1 G. Kotliar's Lecture 1 on LDA+DMFT : Constraining Field Formulation

In the celebrated density functional theory (DFT) approach, the total energy of a solid is expressed as a functional of the charge density of the material. The physical meaning of that functional is that its extrema, gives the physical density of the material and the value of the functional at the stationary point gives the total energy. It turns out that the actual density of the solid can be regarded also as the density of a fictitious set of non interacting particles ("Kohn Sham particles" whose role is to reproduce the density of the solid. Therefore, one can find a potential, called the Kohn Sham potential, such that free particles in this potential have the same density as our fully interacting solid.

It turns out that not only DFT but many other different mean field theories (for example, spectral density functionals such as Dynamical Mean Field Theory (DMFT) DFT+DMFT, GW, GW+DMFT , Baym Kadanoff theory , the "self energy functional " theory, and other static mean field theories such as Hartree Fock LSDA and LDA+U,) can be viewed as special cases of a general construction of a mean field theory. This construction highlights why all these approaches are ultimately mean field constructions in complete analogy with the Weiss mean field theory of spin systems. In this lecture, we will introduce the general formalism first. This will allow us to highlight the similarities and differences between different electronic structure approaches, and will give us a route to construct the Dynamical Mean Field Theory of correlated solids. Finally the abstract construction is a general recipe for constructing mean field theories that can be helpful to the students in his or her research.

The presentation closely follows a recent review [G. Kotliar, S.Savrasov, K. Haule, V.Oudovenko, O. Parcollet, and C.Marianetti, Rev. Mod. Phys. 78, 000865 (2006)] to which the students are referred for further references to the original work and numerous applications. I tried to provide all the intermediate steps, so that this is accessible to everybody.

The general construction consists of the following steps. First a quick overview indicate the steps schematically, and then proceed to write the corresponding equations explicitly. The goal of the lectures (and of the review!) is to provide the students with a roadmap to the different approaches for studying the electronic structure of correlated materials.

1 Select an observable or a set of observables of interest, A_i. Namely, we will be interested in the expectation value of this observables $< A_i >= a_i$. For example in DFT the observables are the charge density in space.

2 Writte down the partition function $Z[J^i]$ of the system, by adding to the action describing the quantum mechanical system in question sources coupled to the observables of interest.

3 Perform a Legendre transformation from $F[J^i] = -Log[Z[J^i]]$ to $\Gamma[a_i]$ therefore eliminating the source J^i in favor of the expectation value of the observables a_i .

4 Divide the action of the problem into two parts. A part that we understand, i.e. our "reference system", and the rest that we multiply by a coupling constant " λ " which we will treat in a formal in perturbation theory around the reference system.

The zeroth order terms in this expansion of the source $J_o(a)$ is the constraining field. $\Gamma_0[a] = \Gamma[a, \lambda = 0] = F_0[J_0(a)] - aJ_0(a)$. The rest of the functional *Gamma* is denoted $\Delta\Gamma$, and it contains a Hartree term and an exchange and correlation part (usually denoted XC).

5 For the exact functional, of for its exchange and correlation piece $\Delta\Gamma_{xc}$ one has formal expressions as either an infinite sum of diagrams or a formal coupling constant integration formula.

So far, no approximations have been made. The success of building a successful mean field theory consist on chosing a clever separation of reference system and "perturbation" so that good approximations can be built to the exchange and correlation part of the functional. There are two ideas which have been very successful successful, one is to evaluate $Delta\Gamma$ in low order systematic perturbation theory in λ. The classic example here is the Weiss mean field theory which is obtained by the lowest order term in a high temperature expansion, while the next order term yields the celebrated Onsager correction. The use some **local** approximation and to request that the approach becomes exact in some limit. The classic example is the Local Density Approximation in LDA where the exchange and correlation functional is assumed to be local and its value is taken so that it gives the exact energy of the uniform electron gas.

6 The final step consist on the extremization of $\Gamma[A]$ to obtain the free energy of the system and the expectation value of A. The stationarity condition of the functional $\Gamma[a]$ results in $J_0(a) = \frac{\delta\Delta\Gamma}{\delta a}$ which together with the definition of $J_0(a)$ gives a closed set of mean field equations.

One can also compute (inverse) correlation functions by further differentiations.

Now a a few details of these steps starting with the functional integral expression for the partition function.

$$Z[J] = \exp(-F[J]) = \int D[\psi^\dagger\psi] e^{-(S+J^i A_i)}. \tag{1}$$

The Legendre transformation is defined

$$\frac{\delta F}{\delta J^i} = a_i \tag{2}$$

$$\Gamma[a] = F[J[a]] - a_i J^i[a_i] \tag{3}$$

Implicit sum over the index i is assumed, and in the future that index will be dropped alltogether, so a will stand for all the a_i's.

$\Gamma[A]$ has several useful properties which follow directly from the definitions, and reflect the stationarity of the functional Γ viewed as a functional of two independent variables a and J_0.

$$\frac{\partial \Gamma}{\partial a_i} = -J^i[a] \tag{4}$$

$$\frac{\partial \Gamma}{\partial \lambda} = \frac{\partial F}{\partial \lambda} \tag{5}$$

where λ is an arbitrary parameter of the action.

The original problem had no source, hence when we set the source to zero we obtain the value of the observable a^* in the state of interest.

$$\frac{\delta \Gamma}{\delta a}[{a^*}_i] = 0 \tag{6}$$

Therefore the value of $\Gamma[a = a^*] = F[J = 0]$ gives us the free energy of the system.

So far the construction is exact but not very useful. A key step to make progress is to separate the action into a part which we understand and serves as a reference system, S_0 and a perturbation. The action is written as $S = S_0 + \lambda S_1$.

A central point is that the system described by $S_0 + AJ_0$ serves as a reference system for the fully interacting problem. It is a **simpler** system which by construction, reproduces the correct value of the observable $\widetilde{A}$. When this observable is properly chosen, other observables of the system can be obtained perturbatively from their values in the reference system. Hence $S_0 + AJ_0$ is a simpler system which allows us to think perturbatively about the physics of a more complex problem. $J_0[A]$ is a central quantity in this formalism and we refer to it as the "constraining field". *It is the source that needs to be added to a reference action S_0 in order to produce a given value of the observable A.*

We now set a systematic expansion of the functional $\Gamma[A]$ to some order in a parameter or coupling constant λ.

$$F[J] = F_0[J] + \lambda F_1[J] + ..., \tag{7}$$

$$\Gamma[A] = \Gamma_0[A] + \lambda \Gamma_1[A] + ... \ , \tag{8}$$

$$J[A] = J_0[A] + \lambda J_1[A] + ... \ . \tag{9}$$

The expansion of Γ at fixed value of a is much better behaved than the expansion of F. For example, in the case of a spin system when a is the magnetization, working at fixed magenetization gives a convergent high temperature expansion for all temperatures, while the naive high temperature expansion of the free energy diverges at the Curie temperature.

The selection of S_0 in the action leads to the separation

$$\Gamma[a] = \Gamma_0[a] + \Delta\Gamma[a] \tag{10}$$

With

$$\Gamma_0[a] = F_0[J_0] - aJ_0 \tag{11}$$

In this equation $J_0 = J_0(a)$ with

$$\frac{\delta F}{\delta {J^i}_0} = a_i \tag{12}$$

is understood

Notice however that we can also consider $\Gamma_0[aJ_0]$ above as a function of two variables and demand stationarity in J_0 which gives back the definition of the constraining field. The same applies to the full functional Γ which can also be regarded as a functional of two variables.

$$\Gamma[a, J_0] = F_0[J_0] - aJ_0 + \Delta\Gamma[a] \tag{13}$$

as a functional which is stationary in two variables, the constraining field J_0 and A. The equation $\frac{\delta\Delta\Gamma}{\delta A} = J_0[A]$, together with the definition of $J_0[A]$ determines the exact constraining field for the problem.

$\Delta\Gamma$ can be given a coupling constant integration representation which is very useful, and has been rediscovered in many different contexts. From eq. 5

$$\Delta\Gamma[A] = \int_0^1 d\lambda \frac{\partial\Gamma}{\partial\lambda} = \int_0^1 d\lambda \langle S_1 \rangle_{J(\lambda),\lambda} \tag{14}$$

In many cases it is useful to decompose $\Delta\Gamma = \Gamma_H + \Gamma_{xc}$, by isolating the Hartree contribution which can usually be evaluated explicitly. The success of the method relies on obtaining good approximations to the "generalized exchange correlation" functional Γ_{xc} as discussed in the outline, and as we will see in the examples.

Differentiating eq. 10 with respect to a, we get the mean field theory equations

$$\frac{\delta\Delta\Gamma}{\delta a} = J_0[a] \tag{15}$$

Together with the definition of the constraining field in eq. 12 it is a non linear set of equations for the observable a.

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One can also use the stationarity condition of the functional (**??**) to express a as a functional of J_0 and to formulate the theory in terms of a functional of the *constraining field alone* (i.e. $\Gamma[J_0] = \Gamma[a[J_0], J_0]$). In the context of the Mott transition problem, this functional was first proposed and used to derive the analytical properties of the free energy underlying the dynamical mean field theory. In the context of Baym Kadanoff theory, this leads to the self energy functional theory.

Comments

The central point is that the choice of observable, and the choice of reference system (i.e. the choice of S_0 which determines J_0) determine the structure of the (static or dynamic) mean field theory to be used.

A mean field theory generally (but not always) starts by identifying a local quantity. In the case of Weiss mean field it is the magnetization, in the case of the density functional theory the local density in the case of DMFT it is the local spectral function. In the case of LDA+DMFT the density and the local spectral function.

The original system with infinite number of degrees of freedom is replaced by an effective system, which yields the same precise exact information for the local quantity selected. The simpler system, contains a "constraining field". It is the field that needs to be added to the simpler system so as to reproduce a given value of the selected local variable. The simpler system is a system of non interacting electrons, for the DFT problem, or a single spin for the ising system or an anderson impurity model for the local problem.

The constraining field depends on the local variable chosen, and there is a non linear equation determining it. These are the mean field equations. Finally even though mean field theories aim at determining a local quantity (density , magnetization etc.) in the process they also gives approximations to the correlation functions, which can be obtained from the functionals via differentiation.

Also other quantities can be obtained from the approach for example the k dependent ARPES spectra in solids or the optical conductivity can be calculated within DMFT.

If we take as our observable the full Greens function of the theory, we will see in the next lecture that we arrive at the Baym Kadanoff theory. In this case the constraining field is the self energy.

There is a representability isssue, namely under which circumstances we can obtain the exact value of the observable A, as an expectation function of a simpler system in the presence of a source, which has been swept under the

rug. In the present formalism it is the problem of invertibility of the Legendre transformations which have been assumed in the approach followed here, but can be proved more rigorously in some special cases.

Finally, notice that the Legendre transformation gives us a functional for which is an extremum for the physical value of a. However in general the extrema is usually a saddle point. In static mean field theories, it is possible to prove that the extrema is actually a minimum, but this is not the case for Dynamical Mean Field Theories. It should be noted that one is free to add terms containing powers higher than one in the source in order to modify the stability conditions of the functional without changing the properties of the saddle points. This freedom has been used to obtain functionals with better stability properties.

In the next lecture we will use this method to map the zoo of electronic structure methods by chosing different a's different Γ_o's and different exchange and correlation functionals Γ_{xc}. All the material of the second lecture and a lot more (in particular what you need to do to solve the key mean field theories of electronic structure!!!! as well as some success stories of the DMFT) can be found in:**G. Kotliar, S.Savrasov, K. Haule, V.Oudovenko, O. Parcollet, and C.Marianetti, Rev. Mod. Phys. 78, 000865 (2006)**