]_{ki} = \sum_k \hat{d}_k^\dagger [\boldsymbol{V}]_{ik}^*$, which is clear from the structure of the Lehmann representation.

$$A[\hat{c}_i, \hat{c}_j^\dagger](\omega) = \sum_k [\boldsymbol{V}]_{ik}[\boldsymbol{V}]_{jl}^* A[\hat{d}_k, \hat{d}_l^\dagger](\omega) = \sum_k [\boldsymbol{V}]_{ik}[\boldsymbol{V}]_{jk}^* \delta(\omega - \epsilon_k). \tag{10}$$

(b) The local spectral function is the case of $i = j$ in which the two defining operators $\hat{c}_i$ and $\hat{c}_i^\dagger$ act on the same spin-orbital. Explain why the local spectral function can be interpreted as the local density of states.

[Solution] We have the local spectral function

$$A[\hat{c}_i, \hat{c}_i^\dagger](\omega) = \sum_k |[\boldsymbol{V}]_{ik}|^2 \delta(\omega - \epsilon_k). \tag{11}$$

From the diagonalization of the single-particle Hamiltonian in Eq. (2), we can interpret $|[\boldsymbol{V}]_{ik}|^2$ as the probability that the particle at site i is in the eigenmode k. Of course, such probabilities are non-negative, $|[\boldsymbol{V}]_{ik}|^2 \geq 0$, and sum up to the unity, $\sum_k |[\boldsymbol{V}]_{ik}|^2 = 1$. Therefore the local spectral function can be interpreted as the local density of states.