GW+EDMFT:
a diagrammatically controlled
ab initio theory of strong correlation
in real materials

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2. partial self-consistency within LQSGW+DMFT
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1. Introduction
One-particle picture (Fermi liquid theory)

- Adiabatic continuity (conservation law unchanged by the interaction)
- Quasiparticles at $|E - E_F| \ll E_F$
- Electron is independent for the requirement of the exclusion principles
- Working horses: DFT and GW

DFT for weakly correlated materials

- Total energy calculation by solving auxiliary non-interacting system

\[
\left\{ \frac{p^2}{2m} + V_{KS}(r) \right\} \psi_i(r) = \varepsilon_i \psi_i(r), \quad \rho(r) = \sum_{i}^{occ} |\psi_i(r)|^2
\]

- For the ground state properties of weakly correlated materials
- Kohn-Sham energy is not a quasiparticle energy.

GW for weakly correlated materials

- The first order expansion of self-energy in $W$
- For the excited state properties of weakly correlated materials

Correlated electron systems: unconventional behavior

- Van der Waals force, excitons, kondo effects, Heavy fermions....
Beyond one-particle picture

Itinerant electrons: bands

• Nondegenerate ground states
• Single Slater determinants

Localized electrons: multiplets

• Degenerate ground states
• Linear combination of many Slater determinants

Electrons in open d and f shell systems are neither localized nor itinerant

Beyond one-particle picture to retain multiplet structure
DMFT and electronic structure theory

- Map solid onto effective atom subject to local interaction and coupled to bath

\[
S = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_s c_s^\dagger(\tau) \Delta(\tau - \tau') c_s(\tau') + U \int_0^\tau n^\uparrow n^\downarrow
\]

\[
G_{\text{imp}} = \langle T c c^\dagger \rangle, \quad \Sigma_{\text{imp}} = \Delta - G_{\text{imp}}^{-1}
\]

- Embed impurity self energy to the lattice green's function and project into correlated subspaces

\[
G_{\text{loc}} = \frac{1}{N_k} \sum_k p_k^\dagger \left\{ G_k^{-1} - p_k (\Sigma_{\text{imp}} - \Sigma_{\text{DC}}) p_k^\dagger \right\}^{-1} p_k
\]

- DMFT Self-consistent equation

\[
G_{\text{loc}} = G_{\text{imp}}
\]

- \( U \) and \( \Sigma_{\text{DC}} \) should be determined by the choice of \( p_k \)

Many successful stories of LDA+DMFT including metal insulator transition in transition metal oxides

Many new features including total energy, forces, exact double-counting energy

Position of La-f, O-p

Non-local correlation is important for many fascinating phenomena including
• Pseudogap in cuprates
• Paramagnon near magnetic phase transition

Nonlocal self-energy: cluster extension

- Correlated orbitals on one site $\rightarrow$ correlated orbitals on several sites (cluster)
- Dynamical cluster approximation (in momentum space) and cellular DMFT (in real space)


Images from O. Parcollet’s slide
Nonlocal self-energy: diagrammatic extension

- GW+EDMFT, TRILEX, QUADRILEX, D\Gamma A, dual fermions, dual boson...
- local approximation to one physical quantity (such as vertex, three point vertex…) and non-local self-energy through Feynman diagrams
- finer momentum resolution is possible than cluster extension.

GW and EDMFT

GW+EDMFT: diagrammatically controlled *ab initio* theory

- a diagrammatical route to calculate on-site strong correlation and non-local correlation
- first-order non-trivial correction to DMFT or local correction to GW

2. GW+EDMFT

Hedin’s equation

\[ \Sigma(1,2) = - \int d(34) G(1,3^+) W(1,4) \Gamma(3,2,4), \] (1)

\[ G(1,2) = G_0(1,2) + \int d(34) G_0(1,3) \Sigma(3,4) G(4,2), \] (2)

\[ \Gamma(1,2,3) = \delta(1-2) \delta(2-3), \]
\[ + \int d(4567) \frac{\partial \Sigma(1,2)}{\partial G(4,5)} G(4,6) G(7,5) \Gamma(6,7,3), \] (3)

\[ \Pi(1,2) = \int d(34) G(1,3) \Gamma(3,4,2) G(4,1^+), \] (4)

\[ W(1,2) = v(1,2) + \int d(34) v(1,3) \Pi(3,4) W(4,2). \] (5)

- If \( \Gamma(1,2,3) \approx \delta(1-2) \delta(2-3) \)

\[ \Sigma^{GW} = -G(1,2) W(1,2) \quad \Pi(1,2) = G(1,2) G(2,1^+) \]

\( \Sigma(k, i\omega_n) = -\int_0^\beta d\tau \sum_R G(R, \tau) \cdot W(R, \tau) e^{i(k \cdot R - \omega_n \tau)} \)

\( P(k, i\omega_n) = \int_0^\beta d\tau \sum_R G(R, \tau) \cdot G(-R, -\tau) e^{i(k \cdot R - \omega_n \tau)} \)

\( G^{-1}(k, i\omega_n) = G_0^{-1}(k, i\omega_n) - \Sigma(k, i\omega_n) \)

\( W^{-1}(k, i\omega_n) = V^{-1}(k) - P(k, i\omega_n) \)

\( G \): fermionic Weiss field
\( U \): bosonic Weiss field
\( G_{imp} \): impurity Green’s function
\( P_{imp} \): impurity polarizability
\( \chi_{imp} \): impurity susceptibility
\( \Sigma_{DC} \): double-counted self-energy
\( P_{DC} \): double-counted polarizability
Extended Dynamical Mean Field Theory for U-V Hamiltonian

• DMFT formalism for models with spatially non-local interactions
• Model Hamiltonian example: U-V Hubbard model

\[ H = -t \sum_{\langle ij \rangle} (c_{i \sigma}^\dagger c_{j \sigma} + \text{H.c.)} - \mu \sum_i n_i + U \sum_i n_{i \uparrow} n_{i \downarrow} + V \sum_{\langle ij \rangle} n_i n_j, \]

• Actions formulation

\[ S[c^*, c] = \int_0^\beta d\tau \left\{ \sum_{ij \sigma} c_{i \sigma}^\dagger(\tau) \left[ \left( \partial_\tau - \mu \right) \delta_{ij} + t_{ij} \right] c_{j \sigma}(\tau) \right. \]
\[ + U \sum_i n_{i \uparrow}(\tau) n_{i \downarrow}(\tau) + \frac{1}{2} \sum_{ij} v_{ij}^{nl} n_i(\tau) n_j(\tau) \left\} \right. \]

• Rewriting the action using the identity \[ n_i n_i = 2n_{i \uparrow} n_{i \downarrow} + n_i \]

\[ S[c^*, c] = \int_0^\beta d\tau \left\{ \sum_{ij \sigma} c_{i \sigma}^\dagger(\tau) \left[ \left( \partial_\tau - \tilde{\mu} \right) \delta_{ij} + t_{ij} \right] c_{j \sigma}(\tau) + \frac{1}{2} \sum_{ij} v_{ij} n_i(\tau) n_j(\tau) \right\} \]

where \[ v_{ij} = U \delta_{ij} + V \delta_{\langle ij \rangle} \] and \[ \tilde{\mu} = \mu + U/2 \]

Extended Dynamical Mean Field Theory

• To map this problem onto single-site impurity model, we need to decouple spatially non-local interactions by using a Hubbard-stratonovich transformation for a real and $\beta$-periodic field.

\[
\exp \left( \frac{1}{2} \int_0^\beta d\tau \, b_i(\tau) A_{ij} b_j(\tau) \right) = \int \mathcal{D}[x_1(\tau), x_2(\tau), \ldots] \frac{1}{\sqrt{(2\pi)^N \det A}} \exp \left( \int_0^\beta d\tau \left\{ \frac{1}{2} x_i(\tau) [A^{-1}]_{ij} x_j(\tau) \mp x_i(\tau) b_i(\tau) \right\} \right)
\]

• Then the action becomes

\[
S[c^*, c, \phi] = \int_0^\beta d\tau \left\{ -\sum_{i,j,\sigma} c_{i\sigma}^*(\tau) \left[ (G_0^H)^{-1} \right]_{ij} c_{j\sigma}(\tau) \right\} + \int_0^\beta d\tau \left\{ \frac{1}{2} \sum_{i,j} \phi_i(\tau) [v^{-1}]_{ij} \phi_j(\tau) + i\alpha \sum_i \phi_i(\tau) n_i(\tau) \right\},
\]

where $[G_0^H]_{ij} = \left[ (-\partial_\tau + \mu + \frac{U}{2}) \delta_{ij} - t_{ij} \right]$.

Bare fermionic and bosonic fields coupled by a local coupling

The physically relevant case corresponds to $\alpha = 1$
Extended Dynamical Mean Field Theory

• By integrating out all sites but one in the action in the infinite dimension limit

\[
S^{\text{EDMFT}} = -\int_0^\beta d\tau d\tau' \sum_\sigma c^*_\sigma(\tau) G^{-1}(\tau - \tau') c_\sigma(\tau') \\
+ \frac{1}{2} \int_0^\beta d\tau d\tau' \phi(\tau) U^{-1}(\tau - \tau') \phi(\tau') \\
+ i \int_0^\beta d\tau \phi(\tau) n(\tau),
\]

Where \( G^{-1} = G^{-1}_\text{imp} + \Sigma_\text{imp} \) and \( U^{-1} = W^{-1}_\text{imp} + P_\text{imp} \)

• by integrating out the \( \phi \) field

\[
S^{\text{EDMFT}} = -\int_0^\beta d\tau d\tau' \sum_\sigma c^*_\sigma(\tau) G^{-1}(\tau - \tau') c_\sigma(\tau') \\
+ \frac{1}{2} \int_0^\beta d\tau d\tau' n(\tau) U(\tau - \tau') n(\tau') - \frac{1}{2} \text{Tr ln} U,
\]

• Green’s function to be computed within EDMFT

\[
G_\text{imp} = -\langle T c(\tau) c^*(0) \rangle \\
W_\text{imp} = \langle T \phi(\tau) \phi(0) \rangle
\]
Extended Dynamical Mean Field Theory

• How to compute $W_{\text{imp}}$

$$W_{\text{imp}} = 2 \frac{\delta \ln Z}{\delta \gamma^{-1}} = 2 \frac{\delta \ln Z}{\delta \gamma} \frac{\delta \gamma}{\delta \gamma^{-1}} = -2 \gamma \frac{\delta \ln Z}{\delta \gamma} \gamma = -\gamma \langle T n(\tau) n(0) \rangle \gamma + \gamma$$

$$W_{\text{imp}} = \gamma - \gamma \chi_{\text{imp}} \gamma$$
EDMFT loop

\[ G^{-1}(\mathbf{k}, i\omega_n) = G_0^{-1}(\mathbf{k}, i\omega_n) - \Sigma_{imp}(i\omega_n) \]
\[ W^{-1}(\mathbf{k}, i\omega_n) = V^{-1}(\mathbf{k}) - P_{imp}(i\omega_n) \]

\[ \Sigma_{imp} = G^{-1} - G_{imp}^{-1} \]
\[ W_{imp} = \mathcal{U} - \mathcal{U} \chi_{imp} \mathcal{U} \]
\[ P_{imp} = \mathcal{U}^{-1} - W_{imp}^{-1} \]

\[ G_{loc}(i\omega_n) = \frac{1}{N_k} \sum_{\mathbf{k}} G(\mathbf{k}, i\omega_n) \]
\[ W_{loc}(i\omega_n) = \frac{1}{N_k} \sum_{\mathbf{k}} W(\mathbf{k}, i\omega_n) \]

\[ G^{-1} = G_{loc}^{-1} + \Sigma_{imp} \]
\[ \mathcal{U}^{-1} = W_{loc}^{-1} + P_{imp} \]

\( G \): fermionic Weiss field
\( U \): bosonic Weiss field
\( G_{imp} \): impurity Green’s function
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\( \chi_{imp} \): impurity susceptibility
\( \Sigma_{DC} \): double-counted self-energy
\( P_{DC} \): double-counted polarizability

G: Green’s function
\( \Sigma \): electron self-energy
P: polarizability
W: screened Coulomb interaction
GW+EDMFT as a electronic structure theory

- Within EDMFT, fermionic as well as bosonic self energy are local.
- A way to restore the non-local self energy by adding the first non-trivial non-local diagrammatic correction

\[
\Sigma(k, i\omega_n) = \Sigma_{GW}(k, i\omega_n) + f_k \left( \tilde{\Sigma}_{imp}(i\omega_n) - \tilde{\Sigma}_{DC}(i\omega_n) \right) f_k^\dagger
\]

\[
P(k, i\nu_n) = P_{GW}(k, i\nu_n) + b_k \left( \tilde{P}_{imp}(i\nu_n) - \tilde{P}_{DC}(i\nu_n) \right) b_k^\dagger
\]

A new Notation from now on

\( A \rightarrow \langle r|A|r' \rangle \)

\( f = \langle r|c_f \rangle \rightarrow \) a orthonormal basis set for correlated orbitals

\( b = \langle r|c_b \rangle \rightarrow \) a orthonormal product basis set composed of correlated orbitals

\( \tilde{A} \rightarrow \langle c_f|A|c_f' \rangle \) for a fermionic quantity and \( \langle c_b|A|c_b' \rangle \) for a bosonic quantity

\[ \Sigma(k, i\omega_n) = \Sigma_{GW}(k, i\omega_n) + f_k \left( \tilde{\Sigma}_{imp}(i\omega_n) - \tilde{\Sigma}_{DC}(i\omega_n) \right) f_k^\dagger \]
\[ P(k, i\nu_n) = P_{GW}(k, i\nu_n) + b_k \left( \tilde{P}_{imp}(i\nu_n) - \tilde{P}_{DC}(i\nu_n) \right) b_k^\dagger \]

\[ \tilde{\Sigma}_{imp} = \tilde{\Sigma}^{-1} - \tilde{\Sigma}_{imp}^{-1} \]
\[ \tilde{W}_{imp} = \tilde{U} - \tilde{U}\tilde{\chi}_{imp}\tilde{U} \]
\[ \tilde{P}_{imp} = \tilde{U}^{-1} - \tilde{W}_{imp}^{-1} \]

\[ G^{-1}(k, i\omega_n) = G_0^{-1}(k, i\omega_n) - \Sigma(k, i\omega_n) \]
\[ W^{-1}(k, i\omega_n) = V^{-1}(k) - P(k, i\omega_n) \]

\[ \tilde{G}_{loc}(i\omega_n) = \frac{1}{N_k} \sum_k f_k^\dagger G(k, i\omega_n) f_k \]
\[ \tilde{W}_{loc}(i\omega_n) = \frac{1}{N_k} \sum_k b_k^\dagger W(k, i\omega_n) b_k \]

**G**: fermionic Weiss field  
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**G_{imp}**: impurity Green’s function  
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**\chi_{imp}**: impurity susceptibility  
**\Sigma_{DC}**: double-counted self-energy  
**P_{DC}**: double-counted polarizability
Functional formulation

• The action after Hubbard-Stranotovich transformation

\[
S[c^*, c, \phi] = \int_0^\beta d\tau \left\{ -\sum_{i,j,\sigma} c^*_i(\tau) \left[ (G_0^H)^{-1} \right]_{ij} c_j(\tau) \right\} + \int_0^\beta d\tau \times \left\{ \frac{1}{2} \sum_{ij} \phi_i(\tau) [v^{-1}]_{ij} \phi_j(\tau) + i\alpha \sum_i \phi_i(\tau) n_i(\tau) \right\},
\]

• Generating function

\[
\Omega \equiv -\ln Z[J_f, J_b] = -\ln \text{Tr} e^{-S[c^*, c, \phi] + S[J_f, J_b]}
\]

where

\[
S[J_f, J_b] = \int_0^\beta d\tau \, d\tau' \sum_{ij} \left\{ J_{f,ij}(\tau, \tau') c_i^*(\tau) c_j(\tau') + \frac{1}{2} J_{b,ij}(\tau, \tau') \phi_i(\tau) \phi_j(\tau') \right\}.
\]

• Baym-Kadanoff functional by a Legendre transformation

\[
\Gamma[G, W] = \Omega[J_f[G], J_b[W]] - \text{Tr} J_f G + \frac{1}{2} \text{Tr} J_b W.
\]

With the reciprocity relation \( J_f = -\frac{\delta \Gamma}{\delta G} \) and \( J_b = 2 \frac{\delta \Gamma}{\delta W} \).
Functional formulation

• Another way to write Baym-Kadanoff functional

\[ \Gamma_{\alpha=1} = \Gamma_{\alpha=0} + \Psi, \]

where

\[ \Gamma_{\alpha=0} = \text{Tr} \ln(-G) - \text{Tr}(G_0^{-1} - G^{-1})G - \frac{1}{2} \text{Tr} \ln W + \frac{1}{2} \text{Tr}(v^{-1} - W^{-1})W \]

and

\[ \Psi \equiv \int_0^1 d\alpha \frac{d\Gamma}{d\alpha} \]

• Stationanarity

\[ \frac{\delta \Gamma}{\delta G} = 0 = \frac{\delta \Gamma_{\alpha=0}}{\delta G} + \frac{\delta \Psi}{\delta G} = G^{-1} - G_0^{-1} + \frac{\delta \Psi}{\delta G} \]

\[ \frac{\delta \Gamma}{\delta W} = 0 = -\frac{1}{2}(W^{-1} - v^{-1}) + \frac{\delta \Psi}{\delta W} \]

• By defining

\[ \Sigma = \frac{\delta \Psi}{\delta G}, \quad \Pi = -2 \frac{\delta \Psi}{\delta W} \]

We get Dyson's equation

\[ G^{-1} = G_0^{-1} - \Sigma, \quad W^{-1} = v^{-1} - \Pi. \]
Functional formulation

- Being “\( \Psi \) derivable,” these self-energies will obey global conservation rules

\[
\Psi^{GW+EDMFT}(G, W) = \text{Tr} G W G + \Psi(G^{\text{loc}}, W^{\text{loc}}) - \text{Tr} G^{\text{loc}} W^{\text{loc}} G^{\text{loc}},
\]

\[\text{GW part}\]

\[\text{double counting}\]

\[\text{impurity diagrams}\]

3. partial self-consistency within LQSGW+DMFT
\[ \Sigma(k, i\omega_n) = \Sigma_{GW}(k, i\omega_n) + f_k \left( \tilde{\Sigma}_{imp}(i\omega_n) - \tilde{\Sigma}_{DC}(i\omega_n) \right) f_k^\dagger \]
\[ P(k, i\nu_n) = P_{GW}(k, i\nu_n) + b_k \left( \tilde{P}_{imp}(i\nu_n) - \tilde{P}_{DC}(i\nu_n) \right) b_k^\dagger \]

\[ \tilde{\Sigma}_{imp} = \tilde{G}^{-1} - \tilde{G}_{imp}^{-1} \]
\[ \tilde{W}_{imp} = \tilde{U} - \tilde{U}\chi_{imp}\tilde{U} \]
\[ \tilde{P}_{imp} = \tilde{U}^{-1} - \tilde{W}_{imp}^{-1} \]

\[ \tilde{G}^{-1}(k, i\omega_n) = G_0^{-1}(k, i\omega_n) - \Sigma(k, i\omega_n) \]
\[ W^{-1}(k, i\omega_n) = V^{-1}(k) - P(k, i\omega_n) \]

\[ \tilde{G}_{loc}(i\omega_n) = \frac{1}{N_k} \sum_k f_k^\dagger G(k, i\omega_n) f_k \]
\[ \tilde{W}_{loc}(i\omega_n) = \frac{1}{N_k} \sum_k b_k^\dagger W(k, i\omega_n) b_k \]

\[ G: \text{ fermionic Weiss field} \]
\[ U: \text{ bosonic Weiss field} \]
\[ G_{imp}: \text{ impurity Green’s function} \]
\[ P_{imp}: \text{ impurity polarizability} \]
\[ \chi_{imp}: \text{ impurity susceptiblity} \]
\[ \Sigma_{DC}: \text{ double-counted self-energy} \]
\[ P_{DC}: \text{ double-counted polarizability} \]
Various simplified approaches to GW+EDMFT

- fixing Bosonic quantities at the GW level
- U from constrained random phase approximation (cRPA) [1] and its extension [2]
- One-shot DMFT approach: G\_\{MF\} is fixed
- For the construction of G\_\{MF\}: one-shot GW [6,7], Screened Exchange [3], QSGW [4] and LQSGW [2], non-local QSGW and LQSGW [5]

*) Multitier-GW+EDMFT [8] approach has been proposed: full GW+EDMFT approach in the low-energy regions

\[
G^{-1}(\mathbf{k}, i\omega_n) = G_{MF}^{-1}(\mathbf{k}, i\omega_n) - f_k \tilde{\Sigma}_{imp}(i\omega_n) f_k^\dagger
\]

\[
G^{-1}(\mathbf{k}, i\omega_n) = \frac{1}{N_k} \sum_{\mathbf{k}} f_{\mathbf{k}} G(\mathbf{k}, i\omega_n) f_{\mathbf{k}}
\]

\[
W_{loc}(i\omega_n) = \frac{1}{N_k} \sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger W(\mathbf{k}, i\omega_n) b_{\mathbf{k}}
\]

LQSGW+DMFT validation on La2CuO4

- LDA+DMFT and LQSGW+DMFT opens a paramagnetic Mott gap
- LQSGW predict a metal in non-magnetic calculation and an insulator in spin-polarized calculation. But its gap is too big (3.4 eV vs ~2 eV)
- LDA predict a metallic phase
- better O-p and La-f position within LQSGW+DMFT

LQSGW+DMFT validation on NiO

• a proper choice of static U gives similar spectral function to Exp and full LQSGW+DMFT
• $U$ and $\Sigma_{DC}$ are self-consistently determined
• Identical Mott gap regardless of the choice of orbitals
• The position of Lower Hubbard band is sensitive to the choice
Linearized Quasiparticle Self-consistent GW (LQSGW)

- Why LQSGW, not one-shot GW or Full GW?

**Electron gas**

- $G_0W_0$: band narrowing (consistent with exp)
- GW: band widening. Worse than $G_0W_0$

**Starting point dependent (PBE vs PBE0)**

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Projector \( \left( f_k \right) \) construction by using Wannier functions

- From tight-binding model

\[
|n_k\rangle = \frac{1}{\sqrt{N_k}} \sum_{\mathbf{R}, \tau} U_{n\tau}(\mathbf{k}) e^{i\mathbf{k} \cdot \mathbf{R}} |\tau \mathbf{R}\rangle
\]

\[
|\tau \mathbf{R}\rangle = \frac{1}{\sqrt{N_k}} \sum_{\mathbf{k}, n} U_{n\tau}^*(\mathbf{k}) e^{-i\mathbf{k} \cdot \mathbf{R}} |n_k\rangle
\]

- One way to construct orthonormal basis set of \(|\tau \mathbf{R}\rangle\) from \(|n_k\rangle\), or to determine \(U_{n\tau}(\mathbf{k})\) → by minimizing total spread

\[
\Omega = \sum_{\tau \mathbf{R}} \langle \mathbf{r}^2 - \langle \mathbf{r} \rangle_{\tau \mathbf{R}}^2 \rangle_{\tau \mathbf{R}} \quad \text{where} \quad \langle A \rangle_{\tau \mathbf{R}} = \langle \mathbf{R}_\tau | A | \mathbf{R}_\tau \rangle
\]

→ Under the constraint that it preserves band eigenvalues \(E_{n\mathbf{k}}\) in the inner (frozen) window

- Our default choice of inner (frozen) window: \(E_F \pm 10\text{eV}\)

- then a projector to correlated orbitals

\[
f_k = \langle \mathbf{r} | \tau \mathbf{k} \rangle = \sum_n U_{n\tau}^*(\mathbf{k}) \langle \mathbf{r} | n_k \rangle
\]
Product basis \((b_k)\) construction by using Wannier functions

- With products of Wannier functions for correlated orbitals

\[
B_{\tau,\tau'}(\mathbf{r}) = W_{\mathbf{R}=0\tau}(\mathbf{r})W_{\mathbf{R}=0\tau'}^*(\mathbf{r})
\]

- Orthonormalized product basis can be represented as a linear combination of the product \(C\)

\[
\langle \mathbf{r}|c_b \rangle = \sum_{\tau,\tau'} X_{\tau,\tau';b} B_{\tau,\tau'}(\mathbf{r})
\]

- The coefficient \(X\) can be calculated by diagonalizing the overlap matrix of \(C\)

\[
O_{\tau_1,\tau_2;\tau_3,\tau_4} = \langle B_{\tau_1,\tau_2}|B_{\tau_3,\tau_4} \rangle
\]

\[
\sum_{\tau_3,\tau_4} O_{\tau_1,\tau_2;\tau_3,\tau_4} D_{\tau_3,\tau_4;b} = F_b D_{\tau_1,\tau_2;b}
\]

\[
X_{\tau_1,\tau_2;b} = \frac{1}{\sqrt{F_b}} D_{\tau_1,\tau_2;b}
\]
Wannier-interpolation of LQSGW bandstructure ($H_{QP}$)

- The more localized orthonormal basis set → the sparser H matrix in the R space
- With localized basis set, hopping energy are essentially 0 beyond a few neighbours.
- If the supercell defined by k-grid is larger than the hopping range, we can interpolate the bands at a arbitrary k point

\[
H_{\tau,\tau'}(k) = \sum_{n,m} \langle \tau k | n k \rangle H_{n,m}(k) \langle m k | \tau' k \rangle
\]

\[
H_{\tau,\tau'}(R) = \frac{1}{N_k} \sum_{k} H_{\tau,\tau'}(k) e^{-ik \cdot R}
\]

\[
H_{\tau,\tau'}(k') = \sum_{R} H_{\tau,\tau'}(R) e^{ik' \cdot R}
\]
Coulomb interaction matrix from cRPA

Suppose that the band-structure of a given solid can be separated into a narrow band near the Fermi level and the rest.

Divide the complete Hilbert space into the subspace for the correlated orbitals and the rest.

Aim: calculate the effective interaction between the correlated orbitals.

This interaction has to be bare with respect to the correlated orbitals but renormalized with respect to the rest.

How to define $P_{QP}^{\text{low}}$

- How to pick bands in the correlated subspace:
  - We pick the same number of bands as the number of correlated orbitals
  - The orbital character of the selected bands are mostly from the correlated orbitals

\[
P_{QP} = P_{QP}^{\text{low}} + P_{QP}^{\text{high}}
\]

\[
P_{QP}^{\text{low}}(\mathbf{r}, \mathbf{r}', \mathbf{k}, i\omega_n) = -N_s \sum_{\mathbf{k}'} \sum_{\text{unocc in the space}} \sum_{\text{occ in the space}} \sum_n \sum_m \\
\psi_{n\mathbf{k}'}(\mathbf{r})\psi^{*}_{m\mathbf{k}'+\mathbf{k}}(\mathbf{r})\psi^{*}_{n\mathbf{k}'}(\mathbf{r}')\psi_{m\mathbf{k}'+\mathbf{k}}(\mathbf{r}') \frac{2(E_{n\mathbf{k}'} - E_{n\mathbf{k}'+\mathbf{k}})}{\omega_n^2 - (E_{n\mathbf{k}'} - E_{n\mathbf{k}'+\mathbf{k}})^2},
\]

\[
W^{-1}_r(\mathbf{k}, i\omega_n) = W^{-1}(\mathbf{k}, i\omega_n) + P_{QP}^{\text{low}}(\mathbf{k}, i\omega_n)
\]

\[
\mathcal{U}(i\omega_n) = W_r(\mathbf{R} = 0, i\omega_n)
\]
Double counting energy

\[ \tilde{\Sigma}_{i,j}^{DC}(i\omega_n) = -\sum_{k,l} 2\tilde{G}_{k,l}(\tau = -\delta)\tilde{U}_{i,j,k,l}(i\nu_n = 0) \]

\[ -\sum_{k,l} \int d\tau \tilde{G}_{k,l}(\tau)\tilde{W}_{loc,i,k,l,j}(\tau) e^{i\omega_n \tau}, \]

\[ \tilde{W}_{i,j,k,l}(i\nu_n) = \tilde{U}_{i,j,k,l}(i\nu_n) + \sum_{m,n,p,q} \tilde{U}_{i,j,m,n}(i\nu_n)\tilde{P}_{m,n,p,q}(i\omega_n)\tilde{W}_{p,q,k,l}(i\omega_n) \]

\[ \tilde{P}_{i,j,k,l}(i\omega_n) = 2 \int d\tau \tilde{G}_{i,l}(\tau)\tilde{G}_{j,k}(-\tau) e^{i\omega \tau} \]
For the GW/LDA part of the GW+DMFT/LDA+DMFT scheme, the code FlapwMBPT was used.

\[ W_r^{-1}(\mathbf{k}, i\omega_n) = W^{-1}(\mathbf{k}, i\omega_n) + P_{QP}^{low}(\mathbf{k}, i\omega_n) \]

\[ \tilde{U}(i\omega_n) = \tilde{W}_r(\mathbf{R} = 0, i\omega_n) \]

\[ \tilde{\Sigma}_{i,j}^{DC}(i\omega_n) = -\sum_{k,l} 2\tilde{G}_{k,l}(\tau = -\delta)\tilde{U}_{i,j,k,l}(i\nu_n = 0) - \sum_{k,l} \int d\tau \tilde{G}_{k,l}(\tau)\tilde{W}_{loc,i,k,l,j}(\tau)e^{i\omega_n\tau} \]
LQSGW+DMFT loop

\[ G^{-1}(k, i\omega_n) = i\omega_n - H_{QP}^{nl}(k) - f_k \tilde{\Sigma}_{imp}(i\omega_n)f_k^\dagger \]
\[ H_{QP}^{nl}(k) = \sqrt{Z_{DC}^{-1}(k)H_{QP}\sqrt{Z_{DC}^{-1}(k) - f_k \tilde{\Sigma}_{DC}(\omega = 0)f_k^\dagger}} \]
\[ Z_{DC}^{-1}(k) = f_k \left(1 - \frac{\partial \Sigma_{DC}(k, \omega = 0)}{i\omega_n}\right)f_k^\dagger \]

\[ \tilde{G}_{loc}(i\omega_n) = \frac{1}{N_k} \sum_k f_k^\dagger G(k, i\omega_n)f_k \]

\[ \tilde{G}^{-1} = \tilde{G}_{loc}^{-1} + \tilde{\Sigma}_{imp} \]

- fixing Bosonic quantities at the GW level
- \( U \) from constrained random phase approximation (cRPA)
- One-shot DMFT approach: \( G_{\{MF\}} \) is fixed
- For the construction of \( G_{\{MF\}} \): non-local LQSGW

Rationale of ComDMFT development (as a part of ComSuite)

For itinerant electron

- DFT
- GW

For correlated electrons

- DMFT
- DFT+DMFT
- GW+EDMFT
- RISB
- DFT+RISB
- GW+RISB

- For **the validation and the theoretical advancement** of each methodology
  → We need **an open-source package**.
- For the **comparison** between different methodologies
  → We need a **package enabling multiple methods**
- For the exascale computing
  → Support for GPU and/or Intel KNL
Rationale of ComDMFT development  
(as a part of Comsuite)

• **Open source package** under GPL  
  (the CPC paper on ComDMFT under review and in arxiv)

• **Multiple methodologies**  
  - ab initio LQSGW+DMFT (a simplified version of GW+EDMFT)  
  - charge self-consistent LDA+DMFT  
  - charge self-consistent LDA+RISB (AKA ComRISB in collaboration with Yongxin)

• **The only open-source package supporting ab initio GW+DMFT,**  
  - ab initio LQSGW+DMFT: **a parameter free method**

• **The only open-source package supporting multiple methodology based on first principles+DMFT**

• **GPU-portied impurity solver** by Kwangmin and Patrick,  
  - Asynchronous CPU-GPU algorithm  
  - 5X speed-up @TITAN, OLCF, **12.5X speed-up @SUMMIT, OLCF**

Physical observables
- single particle Green’s function
- local quantities to correlated orbitals
  Impurity self-energy
  Hybridization function
  Double-counting self-energy (for LQSGW+DMFT)
  Bosonic Weiss field within cRPA (for LQSGW+DMFT)

Paramagnetic phase

For the LQSGW/LDA part of the LQSGW+DMFT/LDA+DMFT scheme, the code FlapwMBPT was used.

Charge self-consistent LDA+DMFT

\[ \tilde{\Sigma}_{\text{imp}} = \tilde{G}^{-1} - \tilde{G}_{\text{imp}}^{-1} \]

\[ G^{-1}(\mathbf{k}, i\omega_n) = G_{\text{MF}}^{-1}(\mathbf{k}, i\omega_n) - f_{\mathbf{k}} \tilde{\Sigma}_{\text{imp}}(i\omega_n) f_{\mathbf{k}}^{\dagger} \]

\[ \tilde{G}^{-1} = \tilde{G}_{\text{loc}}^{-1} + \tilde{\Sigma}_{\text{imp}} \]

\[ \tilde{G}_{\text{loc}}(i\omega_n) = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{k}} f_{\mathbf{k}}^{\dagger} G(\mathbf{k}, i\omega_n) f_{\mathbf{k}} \]

- \( G_{\text{MF}} \) is from double-counting energy compensated LDA Hamiltonian
- Interaction tensor and double-counting energy are supposed to be provided by a user
- New Kohn-Sham potential is constructed from updated \( G \) at every iteration
Ab initio LQSGW+DMFT

\[ \tilde{\Sigma}_{\text{imp}} = \tilde{G}^{-1} - \tilde{G}_{\text{imp}}^{-1} \]

\[ G^{-1}(\mathbf{k}, i\omega_n) = G_{\text{MF}}^{-1}(\mathbf{k}, i\omega_n) - f_\mathbf{k} \tilde{\Sigma}_{\text{imp}}(i\omega_n) f_\mathbf{k}^\dagger \]

\[ \tilde{G}^{-1} = \tilde{G}_{\text{loc}}^{-1} + \tilde{\Sigma}_{\text{imp}} \]

\[ \tilde{G}_{\text{loc}}(i\omega_n) = \frac{1}{N_k} \sum_\mathbf{k} f_\mathbf{k}^\dagger G(\mathbf{k}, i\omega_n) f_\mathbf{k} \]

- \( G_{\text{MF}} \) is from double-counting energy compensated LQSGW Hamiltonian
- Interaction tensor and double-counting energy are calculated (within cRPA and local-GW)
- One-shot DMFT correction to ab initio LQSGW
- a parameter-free method
Code Release and Documentation

• The first release on Sep. 15 at https://www.bnl.gov/comscope/software/comsuite.php

• Online documentation
  - installation instruction
  - online hands-on tutorials to run charge self-consistent LDA+DMFT and ab initio LQSGW+DMFT on MnO
Special Thanks to Chia-Nan Yeh and Jaime Magiera for installing Comsuite in Pauli
Assistant: Siheon Ryee
3. LQSGW+DMFT code tutorial with NiO
Goal

0. Code installation
1. DMFT self-consistent solution (starting from a prerun)
2. DOS and PDOS calculation
3. Spectral function calculation

In this tutorial, commands you should run are marked by red colors
LQSGW+DMFT in COMSUITE

\[
FlapwMBPT
H_{QP} \psi_{nk} = E_{nk} \psi_{nk}
\]

\[
E_{nk}, \psi_{nk}(r)
\]

ComWann
\[
|\tau k\rangle = \sum_n U_{n\tau}^*(k) |n k\rangle
\]

\[
U_{n\tau}(k)
\]

ComDC
\[
\Sigma_{DC} = \tilde{U} \tilde{N} - \tilde{G}_{loc} \tilde{W}_{loc}
\]

\[
\tilde{G}_{loc}
\]

ComLowH
\[
\tilde{g}^{-1} = \tilde{G}_{loc}^{-1} + \tilde{\Sigma}_{imp}
\]

\[
\tilde{\Sigma}_{imp}
\]

ComCoulomb
\[
W_{r}^{-1} = W^{-1} + P_{QP}^{\text{low}}
\]

\[
U
\]

\[
\tilde{g}
\]

CTQMC
\[
\tilde{\Sigma}_{imp} = \tilde{g}^{-1} - \tilde{G}_{imp}^{-1}
\]
Let’s load necessary modules

• Make sure that you logged in to the cluster with “ssh -X” (for the visualization)
  To illustrate:
  ssh -X um180269@pauli.physics.lsa.umich.edu
  For mac
  ssh -Y um180269@pauli.physics.lsa.umich.edu

• Let’s load modules: add these lines in ~/.bashrc
  module purge
  module load Intel python/anaconda-1.4.0 openmpi/openmpi-intel-3.1.3=> for intel compiler, lapack, python, and mpi

  If any other module is loaded in the .bashrc, please delete the line to load the module,

• let’s use the module
  $ source ~/.bashrc
check which module is loaded

$ module list

Currently Loaded Modules:
1) Intel/2018.5.274
2) python/anaconda-1.4.0
3) openmpi/openmpi-intel-3.1.3

If there is any module loaded, please unload it to avoid conflicts.

$ module unload ??? (if necessary)

check which module is loaded

$ module list

Currently Loaded Modules:
1) Intel/2018.5.274
2) python/anaconda-1.4.0
3) openmpi/openmpi-intel-3.1.3
Installation

• get the package
  $ cd ~
  $ cp -r /data/workshop2019/users/um180269/comsuite .

• move into comsuite directory
  $ cd comsuite

• modified arch.mk

```bash
### fortran
F90 = ifort
PF90 = mpi90
compfl = -O3

### phdf5
# USE_HDF5 = defined ### Comment out this line if you don't want to compile with hdf5 (for LDA+RISB, this line should be commented out)
ifdef USE_HDF5
    FPFLAGS += -DUSE_HDF5
    PF90 = h5pfc
endif

### C and C++
CXX = icpc
CXX_MPI = mpicxx

### lapack library
LAPACK_LIB = -mkl

### ComCTQMC
BASE_CPPFLAGS = -DNDEBUG
BASE_LIBS = -ln
CXXFLAGS_CTQMC = -std=c++11 -fexceptions -Wall -O3

### ComRISB
FIX_FORM = -flxed
FREE_FORM = -free
PF90_RISB = h5pfc
CXXFLAGS_RISB = -O2
```
Installation

- **install the package**
  $ make comdmft

- **export the bin directory**: add the following line in ~/.bashrc
  $ export COMSUITE_BIN=$HOME/comsuite/bin

- **let’s update .bashrc**
  $ source ~/.bashrc

- **test the directory naming**
  $ echo $COMSUITE_BIN
Directories

Located at $HOME/comsuite

.
  ..
  arch.mk
  bin
  ComCoulomb
  ComCTQMC
  ComDC
  ComLowH
  ComRISB
  ComWann
  example
  GNUmakefile
  GNUmakefile~
  gw
  README.md
  wannier90_2.1

: where we have all the executables
: program to calculate bosonic Weiss field
: CTQMC impurity solver
: program for double counting self-energy
: program to calculate fermionic Weiss field, DOS, spectral functions
: program for Gutzwiller calculation
: program to construct Wannier functions
: examples
: FlapwMBPT code by Andrey Kutepov
: Wannier90 package
Let's resume our calculations from almost converged results

\[ H_{QP} \psi_{nk} = E_{nk} \psi_{nk} \]

\[ E_{nk}, \psi_{nk}(r) \]

**ComWann**

\[ |\tau k\rangle = \sum_n U^*_{n\tau}(k) |nk\rangle \]

\[ U_{n\tau}(k) \]

**ComDC**

\[ \tilde{\Sigma}_{DC} = \tilde{U} \tilde{N} - \tilde{G}_{loc} \tilde{W}_{loc} \]

\[ \tilde{G}_{loc} \]

\[ \tilde{\Sigma}_{DC} \]

**ComLowH**

\[ \tilde{G}^{-1} = \tilde{G}_{loc}^{-1} + \tilde{\Sigma}_{imp} \]

**ComCoulomb**

\[ W_r^{-1} = W^{-1} + P_{QP}^{low} \]

\[ U \]

\[ \tilde{U} \]

**CTQMC**

\[ \tilde{\Sigma}_{imp} = \tilde{G}^{-1} - \tilde{G}_{imp}^{-1} \]
NiO LQSGW prerun

- It is located at /data/workshop2019/users/um180269/tutorial/NiO/lqsgw:

- you can see the job script (we will use the prerun outputs)

```bash
#!/bin/bash

#SBATCH -J temp
#SBATCH -N 1
#SBATCH -n 32
#SBATCH -c 1
#SBATCH -e temp.%j.err
#SBATCH -o temp.%j.out
#SBATCH -t 2:00:00

srun -n 32 -c 1 --mpi=pmix_v2 $COMSUITET_BIN/rspflapw.exe
```
ini: several important parameters

- **iter_dft**: the number of DFT iteration
- **iter_qp**: the number of QSGW iteration
- **nproc_tau**: total number of MPI processes for the tau parallelization
- **nproc_k**: total number of MPI processes for the k parallelization
- **irel & irel_core**: 0 – non-relativistic
  1 – scalar relativistic
  2 – fully relativistic
- **restart**: F or T

For the more detailed information, please go to https://www.bnl.gov/cmpmsd/flapwmbpt
Ini: several important parameters

<table>
<thead>
<tr>
<th>STRUCTURE</th>
<th>par= 7.92600000</th>
<th>natom= 2</th>
<th>nsort= 2</th>
<th>istruc= 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>is= 1 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>b/a= 1.000000</td>
<td>c/a= 1.000000</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a= 0.000000000000000000 0.500000000000000000 0.500000000000000000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>b= 0.500000000000000000 0.000000000000000000 0.500000000000000000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>c= 0.500000000000000000 0.500000000000000000 0.000000000000000000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>tau= 0.000000000000000000 0.000000000000000000 0.000000000000000000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>tau= 0.500000000000000000 0.500000000000000000 0.500000000000000000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- **par**: the unit to write lattice vectors and the positions of the atoms
- **natom**: the number of atoms in the unit cell
- **nsort**: the number of inequivalent atoms
- **a, b, c**: lattice vector
- **tau**: atomic positions

For the more detailed information, please goto https://www.bnl.gov/cmpmsd/flapwmbpt
Ini: several important parameters

- real space mesh in the interstitial region to represent electron density
- real space mesh in the interstitial region to represent wavefunctions
- crystal momentum vector mesh

REAL SPACE MESHES

mdiv= 14 14 14
nrdiv= 10 10 10

K POINT
ndiv= 6 6 6

For the more detailed information, please go to https://www.bnl.gov/cmpmsd/flapwmbpt
Ini: several important parameters

- **z**: atomic number
- **smt**: muffintin radius
- **lmb**: maximum l number for the wave function expansion
- **lmpb**: maximum l number for the product basis
- **lim_pb_mt**: the number of allowed radial function of muffintin product basis for each l
- **ntle**: the number of allowed radial function of muffintin wavefunction for each l
- **augm**: muffintin wavefunction type
- **ptnl**: potential parameter, related to principle quantum number

For the more detailed information, please goto https://www.bnl.gov/cmpmsd/flapwmbpt
NiO LQSGW+DMFT run

• copy and move to the lqsgw+dmft directory
  $ mkdir ~/NiO
  $ cd ~/NiO
  $ cp -r /data/workshop2019/users/um180269/tutorial/NiO/lqsgw_dmft .
  $ cd lqsgw_dmft

• see the job submission script (llscript) and run the calculation
  $ sbatch llscript

```
#!/bin/bash

#SBATCH -p slurm-16-core
#SBATCH -n 1
#SBATCH -c 1
#SBATCH -e temp.%j.err
#SBATCH -o temp.%j.out
#SBATCH -t 2:00:00

$COMSUITE_BIN/comdmft.py
```
LQSGW+DMFT input file in python dictionary format

- all dictionary keys in small letters
- composed of three python dictionaries of “control”, “wan_hmat” and “imp”
In control

- 'methods': 'lqsgw+dmft'
- 'initial_lattice_dir': '/data/workshop2019/users/um180269/tutorial/NiO/lqsgw'
- the path to LQSGW output directory
- 'impurity_problem': [[2,'d']]  
- a python list to specify correlated orbitals. The first and second indices are for the atom index and shell type.  
- atom index: in the order listed in the “../lqsgw/coord.xsf”

<table>
<thead>
<tr>
<th>PRIMCOORD</th>
</tr>
</thead>
<tbody>
<tr>
<td>O</td>
</tr>
<tr>
<td>Ni</td>
</tr>
<tr>
<td></td>
</tr>
</tbody>
</table>

- shell index: either “d” or “f”
- 'impurity_problem_equivalence': [1]  
- equivalence of each impurity problem.  
- identified by an integer starting from 1. If this value is the same, they are equivalent.  
- If this value is negative, it is the time-reversal symmetry pair to the one with the same absolute value.
- 'spin_orbit': True or False  
- if False, correlated orbitals correspond to cubic spherical harmonics

\[
Y_{lm} = \begin{cases} 
  \frac{i}{\sqrt{2}} Y_l^{-|m|} - (-1)^m Y_l^{|m|}, & m < 0 \\
  Y_l^0, & m = 0 \\
  \frac{1}{\sqrt{2}} Y_l^{-|m|} + (-1)^m Y_l^{|m|}, & m > 0 
\end{cases}
\]

where \( Y_l^m \) is a spherical harmonics.
In control

- if True, correlated orbitals chosen at each correlated atom correspond spin-angular functions $|l,i,m>$

$$\Omega_{l,i=\pm \frac{1}{2},m} = \sum_{s=\pm1/2} C_{i,s}^{l,m} Y_{l}^{m-s}(\hat{r}) u_s$$

where $u_s$ is a spinor, and $C_{i,s}^{l,m} = \langle l, m - s, \frac{1}{2}, s | l + i, m \rangle$.

- 'mpi_prefix': 'srun -n 32 -c 1 --mpi=pmix_v2'
  - MPI prefix commonly used for ComCoulomb, ComDC, ComLowH, ComWann, and CTQMC.
  - If a different MPI prefixs from this prefix is necessary for a program, use 'mpi_prefix_coulomb', 'mpi_prefix_lowh', 'mpi_prefix_dc', 'mpi_prefix_wannier', and 'mpi_prefix_impurity',

- 'restart': True
  - True or False. If True, It will resume the calculation from the prerun.
  - default value: False

- 'mpi_prefix_lowh':
  - MPI prefix for ComLowH
  - default value: control['mpi_prefix']

- 'mpi_prefix_impurity':
  - MPI prefix for the impurity solver
  - default value: control['mpi_prefix']

- 'mpi_prefix_wannier'
  - MPI prefix for ComWann
  - default value: control['mpi_prefix']
In control

- **'mpi_prefix_coulomb'**: MPI prefix for ComCoulomb
  - default value: control['mpi_prefix']
- **'mpi_prefix_dc'**: MPI prefix for ComDC
  - default value: control['mpi_prefix']
- **'sigma_mix_ratio'**: Self-energy linear mixing ratio.
  - default value: 0.1
- **'max_iter_num_impurity'**: maximum iteration for the DMFT self-consistent loop.
  - default value: 50
- **'proj_win_min'**: low-energy cutoff to renormalize the projectors
  - default value: wan_hmat['dis_win_min']
- **'proj_win_max'**: high-energy cutoff to renormalize the projectors
  - default value: wan_hmat['dis_win_max']
Important concepts for wan_hmat

- For Wannier function construction
  - Choice of the inner (frozen) energy window: large energy window in the $E_F \pm 10 \text{eV}$
  - Choice of the outer (disentanglement) energy window: from $E_F - 10 \text{eV}$ to $E_F + 50 \text{eV}$

NiO within LDA

$E - E_F (\text{eV})$

Semicore states

valence + unoccupied states

G X W K G L U W L K
Important concept for wan_hmat

- The choice of initial trial orbitals $|\tau R = 0\rangle_t$
  - MT orbitals with desired angular momentum character
  - Radial function of $|\tau R = 0\rangle_t$ is chosen in such a way which maximize

$$
\frac{1}{N_k} \sum_{n_k}^{E_{\text{inner}} < E_{n_k} < E_{\text{inner}}} |\langle n_k | \tau k \rangle_t|^2
$$

where $|\tau k \rangle_t = \frac{1}{N_k} \sum_R |\tau R \rangle_t e^{ik \cdot R}$

- Among MT orbitals we choose ones

$$
\frac{1}{N_k} \sum_{n_k}^{E_{\text{inner}} < E_{n_k} < E_{\text{inner}}} |\langle n_k | \tau k \rangle_t|^2 > 0.2
$$

- For correlated orbitals, final wannier function $|\tau R = 0\rangle_f$ usually

$$
f \langle \tau R = 0 | \tau R = 0 \rangle_t > 0.95
$$

which means $|\tau R = 0\rangle_f$ is strongly localized and a atom-like wavefunction
Wannier functions and interpolated bandstructure of NiO

- The number of bands in the inner window: 10
- The number of bands in the outer window: 25
- The number of trial orbitals: 12 orbitals (Ni-s, Ni-p, Ni-d, O-p)
In `wan_hmat`

- **'kgrid': [10,10,10],**
  - crystal momentum grid for the wannier interpolation of LQSGW bandstructure

- **'froz_win_min': -15 eV,**
  - lower boundary of the inner (frozen) window in eV

- **'froz_win_max': 10 eV,**
  - upper boundary of the inner (frozen) window in eV

- **'dis_win_min':**
  - lower boundary of the outer (disentanglement) window in eV.
  - default value: `froz_win_min`

- **'dis_win_max':**
  - upper boundary of the outer (disentanglement) window in eV.
  - default value: `froz_win_max` +40.0

- **'num_iter':**
  - the number of minization step for the wannierization process. (gauge dependent part of total spreading)
  - default value: 0

- **'dis_num_iter':**
  - the number of minization step for the disentanglement process. (gauge independent part of total spreading)
  - default value: 100
In imp

• 'temperature': 300
  - simulation temperature in K

• for each distinct impurity problem indexed by the value in control[“impurity_problem_equivalence”]
  - 'impurity_matrix': [
    [1,0,0,0,0],  
    [0,1,0,0,0],  
    [0,0,2,0,0],  
    [0,0,0,1,0],  
    [0,0,0,0,2]  
  ],
  --equivalence of the matrix element of the fermionic Weiss field and impurity self-energy.
  Starting from “1”
  --if these values are the same, the values of the elements will be assumed to be identical.
  --if the element in the matrix is zero, then it will not be sampled by the impurity solver.
  --each column and row corresponds to the Wannier orbitals in the following order.
  --If control['spin_orbit']==False, “m” is sorted in ascending order.
    To illustrate for “d” orbitals, in this order: |xy>,|yz>,|z²>,|xz>, |x²-y²>
  --if control['spin_orbit']==True, the most rapidly changing index is “m” and the next one is “i”. They are sorted in ascending order.
    To illustrate for “f” orbitals, in this order: |3,-0.5, -2.5>,|3,-0.5, -1.5>,|3,-0.5, -0.5>,
    |3,-0.5, 0.5>,|3,-0.5, 1.5>,|3,-0.5, 2.5>, |3,0.5, -3.5>,|3,0.5, -2.5>,|3,0.5, -1.5>,
    |3,0.5, -0.5>,|3,0.5, 0.5>,|3,0.5, 1.5>,|3,0.5, 2.5>, |3,0.5, 3.5>,
    1: t²g
    2: eg
- **'Coulomb': 'full',**
  - 'full' or 'ising' are available. We construct Coulomb matrix in the following way.

\[
U_{m_1,m_2,m_3,m_4} = \sum_{k=0}^{2l,even} \frac{4\pi}{2k + 1} F_l^k \sum_{q=-k}^k \langle Y_{l m_1} | Y_{k q} Y_{l m_4}^* \rangle \langle Y_{l m_2} Y_{k q}^* | Y_{l m_3} \rangle
\]

--If 'full', no additional approximation is considered.
--If 'ising', only $U_{abba}$ or $U_{abab}$ are non-zero.

- **'thermalization_time': 1,**
  - » wall time for the thermalization in minutes

- **'measurement_time': 30,**
  - » wall time for the measurement in minutes

- **'green_cutoff': 50,**
  - » cutoff-energy in eV to sample green's function and self-energy.
  - » values beyond this energy will be provided by analytical equations.

- **'susceptibility_cutoff':**
  - » cutoff-energy to sample susceptibility.
  - » Default value: 300 eV
Output directory

• in lqsgw_dmft directory

- cmd.log
- commdmft.ini
- convergence.log
- coulomb
- dc
- delta.dat
- impurity
- llscript
- lowh
- sig.dat
- sig_dc.dat
- sig_dc_hf.dat
- temp.err
- temp.out
- u_slater.dat
- v_slater.dat
- wannier
- w_slater.dat

→ convergence log file
→ Output of ComCoulomb
→ Output of ComDC
→ hybridization function
→ Output of CTQMC solver
→ Output of ComLowH
→ impurity self-energy
→ double-counting self-energy
→ the high-frequency limit of double-counting self-energy
→ bosonic Weiss-field
→ $V_{\text{loc}}$
→ Output of ComWann
→ $W_{\text{loc}}$
### convergence.log

<table>
<thead>
<tr>
<th>Step</th>
<th>t_imp</th>
<th>causality</th>
<th>static_f0</th>
<th>w_sp_min</th>
<th>w_sp_max</th>
<th>mu</th>
<th>std_sig</th>
<th>n_imp</th>
<th>histo_1</th>
<th>histo_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>wannier</td>
<td>6.97943595685</td>
<td>0.28543421</td>
<td>1.7773025</td>
<td>0.019644259897</td>
<td>3.37592293015</td>
<td>8.13892</td>
<td>104.20317231</td>
<td>113.442465644</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coulomb_1</td>
<td>1</td>
<td>good</td>
<td>0.227452938024</td>
<td>1.76039597987</td>
<td>8.12925</td>
<td>95.5346308627</td>
<td>93.4849387127</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>dc_1</td>
<td>2</td>
<td>good</td>
<td>0.36058436439</td>
<td>0.873908782988</td>
<td>8.12575</td>
<td>93.8121360239</td>
<td>90.1533755051</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>delta_1</td>
<td>3</td>
<td>good</td>
<td>0.438313820721</td>
<td>0.480150872625</td>
<td>8.1247</td>
<td>93.4344592768</td>
<td>89.679114163</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>delta_1</td>
<td>4</td>
<td>good</td>
<td>0.457545535088</td>
<td>0.293644026047</td>
<td>8.12405</td>
<td>93.2885542221</td>
<td>89.2755287147</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- keeping track of convergence of some quantities at each iteration
- causality: causality of hybridization function / self-energy
- \( w_{sp\_min} \): minimum spreading of the Wannier functions
- \( w_{sp\_max} \): maximum spreading of the Wannier functions
- \( \mu \): LQSGW+DMFT chemical potential w.r.t. LQSGW chemical potential
- \( \text{std\_sig} \):
  \[
  \sqrt{\sum_i \left( \sum_j^j (i\omega_n) - \sum_i^{j-1} (i\omega_n) \right)^2 / n_\omega n_{orb}}
  \]
- \( n_{imp} \): occupation in the impurity orbitals
- \( \text{histo\_1} \): the first moment of the perturbation order histogram
- \( \text{histo\_2} \): the second moment of the perturbation order histogram
- \( \text{ctqmc\_sign} \): CTQMC sign
Dynamical U

In “lqsgw_dmft”

- Bosonic Weiss field in u_slater.dat and W_loc in w_slater.dat

<table>
<thead>
<tr>
<th># nu(eV)</th>
<th>1:f0(eV)</th>
<th>1:f2(eV)</th>
<th>1:f4(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000000000000</td>
<td>6.979435956849</td>
<td>9.972684910682</td>
<td>7.626659183780</td>
</tr>
<tr>
<td>0.162432849384</td>
<td>6.991563460566</td>
<td>9.974254718886</td>
<td>7.627439680636</td>
</tr>
<tr>
<td>0.324865698768</td>
<td>6.995381415918</td>
<td>9.974733912820</td>
<td>7.627681553600</td>
</tr>
<tr>
<td>0.487298548153</td>
<td>6.996249914058</td>
<td>9.974825995447</td>
<td>7.627732241701</td>
</tr>
<tr>
<td>0.649731397537</td>
<td>7.003719509740</td>
<td>9.975764279332</td>
<td>7.628170672937</td>
</tr>
<tr>
<td>0.812164246921</td>
<td>7.017060208047</td>
<td>9.977474094269</td>
<td>7.628991575522</td>
</tr>
<tr>
<td>0.974597096305</td>
<td>7.033267110201</td>
<td>9.979588473166</td>
<td>7.630054710525</td>
</tr>
<tr>
<td>1.137029945690</td>
<td>7.051862355810</td>
<td>9.982051407717</td>
<td>7.631340778350</td>
</tr>
<tr>
<td>1.299462759074</td>
<td>7.072740247508</td>
<td>9.984834431675</td>
<td>7.632809228323</td>
</tr>
<tr>
<td>1.461895644458</td>
<td>7.095434905356</td>
<td>9.987388550026</td>
<td>7.634389875835</td>
</tr>
<tr>
<td>1.624328493842</td>
<td>7.120156168285</td>
<td>9.991110737090</td>
<td>7.636007516132</td>
</tr>
<tr>
<td>1.786761343226</td>
<td>7.14702547426</td>
<td>9.99483248404</td>
<td>7.637605923885</td>
</tr>
<tr>
<td>1.949194192611</td>
<td>7.176078015966</td>
<td>9.998305912158</td>
<td>7.639310428276</td>
</tr>
<tr>
<td>2.111627041995</td>
<td>7.206925567288</td>
<td>10.002313799443</td>
<td>7.641264863574</td>
</tr>
<tr>
<td>2.274059891379</td>
<td>7.239487230291</td>
<td>10.00636375810</td>
<td>7.643589514652</td>
</tr>
</tbody>
</table>

- Bare Coulomb interaction in v_slater.dat

<table>
<thead>
<tr>
<th># 1:f0(eV)</th>
<th>1:f2(eV)</th>
<th>1:f4(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.073782938928</td>
<td>12.539899507718</td>
<td>8.587692445309</td>
</tr>
</tbody>
</table>
Dynamical U

- At high frequency, $U$ and $W_{\text{loc}}$ converge to $V_{\text{loc}}$
- In comparison to $F^0$, $F^2$ and $F^4$ shows weaker frequency dependence
Local-GW impurity self-energy

In “lqsgw_dmft”

• “sig_dc.dat”
  » Real and imaginary part of impurity self-energy within local GW approximation are listed

<table>
<thead>
<tr>
<th>#</th>
<th>omega(eV)</th>
<th>Re Sig_{1,1}(eV)</th>
<th>Im Sig_{1,1}(eV)</th>
<th>Re Sig_{1,2}(eV)</th>
<th>Im Sig_{1,2}(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.081216424692</td>
<td>38.849812100573</td>
<td>-0.068546031041</td>
<td>40.025499346945</td>
<td>-0.160998380353</td>
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</tr>
<tr>
<td>0.243649274076</td>
<td>38.843310837938</td>
<td>-0.204087668350</td>
<td>40.019531368126</td>
<td>-0.455870104979</td>
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</tr>
<tr>
<td>0.406082123461</td>
<td>38.830545145097</td>
<td>-0.336860987958</td>
<td>40.009263582673</td>
<td>-0.722950196529</td>
<td></td>
</tr>
<tr>
<td>0.568514972845</td>
<td>38.811894580413</td>
<td>-0.465736619491</td>
<td>39.995967618274</td>
<td>-0.963008760085</td>
<td></td>
</tr>
<tr>
<td>0.730947822229</td>
<td>38.787842093861</td>
<td>-0.589783429676</td>
<td>39.980391178088</td>
<td>-1.17731783712</td>
<td></td>
</tr>
<tr>
<td>0.893380671613</td>
<td>38.758942274676</td>
<td>-0.708323505805</td>
<td>39.963076750413</td>
<td>-1.367777823309</td>
<td></td>
</tr>
<tr>
<td>1.055813520997</td>
<td>38.725785079856</td>
<td>-0.820931932399</td>
<td>39.944463348607</td>
<td>-1.536278967301</td>
<td></td>
</tr>
<tr>
<td>1.218246370382</td>
<td>38.688965464350</td>
<td>-0.927405312935</td>
<td>39.924917597311</td>
<td>-1.685077961169</td>
<td></td>
</tr>
<tr>
<td>1.380679219766</td>
<td>38.649060696289</td>
<td>-1.027719550394</td>
<td>39.904746666450</td>
<td>-1.816380015196</td>
<td></td>
</tr>
<tr>
<td>1.543112069150</td>
<td>38.606616266484</td>
<td>-1.121987778606</td>
<td>39.884206853383</td>
<td>-1.932293825430</td>
<td></td>
</tr>
</tbody>
</table>

• “sig_hf_dc.dat”
  » Real and imaginary part of the Hartree-Fock contribution to the impurity self-energy within local GW approximation are listed

<table>
<thead>
<tr>
<th>#</th>
<th>Re Sig_{1,1}(eV)</th>
<th>Im Sig_{1,1}(eV)</th>
<th>Re Sig_{1,2}(eV)</th>
<th>Im Sig_{1,2}(eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>28.641291666667</td>
<td>0.000000000000</td>
<td>38.254424000000</td>
<td>0.000000000000</td>
<td></td>
</tr>
</tbody>
</table>
Local-GW impurity self-energy

- At high frequency, self-energy converges to Hartree-fock limit
- No divergent self-energy near Fermi-level.
Impurity self-energy

- “lqsgw_dmft/sig.dat”: in the same format as “sig_dc.out”
- Pole in the eg orbital self-energy
Hybridization function

- “lqsgw_dmft/delta.dat”
- in the same format as sig.dat
Analytical continuation

1. We will use the maximum entropy (maxent) method for the analytical continuation. For the purposes of this tutorial, we will use K. Haule’s maxent code.

2. To access maxent code, you should export the path to the executable

   ```
   $ export WIEN_DMFT_ROOT=/data/workshop2019/users/um180269/usr/bini
   ```

4. To run the maxent code, create the maxent directory in the “lqsgw_dmft” directory and then move to it

   ```
   $ mkdir maxent
   $ cd maxent
   ```

5. Let’s copy maxent input file

   ```
   $ cp ../../../maxent_for_comparison/maxent_params_fortutorial.dat maxent_params.dat
   ```
6. By executing ‘maxent_wrapper.py’, we can obtain the self-energy on real axis by calling maxent_run.py:

$ $COMSUITE_BIN/maxent_wrapper.py ../sig.dat

usage: maxent_wrapper.py [-h] sig [error]
call maxent_run.py from EDMFTF package and return self-energy on real axis. If maxent_params.dat is not present in the directory, it generates one. The name of the output file will be sig_realaxis.dat

positional arguments:
  sig  self-energy file on imaginary axis
  error  Errors for the maxent. Optional. Default value=0.05

optional arguments:
  -h, --help  show this help message and exit
Impurity self-energy on real frequency axis

- Divergent self-energy near Fermi level for $e_g$ orbitals
1. move to a directory for the DOS calculation
   
   $ mkdir ../realgrid
   $ cd ../realgrid

2. copy files necessary to calculate DOS and partial DOS by using prepare_realaxis.py
   
   $ $COMSUITE_BIN/prepare_realaxis.py 0.1 ../lowh/ ../wannier/
   ../maxent_for_comparison/sig_realaxis.dat 10 10 10 -m 2

```bash
usage: prepare_realaxis.py [-h] [-m MODE]
broadening lowh_directory wan_directory self_energy
[kmesh_b1_for_dos] [kmesh_b2_for_dos]
[kmesh_b3_for_dos]

prepare inputs of comlowh calculation on real axis

positional arguments:
broadening  broadening
lowh_directory  lowh directory
wan_directory  wannier directory
self_energy  real-axis self-energy
[kmesh_b1_for_dos] finer kmesh along b1 axis for the DOS. Optional
[kmesh_b2_for_dos] finer kmesh along b2 axis for the DOS. Optional
[kmesh_b3_for_dos] finer kmesh along b3 axis for the DOS. Optional

optional arguments:
-h, --help  show this help message and exit
-m MODE, --mode MODE  If 3, code calculates spectral function along the high symmetry line defined in 'kpath.dat'. If it is 2, it calculates projected density of states. Default: 3
```
LQSGW+DMFT DOS

3. prepare job submission script (you can copy it from ..../realgrid_for_comparison)

$ cp ..../realgrid_for_comparison/llscript .

```bash
#!/bin/bash

#SBATCH -J temp
#SBATCH -N 1
#SBATCH -n 32
#SBATCH -c 1
#SBATCH -e temp.%j.err
#SBATCH -o temp.%j.out
#SBATCH -t 2:00:00

srun -n 32 -c 1 --mpi=pmix_v2 $COMSUITE_BIN/ComLowH
```

4. submit the script
   $ sbatch llscript
LQSGW+DMFT DOS

• tdos.dat

<table>
<thead>
<tr>
<th>#</th>
<th>omega (eV)</th>
<th>DOS (1/eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

• pdos.dat
- (atom index, l, m) if spin_orbit==False and (atom index, l, i,m) if spin_orbit==True

<table>
<thead>
<tr>
<th>#</th>
<th>omega(eV)</th>
<th>(1,1,-1)</th>
<th>(1,1,0)</th>
<th>(1,1,1)</th>
<th>(2,0,0)</th>
</tr>
</thead>
<tbody>
<tr>
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<td></td>
</tr>
<tr>
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<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
• energy gap opens due to local strong correlation

```$ cp ../realgrid_for_comparison/pdos_plot.py .
$ ipython
$ %run ./pdos_plot.py
$ exit```

LQSGW+DMFT DOS

[Graphs showing DOS and energy levels]
LQSGW+DMFT spectral function

1. move to a directory for the spectral function calculation
   $ mkdir ../realaxis
   $ cd ../realaxis

2. copy files necessary to calculate spectral functions by using prepare_realaxis.py
   $ $COMSUITE_BIN/prepare_realaxis.py 0.1 ../lowh/ ../wannier/
   ../maxent_for_comparison/sig_realaxis.dat -m 3

usage: prepare_realaxis.py [-h] [-m MODE]
                  broadening lowh_directory wan_directory self_energy
                  [kmesh_b1_for_dos] [kmesh_b2_for_dos]
                  [kmesh_b3_for_dos]

prepare inputs of comlowh calculation on real axis

positional arguments:
  broadening
  lowh_directory
  wan_directory
  self_energy
  kmesh_b1_for_dos
  kmesh_b2_for_dos
  kmesh_b3_for_dos

  broadening
  lowh directory
  wannier directory
  real-axis self-energy
  finer kmesh along b1 axis for the DOS. Optional
  finer kmesh along b2 axis for the DOS. Optional
  finer kmesh along b3 axis for the DOS. Optional

optional arguments:
  -h, --help
  -m MODE, --mode MODE
  show this help message and exit
  If 3, code calculates spectral function along the high symmetry line defined in 'kpath.dat'. If it is 2, it calculates projected density of states. Default: 3
3. create k-path file (kpath.dat)

```
$ cp ../realaxis_for_comparison/kpath.dat .
```
- k points w.r.t. reciprocal lattice vector

<table>
<thead>
<tr>
<th></th>
<th>The number of k points</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00000000</td>
<td>0.00000000 0.00000000</td>
</tr>
<tr>
<td>0.01666667</td>
<td>0.00000000 0.01666667</td>
</tr>
<tr>
<td>0.03333333</td>
<td>0.00000000 0.03333333</td>
</tr>
<tr>
<td>0.05000000</td>
<td>0.00000000 0.05000000</td>
</tr>
<tr>
<td>0.06666667</td>
<td>0.00000000 0.06666667</td>
</tr>
<tr>
<td>0.08333333</td>
<td>0.00000000 0.08333333</td>
</tr>
<tr>
<td>0.10000000</td>
<td>0.00000000 0.10000000</td>
</tr>
<tr>
<td>0.11666667</td>
<td>0.00000000 0.11666667</td>
</tr>
<tr>
<td>0.13333333</td>
<td>0.00000000 0.13333333</td>
</tr>
<tr>
<td>0.15000000</td>
<td>0.00000000 0.15000000</td>
</tr>
<tr>
<td>0.16666667</td>
<td>0.00000000 0.16666667</td>
</tr>
<tr>
<td>0.18333333</td>
<td>0.00000000 0.18333333</td>
</tr>
<tr>
<td>0.20000000</td>
<td>0.00000000 0.20000000</td>
</tr>
<tr>
<td>0.21666667</td>
<td>0.00000000 0.21666667</td>
</tr>
<tr>
<td>0.23333333</td>
<td>0.00000000 0.23333333</td>
</tr>
<tr>
<td>0.25000000</td>
<td>0.00000000 0.25000000</td>
</tr>
<tr>
<td>0.26666667</td>
<td>0.00000000 0.26666667</td>
</tr>
<tr>
<td>0.28333333</td>
<td>0.00000000 0.28333333</td>
</tr>
<tr>
<td>0.30000000</td>
<td>0.00000000 0.30000000</td>
</tr>
<tr>
<td>0.31666667</td>
<td>0.00000000 0.31666667</td>
</tr>
</tbody>
</table>
3. prepare job submission script
   (you can copy it from “..../realaxis_for_comparison/llscript)
   $ cp ../realaxis_for_comparison/llscript .

```bash
#!/bin/bash

#SBATCH -J temp
#SBATCH -N 1
#SBATCH -n 32
#SBATCH -c 1
#SBATCH -e temp.%j.err
#SBATCH -o temp.%j.out
#SBATCH -t 2:00:00

srun -n 32 -c 1 --mpi=pmix_v2 $COMSUITE_BIN/ComLowH
```

4. submit the script
   $ sbatch llscript
LQSGW+DMFT spectral function

- realaxis/spectral.dat

<table>
<thead>
<tr>
<th>#</th>
<th>kpoint</th>
<th>E(eV)</th>
<th>A(1/eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-50.0000000000000</td>
<td>0.000170826963</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>-50.0000000000000</td>
<td>0.000170854205</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>-50.0000000000000</td>
<td>0.000170935102</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>-50.0000000000000</td>
<td>0.000171067293</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>-50.0000000000000</td>
<td>0.000171247218</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>-50.0000000000000</td>
<td>0.000171470600</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>-50.0000000000000</td>
<td>0.000171733002</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>-50.0000000000000</td>
<td>0.000172030282</td>
<td></td>
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<tr>
<td>9</td>
<td>-50.0000000000000</td>
<td>0.000172358869</td>
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</tr>
<tr>
<td>10</td>
<td>-50.0000000000000</td>
<td>0.000172715722</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>-50.0000000000000</td>
<td>0.000173097979</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>-50.0000000000000</td>
<td>0.000173502371</td>
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<tr>
<td>15</td>
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</tr>
</tbody>
</table>
The image shows a graph of the LQSGW+DMFT spectral function. The code snippet includes the following commands:

```bash
$ cp ../realaxis_for_comparison/spectral.py .
$ ipython
$ %run ./spectral.py
$ exit
```

- Charge transfer gap opening
- White line: LQSGW bandstructure
Theories vs experiments

LDA+DMFT details
• a frozen energy window of -10eV < E-Ef < 10eV, T=300K
• $U = 10.0\,\text{eV}$ and $J = 0.9\,\text{eV}$,
• nominal double-counting scheme with d orbital occupancy of 8.
• Different choice of U, J and double-counting scheme may improve LDA+DMFT results