Dynamical Mean Field Theory

Review articles


Thomas Maier, Mark Jarrell, Thomas Pruschke, and Matthias H. Hettler, Rev. Mod. Phys. 77, 1027 (2005)


http://phys.columbia.edu/~millis/MillisTLH.pdf
Dynamical Mean Field Theory

Many-body formalism: analogous to Hohenberg-Kohn

\[ \mathbf{H} = \sum_{\alpha, \beta} E^{\alpha \beta} \psi_\alpha^\dagger \psi_\beta + \sum_{\alpha \beta \gamma \delta} I^{\alpha \beta \gamma \delta} \psi_\alpha^\dagger \psi_\beta^\dagger \psi_\gamma \psi_\delta + \ldots \]

=> Luttinger-Ward functional

\[ \mathcal{F} [\{ \Sigma \}] = \mathcal{F}_{\text{univ}} [\{ \Sigma \}] - \text{Tr} \ln [G_0^{-1} - \Sigma] \]

\( G_0 \): Green function of noninteracting reference problem (contains atomic positions)

\( \mathcal{F}_{\text{univ}} \): determined (formally) from sum of diagrams. Depends only on interactions \( I^{\alpha \beta \gamma \delta} \)

More formalities

\[ \mathcal{F} [\{ \Sigma \}] = \mathcal{F}_{\text{univ}} [\{ \Sigma \}] - \text{Tr} \ln [G_0^{-1} - \Sigma] \]

Diagrammatic definition of \( \mathcal{F}_{\text{univ}} \) =>

\[ \frac{\delta \mathcal{F}_{\text{univ}}}{\delta \Sigma} = G \]

Thus stationarity condition

\[ \frac{\delta \mathcal{F}}{\delta \Sigma} = 0 \Rightarrow G = (G_0^{-1} - \Sigma)^{-1} \]

Difficulties with this formulation:
-- don’t know \( \mathcal{F}_{\text{univ}} \) (exc. perturbatively)
-- can’t do extremization

Example

Second order term

Hubbard model

\[ \Phi_{\text{LW}} [\{ G \}] \text{ defined as sum of all vacuum to vacuum diagrams (with symmetry factors)} \]

\[ \frac{\delta \Phi}{\delta G} = \Sigma \]

\[ \mathcal{F}_{\text{univ}} = \Phi_{\text{LW}} [\{ G \}] - \text{Tr} [\Sigma G] \]

Key first step: infinite d limit

Metzner and Vollhardt, PRL 62 324 (1987)

1992 Breakthrough

Kotliar and Georges found analogue of Kohn-Sham steps: useful approximation for \( \mathcal{F} \) and way to carry out minimization via auxiliary problem
Modern interpretation of Kotliar and Georges idea

Parametrize self energy in terms of small number $N$ of functions of frequency

$$\Sigma^{\alpha\beta}(\omega) = \sum_{ab} f_{ab}^{\alpha\beta} \Sigma_{\text{DMFT}}^{ab}(\omega)$$

$$\alpha = 1...M; \ a = 1...N << M$$

parametrization function $f$ determines ‘flavor’ of DMFT (DFT analogue: LDA, GGA, B3LYP, ....)

Also must truncate interaction $I^{\alpha\beta\gamma\delta}$ “appropriately”

Approximation to self energy + truncated interactions imply approximation to $F_{\text{univ}}$

Specifying the quantum impurity model

Need

--Interactions. These are the ‘appropriate truncation’ of the interactions in the original model

--a noninteracting (‘bare’) Green function $G_0$

Then can compute the Green function and self energy

$$G_{QI} = (G_0^{-1} - \Sigma)^{-1}$$

Approximated functional $F^{\text{approx univ}}$ is functional of finite (small) number of functions of frequency $\Sigma^{ab}(\omega)$ thus is the universal functional of some 0 (space) +1 (time) dimensional quantum field theory. Derivative gives Green function of this model:

$$\frac{\delta F^{\text{approx univ}}}{\delta \Sigma^{ba}(\omega)} = G_{QI}^{ab}(\omega)$$

Analogy:

Density functional $\iff$ ‘Luttinger Ward functional

Kohn-Sham equations $\iff$ quantum impurity model

Particle density $\iff$ electron Green function
Useful to view auxiliary problem as 'quantum impurity model' (cluster of sites coupled to noninteracting bath)

Quantum impurity model is in principle nothing more than a machine for generating self energies (as Kohn-Sham eigenstates are artifice for generating electron density)

As with Kohn Sham eigenstates, it is tempting (and maybe reasonable) to ascribe physical significance to it

In Hamiltonian representation

\[ H_{QI} = \sum_{ab} \langle d_a^\dagger E_{QI}^{ab} d_b \rangle + \text{Interactions} \]

Impurity Hamiltonian

+ \sum_{p, ab} \left( V_{p a}^b d_a^\dagger c_{p b} + H.c. \right) + H_{bath}\left[\{c_{p a}^\dagger c_{p a}\}\right] \]

Coupling to bath

Important part of bath: ‘hybridization function’

\[ \Delta^{ab}(z) = \sum_p V_{p a}^b \left( \frac{1}{z - \epsilon_{p b}} \right) V_{p c}^{b\dagger} \]

Thus

\[ F \rightarrow F_{\text{approx}}^{\text{univ}} \left[ \{\Sigma^{ab}\} \right] - \text{Trln}[G^{-1}_0 - \sum_{ab} f^{\alpha\beta}_a \Sigma^{ab}] \]

and stationarity implies

\[ \frac{\delta F}{\delta \Sigma^{ba}} = G_{QI}^{ab} - \text{Tr}_\alpha f^{\alpha\beta}_a \left[ G^{-1}_0 - \sum_{cd} f^{\alpha\beta}_c \Sigma^{cd} \right]^{-1} = 0 \]

or, using \( G_{QI} = (G^{-1}_0 - \Sigma^{ab})^{-1} \) from ‘impurity solver’

\[ (G^{-1}_0)^{ab} = \Sigma^{ab} + \left( \text{Tr}_\alpha f^{\alpha\beta}_a \left[ G^{-1}_0 - \sum_{cd} f^{\alpha\beta}_c \Sigma^{cd} \right]^{-1} \right)_{ab} \]

so \( G_0 \) is fixed

In practice

Guess hybridization function

Solve QI model; find self energy

Use extremum condition to update hybridization function

Continue until convergence is reached.

This actually works
Technical note

From your ‘impurity solver’ you need G at ‘all’ interesting frequencies. Solution ~uniformly accurate over whole relevant frequency range.

This is challenging.

Severe sign problem if \( \hat{\Delta}, \hat{E} \neq 0 \)

\( \Rightarrow \) reasonably high symmetry desirable so hybridization function commutes with impurity energies

For models with rotationally invariant multiplet interactions, cost grows exponentially with number of orbitals. 5 do-able with great effort more with Ising approximation (typically bad)

For simple 1 band Hubbard model, can access up to 16 orbitals at interesting temperatures.

In formal terms:

--Approximation to full M x M self energy matrix in terms of \( N(N+1)/2 \) functions determined from solution of auxiliary problem specified by self-consistency condition.

--Auxiliary problem: find (at all frequencies) Green functions of N-orbital quantum impurity model.

``Exponential wall” remains:

Question (practical): for feasible N, can you get the physics information you want?

Questions (not addressed here)

• What choices of parametrization function f are admissible
• What kinds of impurity models
• What can be solved
  • Where is the exponential wall (how large can N be?)
  • what kinds of interactions can be included
• What else (besides electron self energy) can be calculated
• Quality of approximation

advantages of method

*‘Moving part’ \( \text{Tr}_p [\phi_a(p) G_{\text{lattice}}(\Sigma_{\text{approx}})] \)

some sort of spatial average over electron spectral function—but still a function of frequency

*Computational task: solve quantum impurity model:
  not necessarily easy, but do-able

=> releases many-body physics from twin tyrannies of
  -- focus on coherent quasiparticles/expansion about well understood broken symmetry state
  -- emphasis on particle density and ground state properties
Single-site (N=1) DMFT of Hubbard model impurity model: One non-degenerate d orbital per unit cell

\[
H = - \sum_{ij} t_{i-j} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}
\]

DMFT impurity model

\[
A = \int dr dr' \left[ d_{r\sigma}(r) G_{0}^{-1}(r-r') d_{r'\sigma}(r') + U \int dr n_{r\uparrow}(r) n_{r\downarrow}(r) \right]
\]

Impurity model is just the Anderson model, with conduction band density of states fixed by self-consistency condition.

Regimes of Anderson model correspond to different physical behavior

Phase diagram and spectral function at n=1

interaction driven MIT via pole splitting

\[
\Sigma(z) \approx \frac{\Delta_1^2}{z - \omega_1} + \frac{\Delta_2^2}{z - \omega_2}
\]

\[
\omega_{1,2} \rightarrow 0 \text{ as } U \rightarrow U_{c2}
\]

\[
\Sigma(z \rightarrow 0) = -\frac{\Delta_1^2 \omega_2 + \Delta_2^2 \omega_1}{\omega_1 \omega_2} - z \left( \frac{\Delta_1^2 \omega_2^2 + \Delta_2^2 \omega_1^2}{\omega_1 \omega_2^2} \right)
\]

\[\mu \text{ renormalization} \quad 0 \text{ if p-h symmetry} \quad \text{'mass' renormalization diverges as approach insulator}
\]

P. Cornaglia data

U=0.85 U_{c2}

doping driven transition:
also coexistence regime;
2 pole structure
Many regimes of behavior

Key Point: theory captures incoherent dynamics at high frequency and crossover to coherent low frequency behavior

Regimes of behavior
configurations of impurity |0>, |1>, |2>, |3>

Strong correlations
generic occupancy
resonance forms: |0>, |2>
fermi liquid: local moment
transport: incoherent transport

T

Strong correlations
integer occupancy
Mott insulator
|0>, |2>
freeze out
local moment
gap opens

T

Orbital degeneracy: t_{2g} orbitals

J=U/6

Mott, magnetic and orbitally ordered phases.
Also "spin freezing"

Chan, Werner, Millis, Phys. Rev. B 80, 235114 (2009)

Spin freezing line: associated with larger spin. =>power law self energy

The power law self energy does not extend to lowest energies


Higher spin: extraordinarily low quasiparticle scale


Third example: nickelate superlattices

Chaloupka-Khalliulin

Bulk LaNiO$_3$ Ni [d]$^7$ (1 electron in two degenerate $e_g$ bands).

In correctly chosen superlattice structure, split $e_g$ bands, get 1 electron in 1 band--"like" high-Tc

Pseudocubic LaNiO$_3$

Relevant orbitals: $e_g$ symmetry Ni-O antibonding combinations

$3z^2-r^2$

Hybridizes strongly along $z$

Hybridizes weakly in $x$-$y$

$x^2-y^2$

Hybridizes strongly along $x$-$y$

Hybridizes very weakly in $z$

2 orbitals transform as doublet in cubic symmetry

Hamada’s result:

Two-fold degenerate $e_g$ band complex

One electron (band theory) physics

Hamada J Phys. Chem Sol 54 1157
Superlattice

Superlattice: La$_2$AlNiO$_6$
LaAlO$_3$ layer: insulating barrier

Question (Khalliulin): how much orbital polarization can we get?

\[ P = \frac{n_{x^2-y^2} - n_{3z^2-r^2}}{n_{x^2-y^2} + n_{3z^2-r^2}} \]

MJ Han, X Wang, C. Marianetti and A. J. Millis, arXiv:1105.0016

Band theory of La$_2$NiAlO$_6$ heterostructure:

La$_2$NiAlO$_6$
2d fermi surface

Hansmann et al PRL 103 016410

LaNiO$_3$
3d fermi surface

Hamada J Phys. Chem Sol 54 1157

No qualitative difference

DFT+DMFT: Correlate frontier orbitals

Map conduction bands to (multiple-orbital) Hubbard model.
Solve with single-site DMFT

\[ e_{c}^{0} = -2(\cos k_{z} + \cos k_{r}) + 2(\cos k_{z} - \cos k_{r}) \]

\[ \times \begin{pmatrix} 0.45 & 0 \cr 0.28 & 0 \cr 0.09 & 0 \cr 0 & 0.15 \end{pmatrix} \]

\[ H_{int} = \sum_{i \neq j} \sum_{\sigma} n_{i\sigma}^{e} n_{j\sigma}^{f} (V - \delta_{i,j} J) n_{i\sigma}^{e} n_{j\sigma}^{f} \]

and Phys. Rev. B 82, 235123 2010
Result: Proximity to Mott insulator=>enhanced polarization

Interactions enhance ‘orbital polarization’

Interactions drive ‘orbitally selective metal-insulator transition’

U=0

U=6eV


Phys. Rev. B 82, 235123 2010

Summary

Dynamical mean field theory:

--approximation to electron self energy obtained from solution of auxiliary quantum impurity problem

--can treat high temperature and incoherent phases;
metal insulator transition and low scales

--limits of accuracy of approximation: subject of different set of lectures

--meshes localized and k-space physics

?how to go beyond phenomenologically defined models?

Green function:

\[ G(r, r'; \omega) = \left\langle \{ \psi(r), \psi^\dagger(r') \} \right\rangle_\omega \]

\[ = \left[ \omega 1 - \hat{H}_0 - \Sigma(r, r'; \omega) \right]^{-1} \]

\[ H_0 = \sum_i \frac{p_i^2}{2m_e} + V_{\text{ext}}(r_i) \]

Bare Hamiltonian:
kinetic energy and lattice potential

DFT: static approximation to self energy

\[ G_{\text{DFT}}(r, r'; \omega) = \left[ \omega 1 - \hat{H}_0 - \Sigma_{\text{DFT}}(r, r') \right]^{-1} \]

Many body theory: supplement DFT self energy with additional terms expressing ‘beyond DFT’ physics

Express beyond DFT physics as ‘dynamical’ self energy

\[ \Sigma(r, r'; \omega) = \Sigma_{\text{DFT}}(r, r') + \Sigma_{\text{dyn}}(r, r'; \omega) \]

Cannot treat many body physics of all electronic degrees of freedom

=>must select subset of states for which dynamical self energy is computed

*different ways to do this
Frontier Orbital Approach

Express $G$ in band basis.
DFT part is diagonal.
Many-body ("dynamical") self energy is in general a matrix

$$
\hat{G}_{DFT}(k, \omega) = \left[ (\omega - \varepsilon_n^{KS}(k)) \delta_{nm} - \Sigma_{dyn}(k, \omega) \right]^{-1}
$$

$$
\Sigma_{dyn}^{nm}(k, \omega) = \int dr dr' \psi_{nk}^{KS}(r) \Sigma_{dyn}(r, r'; \omega) \psi_{mk}^{KS}(r')
$$

*Keep only self-energy and interaction matrix elements within frontier orbital basis.
(Interaction: phenomenological U,J or screened coulomb interaction projected onto these states)

Issues:

Cubic LaNiO$_3$
Fat bands

- Relevant (mainly d) bands entangled with p bands.
- Practical question: how to separate bands.
- Principle question: how important are the O states

``d'' orbital corresponding to the p-d antibonding bands has large spatial extent. Is it reasonable to ascribe just an on-site interaction $U$

Atomic Orbital Approach

alternative: define ‘atomic like’ orbital centered on sites $i$
project self energy onto this basis

$$
\psi_{iat}(r)
$$

$$
\Sigma_{dyn}(r, r'; \omega) \approx \sum_{ij} |\psi_{iat}^i(r)\rangle \Sigma^{ij}_{dyn}(\omega) <\psi_{iat}^j(r')| 
$$

$$
\hat{G}(r, r', \omega) = \left[ \omega - \hat{H}^{KS} - \Sigma_{dyn}(r, r'; \omega) \right]^{-1}
$$

Interaction: intra-d interactions already discussed

In real materials applications

retain only on-site (but orbitally dependent) terms in self energy and only on-site Slater-Kanamori terms in interaction

$$
\Sigma_{dyn}(r, r'; \omega) \rightarrow \sum_{iab} |\psi_{d}^{iA}(r)\rangle \Sigma^{ab}_{dyn}(\omega) <\psi_{d}^{b}(r')| 
$$

$$
\Sigma_{double-count}(r, r') \rightarrow \sum_{iab} |\psi_{d}^{iA}(r)\rangle \Sigma^{ab}_{dc} <\psi_{d}^{b}(r')| 
$$

$$
\hat{G}(r, r', \omega) = \left[ \omega - \hat{H}^{KS} - \Sigma_{dc}(r, r') - \Sigma_{dyn}(r, r'; \omega) \right]^{-1}
$$
Additional step (not often taken in practice):

Full charge self consistency

Recall Kohn-Sham potential $V_{KS}[\{n(r)\}]$ is a functional of density.

=>$\text{need to use density computed from interacting } G$

$$n(r) = \int d\omega \frac{\omega}{\pi} \text{Im} G(r,r,\omega)$$

to construct $V_{KS}$.

Two ways to define atomic orbital

*A priori: simply choose a wave function you think is appropriate (e.g. free atom hartree fock d-wave function)

*Wannier function

If isolated band (index $n$) with wave function $\psi_{nk}(r)$
then real space wave function centered in unit cell $i$ (pos $R_i$)

$$\phi_i(r) = \int_{BZ} (dk) e^{ik \cdot R_i} \psi_{nk}(r)$$

Maximally localized Wannier function

If many bands in a energy window, then many ways to construct Wannier functions--parameterized by family of unitary transformations depending on $k$

$$\phi_{nk}^i(r) = \int_{BZ} (dk) e^{ik \cdot R_i} \sum_n (\hat{U}^{mn}(k)\psi_{nk}(r))$$

Marzari-Vanderbilt: showed how to choose unitary transformation to make wannier functions correspond (as closely as Fourier’s theorem allows) to atomic-like functions centered on particular atoms (e.g. O 2p and Ni 3d)

If you have a set of bands reasonably well separated from other bands (e.g. p-d complex in many transition metal oxides)

Write $G \ H^{KS}$ and self energy as matrices in Wannier basis again retain only terms in dynamical self energy corresponding to orbitals where correlations are important

$$\hat{G}(\omega) = \left[ \omega 1 - \hat{H}_{KS} - \hat{\Sigma}_{dyn}(\omega) \right]^{-1}$$

$$H^{KS}_{ab} = \int dr dr' \phi^*_a(r) \left( \frac{\nabla^2}{2m} + V_{\text{latt}} + \Sigma_{\text{DFT}}(r,r') \right) \phi_b(r')$$

$H^{KS}_{ab}$ is formal definition of tight-binding model corresponding to “ab-initio” wave functions
Note!

All of these procedures assume that the wave functions of band theory have some meaning in the actual correlated material.

What do people do in practice

*DFT+U (Anisimov 1998)

Identify atomic-like d-orbital. Keep on-site d-d self energy arising from Hartree approx to Slater interactions

\[ V_{a\tau} = U < n_{a\tau} > + (U - 2J) \sum_{b \neq a} < n_{b\tau} > + (U - 3J) \sum_{b \neq a} < n_{b\tau} > \]

This calculation "knows" about correlations in the d-multiplet only via ordering. In non-ordered state, shift is same for all orbitals.

As with most Hartree approximations, tendency to order is overestimated.

Crucial physical effect: hartree shift of entire d-multiplet by amount of order \((U-2.5J)\)*n/spin/orbital

Hartree term: shifts d-multiplet relative to p-states.

this is important to the physics!!

atom orbital approach

\[ \sum_{ij} (r, r'; \omega) \approx \sum_{ij} |\psi_{i\tau}^j(r) > \sum_{ij} ^{ij} \omega < \psi_{\tau\tau}^j(r')| \]

will in general lead to hartree shift which moves atomic (here, d) orbitals relative to the p orbitals

Lower energy controls the interesting physics

\[ \Delta > U: \text{Mott-Hubbard} \]

\[ \Delta < U: \text{Charge Transfer} \]

Shift of d relative to p changes the physics
thus the crucial question:

In a beyond-DFT calculation: where is the renormalized d energy, relative to the ligands

This is sometimes called "the double counting problem", based on the idea that DFT includes some of the intra-d interactions and one does not want to count them twice. But the real question is—how much does the d-level shift relative to band theory.

A large literature exists (see, e.g. Karolak et al, Journal of Electron Spectroscopy and related phenomena, 181 (2010) 11–15) but there is as yet no generally agreed upon prescription. Results are sensitive to choice of double counting correction.

p-d covalency

key issue: renormalized d energy, relative to the ligands.

Question: what does "renormalized d energy" mean

My point of view (not universally accepted):
parametrize the renormalized d energy by d occupancy

Unhybridized bands: upper one is pure d. Increase hybridization, increase d-character of occupied states

d-occupancy:

* Intuitive notion: e.g. La$^{3+}$Ni$^{3+}$O$_3^{2-}$ \( \Rightarrow \) Ni$^7$ \( (N_d = 6+1) \)

* Theoretically needed (if you want to put correlations on d-orbital you need to know what this orbital is and how much it is occupied)

* definition:

In terms of exact Green function $G(r, r'; \omega)$ and predefined d-wave function $\phi_d$

$$N_d = \sum_{\alpha, \sigma} \int \frac{d\omega}{\pi} f(\omega) \int d^3r d^3r' \text{ Im} \left[ (\phi_d^{\alpha}(r))^{*} G_{\sigma}(r, r', \omega) \phi_d^{\sigma}(r') \right]$$
Notes

*d occupancy depends on how orbital is defined (as does the entire edifice of DFT+....)

Expect: all reasonable definitions give consistent answers (more on this later)

*should focus only on occupancy of ‘relevant’ orbitals

Notes

*N_d: theoretically precisely defined; experimental measures are indirect

--Intensities in resonant absorption spectra
--Sizes of moments/knight shifts
--peak positions (many-body e_d-e_p)

(.more on this later)

Notes

*Density functional theory only gives you

\[ n(r) = \sum_{\alpha,\sigma} \int \frac{d\omega}{\pi} f(\omega) \int d^3r \text{ Im } [ \mathcal{G}_{\sigma}(r, r, \omega)] \]

Thus even exact density functional, solved exactly, is not guaranteed to give you the exact N_d

But: seems plausible that in most cases DFT is a reasonably good approximation (more on this later)

Notes

In practice:

Available double counting corrections give N_d fairly close to N_d defined from DFT band theory calculations

Example: rare earth nickelates ReNiO_3

LuNiO_3: insulator. 2 inequivalent Ni sites.

Ni1  Ni2
GGA  8.21  8.20
GGA+U  8.24  8.22

Charge fixed by electrostatic effects.
Very robust
**DFT+DMFT (Georges04,Kotliar06,Held06)**

Identify atomic-like d-orbital. Keep on-site d-d self energy arising from single-site DMFT approx using Slater-kanamori interactions.

DMFT self consistency eq:

\[ G_{QI}^{ab} = \langle \psi_d^{ia}(r)|\hat{G}(r, r', \omega)|\psi_d^{ib}(r') \rangle \]

Same double counting issue as in DFT+U

Another example: High Tc cuprates

Green dots: fully charge self-consistent DFT+DMFT calculations for U=7,10eV. Vertical lines: DFT band theory (Wein2K and GGA)

Nickelate superlattices

Frontier orbital approach

U=0

U=6eV


Atomic-like d orbitals


*LaNiO$_3$/LaXO$_3$ (mainly X=Al)

*VASP/Wannier DFT+DMFT (Non-self-consistent)

*Computed ‘orbital polarization’

*Several combinations of U and e$_d$-e$_p$

\[ P = \frac{n_x^2y^2 - n_3z^2r^2}{n_x^2y^2 + n_3z^2r^2} \]
Results 1: Define P by integrating spectral function for superlattice

Results 2: Relation to Nd

Interactions decrease P

Results 2: How many sheets to the Fermi surface

Key point: Ni-O covalency

Band theory: electron moves from O to Ni, configuration is $d^8 \bar{L}$

According to band theory, LaNiO$_3$ and derivatives are close to being negative charge transfer energy materials

$d^8$ is high spin: both orbitals occupied

Occupancy per orbital
\( d^8 \) (high spin) => no distortion

Two electrons in high spin state => no energy gain from distortion

Negligible response to lattice distortion

tetragonal \((c/a) < 1\)

Over wide range of many-body phase space, \( N_d \) is close enough to \( d^8 \) that low-spin J-T state is disfavored

2-band Hubbard model with 1 el/Ni unit cannot represent \( d^8 \) physics

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Covalency in perovskites

Generally important

Band theory or standard double counting indicates that \( \text{La}_2\text{CuO}_4 \) is not a Mott insulator

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Example: \( \text{NiO} \)

Fit full p-d band complex:
Add ‘Slater-Kanamori’ U-J interactions on d-only. Solve.

choice of double counting (covalency) affects results (perhaps less strongly)

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Conclusion

- Wide variety of behaviors
- Important role played by instability of d valence
- Energetics and state of the art of realistic theory of correlated electron materials
- Key (and still ill-understood) role of double counting correction
- Important open question: is the “standard model” (atomic d, local correlation) the most correct and useful description?