Assignment 4: The Metal Insulator Transition in Clean Systems

This the last assignment. It is designed to give you a better understanding of the tricky parts of the Fourier transformation in a simple example of the solution of a many body problem.

The problem is to discretize and solve the discrete version of the following system of DMFT equations for $G(i\omega_n), \omega_n = (2n + 1)\pi T, n = -\infty \ldots \infty$.

1. $G_o(i\omega_n) = [i\omega_n - t^2G(i\omega_n)]^{-1}$
2. $G_o(\tau) = T \sum_{n=\infty}^{\infty} e^{-i\omega_n\tau}G_o(i\omega_n))$
3. $\Sigma(\tau) = -U^2G_o(\tau)^2G_o(-\tau)$
4. $\sum(i\omega_n) = \frac{1}{2} \int_{-\beta}^{\beta} e^{i\omega_n\tau} \Sigma(\tau)d\tau$
5. $G(i\omega_n) = \frac{1}{[G_o(i\omega_n) - \Sigma(i\omega_n)]}$

$U$ and $t$ are parameters whose physical meaning are temperature, interaction strength and hopping integral. $G(i\omega_n) \propto i\omega_n$ means insulating behavior $G(i\omega_n) \approx i(\sigma\omega_n)$ as $\omega_n \rightarrow 0$ means metallic behavior.

You should regard 1 - 5 as a toy model system having the minimal type of non linearities necessary to model a complex physical phenomena, i.e. Mott transition.

We want to explore numerically the full solution of (1) - (5).

However first solve the trivial cases $U = 0$, and $t = 0$ analytically. Discuss the limiting behavior of the self energy $\Sigma$ as the frequency goes to zero.

Then choose a discretization in $\tau$ space $\tau_i$, and a cutoff in frequency space, play with $N$ the number of slices of $[-\beta, \beta]$. See how the results change when $U$ is changed.

You are given the information that $G(o^+) = -\frac{1}{2}, G(o^-) = \frac{1}{2}$, so that $G(\tau)$ has a discontinuity at 0. Furthermore since the frequencies that enter (2) are of the form $(2n + 1)\pi T, G(\tau + \beta) = -G(\tau)$. Also $G(i\omega_n) = -G(-i\omega_n)$.

The strategy for solving the system 1-5 is to first discretize it and then solve it by iteration. Steps (1) (3) and (5) are trivial to implement. Step 2 involves a Fourier transform of a function with a long time tail, transform $[G_o(i\omega_n) - \frac{1}{i\omega_n}]$ numerically and $\frac{1}{i\omega_n}$ analytically $T \sum_n e^{i\omega_n\tau} \frac{1}{i\omega_n} = \{\frac{1}{2} if \beta > \tau > 0 \}$ (Check!) and observe how Fourier trades a long $\frac{1}{i\omega}$ tail for a discontinuity.
Step 4 involves a Fourier transform of a function with a known discontinuity. You first interpolate (linear interpolation is enough) and then Fourier transform the interpolation. Make sure the interpolating function has the right discontinuity and the right boundary values $\sum(-\beta + \sigma)$ and $\sum(\beta - \sigma)$. 

Now you see how Fourier converts discontinuities into long tails. Now explore the high temperature regime set $t = \frac{1}{2}, T = .02$. Start with the $U=0$ solution as an initial guess and solve the system 1-5 for $U = .5, 1, 1.5, 2, 2.5, 3$ then begin with the $t=0$ solution as an initial guess and solve (1-5), for $U = 6, 5, 4, 3$. [When you increase $U$ or decrease $U$, use the previously obtained solution as an initial guess.] Display the $G(i\omega_n)$ vs $i\omega_n$ for different $U$’s in a graph. Is the evolution as a function of $U$ smooth? Now repeat the same steps at much lower temperatures $T = .02$ paying close attention to the neighborhood of the point $U=3$. Is the evolution smooth?