Occupancy Fluctuation Effect on Metal-Insulator Transition in Hubbard Model within Dynamical Mean-Field Theory

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Reference to read DMFT

General references

- ***DMFT, extensions and applications.***
  - A. Georges, G. Kotliar, W. Krauth and M. Rozenberg, Rev. Mod. Phys. 68, 13, (1996).
  - G. Kotliar, S.Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, C.A. Marianetti, Rev. Mod. Phys. 78, 865 (2006)
- ***Metal Insulator transitions.***
  - M. Imada, A.Fujimori, Y.Tokura Rev. Mod. Phys. 70, 1039 (1998)

Hubbard Model

Hubbard model

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$$H = -\sum_{\langle ij\rangle,\sigma=\uparrow,\downarrow} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U n_{i\uparrow} n_{i\downarrow}, \qquad n_{i\sigma} \equiv c^{\dagger}_{i\sigma} c_{i\sigma}$$

$$\delta = 1 - \langle n_{\uparrow} + n_{\downarrow} \rangle$$

Kinetic term

Interaction term
local Coulomb

- A toy-model for strongly correlated systems.
- Plays a role similar to the Ising model in classical statistical physics.
- Parameters :
  - hopping t, frustration t'/t (lattice shape), Coulomb repulsion U
  - doping δ (chemical potential μ), temperature T.
- Half filling : 1 electron/site in average : δ=0

MFT Approach

MFT approach begins by expressing[1]

$$n_{i\uparrow} = \langle n_{i\uparrow} \rangle + (n_{i\uparrow} - \langle n_{i\uparrow} \rangle);$$
$$n_{i\downarrow} = \langle n_{i\downarrow} \rangle + (n_{i\downarrow} - \langle n_{i\downarrow} \rangle)$$

Subtituting these expressions into hubbard hamiltonian. Thus, self-energy matrix element becomes

$$\Sigma_{i\sigma} = U \langle n_{i\sigma'} \rangle n_{i\sigma} \tag{1}$$

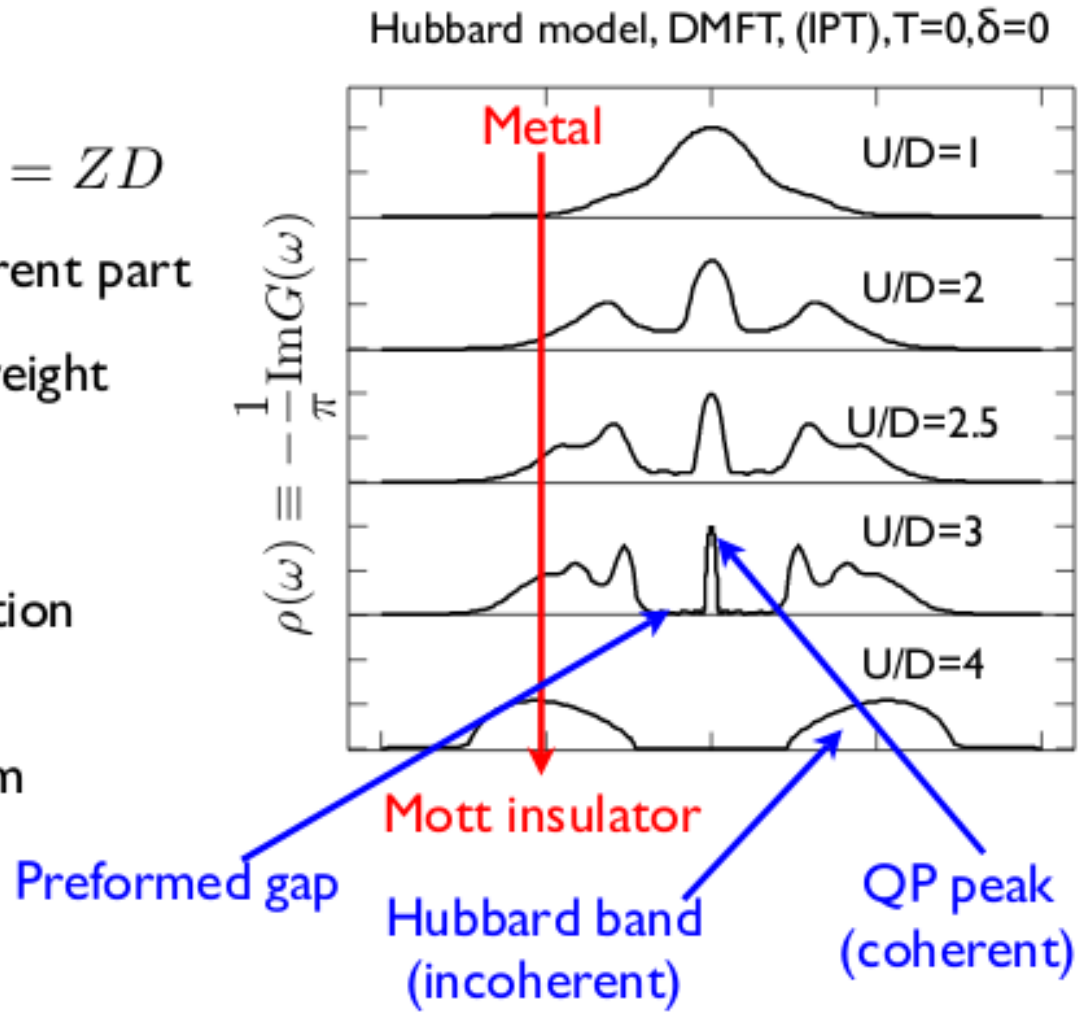
This is also often called as hartree-fock approximation (first order correction)

Because static (no dependencies on energy) self energy, this approach is not good enough for explain for strongly correlated system.

[1] Y Claveau, et.al. 2014 European Journal of Physics 35 035023

Why do we need DMFT?

- Fermi liquid with low coherence scale : $\epsilon_F^* = ZD$
- Coherent and incoherent part
- Transfer of spectral weight from low to high ω
- Beyond a low energy quasi-particle description (slave bosons)
- Price : solve a quantum impurity model.



DMFT: Self Consistent

Solving DMFT : iterative method

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Impurity solver

$$S_{\text{eff}} = -\int_0^\beta c_\sigma^\dagger(\tau)\mathcal{G}_\sigma^{-1}(\tau-\tau')c_\sigma(\tau') + \int_0^\beta d\tau\, U n_\uparrow(\tau) n_\downarrow(\tau)$$

$$G_{\sigma\text{imp}}(\tau) \equiv \left\langle T c_\sigma(\tau) c_\sigma^\dagger(0)\right\rangle_{S_{\text{eff}}}$$

$$\Sigma_{\sigma\text{imp}}(i\omega_n) \equiv \mathcal{G}_\sigma^{-1}(i\omega_n) - G_{\sigma\text{imp}}^{-1}(i\omega_n)$$

$\mathcal{G}$

G_{imp}, Σ_{imp}

Self consistency condition

$$G_{\sigma\text{imp}}[\mathcal{G}](i\omega_n) = \sum_k \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_{\sigma\text{imp}}[\mathcal{G}](i\omega_n)}$$

How to Solve Quantum Impurity Model?

- *Numerical methods :*
  - Quantum Monte-Carlo (Hirsch-Fye, CTQMC).
  - Exact diagonalisation (ED).
  - Renormalization group methods : NRG, DMRG.
- *Analytic methods :*
  - Low energy theories : bosonisation, boundary CFT.
  - Integrability by Bethe Ansatz.
  - Projective method.
- *Approximate methods (fast) :*
  - Iterated Perturbation Theory (IPT)
  - NCA familly (NCA, large-N, SUNCA).

Comparison of impurity solver

- CTQMC :
  - Finite temperature. Flexible
  - Potential sign problem. Imaginary time. "Slow"
- DMRG, NRG :
  - Real time
  - Low T only, limited to 2/3 bands ?
- Approximate solvers : IPT, NCA, Slave Bosons
  - Very fast. To e.g. explore phase diagram.
  - Not exact.

Motivation

- Fast impurity solver
- Better than IPT(Second Order Pertubation Correction)
- No need on analytic continuation

Occupation Fluctuation Approach

In finite temperature, there have been shown temperature dependence on MIT[2] Expressing interaction term as

$$U\sum_j n_{j\uparrow}n_{j\downarrow} = \frac{U}{2}\sum_j n_{j\uparrow}n_{j\downarrow} + n_{j\downarrow}n_{j\uparrow}$$
$$= \frac{U}{2}\sum_j n_{j\uparrow}(\langle n_{j\downarrow}\rangle + \delta_{j\downarrow}) + n_{j\downarrow}(\langle n_{j\uparrow}\rangle + \delta_{j\uparrow})$$

Hence, the self-energy matrix element can be written as

$$\Sigma'_{j\sigma} = \frac{U}{2}(\langle n_{j\sigma'}\rangle + \delta_{j\sigma}) \tag{2}$$

[2] G. Kotliar, et.al. Physical Review Letters 84 22

DMFT Continue

Matsubara green function is

$$G_{j\sigma}(i\omega_n) = \frac{1}{N}\sum_{k}\frac{1}{i\omega_n - \mathcal{E}(\boldsymbol{k}) + \mu - \Sigma_{j\sigma}(\boldsymbol{\delta})} \tag{3}$$

where $\omega_n = (2n+1)\pi T$ is Matsubara fermionic frequency. In the first iteration, we set $\mathbf{\Sigma}(i\omega_n) = 0$. The bath Green's function is then computed,

$$\mathcal{G}(i\omega_n) = [G(i\omega_n)^{-1} + \mathbf{\Sigma}(\boldsymbol{\delta})]^{-1} \tag{4}$$

and the local interacting Green's function is

$$\tilde{G}(i\omega_n, \boldsymbol{\delta}) = [\mathcal{G}(i\omega_n) - \mathbf{\Sigma}'(\boldsymbol{\delta})]^{-1} \tag{5}$$

It is convinient to write Grassman effective action as

$$S_{eff} = -\sum_{n} \ln \det[\mathcal{G}(i\omega_n)\tilde{G}(i\omega_n, \boldsymbol{\delta})] e^{i\omega_n \eta^+} \tag{6}$$

and partition function

$$\mathcal{Z} = \int d\boldsymbol{\delta}_{\alpha\sigma}\ P(\delta_{\alpha\sigma}) \tag{7}$$

where $P(\delta_\sigma)$ as Boltzmann Factor, which is computed as

$$P(\delta_{\alpha\sigma}) = \frac{1}{\mathcal{Z}} \exp\left(-S_{eff}\right) \tag{8}$$

Now, we average the local interacting Green's function over all fluctuation

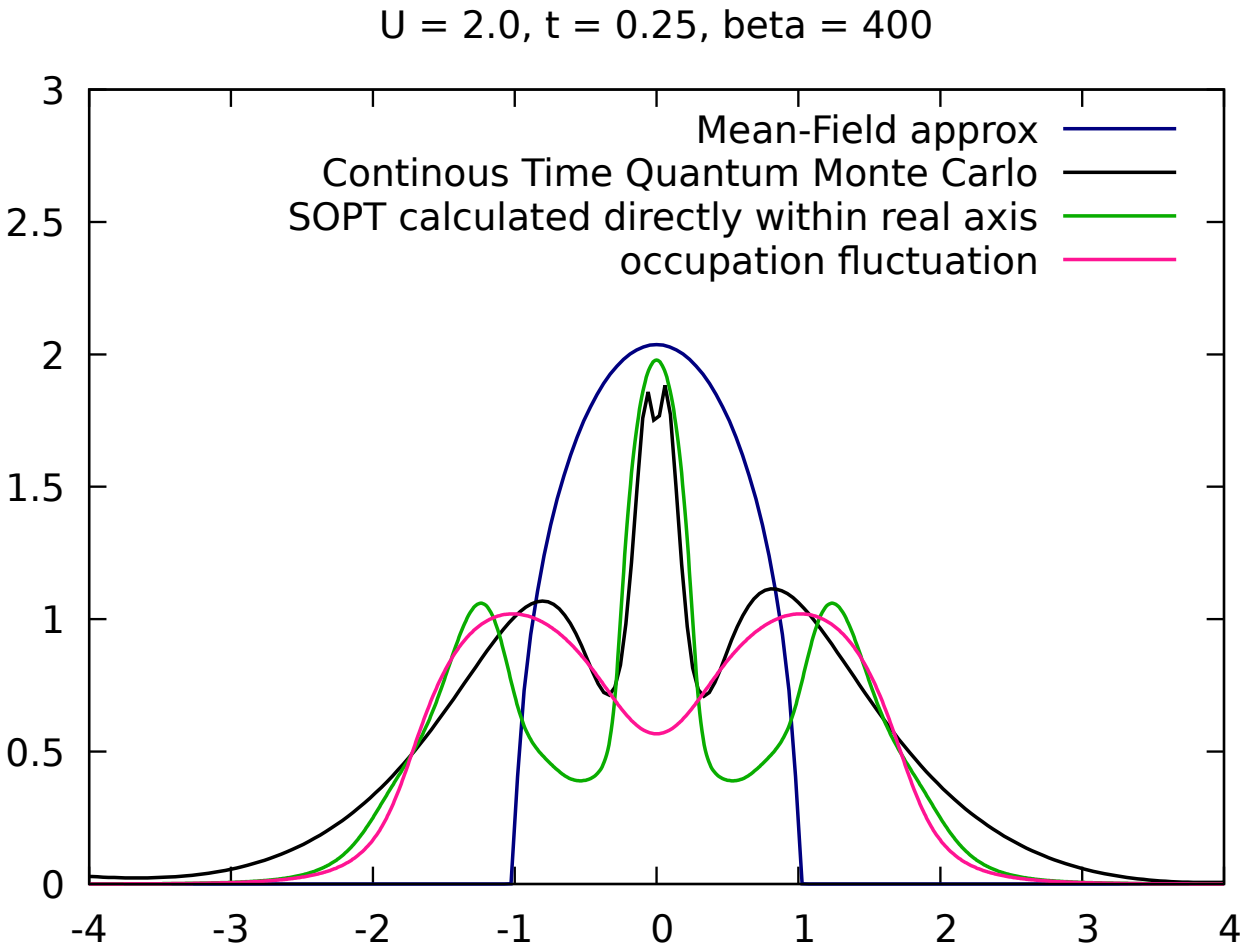
$$G(i\omega_n) = \int d\boldsymbol{\delta}_{\alpha\sigma} P(\delta_{\alpha\sigma}) \tilde{G}_\sigma(i\omega_n, \delta_{\alpha\sigma}) \tag{9}$$

Then we calculate self-energy

$$\boldsymbol{\Sigma}_{\text{calc}}(i\omega_n) = \mathcal{G}^{-1}(i\omega_n) - G^{-1}(i\omega_n) \tag{10}$$

The Self-consistency is eliminated when $\boldsymbol{\Sigma}_{\text{calc}} - \boldsymbol{\Sigma}$ is less than threshold.

Result: Paramagnetic Case



Conclusion

- We have constructed new lower numerical cost (sorry not to show CPU time here, but it is much faster than CT-QMC although little slower than IPT) impurity solver within DMFT. But still not yet enough to show quasi-particle peak at low energy.
- The semiclassical fluctuation generated from mean-field self-energy, next we planned to generated semiclassical fluctuation from second order correction instead mean-field.