561 Fall 2005 Lecture 15

Lattice models for interacting electrons and Dynamical Mean Field Theory - DMFT

Most thorough review to date: A. Georges, G. Kotliar, W. Krauth and M. J. Rozenberg, "Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions"Rev. Mod. Phys. 68, 13-125 (1996).
Recent review: K. Held, et. al. Psi$_k$ highlight (can find on web).
Popular article: G. Kotliar and D. Vollhardt, Physics Today, March 2004. p. 53.

1. Summary

The basic idea of dynamical mean field theory (DMFT) is to take into account correlations explicitly within a local region, treating all effects of the surrounding medium via a *dynamical mean field*. This can be viewed as a generalization of the *Weiss mean field* that embodies average effects of neighbors with thermal fluctuations or the *coherent potential approximation* that represents the average propagation of an electrons through an alloy with random potentials. Like those examples, the dynamical mean field is determined by a self-consistency condition relating the mean field and local expectation values. The generalization to a quantum system requires that the field be *dynamical*, i.e., frequency- or time-dependent, to include the effects of quantum fluctuations. DMFT is naturally formulated in terms of Green's functions and self-energies closely related to those used in the many-body perturbation methods The solution for the local region explicitly include local correlations of the electrons using non-perturbative methods such as exact diagonalizationa and QMC. It is fruitful to see the correspondence to other methods as we develop practical approaches to DMFT in terms of the local approximations. The simplest approximation for the local region is a single site, in which case the theory reduces to a self-consistent version of the Anderson and Kondo impurity models. This approximation is exact in three limits: 1) non-interacting electrons, 2) isolated atoms, and 3) the limit of high dimensions where mean field theory is exact. Studies of Hubbard models have led to dramatic conclusions on metal-insulator transitions, etc., and there have been many applications to problems such as Ce, and transition metal oxides. Dynamical cluster approximation (DCA) approaches take into account additional effects of local correlation and provide an in-principle way to reach the exact solution as the limit of large clusters.

2. Classical static mean field theory

The concept of a mean field plays a central role in all areas of many-body and statistical physics. In the field of electronic structure, mean field approximations for electron-electron interactions are ubiquitous. The Hartree-Fock approximation leads to a potential $V_{HF}(\mathbf{r},\mathbf{r}')$ that is non-local in space, but is local in time, i.e, it is independent of energy. The Kohn-Sham potential $V_{KS}(\mathbf{r})$ is local in both space and time; its value at each point $\mathbf{r}$ in principle is a functional of the density $n(\mathbf{r}')$ everywhere, but practical approximations in terms of the density assume $V_{KS}(\mathbf{r})$ depends only upon the density in a local region near $\mathbf{r}$.

Mean field theory is also the paradigm in statistical mechanics for understanding phase transitions. A simple example is the Ising model for interacting spins

$$H = -\sum_{i,j} J_{ij} S_i S_j - h \sum_i S_i \tag{1}$$

where h is an external magnetic field and J_{ij} are spin interactions. The average spin on each site is the thermal average $m_i \equiv \langle S_i \rangle$. This mean field approach is to assume that each spin S_i acts as if it is is in an effective magnetic field h_{eff} – the Weiss field, introduced by P. Weiss in 1907 – which is the sum of an external field and an average of effects of interactions with neighbors,

$$h_{eff} = h + \sum_j J_{ij} m_j \tag{2}$$

where $\langle S_j \rangle$ denotes a thermal average. If S_i is in thermal equilibrium in the effective field h_{eff}, then it is given by the Brillouin function

$$m_i = tanh(h_{eff}/k_B T) \tag{3}$$

Of course site i is no different from the other sites and the condition that $m_i = m_j \equiv m$ for all j leads to the self-consistent equation

$$m = tanh([h + zJm]/k_B T), \tag{4}$$

where z is the number of neighbors and J is the interaction.

This leads to the well-known mean field approximation for the magnetic phase transitions as a function of temperature.

The mean field equations become exact in the limit of a large number of neighbors z since fluctuations since in that case the neighbors act as a bath in which the fluctuations of the effective field become small. This is formally the case for lattices in which the dimensionality d is allowed to become large, i.e., the $d \to \infty$ limit.

Scattering of waves in disordered media has an even longer history, exemplified by Rayleigh's famous theories of scattering of light and sound waves. In quantum mechanics perhaps the original use is in disordered systems, such as alloys, and the coherent potential approximation (CPA) is an effective potential acting on a site that self-consistently reproduces the average effect of a random distribution of neighbors. See for example review of CPA by R. J. Elliott, J. A. Krumhansl and P. L. Leath in Rev Mod Phys

An important step in many-body physics is the alloy analogy for interacting electrons by Hubbard in the famous Hubbard I approximation.

3. Generalization to quantum dynamical mean field theory

Different lines of reasoning have converged to define a set of approaches to the quantum many-body problem, known variously as "dynamical mean field theory" or dynamical CPA as well as other descriptive terms. We will refer to the general approach as "dynamical mean field theory" (DMFT), and we will denote useful, approximate versions by acronyms "DxA" where "A" serves as a reminder that an approximation has been made.

Generalization of the Hubbard's analogy to alloys - review by Kakehashi[1] - Is the 1992 paper by Kakehashi[1] equivalent to Jarrell and Georges refs. below?

Correlated fermions in infinite dimensions[2] and subsequent work that mapped the Hubbard model onto a self-consistent quantum impurity model and provided effective methods for solution[3, 4]

Review by Georges, et al.[5]

In classical mean-field theory, the local magnetization m_i is assumed to be given by equations for a single spin decoupled from the other spins, except for the effective mean

	MFT	DFT	DMFT
Local Observable	Magnetization m_i at site i	Density $n(\mathbf{x})$ at point $\mathbf{x}$	Green's Func. $G_{ii}(\omega)$ at site i
Equivalent system	Spin in effective field	Electrons in effective potential	Quantum impurity model
Generalised Weiss field	Effective local field	Kohn-Sham potential	Effective hybridization

Table 1: Comparison of theories based on functionals of a local observable, From Georges lecture notes with small modifications.

	Quantum	Classical
Hamiltonian H	$-\sum_{ij\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + \sum_i H_{site}(i)$	$-\sum_{ij} J_{ij} S_i S_j - h \sum_i S_i$
Local Observable	$G_{ii}(z) = - < c^{\dagger}_i(\tau) c_i(0) >_{i\omega_n}$	$m_i = < S_i >$
Effective single-site Hamiltonian	$H_{eff} = H_{site} + \sum_{l\sigma} \tilde{\varepsilon}_k c^{\dagger}_{k\sigma} c_{k\sigma} + + \sum_{l\sigma} \tilde{V}_k (c^{\dagger}_{k\sigma} c_{i\sigma} + h.c)$	$H_{eff} = -h_{eff}\, S$
Effective mean field	$\tilde{\Delta}(z) = \sum_l \frac{\lvert V_l \rvert^2}{z - \tilde{\varepsilon}_l}$ $\mathcal{G}_0^{-1}(z) \equiv z + \mu - \tilde{\Delta}(z)$	h_{eff}
Self-consistency relation	$\sum_{\mathbf{k}} [\tilde{\Delta}(z) + G(z)^{-1} - \varepsilon_{\mathbf{k}}]^{-1} = G(z)$	$h_{eff} = \sum_j J_{ij} m_j + h$

Table 2: Correspondence between the static mean-field theory of a classical system and the dynamical mean-field theory of a quantum system. From Georges lecture notes with small modifications.

field due to the average effects of neighbors, the Weiss field. In a quantum system effective mean fields can be introduced in analogous manner; however, quantum mechanics introduces a dependence upon time or energy because the effective field must take into account the exchange of particles between the site and the neighboring region. This is accomplished through the construction of an *effective action* at the site and a Green's function $\mathcal{G}_0(\tau - \tau')$ that describes creation of a fermion on the central site at time τ (i.e., coming from the other sites that form an "external bath") and destroyed at time τ' (i.e., going to the bath). The function $\mathcal{G}_0(\tau - \tau')$ plays the role of a quantum dynamical mean field and, in the single-site approximation, DMFT corresponds to solving the quantum problem for interacting electrons on the central site in the presence of the dynamical mean field. (It is useful to work with imaginary time $\tau = it$ and the Matsubara formalism.)

1 Dynamical local approximation (DLA): mapping to a quantum impurity problem

CHECK - what is best abbreviation? DLA??

The DMFT approach can be illustrated by the simplest model, the one-band Hubbard model discussed in Sec. **??**. The hamiltonian given in Eq. **??** is repeated here,

$$\hat{H} = \sum_{i \neq j \sigma} t_{i \neq j} c^{+}_{i\sigma} c_{j\sigma} + \sum_{i\sigma} \varepsilon_0 \hat{n}_{i\sigma} + \frac{1}{2} U \sum_{i\sigma} \hat{n}_{i\sigma}, \hat{n}_{i-\sigma}, \tag{5}$$

where i, j label the sites in the lattice and $\hat{n}_{i\sigma} = c^{+}_{i\sigma} c_{i\sigma}$. The interaction U is limited to opposite spin electrons on the same site, and the the single-body kinetic terms t_{ij} lead to dispersion to the electron states. The simplest model assumes the $t's$ are zero except for nearest neighbor hopping terms. (We will also consider t' for second neighbors, which plays an important role in some cases.)

If the mean field is applied to a single site, the problem simplifies in a way analogous to the Weiss mean field of magnetism. The central quantity in the theory is the local Green's function on a given site i

$$G^{\sigma}_{ii}(\tau - \tau') = -\langle T_\tau c_{i\sigma}(\tau) c^{\dagger}_{i\sigma}(\tau') \rangle \tag{6}$$

Since the mean field approach in the single-site approximation considers all other sites as an effective bath, the problem reduces to an Anderson impurity model. All of theoretical understanding and machinery developed for the impurity model can be carried over to DMFT in the single-site approximation. However, there is a crucial difference that the effective dynamical mean field must be self-consistent with the solution on the central site. This "bootstrapping" effect can lead to phase transitions and other physical phenomena qualitatively different from the consequences for an impurity in a host metal.

The hamiltonian for the Anderson impurity model is given by the same expression as before except for changes in notation:

$$\begin{aligned} H &= H_{site} + H_{bath} + H_{hybridization} \\ &= \varepsilon_0 c^{+}_{i\sigma} c_{i\sigma} + U n_{i\uparrow} n_{i\downarrow} + \sum_{k\sigma} \tilde{\epsilon}_k c^{+}_{k\sigma} c_{k\sigma} + \sum_{k\sigma} \tilde{V}_{ki} [c^{+}_{k\sigma} c_{i\sigma} + c^{+}_{i\sigma} c_{k\sigma}]. \end{aligned} \tag{7}$$

The difference in the present case is that the first term the original interacting hamiltonian on site i(which is not really an impurity) and the quantities $\tilde{\epsilon}_k$ and $\tilde{V}_{kL}$ are effective parameters describing the rest of the system as a bath and the hybridization of the site and the bath.

If there were no interaction ($U = 0$) the previous analysis of the AIM shows that the effective Green's function on the site is

$$\mathcal{G}(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_0 - \tilde{\Delta}(i\omega_n)} \tag{8}$$

with

$$\tilde{\Delta}(i\omega_n) = \sum_k \frac{\tilde{V}^2_k}{i\omega_n - \tilde{\epsilon}_k} \rightarrow \sum_l \frac{\tilde{V}^2_l}{i\omega_n - \tilde{\epsilon}_l}. \tag{9}$$

Note that the only way the bath enters the equations is through the function $\tilde{\Delta}(i\omega_n)$. It is not actually needed to express $\tilde{\Delta}(i\omega_n)$ in terms of the $\tilde{V}_k$ and $\tilde{\epsilon}_k$; instead, it can be replaced

by a sum the represents the spectrum on the site. This is the effective function that is varied to find the self-consistent solution as described below.

The solution of the problem involves treating the interaction on the site in the presence of the coupling to the bath and finally achieving a self-consistent solution in which the bath is consistent with the central site. The Green's function on the site can be written (with $G_{ii} = G$ to simplify the notation)

$$G(i\omega_n) = \frac{1}{\mathcal{G}(i\omega_n)^{-}1 - \Sigma_{ii}(i\omega_n)} = \frac{1}{i\omega_n - \varepsilon_0 - \Sigma_{ii}(i\omega_n) + \tilde{\Delta}(i\omega_n)}, \tag{10}$$

where the self-energy $\Sigma_{ii}(i\omega_n)$ must be calculated from a many-body solution of the interacting electron problem for the central site coupled to the bath. There are various methods called "impurity solvers" which vary from quantum Monte Carlo and exact diagonalization algorithms that provide accurate solutions to approximate, but illuminating, solutions such as the large N solution of the impurity problem.

Returning to the original problem, the full Green's function for the original lattice problem has the form

$$G_{\mathbf{k}}(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_0 - \varepsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(i\omega_n)}, \tag{11}$$

where $\varepsilon_{\mathbf{k}} = \sum_j t_{ij} e^{1\mathbf{k}\cdot(\mathbf{R}_i - R_j)}$ is the original band for lattice with $U = 0$ and $\Sigma_{\mathbf{k}}(i\omega_n)$ is the self-energy. The local single-site approximation is that the self-energy $\Sigma_{\mathbf{k}}(i\omega_n)$ is assumed to be local, i.e., it is $\mathbf{k}$-independent and

$$\Sigma_{\mathbf{k}}(i\omega_n) \approx \Sigma_{ii}(i\omega_n). \tag{12}$$

Then the lattice Green's function is

$$G_{\mathbf{k}}(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_0 - \varepsilon_{\mathbf{k}} - \Sigma_{ii}(i\omega_n)}, \tag{13}$$

and the site Green's function is

$$G(i\omega_n) = \sum_{\mathbf{k}} G_{\mathbf{k}}(i\omega_n), \tag{14}$$

This fully specifies the single-site DMFT solution provided a self-consistent solution can be found. Since the only functions that are to be determined are $\Sigma_{ii}(i\omega_n)$ and $\tilde{\Delta}(i\omega_n)$, the steps are:

1. Assume a form for $\tilde{\Delta}(i\omega_n)$
2. Calculate $\Sigma_{ii}(i\omega_n)$ using a many-body "impurity solver" in the presence of the bath represented by the $\tilde{\Delta}(i\omega_n)$
3. Calculate the new $G(i\omega_n)$ and $\tilde{\Delta}(i\omega_n)$ and iterate

It is straightforward to show from the equations that the self-consistency condition can be written

$$G(i\omega_n) = \sum_{\mathbf{k}} \frac{1}{\tilde{\Delta}(i\omega_n) + G(i\omega_n)^{-1} - \varepsilon_{\mathbf{k}}}. \tag{15}$$

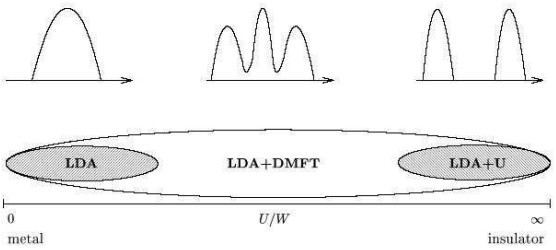

Figure 1: With increasing strength of the local Coulomb repulsion U (relative to the LDA bandwidth W), one observes a weakly correlated metal (left density of states), a strongly correlated metal with a quasiparticle peak at the Fermi energy (middle), and a Mott insulator (right). The weakly correlated metal and the (ordered) Mott insulator are correctly described by LDA and LDA+U, respectively. LDA+DMFT gives the correct answer for all values of U and subsumes the LDA valid for small U/W and the LDA+U results for the Mott insulator appearing at large U/W.

Figure 1: Schematic illustration of DMFT. From Held Psik review - Fig. 1

the relation of DMFT to two types of mean field models: LDA - example of the "usual" DFT that overemphasizes delocalization - LDA+U - example adding local static mean field terms - DMFT that includes the improved treatment of the on-site correlations together with the dynamical mean field.

Methods for solving the self-consistent quantum impurity problem - "Impurity solvers

1. Quantum Monte Carlo - the algorithm made by Hirsch and Fye for the impurity Anderson model - well tested - the most exact approach

2. Exact diagonalization algorithms that solve the problem exactly the impurity embedded in a discrete, finite set of neighbors. Requires extrapolation to a large number of neighbors

3. Approximate, but illuminating, solutions. For example, the such as the large N solution of the impurity problem.

Hubbard Model and metal insulator transitions

Key ideas

Hubbard model is mapped on a self-consistent Anderson lattice model - a low energy scale emerges from the Hubbard model analogous to the Kondo energy scale

Self-consistency can lead to phase transitions - metal-insulator transitions

Finds two types of solutions

Metallic with peak at Fermi energy having weight $Z \to 0$ for $U \to U_{c2}$.

Insulating for $U > U_{c1}$, where $U_{c1} < U_{c2}$. The spectra are shown in Fig. 1.

First order phase transition ending in critical point in range $U_{c1} < U < U_{c2}$, as shon in Fig. 1.

This is very much like the real transition in V_2O_3.

Transition metal oxides - V_2O_3 - prototype metal-insulator transition

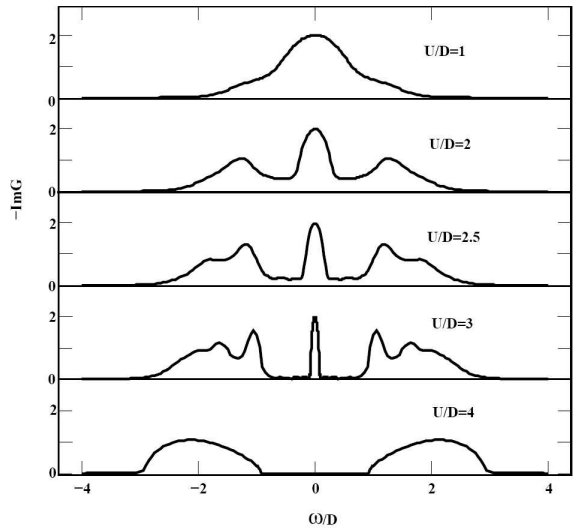

Figure 2: DMFT calculation of the local spectral function for several values of the interaction strength for the half-filled Hubbard model with a semi-circular d.o.s (from Georges RMP review). Close to the transition, there is a clear separation of scales between the quasiparticle peak at the Fermi energy and the distance between Hubbard bands.

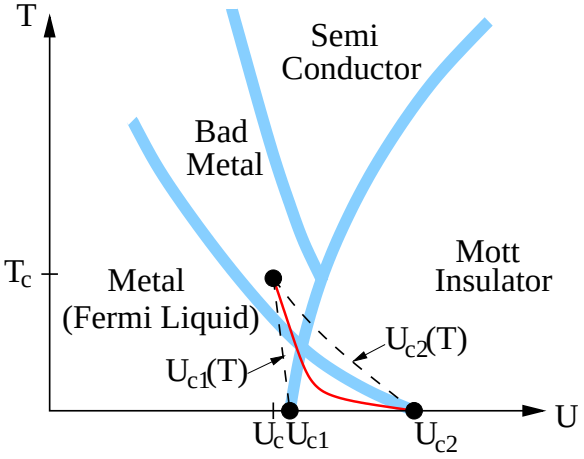

Figure 3: Phases of the Hubbard model within DMFT. Dschematically the spinodal lines of the insulating and metallic mean-field solutions. The first-order transition line is the solid line ending in a critical point. Shaded lines are crossovers for different transport regimes. Magnetic phases are not considered and depend on the lattice and degree of frustration. Figure from review by Georges in 2002.

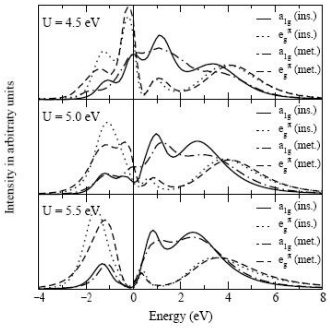

Figure 13: LDA+DMFT(QMC) spectra for paramagnetic $(V_{0.962}Cr_{0.038})_2O_3$ ("ins.") and V_2O_3 ("met.") at $U = 4.5$, 5 and 5.5 eV, and $T = 0.1$ eV = 1160 K [reproduced from Ref.48].

Figure 4: Spectra of showing the metal insulator transition as a function of U. From Held Psik review - Fig. 13

Figure showing results for doped V_2O_3. See Fig. 1.

Anomalous rare earth systems

Materials that are prototype systems for the Anderson and Kondo lattice models.

Results for Ce spectra given in Fig. 1

Also total energies and the volume transition in Ce, Pr, Nd.

Actinides - "band-to-localized" transition in the 5f series

The 5f series presents the difficult challenge of the intermediate case where interaction strengths U are comparable to band widths W

Most problematic element Pu description of the "band-to-localized" transition and the complicated phase diagram

Figure of phonon anomalies calculated before the experiments shown in Fig. 1.

Dynamical cluster approximations - toward a general theory

A general approach to the solution of the many-body problem in extended systems. A systematic approach to treating short range correlations while including long range mean-field effects.

Various approaches being developed.

References

[1] Y. Kakehashi, 'Electron correlations and many-body techniques in magnetism', *Adv. Phys.* 53:497–536, 2004.

[2] Walter Metzner and Dieter Vollhardt, 'Correlated lattice fermions in d = infinity dimensions', *Physical Review Letters* 62(3):324–327, 1989.

[3] A. Georges and G. Kotliar, 'Hubbard model in infinite dimensions', *Phys. Rev. B* 45:6479–6483, 1992.

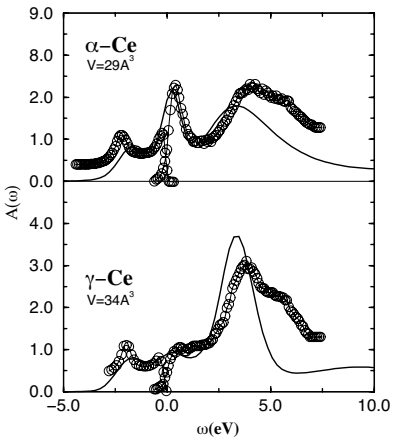

Figure 5: Electron addition/removal spectra for Ce in the alpha phase calculated using DMFT - MaMahan, et al.

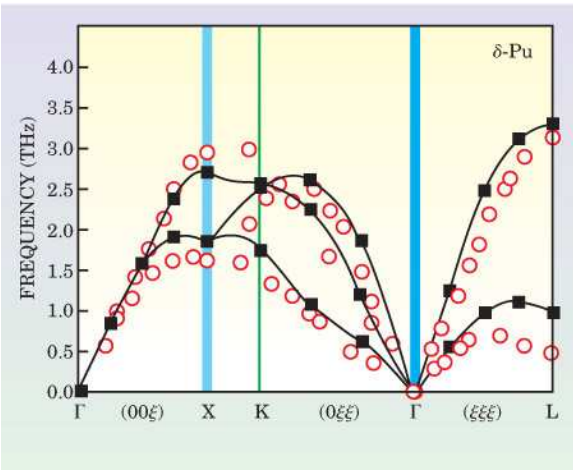

Figure 6: Figure of phonon anomalies calculated before the experiments From Physics Today article.

[4] M. Jarrell, 'Hubbard model in infinite dimensions: A quantum monte carlo study', *Phys. Rev. Lett.* 69:168–171, 1992.

[5] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg, 'Dynamical mean-field theory of strongly correlated fermion systems and the limit of infinite dimensions', *Rev. Mod. Phys.* 68:13–125, 1996.