Hedin equations, *GW*, *GW*+DMFT, and all That

Karsten Held* (TU Wien)

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* with C. Taranto, G. Rohringer, and A. Toschi

1) Introduction

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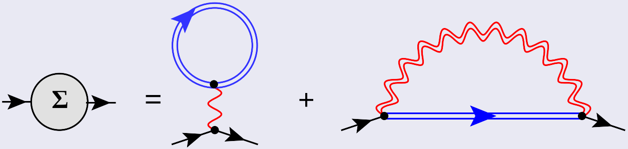
Idea

Alternative to DFT: Hedin's (1965) GW



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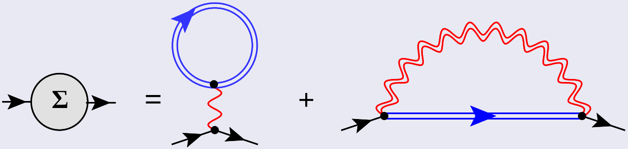

$$\Sigma^{\mathrm{GW}}(\mathbf{r},\mathbf{r}';\omega) = i \int \frac{d\omega'}{2\pi} G(\mathbf{r},\mathbf{r}';\omega+\omega') W(\mathbf{r},\mathbf{r}';\omega') \;.$$

Self energy: Fock-like term but with screened interaction W

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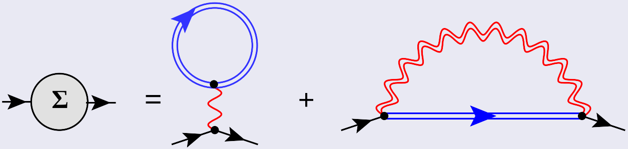

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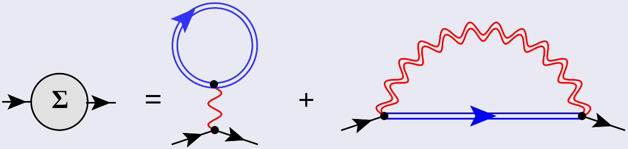

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Self energy: Fock-like term but with screened interaction W

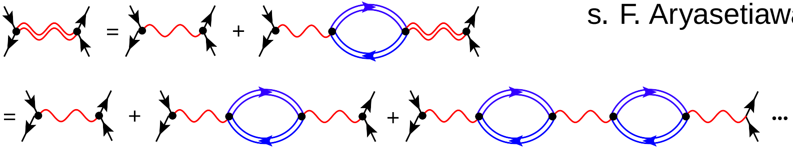
- often similar as LDA
- better if non-local exchange is important

$\rightarrow$ semiconductor band gaps

What kind of diagrams?

Screening within random phase approx (RPA)

s. F. Aryasetiawan's lecture



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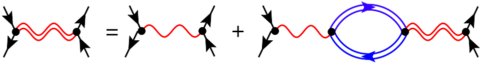

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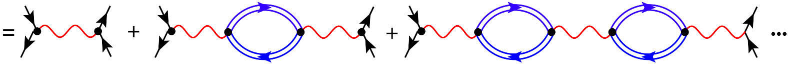

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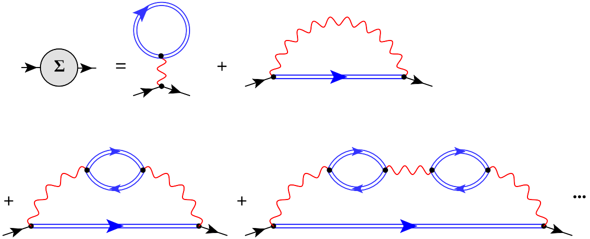

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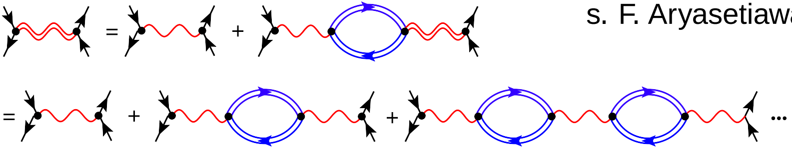

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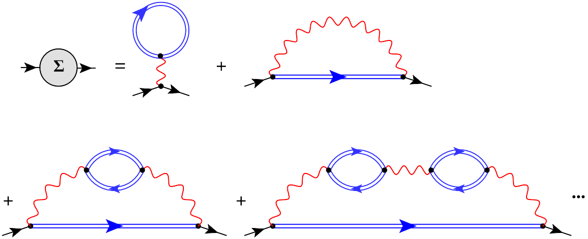

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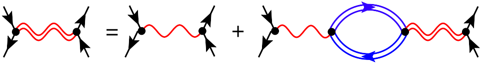

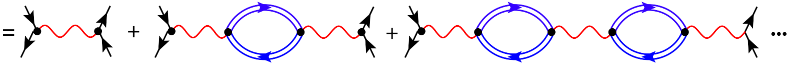

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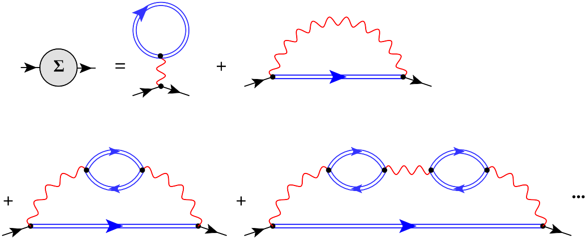

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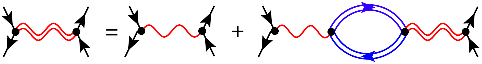

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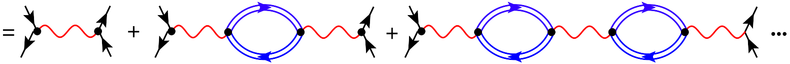

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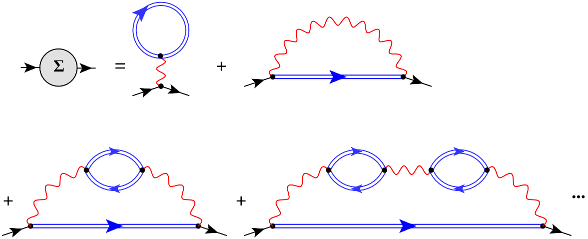

- *GW* exchange "in between" LDA and bare Hartree
- good for exchange cf. hybrid functionals
- no strong correlations (Hubbard bands) $\rightarrow$ DMFT or similar

2) Hedin Equations

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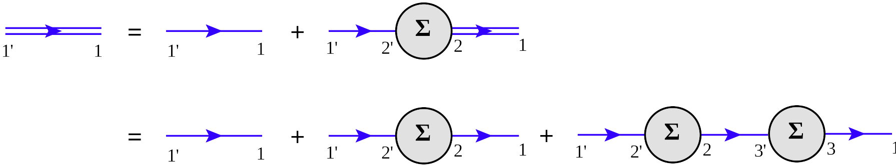
Quote

Hedin (1965): "The results [i.e., the Hedin equations] are well known to the Green function people”

1st Hedin equation: Dyson equation $G \leftrightarrow \Sigma$



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G(11') &= G^0(11') + G(12)\beta\Sigma(22')G^0(2'1') \\
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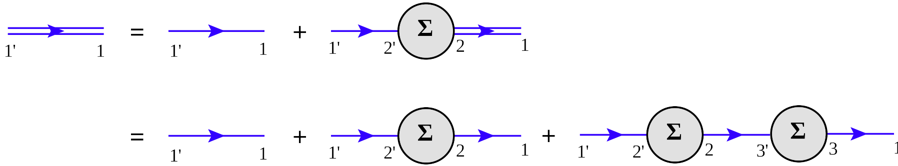

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Short hand notation 1 for $(\mathbf{r}_1, \tau_1, \sigma)$ or (i, m, ω, σ) (Bickers'04)

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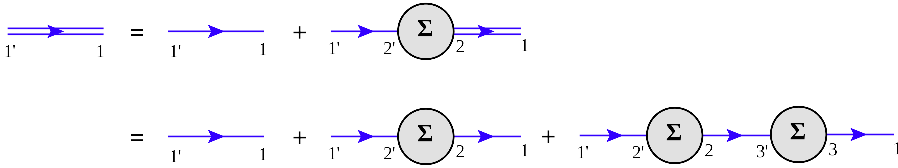

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All Feynman diagrams generated by connecting

1-p irreducible building blocks Σ by GF lines

1-p irreducible: cutting one GF $\Rightarrow$ diagram still connected

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Analogon to Dyson eq.

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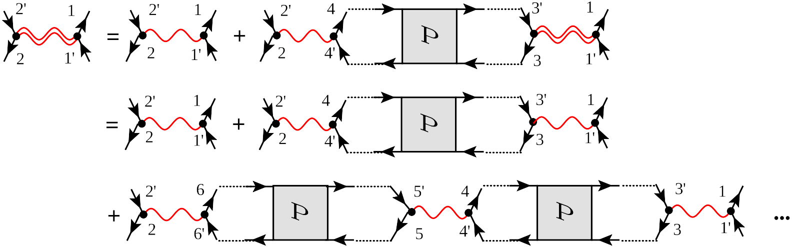
Analogon to Dyson eq.

W: all Feynman diagrams connecting left and rigth by *V*'s

G: all Feynman diagrams connecting left and rigth by G^0's

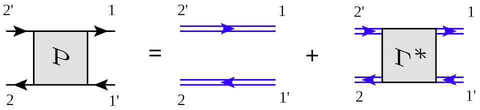


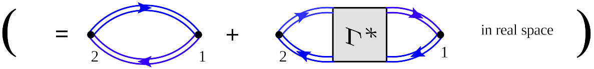
$$W(11';22') = V(11';22') + W(11';33')P(3'3;4'4)V(44';22')\ .$$

P: all diagrams irreducible w.r.t. cutting one *V*

3rd Hedin equation: $P \leftrightarrow$ polarization op. Γ^*

standard relation between 2-p GF (response fct.) and vertex





$$P(11';22') = \beta G(12')G(21') + \beta G(13)G(3'1')\Gamma^*(33';44')\beta G(4'2')G(24)$$

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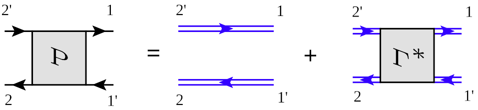

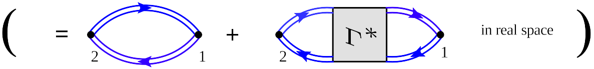

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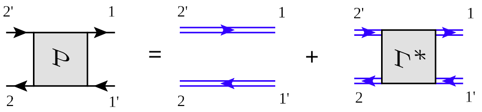

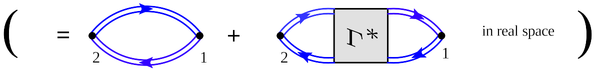

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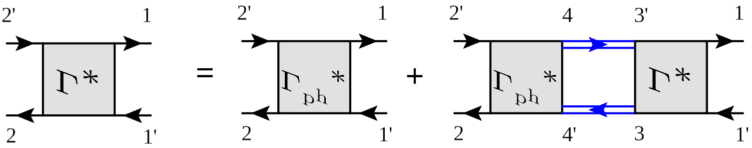
  2nd line: simplifications in real space 2=2', 1=1'

4th Hedin equation: Bethe-Salpeter eq. red. $\Gamma^* \leftrightarrow$ irred. Γ^*_{ph}

Analogon to Dyson eq. but for two-particles



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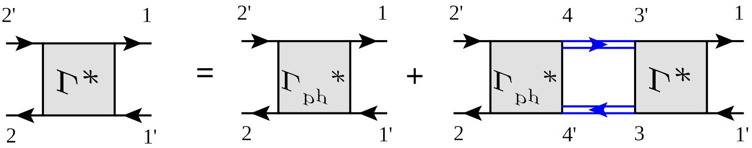

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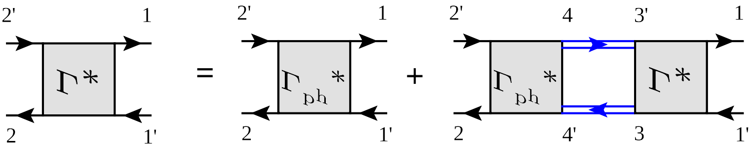

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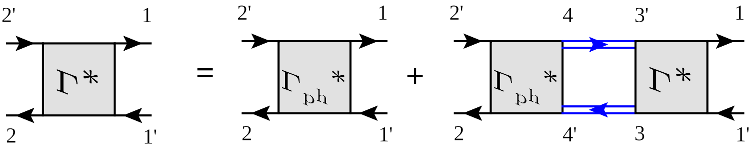

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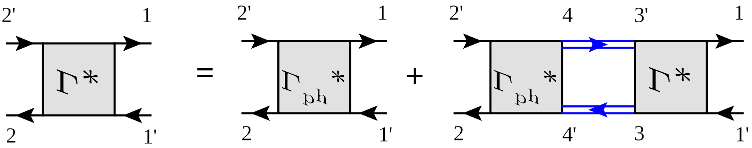

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Hedin: $\Gamma^*_{\mathrm{ph}}(11';22') = \frac{\delta[\Sigma(11') - \Sigma_{\mathrm{Hartree}}(11')]}{\delta G(2'2)}$

5th Hedin equation: (Heisenbeg) equation of motion

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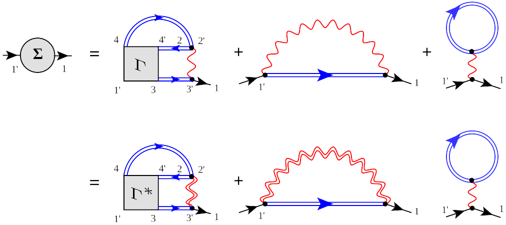

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for details s. Appendix of Lecture Notes

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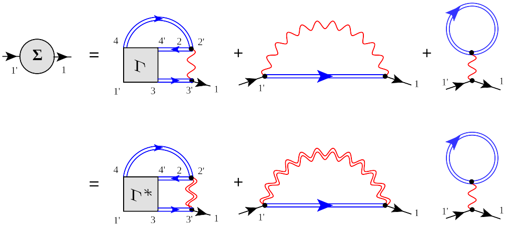

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From Hedin's eq. to *GW*

Complicated part is irreducible vertex

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Dyson equation yields

$$G(11') = G^0(11') + G(12)\beta\Sigma^{\rm GW}(22')G^0(2'1')$$

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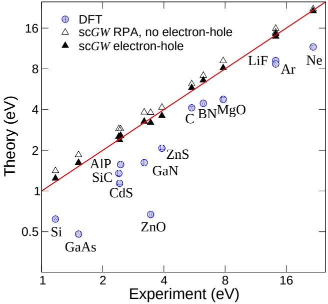
band gaps Shishkin et al.'07



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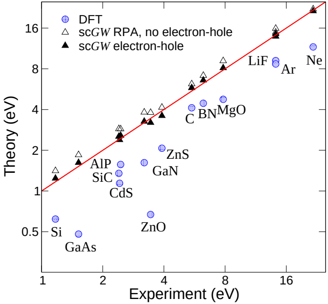
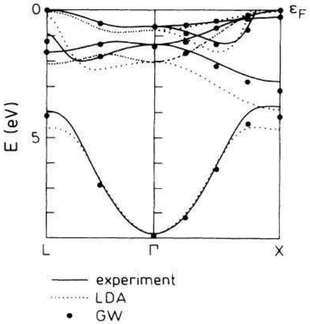




bandstructure of Ni

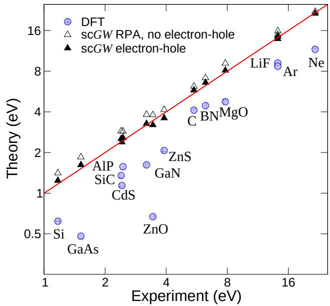
Aryasetiawan'82

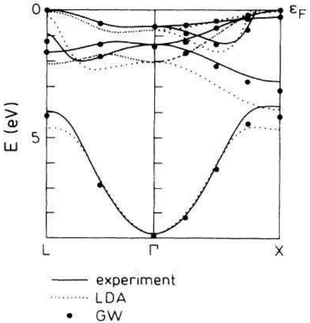
- 1eV less d-bandwidth (exp.: 1.2 eV)
- no -6eV satellite → *DMFT*

Often not self-consistent G_0W_0 – with LDA as starting point
self consistency with (Schilfgaarde,Kontani'04)

$$\bar{\Sigma}_{nn'} = \mathrm{Re}[\Sigma_{nn'}(\epsilon_q, \mathbf{q}) + \Sigma_{n'n}(\epsilon_q, \mathbf{q})]/2$$

band gaps Shishkin et al.'07





bandstructure of Ni
Aryasetiawan'82

- 1eV less *d*-bandwidth (exp.: 1.2 eV)
- no -6eV satellite → *DMFT*

- also finite life times e.g. Ag

4) *GW*+DMFT

Merge *GW* and DMFT self eneries (or energy functionals)

Biermann et al.'03

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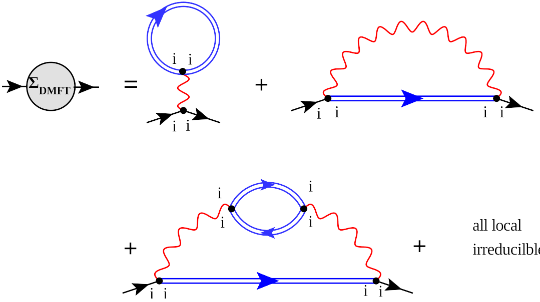


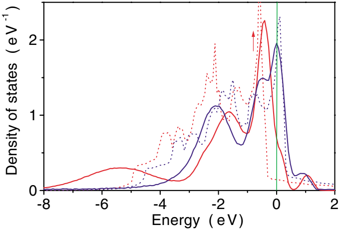
all local
irreducilble diagrams

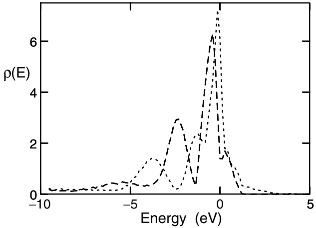
Algorithm

- Do LDA calculation, yielding $\boldsymbol{G}_{\boldsymbol{k}}(\omega)=[\omega\mathbf{1}+\mu\mathbf{1}-\boldsymbol{\epsilon}^{\text{LDA}}(\boldsymbol{k})]^{-1}$.
  - Calculate GW polarization $\boldsymbol{P}^{GW}(\omega)=-2i\int\frac{d\omega'}{2\pi}\boldsymbol{G}(\omega+\omega')\boldsymbol{G}(\omega')$.
  - If DMFT polarization $\boldsymbol{P}^{\text{DMFT}}$ is known (after the 1st iteration), include it
  $$\boldsymbol{P}^{GW+\text{DMFT}}(\boldsymbol{k},\omega)=\boldsymbol{P}^{GW}(\boldsymbol{k},\omega)-\frac{1}{V_{\text{BZ}}}\int d^3k\,\boldsymbol{P}^{GW}(\boldsymbol{k},\omega)+\boldsymbol{P}^{\text{DMFT}}(\omega)\ .$$
  - With this polarization, calculate the screened interaction:
  $$\boldsymbol{W}(\boldsymbol{k};\omega)=\boldsymbol{V}_{\text{ee}}(\boldsymbol{k})[\mathbf{1}-\boldsymbol{V}_{\text{ee}}(\boldsymbol{k})\boldsymbol{P}(\boldsymbol{k};\omega)]^{-1}.$$
  - Calculate $\boldsymbol{\Sigma}^{\text{Hartree}}_{\boldsymbol{k}}=\int\frac{d^3q}{V_{\text{BZ}}}\boldsymbol{G}_{\boldsymbol{q}}(\tau=0^-)\boldsymbol{W}(\boldsymbol{k}-\boldsymbol{q},0)$ and $\boldsymbol{\Sigma}^{\text{Hartree}}_{\text{dc}}$.
  - Calculate $\boldsymbol{\Sigma}^{GW}(\boldsymbol{r},\boldsymbol{r}';\omega)=i\int\frac{d\omega'}{2\pi}\boldsymbol{G}(\boldsymbol{r},\boldsymbol{r}';\omega+\omega')\boldsymbol{W}(\boldsymbol{r},\boldsymbol{r}';\omega')$.
  - Calculate the DMFT self-energy $\boldsymbol{\Sigma}^{\text{DMFT}}$ and polarization $\boldsymbol{P}^{\text{DMFT}}$ as follows:
    - From the local Green function $\boldsymbol{G}$ and old self-energy $\boldsymbol{\Sigma}^{\text{DMFT}}$ calculate
    $$(\boldsymbol{\mathcal{G}}^0)^{-1}(\omega)=\boldsymbol{G}^{-1}(\omega)+\boldsymbol{\Sigma}^{\text{DMFT}}(\omega)\quad \boldsymbol{\Sigma}^{\text{DMFT}}=0 \text{ in 1st iteration.}$$
    - Extract the local screening contributions from $\boldsymbol{W}$:
    $$\boldsymbol{U}(\omega)=[\boldsymbol{W}^{-1}(\omega)-\boldsymbol{P}^{\text{DMFT}}(\omega)]^{-1}.$$
    - With $\boldsymbol{U}$ and $\boldsymbol{\mathcal{G}}^0$, solve impurity problem with effective action
    $$\mathcal{A}=\sum_{\nu\sigma\, lm}\psi^{\sigma*}_{\nu m}(\mathcal{G}^{\sigma 0}_{\nu mn})^{-1}\psi^{\sigma}_{\nu n}+\sum_{lm\sigma\sigma'}\int d\tau\psi^{\sigma*}_{l}(\tau)\psi^{\sigma}_{l}(\tau)\,U_{lm}(\tau-\tau')\psi^{\sigma'*}_{m}(\tau')\psi^{\sigma'}_{m}(\tau'),$$
    resulting in $\boldsymbol{G}$ and susceptibility $\boldsymbol{\chi}$.
    - From $\boldsymbol{G}$ and $\boldsymbol{\chi}$, calculate $\boldsymbol{\Sigma}^{\text{DMFT}}(\omega)=(\boldsymbol{\mathcal{G}}^0)^{-1}(\omega)-\boldsymbol{G}^{-1}(\omega)$, $\boldsymbol{P}^{\text{DMFT}}(\omega)=\boldsymbol{U}^{-1}(\omega)-[\boldsymbol{U}-\boldsymbol{U}\boldsymbol{\chi}\boldsymbol{U}]^{-1}(\omega)$.
  - Combine this to the total GW self-energy:
  $$\boldsymbol{\Sigma}^{GW+\text{DMFT}}(\boldsymbol{k},\omega)=\boldsymbol{\Sigma}^{GW}(\boldsymbol{k},\omega)-\int d^3k\,\boldsymbol{\Sigma}^{GW}(\boldsymbol{k},\omega)+\boldsymbol{\Sigma}^{\text{Hartree}}(\boldsymbol{k})-\boldsymbol{\Sigma}^{\text{Hartree}}_{\text{dc}}+\boldsymbol{\Sigma}^{\text{DMFT}}(\omega).$$
  - From this and $\boldsymbol{G}^0$, calculate $\boldsymbol{G}^{\text{new}}_{\boldsymbol{k}}(\omega)^{-1}=\boldsymbol{G}^0_{\boldsymbol{k}}(\omega)^{-1}-\boldsymbol{\Sigma}_{\boldsymbol{k}}(\omega)$.
- Iterate with $\boldsymbol{G}_{\boldsymbol{k}}=\boldsymbol{G}^{\text{new}}_{\boldsymbol{k}}$ until convergence, i.e. $\|\boldsymbol{G}_{\boldsymbol{k}}-\boldsymbol{G}^{\text{new}}_{\boldsymbol{k}}\|<\epsilon$.

reproduced from Held Adv. Phys. ’07

Results for Ni





LDA+DMFT
Lichtenstein et al.'01

***GW*+DMFT**
Biermann et al.'03

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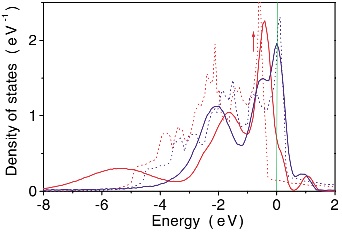

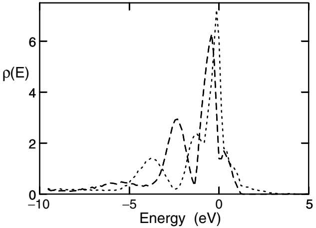

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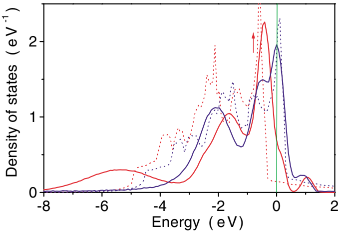

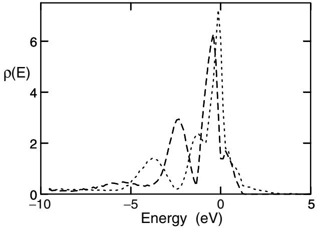

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***GW*+DMFT**
Biermann et al.'03

- satellite at -6eV; both similar
- no self consistency, P^{DMFT} ...
- $W(\omega) \rightarrow W$

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Hedin's eq.: combine *GW* exchange and correlations on 2p level
instead of 1p *GW*+DMFT

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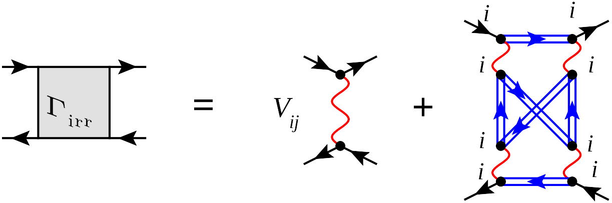

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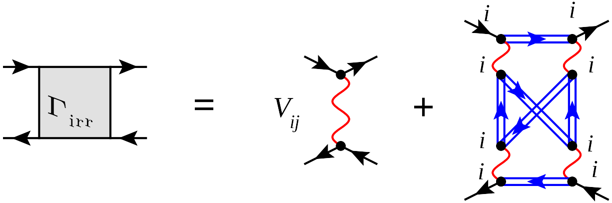

$\rightarrow$ starting point of Hedin eq.