DFT+EMBEDDED DYNAMICAL MEAN FIELD THEORY FROM FUNCTIONAL PERSPECTIVE

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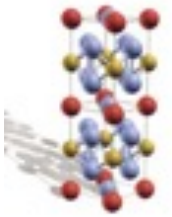
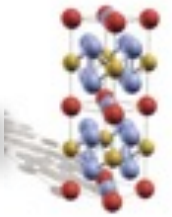
Latest developments



1. Projectors and locality of correlations
2. *Exact double-counting of DFT+EDMFTF* : PRL **115**, 196403 (2015).
3. *Stationary free energy functional (within Embedded DMFT approach) for structural optimization,* PRL**115**, 256402 (2015).
4. Implementation of Forces within E-DMFT functional for optimization of internal structural parameter, arXiv:1602.02819.
5. Some details on the structure of the code.

Reminder: LWF and indirect approach



Basic variable is Green's function:

== dynamic analog of charge density

$$G(\mathbf{r}\tau, \mathbf{r}'\tau') = \langle T_\tau \psi^\dagger(\mathbf{r}'\tau')\psi(\mathbf{r},\tau)\rangle \qquad \rho(\mathbf{r}) = G(\mathbf{r}\tau, \mathbf{r}\tau)$$

Luttinger–Ward functional (1950):

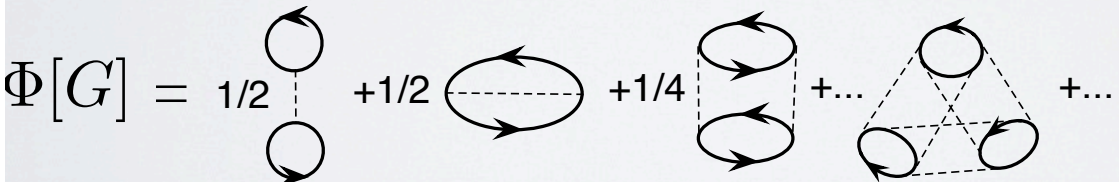
$$\Gamma[\{G\}] = -\mathrm{Tr}((G_0^{-1} - G^{-1})G) + \underbrace{\mathrm{Tr}\log(-G) + \Phi[\{G\}]}$$

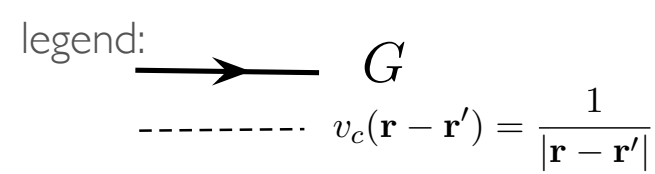
material dependent term

universal functional
independent of material
expressible by the perturbation theory

$$G_0^{-1}(\mathbf{r},\mathbf{r}') = [\omega + \mu + \nabla^2 - V_{ext}(\mathbf{r})]\delta(\mathbf{r}-\mathbf{r}')$$

$\Phi[G]$ *Is a sum of all connected two particle irreducible Feynman diagrams (skeleton diagrams).*



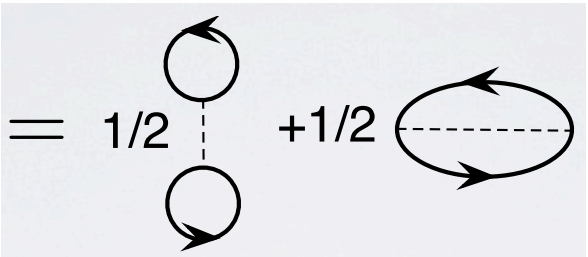


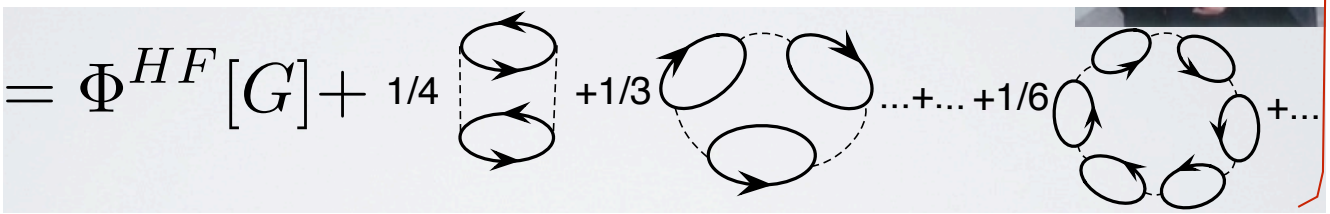
Other approaches in LW language

Density Functional Theory: $\Phi[\{G\}] \rightarrow E_H[\rho] + E_{XC}[\rho]$

Exact DFT appears as
an approximation to the Green's function!

$E_{xc}[\{\rho\}]$ local to a point in 3D space in LDA

Hartree–Fock approximation: $\Phi[\{G\}] =$ 

RPA& GW: $\Phi[\{G\}] = \Phi^{HF}[G] +$ 

Truncation in the real space

Truncation in the space of Feynman diagrams

Dynamical Mean Field Theory: $\Phi[\{G_{ij}\}] \approx E_H[\{\rho\}] + \Phi[\{G_{ii}\}]$

all local Feynman diagrams
(in fully dressed perturbation theory)

Functional Point of view

DMFT for lattice models:

$$\Phi[\{G_{ij}\}] \to \sum_i \Phi[\{G_{ii}\}]$$

i is site or cluster

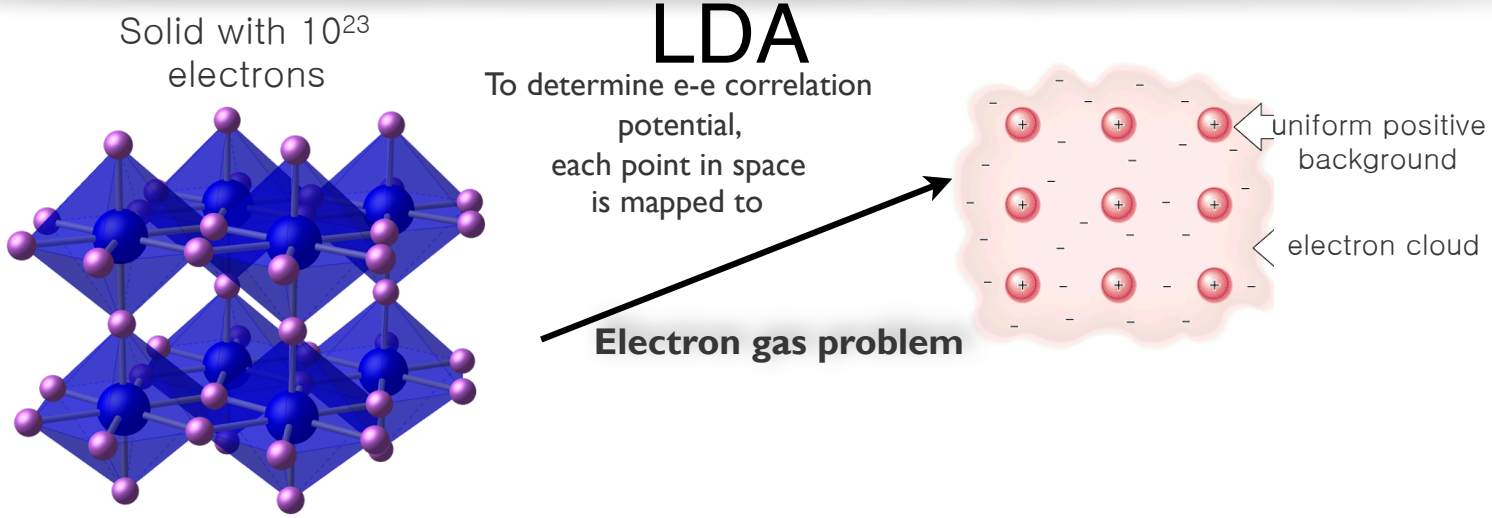
DMFT for continuous problems:

$$\Phi[\{G\}] \to \sum_{\mathbf{R}_i} \Phi[\{\hat{P}_{\mathbf{R}_i} G\}]$$

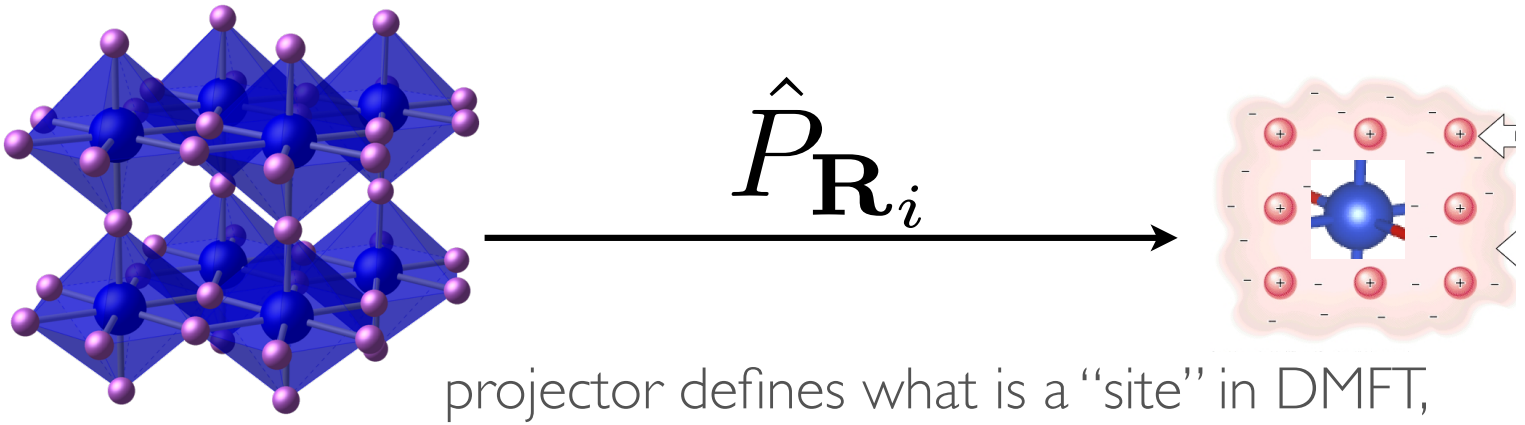
Need to define projector to site (or cluster): $\hat{P}_{\mathbf{R}_i}$

DMFT is projector dependent approximation

How is correlation potential determined?



In DMFT we want to lift the restriction and compute all correlations local to a given site (not given point in space).



projector defines what is a "site" in DMFT, typically an ion with open d of f shell.

The continuos DMFT problem

DMFT approximation: $\Phi[\{G\}] \rightarrow \sum_{\mathbf{R}_i} \Phi[\{\hat{P}_{\mathbf{R}_i} G\}]$

in continuum requires **discretization** of projector,

$$\hat{P}_{\mathbf{R}_i} \rightarrow P_{\mathbf{R}_i}(\alpha\beta) = \int d\mathbf{r} d\mathbf{r}' \mathcal{P}_{\mathbf{R}_i}(\alpha\beta; \mathbf{r}\mathbf{r}')$$

for example: $P_{\mathbf{R}_i}(\alpha\beta) = \int d\mathbf{r} d\mathbf{r}' \phi_\alpha(\mathbf{r} - \mathbf{R}_i) \phi^*_\beta(\mathbf{r}' - \mathbf{R}_i)$

where $\phi_\alpha(\mathbf{r} - \mathbf{R}_i) \equiv \langle \mathbf{r} | \phi^i_\alpha \rangle$ forms a basis on a given atom

so that:

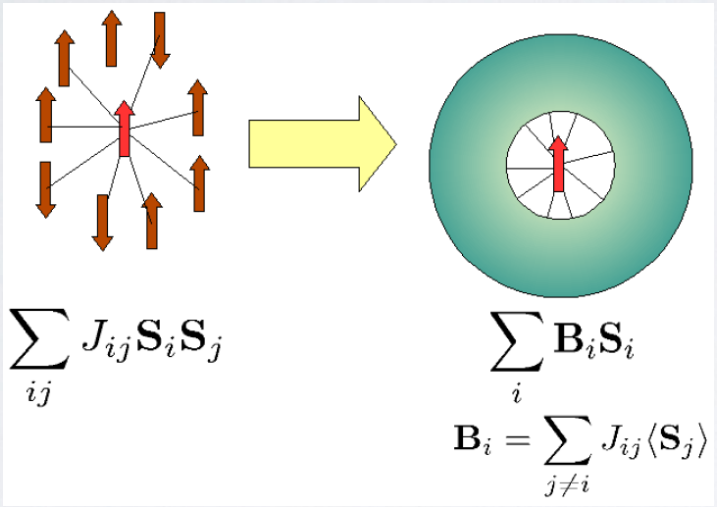
$$G^i_{local}(\mathbf{r}, \mathbf{r}') = \sum_{\alpha\beta} \langle \mathbf{r} | \phi^i_\alpha \rangle \langle \phi^i_\alpha | G | \phi^i_\beta \rangle \langle \phi^i_\beta | \mathbf{r}' \rangle$$

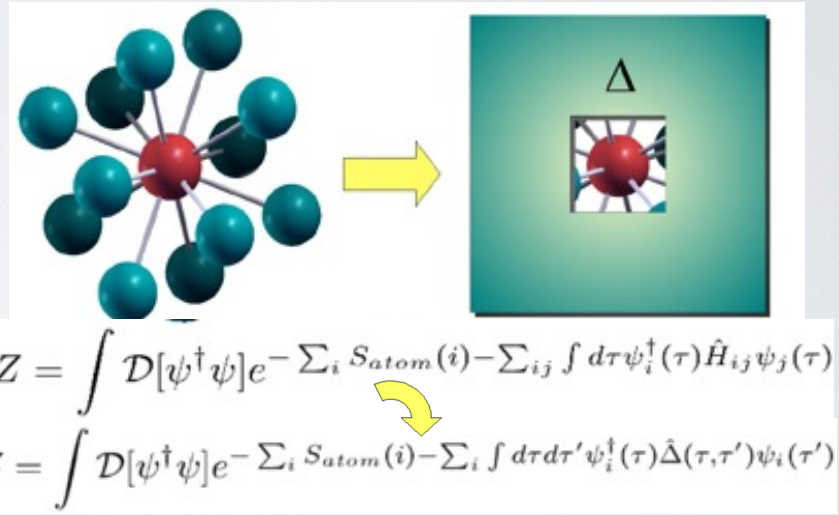
quasi atomic orbitals (locally complete set)

α, β are orbital-spin indices

HOW LOCAL ARE CORRELATIONS?

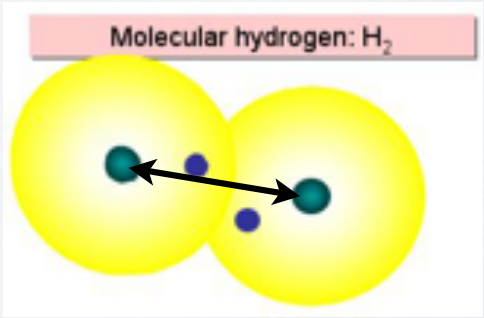
Correlations are local in large d (large connectivity z) where DMFT is exact -- Weiss mean field theory





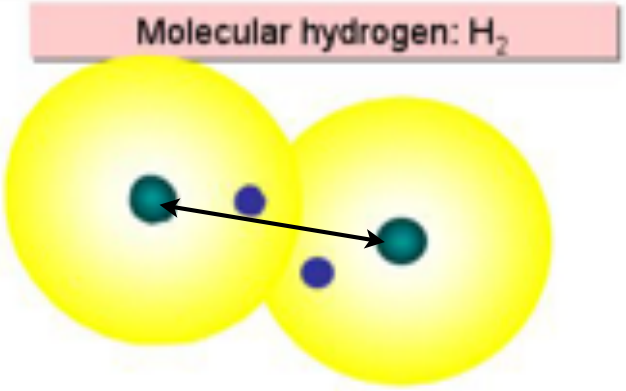
What about finite D? What about 0?

H_2 molecule:

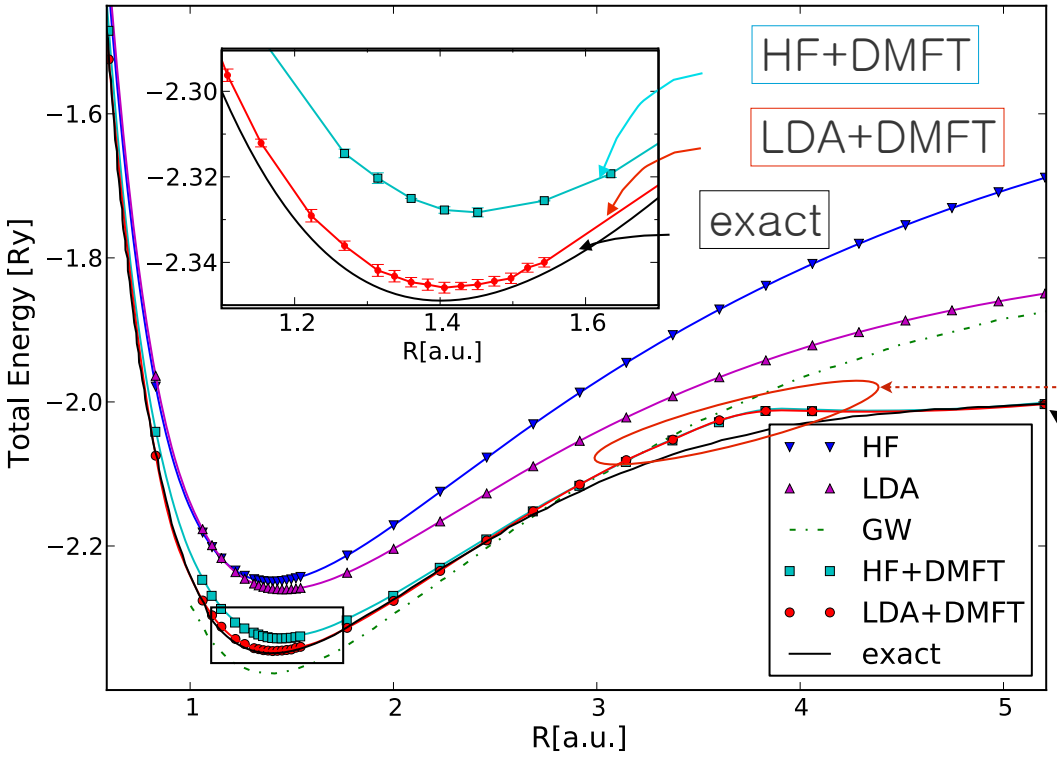


How local are correlations ?
0-D test of the single site DMFT.

Archetypal problem of strong correlations:



DMFT exact in ∞ D, or large connectivity Z
It is not expected to be good for low-D problems
(like H2 molecule)



R-Hartree-Fock fails
(both electrons at the same nucleus)

LDA and GW fail at large R too

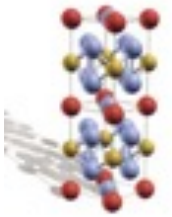
some cluster corrections needed at the breaking point of the molecule

DMFT captures exact atomic limit
accurate at large R!

Error of total energy using LDA+DMFT <0.2%!

Juho Lee, KH, PRB 91, 155144 (2015).

DFT+Embedded Dynamical Mean Field Theory



$$\Gamma[G] = Tr\log G - \mathrm{Tr}((G_0^{-1} - G^{-1})G) + E_{Vc}^{H+XC}[\rho] + \Phi_{V_{DMFT}}^{DMFT}[G_{local}] - \Phi_{V_{DMFT}}^{H+XC}[\rho_{local}]$$

Green's function

$$G_0^{-1} = [i\omega_n + \mu + \nabla^2 - V_{nuc}(\mathbf{r})]\delta(\mathbf{r} - \mathbf{r}')$$

non-interacting part of G

Hartree + XC functional

sum of all "local" Feynman diagrams for correlated ions.

double-counted interaction (we know exactly)

Γ[G] Is stationary and gives free energy of the system.

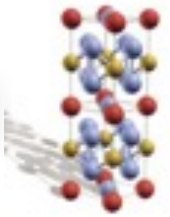
$$\frac{\delta\Gamma[G]}{\delta G} = 0 \quad \text{because} \quad G^{-1} - G_0^{-1} + V_{H+XC}\delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau') +$$

$$+ \hat{P}\frac{\delta\Phi^{DMFT}[G_{local}]}{\delta G_{local}} - \hat{P}\frac{\delta\Phi^{DC}[\rho_{local}]}{\delta\rho_{local}}\delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau') = 0$$

Stationarity : 1st order error in G leads to 2nd order error in free energy.

Note: Migdal-Galitskii formula gives non-stationary total energies in DFT+DMFT.

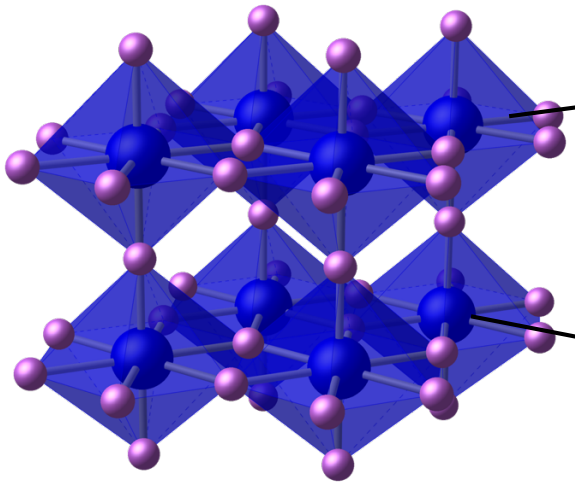
Embedded Dynamical Mean Field Theory Functional



$$\Gamma[G] = Tr\log G - \mathrm{Tr}((G_0^{-1} - G^{-1})G) + E_{Vc}^{H+XC}[\rho] + \Phi_{V_{DMFT}}^{DMFT}[G_{local}] - \Phi_{V_{DMFT}}^{H+XC}[\rho_{local}]$$

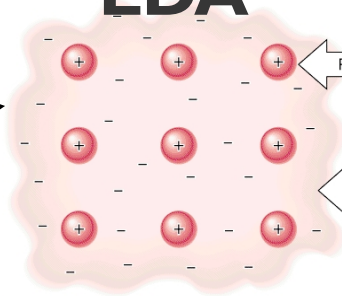
We extremize a DFT-DMFT functional in real space: no need to build tight-binding model Hamiltonian (Wannier orbitals).

Solid with 10^{23} electrons



To determine e-e correlation potential, each point in space is mapped to the uniform electron gas problem.

LDA

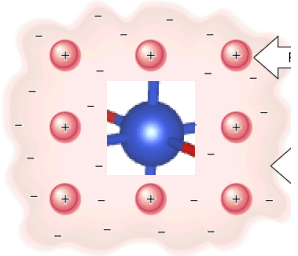


uniform positive background + electron cloud

Auxiliary problem is a non-interacting problem in self-consistent medium

To determine e-e correlation potential, each atom is mapped to auxiliary **quantum impurity** problem

E-DMFT



electron cloud + interacting ion

Auxiliary problem is a "interacting atom" in a self-consistent medium/entanglement

Note: The trick of mapping is used only to determine the exchange-correlation potential, while the *kinetic energy* and *Hartree* term are always treated *exactly*.

Quantum impurity model solved by Monte Carlo

Embedded Dynamical Mean Field Theory Functional

Discretized problem can be handled in similar way as a lattice models.
Extremization:

$$\frac{\delta}{\delta G}\Gamma[\{G\}] = \frac{\delta}{\delta G}(\mathrm{Tr}\log G - \mathrm{Tr}((G_0^{-1} - G^{-1})G)) + \frac{\delta E_{V_c}^{H+XC}[\rho]}{\delta G} + \frac{\delta \sum_{\mathbf{R}_i} \Phi_{V_{DMFT}}[\{\int d\mathbf{r}d\mathbf{r}'\phi_\alpha(\mathbf{r}-\mathbf{R}_i)G(\mathbf{r}\mathbf{r}')\phi^*_\beta(\mathbf{r}'-\mathbf{R}_i)\}]}{\delta G} - \frac{\delta \sum_{\mathbf{R}_i} \Phi^{H+XC}_{V_{DMFT}}[\{\int d\mathbf{r}d\mathbf{r}'\phi_\alpha(\mathbf{r}-\mathbf{R}_i)\rho(\mathbf{r}\mathbf{r}')\phi^*_\beta(\mathbf{r}'-\mathbf{R}_i)\}]}{\delta G}$$

or

$$\frac{\delta}{\delta G}\Gamma[\{G\}] = G^{-1} - G_0^{-1} + \frac{\delta E_{V_c}^{H+XC}[\rho]}{\delta \rho}\delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau') \qquad \left(\rho(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau')G(\mathbf{r}\tau,\mathbf{r}'\tau')\right)$$
$$+\sum_{\alpha\beta}\frac{\delta\Phi_{V_{DMFT}}[\{G^i_{local}\}]}{\delta G^i_{local\,\beta\alpha}}\phi_\alpha(\mathbf{r}-\mathbf{R}_i)\phi^*_\beta(\mathbf{r}'-\mathbf{R}_i)$$
$$-\sum_{\alpha\beta}\frac{\delta\Phi^{H+XC}_{V_{DMFT}}[\{\rho_{local}\}]}{\delta \rho_{local\,\beta\alpha}}\phi_\alpha(\mathbf{r}-\mathbf{R}_i)\delta(\tau-\tau')\phi^*_\beta(\mathbf{r}'-\mathbf{R}_i)\}] = 0$$

finally

$$G^{-1} = G_0^{-1} - V_{H+XC}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau') - \langle\mathbf{r}|\phi^i_\alpha\rangle\,(\Sigma^{imp} - V^{DC})_{\alpha\beta}\,\langle\phi^i_\beta|\mathbf{r}'\rangle$$

where $\Sigma^{imp}_{\alpha\beta} = \frac{\delta\Phi_{V_{DMFT}}[\{G^i_{local}\}]}{\delta G^i_{local\,\beta\alpha}}$ and $V^{DC}_{\alpha\beta} = \frac{\delta\Phi^{H+XC}_{V_{DMFT}}[\{\rho_{local}\}]}{\delta \rho_{local\,\beta\alpha}}\delta(\tau-\tau')$

Embedded Dynamical Mean Field Theory Functional

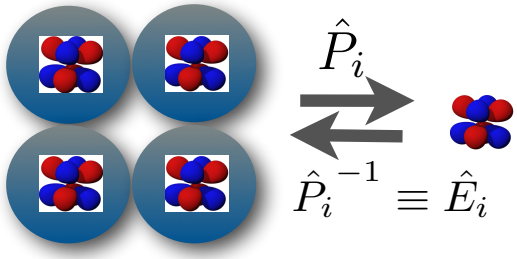
$$G^{-1} = G_0^{-1} - \underbrace{V_{H+XC}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau')}_{DFT} - \underbrace{\langle \mathbf{r}|\phi^i_\alpha\rangle \left(\Sigma^{imp} - V^{DC}\right)_{\alpha\beta} \langle \phi^i_\beta|\mathbf{r}'\rangle}_{\text{quantum impurity S. embedded}}$$

where $\Sigma^{imp}_{\alpha\beta} = \frac{\delta \Phi_{V_{DMFT}}[\{G^i_{local}\}]}{\delta G^i_{local\,\beta\alpha}}$ and $V^{DC}_{\alpha\beta} = \frac{\delta \Phi^{H+XC}_{V_{DMFT}}[\{\rho_{local}\}]}{\delta \rho_{local\,\beta\alpha}}\delta(\tau-\tau')$

On each correlated site $\mathbf{R}_i$ we have to solve a quantum impurity model with $\alpha\beta$ orbitals $\Sigma^{imp}_{\alpha\beta} = \frac{\delta \Phi_{V_{DMFT}}[\{G^i_{local}\}]}{\delta G^i_{local\,\beta\alpha}}$

And **Embed** self-energies to continuum space by $\langle \mathbf{r}|\phi^i_\alpha\rangle \Sigma^{imp}_{\alpha\beta} \langle \phi^i_\beta|\mathbf{r}'\rangle$

Notice that once the projector is defined, embedding is uniquely given by the same matrix elements of $\mathcal{P}_{\mathbf{R}_i}(\alpha\beta;\mathbf{r}\mathbf{r}') = \phi_\alpha(\mathbf{r}-\mathbf{R}_i)\phi^*_\beta(\mathbf{r}'-\mathbf{R}_i)$



REQUIREMENT FOR STATIONARITY

Projector should not depend on the solution

Return to definition of the projector:

$$G_{local,\mathbf{R}_i,\alpha\beta} = \int_{\mathbf{rr}'} \mathcal{P}_{\mathbf{R}_i}(\alpha\beta;\mathbf{rr}')G(\mathbf{rr}')$$

Return to saddle point Eq.:

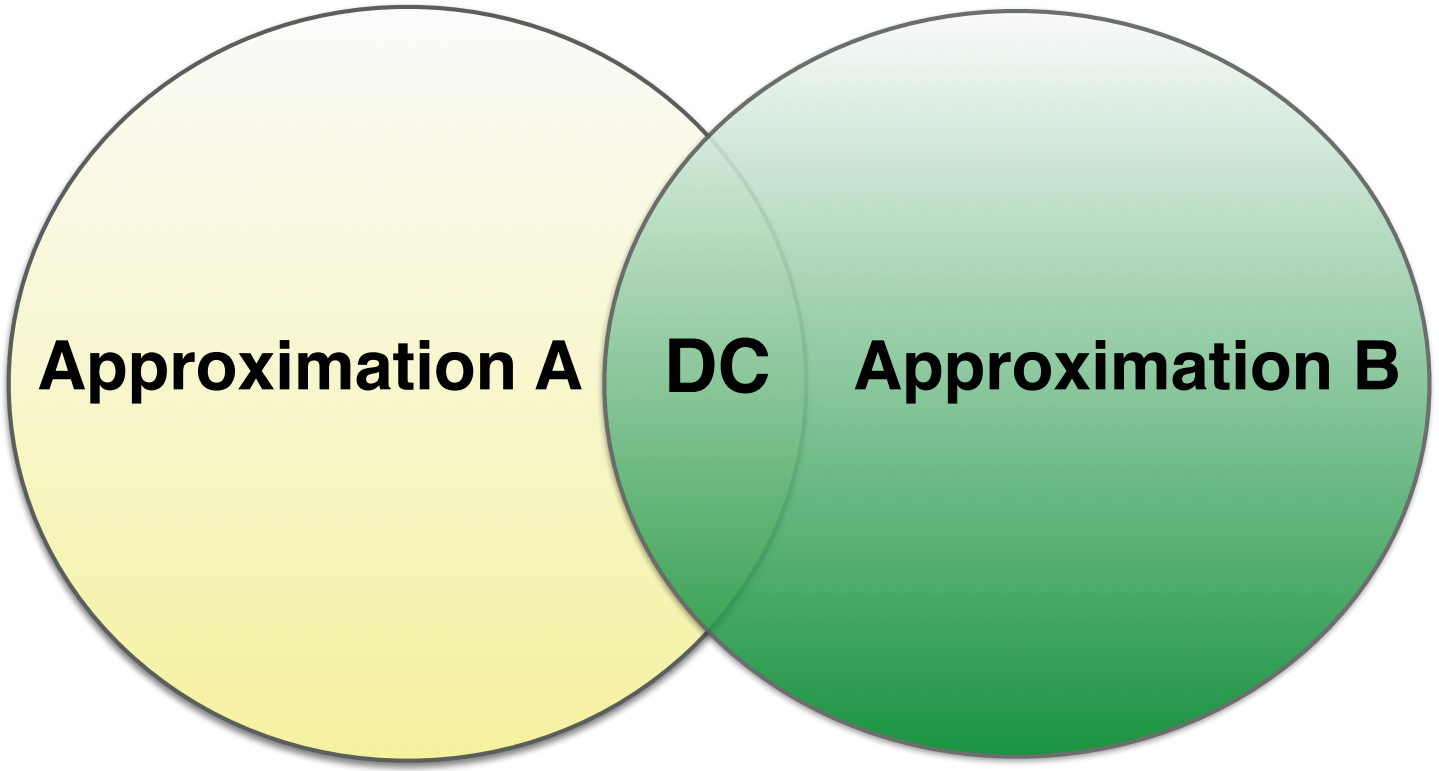
$$\frac{\delta\Phi^{DMFT}[\{G_{local,\mathbf{R}_i}\}]}{\delta G(\mathbf{rr}')} = \sum_{\alpha\beta} \frac{\delta G_{local,\mathbf{R}_i,\alpha\beta}}{\delta G(\mathbf{rr}')} \frac{\delta\Phi[\{G_{local,\mathbf{R}_i}]}{\delta G_{local,\mathbf{R}_i,\alpha\beta}} = \sum_{\alpha\beta} \mathcal{P}_{\mathbf{R}_i}(\alpha\beta;\mathbf{rr}') \frac{\delta\Phi[\{G_{local,\mathbf{R}_i,\alpha\beta}\}]}{\delta G_{local,\mathbf{R}_i,\alpha\beta}}$$

Here we implicitly assumed that $\frac{\delta P}{\delta G} = 0$ or $\frac{\delta\phi_\alpha(\mathbf{r}-\mathbf{R}_i)}{\delta\rho} = 0$

otherwise more complicated terms would appear…

Requirement: $\frac{\delta P}{\delta G} = 0$ is not satisfied with Wannier functions because they essentially depend on the charge, and hence on G.

Double-Counting



Some part of exchange/correlations counted in both approximations.

Double-Counting

$$\Phi[\{G\}] \rightarrow E_{V_c}^{H+XC}[\{\rho\}] + \sum_{\mathbf{R}_i \in corr} \Phi_{V_{DMFT}}[\{G^i_{local}\}] - \Phi^{H+XC}_{V_{DMFT}}[\{\rho^i_{local}\}]$$

Exact functional approximated

LDA functional

Sum of all skeleton diagrams local to correlated ions

DC : intersection of DMFT and LDA approximation

Hartree: $E^H_{V_C}[\{\rho\} = \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' V_C(|\mathbf{r}-\mathbf{r}'|)\rho(\mathbf{r})\rho(\mathbf{r}')$

LDA-XC: $\Phi_{V_C}[\{G\}] \rightarrow E^{LDA}_{XC}[\{\rho\}] = \int d\mathbf{r}\rho(\mathbf{r})\varepsilon^{XC}_{V_C}(\rho(\mathbf{r}))$

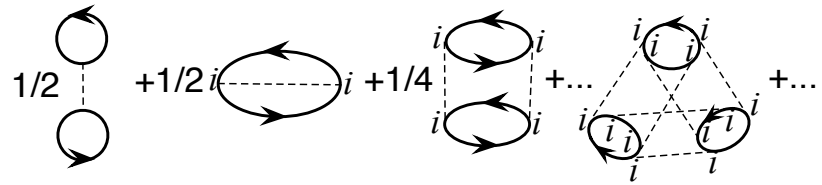
DMFT: $\Phi_{V_C}[\{G\}] \rightarrow \Phi_{V_{DMFT}}[\{G_{local}\}]$

Φ^{DMFT} sums all Feyn. graphs (just like the exact Φ) but uses only G_{local} and screened interaction instead of full G and V_C

$$V_{DMFT}(\mathbf{r}-\mathbf{r}') = \frac{e^{-\lambda|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$$

example of screened Coulomb repulsion

$\Phi[G_{local,\mathbf{R}_i}] =$



Double-Counting of Hartree

Exact Hartree: $E^H_{V_C}[\rho] = \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' V_C(|\mathbf{r}-\mathbf{r}'|)\rho(\mathbf{r})\rho(\mathbf{r}')$

LDA *approximation*

Exact Hartree Hartree term included

$$E^H_{V_C}[\rho] = \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' V_C(|\mathbf{r}-\mathbf{r}'|)\rho(\mathbf{r})\rho(\mathbf{r}')$$

DMFT *approximation*

density projected & interaction screened

$\rho \to \hat{P}\rho$ & $V_C \to V_{DMFT}$

$$E^H_{DMFT}[\rho] = \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' (\hat{P}\rho(\mathbf{r}))(\hat{P}\rho(\mathbf{r}'))V_{DMFT}(\mathbf{r}-\mathbf{r}')$$

This approximation for Hartree term appears in Φ^{DMFT}

Double counting to subtract is the DMFT approximation for the Hartree term:

$$\Phi^{DC,Hartree}_{DMFT}[\{\rho\}] = \frac{1}{2}\int d\mathbf{r}d\mathbf{r}' (\hat{P}\rho(\mathbf{r}))(\hat{P}\rho(\mathbf{r}'))V_{DMFT}(\mathbf{r}-\mathbf{r}')$$

Double-Counting of Exchange

Exact Exchange:

$$E^X[\rho] = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\rho(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}',\mathbf{r})V_C(|\mathbf{r}-\mathbf{r}'|)$$

LDA *approximation:* exchange of electron gas, matching electron density

$$E_F = (2\pi^2\rho)^{2/3}/(2m) \quad \textit{and}$$

$$\rho^0_\sigma(\mathbf{r},\mathbf{r}') = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} f(\frac{k^2}{2m} - E_F)$$

$$E^X_{LDA}[\rho] = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\rho^0(\mathbf{r},\mathbf{r}')\rho^0(\mathbf{r}',\mathbf{r})V_C(|\mathbf{r}-\mathbf{r}'|)$$

$$E^X_{LDA}[\rho] = -\frac{0.9163\,\mathrm{Ry}}{\left(\frac{3}{4\pi}\rho\right)^{1/3}}$$

DMFT *approximation:* density projected & interaction screened

$$\rho \to \hat{P}\rho \;\;\&\;\; V_C \to V_{DMFT}$$

$$E^X_{V_{DMFT}}[\rho] = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'(\hat{P}\rho(\mathbf{r},\mathbf{r}'))(\hat{P}\rho(\mathbf{r}',\mathbf{r}))V_{DMFT}(|\mathbf{r}-\mathbf{r}'|)$$

$$E^X_{V_{DMFT}}[\{\rho\}] = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}' \left(\sum_{mm'} \langle\mathbf{r}|\phi^i_m\rangle\langle\phi^i_m|\,\rho\,|\phi^i_{m'}\rangle\langle\phi^i_{m'}|\mathbf{r}'\rangle\right)\left(\sum_{m''m'''} \langle\mathbf{r}'|\phi^i_{m''}\rangle\langle\phi^i_{m''}|\,\rho\,|\phi^i_{m'''}\rangle\langle\phi^i_{m'''}|\mathbf{r}\rangle\right) V_{DMFT}(\mathbf{r}-\mathbf{r}')$$

$$= -\frac{1}{2}\sum_{m,m',m'',m''} \langle\phi^i_m|\rho|\phi^i_{m'}\rangle\langle\phi^i_{m''}|\rho|\phi^i_{m'''}\rangle \int d\mathbf{r}d\mathbf{r}'\phi^{i*}_{m'''}(\mathbf{r})\phi^{i*}_{m'}(\mathbf{r}')V_{DMFT}(\mathbf{r}-\mathbf{r}')\phi^i_{m''}(\mathbf{r}')\phi^i_m(\mathbf{r})$$

$$= -\frac{1}{2}\sum_{m,m',m'',m''} \rho^i_{mm'}\rho^i_{m''m'''}\langle\phi^i_{m'''}\phi^i_{m'}|V_{DMFT}|\phi^i_{m''}\phi^i_m\rangle$$

Double-Counting of Exchange

Exact Exchange: $E^X[\rho] = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\rho(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}',\mathbf{r})V_C(|\mathbf{r}-\mathbf{r}'|)$

LDA *approximation:* *exchange of electron gas, matching electron density*

$E_F = (2\pi^2\rho)^{2/3}/(2m)$ *and*

$$\rho^0_\sigma(\mathbf{r},\mathbf{r}') = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} f(\frac{k^2}{2m} - E_F)$$

$$E^X_{LDA}[\rho] = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\rho^0(\mathbf{r},\mathbf{r}')\rho^0(\mathbf{r}',\mathbf{r})V_C(|\mathbf{r}-\mathbf{r}'|)$$

DMFT *approximation* *density projected & interaction screened*

$\rho \to \hat{P}\rho$ & $V_C \to V_{DMFT}$

$$E^X_{V_{DMFT}}[\rho] = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'(\hat{P}\rho(\mathbf{r},\mathbf{r}'))(\hat{P}\rho(\mathbf{r}',\mathbf{r}))V_{DMFT}(|\mathbf{r}-\mathbf{r}'|)$$

Intersection of both approximations: apply ***both approximations*** to the functional

1) Interaction is screened in DC term
2) Use projected density in DC term
3) Replace exact expression by electron gas expression

Result is: $\Phi^{DC,X} = -\frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\rho^0(\mathbf{r},\mathbf{r}')\rho^0(\mathbf{r}'\mathbf{r})V_{DMFT}(\mathbf{r}-\mathbf{r}')$

$$\rho^0(\mathbf{r},\mathbf{r}') = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} f(\frac{k^2}{2m} - E_F)$$

$$E_F = \left(2\pi^2(\hat{P}\rho)^{2/3}\right)/(2m)$$

Double-Counting of Correlations

KH, PRL **115**, 196403 (2015).

$$\Phi^{exact}[G, V_C]$$ (beyond Hartree)

***LDA** approximation*

map to electron gas problem point by point

$$E^{electron-gas}[\rho, V_C] = \int d\mathbf{r}\rho(\mathbf{r})\varepsilon_{xc}^{V_C}(\rho(\mathbf{r}))$$

***DMFT** approximation*

in exact Φ replace $G \to \hat{P}G$, $V_C \to V_{DMFT}$

$$\Phi_{V_{DMFT}}[\{G_{local}\}]$$

intersection of both approximations:
electron gas problem with
projected density and screened interaction

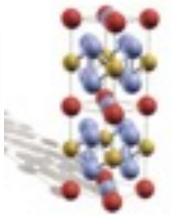
$$E^{electron-gas}[\hat{P}\rho = \rho_{loc}, V_{DMFT}] = \int d\mathbf{r}\rho_{loc}(\mathbf{r})\varepsilon_c^{V_{DMFT}}(\rho_{loc}(\mathbf{r}))$$

Double counting:

$$\Phi^{DC}[\rho_{local}] = \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\rho_{local}(\mathbf{r})V_{DMFT}(\mathbf{r}-\mathbf{r}')\rho_{local}(\mathbf{r}') + \int d\mathbf{r}\rho_{local}(\mathbf{r})\epsilon_{xc}^{V_{DMFT}}[\rho_{local}(\mathbf{r})]$$

electron gas interacting with screened Coulomb interaction

Stationary Free Energy Functional



$$\delta\Gamma[G]/\delta G = 0$$

For numeric stability, the stationary DFT+DMFT functional is needed but the implementation is challenging.

$$\Gamma[G] = \mathrm{Tr}\log G - \mathrm{Tr}[(G_0^{-1} - G^{-1})G] + E^H[\rho] + E^{xc}[\rho] + \Phi^{\mathrm{DMFT}}[\hat{P}G] - \Phi^{\mathrm{DC}}[\hat{P}\rho] + E_{\text{nuc-nuc}}$$

Can be computed from frequency dependent band structure $\varepsilon_{\mathbf{k}\omega_n,i}$

Very hard to compute

Idea : Use the free energy F_{imp} of the auxiliary impurity problem:

$$F_{imp} = \mathrm{Tr}\log G_{imp} - \mathrm{Tr}(\Sigma_{imp}G_{imp}) + \Phi[G_{imp}] \quad \textbf{and} \quad \Phi[G_{imp}] == \Phi[\hat{P}G]$$

$$F_{solid} = F_{imp} + \mathrm{Tr}\log G - \mathrm{Tr}\log G_{imp} + E^H + E^{XC} + E_{nuc-nuc} - \Phi^{DC}[\{\hat{P}\rho\}]$$

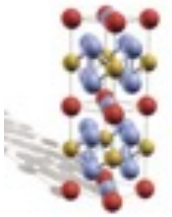
For the impurity problem we can compute with CTQMC very precisely all necessary quantities

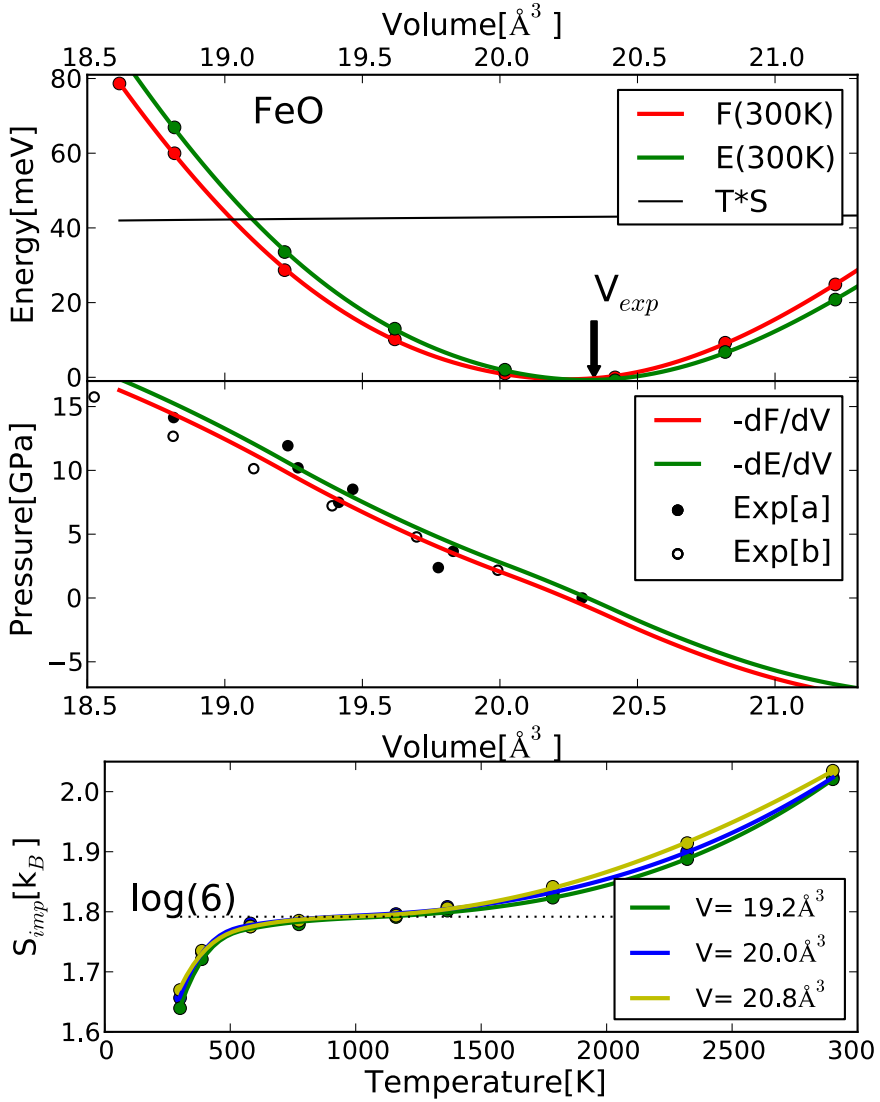
$$F_{imp} = \mathrm{Tr}((\Delta + \varepsilon_{imp} - \omega_n \frac{d\Delta}{d\omega_n})G_{imp}) + E_{imp}^{potential} - T\,S_{imp}$$

$$S_{imp}(T) = S_{imp}(T_>) - \frac{E_{imp}(T_>)}{T_>} + \frac{E_{imp}(T)}{T} - \int_{1/T_>}^{1/T} E_{imp}(1/\beta)d\beta$$

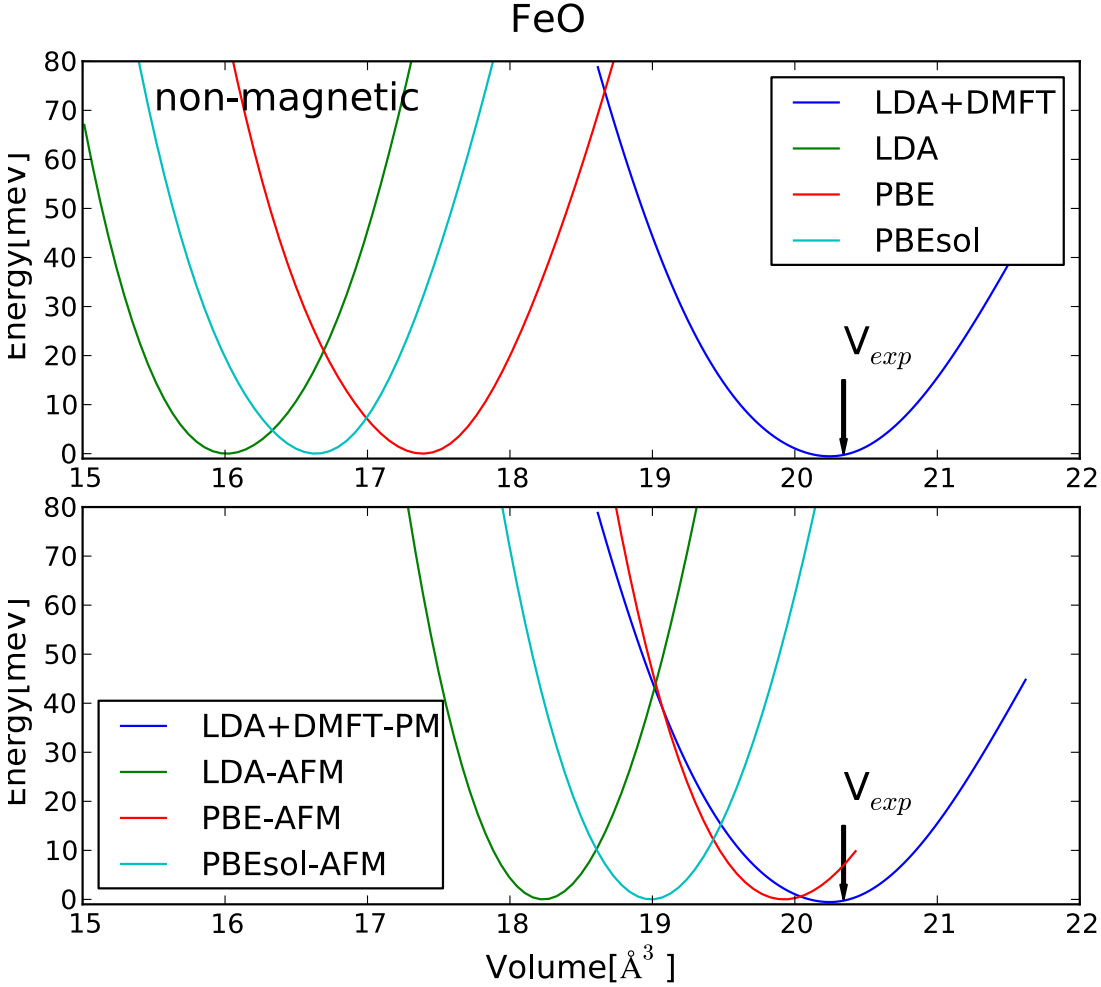
*Details of the implementation in supplementary of PRL**115**, 256402 (2015).*

paramagnetic Mott insulator FeO

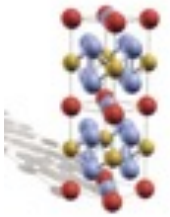




comparison with other functionals



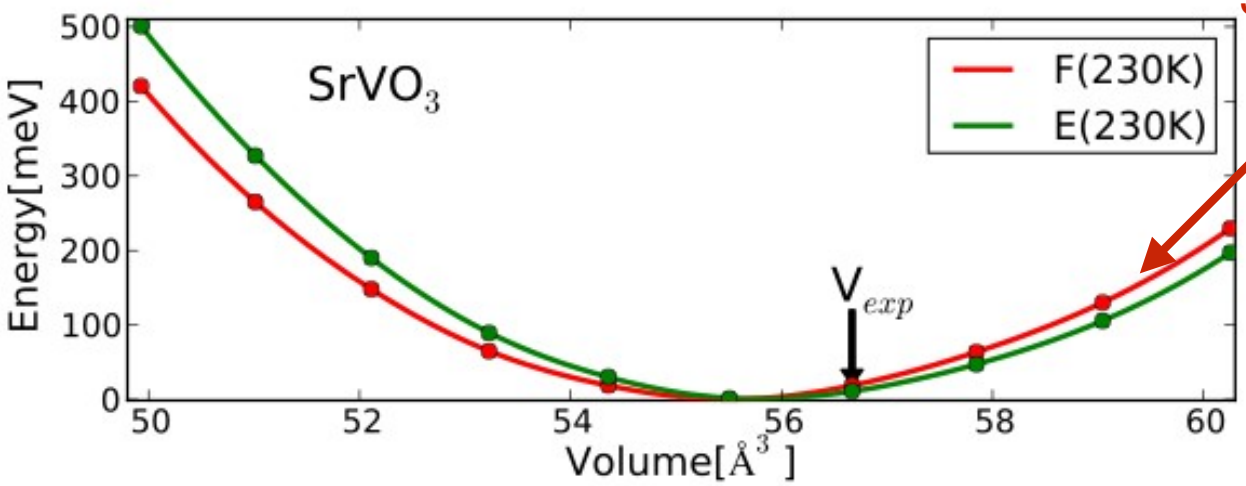
Example $SrVO_3$

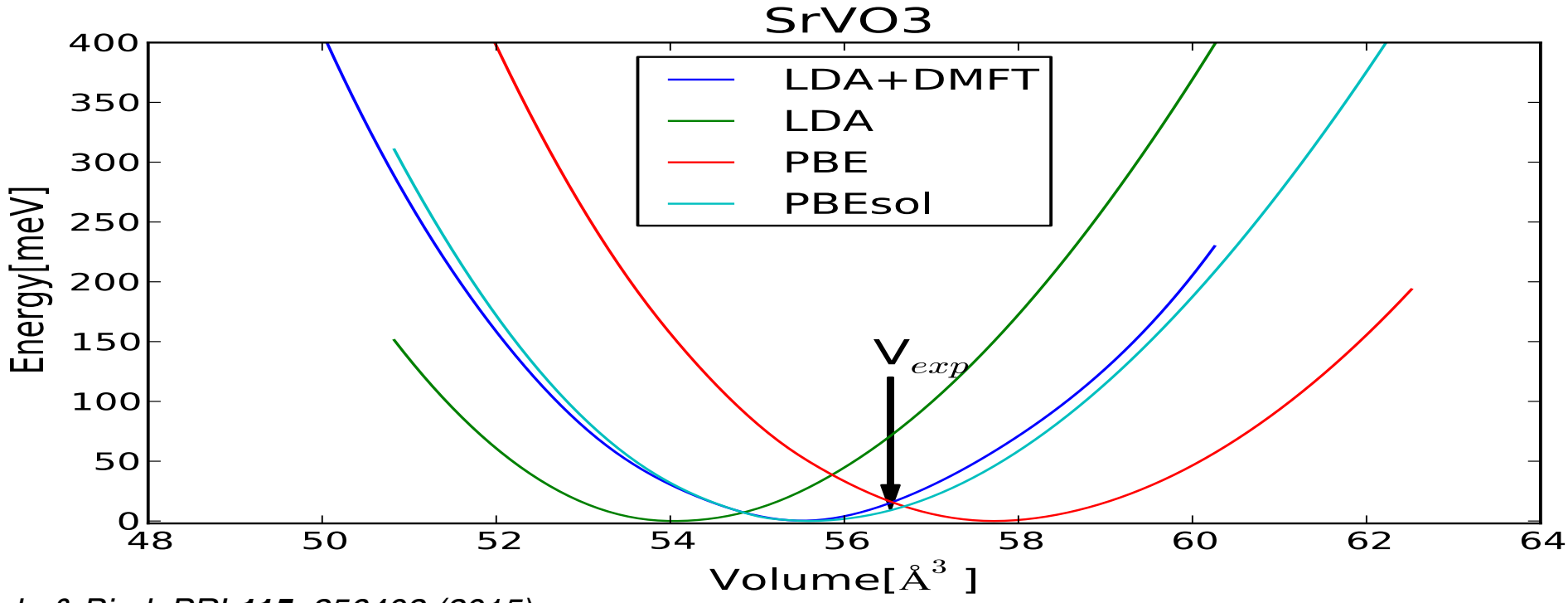


Stationary free energy

E**DMFT**F

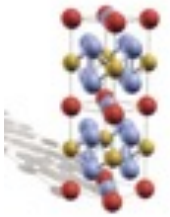
U = 8 eV



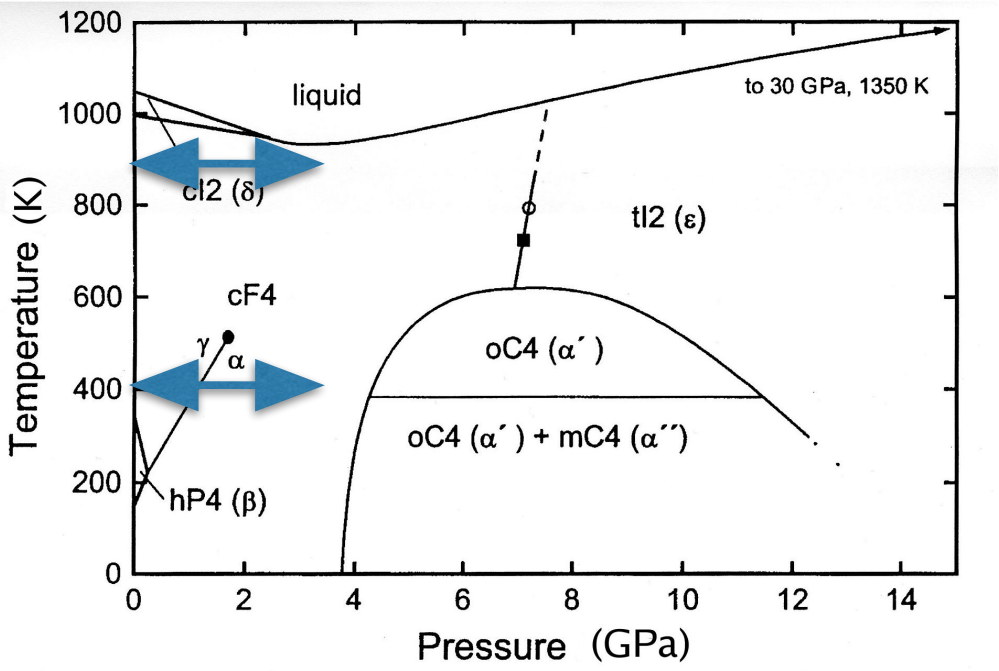


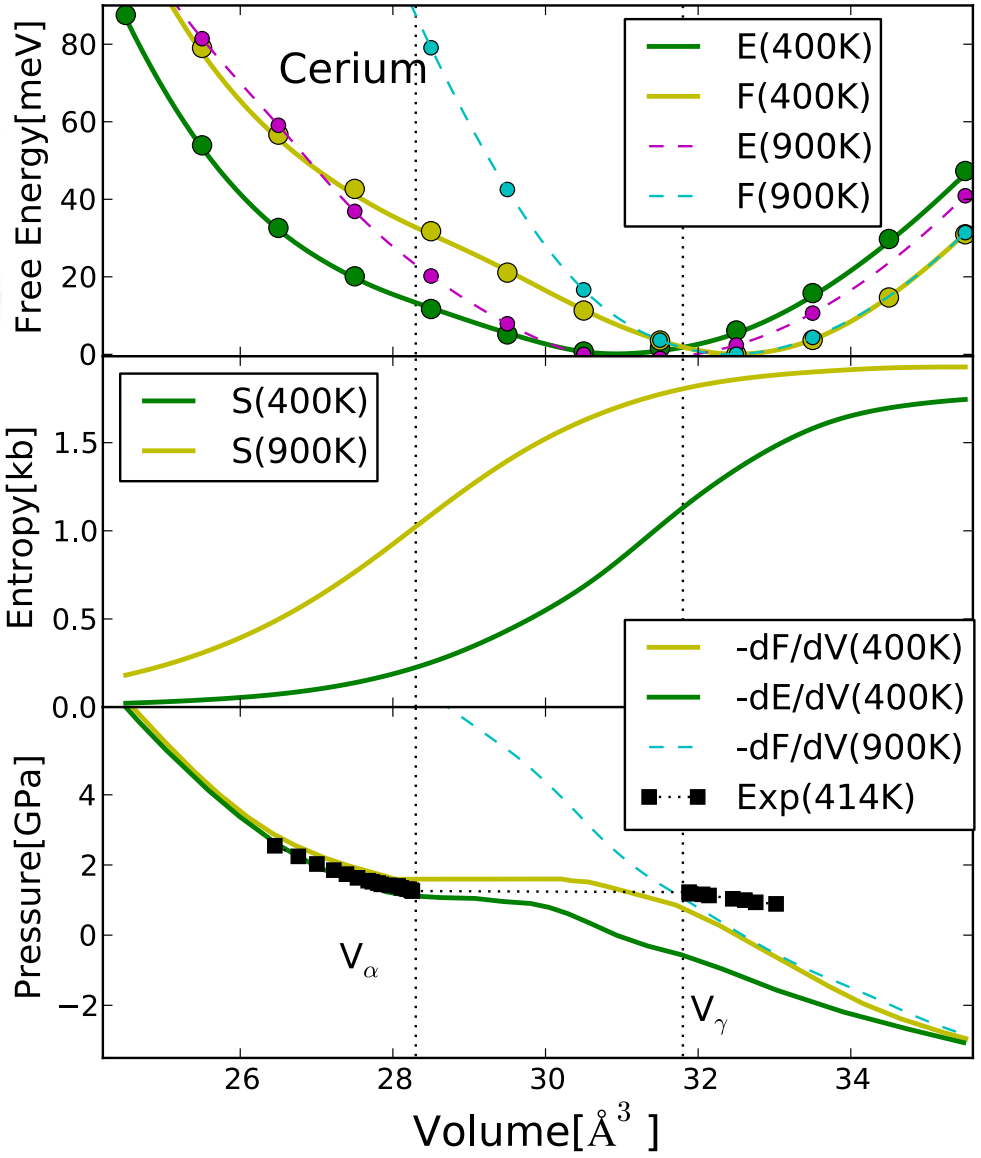
*Haule & Birol, PRL**115**, 256402 (2015).*

Isostructural transition in elemental Cerium

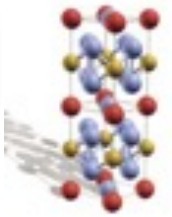


First order (entropy driven) transition





Embedded Dynamical Mean Field Theory Functional



Stationary Embedded DMFT functional extremized in real space.

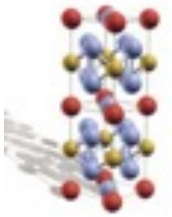
↓

Free energy functional can be analytically differentiated to give forces on all atoms.

↓

Can predict complex crystal structures

Force on all atoms from derivative of the functional



$$\frac{\delta\Gamma[G]}{\delta\mathbf{R}_\mu} = \frac{\delta G}{\delta\mathbf{R}_\mu}\left(\frac{\partial\Gamma[G]}{\partial G}\right)_{R_\mu} + \left(\frac{\partial\Gamma[G]}{\partial\mathbf{R}_\mu}\right)_G$$

vanishes

$$\begin{aligned}\frac{\delta\Gamma[\{G\}]}{\delta\mathbf{R}_\mu} &= \frac{\partial}{\partial\mathbf{R}_\mu}\left(\mathrm{Tr}\log(G) - \mathrm{Tr}((G_0^{-1} - G^{-1})G) + \Phi[\{G\}] + E_{nuc-nuc}\right)_G \\ &= \frac{\partial}{\partial\mathbf{R}_\mu}\left(-\mathrm{Tr}\left([i\omega + \mu + \nabla^2 - V_{nuc}(\mathbf{r})]\delta(\mathbf{r}-\mathbf{r}')G\right) + E_{nuc-nuc}\right) \\ &= \mathrm{Tr}(\rho\frac{\partial}{\partial\mathbf{R}_\mu}V_{nuc}) + \frac{\partial}{\partial\mathbf{R}_\mu}E_{nuc}\end{aligned}$$

$$\mathbf{F}^{HF} = -\mathrm{Tr}(\rho\frac{\partial V_{nuc}}{\partial\mathbf{R}_\mu}) - \frac{\partial E_{nuc}}{\partial\mathbf{R}_\mu}$$

The Hellman-Feynman force

Force on all atoms from derivative of the functional

But the LAPW basis set, and the DMFT projector, are not fixed in space, but rather move with the atom.

→ **"Pulay forces"** appear

We need to differentiate the implemented expression for the free energy.

Free energy expression again

Recall:

$$\Gamma[\{G\}] = \mathrm{Tr}\log G - \mathrm{Tr}((G_0^{-1} - G^{-1})G) + E_{V_C}^{H+XC}[\rho] + \sum_{\mathbf{R}_i \in corr} \Phi_{V_{DMFT}}^{DMFT}[G_{loc}^i] - \Phi_{V_{DMFT}}^{DC}[\rho_{loc}^i]$$

at the DMFT solution the Dyson Eq. is satisfied

$$G^{-1} = G_0^{-1} - V_{H+XC}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau') - \langle \mathbf{r}|\phi_\alpha^i\rangle \left(\Sigma^{imp} - V^{DC}\right)_{\alpha\beta} \langle \phi_\beta^i|\mathbf{r}'\rangle$$

hence the free can be computed by

$$F = \mathrm{Tr}\log(G) - \mathrm{Tr}(V_{H+XC})\rho) + E^{H+XC}[\rho]$$
$$+ \sum_{\mathbf{R}_i} \left\{ -\mathrm{Tr}((\Sigma^{imp} - V^{DC})G_{loc}^i) + \Phi^{DMFT}[G_{loc}^i] - \Phi^{DC}[\rho_{loc}^i] \right\}$$

nuclear-nuclear energy is added;
canonical ensemble needs +μ N

Free energy expression implementation

To implement $\mathrm{Tr}\log G$ we compute generalized Kohn-Sham orbitals:

$$\langle\psi_{j\mathbf{k}\omega_n}|\left(T+V_{nuc}+V_{H+XC}+\sum_{mm',\mathbf{R}_\mu}|\phi^\mu_m\rangle\langle\phi^\mu_m|\Sigma_{i\omega_n}-V_{DC}|\phi^\mu_{m'}\rangle\langle\phi^\mu_{m'}|\right)|\psi_{i\mathbf{k}\omega_n}\rangle=\delta_{ij}\varepsilon_{\mathbf{k}\omega_n,i}$$

so that $\langle\psi_{j\mathbf{k}\omega_n}|G|\psi_{i\mathbf{k}\omega_n}\rangle=\dfrac{\delta_{ij}}{i\omega_n+\mu-\varepsilon_{\mathbf{k}\omega_n,i}}$,i.e., G is diagonalized

then

$$\mathrm{Tr}\log(-G)=-\mathrm{Tr}\log(-i\omega_n-\mu+\varepsilon_{\mathbf{k}\omega_n})$$

and

$$F=-\mathrm{Tr}\log(-i\omega_n-\mu+\varepsilon_{\mathbf{k}\omega_n})-\mathrm{Tr}(V_{H+XC})\rho)+E^{H+XC}[\rho]+E_{nuc-nuc}+\mu N$$
$$+\sum_{\mathbf{R}_i}\left\{-\mathrm{Tr}((\Sigma-V_{DC})G^i_{loc})+\Phi^{DMFT}[G^i_{loc}]-\Phi^{DC}[\rho^i_{loc}]\right\}$$

Derivative of the free energy

The free energy :

$$F = -\mathrm{Tr}\log(-i\omega_n - \mu + \varepsilon_{\mathbf{k}\omega_n}) - \mathrm{Tr}(V_{H+XC})\rho) + E^{H+XC}[\rho] + E_{nuc-nuc} + \mu N + \sum_{\mathbf{R}_i}\{-\mathrm{Tr}((\Sigma - V_{DC})G^i_{loc}) + \Phi^{DMFT}[G^i_{loc}] - \Phi^{DC}[\rho^i_{loc}]\}$$

$$\frac{\delta F}{\delta \mathbf{R}_\mu} = \mathrm{Tr}\left(\frac{1}{i\omega + \mu - \varepsilon_{\mathbf{k}\omega_n}}\frac{\delta(\varepsilon_{\mathbf{k}\omega_n} - \mu)}{\delta \mathbf{R}_\mu}\right) - \mathrm{Tr}(\rho\frac{\delta V_{H+XC}}{\delta \mathbf{R}_\mu}) + \frac{\delta E_{nuc-nuc}}{\delta \mathbf{R}_\mu} + N\frac{\delta \mu}{\delta \mathbf{R}_\mu}$$

$$-\mathrm{Tr}\left(G_{loc}\frac{\delta\Sigma - \delta V_{DC}}{\delta \mathbf{R}_\mu}\right)$$

$$\frac{\delta F}{\delta \mathbf{R}_\mu} = \mathrm{Tr}\left(\frac{1}{i\omega + \mu - \varepsilon_{\mathbf{k}\omega_n}}\frac{\delta(\varepsilon_{\mathbf{k}\omega_n})}{\delta \mathbf{R}_\mu}\right) - \mathrm{Tr}(\rho\frac{\delta(V_{KS})}{\delta \mathbf{R}_\mu})$$

$$-\mathrm{Tr}\left(G_{loc}\frac{\delta\Sigma - \delta V_{DC}}{\delta \mathbf{R}_\mu}\right)$$

Recall: $\mathbf{F}^{HF} = -\mathrm{Tr}(\rho\frac{\partial V_{nuc}}{\partial \mathbf{R}_\mu}) - \frac{\partial E_{nuc}}{\partial \mathbf{R}_\mu}$

Derivative of the free energy

$$\mathbf{F}_{\mu}^{Puly} = -\mathrm{Tr}\left(\frac{1}{i\omega_n + \mu - \varepsilon_{\mathbf{k}\omega_n}}\frac{\delta\varepsilon_{\mathbf{k}\omega_n}}{d\mathbf{R}_{\mu}}\right) + \mathrm{Tr}\left(\rho\frac{\delta V_{KS}}{\delta\mathbf{R}_{\mu}}\right) + \mathrm{Tr}\left(G_{loc}\frac{\delta\Sigma - \delta V_{DC}}{\delta\mathbf{R}_{\mu}}\right)$$

$\delta\Sigma(\omega)$ very hard to compute.

appears in two terms.

But: Functional is stationary, and $\delta\Sigma(\omega)$ *cancel out.*

KH, arXiv:1602.02819.

Derivative of the free energy

To prove that $\delta(\Sigma - V_{DC})$ cancels, we recall eigenvalue Eq.

$$\langle\psi_{i\mathbf{k}\omega_n}|\left(T + V_{nuc} + V_{H+XC} + \sum_{mm',\mathbf{R}_\mu} |\phi^\mu_m\rangle\langle\phi^\mu_m|\Sigma_{i\omega_n} - V_{DC}|\phi^\mu_{m'}\rangle\langle\phi^i_{m'}|\right) - \varepsilon_{\mathbf{k}\omega_n,i}|\psi_{i\mathbf{k}\omega_n}\rangle = 0$$

which is satisfied for each atomic position $\mathbf{R}_\mu$ hence

$$\langle\psi_{i\mathbf{k}\omega_n}|\left(\delta(T + V_{nuc} + V_{H+XC}) + \sum_{mm',\mathbf{R}_\mu} \delta(|\phi^\mu_m\rangle\langle\phi^\mu_m|\Sigma_{i\omega_n} - V_{DC}|\phi^\mu_{m'}\rangle\langle\phi^i_{m'}|)\right) - \delta\varepsilon_{\mathbf{k}\omega_n,i}|\psi_{i\mathbf{k}\omega_n}\rangle = 0$$

therefore $\delta\varepsilon_{\mathbf{k}\omega_n,i} = \sum_{\mathbf{R}_\mu,mm'} \langle\psi_{i\mathbf{k}\omega_n}|\phi^\mu_m\rangle\langle\phi^\mu_m|\delta(\Sigma - V_{DC})|\phi^\mu_{m'}\rangle\langle\phi^\mu_{m'}|\psi_{i\mathbf{k}\omega_n}\rangle + \ldots$

….+derivative of the projector+DFT terms

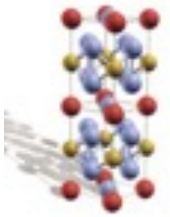
hence

$$\mathrm{Tr}\left(\frac{\delta\varepsilon_{\mathbf{k}\omega_n}}{i\omega + \mu - \varepsilon_{\mathbf{k}\omega_n}}\right) = \mathrm{Tr}\left(|\psi_{i\mathbf{k}\omega_n}\rangle \frac{1}{i\omega + \mu - \varepsilon_{\mathbf{k}\omega_n}} \langle\psi_{i\mathbf{k}\omega_n}| \sum_{\mathbf{R}_\mu,mm'} |\phi^\mu_m\rangle\langle\phi^\mu_m|\delta(\Sigma - V_{DC})|\phi^\mu_{m'}\rangle\langle\phi^\mu_{m'}|\right) + \ldots$$

$$= \mathrm{Tr}\left(G \sum_{\mathbf{R}_\mu,mm'} |\phi^\mu_m\rangle\langle\phi^\mu_m|\delta(\Sigma - V_{DC})|\phi^\mu_{m'}\rangle\langle\phi^\mu_{m'}|\right) + \ldots$$

$$\mathbf{F}^{Puly}_\mu = -\mathrm{Tr}\left(\frac{1}{i\omega_n + \mu - \varepsilon_{\mathbf{k}\omega_n}} \frac{\delta\varepsilon_{\mathbf{k}\omega_n}}{d\mathbf{R}_\mu}\right) + \mathrm{Tr}\left(\rho\frac{\delta V_{KS}}{\delta\mathbf{R}_\mu}\right) + \mathrm{Tr}\left(G_{loc}\frac{\delta\Sigma - \delta V_{DC}}{\delta\mathbf{R}_\mu}\right) = \mathrm{Tr}(G_{loc}\delta(\Sigma - V_{DC})) + \ldots$$

Final results for forces in a mixed basis set



Pulay force in mixed basis:

DFT-like terms

$$\mathbf{F}_{\mu}^{Puly} = -\mathrm{Tr}\left(\widetilde{\rho} A^{0\dagger} \frac{\delta H^0}{\delta \mathbf{R}_\mu} A^0 - \widetilde{(\rho\varepsilon)} A^{0\dagger} \frac{\delta O}{\delta \mathbf{R}_\mu} A^0\right) + \mathrm{Tr}\left(\rho \frac{\delta V_{KS}}{\delta \mathbf{R}_\mu}\right)$$

$$-\frac{1}{\beta}\sum_{i\omega_n}\sum_{\mathbf{K}\mathbf{K}',m'm} \bar{G}_{\mathbf{K}\mathbf{K}'}(\Sigma - V_{DC})_{m'm} \frac{\delta\left(\langle\chi_{\mathbf{K}'}|\phi_{m'}\rangle\langle\phi_m|\chi_{\mathbf{K}}\rangle\right)}{\delta\mathbf{R}_\mu}$$

derivative of the DMFT projector, because the DMF basis moves with the atom

depends on the DMFT density matrices

$$\widetilde{\rho} \equiv \frac{1}{\beta}\sum_{i\omega_n} B^R_{\omega_n} \frac{1}{i\omega_n + \mu - \varepsilon_{\mathbf{k}\omega_n}} B^L_{\omega_n}$$

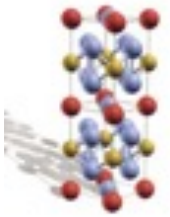
$$\widetilde{(\rho\varepsilon)} \equiv \frac{1}{\beta}\sum_{i\omega_n} B^R_{\omega_n} \frac{\varepsilon_{\mathbf{k}\omega_n}}{i\omega_n + \mu - \varepsilon_{\mathbf{k}\omega_n}} B^L_{\omega_n}$$

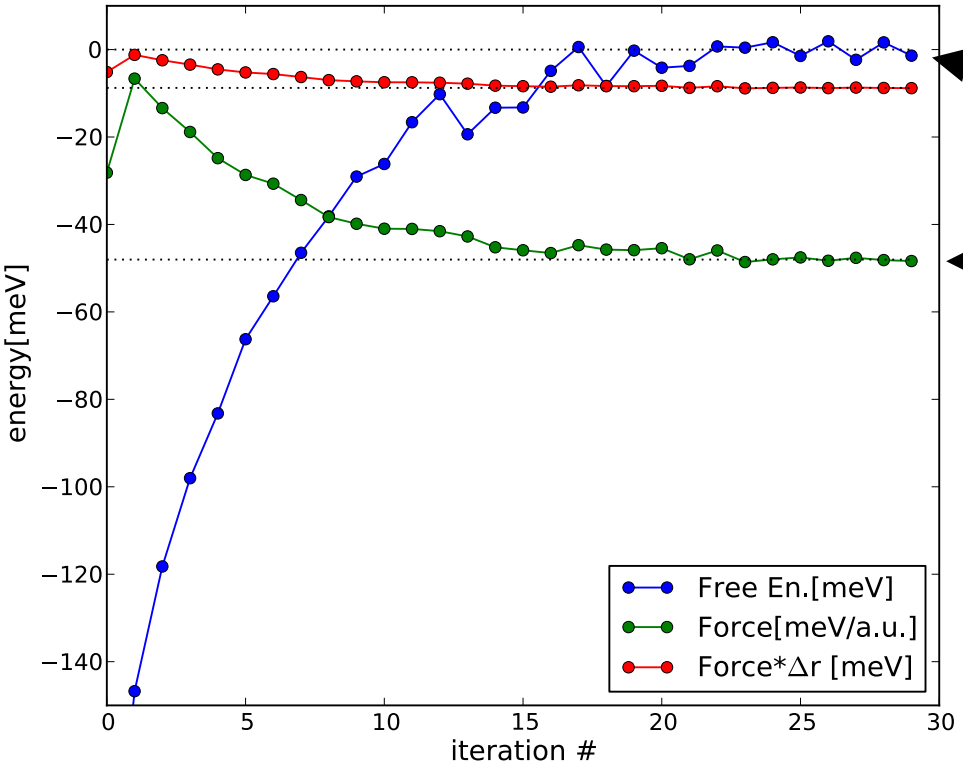
Success: Forces do not depend on $\Phi[G]$ or $\delta\Sigma/\delta G = \delta^2\Phi/\delta G^2$

which are hard to compute.

KH, arXiv:1602.02819.

Forces more stable than free energies





MC noise at constant statistics

free energy noise ~1meV

force noise ~ 0.2 meV/a.u.

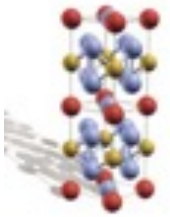
Forces very stable!

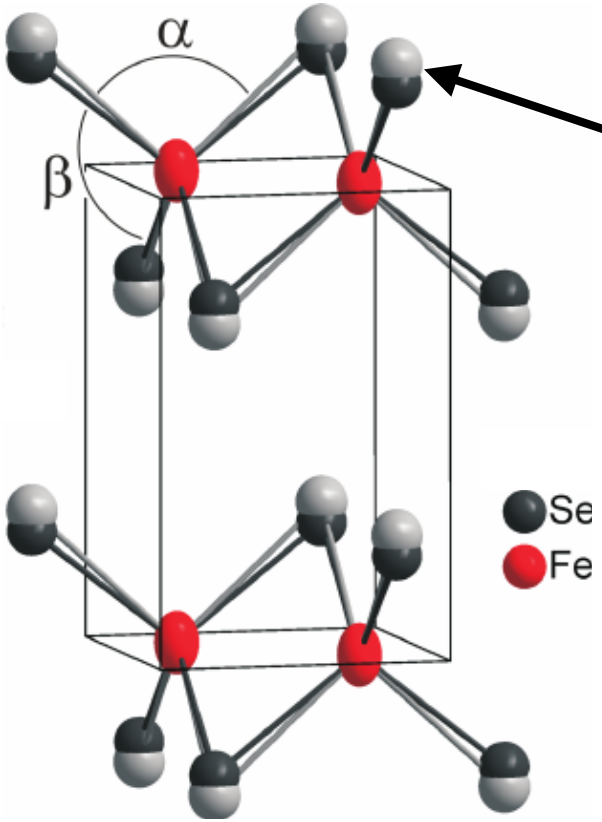
$\Phi[G]$ hard to compute (needed for free energy)

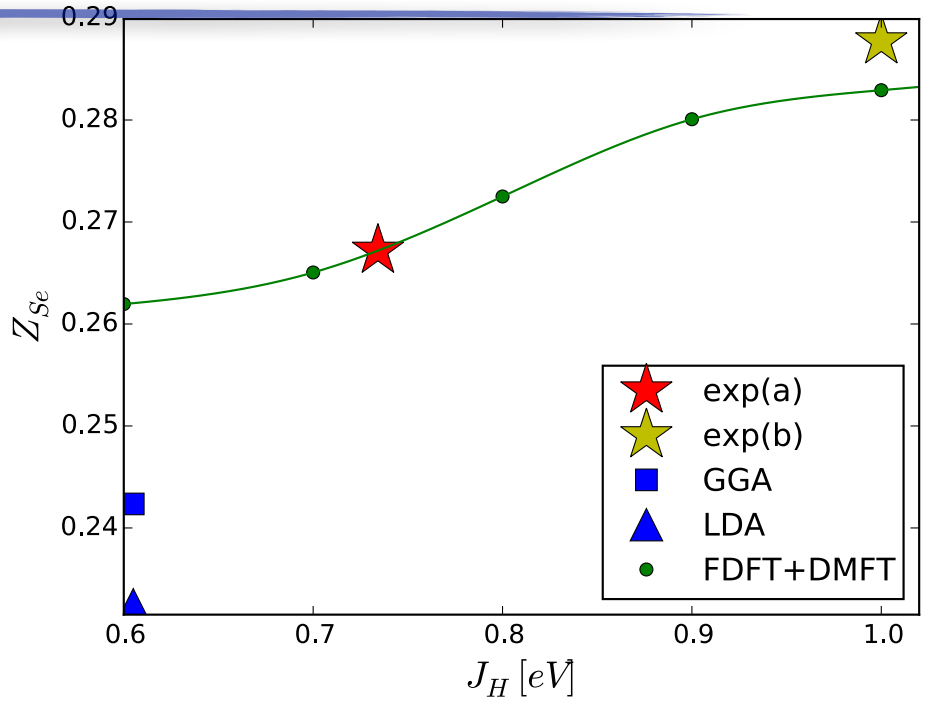
$\Sigma = \delta\Phi[G]/\delta G$ easy to compute
only this is needed for the force

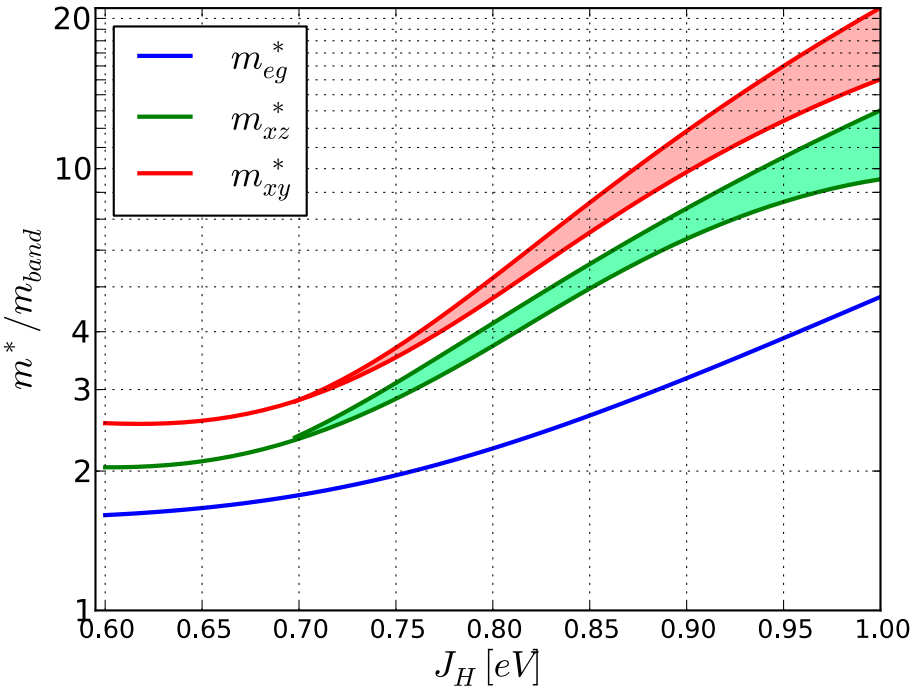
$\delta^2\Phi[G]/\delta G^2$ hard to compute (needed for dynamical matrix)

Optimizing FeSe structure - Hunds metal





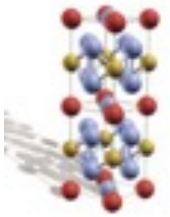




exp(a): T. M. McQueen, … R.J.Cava, PRB 79, 014522 (2009).

exp(b): R. S. Kumar, … C. Chen, The Journal of Physical Chemistry B 114, 12597 (2010).

Electronic structure package: EDMFTF



Download: http://hauleweb.rutgers.edu/tutorials

Some tutorials:

DMFT_W2K Tutorials and Installation Instructions

- Installation
- Overview
- Tutorial on single band Hubbard model
- Tutorial 1 on $SrVO_3$
- Tutorial 2 on $LaVO_3$
- Tutorial 3 on elemental Cerium
- Tutorial 4 on Sr_2IrO_4

- Projection & Embedding instead of downloading in the full potential (APW+lo,LAPW) basis.
- Continuous time quantum Monte Carlo, OCA, NCA…
- Stationary implementation of free energy
- Forces on all atoms

Database:

http://hauleweb.rutgers.edu/

Download the DMFT-Wien2K source code

dmft_w2k.tgz (version 2012)

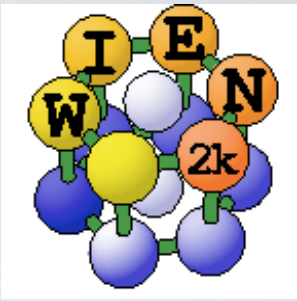
dmft_w2k.tgz (version 2015)

DFT PART

init_lapw : $\rho^{atom}(\mathbf{r})$

run_lapw ==

x lapw0 : $V_{ext}(\mathbf{r})\ \rho(\mathbf{r}) \rightarrow V_{KS}(\mathbf{r})$



x mixer: $\rho^{val} + \rho^{core}, \rho^{old}(\mathbf{r}) \rightarrow \rho^{new}(\mathbf{r})$

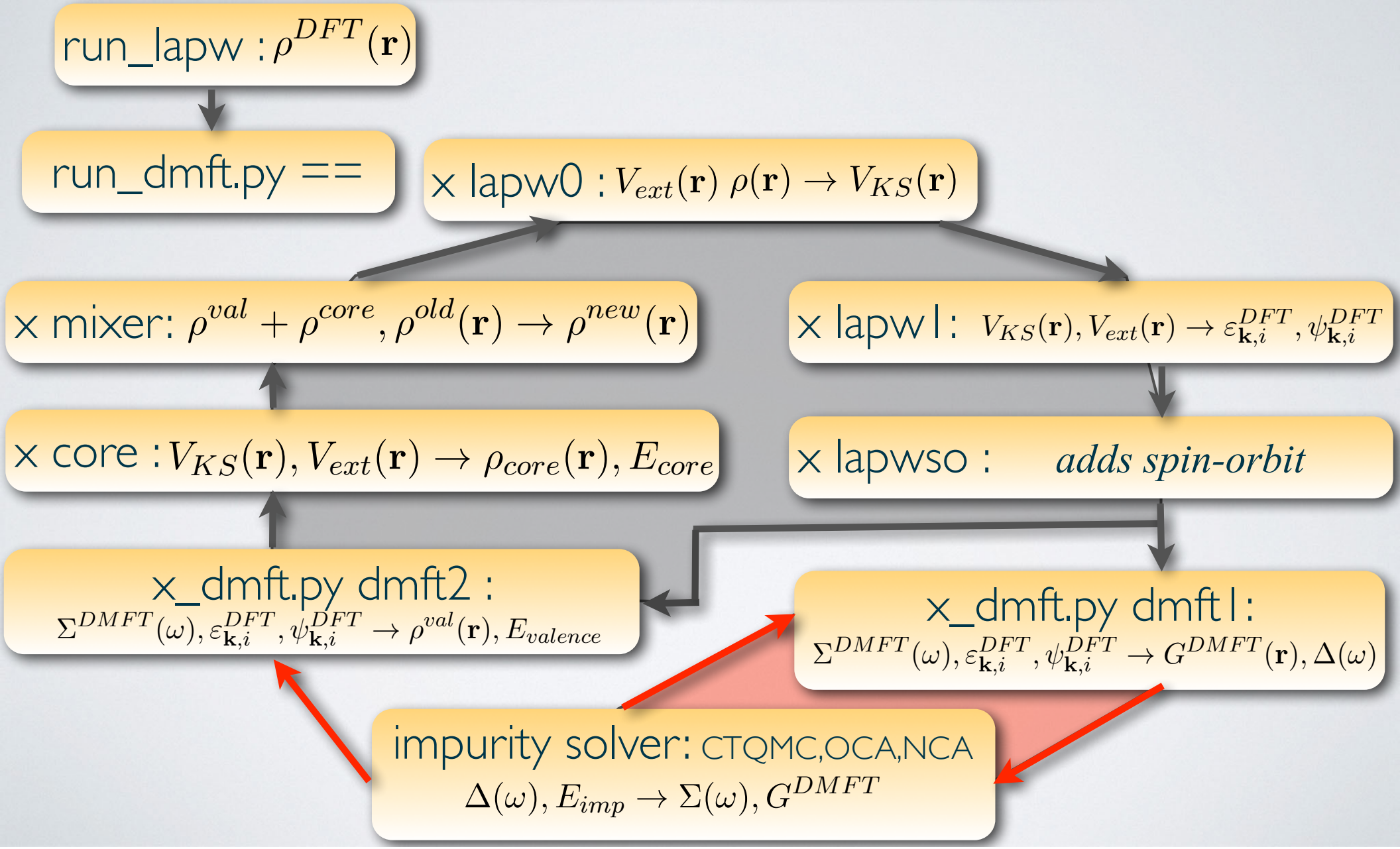
x lapw1 : $V_{KS}(\mathbf{r}), V_{ext}(\mathbf{r}) \rightarrow \varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i}$

x core : $V_{KS}(\mathbf{r}), V_{ext}(\mathbf{r}) \rightarrow \rho_{core}(\mathbf{r}), E_{core}$

x lapwso : *adds spin-orbit*

x lapw2: $\varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i} \rightarrow \rho^{val}(\mathbf{r}), E_{valence}$

DFT+DMFT COMBINED



x_dmft.py dmft1:

$\Sigma^{DMFT}(\omega), \varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i} \rightarrow G^{DMFT}(\mathbf{r}), \Delta(\omega)$

input → **output**

$\Sigma(\omega), \varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i}(\mathbf{r}) \longrightarrow G_{local}(\omega), \Delta(\omega), E_{imp}, n_{local}$

1) Construct projector: $P(\mathbf{r}\mathbf{r}', \mathbf{R}_\mu, mm') = \langle \mathbf{r}|\phi^\mu_m\rangle \langle \phi^\mu_{m'}|\mathbf{r}'\rangle$

where $\langle \mathbf{r}|\phi^\mu_m\rangle = u_l(|\mathbf{r}-\mathbf{R}_\mu|)Y_{lm}(\widehat{\mathbf{r}-\mathbf{R}_\mu})$

2) Embed self-energy: $\bar{\Sigma}_{ij}(\mathbf{k},\omega) = \sum_{\mathbf{R}_\mu} \langle \psi^{DFT}_{\mathbf{k},i}|\phi^\mu_m\rangle \left(\Sigma^\mu_{mm'}(\omega) - V^\mu_{DC}\right) \langle \phi^\mu_{m'}|\psi^{DFT}_{\mathbf{k},j}\rangle$

3) Calculate local Green's function, hybridization, imp. levels:

$$G^\mu_{local\ mm'} = \sum_{\mathbf{k},ij} \langle \phi^\mu_m|\psi^{DFT}_{\mathbf{k},i}\rangle \left(\omega + \mu - \varepsilon_{\mathbf{k}} - \bar{\Sigma}(\mathbf{k},\omega)\right)^{-1}_{ij} \langle \psi^{DFT}_{\mathbf{k},j}|\phi^\mu_{m'}\rangle = \left(\frac{1}{\omega - E^\mu_{imp} - \Sigma^\mu(\omega) - \Delta^\mu(\omega)}\right)_{mm'}$$

symmetrization over all group operations is performed

x_dmft.py dmft2 :

$$\Sigma^{DMFT}(\omega), \varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i} \rightarrow \rho^{val}(\mathbf{r}), E_{valence}$$

input $\Sigma(\omega), \varepsilon^{DFT}_{\mathbf{k},i}, \psi^{DFT}_{\mathbf{k},i}(\mathbf{r})$ ⟶ **output** $\rho^{DMFT}_{val}(\mathbf{r}), E_{valence}, F_{valence}, \mathbf{F}^{\mathbf{R}_\mu}$

1) Construct projector: $P(\mathbf{r}\mathbf{r}', \mathbf{R}_\mu, mm') = \langle \mathbf{r}|\phi^\mu_m\rangle \langle \phi^\mu_{m'}|\mathbf{r}'\rangle$

where $\langle \mathbf{r}|\phi^\mu_m\rangle = u_l(|\mathbf{r}-\mathbf{R}_\mu|) Y_{lm}(\widehat{\mathbf{r}-\mathbf{R}_\mu})$

2) Embed self-energy: $\bar{\Sigma}(\mathbf{r},\mathbf{r}') = \sum_{\mathbf{R}_\mu} \langle \mathbf{r}|\phi^\mu_m\rangle \left(\Sigma^\mu_{mm'}(i\omega) - V^\mu_{DC}\right) \langle \phi^\mu_{m'}|\mathbf{r}'\rangle$

3) Solve the Dyson Eq.: $\left(-\nabla^2 + V_{KS} + \bar{\Sigma}\right)|\psi_{\mathbf{k},i\omega_n,i}\rangle = |\psi_{\mathbf{k},i\omega_n,i}\rangle \varepsilon^{DMFT}_{\mathbf{k},i\omega_n,i}$

or $(\varepsilon^{DFT}_{\mathbf{k},i_1}\delta_{i_1,i_2} + \langle \psi^{DFT}_{\mathbf{k},i_1}|\bar{\Sigma}|\psi^{DFT}_{\mathbf{k},i_2}\rangle) \langle \psi^{DFT}_{\mathbf{k},i_2}|\psi_{\mathbf{k},i\omega,i}\rangle = \langle \psi^{DFT}_{\mathbf{k},i_1}|\psi_{\mathbf{k},i\omega_n,i}\rangle \varepsilon^{DMFT}_{\mathbf{k},i\omega_n,i}$

4) Determine the chemical potential: $N_{val} = T \sum_{i\omega_n,\mathbf{k},i} \frac{1}{i\omega + \mu - \varepsilon_{\mathbf{k},i\omega_n,i}}$

5) Calculate DMFT electronic charge in space:

$$\rho^{DMFT}_{val}(\mathbf{r}) = \sum_{\mathbf{k},ij} \psi^{DFT}_{\mathbf{k},i}(\mathbf{r})\, T \sum_{i\omega_n} \left[(i\omega + \mu - \varepsilon^{DFT}_{\mathbf{k}} - \bar{\Sigma}_{\mathbf{k}}(\omega))^{-1}\right]_{ij} \psi^{DFT*}_{\mathbf{k},j}(\mathbf{r})$$

6) Calculate DMFT free energy and forces on all atoms

symmetrization over group operations not performed

http://summer2016.ccs.usherbrooke.ca/dmft/

Initialize the DMFT calculation

```
$> ssh -X stud[..]@summer2016.ccs.usherbrooke.edu
$> qsub -I -X                                    start interactive session
$> module load edmftf                            load the module
$> export OMP_NUM_THREADS=2                      don't use too many cores!
$> cd MnO
$> init_dmft.py                                  this sets up DMFT projector
```

To answer the questions, look at:

http://hauleweb.rutgers.edu/tutorials/ click: Tutorial 1 on MnO

Continue… initialize the DMFT calculation

```
$> mkdir ../DMFT_MnO; cd ../DMFT_MnO      fresh start in new dir
$> dmft_copy.py ../MnO                    copy necessary files here
$> x kgen -f MnO                          increase number of k-points
          2000
$> cp $RESULT/MnO/params.dat  .           get params file
$> szero.py -e 38.22 -T 0.025853 create blank Sigma (T=1/beta=1/38.68)
$> cp $RESULT/submit2.sh .                obtain submission script
$> exit                                   stop interactive session
$> cd DMFT_MnO                            return to the current dir
$> qsub  submit2.sh                       submit to the queue
```

Monitor the job

```
$> less dmft_info.out                          check the master log file
$> less ':log'                                 check execution log
$> plot -u1:3,1:5 -x:10  MnO.dlt1              plot hybridization function
$> plot -x:20 -g -u1:3,1:5 imp.0/Gf.out.?.1    plot the DMFT output G
$> less info.iterate                           see current energy/mu/Vdc/…
$> plot -g -u1:9,1:10 info.iterate             plot lattice & impurity occupancy
$> grep ':CHARGE' MnO.dayfile                  how well is charge converged
```

it might take too much time to converge…

After some time you should kill your job, and continue with postprocessing

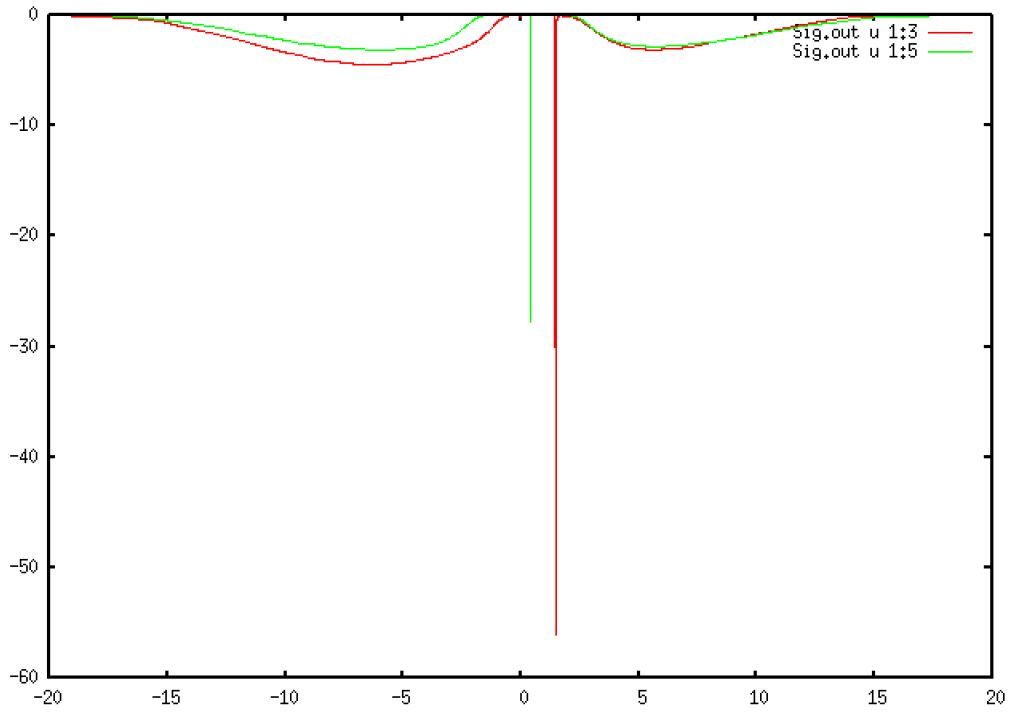
To kill your job, type

```
$> qstat                find your job ID
$> qdel  <Job ID>
```

Postprocessing maxent

```
$> mkdir maxent; cd maxent                                  new directory
$> saverage.py $RESULT/MnO/sig.inp.1?.1                     average over a few MC steps
$> cp $RESULT/MnO/maxent/maxent_params.dat .                parameters for maxent
$> qsub -I -X                                               interactive session
$> module load edmftf
$> cd DMFT_MnO/maxent                                       go back to the new dir
$> maxent_run.py sig.inpx                                   run maxent
$> plot -u1:3,1:5 Sig.out                                   plot Sigma on real axis
```

you should get:



Postprocessing DOS

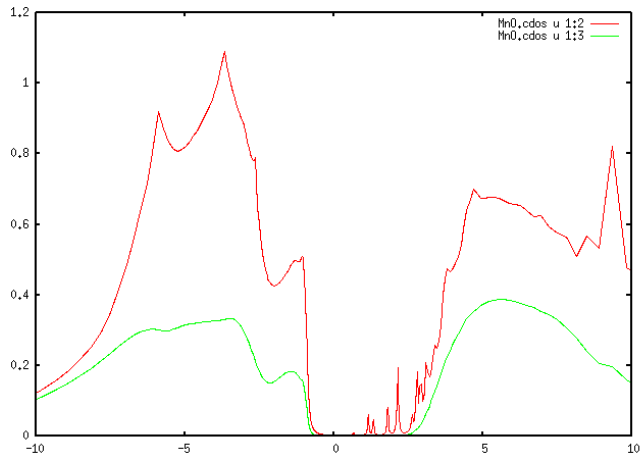
```
$> mkdir ../onreal; cd ../onreal          new directory
$> dmft_copy.py  $RESULT/MnO              copy converged DMFT outputs
$> cp ../maxent/Sig.out sig.ip            replace Sigma(iom) with Sigma(om)
```

*edit the second line of **MnO.indmfl** file and change the flag **matsubara** to 0*

```
    0 0.025 0.025 200 -3.000000 1.000000  # matsubara,..
```

```
$> x lapw0 -f MnO                         recompute KS potential
$> x lapw1 -f MnO                         recompute KS eigensystem
$> x_dmft.py dmft1                        compute DOS and G on real axis
$> plot -x-10:10 -uall MnO.cdos           plots partial DOS
$> plot -x-10:10 -u1:3,1:5 MnO.gc1        plots local G(omega)
```

you should get:



Post-processing band structure

$> cp $RESULT/MnO/onreal/MnO.klist_band . `get k-path`

$> x lapw1 -f MnO -band `KS eigvals on k-path`

*edit the second line of **MnO.indmfl** file and change **omega_min, omega_max** to -6 6*

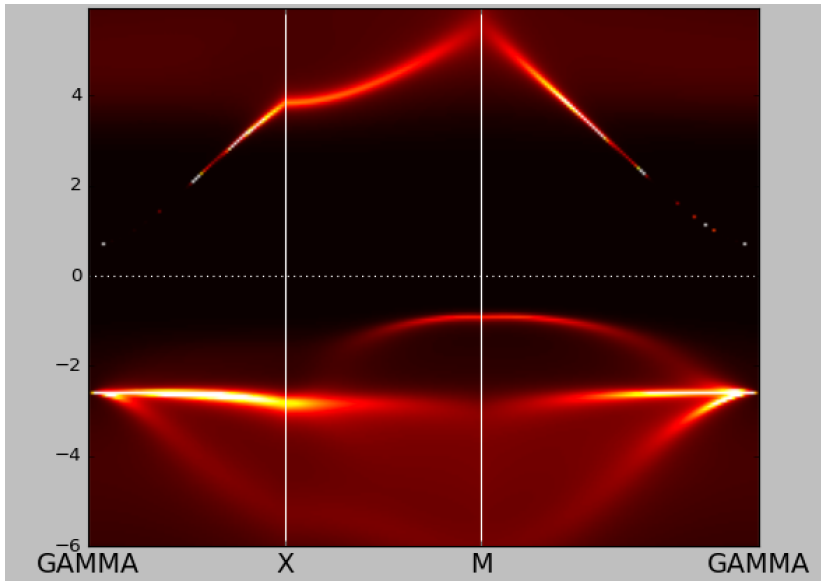
```
    0 0.025 0.025 200 -6.000000 6.000000  # matsubara,..
```

$> x_dmft.py dmftp `compute dmft eigvals`

$> cp $RESULT/MnO/EF.dat . `get final EF`

$> wakplot.py 0.02 `plot spectral function`

`you should get:`



FeSe

`Repeat all above steps for FeSe reading the tutorial at:`

http://hauleweb.rutgers.edu/tutorials/ `click:` Tutorial 2 on FeSe

Thank you!