May 29, 2014.

Introduction to realistic treatments of solids using DMFT
(LDA + DMFT)

LDA+DMFT: introduced in 1997,

Anisimov et al. J. phys. 9, 7359 (1997) (LDA+DMFT)

RMP 68, 13 (1996) Georges et. al. (DMFT)

RMP 78, 865 (2006) Kotliar et. al.

Outline:

1) Model Hamiltonians — First principle methods.
— Why we need both?

2) Simple ~~deri~~ derivation of DMFT: Quantum Weiss field $\Delta(i\omega)$
Embedding — Truncation.

3) Basis sets. $-\nabla^2 + V(r) \rightarrow H_{ij}$
- Muffin tin spheres
- Augmentation.

4) A quick review of Atomic physics.
- What is U?
- How to calculate U?
- GW, constrained RPA.

5) Motivation for LDA+DMFT. (heuristic derivation)

6) Example: Iron Pnictides. — high T_c. $T_c \sim 50K$

7) Deconstructing LDA+DMFT: functionals.
[DFT (LDA, LSDA), GW, DMFT
within one framework.]
- DFT: ρ, $T[\rho]$, $T[\rho_\uparrow, \rho_\downarrow]$.

- DMFT: $\Gamma[G,W]$, Baym-Kadanoff.

8) Possible direction.

1) Theory of everything. (T.O.E)

$$H = \sum_i \nabla_i^2 + \sum_\alpha \frac{1}{2M_\alpha} \nabla_\alpha^2 + \sum_{\alpha,i} \frac{Z_\alpha}{|R_i - R_\alpha|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{|R_i - R_j|} + \frac{1}{2} \sum_{\alpha \neq \beta} \frac{Z_\alpha Z_\beta}{|R_\alpha - R_\beta|}$$

+ relativistic effects. $\left(\sum_i \frac{l_i s_i}{R_i^3} + \dots \text{many body terms} \right)$

- Ignore the relativistic effects.
- Treat ions as they are very heavy. (Adiabatic approximation).
  - $-\sum_\alpha \nabla_\alpha^2$ is a number
  - $-\sum_{\alpha,i} \frac{Z_\alpha}{|R_\alpha - R_i|}$ becomes external potential for electrons.
- 'Z_α, R_α' are input.

Model Hamiltonians: [Hubbard model, Andeson Lattice model, ...]

$$H = \sum_{R,R'} C^\dagger_{\alpha R} t_{\alpha\beta}(R,R') C_{\beta R'} + U^{\alpha\beta\gamma\delta} C^\dagger_{\alpha R} C^\dagger_{\beta R} C_{\gamma R} C_{\delta R}$$

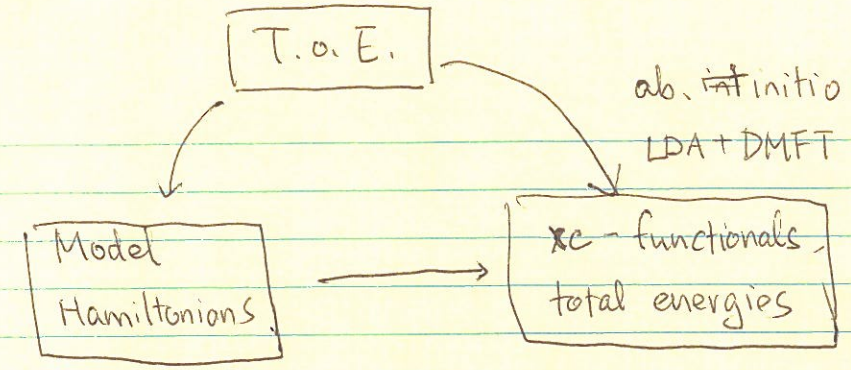
- Models select some degree of freedoms.

From <u>T.O.E.</u> to <u>Models</u>:

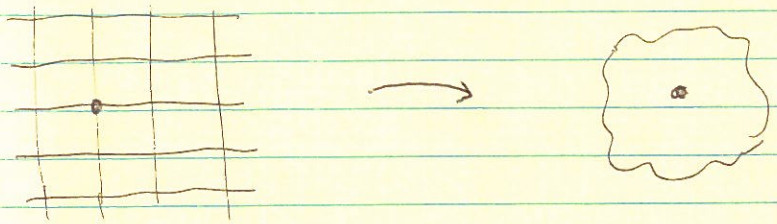
a) Write T.O.E. in second quantization.

b) Eliminate (Integrate out) degrees of freedom of no interest.

c) Screening of Coulomb interaction.

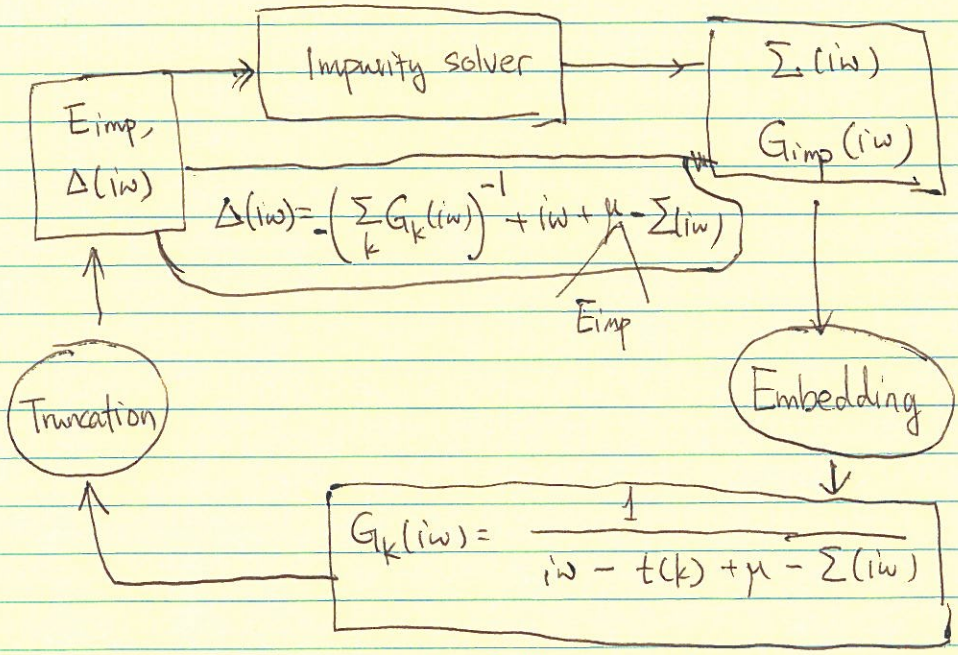


2) DMFT (Weiss field)



Lattice model ⇝ Impurity model ; E_{imp}, $\Delta(i\omega)$

$$\Delta(i\omega) = \sum_\alpha \frac{V_\alpha^2}{i\omega - \varepsilon_\alpha}$$



SC Self-consistent

$J_{ij} S_i S_j + \sum_i h_i S_i \longrightarrow h_{eff} \cdot S_0$, $\underline{\text{th}\,\beta \sum_j J_{ij} S_j = m}$ (MF)

Hubbard ⟶ Impurity model: E_{imp}, Δ (DMF)

($h_{eff} \leftrightarrow \Delta(i\omega)$)
($S \leftrightarrow G_{loc}(i\omega)$)

$$\underline{i\omega_n + \mu - \Delta(i\omega) - \Sigma(i\omega) = \left[\sum_k G_k(i\omega)\right]^{-1}}$$

Self-consistent

3) Basis sets.

$$\left[-\nabla^2 + V_{KS}(r)\right]\psi_{kj} = \varepsilon_{kj}\psi_{kj}$$

$$\psi_k = \sum_i c_i \chi_j$$

$$\langle \chi_j | H | \psi_k \rangle = \sum_i c_i \langle \chi_j | H | \chi_i \rangle = \varepsilon_k \sum_i c_i \langle \chi_j | \chi_i \rangle$$

$$\sum_i h_{ji} c_i = \varepsilon_k \sum_i O_{ji} c_i,$$

$$\begin{cases} h_{ji} = \langle \chi_j | \hat{H} | \chi_i \rangle = \langle \chi_j | -\nabla^2 + V_{KS} | \chi_i \rangle \\ O_{ji} = \langle \chi_j | \chi_i \rangle \quad \text{Overlap matrix.} \end{cases}$$

$$\left[-\nabla^2 + V_{av}(R)\right]\phi_{LM}(r,\varepsilon) = \varepsilon\,\phi_{LM}(r,\varepsilon)$$

$$\phi_{LM}(r,\varepsilon) = R_L(r)\,Y_{LM}(r,\varepsilon)$$

Linearization: $\phi_{LM}(r,\varepsilon) = \phi_{LM}(r,E_v) + (\varepsilon - E_v)\dot{\phi}_{LM}(r,E_v)$

$$\left[-\nabla^2 + V_{av}(R)\right]\dot{\phi}_{LM} = \phi_{LM}$$

Basis sets include $\phi_{LM}(r,E_v)$ and $\dot{\phi}_{LM}(r,E_v)$

Envelope — Augmentation.

LAPW:

$$\chi_{k,G}(\vec{r}) = \begin{cases} e^{i\vec{k}\cdot\vec{r}}\, e^{i\vec{G}\cdot\vec{r}} & (\vec{r} \in I) \\ \sum_{LM} a_{LM}(k)\,\phi_{LM} + b_{LM}(k)\,\dot{\phi}_{LM}, & (\vec{r} \in MT) \end{cases}$$

LMTO: Use Hankel functions in the muffin-tin.

4) Atomic physics.

What is U ? (in Atom and Solid)

Write a model of an atom

$U\hat{N}^2 + J\hat{S}^2$

In second quantization:

$$\frac{1}{2}\int \psi^\dagger_\sigma(\vec{r})\,\psi^\dagger_{\sigma'}(\vec{r}')\,\frac{1}{|\vec{r}-\vec{r}'|}\,\psi_{\sigma'}(\vec{r}')\,\psi_\sigma(\vec{r})$$

$$= \frac{1}{2}\sum_{\alpha\beta\gamma\delta} c^\dagger_{\alpha\sigma}\, c^\dagger_{\beta\sigma'} \langle\alpha\beta|V|\delta\gamma\rangle\, c_{\delta\sigma'}\, c_{\gamma\sigma}$$

$$\langle\alpha\beta|V|\gamma\delta\rangle = \int dr_1 dr_2\, \phi^*_\alpha(r_1)\,\phi^*_\beta(r_2)\,\frac{1}{|r_1-r_2|}\,\phi_\delta(r_2)\,\phi_\gamma(r_1)$$

Using $\phi(r,\theta,\phi) = R_L(r)\,Y_{LM}(\theta,\phi)$

$$\frac{1}{|r-r'|} = \sum_{k=0}^{\infty} \frac{r_<^k}{r_>^{k+1}}\,\frac{4\pi}{(2k+1)}\sum_{q=-k}^{k} Y^*_{kq}(r)\,Y_{kq}(r'),$$

d - shell.

$$c^\dagger_{m_1\sigma}\, c^\dagger_{m_2\sigma'}\, c_{m_3\sigma'}\, c_{m_4\sigma} \sum_k \sum_{q=-k}^{k} \int dr_1\, \phi^*_{m_1}(r_1)\,\phi_{m_4}(r_1)\,Y^*_{kq}(r_1) \times \int dr_2\, \phi^*_{m_2}(r_2)\,\phi_{m_3}(r_2)\,Y_{kq}(r_2) \times \frac{r_<^k}{r_>^{k+1}}$$

$$U_{m_1 m_2 m_3 m_4} = \sum_k F_k \sum_q \langle Y_{m_1}|\,Y^*_{kq}\,|Y_{m_4}\rangle \langle Y_{m_2}|\,Y_{kq}\,|Y_{m_3}\rangle \left(\frac{4\pi}{2k+1}\right)$$

$$F_k = \int dr_1\, r_1^2 \int dr_2\, r_2^2\, \frac{r_<^k}{r_>^{k+1}}\, R_L^2(r_1)\, R_L^2(r_2)$$

The Coulomb-U is F_0 in atom.

$$F_2 = \frac{14}{1.6}\,J, \qquad F_4 = \frac{0.6}{1.6}\,J.$$

- Absence of $F_1, F_3, F_5, \cdots$
  (Parity symmetry)

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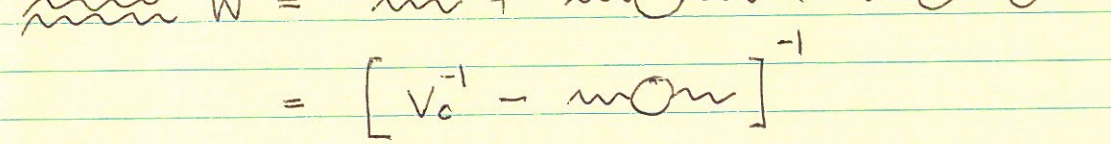
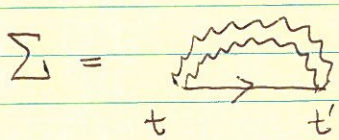
For F_0: $U_{m_1 m_2 m_3 m_4} \sim F_0 \delta_{m_1 m_4} \delta_{m_2 m_3}$

$$\sim H_I \simeq F_0 \sum_{m,m'} \left(c^\dagger_{m\sigma} c_{m\sigma}\right)\left(c^\dagger_{m'\sigma'} c_{m'\sigma'}\right)$$

- Screening


g_0,


$$= \left[V_c^{-1} - \text{bubble}\right]^{-1}$$



$$= W(t,t')\, g_0(t,t') \qquad \text{(GW method)}$$


$$= T \sum_{i\omega} \frac{1}{i\omega - \epsilon_k} \cdot \frac{1}{i\omega - \epsilon_{k+q}}$$

$$= \sum_k \frac{f(\epsilon_{k+q}) - f(\epsilon_k)}{\epsilon_{k+q} - \epsilon_k} \simeq \sum_k \left(-\frac{\partial f}{\partial \epsilon_k}\right) \simeq$$

$$\simeq \sum_k \delta(\epsilon_k) \simeq \rho_{DOS}.$$

Then $$W = \frac{V_q}{1 + V_q \rho_{DOS}} \sim \frac{1}{q^2 + \left(4\pi e^2 \rho_{DOS}\right)}$$

GW

$$\Pi = \bigcirc = g_0 g_0$$

$$(\sim)^{-1} = [v_{col}^{-1} - \bigcirc]$$

$$\Sigma = g_0 W$$

$$g^{-1} = g_0^{-1} - \Sigma$$

- $g_0^{-1} = i\omega_n + \mu + \nabla^2 - V_H - V_{LDA}^{XC}$ (One shot GW)
- $g_0 = g$ (SC - GW, Hedin)
- $g_0^{-1} = i\omega_n + \mu + \nabla^2 - V_H - V_{QPGW}^{XC}$ (Quasi-particle GW)

— Minimize $\| \Sigma_{GW} - V_{QPGW}^{XC} \|$

T.o.E. ⟨1⟩	Model ⟨2⟩

— Principle of uniform matching

1) Chose an approximate method.

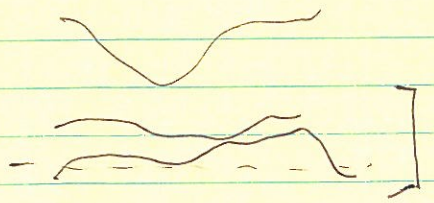
2) Apply the method to ⟨1⟩ and ⟨2⟩.

3) Match enough quantities to determine (over-determine) a few physical observables.

constrained - RPA

- $W = \dfrac{v}{1 + v\Pi}$

$$W_{model} = \frac{v}{1 + v\Pi_{model}}$$



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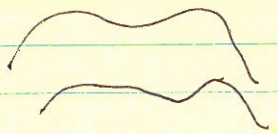
of interest.



$$W_{model} = \frac{U}{1 + U\Pi_{model}}$$

$$W = \frac{V}{1 + V(\Pi_{model} + \Pi_{rest})}$$

To enforce $W_{model} = W$,

$$\frac{U}{1 + U\Pi_{model}} = \frac{V}{1 + V(\Pi_{model} + \Pi_{rest})}$$

$$U = \frac{V}{1 + V\Pi_{rest}}$$

(constrained RPA, PRB 70, 195104 (2004))

— $U(w; r, r')$ is a function of w, r, and r'.

More requirement:

$$\begin{cases} W_{loc} = (W_{model})_{loc} ; \\ \Pi_{loc} = (\Pi_{model})_{loc} ; \\ W_{loc}^{-1} = U^{-1} + \Pi_{loc} ; \end{cases}$$