QuasiParticle Self-Consistent GW + DMFT for Magnetic Systems

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Motivation:

By far the largest many-body effects have to do with screening of the bare coulomb interaction.

Strong correlations beyond the screening tend to be local

Observation:

RPA screening is reasonably good

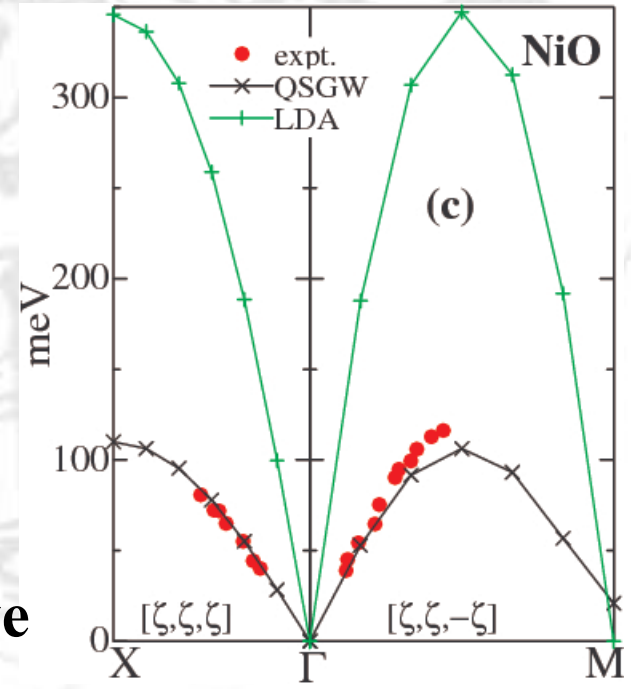
Strong correlations tend to be local.

Example: magnetic susceptibility

$$\chi^{-1} = \chi_0^{-1} - I$$

Nonlocal … independent particle picture sufficient

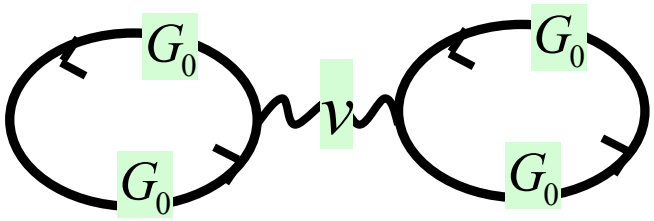
Site local effective interaction



spin waves in NiO

Properties of the GW Approximation

☑ ω-dependent W and Σ – outside one-electron picture.
☑ Nonlocal W and Σ --- very important.
☑ Van der Waals treated exactly.



☒ W screens v in the charge channel only … its dynamical fluctuations are plasmons.
☒ Σ knows has spin through the Fock exchange only.
☒ Other interactions (particle-particle) are missing

Conclusion:
If correlations are not strong, GW should be sufficient.
If dominant higher order correlations are local,
DMFT should address the primary weaknessess of GW

Characteristics of Dynamical Mean Field Theory

Dynamical Mean Field Theory: Many body approach that goes beyond low-order diagrammatic theory

☑ Nonperturbative theory. Diagrams taken to all orders
- A veritable soup of low-order diagrams! Hard to determine which diagrams are dominant if any.

☑ ω dependence of $\Sigma(k,\omega)$ is handled very well.

☑ LDA+DMFT : primary approach to strong correlations today

☒ Select out subspace of the full Hilbert space.
- Answer depends on choice of subspace

☒ Ambiguities in both effective interaction and (especially) double counting … difficult to fix.

☒ Single site approximation : nonlocality on-site only.
- $\Sigma(k,\omega)$ has no k-dependence … Nor does LDA!

☒ ω dependence on Matsubara frequencies

GW Approximation and Starting Point

G and Σ are usually generated from some effective noninteracting one-body hamiltonian H_0, usu. $H_0=H_{\rm LDA}$

But this description is often problematic … particularly when magnetism is present

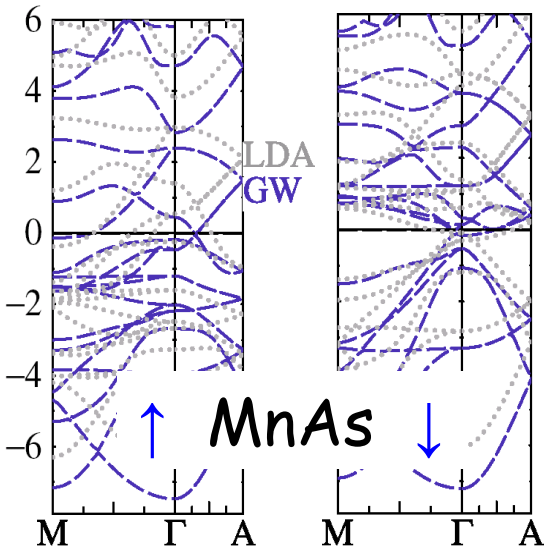
$$P(1,2) = -iGG, \quad \Sigma = iGW$$

GW neglects vertex

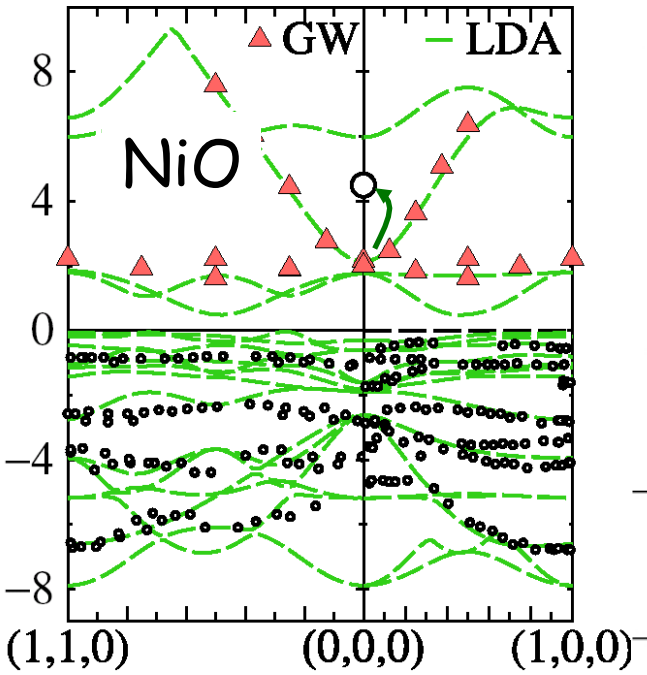
$$(h + V_H + V_x)\psi_s = \varepsilon_s \psi_s$$

$$G = \sum_s \frac{\psi_s \psi_s^*}{\omega - \varepsilon_s \pm i\delta}$$

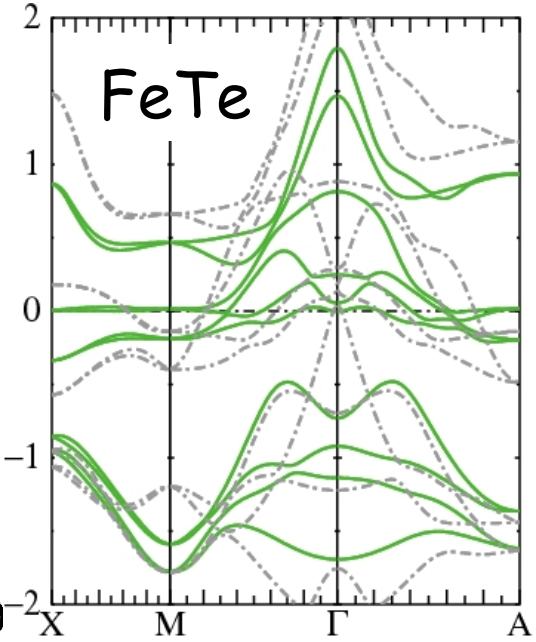
Nonsensical M, E_x



Severe gap errors



Nonsensical FS



Fully self-consistent GW

Iterate G to self-consistency to remove starting-point dependence

$G_0 \rightarrow \Sigma \rightarrow$

$G \rightarrow \Sigma \rightarrow G \rightarrow \Sigma \ldots$

True self-consistent GW looks good as formal theory:

→ Based on Luttinger-Ward functional.

→ Keeps symmetry for G

→ Conserving approximation

But poor in practice, even for the electron gas

B. Holm and U. von Barth, PRB57, 2108 (1998)

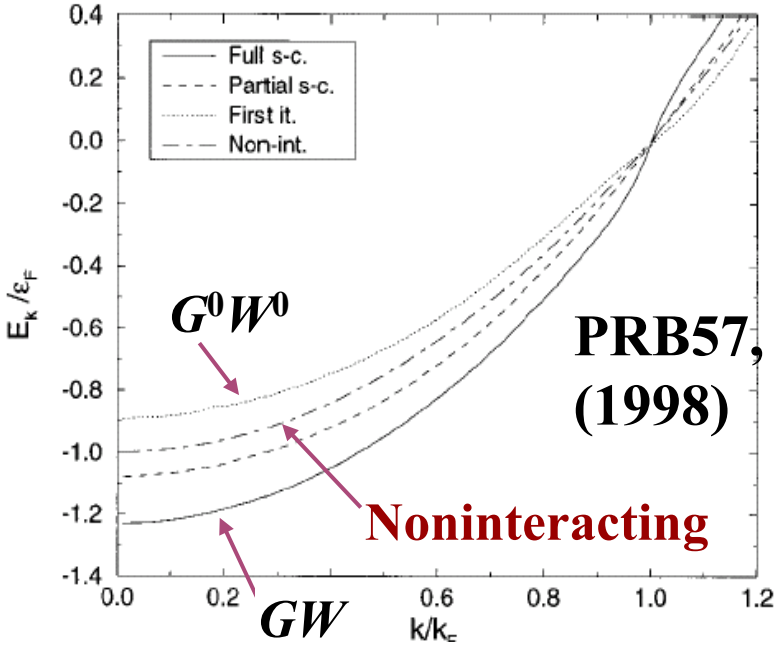
calculations with partial self-consistency using a fixed W. The quasiparticle bandwidth is larger than that of free electrons and the satellite structure is broad and featureless; both results clearly contradict the experimental evidence. The total energy, though, is as accurate as that from quantum Monte Carlo calculations, and its derivative with respect to particle number agrees with the Fermi energy as obtained directly from the pole of the Green's function at the Fermi level. Our results indicate that, unless vertex corrections are included, non-self-consistent results are to be preferred for most properties except for the total energy.

Bandwidths in scGW

Holm and von Barth compared *scGW* to G^0W^0 in the homogeneous electron gas.

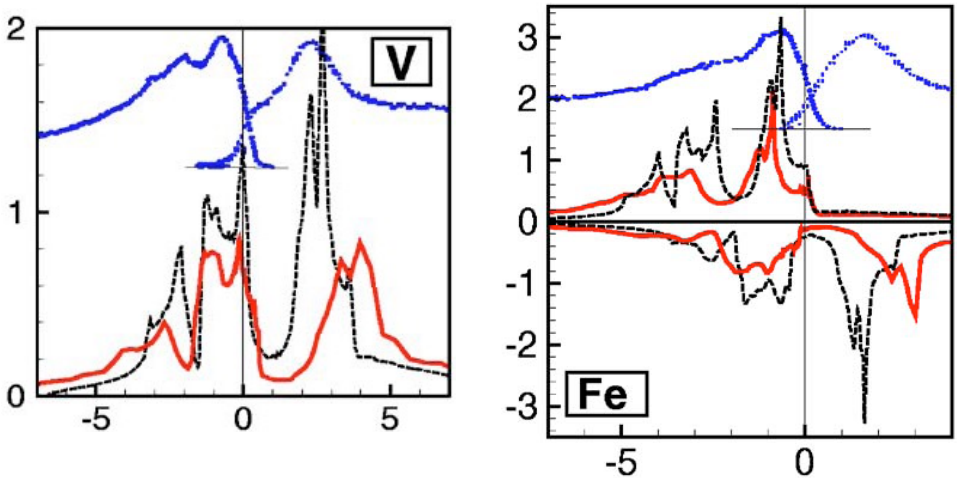
The G^0W^0 bandwidth *narrows* noninteracting by ~10%.

The *scGW* bandwidth *widens* it by ~20% (30% error)



PRB57, 2108 (1998)

Spectral functions in real materials broaden too much and get washed out. Often worse than LDA!



From Belashchenko et al, PRB 73, 073105

Quasiparticle self-consistent GW Approximation

Fully self-consistent many-body perturbation theory is problematic in many contexts …

PRL 114, 156402 (2015) PHYSICAL REVIEW LETTERS week ending 17 APRIL 2015

Nonexistence of the Luttinger-Ward Functional and Misleading Convergence of Skeleton Diagrammatic Series for Hubbard-Like Models

Evgeny Kozik,[1,2,*] Michel Ferrero,[2] and Antoine Georges[3,2,4]

The problem appears to be connected with limits to the domain of the fully interacting G.

Stick with perturbation theory around some noninteracting G_0 . How to find the best possible G_0?

Key: minimize the difference between the full G and G_0 (requires a definition of norm measuring the difference)

QSGW : a self-consistent perturbation theory where self-consistency determines the best G_0 (within the GW approximation) PRL 96, 226402 (2006)

Optimal G_0

Start with some trial V_{xc} (e.g. from LDA, or …). Defines G_0 :

$$H_0 = \frac{-1}{2m}\nabla^2 + V^{\text{ext}}(\mathbf{r}) + V^{\text{H}}(\mathbf{r}) + V^{\text{xc}}(\mathbf{r},\mathbf{r}')$$

$$H_0\psi_i = E_i\psi_i \longrightarrow G_0(\mathbf{r},\mathbf{r}',\omega) = \sum_i \frac{\psi_i(\mathbf{r})\psi_i^*(\mathbf{r}')}{\omega - E_i}$$

GWA determines ΔV and thus H :

$$G_0 \xrightarrow{RPA} \varepsilon(iG_0G_0) \xrightarrow{GWA} \Sigma(\mathbf{r},\mathbf{r}',\omega) = iG_0W; \qquad \Delta V = \Sigma - V^{\text{xc}}$$

Find a new V^{xc} that minimizes norm M, a measure of $\Delta V\, G_0$.

$$V^{\text{xc}} = \frac{1}{2}\sum_{ij}\langle\psi_i|\text{Re}\left(\Sigma(E_i)+\Sigma(E_j)\right)|\psi_j\rangle$$

(approximate) result of min M

Iterate to self-consistency. At self-consistency, E_i of G matches E_i of G_0 (real part). See Phys. Rev. B76, 165106.

skip

Z-factor cancellation

Exact $\Sigma = iGW\Gamma$. Suppose W is exact. Then

$$G = \frac{1}{\omega - H_0 - \left[-V^{xc} + \Sigma(\omega_0) + (\partial\Sigma/\partial\omega)_{\omega_0}(\omega - \omega_0)\right] + i\delta}$$

$$Z = (1 - \partial\Sigma/\partial\omega)^{-1}$$

Residual of this pole (loss of QP weight) is reduced by Z

Write G as $G = ZG^0 + (\text{incoherent part})$ Ward identity

$\therefore GW\Gamma \approx G^0 W + (\text{incoherent part})$ $\Gamma \to Z^{-1}$ for $q', \omega' \to 0$

Similar argument for W. Ishii et al (arxiv 1003.3342)
reversed argument: postulate Γ that satisfies Ward Identity

$$\Gamma_{WI}(p, p+q) \equiv \frac{G(p+q)^{-1} - G(p)^{-1}}{G_0(p+q)^{-1} - G_0(p)^{-1}}$$

Results from $GW\Gamma_{WI}$ similar to G_0W_0.

Formal Justification of QSGW

Original justification for QSGW: find the G_0 which miminizes the difference $\langle G-G_0 \rangle$, according to some definition of $\langle \ldots \rangle$, within the GW approximation.

Why not just find G_0 that minimizes the RPA total energy E^{RPA} ?

$$\frac{\delta E^{\mathrm{RPA}}}{\delta G_0} = 0$$

Not possible … there is no lower bound (PRB76, 165106).

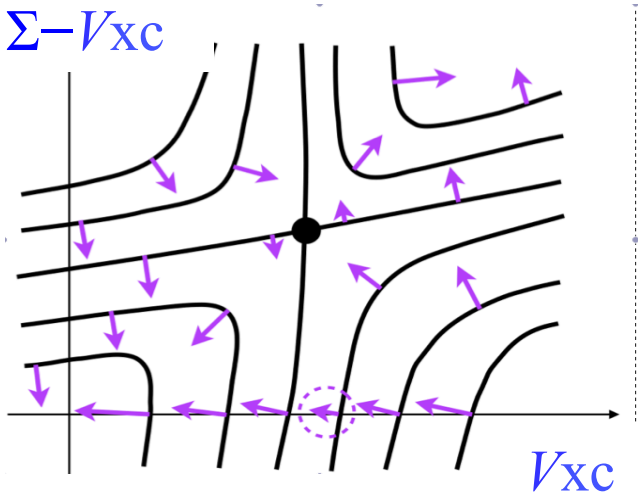
Justifying quasiparticle self-consistent schemes via gradient optimization in Luttinger-Ward theory

arXiv:1406.0772

Sohrab Ismail-Beigi

A *different* justification (Ismail-Beigi)
Minimize square of *gradient* of Luttinger Ward energy

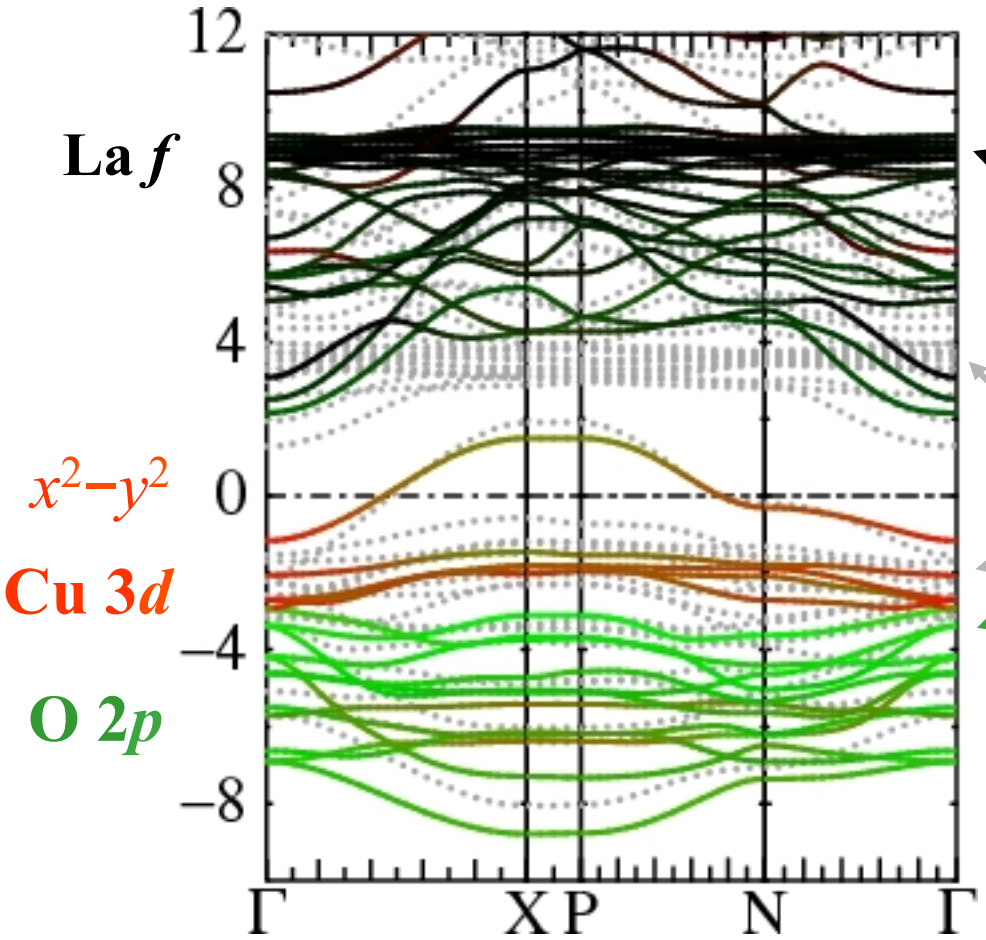
$$|D|^2 \rightarrow \min \quad \text{where} \quad D = \frac{\delta F[G_0]}{\delta \Sigma}$$



Why not 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)]

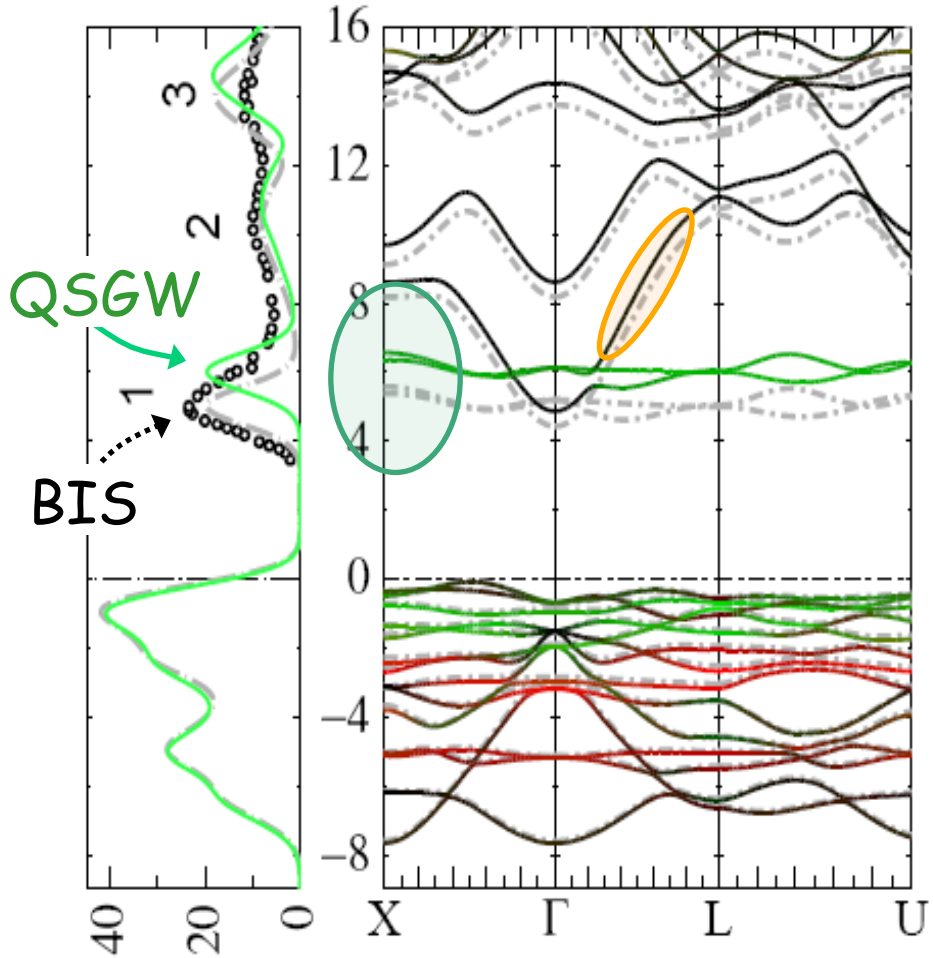
Too much O $2p$ admixes into Cu x^2-y^2 .

- Ordered antiferro state is still a metal

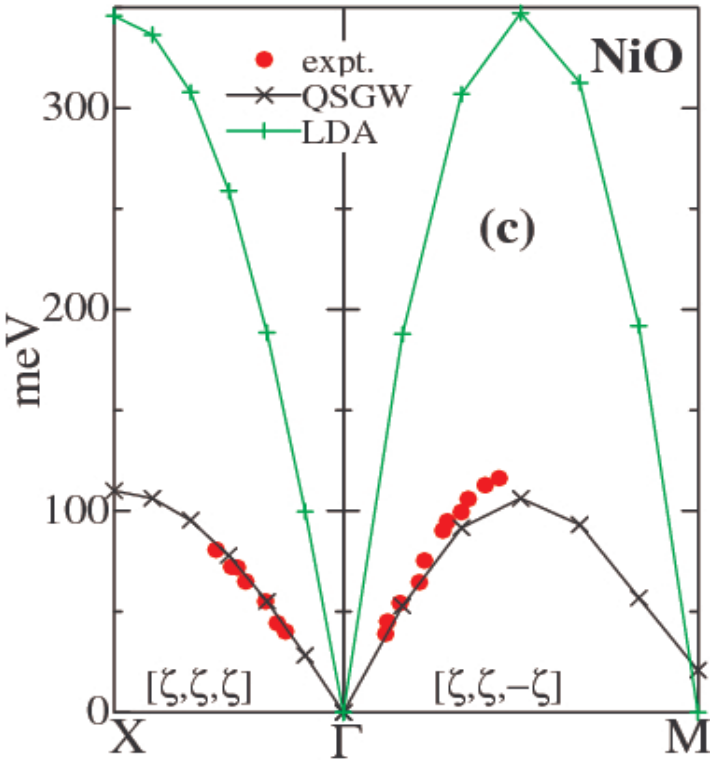
Significant intermixing of O $2p$ with Cu $3d$.

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

Quasiparticle Self-Consistency for NiO



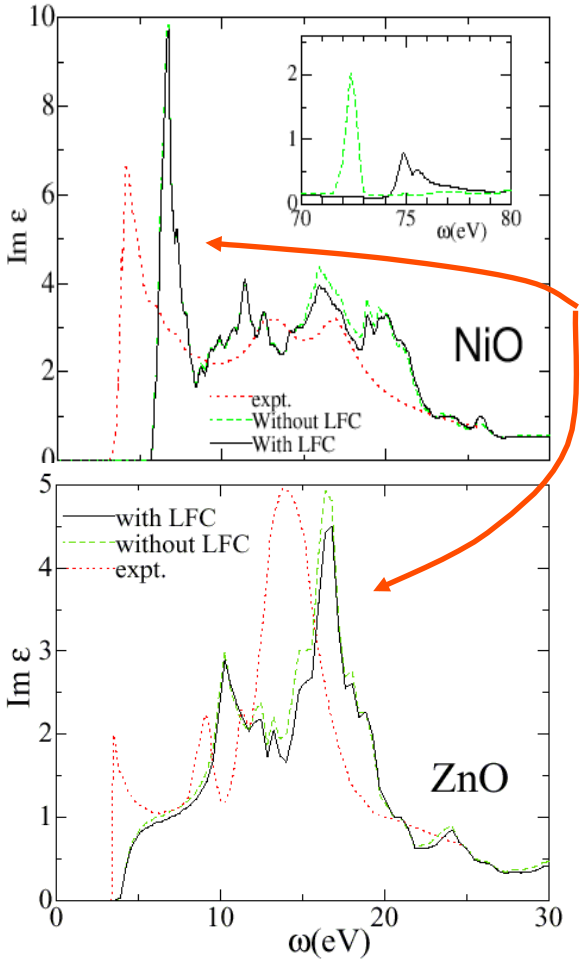
NiO looks ok, but gaps too big! (clear marker of RPA overestimating W)



J. Phys. Cond. Matt. 20, 95214

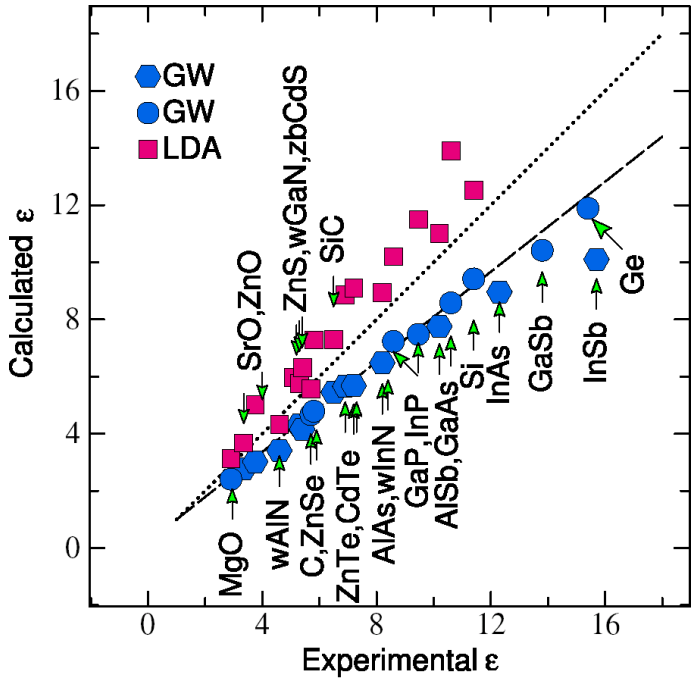
Spin waves in MnO and NiO very well described. Nothing adjustable, all electrons on same footing.

Why the NiO Bandgap is too large

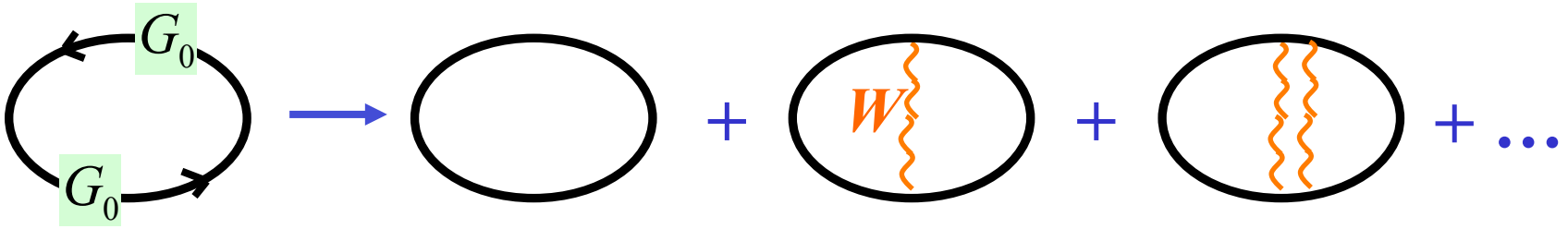


Plasmon peaks in Im $\varepsilon(\omega)$ are too high

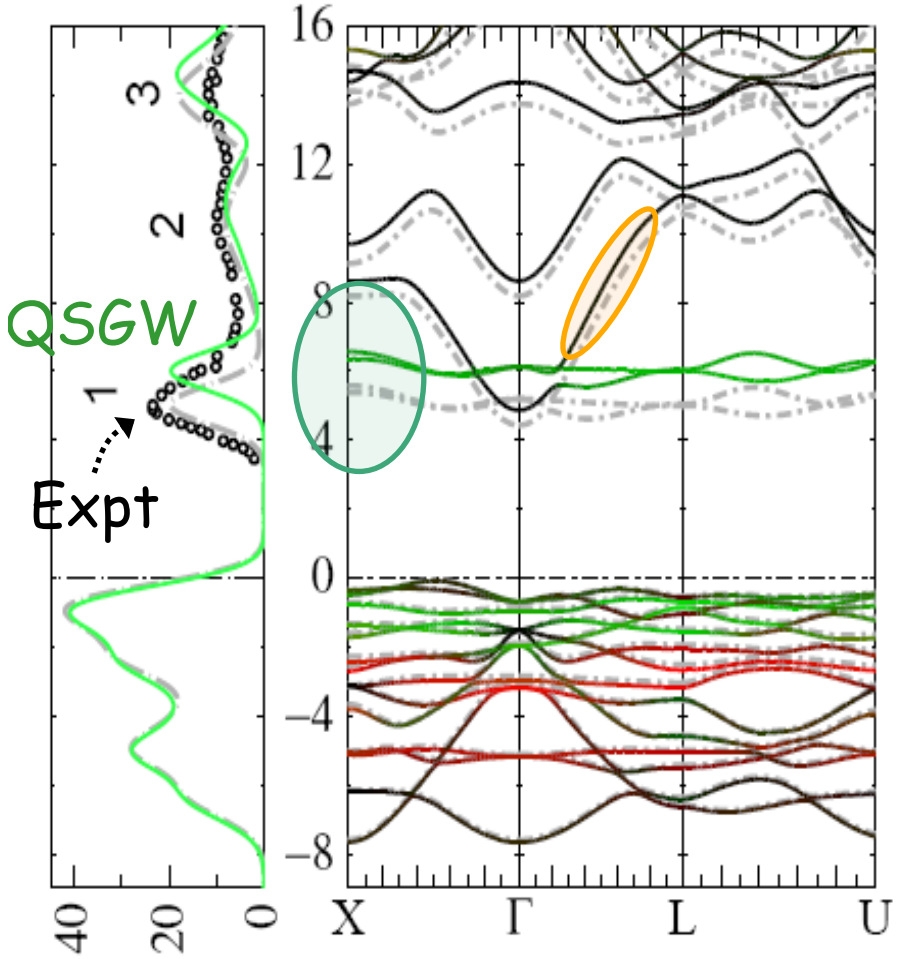
This makes $\varepsilon_\infty = \mathrm{Re}\,\varepsilon(0)$ too small

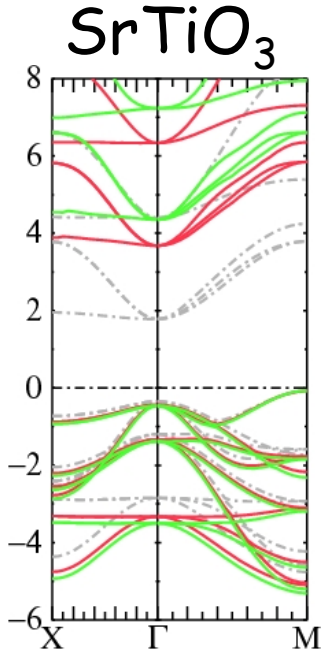


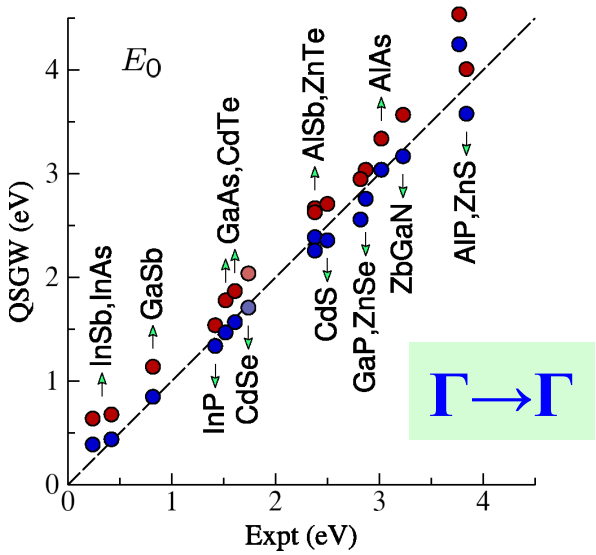
ε_∞ is *universally* 20% too small in insulators (missing ladders)



Better screening in the charge channel fixes much







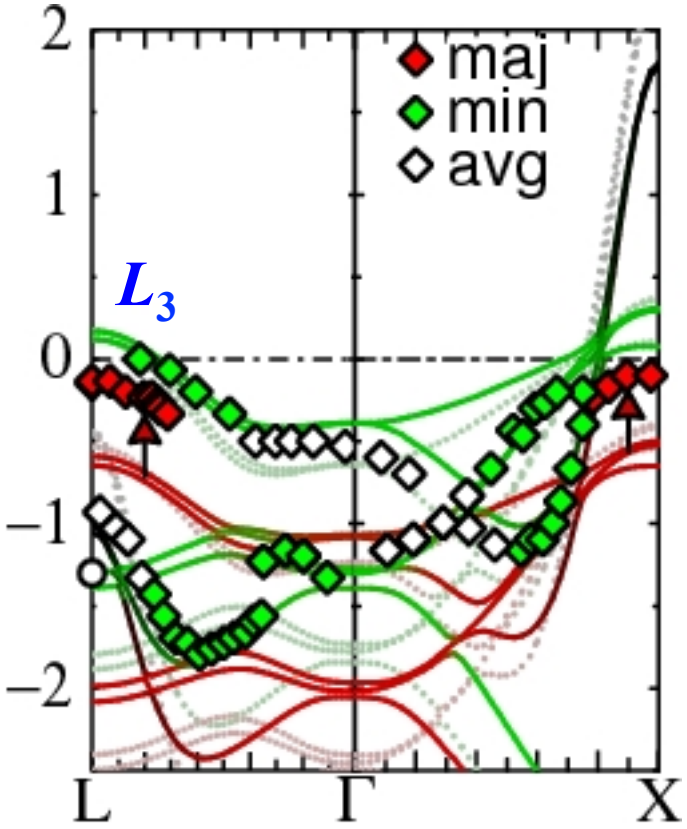
Estimate error

$W \sim [\varepsilon_\infty^{-1}(\text{expt})/\varepsilon_\infty^{-1}(\text{QS}GW)]\, W^{\text{RPA}}$

Result: spectra aligns almost exactly with BIS. Peaks 1, 2, 3 shift different amounts

Seen in most TM oxides and universally seen in *sp* systems

ARPES Measurements of Ni



W^{RPA} is screened in the charge channel only … no spin fluctuations.

QSGW : vast improvement over LDA for TM in general. But for Ni, problems appear

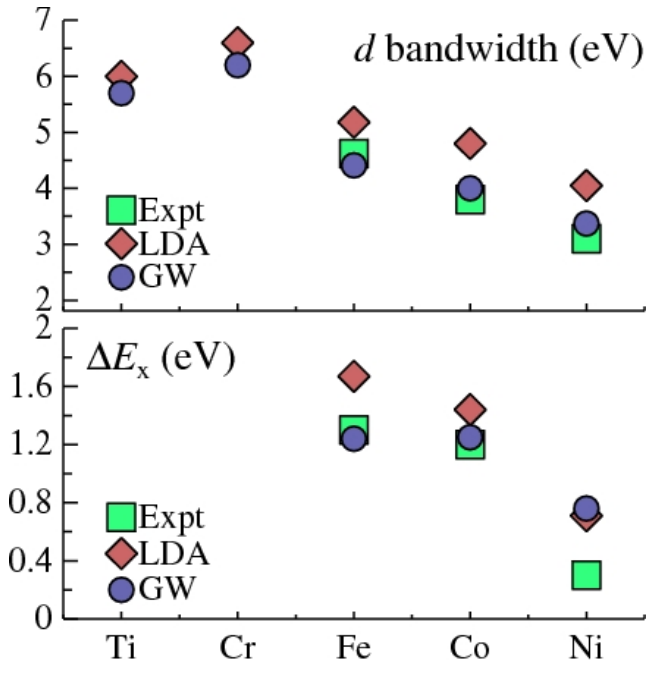
Calculated ΔE_x :

QSGW	LDA
0.76	**0.71**

Calculated M :

QSGW	LDA
0.76	**0.60**

Trends in 3*d* series

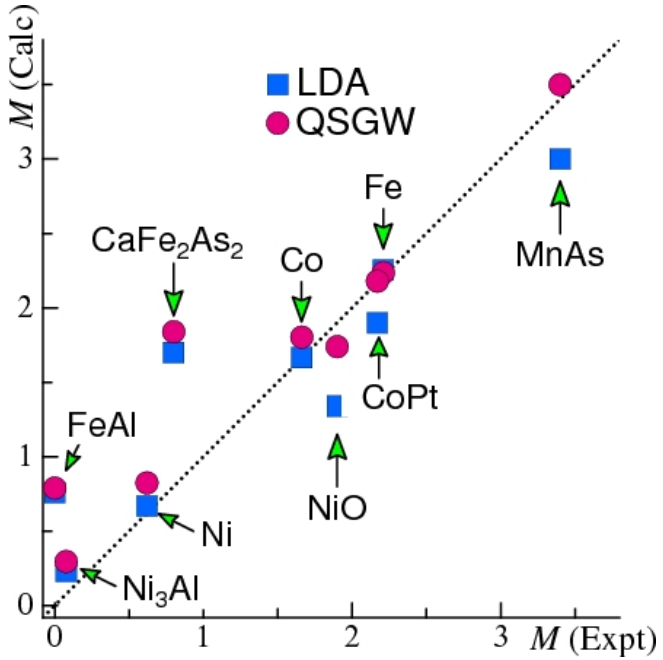


QSGW misses a satellite at -6 eV seen in photoemission

Spin Fluctuations

In Ni spin fluctuations are important (Nolting et al, 1989)
Quite generally, QSGW appears to:

- predict M in local-moment systems very well
- overestimate M in itinerant systems.

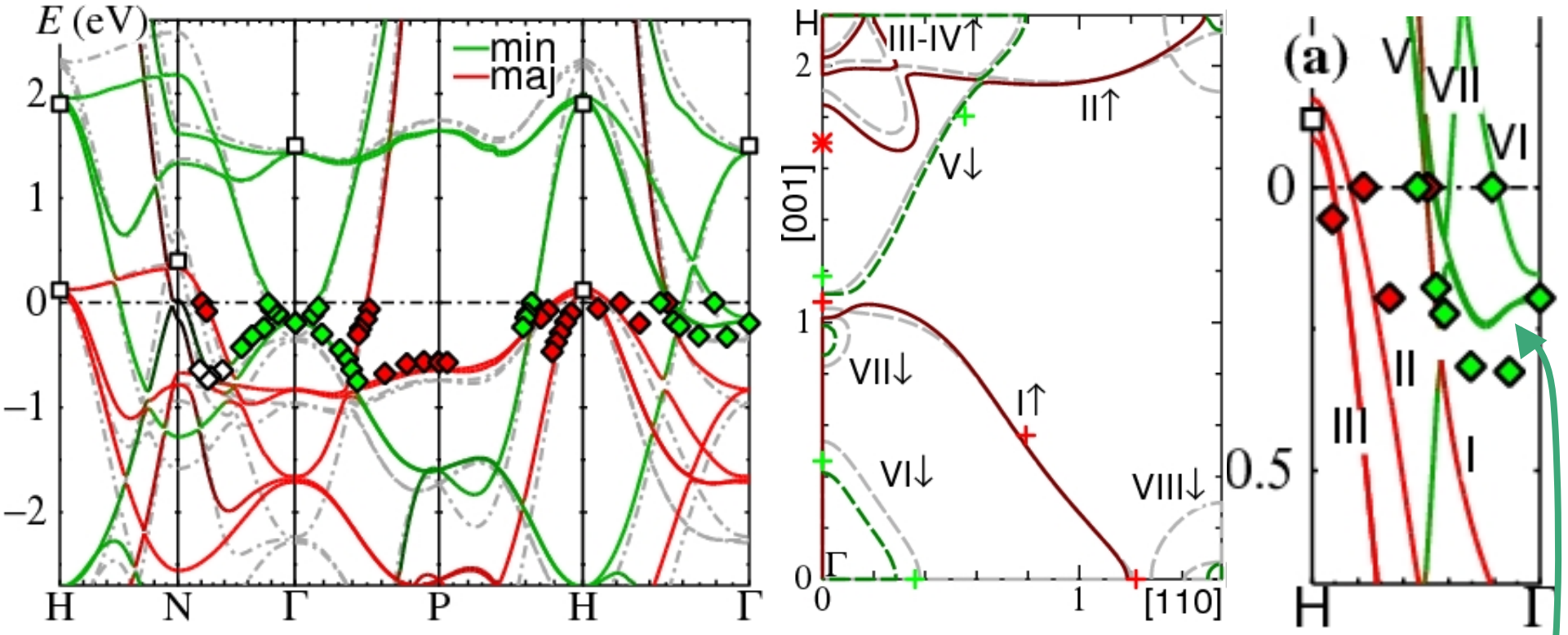


LDA has two distinct errors:
$\langle M \rangle$ is too large in itinerant materials.
$\langle M \rangle$ is too small in local-moment systems (CoPt, MnAs)
In Ni the errors cancel … $\langle M \rangle$ is fortuitously good!

Spin fluctuations reduce $\langle M \rangle$. Moriya estimated $\langle \Delta M \rangle$ from FD theorem. Requires $\int d\omega \, \mathrm{Im}\chi$ (Mazin et al PRL 2004).
… Better fluctuations are built into higher order diagrams.

Spin Fluctuations in Fe are not important

QS*GW* matches ARPES and inverse PE (Santoni & Himpsel, Phys. Rev. B 1991) extremely well …



Much better than LDA. Small discrepancies at ~0.1 eV scale: e.g. the VI ↓ dispersion near **k**=0 … But it turns out that differences are largely artifacts of final-state effects in PE!

QSGW + "Magnetic" DMFT

- $\Sigma^{GW}(k,\omega)$ mainly misses spin fluctuations
- DMFT should treat spin fluctuations well, but no $\Sigma(k)$.

Basic idea : combine charge $\Sigma^{QSGW}(k)$ with spin $\Sigma^{DMFT}(\omega)$.

$$\Sigma^{\pm} = \bar{\Sigma}^{QSGW}(k) + \Sigma^{DMFT,\pm}(\omega)$$

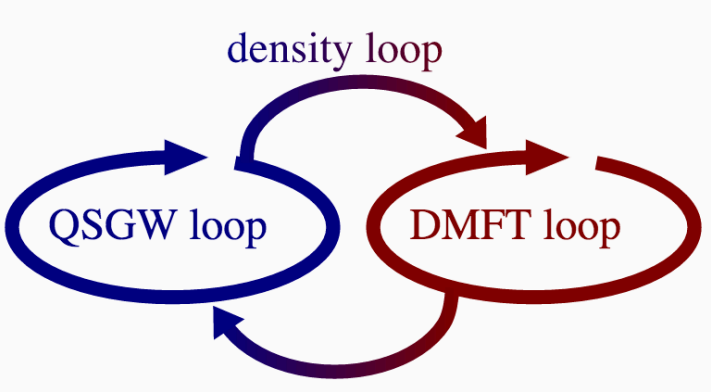
$$\bar{\Sigma}^{QSGW} = [\Sigma^{+}(k) + \Sigma^{-}(k)]/2$$

$$\Sigma^{DMFT,\pm} = \pm[\Sigma^{+}(\omega) - \Sigma^{-}(\omega)]/2$$

Avoids double counting

Complications :
$\Sigma^{GW}(k,\omega)$ on the real axis, for the full hilbert space
$\Sigma^{DMFT}(\omega)$ at the Matsubara frequencies for the *d* subspace

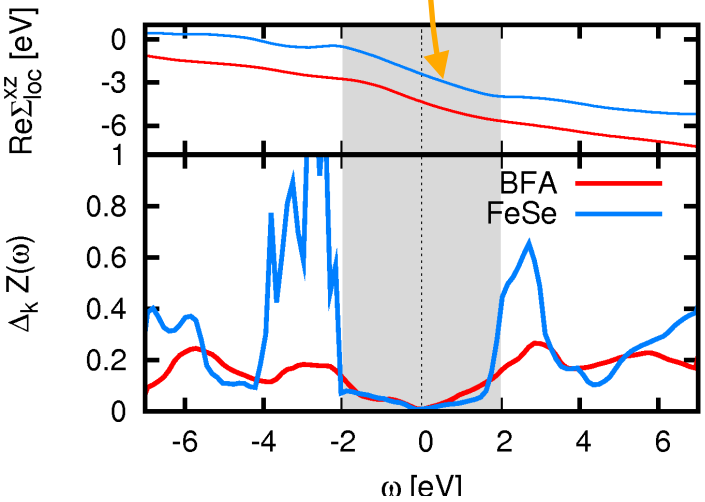
How to quasiparticlize Σ?
What kind of self-consistency?



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

Consider the superconductor $BaFe_2As_2$.
Restrict consideration to the the Fermi liquid regime (~ $E_F \pm 2eV$)
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 $\Sigma^s(k)$. See Phys. Rev. Lett. 109, 237010 (2012)

Implementation of QSGW + "magnetic DMFT"

1. Make QSGW $\Sigma^{\mathrm{GW}}(k,\omega) \Rightarrow$ quasiparticlize $\Rightarrow \Sigma^{\mathrm{QSGW}}(k)$
2. Projectors from d partial waves in augmentation sphere.
3. Calculate U_{ijkl} within constrained RPA (For now just pick U, J)

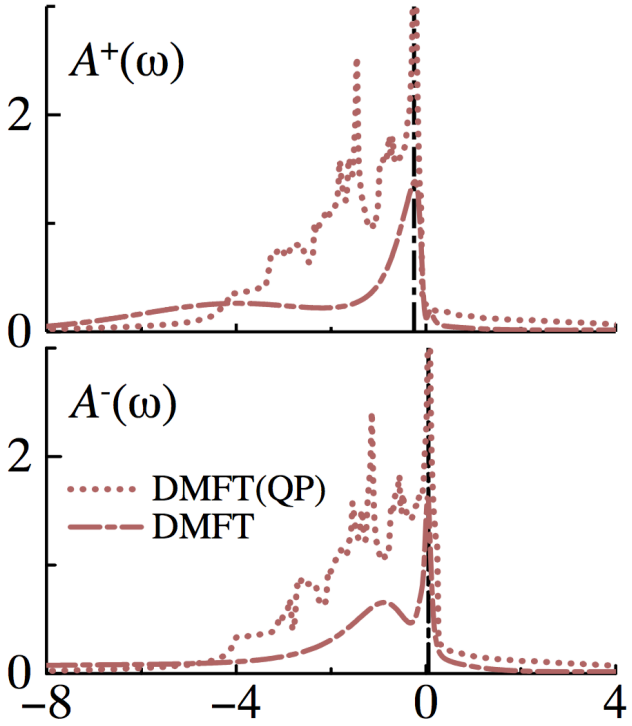
--- Iterate the following nested loops to self-consistency ---

1. Make $\Sigma^{\pm} = \overline{\Sigma}^{\mathrm{QSGW}}(k) + \Sigma^{\mathrm{DMFT},\pm}(\omega)$ **(Initially 0)**
2. Project $G \rightarrow G^{\mathrm{loc}}$; with U, J generate Σ^{DMFT} from CTQMC.
3. Construct a new G, new density and Hartree potential
4. Quasiparticlize† $G \rightarrow G^0$ to generate new $\Sigma^{\mathrm{GW}}(k,\omega)$, $\Sigma^{\mathrm{QSGW}}(k)$.

†We use static limit of Σ^{DMFT} for now

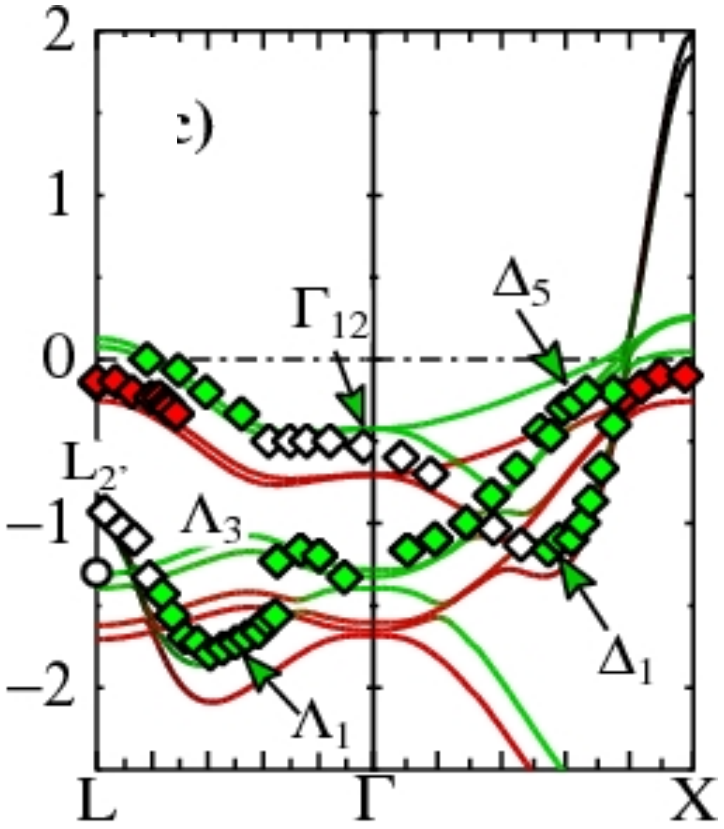
QSGW + Magnetic DMFT, ARPES

	ΔE_x	M:
LDA	**0.71**	**0.60**
QSGW	**0.76**	**0.76**
QSGW+DMFT	**0.3**	**0.51**
QSGW+DMFT(QP)	**0.3**	**0.55**
Experiment	**0.3**	**0.57**



Dynamical Σ washes out DOS

QP weight pushed to a plasmon near -4.5 eV



Exchange splitting well described by QP

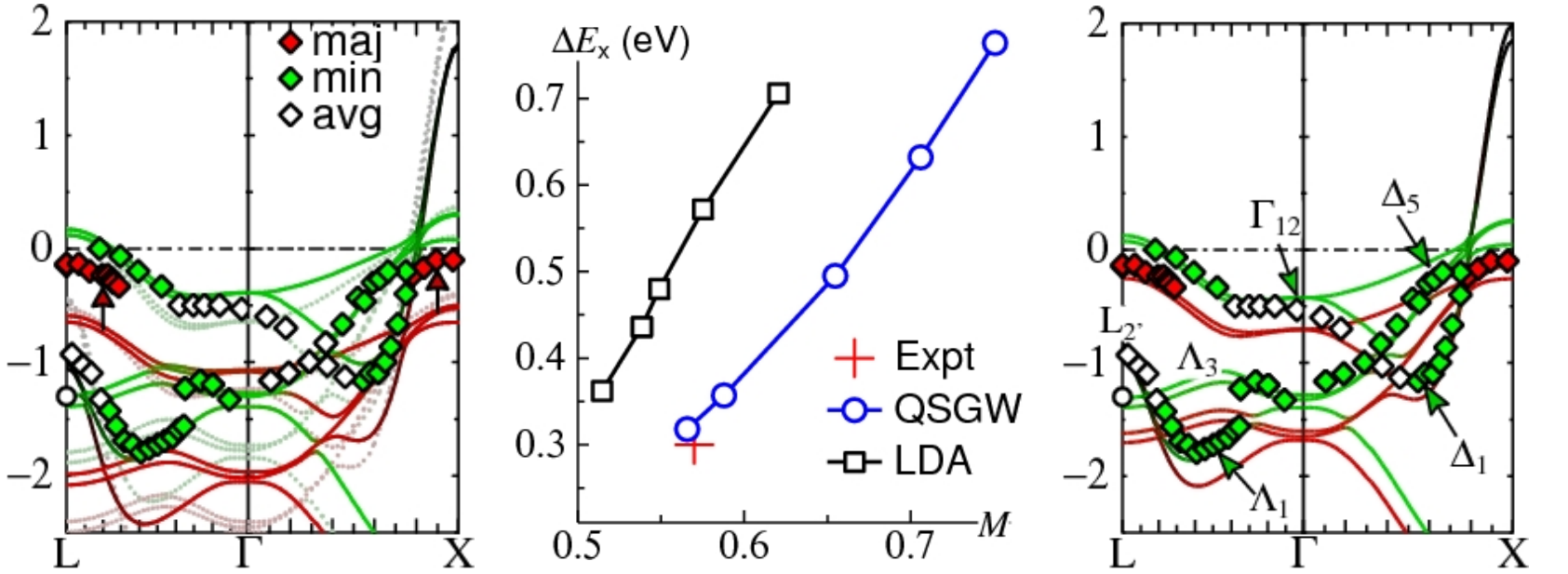
Self-consistency has minimal effect

Renormalization of ΔE_x by effective field

If Ni is reasonably described by a QP picture, fluctuations will modify the static (QS*GW*) 1-body $\mathbf{B}^{sf}$.

Simulate DMFT Σ with an external static $\mathbf{B}^{sf}$ added to Σ^{QSGW}.

Iterate QS*GW* + $\mathbf{B}^{sf}$ to self-consistency.

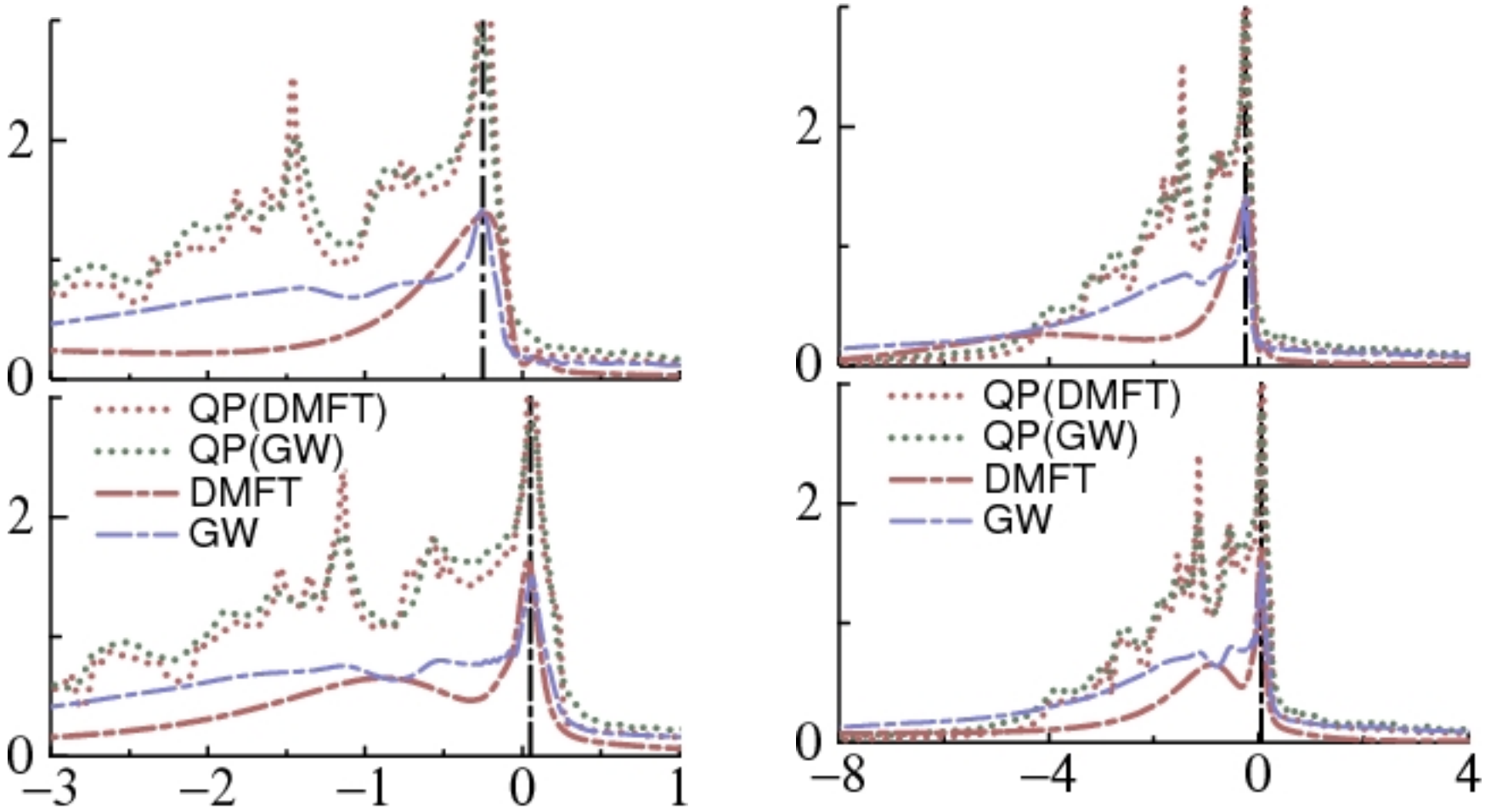


$\mathbf{B}^{sf}=0$

Result almost identical to QSGW+magnetic DMFT

$\mathbf{B}^{sf}$ at $\langle \boldsymbol{M} \rangle = \langle \boldsymbol{M}^{expt} \rangle$

Spectral functions, QSGW+B^{SF} and QSGW+DMFT



DMFT more strongly suppresses QP weight, pushes to satellite deeper in energy.

Spin Waves in QSGW

$$\chi^{-1}(\mathbf{q},\mathbf{r},\mathbf{r}',\omega) = \chi_0^{-1}(\mathbf{q},\mathbf{r},\mathbf{r}',\omega) - I(\mathbf{q},\mathbf{r},\mathbf{r}',\omega)$$

Transverse spin susceptibility

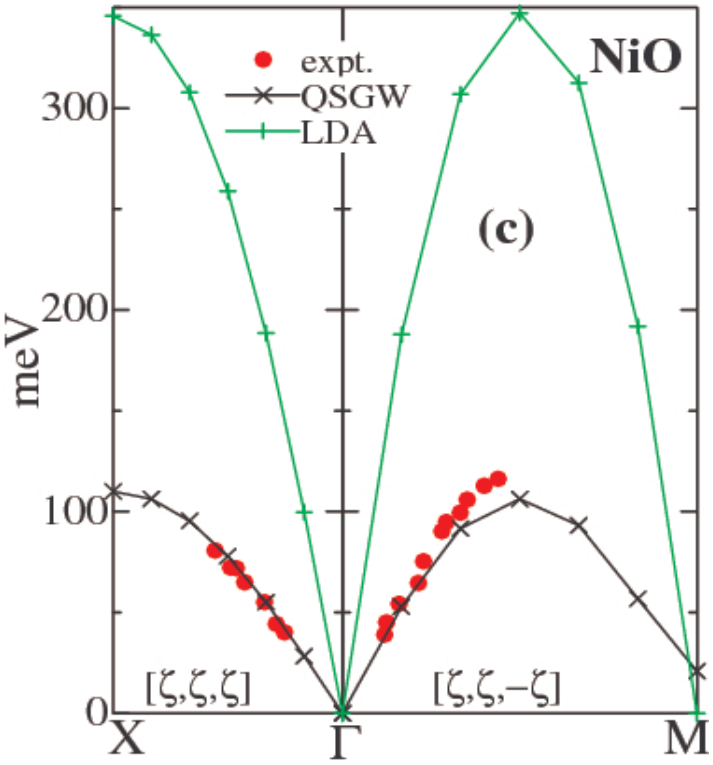
Assume spin $|\mathbf{m}(\mathbf{r})\rangle$ rotates rigidly. Then

$$\chi^{-1}(\mathbf{q},\mathbf{r},\mathbf{r}',\omega) \propto |\mathbf{m}(\mathbf{r})\rangle\langle\mathbf{m}(\mathbf{r}')|$$

Assume further I is static and site-local. Then I can be can be inferred from condition that the pole go to zer for $\mathbf{q} \to 0$:

$$\langle\mathbf{m}|\,\chi_0^{-1}(\mathbf{q}=0,\omega=0)\,|\mathbf{m}\rangle = \langle\mathbf{m}|\,I\,|\mathbf{m}\rangle$$

Find SW's from pole in χ^{-1}.
Avoid "hard" problem of calculating effective (Stoner) interaction.
Works very well in NiO, MnO, MnAs (local-moment systems) ...



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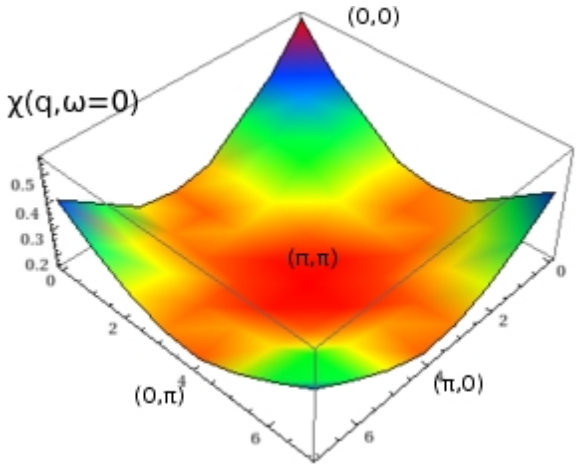
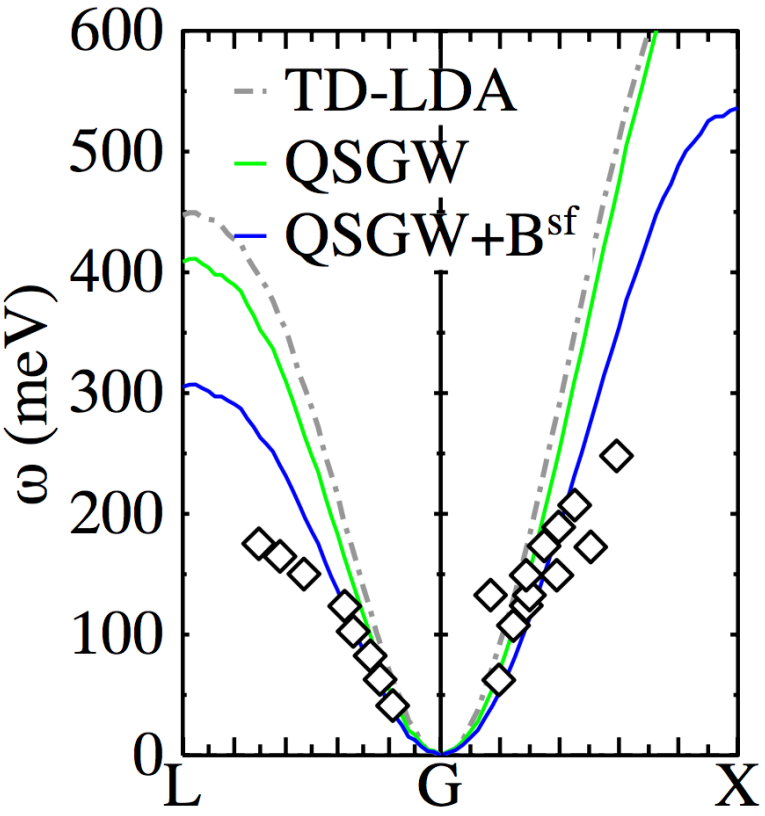
Spin Waves in Ni

For larger $\mathbf{q}$, $\omega(\mathbf{q})$ is too high.
Similar to conclusions by Karlsson and Aryasetiawan (J Phys C12, 7617) -- vertex $\delta\Sigma/\delta\varphi$ calculated in GW-ASA

They got better agreement by scaling matrix elements to reduce ΔE_x.
Similar improvement with QSGW + B^{sf}
(RSA ⇒ no optical mode)



In progress:
(Swagata Acharya)
Use DMFT to calculate I.



Adopt approach by Park, Haule, and Kotliar (PRL 107, 137007)

Community Code: Questaal Package

CCP9 Flagship code: transform our electronic structure code into a community code (CCP9 flagship) with wide user base

Join with the "real materials" part of the Simons Foundation : collaboration on the many-electron problem

SIMONS FOUNDATION

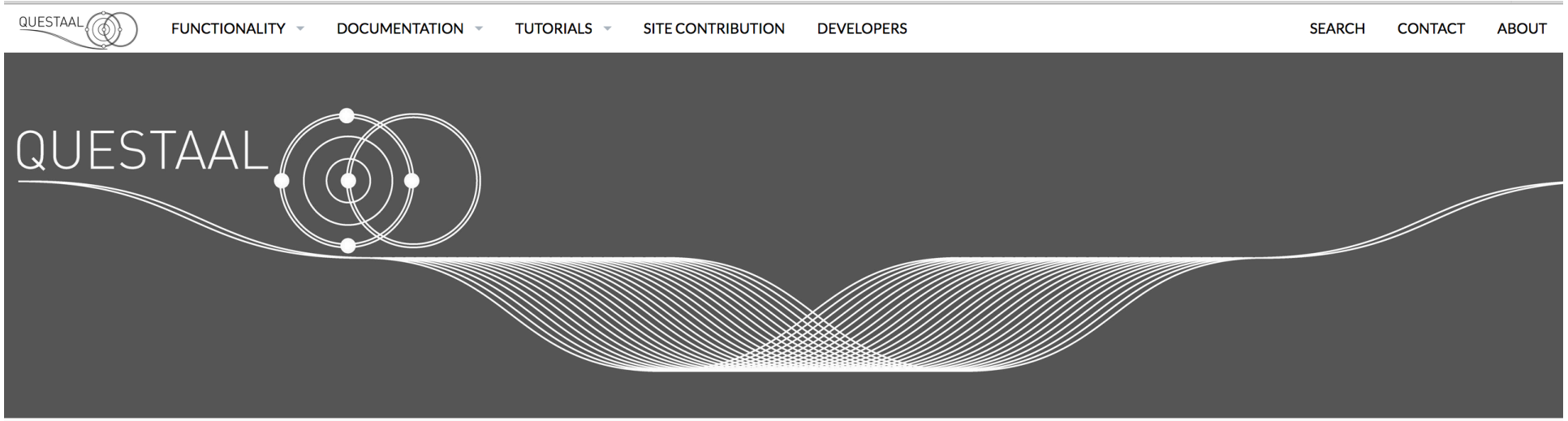
Advancing Research in Basic Science and Mathematics

Simons Collaboration on the Many Electron Problem

The Simons Collaboration on the Many Electron Problem brings together a group of scientists focused on developing new ways to solve the quantum mechanical behavior of systems

Questaal Website

Community Aspects



Web site with documentation, tutorials, ticketing system.

Parts are working; still under development (time consuming!)

Website temporarily at: https://lordcephei.github.io/

Download the package at https://bitbucket.org/lmto

Unique Features of Questaal Pacakge

- A long and venerable tradition: descendant of O.K.Andersen (Stuttgart) LMTO-ASA (1980's) and first all-electron GW evolved from Aryasetiawan's GW-ASA (1990's)

Unique Attributes

- A very accurate but minimal and short-range basis – essentially optimal 1-particle basis for given hamiltonian rank (Pashov) ⇒ LAPW accuracy, Siesta size (next page)
- QSGW, and QSGW+BSE (Myrta Gruening)
- QSGW + electron phonon interaction from MBPT (N. Bonini)
- Interface to K Haule's DMFT plans to link to other engines

Future :

- basis + algorithmic improvements : much faster, more accurate
- Diagrammatic Monte Carlo, FCIQMC

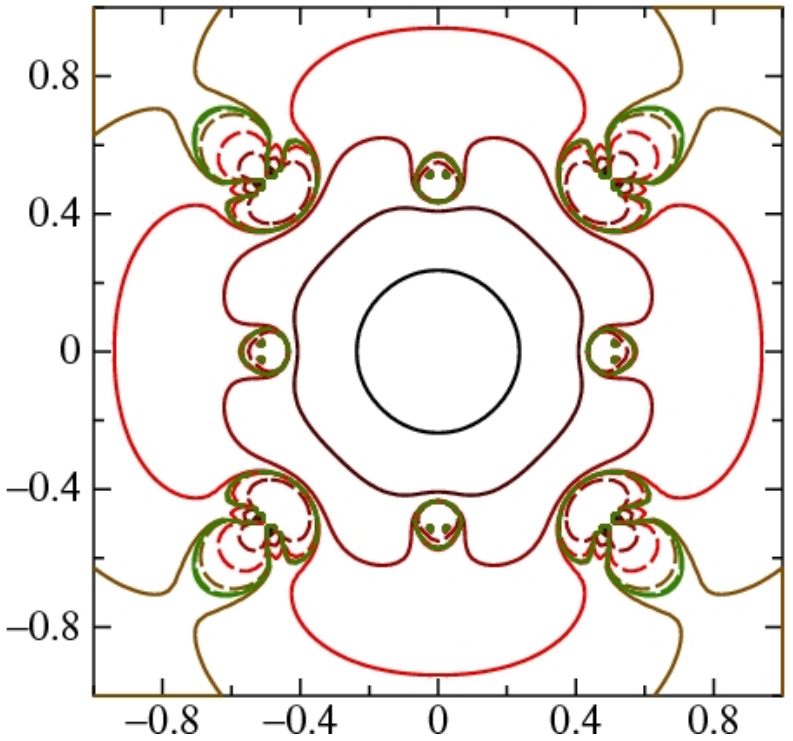
One-Particle Basis : Jigsaw Puzzle Orbitals

One-particle basis sets play a key role in this business.
Today these are normally Wannier functions or partial waves.

JPO functions satisfy $(-\Delta + V)\chi = 0$ except where it is centred

1. Division of labor: 1 partial wave carries nearly entire ψ at a point
   Solves the SE with minimum number of basis functions for a given accuracy in the four dimensions $(\mathbf{r}, E)$
2. Very short ranged
3. Atom centered with a fixed l

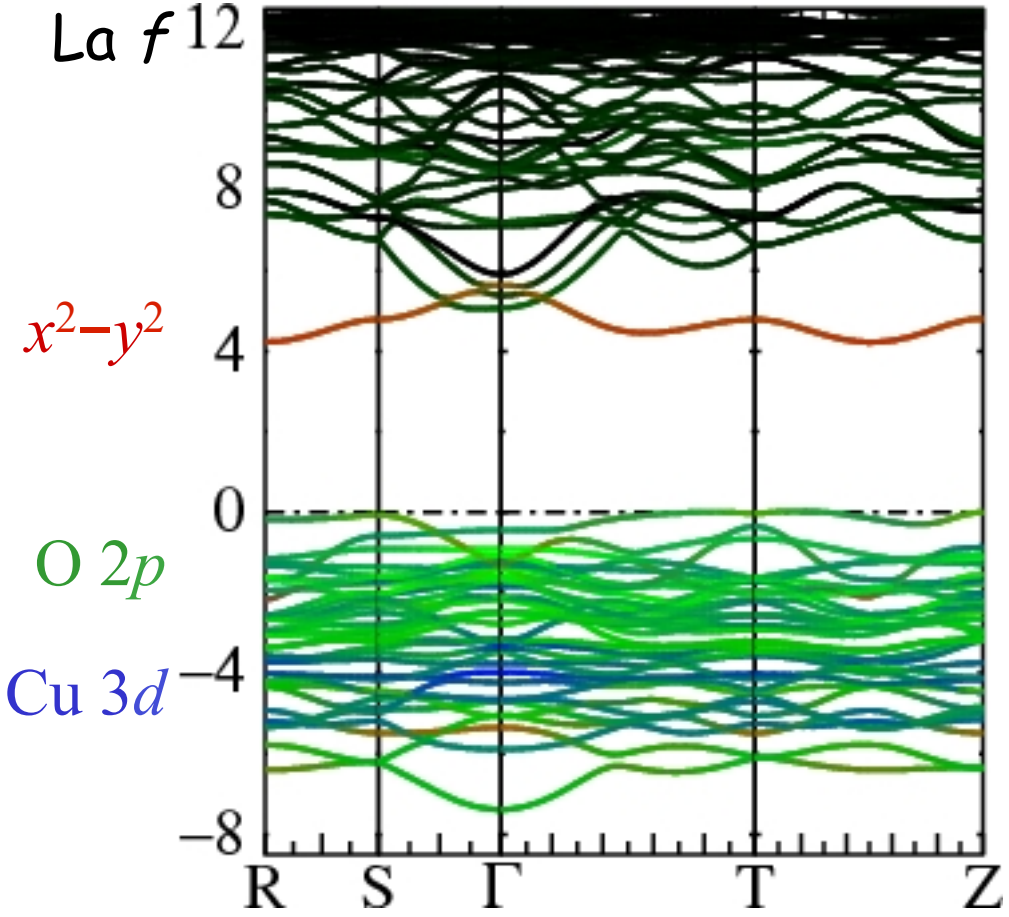
Very efficient framework both for DFT and many-body theories.



QSGW La_2CuO_4 ordered antiferromagnetic state

Low T° phase: AFM with (π, π) ordering

QSGW: insulating state with E_g~4eV.



Results:

- Lowest CB is Cu x^2-y^2 with significant O $2p$ admixed.
- VBM is O $2p$.
- Cu x^2-y^2 ↑ and ↓ split by ~10eV
- Remaining Cu d pushed below O $2p$.
- Magnetic moment M~0.8.

Failings:

- Gap ~4eV >> expt (2 eV)
- Disorder is expensive

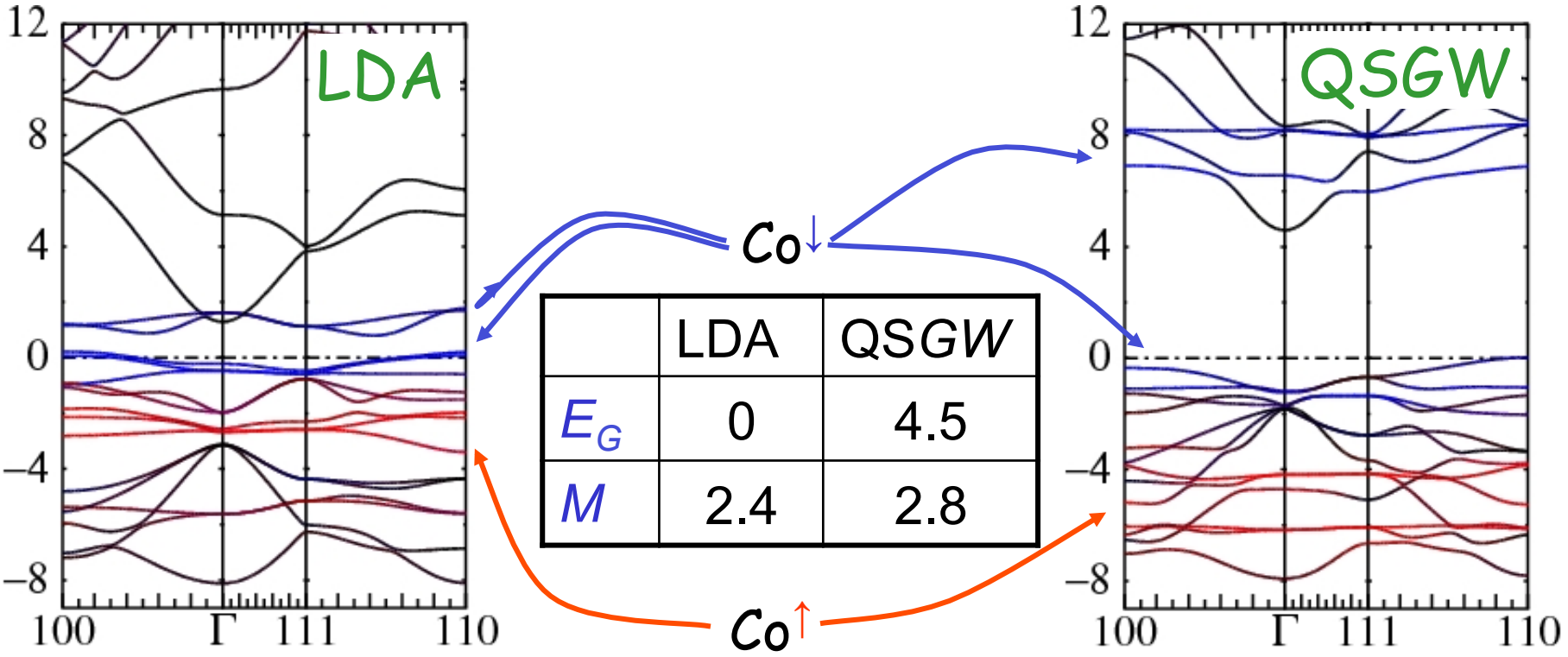
CoO shows a pattern very similar to La_2CuO_4 ….

AFM II spin configuration:

The 5 $Co^{\uparrow}$ states are filled

The 5 $Co^{\downarrow}$ states split into 3(occ)+2(unocc) separated by a gap.

The QS*GW* gap (4.4 eV) is 2 eV too big (experiment ~2.4 eV).

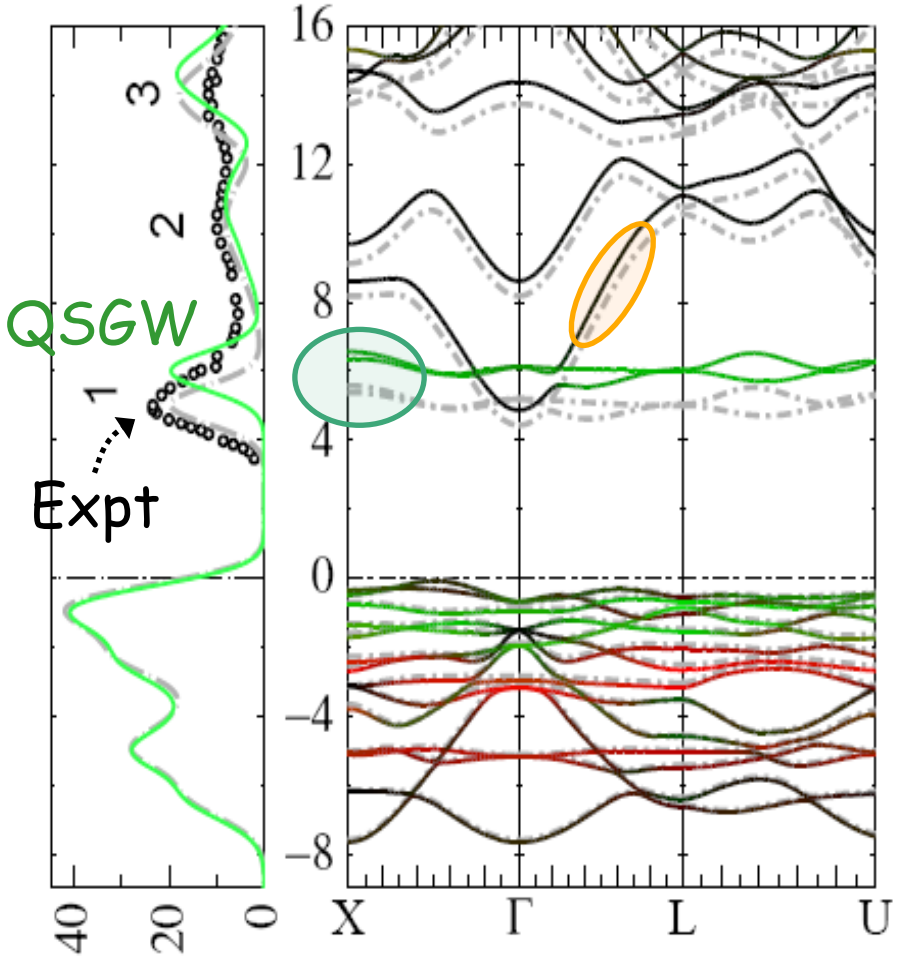


	LDA	QS*GW*
E_G	0	4.5
M	2.4	2.8

LDA: a stable AFM state with no gap (TR symmetry).

The O(2p) – Cu (3d) alignment is ~2 eV different from GW

… where NiO does not



The BIS spectra show 3 distinct peaks:

- 1 near 4.5 eV (Ni *d*)
- 2 near 10 eV (O *sp*)
- 3 near 14 eV (mixed)

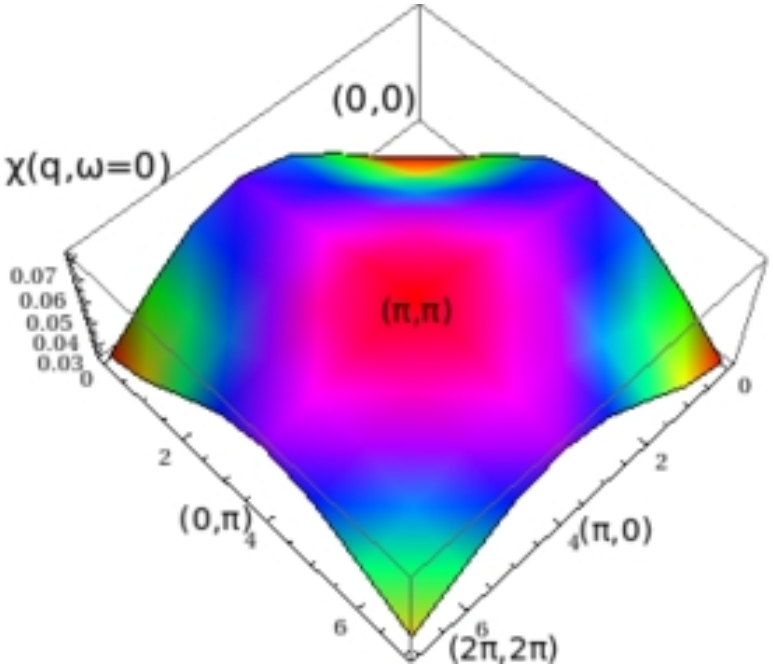
QSGW overestimates :

- 1 by ~1.1 eV (similar to $SrTiO_3$ and many nonmagnetic TM oxides)
- 2 by 0.3 eV (similar to *sp* semiconductors)
- 3 by 0.5 eV.

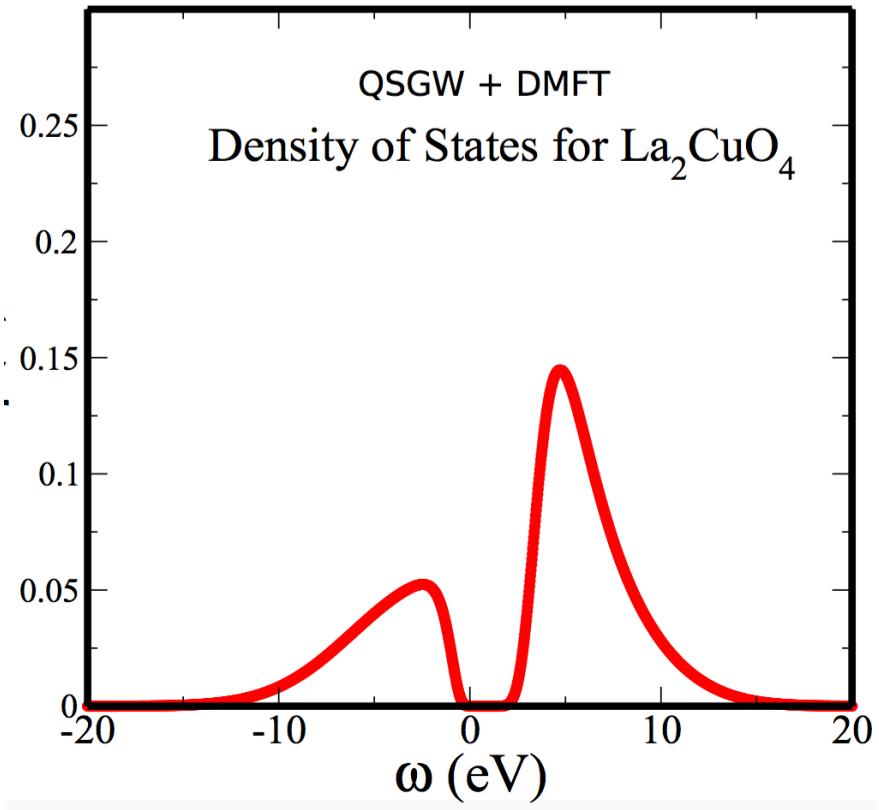
Conclusion:
For NiO spin fluctuations less important than in LSCO and CoO,

Spin fluctuations in LSCO

Conclusion:
For NiO spin fluctuations less important than in LSCO and CoO,



Static χ in LSCO

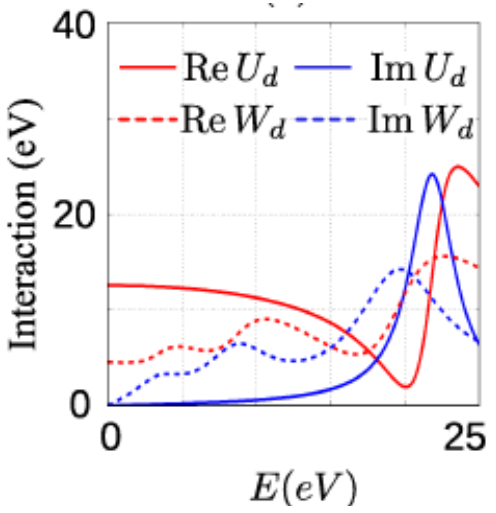


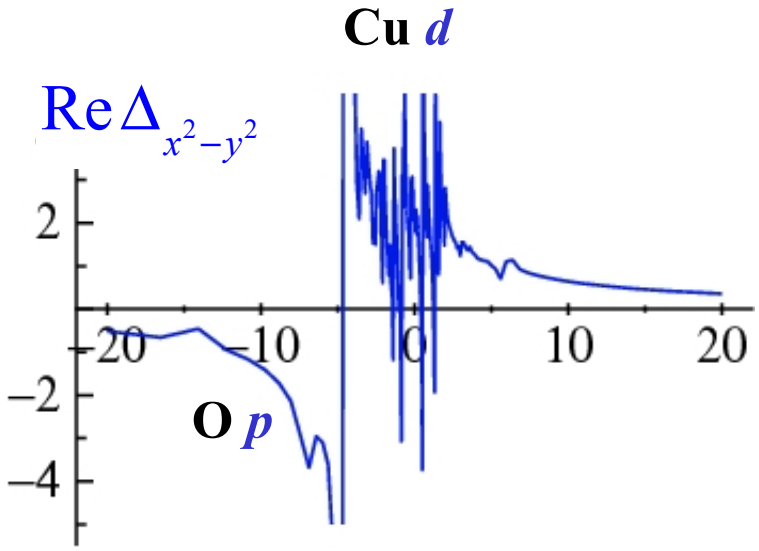
DMFT, χ calculation by Swagata Acharya. Gap ~2.6 eV.

Novel features of the "Haule" DMFT Philosophy

Use a wide energy window (20 eV) so :

- the orbitals are highly localized (>90% overlap with Cu atomic d orbital)
- The screening from the bath is greatly reduced so the effective interaction $U(\omega)$ becomes weakly ω-dependent. Replace with $U(\omega)$ with $U(0)$ for the DMFT solver (CTQMC)
- The hybridization function has an additional contribution (mostly O 2p) which substitutes for the missing screening of U





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A Q(P,S)GW+DMFT study of La_2CuO_4

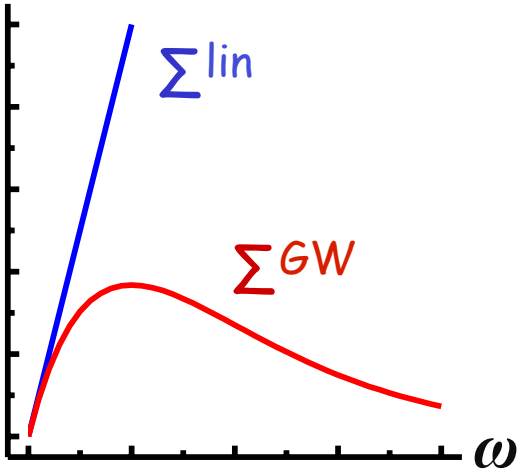
- QPGW+DMFT performed at Rutgers See NPJ Quantum Materials 1, 16001 (2016). Compare to QSGW+DMFT (KCL)
- QPGW is intermediate between COHSEX and QSGW

$\Sigma(\omega)$ is linearized: $\Sigma^{lin}(\omega) = \Sigma(0) + \omega\,\Sigma'(0)$

COHSEX Linear term

Quasiparticlize $\Sigma^{lin}(\omega) \rightarrow [\Sigma^{lin}(\omega_i) + \Sigma^{lin}(\omega_j)]/2$

Σ^{lin} increases without bound ⇒ QPGW should underestimate gaps , while COHSEX should overestimate them



	QSGW	scGW	QPGW
E_G	4.0	4.0	3.5
M	0.8	0.8	0.8

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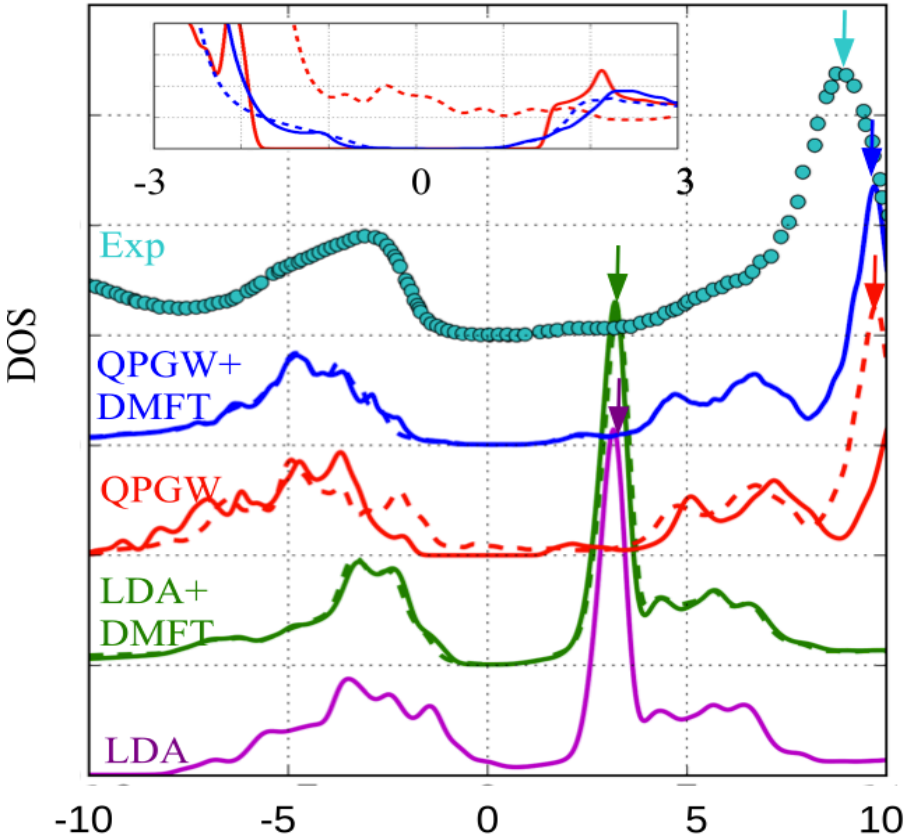
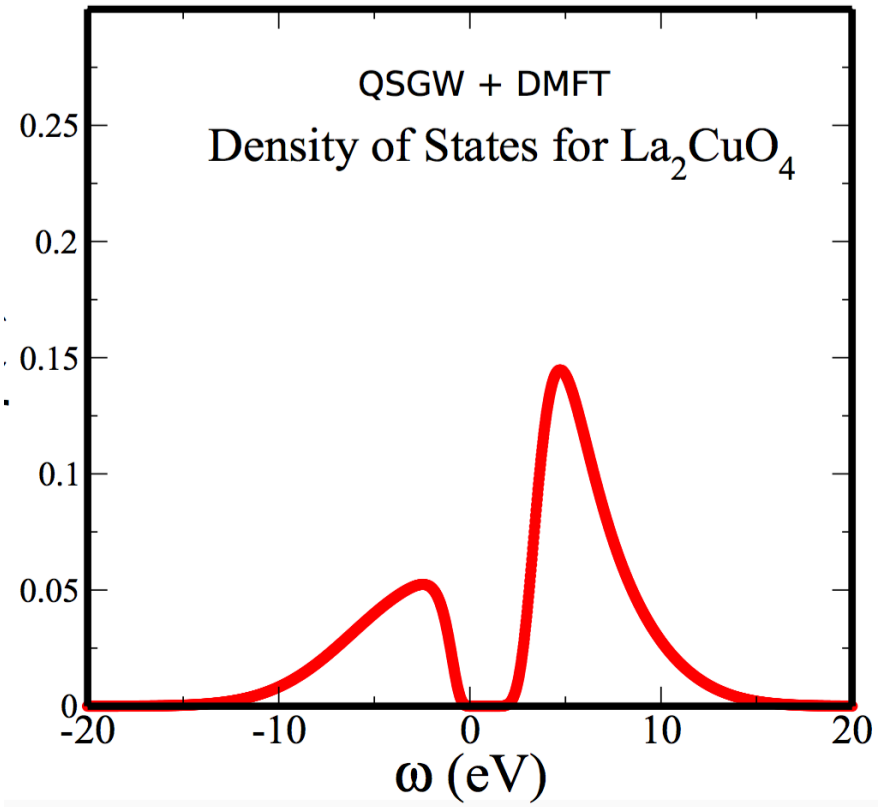
La_2CuO_4 within QPGW+DMFT

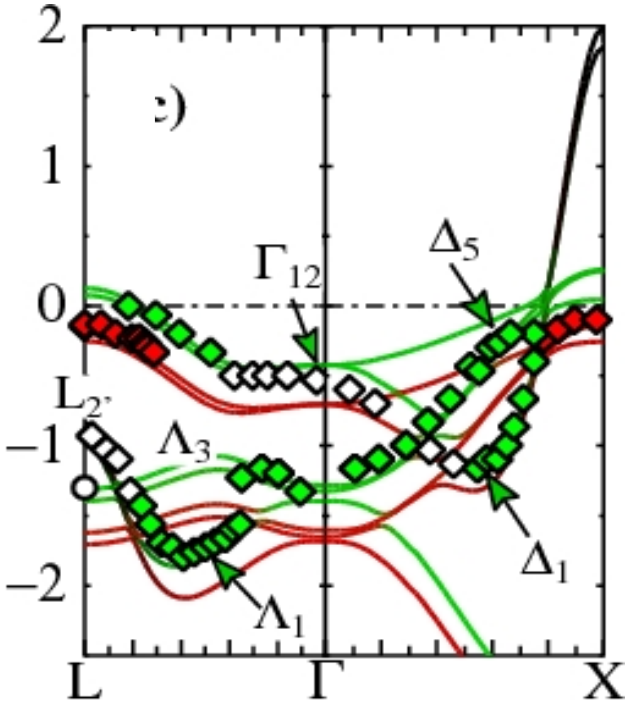




	QP*GW*(A)	QP*GW*(A) +DMFT	QP*GW*(N) +DMFT	QSGW(A)	QSGW +DMFT	Expt
E_G	3.5	1.6	1.5	4.0	2.6	~2
M	0.7	0.8	0.8	0.8	0.8	0.4-0.8

Conclusions

1. *GW* provides an *ab initio* framework for optimal G_0, through QS*GW*. QS*GW* dramatically improves the consistency and reliability of G_0 and is universally applicable.
2. QS*GW* alone sometimes sufficient. (ARPES in Fe, SW in NiO, MnO). But spin fluctuations are missing and they can be important (Ni, CoO, La_2CuO_4)
3. LDA+DMFT has been highly successful but LDA is has serious weaknesses. Results should be much better using QSGW (optimal G_0) for bath.
4. A new QSGW+"magnetic" DMFT approach was developed and applied to Ni.
5. QSGW+DMFT seems a bit different from QPGW+DMFT ($LaCu_2O_4$)



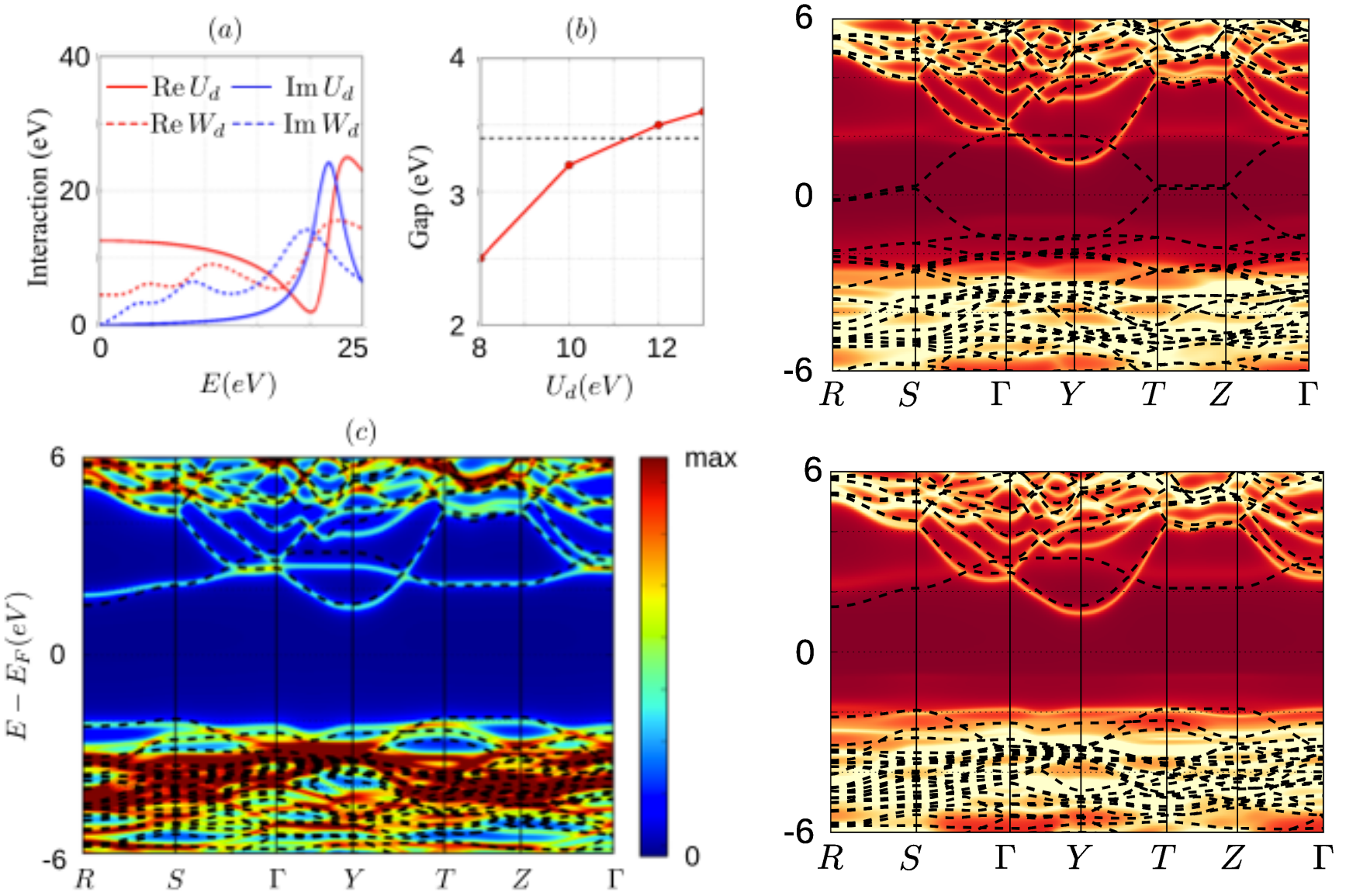
On the QSGW+DMFT Implementation

1. Local orbitals from *d* partial waves in augmentation sphere.
2. From quasiparticlized G_0 calculate U_{ijkl} within constrained RPA and extract static U and J. (For now just pick U and J)

--- The following steps are iterated to self-consistency ---

1. Make QSGW $\Sigma^{\mathrm{GW}}(k,\omega)$ and quasiparticlized $\Sigma^{\mathrm{QSGW}}(k)$.
2. Project G onto G^{loc} (initially G is the quasiparticlized G^0). Use G^{loc}, U, J as inputs to generate Σ^{DMFT} from DMFT.
5. From Σ^{DMFT} calculate Σ^{DC} (Here, use $\Sigma^{\mathrm{DC}}=U(n-1/2)-J(n-1)/2$)
6. Embed ($\Sigma^{\mathrm{DMFT}}-\Sigma^{\mathrm{DC}}$) into the quasiparticlized G_0 to construct a new G and generate a new density and Hartree potential.
7. Quasipoarticlize

QPGW+DMFT(RPA)



QPGW on an Imaginary Frequency axis

skip

$$\widetilde{G}_{QP}(i\omega_n) = (i\omega_n + \mu - \widetilde{H}_{QP})^{-1}$$

$$\widetilde{\chi}(i\omega_n) = 2\int d\tau \widetilde{G}_{QP}(\tau) \circ \widetilde{G}^t_{QP}(-\tau) e^{i\omega_n \tau}$$

$$\widetilde{H}_{QP} = \widetilde{Z}^{1/2}\left(\widetilde{H}_H + \widetilde{\Sigma}(i\omega_n = 0)\right)\widetilde{Z}^{1/2}$$

$$\widetilde{Z} = \left(1 - \frac{\widetilde{\Sigma}(i\omega_n = 0)}{\partial(i\omega_n)}\right)^{-1}$$

$$\widetilde{W}^{-1}(i\omega_n) = \widetilde{V}^{-1} - \widetilde{\chi}(i\omega_n)$$

$$\widetilde{\Sigma}(i\omega_n) = -\int d\tau \widetilde{G}_{QP}(\tau) \circ \widetilde{W}(\tau) e^{i\omega_n \tau}$$

$$\simeq \widetilde{\Sigma}(i\omega_n = 0) + i\omega_n \frac{\widetilde{\Sigma}(i\omega_n = 0)}{\partial(i\omega_n)}$$

[1] A. Kutepov, K. Haule, S. Y. Savrasov, and G. Kotliar, Phys. Rev. B 85, 155129 (2012).
[2] A. Kutepov, S. Y. Savrasov, and G. Kotliar, Phys. Rev. B 80, 041103 (2009).

Self-consistent DMFT from QPGW

$$\widetilde{G}_{QP}(\mathbf{k}, i\omega_n) = (i\omega_n + \mu - \widetilde{H}_{QP}(\mathbf{k}))^{-1}$$

$\widetilde{P}(\mathbf{k})$ Using MLWF, U and J from cRPA

$$G_{loc}(i\omega_n) = \frac{1}{N_k} \sum_{\mathbf{k}} \widetilde{P}(\mathbf{k}) \left\{ \widetilde{G}^{-1}_{QP}(\mathbf{k}, i\omega_n) - \widetilde{P}^{\dagger}(\mathbf{k}) \left(\widetilde{\Sigma}_{imp}(s, i\omega_n) - \widetilde{\Sigma}_{DC}(i\omega_n) \right) \widetilde{P}(\mathbf{k}) \right\}^{-1} \widetilde{P}^{\dagger}(\mathbf{k})$$

$\Sigma_{imp}(i\omega_n)$ From CTQMC impurity solver

[1] P. Werner, et.al., Phys. Rev. Lett. 97, 076405 (2006).
[2] K. Haule, Phys. Rev. B 75, 155113 (2007).