organization of the lecture

- introduction
- from DMFT to LDA+DMFT
  - Hubbard dimer
  - one-band Hubbard model
  - multi-band Hubbard model
- building materials-specific models
  - model construction
  - basis localization and interaction range
  - spin orbit & double counting
- conclusion
introduction

strong correlations: what are they?
all of physics and chemistry is correlation

Born-Oppenheimer approximation, non-relativistic

\[
\hat{H}_e = -\frac{1}{2} \sum_i \nabla_i^2 + \frac{1}{2} \sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2} \sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}
\]

electron-electron interaction

why is it a problem?

simple interactions among many particles lead to unexpected emergent co-operative behavior

more is different

Philip Warren Anderson
4 August 1972, Volume 172, Number 4047
emergence in social media

formation of polarized opinion-bubbles

yes yes yes yes yes yes yes yes yes yes

no no no no no no no no no no

idiot! idiot!
emergence in solid-state systems

superconductivity

high-Tc superconductivity

non-conventional superconductivity

Mott transition


orbital order


magnetism

bad news: the exact solution is not an option

\[ \hat{H}_e = -\frac{1}{2} \sum_i \nabla_i^2 + \frac{1}{2} \sum_{i \neq i'} \frac{1}{|r_i - r_i'|} - \sum_{i,\alpha} \frac{Z_\alpha}{|r_i - R_\alpha|} + \frac{1}{2} \sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|R_\alpha - R_{\alpha'}|} \]

electron-electron interaction

\[ \hat{H}_e \Psi_\alpha(r_1, r_2, \ldots, r_N) = E_\alpha \Psi_\alpha(r_1, r_2, \ldots, r_N) \]
quantum N-body problem

1 body is difficult

- uncertainty principle: \( \Delta x \Delta \nu \geq \frac{1}{2} \frac{\hbar}{m} \)
- described via wavefunction \( \Psi(r) \)
- eigenvalue problem & discrete energies

2-bodies non interacting

- particles are identical \textbf{and} indistinguishable
- fermions: \( \psi(r_1)\psi(r_2) - \psi(r_2)\psi(r_1) \)

\[ \hat{H}_0 = \sum_i \hat{H}_i^0 \]

Slater determinant
quantum N-body problem, no interaction

\[ \hat{H}_0 = \sum_i \hat{H}_i^0 \]

\[ \hat{H}_i^0 \Psi(r_i) = \varepsilon_i \Psi(r_i) \]

\[ E = \sum_i \varepsilon_i \]

\[ \Psi = \Psi(r_1) \Psi(r_2) \ldots \Psi(r_N) \]

(classical/mean field)

+ antisymmetrization

(Slater determinant)

Fermi gas

neutron stars
bad news: the exact solution is not an option

\[ \hat{H}_e = -\frac{1}{2} \sum_i \nabla_i^2 + \frac{1}{2} \sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2} \sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|} \]

**kinetic energy** | **potential energy** | **constant**
---|---|---
\[ -\frac{1}{2} \sum_i \nabla_i^2 \] | \[ - \sum_{i,\alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} \] | \[ + \frac{1}{2} \sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|} \]

**electron-electron interaction**

\[ \hat{H}_e \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = E_\alpha \Psi_\alpha(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \]
good news: it would be anyway useless

On the other hand, the exact solution of a many-body problem is really irrelevant since it includes a large mass of information about the system which although measurable in principle is never measured in practice.

[...] An incomplete description of the system is considered to be sufficient if these measurable quantities and their behavior are described correctly.
what can be done then?
Inhomogeneous Electron Gas

P. Hohenberg
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and

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and

University of California at San Diego, La Jolla, California

(Received 18 June 1964)

This paper deals with the ground state of an interacting electron gas in an external potential \( v(r) \). It is emphasized that the electronic density \( n(r) \) plays a central role and in theoretical considerations is a description of this. We want to emphasize that the simple methods that are here proposed are uncomprehensive and that all previously developed refinements of the Thomas-Fermi and the Slater exchange interactions and as a result there has been little recent progress.

In Part I, we develop an exact formal variational method of Thomas-Fermi and the Slater exchange and correlation effects. They require only a knowledge of the true chemical potential, \( \mu(n) \), of a uniform electron gas. This procedure will describe correctly the local effective potentials in these methods. The methods proposed here offer the hope of new and refined treatments of inhomogeneous systems. The well-known Thomas-Fermi method has failed to include these.

In Part II, we obtain an expression for the ground-state energy in a given external potential.

\[ \mu(n) = \frac{1}{2} \int n(r) \left( \frac{e^{-\beta v(r)}}{e^{-\beta v(r)}} + 1 \right) dr \]

The expansion \( \mu(n) = \frac{1}{2} \int n(r) \left( \frac{e^{-\beta v(r)}}{e^{-\beta v(r)}} + 1 \right) dr \) is the variable functional, \( PL_{tr}(r) \), which applies to homogeneous systems like atoms and impurities in metals. This approach has been useful, up to the 1970's a different approach, represented by the Thomas-Fermi method and its refinements, in which the electronic density \( n(r) \) plays a central role and in which the system of electrons is pictured more like a classical liquid. This approach has been useful, up to now, for simple though crude descriptions of inhomogeneous systems like atoms and impurities in metals.

Recently, however, there has been some important advances along this second line of approach, such as the work of Kompaneets and Pavlovski, Koehn, Lewis, Baraff and Borowitz, Baraff, and DuBois and Kivelson. The present paper represents a contribution in the same area.

In Secs. III and IV, we describe the necessary modifications to deal with the finite-temperature properties and with the spin paramagnetism of an inhomogeneous electron gas.

Of course, the simple methods which are here proposed in general involve errors. These are of two general origins: a too rapid variation of density and, for finite systems, boundary effects. Refinements aimed at reducing the first type of error are briefly discussed in Appendix II.

II. THE GROUND STATE

In recent years a great deal of attention has been given to the problem of a homogeneous gas of interacting electrons and its properties have been established with a considerable degree of confidence over a wide range of densities. Of course, such a homogeneous gas represents only a mathematical model, since in all real systems (atoms, molecules, solids, etc.) the electronic density is nonuniform.

It is then a matter of interest to see how properties of the homogeneous gas can be utilized in theoretical investigations of the electron gas in solid state physics.
1998: Nobel Prize in Chemistry to Walter Kohn
In my view DFT makes two kinds of contribution to the science of multi-particle quantum systems, including problems of electronic structure of molecules and of condensed matter:

The first is in the area of fundamental understanding. Theoretical chemists and physicists, following the path of the Schroedinger equation, have become accustomed to think in a truncated Hilbert space of single particle orbitals. The spectacular advances achieved in this way attest to the fruitfulness of this perspective. However, when high accuracy is required, so many Slater determinants are required (in some calculations up to ~ $10^9$!) that comprehension becomes difficult. DFT provides a complementary perspective. It focuses on quantities in the real, 3-dimensional coordinate space, principally on the electron density $n(r)$ of the groundstate. Other quantities of great interest
The main fallacy in this kind of thinking is that the reductionist hypothesis does not by any means imply a “constructionist” one: the ability to reduce everything to simple fundamental laws does not imply the ability to start from those laws and reconstruct the universe. In fact, the more the ele-

There is a school which essentially accepts the idea that nothing further is to be learned in terms of genuine fundamentals and all that is left for us to do is calculate. . . . [..] This is then the idea that I call “The Great Solid State Physics Dream Machine”…

. . . In other words the better the machinery, the more likely it is to conceal the workings of nature, in the sense that it simply gives you the experimental answer without telling you why the experimental answer is true (1980)

(RO Jones, DFT for emergents, Autumn School on Correlated Electrons 2013)
a way out: density-functional theory

\[ \hat{H} = -\frac{1}{2} \sum \nabla_i^2 + \frac{1}{2} \sum_{i \neq i'} \frac{1}{|r_i - r_{i'}|} - \sum_{i, \alpha} \frac{Z_\alpha}{|r_i - R_\alpha|} - \sum_\alpha \frac{1}{2M_\alpha} \nabla_\alpha^2 + \frac{1}{2} \sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|R_\alpha - R_{\alpha'}|} \]

from the ground-state wave-function to the electron density

**Kohn-Sham auxiliary Hamiltonian**

\[ \hat{h}_e = \sum_i \left[ -\frac{1}{2} \nabla_i^2 + v_R(r_i) \right] = \sum_i \hat{h}_e(r_i) \]

\[ v_R(r) = -\sum_\alpha \frac{Z_\alpha}{|r - R_\alpha|} + \int dr' \frac{n(r')}{|r - r'|} + \frac{\delta E_{xc}[n]}{\delta n} = v_{en}(r) + v_H(r) + v_{xc}(r) \]

(in practice: LDA, GGA, …)
unexpected successes of DFT

Kohn-Sham eigenvalues as elementary excitations!

band structures, material trends, prediction
unexpected successes of DFT

“the labours and controversies . . . in understanding the chemical binding in materials had finally come to a resolution in favour of ‘LDA’ and the modern computer” (1998)

Philip Warren Anderson

but “very deep problems” remain (1998)

origin of failures: one-electron picture

(R.O. Jones, DFT for emergents, Autumn School on Correlated Electrons 2013)
Experiments: it is an insulator! and above 40 K a **paramagnetic** insulator
strongly correlated systems

paramagnetic Mott insulators are either metals or magnetically ordered insulators in the Kohn-Sham picture

Coulomb-induced metal-insulator transition
heavy-Fermions
unconventional superconductivity
spin-charge separation
$ab$-$initio$ methods fail...
but it can be explained with simple models!

The Hubbard model at half a century

Models are abundant in virtually all branches of physics, with some achieving iconic status. The Hubbard model, celebrating its golden jubilee this year, continues to be one of the most popular contrivances of theoretical condensed-matter physics.

Capturing the essence of a phenomenon while being simple: the ingredients of a top model in physics. Since the early days of quantum mechanics, many models, Hamiltonians and theories aiming to provide a deeper understanding of various properties of condensed matter have been put forward — with varying degrees of success and fame. One truly legendary model is the Hubbard model, independently conceived by Martin Gutzwiller¹, Junjiro Kanamori² and, of course, John Hubbard³ — their original papers all appearing in 1963. The refine his model. His ‘Electron correlations in narrow energy bands’ would eventually comprise six installments. ‘Hubbard III’⁴ became especially important as it showed that for one electron per lattice site — the Hubbard model at half filling — the Mott (or Mott–Hubbard) transition is reproduced. This is a type of metal–insulator transition that could not be understood in terms of conventional band theory (which predicts that a half-filled band always results in a conducting state).

The simplicity of the Hubbard model, when written down, is deceptive. Not only when the field of cold-atom optical trapping had advanced so far that experimental realizations of the Hubbard model could be achieved. A landmark experiment demonstrated how a lattice of bosonic atoms displays a transition from a superfluid to a Mott insulator⁵, a result accounted for by the Bose–Hubbard model (the Hubbard model for bosons). Many other variants of the Hubbard model, including the original model for fermions⁶, have been experimentally realized by now, a development that nicely illustrates how a model can become the target of experiments.
Hubbard model at half-filling

\[ \hat{H} = \varepsilon_d \sum_i \sum_{\sigma} c^\dagger_{i\sigma} c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_{\sigma} c^\dagger_{i\sigma} c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = \hat{H}_d + \hat{H}_T + \hat{H}_U \]

1. \( t=0 \): collection of atoms, **insulator**
2. \( U=0 \): half-filled band, **metal**

**canonical model for Mott transition**
Mott systems: two irreconcilable philosophies?

• improve exchange-correlation functional
  ▶ materials-specific aspects are key

• give up DFT and use canonical models
  ▶ generic mechanism-specific aspects are key

both right and wrong
how do we connect canonical models and DFT?
let us go back to the basics

\[
\hat{H}_e = -\frac{1}{2} \sum_i \nabla_i^2 + \frac{1}{2} \sum_{i \neq i'} \frac{1}{|\mathbf{r}_i - \mathbf{r}_{i'}|} - \sum_{i, \alpha} \frac{Z_\alpha}{|\mathbf{r}_i - \mathbf{R}_\alpha|} + \frac{1}{2} \sum_{\alpha \neq \alpha'} \frac{Z_\alpha Z_{\alpha'}}{|\mathbf{R}_\alpha - \mathbf{R}_{\alpha'}|}
\]

electronic Hamiltonian in 2nd quantization

\[
\hat{H}_e = -\sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{aa' bb'} U_{aa' bb'} c_a^\dagger c_{a'}^\dagger c_{b'} c_b
\]

complete one-electron basis set!
parameters

\[
t_{ab} = - \int dr \ \phi_a(r) \left( -\frac{1}{2} \nabla^2 - \sum_{\alpha} \frac{Z_{\alpha}}{|r - \mathbf{R}_{\alpha}|} \right) \phi_b(r)
\]

hopping integrals

\[
U_{aa'bb'} = \int dr_2 \int dr_2 \ \phi_a(r_1) \overline{\phi_{a'}(r_2)} \ \frac{1}{|r_1 - r_2|} \ \phi_{b'}(r_2) \ \phi_b(r_1)
\]

Coulomb integrals
in theory all basis are identical

in practice some bases are better than others

\[
\hat{H}_e = -\sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{aa'bb'} U_{aa'bb'} \ c_a^\dagger c_{a'}^\dagger c_b c_b
\]

\[
\hat{H}_0 \quad \hat{H}_U
\]

Kohn-Sham orbitals

\[
\hat{H}_e = -\sum_{ab} \tilde{t}_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{aba'b'} \tilde{U}_{aa'bb'} \ c_a^\dagger c_{a'}^\dagger c_b c_b - \hat{H}_{DC}
\]

\[
\hat{H}_0 = \hat{H}_e^{\text{LDA}} \quad \Delta \hat{H}_U
\]
what do the parameters contain?

\[ \tilde{t}_{ab} = -\int d\mathbf{r} \ \overline{\phi_a^{KS}}(\mathbf{r}) \left( -\frac{1}{2} \nabla^2 + v_R(\mathbf{r}) \right) \phi_b^{KS}(\mathbf{r}) \]

- Hartree
- potential
- exchange-correlation

\[ v_R(\mathbf{r}) = -\sum_\alpha \frac{Z_\alpha}{|\mathbf{r} - \mathbf{R}_\alpha|} + \int d\mathbf{r}' \ \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{\delta E_{xc}[n]}{\delta n} = v_{en}(\mathbf{r}) + v_H(\mathbf{r}) + v_{xc}(\mathbf{r}) \]

Walter Kohn

Nobel Prize in Chemistry (1998)

Kohn-Sham equations

understand and predict properties of solids, molecules, biological systems, geological systems...
weakly-correlated systems

one-electron approximation

\[ \hat{H}_e = -\sum_{ab} \tilde{t}_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{aba'b'} \tilde{U}_{aa'bb'} c_a^\dagger c_{a'}^\dagger c_{b'} c_b - \hat{H}_{DC} \]

\[ \hat{H}_0 = \hat{H}_e^{LDA} \]

\[ \Delta \hat{H}_U \]

\[ \hat{H}_{\text{eff}} \sim \hat{S}^{-1} \hat{H}_e \hat{S} \sim \hat{H}_e^{LDA} \]

very good approach for weakly correlated systems
why not also for Mott systems?

\[
\hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{cd, cd'} U_{cdcd'} c_c^\dagger c_d^\dagger c_{c'} c_{d'}
\]

\[
\hat{H}_e = \sum_{ab} \tilde{t}_{ab} c_a^\dagger c_b
\]

one-electron approximation
Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_c \text{max}$

E. Pavarini, I. Dasgupta, a T. Saha-Dasgupta, b O. Jepsen, and O. K. Andersen
Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany
(Received 4 December 2000; published 10 July 2001)

By calculation and analysis of the bare conduction bands in a large number of hole-doped high-temperature superconductors, we have identified the range of the intralayer hopping as the essential, material-dependent parameter. It is controlled by the energy of the axial orbital, a hybrid between Cu 4s, apical-oxygen 2p$_z$, and farther orbitals. Materials with higher $T_c \text{max}$ have larger hopping ranges and axial orbitals more localized in the CuO$_2$ layers.
electron counting argument

one electron per site

\[ \varepsilon_k = -2t \left[ \cos k_x + \cos k_y \right] \]

\[ \frac{t'}{t} = 0.2 \quad \frac{t'}{t} = 0.4 \]
to open a gap we must lower the symmetry
methods to lower the symmetry

magnetic/orbital/charge order

spin-glass

Mott insulators have different properties than Slater insulators

the gap is only one of them

it is not only about the gap
strongly-correlated systems

\[
\hat{H}_e = -\sum_{ab} \tilde{t}_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{aba'b'} \tilde{U}_{aa'bb'} c_a^\dagger c_{a'}^\dagger c_b c_{b'} - \hat{H}_{DC}
\]

\[
\hat{H}_0 = \hat{H}_e^{LDA}
\]

\[
\Delta \hat{H}_U
\]

\[
\hat{H}_{\text{eff}} \sim \hat{S}^{-1} \hat{H}_e \hat{S} \sim \hat{H}_{\text{Hubbard-like}}
\]

it is the local Coulomb interaction that matters

minimal model for a given class of phenomena

as system-specific as possible
we have to **build & solve** materials-specific Hubbard-like models

let us discuss first how to **solve** them
Hubbard model

\[
\hat{H} = \epsilon_d \sum_i \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_{\sigma} c_{i\sigma}^\dagger c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = \hat{H}_d + \hat{H}_T + \hat{H}_U
\]

at half filling:
1. \( t=0 \): collection of atoms, \textbf{insulator} \\
2. \( U=0 \): half-filled band, \textbf{metal}

\textbf{how do we solve it?}
1989-1992: dynamical mean-field theory

map LATTICE problem to QUANTUM IMPURITY problem

local self-energy approximation

1989-1992: dynamical mean-field theory

Hubbard model

$$\hat{H} = \varepsilon_d \sum_i \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_{\sigma} c_{i\sigma}^\dagger c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

self-consistent quantum-impurity model

$$G^{-1} = G^{-1} + \Sigma$$
$$G = G^{i,i}$$

main difficulty: solve self-consistent quantum impurity problem

dynamical mean-field theory

\[ \hat{H} = \varepsilon_d \sum_i \sum_{\sigma} c_{i\sigma} \dagger c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_{\sigma} c_{i\sigma} \dagger c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Bethe Lattice

W: band width

DMFT for real materials

realistic models

\[ \hat{H}_e = \sum_{ab} t_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{c d c' d'} U_{c d c' d'} c_c^\dagger c_c^\dagger c_{c'} c_{d'} \]

realistic self-consistent quantum-impurity (QI) model
how does it work?
DMFT for the Hubbard dimer

this is a toy model: coordination number is one

DMFT is exact for $t=0$, $U=0$ and in the infinite dimension limit
the Hubbard dimer
the Hubbard dimer

\[ \hat{H} = \varepsilon_d \sum_{i\sigma} \hat{n}_{i\sigma} - t \sum_{\sigma} \left( c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \]
\( t=0: \) exact diagonalization

| \(|N, S, S_z\rangle\) | \(|0\rangle\) | \(N\) | \(S\) | \(E(N, S)\) |
|-----------------|-----------------|---|---|---|
| \(|0, 0, 0\rangle\) | \(|0\rangle\) | 0 | 0 | 0 |
| \(|1, 1/2, \sigma\rangle_1\) | \(c_{1\sigma}^\dagger|0\rangle\) | 1 | 1/2 | \(\varepsilon_d\) |
| \(|1, 1/2, \sigma\rangle_2\) | \(c_{2\sigma}^\dagger|0\rangle\) | 1 | 1/2 | \(\varepsilon_d\) |
| \(|2, 1, 1\rangle\) | \(c_{2\uparrow}^\dagger c_{1\uparrow}^\dagger|0\rangle\) | 2 | 1 | 2\(\varepsilon_d\) |
| \(|2, 1, -1\rangle\) | \(c_{2\downarrow}^\dagger c_{1\downarrow}^\dagger|0\rangle\) | 2 | 1 | 2\(\varepsilon_d\) |
| \(|2, 1, 0\rangle\) | \(\frac{1}{\sqrt{2}} \left[ c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger + c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger \right] |0\rangle\) | 2 | 1 | 2\(\varepsilon_d\) |
| \(|2, 0, 0\rangle_0\) | \(\frac{1}{\sqrt{2}} \left[ c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger - c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger \right] |0\rangle\) | 2 | 0 | 2\(\varepsilon_d\) |
| \(|2, 0, 0\rangle_1\) | \(c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger|0\rangle\) | 2 | 0 | 2\(\varepsilon_d + U\) |
| \(|2, 0, 0\rangle_2\) | \(c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger|0\rangle\) | 2 | 0 | 2\(\varepsilon_d + U\) |
| \(|3, 1/2, \sigma\rangle_1\) | \(c_{1\sigma}^\dagger c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger|0\rangle\) | 3 | 1/2 | 3\(\varepsilon_d + U\) |
| \(|3, 1/2, \sigma\rangle_2\) | \(c_{2\sigma}^\dagger c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger|0\rangle\) | 3 | 1/2 | 3\(\varepsilon_d + U\) |
| \(|4, 0, 0\rangle\) | \(c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger|0\rangle\) | 4 | 0 | 4\(\varepsilon_d + 2U\) |
### finite $t$: exact diagonalization

| $|1, S, S_z\rangle_\alpha$ | $E_\alpha(1, S)$ | $d_\alpha(1, S)$ |
|---------------------------|----------------|------------------|
| $|1, 1/2, \sigma\rangle_+ = \frac{1}{\sqrt{2}} (|1, 1/2, \sigma\rangle_1 - |1, 1/2, \sigma\rangle_2)$ | $\varepsilon_d + t$ | 2 |
| $|1, 1/2, \sigma\rangle_- = \frac{1}{\sqrt{2}} (|1, 1/2, \sigma\rangle_1 + |1, 1/2, \sigma\rangle_2)$ | $\varepsilon_d - t$ | 2 |

#### Diagram:

- **$k=\pi$**
  - $\varepsilon_\pi = \varepsilon_d + t$
  - $k=\pi$
- **$k=0$**
  - $\varepsilon_0 = \varepsilon_d - t$
  - $k=0$
finite \( t \): exact diagonalization

half filling (N=2)

| \( |2, S, S_z\rangle_\alpha \) | \( E_\alpha(2, S) \) | \( d_\alpha(2, S) \) |
|---|---|---|
| \( |2, 0, 0\rangle_+ = b_1 |2, 0, 0\rangle_0 - \frac{b_2}{\sqrt{2}} (|2, 0, 0\rangle_1 + |2, 0, 0\rangle_2) \) | \( 2\epsilon_d + \frac{U}{2} + \frac{1}{4}(U + 2\Delta(t, \frac{U}{2})) \) | 1 |
| \( |2, 0, 0\rangle_o = \frac{1}{\sqrt{2}} (|2, 0, 0\rangle_1 - |2, 0, 0\rangle_2) \) | \( 2\epsilon_d + U \) | 1 |
| \( |2, 1, m\rangle_o = |2, 1, m\rangle \) | \( 2\epsilon_d + \frac{U}{2} \) | 3 |
| \( |2, 0, 0\rangle_- = b_2 |2, 0, 0\rangle_0 + \frac{b_1}{\sqrt{2}} (|2, 0, 0\rangle_1 + |2, 0, 0\rangle_2) \) | \( 2\epsilon_d + \frac{U}{2} + \frac{1}{4}(U - 2\Delta(t, \frac{U}{2})) \) | 1 |

U=0
finite $t$: exact diagonalization

\[ |3, S, S_z\rangle_{\alpha} \]

\[
|3, 1/2, \sigma\rangle_+ = \frac{1}{\sqrt{2}}(|1, 1/2, \sigma\rangle_1 + |1, 1/2, \sigma\rangle_2) \\
|3, 1/2, \sigma\rangle_- = \frac{1}{\sqrt{2}}(|1, 1/2, \sigma\rangle_1 - |1, 1/2, \sigma\rangle_2)
\]

<table>
<thead>
<tr>
<th>[E_{\alpha}(3)]</th>
<th>[d_{\alpha}(3, S)]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$3\varepsilon_d + U + t$</td>
<td>2</td>
</tr>
<tr>
<td>$3\varepsilon_d + U - t$</td>
<td>2</td>
</tr>
</tbody>
</table>

U=0

[Diagram with states A and B labeled]
the local Green function

Lehmann representation

\[ G_{i,i}^{\sigma}(i\nu_n) = \frac{1}{4} \left( \frac{1 + w(t, U)}{i\nu_n - (E_0(2) - \varepsilon_d + t - \mu)} + \frac{1 - w(t, U)}{i\nu_n - (E_0(2) - \varepsilon_d - t - \mu)} \right) \]

\[ \left| \langle 1 | c_\sigma | 2 \rangle \right|^2 \]

\[ \left| \langle 3 | c_\sigma^\dagger | 2 \rangle \right|^2 \]

\[ G_{i,i}^{\sigma}(i\nu_n) = \frac{1}{4} \left( \frac{1 - w(t, U)}{i\nu_n - (-E_0(2) + U + 3\varepsilon_d + t - \mu)} + \frac{1 + w(t, U)}{i\nu_n - (-E_0(2) + U + 3\varepsilon_d - t - \mu)} \right) \]
the local spectral function

$W=2t$

$t=1$

$U=0$

$U=4$

$\omega$
the local Green function

Lehmann representation

\[ G^{\sigma}_{i,i}(i\nu_n) = \frac{1}{4} \left( \frac{1 + w(t,U)}{i\nu_n - (E_0(2) - \epsilon_d + t - \mu)} + \frac{1 - w(t,U)}{i\nu_n - (E_0(2) - \epsilon_d - t - \mu)} \right) \]

\[ \left| \langle 1 | c_{\sigma} | 2 \rangle \right|^2 \]

\[ \left| \langle 3 | c_{\sigma}^\dagger | 2 \rangle \right|^2 \]

\[ \left( + \frac{1 - w(t,U)}{i\nu_n - (-E_0(2) + U + 3\epsilon_d + t - \mu)} + \frac{1 + w(t,U)}{i\nu_n - (-E_0(2) + U + 3\epsilon_d - t - \mu)} \right) \]

E(2)-E(1) \rightarrow d^1 \rightarrow d^0 \\
E(3)-E(2) \rightarrow d^2 \rightarrow d^1
the local Green function

change basis

\[ c_{k\sigma} = \frac{1}{\sqrt{2}} (c_{1\uparrow} \mp c_{2\uparrow}) \]

\[
G^\sigma_{i,i}(i\nu_n) = \frac{1}{2} \left( \frac{1}{i\nu_n + \mu - \varepsilon_d + t - \Sigma^\sigma(0,i\nu_n)} + \frac{1}{i\nu_n + \mu - \varepsilon_d - t - \Sigma^\sigma(\pi,i\nu_n)} \right)
\]

\[
\Sigma^\sigma(k, i\nu_n) = \frac{U}{2} + \frac{U^2}{4} \frac{1}{i\nu_n + \mu - \varepsilon_d - \frac{U}{2} - e^{ik} 3t}.
\]
local Green function

\[ G_{11}^{0\sigma}(i\nu_n) = \frac{1}{2} \sum_k \frac{1}{i\nu_n - (\varepsilon_k - \mu)} = \frac{1}{i\nu_n - (\varepsilon_d + F^0(i\nu_n) - \mu)}, \]

\[ G_{11}^{\sigma}(i\nu_n) = \frac{1}{2} \sum_k \frac{1}{i\nu_n - (\varepsilon_k + \Sigma^\sigma(k, i\nu_n) - \mu)} = \frac{1}{i\nu_n - (\varepsilon_d + \Sigma^\sigma(i\nu_n) + F^\sigma(i\nu_n) - \mu)} \]

hybridization function

\[ F^0(i\nu_n) = \frac{t^2}{i\nu_n - (\varepsilon_d - \mu)}, \]
the local Green function

**local self-energy**

\[
\Sigma_i^\sigma(i\nu_n) = \frac{1}{2} \left( \Sigma^\sigma(\pi, i\nu_n) + \Sigma^\sigma(0, i\nu_n) \right) = \frac{U}{2} + \frac{U^2}{4} \frac{i\nu_n + \mu - \varepsilon_d - \frac{U}{2}}{(i\nu_n + \mu - \varepsilon_d - \frac{U}{2})^2 - (3t)^2}
\]

**non-local self-energy**

\[
\Delta \Sigma_i^\sigma(i\nu_n) = \frac{1}{2} \left( \Sigma^\sigma(\pi, i\nu_n) - \Sigma^\sigma(0, i\nu_n) \right) = \frac{U^2}{4} \frac{3t}{(i\nu_n + \mu - \varepsilon_d - \frac{U}{2})^2 - (3t)^2}
\]

**modified hybridization function**

\[
F^\sigma(i\nu_n) = \frac{(t + \Delta \Sigma_i(i\nu_n))^2}{i\nu_n - (\varepsilon_d - \mu + \Sigma_i^\sigma(i\nu_n))}.
\]
the local Green function

hybridization function

$$F^0(i\nu_n) = \frac{t^2}{i\nu_n - (\varepsilon_d - \mu)},$$

modified hybridization function

$$F^\sigma(i\nu_n) = \frac{(t + \Delta \Sigma_l(i\nu_n))^2}{i\nu_n - (\varepsilon_d - \mu + \Sigma_l^\sigma(i\nu_n))}.$$
map to a quantum impurity model?

the Anderson molecule

\[
\hat{H}^A = \varepsilon_s \sum_{\sigma} \hat{n}_{s\sigma} - t \sum_{\sigma} \left( c_{d\sigma}^{\dagger} c_{s\sigma} + c_{s\sigma}^{\dagger} c_{d\sigma} \right) + \varepsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}
\]

~ same local Green function?
### Self-consistency

#### Hubbard

The Hubbard Hamiltonian for the dimer can be represented as:

\[
\hat{H}_2(\epsilon_d, U, t) = \begin{pmatrix}
2\epsilon_d & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2\epsilon_d & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2\epsilon_d & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2\epsilon_d & -\sqrt{2}t & -\sqrt{2}t & 0 \\
0 & 0 & 0 & -\sqrt{2}t & 2\epsilon_d + U & 0 & 0 \\
0 & 0 & 0 & -\sqrt{2}t & 0 & 2\epsilon_d + U & 0 \\
\end{pmatrix}
\]

#### Anderson

The Anderson Hamiltonian for the dimer can be represented as:

\[
\hat{H}^A_2(\epsilon_d, U, t; \epsilon_s) = \begin{pmatrix}
\epsilon_d + \epsilon_s & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \epsilon_d + \epsilon_s & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \epsilon_d + \epsilon_s & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \epsilon_d + \epsilon_s & -\sqrt{2}t & -\sqrt{2}t & 0 \\
0 & 0 & 0 & -\sqrt{2}t & 2\epsilon_d + U & 0 & 0 \\
0 & 0 & 0 & -\sqrt{2}t & 0 & 2\epsilon_s & 0 \\
\end{pmatrix}
\]

The Hamiltonians show the same occupations of Hubbard dimer.

\[\epsilon_s = \epsilon_d + U/2 = \mu\]
solution: Hubbard vs Anderson

Anderson molecule

\[ G_{dd}^\sigma(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_d - \mu + \Sigma_l^\sigma(i\nu_n) + F_0^\sigma(i\nu_n))} \]

Hubbard dimer

\[ G_{11}^\sigma(i\nu_n) = \frac{1}{i\nu_n - (\varepsilon_d - \mu + \Sigma_l^\sigma(i\nu_n) + F^\sigma(i\nu_n))} \]

let us neglect the non-local self-energy
hybridization function

\[ F^0(i\nu_n) = \frac{t^2}{i\nu_n - (\varepsilon_d - \mu)}, \]

modified hybridization function

\[ F^\sigma(i\nu_n) = \frac{(t + \Delta \Sigma_l(i\nu_n))^2}{i\nu_n - (\varepsilon_d - \mu + \Sigma^\sigma_l(i\nu_n))}. \]
Green function $U=4t$

Anderson vs Hubbard

only **local** self-energy

exact

1 2
DMFT for the dimer

\[ \hat{H} = \epsilon_d \sum_{i\sigma} \hat{n}_{i\sigma} - t \sum_{\sigma} \left( c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \]

map to quantum impurity model (QIM) in local self-energy approximation

\[ \hat{H}^A = \epsilon_s \sum_{\sigma} \hat{n}_{s\sigma} - t \sum_{\sigma} \left( c_{d\sigma}^\dagger c_{s\sigma} + c_{s\sigma}^\dagger c_{d\sigma} \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \]

QIM solver

self-consistency loop
\[ \Sigma(k, \omega) \rightarrow \Sigma_d(\omega) \]

non-local self-energy terms vs non-local interaction

\[ U_{ijij} \]
non-local Coulomb terms

how important are they?

\[ \hat{H} = \varepsilon_d \sum_{i\sigma} \hat{n}_{i\sigma} - t \sum_{\sigma} \left( c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma} \right) + U \sum_{i=1,2} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \]

\[ + \sum_{\sigma \sigma'} (V - 2J_V - J_V \delta_{\sigma \sigma'}) \hat{n}_{1\sigma} \hat{n}_{2\sigma'} - J_V \sum_{i \neq i'} \left( c_{i\uparrow}^{\dagger} c_{i\downarrow}^{\dagger} c_{i'\downarrow} c_{i'\uparrow} + c_{i\uparrow}^{\dagger} c_{i'\downarrow}^{\dagger} c_{i'\uparrow} c_{i\downarrow}^{\dagger} \right) \]
non-local Coulomb terms

\[ \hat{H}_2(\varepsilon_d, U, t) = \begin{pmatrix}
2\varepsilon_d & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2\varepsilon_d & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2\varepsilon_d & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2\varepsilon_d & -\sqrt{2}t & -\sqrt{2}t & 0 \\
0 & 0 & 0 & -\sqrt{2}t & 2\varepsilon_d + U & 0 & 0 \\
0 & 0 & 0 & -\sqrt{2}t & 0 & 2\varepsilon_d + U & 0 \\
\end{pmatrix} \]

Hubbard

\[ \hat{H}_2^{NL} = \begin{pmatrix}
2\varepsilon_d + V - 3J_V & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2\varepsilon_d + V - 3J_V & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 2\varepsilon_d + V - 3J_V & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2\varepsilon_d + V - J_V & -\sqrt{2}t & -\sqrt{2}t & 0 \\
0 & 0 & 0 & -\sqrt{2}t & 2\varepsilon_d + U & -J_V & 0 \\
0 & 0 & 0 & -\sqrt{2}t & -J_V & 2\varepsilon_d + U & 0 \\
\end{pmatrix} \]

Hubbard + non-local

Setting for simplicity \( J_V = 0 \), we can notice that \( \hat{H}_2^{NL} \) equals \( \hat{H}_2(\varepsilon'_d, U', t) \), the Hamiltonian of the \( J_V = V = 0 \) Hubbard dimer, with parameters \( \varepsilon'_d = \varepsilon_d + V/2 \) and \( U' = U - V \).
non-local Coulomb terms

\[ U=V: \ N=2, \ \text{effective non-correlated dimer} \]

Strong-correlation effects appear when the local electron-electron repulsion dominates over non-local terms.

If Coulomb interaction independent on site distance map to effective weakly correlated model.
quantum-impurity solvers
DMFT for the dimer

\[ \hat{H} = \varepsilon_d \sum_{i \sigma} \hat{n}_{i\sigma} - t \sum_{\sigma} \left( c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \]

map to quantum impurity model (QIM) in local self-energy approximation

\[ \hat{H}^A = \varepsilon_s \sum_{\sigma} \hat{n}_{s\sigma} - t \sum_{\sigma} \left( c_{d\sigma}^{\dagger} c_{s\sigma} + c_{s\sigma}^{\dagger} c_{d\sigma} \right) + \varepsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \]

QIM solver

self-consistency loop
quantum-impurity solver

\[ \hat{H}^A = \varepsilon_s \sum_\sigma \hat{n}_{s\sigma} - t \sum_\sigma \left( c_{d\sigma}^\dagger c_{s\sigma} + c_{s\sigma}^\dagger c_{d\sigma} \right) + \varepsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \]

\[ \begin{align*}
&\hat{H}_{bath} \\
&\hat{H}_{hyb} \\
&\hat{H}_{loc}
\end{align*} \]

hybridization-expansion CT-QMC
hybridization expansion

\[ Z = \text{Tr} \left( e^{-\beta (\hat{H}_0 - \mu \hat{N})} \hat{V}(\beta) \right) \]

\[ \hat{V}(\beta) = e^{\beta (\hat{H}_0 - \mu \hat{N})} e^{-\beta (\hat{H}_0 + \hat{H}_{\text{hyb}} - \mu \hat{N})} = \sum_m \int_0^\beta d\tau_1 \cdots \int_{\tau_{m-1}}^\beta d\tau_m (-1)^m \prod_{l=m}^1 \hat{H}_{\text{hyb}}(\tau_l) \]

only even orders survive \((m=2k)\)
\[ \frac{Z}{Z_{\text{bath}}} = \sum_k \int^k d\tau \int^k d\bar{\tau} \sum_{\sigma, \bar{\sigma}} d^k_{\sigma, \sigma} (\tau, \bar{\tau}) t^k_{\sigma, \bar{\sigma}} (\tau, \bar{\tau}) \]

\[ d^k_{\sigma, \sigma} (\tau, \bar{\tau}) = (t)^{2k} \text{Tr}_{\text{bath}} \left( e^{-\beta(\hat{H}_{\text{bath}} - \mu \hat{N}_s)} \mathcal{T} \prod_{i=k}^{1} c^\dagger_{s \sigma_i} (\tau_i) c_{s \bar{\sigma}_i} (\bar{\tau}_i) \right) / Z_{\text{bath}} \]

\[ t^k_{\sigma, \bar{\sigma}} (\tau, \bar{\tau}) = \text{Tr}_{\text{loc}} \left( e^{-\beta(\hat{H}_{\text{loc}} - \mu \hat{N}_d)} \mathcal{T} \prod_{i=k}^{1} c_{d \sigma_i} (\tau_i) c^\dagger_{d \bar{\sigma}_i} (\bar{\tau}_i) \right) , \]
quantum-impurity solver

bath-impurity decoupling

\[
\frac{Z}{Z_{\text{bath}}} = \sum_k \int^k d\tau \int^k d\bar{\tau} \sum_{\sigma, \bar{\sigma}} d^k_{\bar{\sigma}, \sigma}(\tau, \bar{\tau}) t^k_{\sigma, \bar{\sigma}}(\tau, \bar{\tau})
\]

bath

\[
d^k_{\bar{\sigma}, \sigma}(\tau, \bar{\tau}) = \det \left( F^k_{\bar{\sigma}, \sigma}(\tau, \bar{\tau}) \right)
\]

non-interacting hybridization function

the difficult part: the local trace

\[
t^k_{\sigma, \bar{\sigma}}(\tau, \bar{\tau})
\]
define configurations

\[ t_{\sigma, \bar{\sigma}}^k (\tau, \bar{\tau}) = \left( \prod_{\sigma} s_{\sigma}^k \right) e^{-\sum_{\sigma \sigma'} ((\varepsilon_d - \mu) \delta_{\sigma \sigma'} + \frac{U}{2} (1 - \delta_{\sigma, \sigma'})) l_{\sigma, \sigma'}} \]
quantum-impurity solver

hybridization-expansion CT-QMC

\[ Z = \sum_c w_c = \sum_c |w_c| \text{sign } w_c \]

configuration \( c \): expansion order & segments

\[ w_c = d\tau_c \, d_c \, t_c \]

moves: addition & removal of segments, antisegments, or complete lines
DMFT for the one-band Hubbard model

\[ H = \varepsilon_d \sum_i \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_\sigma c_{i\sigma}^\dagger c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U \]
dynamical mean-field theory

\[ G^{-1} = G^{-1} + \Sigma \]
\[ G = G^{i,i} \]

Metzner and Vollhardt, PRL 62, 324 (1989); Georges and Kotliar, PRB 45, 6479 (1992)
self-consistency loop

\[ H = \varepsilon_d \sum_i \sum_{\sigma} c_{i\sigma}^\dagger c_{i\sigma} - t \sum_{\langle ii' \rangle} \sum_{\sigma} c_{i\sigma}^\dagger c_{i'\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} = H_d + H_T + H_U \]

quantum impurity model (QIM)

\[ \hat{H}^A = \sum_{k\sigma} \varepsilon_k^S \hat{n}_{k\sigma} + \sum_{k\sigma} \left( V_{k\sigma}^S c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) + \varepsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \]

\[ \hat{H}_{\text{bath}} + \hat{H}_{\text{hyb}} + \hat{H}_{\text{imp}} \]

QIM solver: QMC, ED, NRG, DMRG,...

self-consistency loop \( G_{dd} = G_{ii} \)
a real-system case: VOMoO$_4$

a real-system: VOMoO$_4$
why this cannot be obtained with static mean-field methods?
comparison to Hartree-Fock (LDA+$U$)

Hartree-Fock Hamiltonian and bands

$$U \hat{n}_i \uparrow \hat{n}_i \downarrow \rightarrow U (\bar{n}_i \uparrow \hat{n}_i \downarrow + \hat{n}_i \uparrow \bar{n}_i \downarrow - \bar{n}_i \uparrow \bar{n}_i \downarrow)$$

ferromagnetic Hartree-Fock

$$\hat{H}_{MF} = \sum_{k\sigma} \left[ \varepsilon_k + U \left( \frac{1}{2} - \sigma m \right) \right] \hat{n}_{k\sigma}$$

self-energy

m: magnetization
2d-tight binding model

\[ \varepsilon_{k} = -2t[\cos k_x + \cos k_y] \]

\[ \Sigma^\sigma(k, i\nu_n) = U\left(\frac{1}{2} - \sigma m\right) \]
antiferromagnetic case

CuO$_2$

\[ \text{energy (eV)} \]

\begin{align*}
\text{mU}=0 & \quad & \text{mU}=0.5t \\
\end{align*}

\[ \begin{array}{c}
\Gamma \quad X \quad M \quad \Gamma \\
\end{array} \]

\[ \begin{array}{c}
\Gamma \quad X \quad M \quad \Gamma \\
\end{array} \]
Mott transition: HF vs DMFT

LDA+\(U\)
Hartree-Fock

LDA+DMFT
DMFT

see also my lecture notes in correl17
multi-band Hubbard model
DMFT for multi-band models

\[ \hat{H}_e = - \sum_{ab} t_{ab} c_a^{\dagger} c_b + \frac{1}{2} \sum_{cd'c'd'} U_{cd'c'd'} c_{c'} c_{c'}^{\dagger} c_{c'} c_{d'} \]
in theory, more indices

\[ H_{LDA}^k = \begin{pmatrix} H_{i_c,i_c}^k & H_{i_c,i_c'}^k & \cdots \\ H_{i_c,i_c}^k & H_{i_c,i_c'}^k & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \]

\[ U_{m\alpha m\beta m'_\alpha m'_\beta} \]

\[ G_{i_c m_\alpha, i'_c m'_\alpha}(i\nu_n) = \frac{1}{N_k} \sum_k \left[ \frac{1}{i\nu_n I - H_{LDA}^k - \Sigma(i\nu_n) + H_{DC}} \right]_{i_c m_\alpha, i'_c m'_\alpha} \]

\[ G_{m_\alpha, m'_\alpha}(i\nu_n) = G_{i_c m_\alpha, i_c m'_\alpha}(i\nu_n) \]

\[ G^{-1}(i\nu_n) = G^{-1}(i\nu_n) + \Sigma^{i_c}(i\nu_n) \]

\[ \nu_n \rightarrow \tau \quad G(\tau) \]

QMC

\[ G(\tau) \quad \tau \rightarrow \nu_n \]

\[ \Sigma^{i_c}(i\nu_n) = G^{-1}(i\nu_n) - G^{-1}(i\nu_n) \]

\[ \Sigma = \begin{pmatrix} \Sigma^{i_c} & 0 & \cdots \\ 0 & \Sigma^{i_c} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \]

converged? NO YES

Jolly good show! You converged

\[ \Sigma(i\nu_n) \]

\[ G(i\nu_n) \]
in practice, **QMC**-based solvers

- computational time
  - *limited* number of orbitals/site
  - *finite* temperature
- sign problem
  - some *interactions* are worse than others
  - some *bases* are worse than others

we need **minimal** material-specific models
strongly-correlated systems

\[ \hat{H}_e = - \sum_{ab} \tilde{t}_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{aba'b'} \tilde{U}_{aa'bb'} c_a^\dagger c_{a'}^\dagger c_{b'} c_b - \hat{H}_{DC} \]

\[ \hat{H}_0 = \hat{H}_e^{LDA} \]

\[ \Delta \hat{H}_U \]

\[ \hat{H}_{\text{eff}} \sim \hat{S}^{-1} \hat{H}_e \hat{S} \sim \hat{H}_{\text{Hubbard-like}} \]

minimal model for a given class of phenomena

as system-specific as possible

build & solve these models
model building
chose the one-electron basis

LDA Wannier(-like) functions

\[ \hat{H}_e = - \sum_{ab} \tilde{t}_{ab} c_a^\dagger c_b + \frac{1}{2} \sum_{aba'b'} \tilde{U}_{aa'bb'} c_a^\dagger c_{a'}^\dagger c_b c_{b'} - \hat{H}_{\text{DC}} \]

\[ \hat{H}_0 = \hat{H}_e^{\text{LDA}} \]

\[ \Delta \hat{H}_U \]

LDA, GGA & so on: minor differences in this context
why LDA Wannier functions?

span exactly the one-electron Hamiltonian
can be constructed site-centered & orthogonal & localized
natural basis for local Coulomb terms
very good for weakly correlated systems
information on lattice and chemistry
why LDA Wannier functions?

\[ \hat{H}_e = \hat{H}_0 + \hat{H}_U \rightarrow \hat{H}^{\text{LDA}} + [\hat{H}_U - \hat{H}_{\text{dc}}] \]

if long range Hartree and mean-field exchange-correlation already are well described by LDA (GGA,..), \( \Delta U \) is local
heavy electrons, light electrons

light electrons

DFT (LDA, GGA, ...)

heavy electrons

$\Delta U$ correction, DMFT
self-consistency loop

\[ H_{k}^{\text{LDA}} = \left( \begin{array}{ccc} H_{k}^{i_{c},i_{c}} & H_{k}^{i_{c},i_{c}'} & \cdots \\ H_{k}^{i_{c}',i_{c}} & H_{k}^{i_{c}',i_{c}'} & \cdots \\ \vdots & \vdots & \ddots \end{array} \right) \]

\[ U_{m_{\alpha} m_{\beta} m'_{\alpha} m'_{\beta}} \]

\[ G_{i_{c} m_{\alpha},i_{c}' m'_{\alpha}}(i\nu_{n}) = \frac{1}{N_{k}} \sum_{k} \left[ \frac{1}{i\nu_{n} I - H_{k}^{\text{LDA}} - \Sigma(i\nu_{n}) + H_{\text{DC}}} \right]_{i_{c} m_{\alpha},i_{c}' m'_{\alpha}} \]

\[ G_{m_{\alpha},m'_{\alpha}}(i\nu_{n}) = G_{i_{c} m_{\alpha},i_{c} m'_{\alpha}}(i\nu_{n}) \]

\[ G^{-1}(i\nu_{n}) = G^{-1}(i\nu_{n}) + \Sigma(i\nu_{n}) \]

QMC

\[ \nu_{n} \to \tau \quad G(\tau) \]

\[ \tau \to \nu_{n} \quad G(\tau) \]

\[ \Sigma(i\nu_{n}) = G^{-1}(i\nu_{n}) - G^{-1}(i\nu_{n}) \]

\[ \Sigma = \left( \begin{array}{ccc} \Sigma^{i_{c}} & 0 & \cdots \\ 0 & \Sigma^{i_{c}} & \cdots \\ \vdots & \vdots & \ddots \end{array} \right) \]

converged?

NO

YES

Jolly good show!

You converged

\[ \Sigma(i\nu_{n}) \]

\[ G(i\nu_{n}) \]
to downfold or not to downfold?

KCuF₃

energy (eV)

integrate out light electrons

rest

eg

t₂g

eg
massive downfolding: no DC correction

around mean-field approximation

\[
\hat{H}_U = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}
\]

\[
\hat{H}_{\text{DC}} = U \sum_i \left( \hat{n}_{i\uparrow} \bar{n}_{i\downarrow} + \bar{n}_{i\uparrow} \hat{n}_{i\downarrow} - \bar{n}_{i\uparrow} \bar{n}_{i\downarrow} \right)
\]

\[
\bar{n}_{i\sigma} = n/2
\]

\[
\hat{H}_{\text{DC}} = \frac{n}{2} U \sum_i \left( \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} - \frac{n}{2} \right) = \delta \mu \hat{N} - \text{const}
\]
should we downfold light electrons?

**no downfolding**

- More parameters & $H_{DC}$
- WF more localized

**massive downfolding**

- Fewer parameters & no $H_{DC}$
- WF less localized
how important is the basis localization?

\[ \hat{H}_e = \hat{H}_0 + \hat{H}_U \rightarrow \hat{H}_\text{LDA} + \hat{H}_U - \hat{H}_\text{dc} \]

local or almost local
strong correlations arise from strong local Coulomb

\[ U_{np n'p'}^{ij i'j'} = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \frac{\psi_{i n \sigma}(\mathbf{r}_1)\psi_{j p \sigma'}(\mathbf{r}_2)}{\psi_{i' n' \sigma'}(\mathbf{r}_2)\psi_{i' n' \sigma}(\mathbf{r}_1)}. \]

\[ \psi_{i m \sigma}(\mathbf{r})\psi_{i' m' \sigma'}(\mathbf{r}) \sim \delta_{i, i'} \delta(\mathbf{r} - \mathbf{T}_i) \]

\[ U_{mp m'p'}^{ij i'j'} \propto \frac{\delta_{i, i'} \delta_{j, j'}}{|\mathbf{T}_i - \mathbf{T}_j|}. \]
extreme localization

\[ \psi_{im\sigma}(r)\overline{\psi_{i'm'\sigma'}}(r) \sim \delta_{i,i'}\delta(r - T_i) \]

methods based on space tiling functions inside the sphere?
screening effects

\[ U_{np \bar{n}'p'}^{ijij'} = \int dr_1 \int dr_2 \frac{1}{|r_1 - r_2|} \psi_{jn\sigma}(r_1) \psi_{jp\sigma}(r_2) \frac{\psi_{j'n'\sigma'}(r_2)}{\psi_{ijn\sigma}(r_1)} \]

- Light electrons \( \rightarrow \) DFT (LDA, GGA, …)
- Heavy electrons \( \rightarrow \) \( \Delta U \) correction, DMFT

Screening: approximate schemes such as cRPA, cLDA
LDA+DMFT

\[ H_{\mathbf{k}}^{\text{LDA}} = \begin{pmatrix} H_{\mathbf{k}}^{i_c,i_c} & H_{\mathbf{k}}^{i_c,i'}_c & \ldots \\ H_{\mathbf{k}}^{i',i_c} & H_{\mathbf{k}}^{i',i'}_c & \ldots \\ \vdots & \vdots & \ddots \end{pmatrix} \]

\[ U_{m\alpha m\beta m'_\alpha m'_\beta} \]

\[ G_{i_c m\alpha, i'_c m'_\alpha} (i\nu_n) = \frac{1}{N_k} \sum_{\mathbf{k}} \left[ \frac{1}{i\nu_n I - H_{\mathbf{k}}^{\text{LDA}} - \Sigma (i\nu_n) + H_{\text{DC}}} \right]_{i_c m\alpha, i'_c m'_\alpha} \]

\[ G_{m\alpha, m'_\alpha} (i\nu_n) = G_{i_c m\alpha, i'_c m'_\alpha} (i\nu_n) \]

\[ G^{-1} (i\nu_n) = G^{-1} (i\nu_n) + \Sigma (i\nu_n) \]

\[ \nu_n \rightarrow \tau \quad G(\tau) \]

QMC

\[ G(\tau) \quad \tau \rightarrow \nu_n \]

\[ \Sigma (i\nu_n) = G^{-1} (i\nu_n) - G^{-1} (i\nu_n) \]

\[ \Sigma = \begin{pmatrix} \Sigma_{i_c} & 0 & \ldots \\ 0 & \Sigma_{i_c} & \ldots \\ \vdots & \vdots & \ddots \end{pmatrix} \]

converged?

YES

Jolly good show!

You converged

\[ \Sigma (i\nu_n) \]

\[ G (i\nu_n) \]
what can we be done?

orbital order

Fermi surface

spin-orbit

conductivity

response functions

spin waves
do we need it?
details matter!

Mott Transition and Suppression of Orbital Fluctuations in Orthorhombic 3d$^1$ Perovskites

E. Pavarini, 1 S. Biermann, 2 A. Poteryaev, 3 A. I. Lichtenstein, 3 A. Georges, 2 and O. K. Andersen 4

$\Delta=200-300$ meV a small crystal field plays a key role
our DMFT codes for materials

\[
H = - \sum_{ii'} \sum_{mm'} \sum_{\sigma} t_{im'm'}^{ii'} c_{im\sigma}^\dagger c_{i'm'\sigma}^\dagger \\
+ U \sum_{im} n_{im\uparrow} n_{im\downarrow} \\
+ \frac{1}{2} \sum_{im \neq m' \sigma'} (U - 2J - J\delta_{\sigma\sigma'}) n_{im\sigma} n_{im'\sigma'} \\
- J \sum_{m \neq m'} (c_{m\uparrow}^\dagger c_{m\downarrow}^\dagger c_{m'\uparrow}^\dagger c_{m'\downarrow} + c_{m\uparrow}^\dagger c_{m\downarrow}^\dagger c_{m'\uparrow} c_{m'\downarrow})
\]

DMFT and cDMFT

quantum impurity solvers:
- general HF QMC
- general CT-INT QMC
- general CT-HYB QMC

...PHYSICAL REVIEW B...

...K...K-t...S...K-t

...QMC time/iteration (a.u.)...β (eV⁻¹)...
an example:

Sr$_2$RuO$_4$

and its Fermi surface
the case of $\text{Sr}_2\text{RuO}_4$

\[ \hat{H}_e = - \sum_{ab} \tilde{t}_{ab} \, c_a^\dagger \, c_b + \frac{1}{2} \sum_{aba'b'} \tilde{U}_{aa'bb'} \, c_a^\dagger \, c_a', c_b, c_b - \hat{H}_{\text{DC}} \]

\[ \hat{H}_0 = \hat{H}_e^{\text{LDA}} \]

\[ \Delta \hat{H}_U \]

QI size: 3x3

\[ \hat{H} = - \sum_{\sigma} \sum_{i \neq i'} \sum_{mm'} t^{i,i'}_{m,m'} \, c_{i m \sigma}^\dagger \, c_{i' m' \sigma}^\dagger + U \sum_{im} \hat{n}_{im\uparrow} \hat{n}_{im\downarrow} + \frac{1}{2} \sum_{i \sigma \sigma'} (U - 2J - J\delta_{\sigma,\sigma'}) \hat{n}_{im \sigma} \hat{n}_{im' \sigma'} \]

\[ - J \sum_{im \neq m'} \left( c_{im \uparrow}^\dagger \, c_{im \downarrow} \, c_{im' \uparrow} \, c_{im' \downarrow} + c_{im \uparrow} \, c_{im \downarrow} \, c_{im' \uparrow} \, c_{im' \downarrow} \right) \]

derivation: www.cond-mat.de/events/correl11/manuscripts/pavarini.pdf
however, spin-orbit interaction important

\[
H = - \sum_{\sigma\sigma'} \sum_{mm'} \sum_{ii'} t_{m\sigma,m'\sigma'}^{i,i'} c_{im\sigma}^{\dagger} c_{i'm'\sigma'} \\
+ \frac{1}{2} \sum_{\sigma\sigma'} \sum_{mm' pp'} \sum_{i} U_{mm' pp'} c_{im\sigma}^{\dagger} c_{im'\sigma'}^{\dagger} c_{ip'\sigma'} c_{ip\sigma}
\]

local spin-orbit interaction

\[
H_{SO} = \sum_{i\mu} H_{SO}^{i\mu} = \sum_{i\mu} \sum_{m\sigma m'\sigma'} \lambda_{i\mu}^{i\mu} \xi_{m\sigma m'\sigma'}^{i\mu} c_{im\sigma}^{\dagger} c_{im'\sigma'}
\]
with SO, everything more difficult

larger (6x6) Green function matrices, QMC sign problem

basis that diagonalizes on-site Hamiltonian/Green function reduces sign problem

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<th>m (T)</th>
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<tr>
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Fermi surface $\text{Sr}_2\text{RuO}_4$
DMFT — Fermi surface $\text{Sr}_2\text{RuO}_4$

Effective crystal-field

$$\varepsilon_{\text{CF}} = \varepsilon_{xz/yz} - \varepsilon_{xy} > 0$$

Effective spin-orbit coupling

$$\lambda_{xy} \quad \lambda_z$$

$$\Delta$$ changes local Hamiltonian

$$\Sigma(0)$$
the LDA+DMFT Fermi surface

Is the Coulomb interaction spherical?

the bare Coulomb interaction is spherical
but the screened interaction has the symmetry of the site

\[ \varepsilon_{\text{CF}} + \Delta' \varepsilon_{\text{CF}} \sim \varepsilon_{\text{CF}} \]

reduced crystal-field enhancement

\( \Delta U = U_{xy,xy} - U_{xz,xz} \)

\( \varepsilon_{CF} + \Delta' \varepsilon_{CF} \sim \varepsilon_{CF} \)

\( \lambda + \Delta\lambda \sim 2\lambda \)

DMFT

dimer

one band

multiband

strong-correlations are local

$U=V$

DMFT vs HF

Hartree-Fock

DMFT
DMFT for materials

basis choice

light & heavy electrons

downfolding, localization, double counting & screening

spin-orbit coupling & non-spherical U
thank you!