Approach to Strong Correlations

- Strong correlations in many body perturbation theory
- Strong correlations in a local subspace + bath: partitioning
- Ingredients required for subspace : G^{loc} and W^{loc} .
- Ingredients required for bath. Importance of nonlocality
- Outline of general procedure to solve coupled (local, bath) problem.

Strong Correlations, MBPT

Many Body Perturbation Theory

Lowest-order diagrammatic expansion misses important physics.

Some strategies exist to incorporate next higher orders in a partial way. You saw Bethe-Salpeter and T-matrix.

A few alternate strategies can partially incorporate still high order diagrams.

One very ambitious strategy: Diagrammatic Monte Carlo. Really try to solve entire problem!

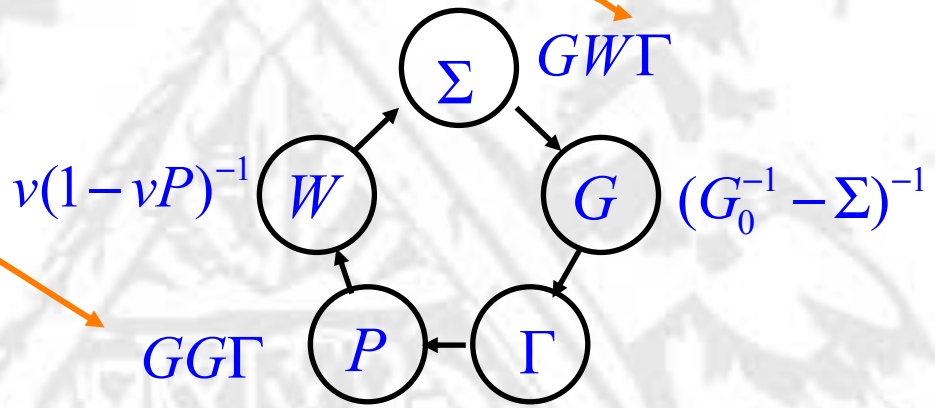
Samples many higher order diagrams stochastically (up to say 10^{th} order), using Monte Carlo methods [Kozik et al, Euro. Phys. Lett. 90 10004]. Large computational challenges,,,

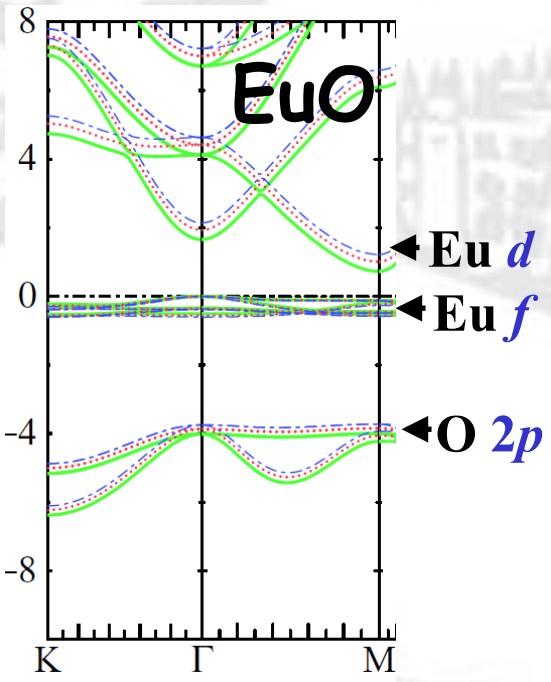
So far applied to model systems only (mainly 1 band Hubbard)

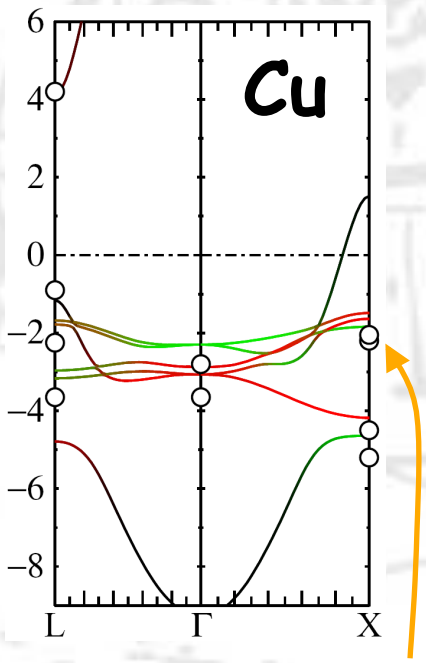
MBPT Route: GW in the Self-Energy

In Hedin's equations, Γ appears in 2 places:

1. Modify Σ
2. Modify P







Expect that Σ=GW→ GWΓ pushes levels down. The more localized the state the larger the effect

Physical Interpretation of Vertex GW→ GWΓ

W represents the screening of classical ("test" charges. But an electron is a fermion, not a classical test charge. Assuming W is exact ($W^{Tc-Tc)}$, the difference between GW and GWΓ is that GW is the potential a classical test charge would see, while GWΓ is the potential that accounts for the fermionic nature of the electron.

This vertex is much less studied. Vertex in W (P=GGΓ) is easier because we could contract it into something that contains only 2 points. Now, the vertex is inherently 3-point:

$$\Sigma_{xc}(1,2) = i\int d3G\left(1,3^{+}\right)\int d4W\left(1,4\right)\Gamma\left(3,2;4\right)$$

One cheap route to slip in vertex corrections at little cost
Example: cumulant expansions (next slide)

Cumulant Expansion

$$G^{-1} - G_0^{-1} = -v - iv\frac{\delta G}{\delta\phi}G^{-1}$$

Since G^{-1} is the hamiltonian,
$G^{-1} - G_0^{-1}$ is an effective potential

This identifies as Σ_{xc} as :

$$\Sigma_{xc} = iv\frac{\delta G}{\delta\phi}G^{-1} = -ivG\frac{\delta G^{-1}}{\delta\phi}$$

Note

$$\frac{\delta G}{\delta\phi}G^{-1} = \frac{\delta \ln G}{\delta\phi}$$

This hints at an exponential form for G with $i\Sigma_{xc} \rightarrow \exp(i\Sigma_{xc})$

Cumulant expansions basically use this trick to include higher order diagrams with little extra effort.
Define a cumulant C in terms of the Green's function:

$$G(k,t) = ie^{-i\varepsilon_s t + C(k,t)} = G^0(k,t)e^{C(k,t)} = G^0[1 + C + \frac{1}{2}C^2 + \ldots]$$

Compare to Dyson eqn

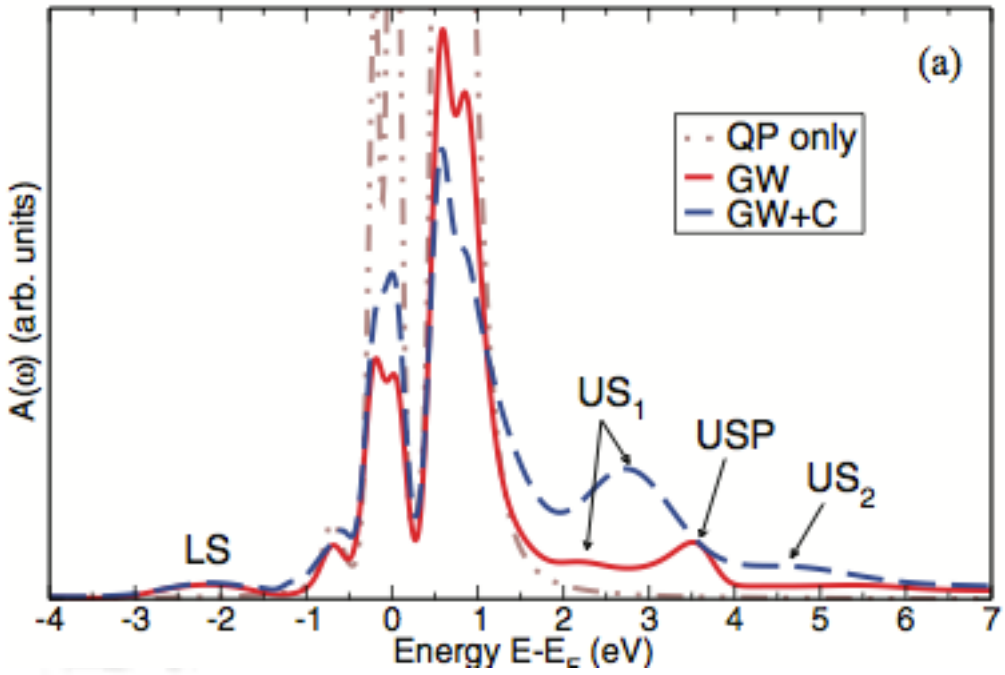
$$G = G^0 + G^0\Sigma G^0 + G^0\Sigma G^0\Sigma G^0 + \ldots$$

Cumulant Expansion II

$$G(k,t) = G^0[1 + C + \frac{1}{2}C^2 + \ldots] = G^0 + G^0\Sigma G^0 + G^0\Sigma G^0\Sigma G^0 + \ldots$$

Equating the 2 forms establishes a connection between C and Σ_{xc}. Roughly, $i\Sigma_{xc} \rightarrow \exp(i\Sigma_{xc})$. The exponential form yields plasmon satellites. The details are worked out very nicely in Aryasetiawan, Phys. Rev. Lett. 77, 2268

A recent application demonstrating low-energy plasmon satellites in $SrVO_3$ was done by Gatti and Guzzo, PhysRevB87, 155147. Was previously identified as a "Hubbard band" in a DMFT calc.



The GWΓ$^{(1)}$ Approximation

To lowest order, the vertex may be written

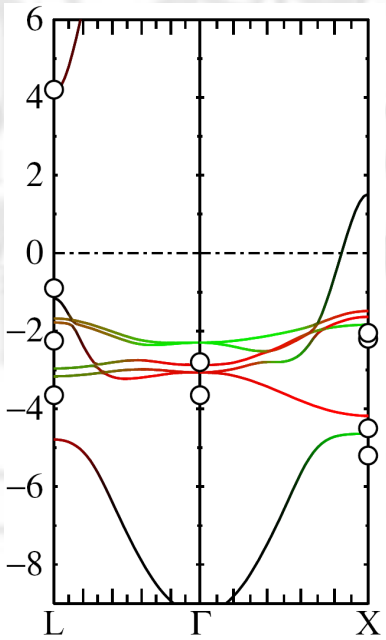
$$\tilde{\Gamma}(1,2;3) = \delta(12)\delta(23) + \frac{\delta\Sigma_{xc}(1,2)}{\delta G(\bar{4},\bar{5})} G^0(\bar{4},3) G^0(3,\bar{5})$$

Also use $\delta\Sigma_{xc}/\delta G \cong iW$. Γ with these approximations is called $\Gamma^{(1)} = 1 + GGW$. Grüneis et al [PRL 112, 096401] evaluated $\Gamma^{(1)}$ for some *sp* semiconductors.

They found:

1. Ionization potentials deepened a little, while:
2. Bandgaps changed little
3. Localized *d* states (eg on Cu, CdTe) pushed down ~0.5 eV

Tallies with universal QSGW semicore d state misalignment of ~0.4 eV



Strong Correlations in a subspace

Idea: select out a few degrees of freedom to handle in the strongly correlated subspace at a higher level of approximation

Partition a Hamiltonian H into "Subsystem" and "Rest."

$$H = \begin{pmatrix} H_{ss} & H_{sr} \\ H_{rs} & H_{rr} \end{pmatrix}$$

Dynamical Mean Field Theory

Subspace is an atom, or some strongly correlated orbitals on an atom.

Embed it in the "rest" (traditionally LDA) , and solve the SE in the subspace nonperturbatively, essentially exactly!

* Note: the self-energy is nonlocal within the atom, but nonlocality does not extend outside. Then: $\Sigma(\mathbf{k},\omega)$ does not depend on $\mathbf{k}$.

A very important point!

Strong correlations: partitioning

A universal theory that handles all electrons on an even footing is not feasible. So … we do higher level physics in subspace where correlations are strong. What is required?

1. A starting noninteracting hamiltonian (or G^0) with a family of states $\{i\}$ and a subspace of it (this will explained later)
2. We saw that we could partition G into a subspace G_{ss} and the "rest", and that the effect of the "rest" on G_{ss} can be cast in terms of a self-energy

$$G_{ss} = G^0_{ss} + G^0_{ss}\Sigma_{\text{rest}}G_{ss}$$

3. We need the effective interaction W^{eff} in the subspace. If the subspace were the full space, W^{eff} would be just the bare Coulomb v. If you could solve the full problem exactly, the solver would determine its own screening internally.

Dyson Equation for W

Remember that we developed a formula for W in the RPA.

$$W = (1 - vP^0)^{-1} v = \varepsilon^{-1} v$$

This formula carries over to the exact many-body system with a suitable redefinition of P.

W can be equivalently expressed as a Dyson equation

$$W = (1 - vP)^{-1} v = v + vPW$$

If P is divided into separate contributions $P = P^{(1)} + P^{(2)}$, then W can be similarly partitioned

$$W^{(1)} = v + vP^{(1)}W^{(1)}$$

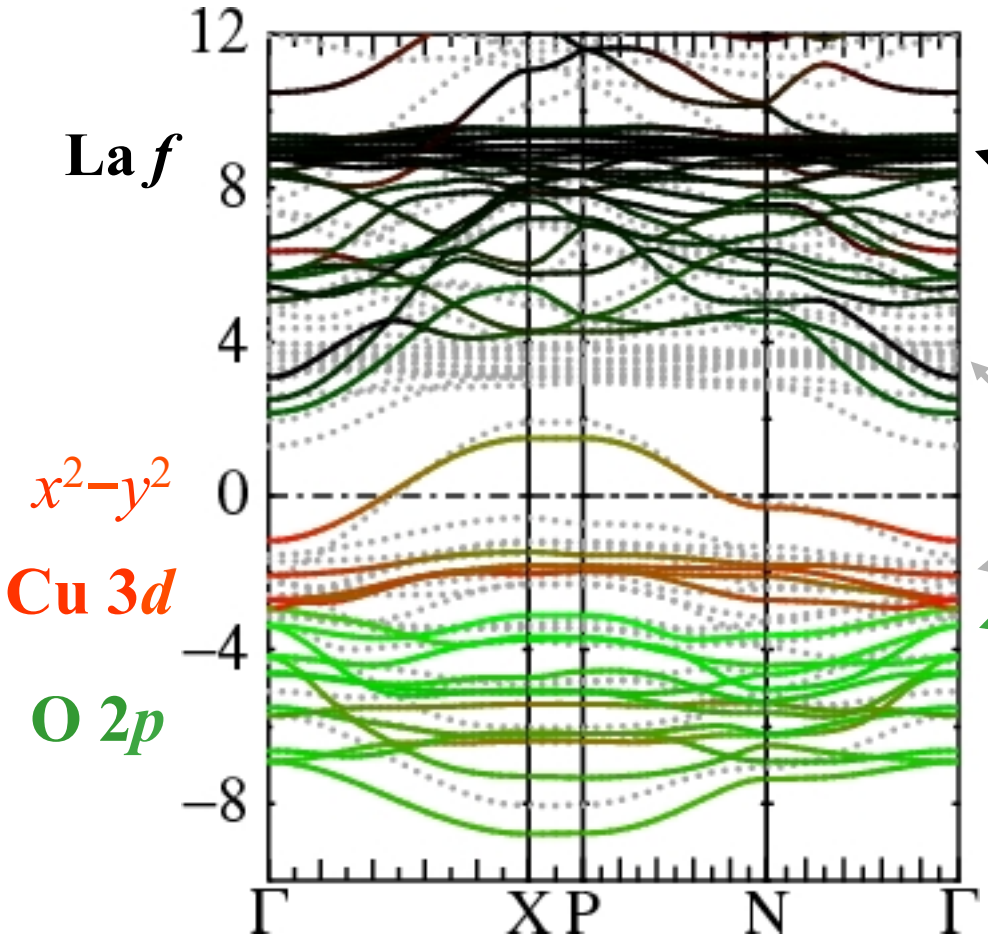
$$W^{(2)} = W^{(1)} + W^{(1)}P^{(2)}W^{(2)}$$

So … if $W^{(1)}$ is W from a low-level theory like GW, we can calculate $W^{(2)}$ if we can calculate $P^{(2)}$. We will see that $P^{(2)}$ can be obtained from a pair correlation function.

Note: no one actually does this today, but it tells you what to do in principle.

Traditional approach : LDA + DMFT

La_2CuO_4 : antiferromagnetic insulator, gap ~2 eV
Nonmagnetic calculation: LSCO is metal with Cu x^2-y^2 at E_F.



Failings of LDA:

- La $4f$ states much too low.
- O $2p$ ~1.3 eV too shallow [typical; see Dang et al, PRB90, 125114 (2014)]

Too much O $2p$ admixes into Cu x^2-y^2 .

- Ordered antiferro state is still a metal

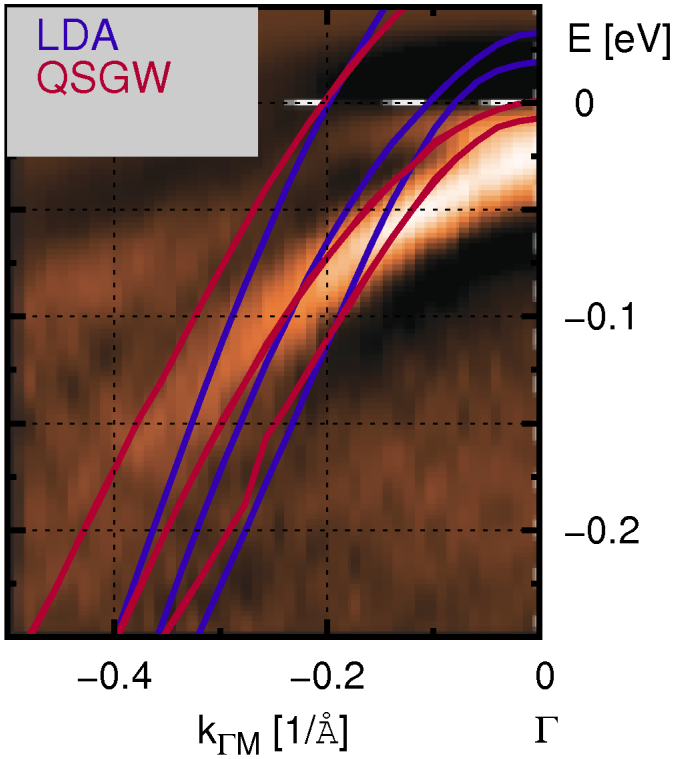
Significant intermixing of O $2p$ with Cu $3d$.

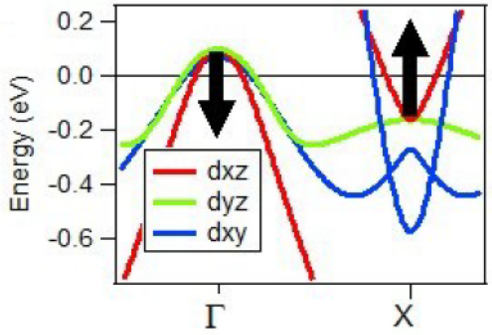
LDA+DMFT: Opens a gap of 1.5-1.8 eV

Fe Superconductor: Paramagnetic $Ba_{0.85}Co_{0.15}Fe_2As_2$

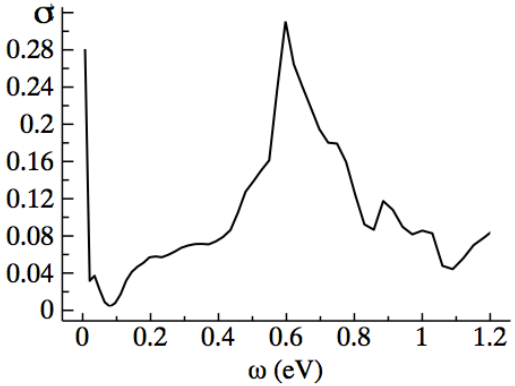
✔ QSGW improves on LDA Fermi surface pockets (k-dependent shift)

✖ QSGW m^* too small





σ(ω) well described: similar in QSGW and DMFT (LDA is poor)



Band and Mass Renormalization revisited

$$v_F \equiv \frac{d\omega^*}{dk} = \frac{d\omega^j}{dk} + \frac{d}{dk} Z^j \left(\mathrm{Re}\Sigma(k,\omega^j) - V_{xc}^j(k,\omega^j) \right)$$

In *general*, $\omega^* \neq \omega^j$. But QS*GW* is *different*: $(..)$ vanishes by construction --- *no* band mass renormalization.

Thus "renormalization" is an artifact of how H_0 is chosen --- *not* a true many-body effect.

QS*GW* QP levels should track peaks in the spectral function: to the extent ARPES is a true measure of $A(\omega)$ its peaks should be described by QSGW eigenvalues.

ARPES is widely used to measure both the Fermi surface and the velocity at E_F … we will check both.

Note: in general Σ *does* depend on k … both affect m^*.
Nonlocality of Σ is omitted in *both* LDA and DMFT.
Is it important?

Z factors and FS velocity

	QSGW $\frac{m^{QSGW}}{m^{LDA}}$	QSGW $1/Z^{QSGW}$		[AR]PES m^*/m^{LDA}		DMFT $1/Z^{DMFT}$ [Yin, Ferber, Aichhorn]	
		xy	xz/yz	xy	xz/yz	xy	xz/yz
$CaFe_2As_2$	1.05	2.2	2.1	2.5[1]		2.7	2.0
$SrFe_2As_2$	1.13	2.3	2.0	3.0[2]		2.7	2.6
$BaFe_2As_2$	1.16	2.2	2.2	2.7	2.3 [3]	3.0	2.8
LiFeAs	1.15	2.4	2.1	3.0[4]		3.3/2.8	2.8/2.4
FeSe	1.22	2.4	2.2	3.6[5]		3.5/5.0	2.9/4.0
FeTe	1.17	2.6	2.3	6.9[6]		7.2	4.8

Z factors ($1/Z = 1 - \partial\Sigma(k,\omega)/\partial\omega$) manifest as renormalization of band velocities, band widths: key measure of correlation

1. The Z factors in DMFT and QSGW are similar for weakly correlated cases, but diverge where correlations are known to be large (FeTe). Limits to adequacy of QSGW.

Z factors and FS velocity

	QS*GW* $\frac{m^{QSGW}}{m^{LDA}}$	QS*GW* $1/Z^{QSGW}$		[AR]PES m^*/m^{LDA}		DMFT $1/Z^{DMFT}$ [Yin, Ferber, Aichhorn]	
		xy	xz/yz	xy	xz/yz	xy	xz/yz
$CaFe_2As_2$	1.05	2.2	2.1	2.5[1]		2.7	2.0
$SrFe_2As_2$	1.13	2.3	2.0	3.0[2]		2.7	2.6
$BaFe_2As_2$	1.16	2.2	2.2	2.7	2.3 [3]	3.0	2.8
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FeTe	1.17	2.6	2.3	6.9[6]		7.2	4.8

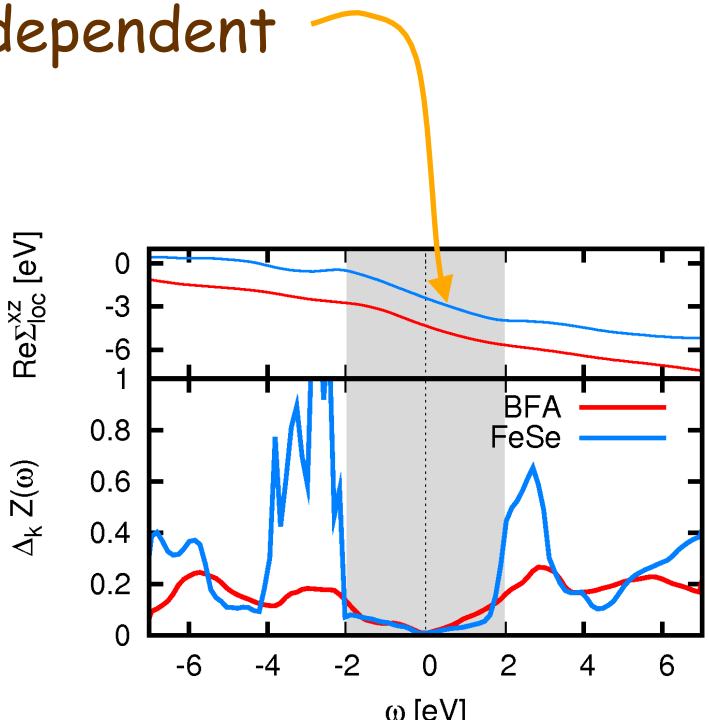
1. The Z factors in DMFT and QS*GW* are similar for weakly correlated cases, but diverge where correlations are known to be large (FeTe).
2. Renormalization of v_F relative to LDA does not match Z! Implies k-dependence of Σ is comparable to ω dependence. A high degree of cancellation between these effects.

Implies LDA+DMFT *should not describe* ARPES correctly in these compounds … since nonlocality is absent

Parititioning of k and ω Dependence of $\Sigma(k,\omega)$

Restrict consideration to the the Fermi liquid regime (~ $E_F \pm 2\text{eV}$)
At least in $BaFe_2As_2$, Z is nearly k-independent

$$\Omega \int_{BZ} dk \left[(Z - \bar{Z})^2 \right] < 0.005 < \bar{Z}/10$$



If $\partial\Sigma(k,\omega)$ is independent of k, then $\Sigma(k,\omega)$ becomes vastly simpler … it implies that Σ can be partitioned into a sum of k dependent and ω dependent terms:

$$\Sigma(k,\omega) \simeq \Sigma^s(k) + \frac{\partial\Sigma}{\partial\omega} f(\omega)$$

… If partitioning is valid, it "saves the day" for DMFT *provided* DMFT is built around a framework that generates a suitable $\Sigma^s(k)$.

QS(GW+DMFT)

QS*GW* provides an ideal framework for DMFT.

Constructs an optimally chosen static potential, which "folds in" the best static approximation to the ω dependent Σ.

There is self-consistency in the QP sense: the QP potential is improved beyond RPA by an ω-dependent, but local, potential generated nonperturbatively from DMFT. It affects charge densities, QP levels, etc.

General Framework for the Many-Body Problem

Partition using the "dual Dyson equation" for G and W

$$G^{(1)} = G^{(0)} + G^{(0)}\Sigma^{(1)}G^{(1)} \qquad W^{(1)} = v + vP^{(1)}W^{(1)}$$

$$G^{(2)} = G^{(1)} + G^{(1)}\Sigma^{(2)}G^{(2)} \qquad W^{(2)} = W^{(1)} + W^{(1)}P^{(2)}W^{(2)}$$

Treat entire system at a low level approximation (for definiteness, take this approximation as GW) and deal with the interactions of a subsystem at a higher level.

Note $G^{(2)} = G^{(1)} + G^{(1)}\Sigma^{(2)}G^{(1)} + G^{(1)}\Sigma^{(2)}G^{(1)}\Sigma^{(2)}G^{(1)} + \ldots$

0. Begin with a noninteracting $H_0 \Rightarrow G^{(0)} = \omega - H_0$

   Make P and $\Sigma^{(1)}$ and for the entire system.

   - At the GW level, $P \to P^0 = G^0G^0$ and $\Sigma^{(1)} \to iG_0W$.
   - This defines an initial $G^{(1)} = (\omega - H_0 - \Sigma^{(1)})^{-1}$
   - Note: this is typically performed in k-space .

Prescription II

1. Choose a subspace, defined by one-particle orbitals $|j\rangle$.

Make the projection of $G^{(1)}$, $P^{(1)}$, $W^{(1)}$ onto this subspace, e.g. projections $G_{ij} = \langle i|G|j\rangle$, $W_{ijkl} = \langle ij|W|kl\rangle$, $P_{ijkl} = \langle ij|P|kl\rangle$

2. Build the effective interaction U_{ijkl} for the subspace.

If the "rest" (what is outside the subspace) didn't screen the coulomb interaction at all, the effective interaction would be the bare $v = \langle ij|v|kl\rangle$

The "rest" *does* screen the subspace, resulting in W_{ijkl} (i.e. W projected onto the subspace) but we must avoid double-counting because the higher-level (eg DMFT) calculation will also screen v within its own subspace.

Recall the relation between W and the polarizability P:

$$W = (1 - vP)^{-1} v \Rightarrow W^{-1} = v^{-1} - P \Rightarrow v^{-1} = W^{-1} + P$$

Prescription III

Full system $v^{-1} = W^{-1} + P$ ← P removes screening from W

P partitions into $P = P_{\text{rest}} + P_{ijkl}$. Remove P_{ijkl} part of screening in W_{ijkl} to get effective interaction partially screened by the "rest." Interaction is customarily called U.

$$U^{-1} = W_{\text{rest}}^{-1} = W_{ijkl}^{-1} + P_{ijkl}$$

3. $G_{ij}^{(1)}$ and $U^{(1)}$ define the many-body hamiltonian for the system. Use a high-level solver (e.g. DMFT) to obtain $\Sigma_{ij}^{(2)}$ and $G_{ij}^{(2)} = (G_{ij}^{(1)} - \Sigma_{ij}^{(2)})^{-1}$

4. (Never done in practice, but possible in principle).
Subsystem's update of $U = W_{\text{rest}}$. Make reducible polarizability χ_{ijkl} --- relation is $W_{ijkl} = (U + U\chi U)_{ijkl}$.
Obtain an improved P_{ijkl} from $P_{ijkl} = U^{-1} - W_{ikjl}^{-1}$

Prescription IV

5. (Never done in practice, but possible in principle).

Update of full system's P and W. We have three quantities:

$P^{(1)}$ Polarizability of whole system at low level, eg. GW, approx

$P^{(1)}{}_{ijkl}$ projection of $P^{(1)}$ onto subsystem

P_{ijkl} A better calculation of P in the subsystem.

Improve the system P with the construction

$$P^{(1,\mathrm{new})} = P^{(1,\mathrm{old})} + \mathrm{P}_{\mathrm{ijkl}} - P^{(1,\mathrm{old})}{}_{ijkl}$$

From $P^{(1,\mathrm{new})}$, obtain $W^{(1,\mathrm{new})}$ from Dyson's equation for W.

6. Determine a better $\Sigma^{(1)}$ in the same manner

$$\Sigma^{(1,\mathrm{new})} = \Sigma^{(1,\mathrm{old})} + \Sigma - \Sigma^{(1,\mathrm{old})}$$

This determines a new G.

7. (Never done in practice, but possible in principle).

Update the low-level (e.g. GW) $\Sigma^{(1,\mathrm{new})} = i$

Prescription V

Approximately this procedure was outlined in Phys Rev Lett 90, 086402 (Aryasetiawan, Biermann and Georges)

Practical algorithms iterate only parts the entire cycle:
The pair (Σ,P) gets successively refined

Standard practice today: LDA+DMFT.

It fits with this formalism with the substitution $\Sigma_{xc}^{(1)} = V_{xc}^{\mathrm{LDA}}$.

Self-consistency from (3) above: $G_{ij}^{(2)} = (G_{ij}^{(\mathrm{LDA})} - \Sigma_{ij}^{(2)})^{-1}$ ...
This updates the hybridization function and (possibly) the Hartree potential

Summary

- Perturbative approach to strong correlations.
  - A variety of approaches, e.g. cumulants.
  - *Systematic* improvement very difficult
- Nonperturbative approach : DMFT
  - Handles strong *local* correlations very well!
  - Nonlocality comparable in size to local correlations (at least in Fe superconductors), but some evidence not strongly ω dependent in Fermi liquid regime.
  - For solution to be accurate, bath must reliably describe k-dependence of Σ. Rules out LDA!
  - QSGW+DMFT is a good candidate for this.
- Rudiments on how to set and solve partitioned problem in terms of linked equations for (G,W).