Functionals for DMFT and DFT+DMFT

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Contents

1 Introduction

In these notes, I gather derivations of DFT[1, 2, 3, 4, 5], DMFT[3, 5, 6] and DFT+DMFT [3, 5, 7] using a Legendre transformation. The aim is to highlight the physical or formal connections between the different theories and approximations.

2 Density Functional Theory

In this section, we rederive some basic equations of Density Functional Theory, as presented in the lecture of Julien Toulouse, using a Legendre transformation. We use mainly the notations of [3] with some minor reformulations.

2.1 A functional of the density

The electronic Hamiltonian H is composed of a non interacting part H_0 and an interaction part H_{int} :

$$H = H_0 + H_{\text{int}} = \sum_i \left(\frac{\nabla_i^2}{2} + V_{\text{ext}}(\mathbf{r}_i) \right) + \frac{1}{2} \sum_{ij} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{1}$$

In second quantization

$$H = \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \left(\frac{\nabla^2}{2} + V_{\text{ext}}(\mathbf{r}) \right) \Psi(\mathbf{r}) + \frac{1}{2} \int \Psi^\dagger(\mathbf{r}) \Psi^\dagger(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} \Psi(\mathbf{r}') \Psi(\mathbf{r}) d\mathbf{r} d\mathbf{r}' \tag{2}$$

For later use, we define an Hamiltonian with a rescaled interaction such that $H_\alpha = H_0 + \alpha H_{\text{int}}$. In this paragraph, however, we use $\alpha = 1$, so α does not play a role yet.

Moreover, we couple the system to a supplementary one body potential λ, the total Hamiltonian is thus $H_\alpha + \int d\mathbf{r} \lambda(\mathbf{r}) \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r})$.

We thus define the partition function Z_α and the free energy Ω_α for this Hamiltonian as a function of λ:

$$\widehat{\Omega}_\alpha[\lambda(\mathbf{r})] = -\frac{1}{\beta} \ln \widehat{Z}_\alpha[\lambda(\mathbf{r})] = -\frac{1}{\beta} \ln \mathrm{Tr}[\exp^{-\beta(H_\alpha + \int d\mathbf{r} \lambda(\mathbf{r}) \Psi^\dagger(\mathbf{r}) \Psi(\mathbf{r})))}] \tag{3}$$

The trace is a sum over all many-body eigenstates. We note that this expression gives the exact free energy $\mathcal{F}$ of the system if $\alpha = 1$ and $\lambda = 0$: $\mathcal{F} = \widehat{\Omega}_{\alpha=1}[\lambda(\mathbf{r}) = 0]$.

We can compute the exact density $n_\alpha(\mathbf{r})$ for the Hamiltonian $H_\alpha + \lambda$ with:

$$\frac{\delta \widehat{\Omega}_\alpha[\lambda(\mathbf{r})]}{\delta \lambda(\mathbf{r})} = \widehat{n}_\alpha(\mathbf{r})[\lambda(\mathbf{r})] \tag{4}$$

We now use the concavity of the functional $\widehat{\Omega}_\alpha[\lambda(\mathbf{r})]$ as a function of $\lambda(\mathbf{r})$[1].

From the concavity of the functional, we have the monotonous behavior of its first derivative, namely $\widehat{n}_\alpha(\mathbf{r})[\lambda(\mathbf{r})]$. We can thus inverse this relation so that λ is now a functional of $n(\mathbf{r})$: $\widehat{\lambda}_\alpha(\mathbf{r})[n(\mathbf{r})]$. The physical meaning of this functional is the following: For a given density $n(\mathbf{r})$, it gives the value of λ which is necessary to add to H_α in order that the density of Hamiltonian $H_\alpha + \lambda$ is $n(\mathbf{r})$.

We can thus define the following functional of the density (which is the Legendre transform of $\widehat{\Omega}_\alpha[\widehat{\lambda}(\mathbf{r})]$):

$$\widehat{\Gamma}_\alpha[n(\mathbf{r})] = \widehat{\Omega}_\alpha[\widehat{\lambda}_\alpha[n(\mathbf{r})]] - \mathrm{Tr}[n(\mathbf{r}) \lambda_\alpha[n(\mathbf{r})]] \tag{7}$$

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[1] For simplicity we show it at T=0K: Let us suppose that the system has a Hamiltonian $H + \beta\lambda_1 n(\mathbf{r}) + (1-\beta)\lambda_2 n(\mathbf{r})$ and the we call the ground state Ψ_β, thus, using the Ritz principle, we have:

$$\begin{aligned} \langle \Psi | H + \beta\lambda_1 n(\mathbf{r}) + (1-\beta)\lambda_2 n(\mathbf{r}) | \Psi \rangle &= \beta \langle \Psi | H + \lambda_1 n(\mathbf{r}) | \Psi \rangle (1-\beta) \langle \Psi | H + \lambda_2 n(\mathbf{r}) | \Psi \rangle & (5) \\ &\geq \beta E_{\text{GS}}(H_\alpha + \lambda_1) + (1-\beta) E_{\text{GS}}(H_\alpha + \lambda_2) & (6) \end{aligned}$$

where $E_{\text{GS}}(H)$ is the ground state energy for Hamiltonian H. The last line is the definition of concavity. (See Ref. [6] for a generalization to finite temperature)

2.2 The non interacting system: $\alpha = 0$.

Let's use this functional for $\alpha = 0$. We have thus:

$$\widehat{\Gamma}_0[n(\mathbf{r})] = \widehat{\Omega}_0[\widehat{\lambda}_0[n(\mathbf{r})]] - \mathrm{Tr}[n(\mathbf{r})\widehat{\lambda}_0[n(\mathbf{r})]] \tag{8}$$

We thus use Eq. 4, to obtain:

$$n(\mathbf{r}) = \frac{\delta\widehat{\Omega}_0}{\delta\lambda_0(\mathbf{r})}[\widehat{\lambda}_0[n(\mathbf{r})]] \tag{9}$$

In other word, the density is the density of a non interacting system ($\alpha = 0$) in an effective potential λ_0. So the density can be computed simply with the sum of individual wavefunctions which are the eigenvectors of the Hamiltonian $H + \lambda_0$. In other words, we know the functional $\frac{\delta\widehat{\Omega}_0}{\delta\lambda_0(\mathbf{r})}[\lambda_0]$. [2]

At this stage, λ_0 is a parameter.

2.3 The real system: $\alpha = 1$.

The functional of the density is:

$$\widehat{\Gamma}_1[n(\mathbf{r})] = \widehat{\Omega}_1[\widehat{\lambda}_1[n(\mathbf{r})]] - \mathrm{Tr}[n(\mathbf{r})\lambda_1[n(\mathbf{r})]] \tag{10}$$

We can compute the functional derivative with respect to $n(\mathbf{r})$ with:

$$\frac{\delta\widehat{\Gamma}_1}{\delta n(\mathbf{r})} = \frac{\delta\widehat{\Gamma}_1}{\delta\lambda_1(\mathbf{r})}\frac{\delta\lambda_1(\mathbf{r})}{\delta n(\mathbf{r})} + \left.\frac{\delta\widehat{\Gamma}_1}{\delta n(\mathbf{r})}\right|_{\lambda_1} = 0 + \lambda_1[n(\mathbf{r})] \tag{11}$$

(The first derivative disappears because of Eq. 4)

Now, we *choose* $\lambda_1 = 0$. We make this choice, because, using Eq. 10, if $\lambda_1 = 0$, then $\widehat{\Gamma}_1[n(\mathbf{r})] = \widehat{\Omega}_1[\lambda_1 = 0]$ is the exact free energy $\mathcal{F}$ of the real system by definition of $\widehat{\Omega}_1[\lambda_1 = 0]$. Thus, using Eq. 11, the functional $\widehat{\Gamma}_1[n(\mathbf{r})]$ is stationary for the exact density $n_{\mathrm{GS}}(\mathbf{r})$.

$$\frac{\delta\widehat{\Gamma}_1}{\delta n(\mathbf{r})}[n_{\mathrm{GS}}(\mathbf{r})] = 0 \tag{12}$$

and for this density, the functional is the exact free energy $\mathcal{F}$.

So we have a functional of the density which is stationary for the exact density, and for the exact density, the functional is the exact free energy.

2.4 The adiabatic connection

Let us now compute the derivative of $\widehat{\Gamma}$ as a function of α:

$$\frac{\partial\widehat{\Gamma}_\alpha[n(\mathbf{r})]}{\partial\alpha} = \frac{\delta\widehat{\Gamma}_\alpha[n(\mathbf{r})]}{\delta\lambda_\alpha(\mathbf{r})}\frac{\partial\lambda_\alpha}{\partial\alpha} + \left.\frac{\delta\widehat{\Gamma}_\alpha}{\delta\alpha}\right|_{\lambda_\alpha} = \left.\frac{\delta\widehat{\Gamma}_\alpha}{\delta\alpha}\right|_{\lambda_\alpha} = \langle H_{\mathrm{int}}\rangle_{\lambda_\alpha[n(\mathbf{r})]} \tag{13}$$

By integration, we have:

$$\Rightarrow \widehat{\Gamma}_1[n(\mathbf{r})] = \widehat{\Gamma}_0[n(\mathbf{r})] + \int_0^1 \langle H_{\mathrm{int}}\rangle_{\lambda_\alpha[n(\mathbf{r})]} d\alpha \tag{14}$$

$$= \widehat{\Omega}_0[\widehat{\lambda}_0[n(\mathbf{r})]] - \mathrm{Tr}[n(\mathbf{r})\widehat{\lambda}_0[n(\mathbf{r})]] + \int_0^1 \langle H_{\mathrm{int}}\rangle_{\lambda_\alpha[n(\mathbf{r})]} d\alpha \tag{15}$$

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[2] Indeed, the functional $\widehat{\Omega}_0[\widehat{\lambda}_0]$ can be practically evaluated. First one needs to solve the Schrödinger equation for the potential $v_{\mathrm{ext}} + \lambda_0$, then, using the eigenvalues $\epsilon_i[\lambda_0]$, one can compute the partition function functional as $\widehat{Z} = \prod_i [1 + \exp(-\beta(\epsilon_i - \mu))]$, and the free energy functional is thus $\widehat{\Omega} = -\frac{1}{\beta}\sum_i \ln[1 + \exp(-\beta(\epsilon_i - \mu))]$

To derive 15 from 14, we used Eq. 8.

Using $H_{\rm int} = \int \Psi^\dagger(\mathbf{r})\Psi^\dagger(\mathbf{r}')\frac{1}{|\mathbf{r}-\mathbf{r}'|}\Psi(\mathbf{r}')\Psi(\mathbf{r})d\mathbf{r}d\mathbf{r}'$, we can write the last term as[3]:

$$\int_0^1 \langle H_{\rm int}\rangle_{\lambda_\alpha[n(\mathbf{r})]}d\alpha = \widehat{E}_{\rm Ha}[n(\mathbf{r})] + \widehat{E}_{\rm xc}[n(\mathbf{r})] \tag{16}$$

It can be viewed as an alternative definition of $E_{\rm xc}$ with a coupling constant integration (see Refs [8, 3]). Then, we use eq. 12 with the expression of eq. 15 (in which all terms are known), to show that λ_0 is such that:

$$\widehat{\lambda}_0[n(\mathbf{r})] = \widehat{v}_{\rm Ha}[n(\mathbf{r})] + \widehat{v}_{\rm xc}[n(\mathbf{r})] \tag{17}$$

We can now identify λ_0 with the effective Kohn Sham potential.

Finally, in order to compare to the more familiarly $T = 0$ K case, we can write Eq. 15 as:

$$\widehat{E}[n(\mathbf{r})] = \widehat{E}_0[\widehat{v}_{\rm Ha+xc}[n(\mathbf{r})]] - \int d\mathbf{r}n(\mathbf{r})\widehat{v}_{\rm Ha+xc}[n(\mathbf{r})] + \widehat{E}_{\rm Ha+xc}[n(\mathbf{r})] \tag{18}$$

It is the usual expression for the total energy of the system as a function of the density. Where $E_0[\hat{v}_{\rm Ha+xc}[n(\mathbf{r})]]$ is the energy of a non interacting system with the potential $v_{\rm eff} = v_{\rm ext} + v_{\rm Ha+xc}$, namely the sum over the Kohn Sham eigenvalues.

To sum up, Eq. 9 shows that the density can be computed from a non interacting system. Eq. 17 shows that this effective potential is the Kohn Sham potential and Eq. 18 is the DFT total energy.

3 Functional of the Green's function

In this section, we will follow exactly the same lines to derive the Green's function functional theory (the Luttinger Ward or Baym Kadanoff Functional)[9, 10, 3, 5], which is the analogue of DFT, but for a functional of the Green's function. We will then show that DMFT is an approximation to this theory, as LDA is an approximation for DFT.

3.1 A functional of the Green's function

We will follow a similar path to the derivation made in the first section. This derivation follows closely Ref. [5], see also [3] or [11]. For simplicity, we will use the Hubbard model:

$$H_\alpha = \sum_{ij\sigma} t c^\dagger_{i\sigma}c_{j\sigma} + \alpha U \sum_i n_{i\uparrow}n_{j\downarrow} \tag{19}$$

At finite temperature, the Green's function is conveniently defined as:

$$G_{ij}(\tau) = \frac{\mathrm{Tr}[\mathrm{e}^{-\beta H}T_\tau c_i(\tau)c^\dagger_j(0)]}{\mathrm{Tr}[\mathrm{e}^{-\beta H}]} \tag{20}$$

where τ is an imaginary time. In the following, we will forget the atom index i, j and time for simplicity in the following. For simplicity in the following, we will use the real time and frequency, even if the quantities that are extracted here have to be computed in imaginary time and frequency[12].

First, we have to build a way to extract the Green's function from a free energy as the density was extracted in Eq. 4. Whatever the formulation (finite temperature or zero temperature), the Green's function is non local both in time and in space. In particular, the Green's function contains memory effect from previous time. As a consequence, the source term J, from which it can be extracted (in a similar way to λ in Eq. 4) has to be non local in time and in space. It cannot be formulated in an

Hamiltonian formulation, and a functional path integral has to be used[12] to define the free energy $\widehat{\Omega}_\alpha[J]$. Using such a formulation[12, 6, 5], one can show that:

$$\frac{\delta\widehat{\Omega}_\alpha}{\delta J}[J] = \widehat{G}[J] \tag{21}$$

There is no proof of the global concavity of this functional (see discussion in Ref. [11]). Let us however suppose that we can invert $\widehat{J}[G]$ to define the following functional: $\widehat{J}[G]$. As a consequence, we can write the Legendre transformation which is a functional of G

$$\widehat{\Gamma}_\alpha[G] = \widehat{\Omega}_\alpha[\widehat{J}_\alpha[G]] - \mathrm{Tr}[G\widehat{J}_\alpha[G]] \tag{22}$$

3.2 The non interacting system $\alpha = 0$

We have thus

$$\widehat{\Gamma}_0[G] = \widehat{\Omega}_0[\widehat{J}_0[G]] - \mathrm{Tr}[G\widehat{J}_0[G]] \tag{23}$$

We have (in a similar way to Eq. 9):

$$G = \frac{\delta\widehat{\Omega}_0}{\delta\widehat{J}_0}[\widehat{J}_0[G]] \tag{24}$$

In other word, the Green's function is the local Green's function of a non interacting system ($\alpha = 0$) but with a non local frequency dependent effective potential J_0.

We emphasize that this last equation is obtained from the functional Γ_0. It thus expresses the Green's function of a non interacting system $\alpha = 0$ as the derivative of the free energy for the non interacting system Γ_0. We could compute the derivative, but in fact the solution is known, the Green's function of a non interacting system in a non local, frequency dependant potential is :

$$G_{\mathbf{k}}(\omega) = \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - J_{0\,\mathbf{k}}(\omega)} \tag{25}$$

3.3 The real system: $\alpha = 1$

For $\alpha = 1$, we have:

$$\widehat{\Gamma}_1[G] = \widehat{\Omega}_0[\widehat{J}_1[G]] - \mathrm{Tr}[G\widehat{J}_1[G]] \tag{26}$$

We can choose that $J_1 = 0$. The same derivations as above lead to the stationarity of the functional $\widehat{\Gamma}[G]$ as a function of the local Green's function G, for the physical local Green's function $G_{\mathrm{GS}}(\tau)]$, and for this Green's function, the functional is the exact free energy $\mathcal{F}$.

$$\frac{\delta\widehat{\Gamma}_{\alpha=1}}{\delta G}[G = G_{\mathrm{GS}}] = 0 \tag{27}$$

We will use this result below.

3.4 The adiabatic connection

In a similar way, one can show, similarly to Eq. 15 that

$$\begin{aligned}\widehat{\Gamma}_1[G] &= \widehat{\Gamma}_0[G] + \int_0^1 \langle H_{\mathrm{int}}\rangle_{\widehat{J}_\alpha[G]} d\alpha &(28)\\ &= \widehat{\Omega}_0[\widehat{J}_0[G]] - \mathrm{Tr}[G\widehat{J}_0[G]] + \int_0^1 \langle H_{\mathrm{int}}\rangle_{\widehat{J}_\alpha[G]} d\alpha &(29)\end{aligned}$$

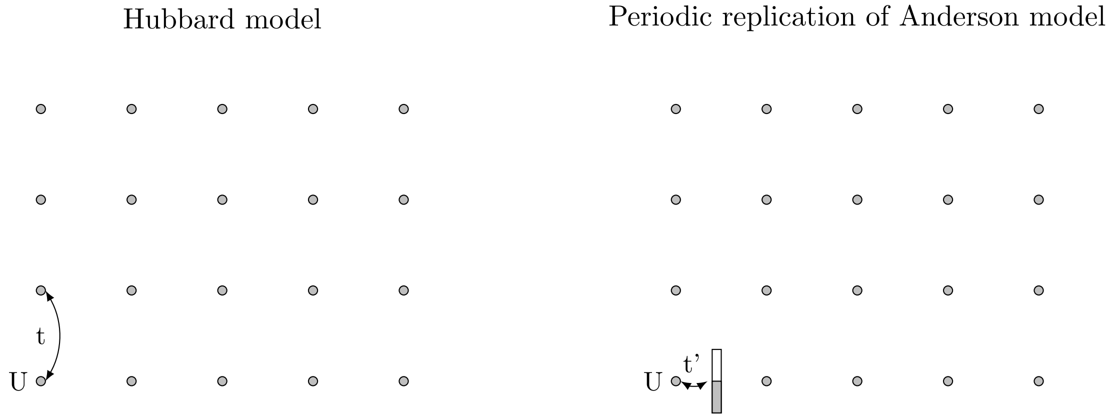

Figure 1: Two different models with the same interaction part in the Hamiltonian, and thus the same functional $\widehat{\Phi}_U[G]$

Using, Eq. 27, we thus show that J_0 is the functional derivative of $\widehat{\Phi}[G] = \int_0^1 \langle H_{\text{int}} \rangle_{\widehat{J}_\alpha[G]} d\alpha$

$$\widehat{J}_0[G] = \frac{\delta \widehat{\Phi}[G]}{\delta G} \tag{30}$$

This is the equation similar to Eq. 17.

To sum up, Eq. 25 shows that the Green's function can be computed from a non interacting system with a non local, frequency dependent potential J_0. We can use the notation $J_0 = \Sigma$ and call it the self energy. Eq. 30 shows that this non local, energy dependent potential is the functional derivative of the Luttinger Ward functional and finally Eq. 29 is the famous Luttinger Ward functional for the free energy.

3.5 The Dynamical Mean Field Theory (or Approximation)

The derivation presented here was proposed by M Potthoff[13, 6]. We first write the Luttinger Ward functional in the particular case of the Hubbard model. The Hubbard model is

$$H = \sum_{i,j} t_{ij} c_i^\dagger c_j + \sum_i U n_{i,\uparrow} n_{i,\downarrow}$$

The LW functional can thus be written

$$\Gamma_{t,U}[G] = \Omega_{0\,t}[\widehat{\Sigma}_U[G]] - \text{Tr}[G\widehat{\Sigma}_U[G]] + \widehat{\Phi}_U[G] \tag{31}$$

Indeed, it can be shown (see e.g. [6] or [5]) that the functional $\widehat{\Phi}_U[G]$ does only depend on the interaction part and not on t. Thus as the functional $\widehat{\Sigma}[G] = \widehat{J}_0[G]$ is the functional derivative of $\widehat{\Phi}_U[G]$, it depends only of U and not t. Thus the only t dependence is in the non interacting part $\Omega_{0\,t}$.

This functional can be written for the Hubbard model. We also build another model which is a periodization of the Anderson model (see Fig. 3.5): it is just a collection of disconnected Anderson model (this is not the so called periodic Anderson model). The functional for this replication of Anderson models is:

$$\widehat{\Gamma}_{t',U}[G] = \widehat{\Omega}_{0\,t'}[\widehat{\Sigma}_U[G]] - \text{Tr}[G\widehat{\Sigma}_U[G]] + \widehat{\Phi}_U[G] \tag{32}$$

Here t' is a symbol to express the non interacting part of the periodic model. By definition, all the non interacting part is contained in $\Omega_{0\,t'}$.

Interestingly the two functionals (Eqs. 31 and 32) contains the same interacting part $\widehat{\Phi}_U[G]$, because the interacting part of the two models are the same ($\sum_i U n_{i,\uparrow} n_{i,\downarrow}$). As a consequence, the functionals $\widehat{\Sigma}_U[G]$ are also the same, as well as the inverse functional $\widehat{G}_U[\Sigma]$.

Now, we express Eq. 24 with the current notation, it writes

$$G = \frac{\delta \widehat{\Omega}_{0,t}[\widehat{\Sigma}_U[G]]}{\delta \Sigma} \tag{33}$$

which can be written as a function of Σ:

$$\widehat{G}_U[\Sigma] = \frac{\delta \widehat{\Omega}_{0,t}[\Sigma]}{\delta \Sigma} \tag{34}$$

The left part of this equation is a complex functional of Σ which comes from the derivative of the interaction functional, whereas the right part is a very simple function of the self energy (Eq. 25)

The DMFT approximation consists to use in this equation the self energy of the Anderson model for the same U

$$\Sigma = \Sigma_{U,t'} \tag{35}$$

Putting this in Eq. 49 gives for the left part:

$$\widehat{G}_U[\Sigma_{U,t'}] = G_{t',U}(\omega) \tag{36}$$

thus the equation gives:

$$\widehat{G}_U[\Sigma_{U,t'}] = G_{t',U}(\omega) = \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma_{t',U}(\omega)} \tag{37}$$

This equation can only be fulfilled locally thus

$$G_{t',U}(\omega) = \frac{1}{N_k} \sum_k \frac{1}{\omega + \mu - \epsilon_{\mathbf{k}} - \Sigma_{t',U}(\omega)} \tag{38}$$

We thus recover the DMFT Self consistency equation: The impurity Anderson Green's function $G_{t',U}$ is equal to the local Green's function of the lattice $\sum_k \frac{1}{\omega+\mu-\epsilon_{\mathbf{k}}-\Sigma_{t',U}(\omega)}$.

4 Comparison of density and Green's function functional theories

Finally we sum up in the table below the comparison between the density and Green's function approaches

Exact Theory	DFT	Green's fct Functional Theory
Equivalent exact system	non interacting system with a potential	non interacting with a self energy
Interaction functional	$E_{\text{Ha+xc}}[n(\mathbf{r})]$	$\widehat{\Phi}_U[G]$
Interaction potential	$v_{\text{Ha+xc}}$	Self energy Σ
Reference system	Homogeneous electron gas	Anderson Impurity model
Approximation	LDA	DMFT

5 Functional of $n(\mathbf{r})$ and G_{loc} and the DFT+DMFT method

We can now combine the DFT and DMFT derivation with the following Hamiltonian[3]:

$$H = H_{\text{exact}} + H_{\text{correlated electrons}}. \tag{39}$$

$$H_{\text{exact}} = \sum_i \left(\frac{\nabla_i^2}{2} + V_{\text{ext}}(\mathbf{r}_i) \right) + \frac{\alpha}{2} \sum_{ij} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \tag{40}$$

$$H_{\text{correlated electrons}} = \theta(\sum_{m_1,m_2,m_3,m_4,\mathbf{R}} (U^{\mathbf{R}}_{m_1,m_2,m_3,m_4} c^{\mathbf{R}\dagger}_{m_1} c^{\mathbf{R}\dagger}_{m_2} c^{\mathbf{R}}_{m_3} c^{\mathbf{R}}_{m_4} - H_{\text{DC}}[N_{\mathbf{R}}])) \tag{41}$$

Let's now make a double Legendre transformation to have a functional of both the density and the local Green's function.

$$\widehat{\Gamma}[n, G_{\text{loc}}] = \widehat{\Omega}[\widehat{\lambda}[n, G_{\text{loc}}], \widehat{J}[n, G_{\text{loc}}]] - \text{Tr}[n\widehat{\lambda}[n, G_{\text{loc}}]] - \text{Tr}[G_{\text{loc}}\widehat{J}[n, G_{\text{loc}}]] \tag{42}$$

5.1 The non interacting system

In this case

$$\widehat{\Gamma}_{00}[n, G_{\text{loc}}] = \widehat{\Omega}_{00}[\widehat{\lambda}_0[n, G_{\text{loc}}], \widehat{J}_0[n, G_{\text{loc}}]] - \text{Tr}[n\widehat{\lambda}_0[n, G_{\text{loc}}]] - \text{Tr}[G_{\text{loc}}\widehat{J}_0[n, G_{\text{loc}}]] \tag{43}$$

We can write, as above, the density and the Green's function as a function of the non interacting free energy:

$$\widehat{n}[\lambda_0, J_0] = \frac{\delta\widehat{\Omega}_{00}}{\delta\lambda_0}[\lambda_0, J_0] \tag{44}$$

$$\widehat{G}_{\text{loc}}[\lambda_0, J_0] = \frac{\delta\widehat{\Omega}_{00}}{\delta J_0}[\lambda_0, J_0] \tag{45}$$

As a consequence we have to write the density and the local Green's function for a system of non interacting electrons with an external potential λ_0 and a local frequency dependent self energy J_0. By definition, this Green's function is the lattice Green's function that we have written above in the first lecture.

$$G^{\mathbf{R}}_{\text{loc}\,mm'}(\omega) = \sum_{\mathbf{k}} \langle \chi^{\mathbf{R}}_{\mathbf{k}m} | \Psi_{\mathbf{k}n} \rangle G_{nn'}(\mathbf{k}, \omega) \langle \Psi_{\mathbf{k}n'} | \chi^{\mathbf{R}}_{\mathbf{k}m'} \rangle \tag{46}$$

with

$$G_{nn'}(\mathbf{k}, \omega) = [(\omega + \mu)I - \epsilon_{\mathbf{k}n} - J_{0nn'}(\mathbf{k}, \omega)]^{-1} \tag{47}$$

with $\epsilon_{nk} = \langle \Psi_{\mathbf{k}n} | - \nabla^2/2 + v_{\text{ext}} + \lambda_0 | \Psi_{\mathbf{k}n} \rangle$. and

$$J_{0nn'}(\mathbf{k}, \omega) = \sum_{m,m',\mathbf{R}} \langle \Psi_{\mathbf{k}n'} | \chi_{\mathbf{k}m} \rangle J^{\mathbf{R}}_{0mm'}(\omega) \langle \chi_{\mathbf{k}m'} | \Psi_{\mathbf{k}n} \rangle \tag{48}$$

From Eq. 44, The density can be obtained from the Green's function of a non interacting system with J_0, so:

$$n(\mathbf{r}) = -i \sum_{n,\mathbf{k}} \Psi_{\mathbf{k}n}(\mathbf{r}) G_{\nu\nu'}(\mathbf{k}, t - t' = 0^-) \Psi_{\mathbf{k}n'}(\mathbf{r}) \tag{49}$$

We emphasize that the four preceding equations are just the definition of the local Green's function, the full lattice Green's function, the $J_0 = \Sigma$ in the Kohn Sham basis, and the local density as a function of the full lattice Green's function, for non interacting electrons in the potential $\lambda_0 + J_0$.

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[3] For simplicity we write for the second part of the Hamiltonian the interaction of a simple one band Hubbard model, but the results are general and are also valid for the multiorbital case with a completely general interaction.

5.2 The interacting system

We show similarly to other cases, that the functional $\Gamma_{11}[n, G]$ is stationary with respect to n and G, and is the exact free energy if we choose $\lambda_1 = 0$ and $\Sigma_1 = 0$.

5.3 The adiabatic connection

We have

$$\widehat{\Gamma}_{11}[n, G_{\text{loc}}] = \widehat{\Omega}_{00}[\widehat{\lambda}_0[n, G_{\text{loc}}], \widehat{J}_0[n, G_{\text{loc}}]] - \text{Tr}[n\widehat{\lambda}_0[n, G_{\text{loc}}]] - \text{Tr}[G_{\text{loc}}\widehat{J}_0[n, G_{\text{loc}}]] + \widehat{\Psi}[n, G_{\text{loc}}] \tag{50}$$

Where Ω_{00} is the free energy of a non interacting electron system in the fields λ_0 and J.

5.4 The LDA+DMFT approximation

The LDA+DMFT approximation consists of using for $\widehat{\Psi}[n, G_{\text{loc}}]$, the sum of the LDA approximation for the exchange and correlation functional, and the Luttinger Ward functional for a local interaction U. Moreover, we have to restrict the domain of variation of G_{loc} to solution of an Anderson impurity model $G_{t',U}$ in Eq. 50.

$$\widehat{\Psi}[n, G_{t'U}] = \widehat{\Gamma}_{\text{Ha+xc}}[n] + \widehat{\Phi}_U[G_{t'U}] - \widehat{\Phi}_{\text{DC}}[G_{t'U}] \tag{51}$$

$\widehat{\Phi}_{\text{DC}}$ is here to compensate for the double counting of the interaction between correlated electrons.

Using the stationary conditions with respect to n and G_{loc}, we have:

$$\widehat{\lambda}_0[n(\mathbf{r})] = v_{\text{Ha+xc}}[n(\mathbf{r})] \tag{52}$$

$$\widehat{\Sigma}_U[G_{t'U}] = \widehat{J}_0[G_{t'U}] = \frac{\delta(\widehat{\Phi}_U - \widehat{\Psi}_{\text{DC}})}{\delta G_{\text{loc}}}[G_{t'U}] \tag{53}$$

5.4.1 The DMFT self-consistency equation

We can rewrite Eq. 45 as

$$G_{t'U} = \frac{\delta\widehat{\Omega}_{00}}{\delta J_0}[\widehat{\lambda}_0[n(\mathbf{r})], \Sigma_{t'U}] \tag{54}$$

because G_{loc} is imposed to be a Green's function of an impurity Anderson model. As the right part is the local Green's function of the lattice (Eq. 46) with self energy $\Sigma_{t'U}$, this equation expresses the self consistency equation in DFT+DMFT.

5.4.2 The DFT self-consistency equation

Finally, Eq. 44 expresses the DFT self consistent equation (Eq. 49) in the DFT+DMFT framework as discussed in the first lecture on DMFT.

6 Conclusion

We have presented derivations of DFT, DMFT and DFT+DMFT from a free energy functional using a Legendre transform. Extension of DMFT towards non local correlations (e.g. Cluster DMFT) can be derived using the same ideas as presented above[6]. The so called GW+DMFT scheme, which allows for the self-consistent calculation of the dynamical screened interaction, can also be derived from a free energy functional formulation[5, 14].

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