"GW + DMFT"

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Cf. early related ideas by
P. Sun, G. Kotliar, S. Savrasov, A. Lichtenstein

Motivation :

* DMFT local : $\Sigma(\cancel{k}, \omega)$
* "realistic interactions" ?

  "LDA + DMFT" :

  $H = H_{LDA}$ + Hubbard-U − Double counting

  Reality :

  long-range interactions, screening ...

Basic idea :

* { local physics → DMFT
  nonlocal aspects → GW
* interactions from GW / E-DMFT

Functional point of view

[R. Chitra & G. Kotliar, PRB 63, 115110 (2001),

C.O. Almbladh et al., J. Mod. Phys. B 13, 535 (1999)]

Free energy:

$$\Gamma[G,W] = \mathrm{Tr}\ln G - \mathrm{Tr}[(G_0^{-1} - G^{-1})G] - \frac{1}{2}\mathrm{Tr}\ln W + \frac{1}{2}\mathrm{Tr}[(V^{-1} - W^{-1})W] + \Psi[G,W]$$

is a functional of $G = \langle \psi \psi \rangle$

and $W = V - V\chi V$

with

$$\Psi[G,W] = i\int_0^1 d\alpha \int dr\, d\tau \, \langle \phi(r,\tau)\left(\psi^+(r,\tau)\psi(r,\tau) - n(r)\right)\rangle$$

Construction of $\Psi[G,W]$

$$H = -\frac{1}{2}\sum_i \left[\nabla_i^2 + v_{ext}(r_i)\right] + \frac{1}{2}\sum_{i\neq j} V(r_i - r_j)$$

$$Z = \int \mathcal{D}\psi \mathcal{D}\psi^+ \, e^{-S}$$

$$S = -\int \psi^+(i\omega - H_0 - V_{Hartree})\psi + \frac{1}{2}\int :\hat{n}(r): V(r-r') :\hat{n}(r'):$$

Introduce:
- Hubbard-Stratonovich field $\varphi(r,\tau)$
- coupling constant α
- source terms $\int \Sigma \psi^+\psi + \frac{1}{2}\int P\varphi\varphi$

Define $G = -\langle T\psi\psi^+\rangle$

$W = \langle T\varphi\varphi\rangle$

$$\mathcal{F}[\Sigma,P] = \ln \int \mathcal{D}\psi\mathcal{D}\psi^+\mathcal{D}\varphi \; e^{-S[\Sigma,P]}$$

$$S[\Sigma,P] = -\int \psi^+ G_0^{-1}\psi + \frac{1}{2}\int \varphi V^{-1}\varphi - i\alpha\int \varphi(\psi^+\psi - n) + \int \Sigma\psi^+\psi + \frac{1}{2}\int P\varphi\varphi$$

Legendre transf. w.r.t. $G = -\frac{\delta \mathcal{F}}{\delta \Sigma}$, $W = 2\frac{\delta \mathcal{F}}{\delta P}$

$$\Gamma[G,W] = \mathcal{F} + \mathrm{tr}[\Sigma G] - \frac{1}{2}\mathrm{tr}[PW]$$

$$\equiv \Gamma_{\alpha=0}[G,W] + \Psi[G,W]$$

Approximations ?

E - DMFT : $\Psi = \Psi_{imp}$

GW : $\Psi_{GW} = -\frac{1}{2}\,\mathrm{Tr}\,GWG$

"GW + DMFT" : $\Psi = \Psi_{local} + \Psi_{nonlocal}$

$$= \Psi_{imp} + \Psi_{GW}^{nonlocal}$$

E - DMFT (Chitra & Kotliar ; Si & Smith ...)

Ψ_{imp} from local impurity model :

$$S_{imp} = \int d\tau\, d\tau' \Big[-\sum c_L^{+}(\tau)\, \mathcal{G}_{LL'}^{-1}(\tau-\tau')\, c_{L'}(\tau')$$

$$+ \frac{1}{2} \sum : c_{L_1}^{+}(\tau)\, c_{L_2}(\tau) : \mathcal{U}_{L_1L_2L_3L_4}(\tau-\tau') : c_{L_3}^{+}(\tau')\, c_{L_4}(\tau') : \Big]$$

$$G_{imp}(\tau) = -\langle T\, c(\tau)\, c^{+}(0) \rangle_{S_{imp}}$$

$$\Sigma_{imp} = \mathcal{G}_0^{-1} - G_{imp}^{-1}$$

GW (L. Hedin)

$$\Psi = -\frac{1}{2}\,\mathrm{Tr}\,GWG$$

$$\Sigma = \frac{\delta\Psi}{\delta G} = -GW$$

$$P = -\frac{\delta\Psi}{\delta W} = GG$$

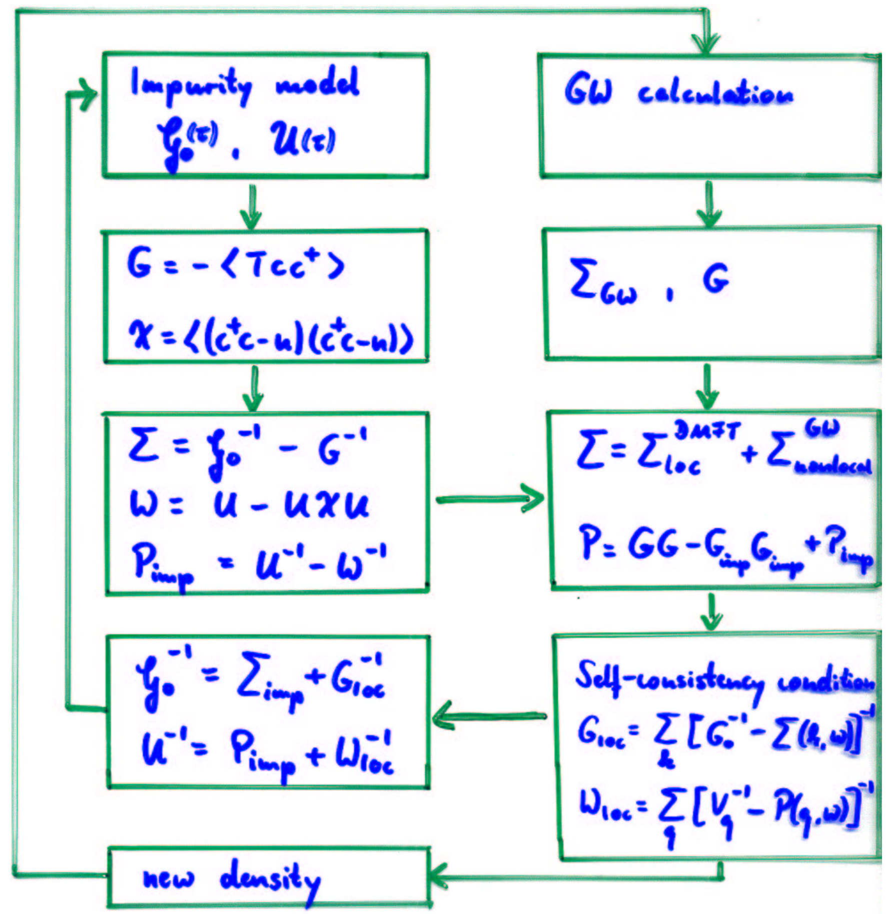
"GW + DMFT"

$$\Psi = -\frac{1}{2}\int d\tau \sum_{L_1 \dots L_2'} \sum_{R \neq R'} G^{RR'}_{L_1 L_1'}(\tau)\, W^{RR'}_{L_1 L_2 L_1' L_2'}(\tau)\, G^{R'R}_{L_2' L_2}(-\tau)$$

$$+ \Psi_{imp}$$

$$= \Psi_{GW} - \Psi^{local}_{GW}[G^{RR}, W^{RR}] + \Psi_{imp}$$

$$\Rightarrow \begin{cases} \Sigma^{xc}(k, i\omega) = \Sigma^{xc}_{GW}(k, i\omega) - \sum_{k} \Sigma^{xc}_{GW} + \Sigma_{imp}(i\omega) \\ P(q, i\nu_n) = P^{GW}(q, i\nu_n) - \sum_{q} P^{GW}(q, i\nu_n) + P_{imp}(i\nu_n) \end{cases}$$



Technical aspects

* dynamical impurity model
  - P. Sun & G. Kotliar
  - S. Florens, work in progress

here: static approximation

* "local" = "onsite" in LMTO sense

* "two-particle basis"

$$E.g.\ \ W(r,r') = \sum_{RR'} \sum_{\alpha\beta} B_\alpha^R(r)\, W_{\alpha\beta}^{RR'}(\omega)\, B_\beta^{R'}(r')^*$$

B = linear combination of $\phi_L(r)\phi_{L'}(r)$

Simplified implementation

$$G_{loc}(i\omega) = \sum_k \left[G_0^{-1} - \Sigma(k, i\omega) \right]^{-1}$$

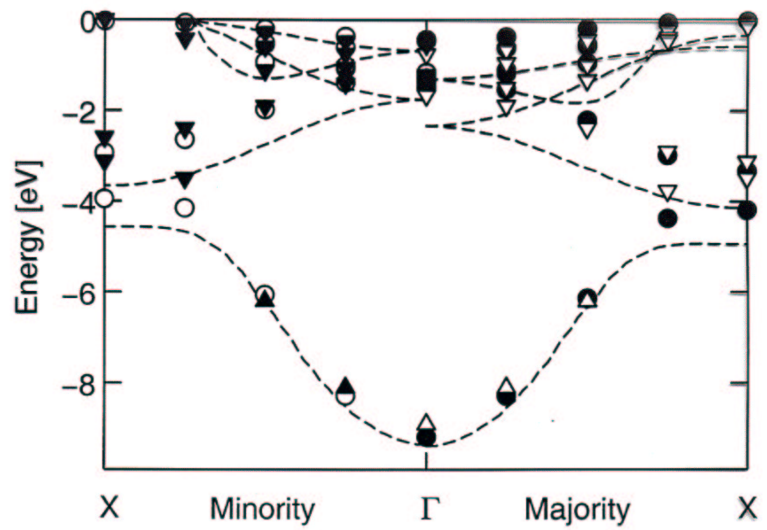
$$= \sum_k \left[\overbrace{i\omega + \mu - H_{LDA} + V_{xc}^{LDA}} - \overbrace{\Sigma_{GW}^{nonlocal} - \Sigma_{DMFT}} \right]^{-1}$$

replaced by

$$\sum_k \left[\overbrace{i\omega + \mu - H_{LDA} + V_{xc}^{LDA}\Big|_{nonlocal} + \Sigma_{\substack{double\\counting}}} - \Sigma_{GW}^{nonlocal} - \Sigma_{DMFT} \right]^{-1}$$

=> Non-selfconsistent GW + local Σ from static impurity model

Ni bands from "$\Sigma_{GW}^{nonlocal} + \Sigma_{imp}$"



Circles : "GW + DMFT"

dashed : LDA

triangles : experiment (Bünemann et al. '02, & Mårtensson & Nilsson, 1984)

$\Sigma_{GW}^{nonlocal} + \Sigma_{imp}$