between the localized moment and the conduction electrons, we use for the latter operators $c, c^\dagger$, e.g. $n_{\mathbf{k},\sigma} = c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$. The energy $\epsilon_{\mathbf{k}}$ can be computed as the Fourier transform of the tunneling coefficient t_{ij} of the Hubbard model $\epsilon_{\mathbf{k}} = \sum_{<i,j>} t_{i,j} e^{-i\mathbf{k}.(\mathbf{r}_i - \mathbf{r}_j)}$. The second term H takes care of the mixing between the localized f-state and the degenerate band-electrons in which it is embedded. $V(\mathbf{k})$ describes the hybridization between the impurity potential and a plane wave.

$$V(\mathbf{k}) = < \mathbf{k}|V_{impurity}|f> = \int d^3x e^{-i\mathbf{k}.\mathbf{x}} V_{impurity}(\mathbf{x}) \psi_f(\mathbf{x}) \tag{5}$$

The Matsubara Green's function of this model, defined as $G_{imp}(\tau) = - < \hat{T} f(\tau) f^\dagger(0) >$, with $\hat{T}$ the time-ordering operator, is entirely determined by U, ϵ_f and the hybridization function Δ:

$$\Delta(i\omega_n) = \frac{1}{\Omega_0} \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{i\omega_n - \epsilon_{\mathbf{k}}} \tag{6}$$

where $\omega_n = \frac{(2n+1)\pi}{\beta}$, $\beta = \frac{1}{k_B T}$ and T the temperature of the system. The hybridization describes the dynamics of electrons going in and out of the bath.

C. DMFT

1. The Green's functions

The DMFT method is based on the computations of the one particle Green's function $G_{ij}(\tau - \tau') = - < T c_{i,\sigma}(\tau) c^\dagger_{j,\sigma}(\tau') >$, where τ is the imaginary time, of the Hubbard model and the one associated to the Anderson impurity model G_{imp}. The self-consistency condition requires that the impurity Green's function G_{imp} coincides with the local lattice Green's function

$$G_{loc}(i\omega_n) = G_{ii}(i\omega_n) = \sum_{\mathbf{k}} \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, i\omega_n)} \tag{7}$$

with $\omega_n = \frac{(2n+1)\pi}{\beta}$ the imaginary frequency, $\beta = \frac{1}{k_B T}$, T the temperature of the system, $\Sigma(\mathbf{k}, i\omega_n)$ the self-energy and the following Fourier transform:

$$G(i\omega_n) = \int_0^\beta d\tau G(\tau) e^{i\omega_n \tau} \tag{8}$$

The local approximation consist to neglect the spatial fluctuations of the self-energy by considering it equals to the impurity self-energy

$$\Sigma(\mathbf{k}, i\omega_n) = \Sigma_{imp}(i\omega_n) \tag{9}$$

This approximation becomes exact in the limit of lattices with infinite coordination, that is when the number of neighbors of each site is infinite [1, 5]. Indeed, one can show that in the diagrammatic expansion of the lattice self-energy, only local diagrams survive when one goes into the infinite coordination limit.

Thus, as in classical mean-field theories, DMFT is supposed to get more accurate as the dimensionality (and thus the number of neighbors) increases. Put differently, for low dimensions, spatial fluctuations will render the DMFT approximation less reliable, especially to determine accurately the critical order parameters of phase transitions.

2. The numerical scheme

Most of the computation are done in the imaginary-frequency space before going back in the real-frequency space after convergence of the recursive numerical scheme.

1. Make a guess for Σ_{imp}. Usually there is 2 choices, either one start with $\Sigma_{imp} = 0$ which is a metallic initial condition or one start with $\Sigma_{imp} \propto -\frac{1}{i\omega_n}$ which is an insulator initial condition.

2. Obtain the local Green's function:

$$G_{loc}(i\omega_n) = \frac{1}{N_k} \sum_{\mathbf{k}} \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} - \Sigma_{imp}(i\omega_n)}, \tag{10}$$

where N_k is the number of k-points. For instance, for a two-dimensional square lattice:

$$G_{loc}(i\omega_n) = \frac{1}{N_x N_y} \sum_{k_x, k_y}^{N_x, N_y} \frac{1}{i\omega_n - \epsilon_{k_x, k_y} - \Sigma_{imp}(i\omega_n)}. \tag{11}$$

If only the density of state in energy $\rho(e)$ is known, we can use the following formula:

$$G_{loc}(i\omega_n) = \frac{1}{N_e} \sum_e \frac{\rho(e)}{i\omega_n - e - \Sigma_{imp}(i\omega_n)}, \tag{12}$$

Where N_e is the number of energy points.

3. Use the Dyson equation to compute the non-interacting Green's function :

$$G_0(i\omega_n) = \frac{1}{G_{loc}^{-1}(i\omega_n) + \Sigma_{imp}(i\omega_n)} \tag{13}$$

4. A solver is needed in order to compute the new impurity self-energy. We use the Impurity Perturbative Theory (IPT) solver [6], which is an expansion of the self energy up to the order U^2:

$$\Sigma'_{imp}(i\omega_n) = U^2 \int_0^\beta G_0(\tau)^3 e^{i\omega_n \tau} d\tau$$
$$= U^2 \sum_{j=1}^N G_0\left(j\frac{\beta}{N}\right)^3 e^{i\omega_n(j\frac{\beta}{N})} \frac{\beta}{N} \tag{14}$$

Where one have to be careful on the computation of $G_0(\tau)$ the inverse Fourier transform of $G_0(i\omega_n)$, because it is expected that $G_0(i\omega_n) \sim \frac{1}{i\omega_n}$ and $\int_{-\infty}^{+\infty} d\omega \frac{e^{-i\omega\tau}}{i\omega}$ converges very badly:

$$
\begin{aligned}
G_0(\tau) &= \int_{-\infty}^{+\infty} G_0(i\omega_n)e^{-i\omega_n\tau}d\omega \\
&= \int_{-\infty}^{+\infty} (G_0(i\omega_n) - \frac{1}{i\omega_n} + \frac{1}{i\omega_n})e^{-i\omega_n\tau}d\omega
\end{aligned}
\tag{15}
$$

By writing $G'(i\omega_n) = G_0(i\omega_n) - \frac{1}{i\omega_n}$, 2 integrals have to be computed. The first one converges better as $G' = \mathcal{O}\left(\frac{1}{(i\omega_n)^2}\right)$, we can thus use its discrete form. The second one is a well known integral which can be calculated analytically (its value is $\frac{\text{sign}(\tau)}{2}$)

$$
\begin{aligned}
G_0(\tau) &= \frac{1}{\beta} \sum_{n=-N}^{N-1} (G'(i\omega_n))e^{-i\omega_n\tau} - \frac{\text{sign}(\tau)}{2} \\
&= \frac{2}{\beta} \sum_{n=0}^{N-1} Re(G'(i\omega_n)e^{-i\omega_n\tau}) - \frac{\text{sign}(\tau)}{2}
\end{aligned}
\tag{16}
$$

using the fact that $\omega_{-n} = -\omega_{n-1}$ and $G'(-i\omega_n) = G'^*(i\omega_{n-1})$.

5. Get the impurity Green's function using Dyson equation:

$$
G_{imp}(i\omega_n) = \frac{1}{G_0^{-1}(i\omega_n) + \Sigma'_{imp}(i\omega_n)}
\tag{17}
$$

6. Perform the Self-consistent test : Is $G_{imp} = G_{loc}$? Compute the following in order to know if the convergence has been reached:

$$
D = \sqrt{\sum_n (G_{imp}(i\omega_n) - G_{loc}(i\omega_n))}
\tag{18}
$$

Is $D < \delta$? with δ a small parameter (typically $\delta = 10^{-10}$). If no, go back to step 2 with Σ'_{imp}. If yes, go the following step.

7. Perform the Padé approximation in order to go from the imaginary-frequency axis to the real-frequency axis. The idea is to make an analytic continuation of the complex axis to obtain the real axis. One way to do this is to use the Padé approximation, which is an approximation of a discrete set of points by a rational function. It is a better than a regular polynomial approximation because:

   - We can choose the function to go to 0 (the polynomial approximation always diverges).
   - The approximation take into account the eventual poles of the function, which are very important for analytic continuation.

   - The approximation is more precise than the polynomial one.
   - The form of the Green function is always close to be rational.

8. Compute the spectral function $A(\omega) = -\frac{1}{\pi}Im(G_{imp}(\omega))$ and we can deduce, for example, if the system is an insulator or a metal.

III. RESULTS

A. The Mott insulator to metal phase transition

Mott insulators are a class of materials presenting a conductor phase as predicted by usual band theory and an insulator phase (particularly at low temperatures) which is not well described by band theory due to strong electron-electron interactions. The Mott insulator to metal phase transition can be captured by the Hubbard model and its associated Anderson Impurity model [7].

To test the algorithm we can work with the 2D Hubbard model with a density of state given by:

$$
\epsilon_{\vec{k}} = -2t\left(\cos(k_x a) + \cos(k_y a)\right),
\tag{19}
$$

where $a = 1$ is the lattice spacing and $t = 1$ is the hopping integral between nearest neighbour. The bandwidth is then $D = 4t$ and will be our energy reference. The calculation of the Green function was made at low temperature $T/D = 0.01$ and the spectral function can be deduce by the formula:

$$
A(\omega) = -\frac{Im(G(\omega))}{\pi},
\tag{20}
$$

for different value of the interaction U. The result of these calculation are plotted in (1). The calculation stopped when the difference between the Green-function of two steps is below a threshold (here 10^{-10}). The initial condition is $\Sigma(\omega) = 0$, which correspond to a metallic state. We will study later the influence of such a choice on the result, especially close to the transition.

Without interaction, the density of state of a regular 2D tight binding model is recovered as expected. The system is a metal as far as $A(0)$, the density of state at the Fermi energy, is non zero (at half filling). On the contrary for large interaction, the system become an insulator (a Mott insulator) as $A(0)$ vanishes. In between, there is a three-peak structure and the system stay metallic, because of the central peak, the quasi-particle band, which assure $A(0)$ to be non zero in this regime.

These two state are the two state one could expect for such a system, and thus using the value of the spectral function on the Fermi surface, it is possible to obtain the phase diagram of the system.