LDA+DMFT

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OUTLINE

- Review – ab initio models DMFT
- Functionals and constraining fields
- LDA+DMFT intuitive derivation
- LDA+DMFT - functional - further topics - U's
- Application to iron pnictides

CORRELATIONS IN AB INITIO MODELS

What do we mean when we refer to correlations? Confusing because different people mean different things. My view is as follows: we want to compute the Green's function

$$G(\mathbf{r},\mathbf{r}';i\omega)=\frac{1}{i\omega+\nabla^2/(2m)+\mu-V_{\rm model}(\mathbf{r})-V_{\rm Coul}(\mathbf{r})-\Sigma(\mathbf{r},\mathbf{r}')}. \tag{1}$$

When are correlations small?

- A chemist would say correlations are small when $|\Sigma(\omega)-\Sigma_{\rm HF}|$ is large.
- A physicist would say correlations are small when $|\Sigma(\omega)-V_{\rm xc}^{\rm LDA}|$ is small (at low frequencies).

We will take the physics definition. Thus, systems are strongly correlated if they depart from this criteria.

How do we treat correlations? Using dynamical mean-field theory (DMFT). Consider a Hubbard model:

$$H=-t\sum_{ij}t_{ij}c_i^\dagger c_j+\sum_i Un_{i\uparrow}n_{i\downarrow} \tag{2}$$

In a nutshell, DMFT is:

- Begin with lattice problem.
- *Truncate* to a correlated subspace to get a single-site problem, which is an Anderson impurity model, with the rest of the environment captured by a hybridization function $\Delta(i\omega)$.
- Solve this model for its self-energy $\Sigma_{\rm imp}=\Sigma_{\rm imp}[\Delta]$, which depends on the hybridization function.
- *Embed* this self-energy back in the lattice.

We approximate the lattice self-energy as:

$$\Sigma_{RR'}=\begin{pmatrix}\Sigma_{\rm imp} & & \\ & \Sigma_{\rm imp} & \\ & & \ddots\end{pmatrix} \tag{3}$$

and the Green's function is

$$G_{\rm imp}(i\omega) = G(\mathbf{k}, i\omega) = \sum_k \frac{1}{i\omega + t(k) + \mu - \Sigma(i\omega)[\Delta]}. \tag{4}$$

These are the self-consistent equations to solve.

A note on models: models are great for a first-pass at capturing the basic qualitative physics. However, models are often too simply and they have parameters which need to be determined. We'd like to go beyond models and quantitatively describe realistic systems.

FUNCTIONALS

Begin with the Baym-Kadanoff-Klein functional, which I like to consider as a functional of two variables:

$$\Gamma[G, \Sigma] = -\operatorname{tr}\log(G_0^{-1} - \Sigma) - \operatorname{tr}\Sigma G + \Phi[G], \tag{5}$$

where Φ is the sum of 2PI (two-particle irreducible) graphs. Most people look at it in terms of one variable:

$$\Gamma[G] = -\operatorname{tr}\log G^{-1} - \operatorname{tr}(G_0^{-1} - G^{-1})G + \Phi[G] \tag{6}$$

where G_0 specifices the non-interacting system.

LDA+DMFT INTUITIVE DERIVATION

There are two approaches:

- View the exact functional as a function of the local Green's function $G^{\rm loc}$, then approximate it.

- Start with higher level theory (Baym-Kadanoff), and approximate it to produce DMFT as an approximation ("restriction").

Let's take the second viewpoint. The approximation (restriction) we make is

$$\Phi^{\rm DMFT}[G_{ii}] = \Phi^{\rm BK}[G_{ii}, G_{i\neq j} = 0]. \tag{7}$$

Let's extremize the functional. Taking the derivative with respect to the off-diagonal terms ($i \neq j$) gives:

$$\frac{\delta\Gamma}{\delta G_{ij}} = \Sigma_{ij} = 0 \tag{8}$$

For the diagonal components:

$$\frac{\delta\Phi(G_{ii})}{\delta G_{ii}} = \Sigma_{ii} = \text{1PI local graphs} \tag{9}$$

and $G^{-1} = G_0^{-1} - \Sigma$ and G_0 describes the bandstructure of the model under consideration.

References:

- RMP 78, 865 (2006) functionals

- LDA+DMFT J. Phys. Cond. Matt. 9, 7354 (1997)

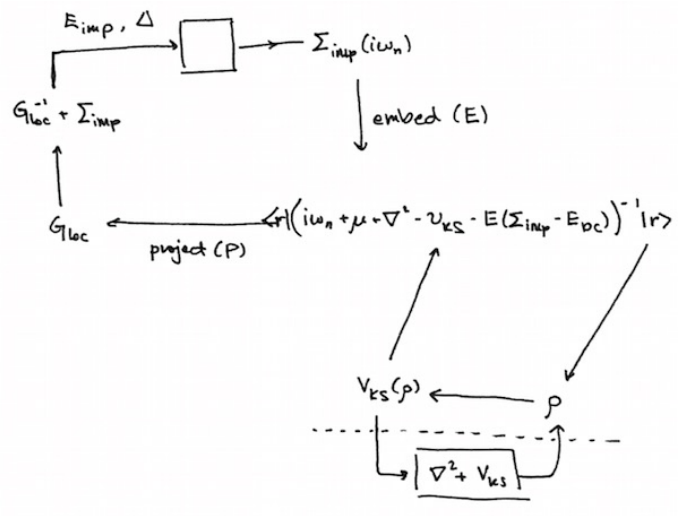

FIG. 1. Schematic of LDA+DMFT loops.

LDA+DMFT INTUITIVE DERIVATION

Focus on correlated shell (e.g. 3d shell for Fe or Ni, or 4f for Cerium). Treat that with DMFT. Rest is treated with LDA. Pick correlated orbitals for the shell.

$$\phi(r) = R(r)Y_{lm}(\theta, \phi) \tag{10}$$

and we get

$$G^{\mathrm{LDA+DMFT}}(\mathbf{r}, \mathbf{r}')(i\omega) = \frac{1}{i\omega + \nabla^2 + \mu - V_{\mathrm{KS}}(\mathbf{r}) - \sum_{Rab}(\Sigma^{\mathrm{imp}}_{RRab}(i\omega) - E^{\mathrm{dc}}\phi^*_{Ra}(r)\phi_{Rb}(r'))} \tag{11}$$

When we map to the impurity, we get the following action:

$$S_{\mathrm{imp}} = \int d\tau \int d\tau' d^\dagger_{a\sigma}(\tau)(\partial_\tau - E_{\mathrm{imp}} - \Delta_{ab}(\tau - \tau'))d_{b\sigma}(\tau) + \int d\tau d^\dagger_{a\sigma}(\tau)d^\dagger_{b\sigma'}(\tau)d_{c\sigma'}(\tau)d_{d\sigma}(\tau)U_{abdc} \tag{12}$$

The DMFT loop is shown in Fig. 1.

OUTLINE

- R. Chitra and GK, PRB 62, 12715 (2000)
- S. Savrasov and GK PRB 69, 245101 (2001)
- RMP 78, 865 (2006) GK, Savrasov, Haule, Udovenko, Parcollet, Marianetti
- Spectral density functional
- U's
- Iron pnictides: work with K. Haule and Zhiping Yin

Begin with path integral for the partition function:

$$e^{F[J]} = Z[J] = \int d\bar{\psi}d\psi e^{-[S(\bar{\psi},\psi)+JA]} \tag{13}$$

where A is an arbitrary observable. To compute $\langle A \rangle$, we take the derivative

$$\partial F/\partial J = \langle A \rangle_J = a(J) = a \tag{14}$$

Here $a = G$. Invert $J = J(a)$ and define $\Gamma(a) = F[J(a)] - aJ(a)$. Taking

$$\partial\Gamma(a)/\partial a|_{a^*} = 0 \tag{15}$$

at the correct physical solution and $\Gamma(a^*)$ is the free energy (in units of kT).

Now take $S = S_0 + \lambda S_1$ and write

$$\Gamma_0(a) = G[J_0(a)] - J_0(a)a \tag{16}$$

Here J_0 is called the constraining field. We can expand in powers of λ:

$$\Gamma[a] = \Gamma_0(a) + \lambda\Gamma_1 + \lambda^2\Gamma_2 + \cdots \tag{17}$$
$$J(\lambda) = J_0(a) + \lambda J_1 + \cdots \tag{18}$$
$$\Gamma(a) = F[J_0(a)] - J_0(a)a + \Delta\Gamma(a) \tag{19}$$
$$\tag{20}$$

Let's ask for the following quantity:

$$\int_0^1 \frac{\partial F(a)}{\partial\lambda} = \int_0^1 \frac{\partial F}{\partial\lambda} = \int_0^1 \langle S_1\rangle_{\lambda,J(\lambda,a)} d\lambda = \Delta\Gamma(a) \tag{21}$$

THE CALCULATION OF U

The U matrix is difficult to understand because it has 4 indices. We make approximations to parameterize this matrix: there are two main formulations:

- Kanamori parameterization
- Slater parameterization: pretend we are in the atom