Appendix A

Zero temperature Greens function in frequency domain

The impurity retarded Green's function (assuming the Hamiltonian to be time-independent, which it is) is defined as

$$G^{\sigma}_{dd}(t) = -i\theta(t)\left\langle\left\{\mathcal{O}_\sigma(t), \mathcal{O}^\dagger_\sigma\right\}\right\rangle \tag{A.0.1}$$

where the average $\langle\rangle$ is over a canonical ensemble at temperature T, and $\mathcal{O}_\sigma = c_{d\sigma} + S^-_d c_{0\overline{\sigma}} + S^z_d c_{0\sigma}$ is the excitation whose spectral function we are interested in. The excitations defined in $\mathcal{O}$ incorporates both single-particle excitations brought about by the hybridisation as well as two-particle spin excitations brought about by the spin-exchange term. What follows is a standard calculation where we write the Green's function in the Lehmann representation. The ensemble average for an arbitrary operator $\hat{M}$ can be written in terms of the exact eigenstates of the fixed point Hamiltonian:

$$H^* |n\rangle = E^*_n |n\rangle, \quad \left\langle \hat{M} \right\rangle \equiv \frac{1}{Z}\sum_n \langle n| \hat{M} |n\rangle e^{-\beta E^*_n} \tag{A.0.2}$$

where $Z = \sum_n e^{-\beta E^*_n}$ is the fixed point partition function and $\left\{|n\rangle\right\}$ is the set of eigenfunctions of the fixed point Hamiltonian. We can therefore write

$$\begin{aligned}
&\left\langle\left\{\mathcal{O}_\sigma(t), \mathcal{O}^\dagger_\sigma\right\}\right\rangle \\
&= \frac{1}{Z}\sum_m e^{-\beta E_m} \langle m| \left\{\mathcal{O}_\sigma(t), \mathcal{O}^\dagger_\sigma\right\} |m\rangle \\
&= \frac{1}{Z}\sum_{m,n} e^{-\beta E_m} \langle m| \Big(\mathcal{O}_\sigma(t) |n\rangle \langle n| \mathcal{O}^\dagger_\sigma + \mathcal{O}^\dagger_\sigma |n\rangle \langle n| \mathcal{O}_\sigma(t)\Big) |m\rangle \qquad \left[\sum_n |n\rangle\langle n| = 1\right] \\
&= \frac{1}{Z}\sum_{m,n} e^{-\beta E_m} \langle m| \Big(e^{iH^*t}\mathcal{O}_\sigma e^{-iH^*t} |n\rangle \langle n| \mathcal{O}^\dagger_\sigma + \mathcal{O}^\dagger_\sigma |n\rangle \langle n| e^{iH^*t}\mathcal{O}_\sigma e^{-iH^*t}\Big) |m\rangle \\
&= \frac{1}{Z}\sum_{m,n} e^{-\beta E_m} \Big(e^{i\left(E_m - E_n\right)t} \langle m| \mathcal{O}_\sigma |n\rangle \langle n| \mathcal{O}^\dagger_\sigma |m\rangle + e^{i\left(E_n - E_m\right)t} \langle m| \mathcal{O}^\dagger_\sigma |n\rangle \langle n| \mathcal{O}_\sigma |m\rangle\Big) \\
&= \frac{1}{Z}\sum_{m,n} e^{i\left(E_m - E_n\right)t} || \langle m| \mathcal{O}_\sigma |n\rangle ||^2 \left(e^{-\beta E_m} + e^{-\beta E_n}\right)
\end{aligned} \tag{A.0.3}$$

The time-domain impurity Green's function can thus be written as (this is the so-called Lehmann representation)

$$G^{\sigma}_{dd} = -i\theta(t)\frac{1}{Z}\sum_{m,n} e^{i\left(E_m - E_n\right)t} || \langle m| \mathcal{O}_\sigma |n\rangle ||^2 \left(e^{-\beta E_m} + e^{-\beta E_n}\right) \tag{A.0.4}$$

We are interested in the frequency domain form.

$$\begin{aligned} G^{\sigma}_{dd}(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} G^{\sigma}_{dd}(t) \\ &= \frac{1}{Z}\sum_{m,n} || \langle m| \mathcal{O}_\sigma |n\rangle ||^2 \left(e^{-\beta E_m} + e^{-\beta E_n}\right)\left(-i\right)\int_{-\infty}^{\infty} dt \theta(t) e^{i\left(\omega + E_m - E_n\right)t} \end{aligned} \tag{A.0.5}$$

To evaluate the time-integral, we will use the integral representation of the Heaviside function:

$$\theta(t) = \frac{1}{2\pi i}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\frac{1}{x - i\eta} e^{ixt} dx \tag{A.0.6}$$

With this definition, the integral in $G^{\sigma}_{dd}(\omega)$ becomes

$$\begin{aligned} \left(-i\right)\int_{-\infty}^{\infty} dt\theta(t) e^{i\left(\omega+E_m-E_n\right)t} &= \left(-i\right)\frac{1}{2\pi i}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty} dx \frac{1}{x - i\eta}\int_{-\infty}^{\infty} dt e^{i\left(\omega + E_m - E_n + x\right)t} \\ &= \left(-i\right)\frac{1}{2\pi i}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty} dx\frac{1}{x-i\eta} 2\pi\delta\left(\omega + E_m - E_n + x\right) \\ &= \left(-i\right)\frac{1}{i}\lim_{\eta\to 0^+}\frac{-1}{\omega + E_m - E_n - i\eta} \\ &= \frac{1}{\omega + E_m - E_n} \end{aligned} \tag{A.0.7}$$

The frequency-domain Green's function is thus

$$G^{\sigma}_{dd}(\omega) = \frac{1}{Z}\sum_{m,n} || \langle m| \mathcal{O}_\sigma |n\rangle ||^2 \left(e^{-\beta E_m} + e^{-\beta E_n}\right)\frac{1}{\omega + E_m - E_n} \tag{A.0.8}$$

The zero temperature Green's function is obtained by taking the limit of $\beta \to \infty$. In both the partition function as well as inside the summation, the only term that will survive is the exponential of the ground state energy E_0.

$$Z \equiv \sum_m e^{-\beta E_m} \implies \lim_{\beta\to\infty} Z = d_0 e^{-\beta E_0}, \quad E_0 \equiv \min\left\{E_n\right\}$$

where d_0 is the degeneracy of the ground state. The Greens function then simplifies to

$$\begin{aligned} G^{\sigma}_{dd}(\omega, \beta\to\infty) &= \frac{1}{d_0 e^{-\beta E_0}}\sum_{m,n} || \langle m| \mathcal{O}_\sigma |n\rangle ||^2 \left[e^{-\beta E_m}\delta_{E_m,E_0} + e^{-\beta E_n}\delta_{E_n,E_0}\right]\frac{1}{\omega + E_m - E_n} \\ &= \frac{1}{d_0}\sum_{n,0}\left[|| \langle 0| \mathcal{O}_\sigma |n\rangle ||^2 \frac{1}{\omega + E_0 - E_n} + || \langle n| \mathcal{O}_\sigma |0\rangle ||^2 \frac{1}{\omega - E_0 + E_n}\right] \end{aligned} \tag{A.0.9}$$

The label 0 sums over all states $|0\rangle$ with energy E_0. The spectral function is the imaginary part of this Green's function. To extract the imaginary part, we insert an infinitesimal imaginary part in the denominator:

$$G^{\sigma}_{dd}(\omega, \eta) = \frac{1}{d_0}\lim_{\eta\to 0^-}\sum_{n,0}\left[|| \langle 0| \mathcal{O}_\sigma |n\rangle ||^2 \frac{1}{\omega + E_0 - E_n + i\eta} + || \langle n| \mathcal{O}_\sigma |0\rangle ||^2 \frac{1}{\omega - E_0 + E_n + i\eta}\right] \tag{A.0.10}$$

The spectral function at zero temperature can then be written as

$$
\begin{aligned}
\mathcal{A}(\omega) &= -\frac{1}{\pi}\ \mathrm{Im}\ \left[G^{\sigma}_{dd}\left(\omega\right)\right] \\
&= \frac{1}{d_0}\frac{1}{\pi}\ \mathrm{Im}\ \left[\lim_{\eta\to 0^-}\sum_{n,0}\left(\frac{-i\eta||\left\langle 0\right|\mathcal{O}_\sigma\left|n\right\rangle||^2}{\left(\omega+E_0-E_n\right)^2+\eta^2}+\frac{-i\eta||\left\langle n\right|\mathcal{O}_\sigma\left|0\right\rangle||^2}{\left(\omega-E_0+E_n\right)^2+\eta^2}\right)\right] \\
&= \frac{1}{d_0}\frac{1}{\pi}\sum_{n,0}\left[||\left\langle 0\right|\mathcal{O}_\sigma\left|n\right\rangle||^2\pi\delta\left(\omega+E_0-E_n\right)+||\left\langle n\right|\mathcal{O}_\sigma\left|0\right\rangle||^2\pi\delta\left(\omega-E_0+E_n\right)\right] \\
&= \frac{1}{d_0}\sum_{n,0}\left[||\left\langle 0\right|\mathcal{O}_\sigma\left|n\right\rangle||^2\delta\left(\omega+E_0-E_n\right)+||\left\langle n\right|\mathcal{O}_\sigma\left|0\right\rangle||^2\delta\left(\omega-E_0+E_n\right)\right]
\end{aligned}
\tag{A.0.11}
$$