Assignment 4: The Metal Insulator Transition in Clean Systems (corrected version)

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  $G(i\omega_n), \omega_n = (2n+1)\pi T, n = -\infty \dots \infty$ .

- 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.  $\Sigma(\tau) = -U^2 G_o(\tau)^2 G_o(-\tau)$
- 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  $\omega_n \to 0$  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 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  $T\sum_n \frac{e^{i\omega_n\tau}}{i\omega_n} = \begin{cases} \frac{1}{2} & \beta > \tau > o \\ \frac{1}{2} & -\beta < \tau < o \end{cases}$  (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, 1.5, 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?