Solution for Homework 2

Problem 1.

We consider the symmetric ($\epsilon_f = -\frac{U}{2}$) Anderson impurity model:

$$H = \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k\sigma} (V_k c^\dagger_{k\sigma} f_\sigma + V_k^* f^\dagger_\sigma c_{k\sigma}) + \epsilon_f (n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow$$

Evaluating the impurity Greens function $G_\sigma(\tau) = \langle f_\sigma(\tau) f^\dagger_{sigma}(0)\rangle$ we can integrate out the conduction electrons $c_{k\sigma}$ to end up with:

$$G(i\omega) = \frac{1}{i\omega - \epsilon_f - \Delta(i\omega) - \Sigma(i\omega)}$$

where the the hybridization function is

$$\Delta(i\omega_n) = \sum_k \frac{|V_k|^2}{i\omega_n - \epsilon_k} = -i\Gamma \mathrm{sign}(\omega_n)$$

and $\Gamma = V^2\rho = 1$. In the symmetric case the Hartrey term in the self energy cancels ϵ_f and we only need to consider the second order term, so:

$$G(i\omega) = \frac{1}{G_0^{-1}(i\omega) - \Sigma_2(i\omega)} \tag{1}$$

where $G_0^{-1}(i\omega) = i\omega + i\Gamma\mathrm{sign}(\omega_n)$. In bare perturbation theory the self energy can be written as a convolution type integral in frequency representation:

$$\Sigma_2(i\omega) = U^2 T^2 \sum_{i\omega', i\Omega} G_0(i\omega + i\Omega) G_0(i\omega') G_0(i\omega' + i\Omega) \tag{2}$$

or as a product of Green's function in time representation:

$$\Sigma_2(\tau) = U^2 G_0^3(\tau) \tag{3}$$

In selfconsistent perturbation theory the free Green's function G_0 in the above two equations should be substituted by the full Green's function defined in Eq.(1) and equations solved selfconsistently.

When solving equations numerically we discretize variables and store functions as arrays (lists). The analog of the Fourier transformation of the continues function $a(\tau)$ is the discrete Fourier transformation of the discrete function a_r will be:

$$\begin{aligned} b_s &= \frac{c}{N} \sum_{r=-n}^{r=n} a_r \mathrm{e}^{2\pi i r s/N} \\ a_r &= c^{-1} \sum_{s=-n}^{s=n} b_s \mathrm{e}^{-2\pi i s r/N} \end{aligned} \tag{4}$$

where the second line is the inverse transformation, c is an arbitrary constant and $N = 2n{+}1$. To make correspondence to Matsubara frequencies we set:

$$\omega_s = \pi T s, \quad \tau_r = 2\beta r/N, \quad c = \beta$$

In the limit $N \to \infty$ Eq.(4) becomes:

$$\begin{aligned} a(i\omega) &= \frac{1}{2}\int_{-\beta}^{\beta} d\tau a(\tau) \mathrm{e}^{i\omega_n \tau} \\ a(\tau) &= T \sum_{i\omega_n} a(i\omega) \mathrm{e}^{-i\omega_n \tau} \end{aligned} \tag{5}$$

Frequencies $s = \pm 1, \pm 3, ...$ are relevant in Fermi statistics, while $s = 0, \pm 2, \pm 4, ...$ are relevant in Bose statistics.

Two-point functions in perturbation theory have (slowly decaying) asymptotics: $C(i\omega)\ 1/(i\omega)$. On the other hand, number of matsubara frequencies which we can sum up using a computer is quite finite. To handle this problem we use the knowledge of the function's asymptotics to separate it into a slowly decaying part, which can be summed analytically, and a fast decaying part, which can be easily summed numerically. For example, to Fourier transform a Green's function we do:

$$G(i\omega) = \{G(i\omega) - (i\omega)^{-1}\} + (i\omega)^{-1}$$

The first term (curly brackets) has asymptotics $\ \omega^{-2}$ and can be Fourier transformed numerically. For the last term we have:

$$T \sum_{i\omega_n} \frac{1}{i\omega} \mathrm{e}^{-i\omega_n \tau} = -\frac{1}{2}\Theta(\tau)$$

In case of the real frequencies, similarly:

$$\begin{aligned} G(i\omega) &= \{G(\omega) - \omega^{-1}\} + \omega^{-1} \\ \mathcal{P}\int \frac{d\omega}{2\pi}\omega^{-1}\mathrm{e}^{-i\omega\tau} &= -\frac{i}{2}\Theta(\tau) \end{aligned}$$

In general, a convolution type transformation, like Fourier transformation, if implemented effectively, can be performed in $O(N \ln N)$ time, much faster than a naive $O(N^2)$ estimate. If one computes self energy straitforwardly in frequency domain, like prescribed by Eq.(2), one would need $O(N^2)$ time. Therefor we chose to resort to time domain Eq.(3), price for that is Fourier transformations, which can be done in $O(N \ln N)$. Here is the algorithm:

$$G(i\omega) \xrightarrow{\text{InvFT}} G(\tau) \to \Sigma(\tau) \xrightarrow{\text{FT}} \Sigma(i\omega) \to G(i\omega)$$

In the bare perturbation theory we start with $G = G_0$ and iterate this loop once, while in selfconsistent approach the loop is iterated until convergence is reached.

To compute the spectral function $A(\omega)$ at $T = 0$ we compute Green's function in real frequency $G(\omega)$ and take the imaginary part:

$$A(\omega) = -\mathrm{Im}G_R(\omega) = -\mathrm{Im}G(\omega + i\delta) \tag{6}$$

The computation of finite T spectral function is more involved. We first derive the expression of the self energy in terms of the spectral functions. We use the following representation of the Green's function:

$$G(\omega) = -\frac{1}{\pi}\int d\omega' \frac{A(\omega')}{\omega' - \omega}$$

to write:

$$\Sigma_2(i\omega) = -U^2T^2 \sum_{i\omega', i\Omega} \int \frac{dxdydz}{\pi^3} \frac{1}{(x - i\omega')(y - i\omega' - i\Omega)(z - i\omega - i\Omega)}$$

Performing standard Matsubara frequency summation, continuing to real frequencies $i\omega \to \omega + i\delta$ and taking the imaginary part of the expression we find:

$$\mathrm{Im}\Sigma(\omega + i\delta) = -U^2 \int \frac{dxdy}{\pi^2}[b(y) + f(y + \omega)][f(x) - f(x + y)]A(x)A(x + y)A(y + \omega) \tag{7}$$

where $f(x)$ and $b(x)$ are Fermi and Bose functions. In principle, we could use the Kramers-Kronig relation to compute $\Sigma(\omega)$ from its imaginary part and then use Eq.(6) to close the loop. However direct use of Eq.(7) or Kramers Kronig requires $O(N^2)$ of computational time. We will show how one can do all calculations in $O(N \ln N)$.

Using relation $b(y)[f(x) - f(x + y)] = f(-x)f(x + y)$ we rewrite Eq.(7) as:

$$\begin{aligned}\mathrm{Im}\Sigma(\omega + i\delta) = -U^2 \int \frac{dxdy}{\pi^2}\\ [A_2(x)A_1(x + y)A(y + \omega) + A_1(x)A(x + y)A_1(y + \omega) - A(x)A_1(x + y)A_1(y + \omega)]\end{aligned} \tag{8}$$

where

$$A_1(x) = A(x)f(x), \quad A_2(x) = A(x)f(-x)$$

In time representation Eq.(8) becomes

$$\mathrm{Im}\Sigma(t) = -4U^2[A_2(t)A_1(-t)A(t) + A_1(t)A(-t)A_1(t) - A(t)A_1(-t)A_1(t)]$$

We should how to compute $\mathrm{Im}\Sigma$ by using Fourier transform and regular multiplication. Instead of using Kramers Kronig we can compute real part of self energy in the same way as we did for real part. For that we use a slightly different representation for one out of three Green's functions in Eq.(2):

$$G(\omega) = -\frac{i}{\pi}\int d\omega' \frac{B(\omega')}{\omega' - \omega}$$

where $B(\omega)$ is defined as

$$B(\omega) = \mathrm{Re}G(\omega + i\delta)$$

Then for the real part of Σ we find:

$$\mathrm{Re}\Sigma(\omega) = U^2 \int \frac{dxdy}{\pi^2} \\ [A_2(x)A_1(x+y)B(y+\omega) - A_1(x)B(x+y)A_1(y+\omega) - B(x)A_1(x+y)A_1(y+\omega)] \quad (9)$$

or in time representation:

$$\mathrm{Re}\Sigma(t) = 4U^2[A_2(t)A_1(-t)B(t) + A_1(t)B(-t)A_1(t) - B(t)A_1(-t)A_1(t)]$$

This completes calculation of $\Sigma = \mathrm{Re}\Sigma + i\mathrm{Im}\Sigma$.

In the attached Mathematica notebook file we implement algorithm we outlined above. All computations are done in $O(N \ln N)$ time.