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

T 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 $G(i\omega_n) \simeq i(sig\omega_n)$ 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 Σ as the frequency goes to zero.

Then choose a discretization in τ space τ_i, and a cuttoff 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 $\frac{1}{i\omega_r}$ analytically $T\sum_n \frac{e^{i\omega_n \tau}}{i\omega_n} = \{ \begin{smallmatrix} \frac{1}{2} & \beta>\tau>o \\ \frac{1}{2} & -\beta<\tau<o \end{smallmatrix}$ (Check!) and observe how Fourier trades a long $\frac{1}{i\omega}$ tail for a discontinuity.

Step 4 involves a Fourrier 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 $\sum(-\beta + o)$ and $\sum(\beta - o)$. $(\sum(\tau + \beta) = -\sum(\tau))$. Now you see how Fourier converts discontinuities into long $\frac{1}{i\omega}$ tails. Now explore the high temperature regime set $t = \frac{1}{2}$, $T = .02$. Start with the U=o solution as an initial guess and solve the system 1-5 for U = .5, 1, l.5, 2, 2.5, 3 then begin with the t=o 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?