ComRISB--tutorials

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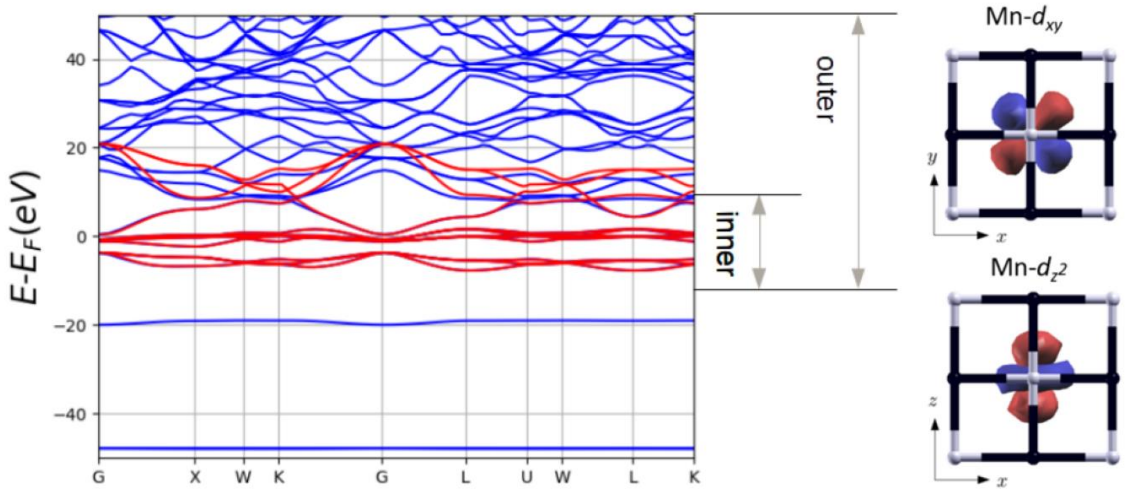
Important technical details

- Local projector
- Double counting
- Flow chart for implementation

Local Projector

The choice of local projectors can be crucial!
Candidates:

- Maximally Localized Wannier Function
  a) sufficiently large energy window
  b) optimized initial guess (centered at atoms)
- Projected Wannier Function
- Quasi-Atomic Minimal basis set orbitals



Caveat: local projectors are NOT born equal and they define "correlated manifold", therefore calculation results can differ. Important to compare results with common interface.

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- V. I. Anisimov, D. E. Kondakov, A. V. Kozhevnikov, I. A. Nekrasov, Z. V. Pchelkina, J. W. Allen, S.-K. Mo, H.-D. Kim, P. Metcalf, S. Suga, A. Sekiyama, G. Keller, I. Leonov, X. Ren, and D. Vollhardt. Phys. Rev. B 71, 125119 (2005)
- Kristjan Haule, Chuck-Hou Yee, and Kyoo Kim, Phys. Rev. B **81**, 195107 (2010)
- T.-L. Chan, Y. X. Yao, C. Z. Wang, W. C. Lu, J. Li, X. F. Qian, S. Yip, and K. M. Ho, Phys. Rev. B **76**, 205119 (2007)
- X. Qian, J. Li, L. Qi, C. Wang, T. Chan, Y. Yao, K. Ho, and S. Yip, *Quasiatomic Orbitals for Ab Initio Tight-Binding Analysis*, Phys. Rev. B **78**, (2008).

Double counting

Kohn-Sham-Hubbard scheme:

$$\begin{cases} \mathscr{E}[\rho] = T_{KSH}[\rho] + E_{HXC}[\rho] + \int \mathbf{dr}\, V(\mathbf{r})\,\rho(\mathbf{r}) + \sum_{i\geq 1} E_{dc}^{U_i J_i}\left(\langle \Psi_G | \hat{N}_i | \Psi_G \rangle\right) \\ T_{KSH}[\rho] = \min_{\Psi_G \to \rho} \langle \Psi_G | \hat{T} | \Psi_G \rangle + \sum_{i\geq 1} \hat{H}_i^{U_i J_i} \end{cases}$$

Projectors over "correlated" degrees of freedom

$$\min_{\rho} \mathscr{E}[\rho] = \min_{\Psi_G} \Big[\langle \Psi_G | \hat{T} + \int \mathbf{dr}\, V(\mathbf{r})\,\hat{\rho}(\mathbf{r}) + \sum_{i\geq 1} \hat{H}_i^{U_i J_i} | \Psi_G \rangle + E_{HXC}\left[\langle \Psi_G | \hat{\rho} | \Psi_G \rangle\right] + E_{dc}^{U,J}\left(\langle \Psi_G | \hat{N}_i | \Psi_G \rangle\right) \Big]$$

- "Fully Localized Limit" DC

$$\mu_{dc}^{FLL} = U(N_{\text{imp}} - 1/2) + J(N_{\text{imp}}^{\sigma} - 1/2),$$

- "Around Mean Field" DC

$$\mu_{dc}^{AMF} = \sum_{m'} U_{mm'} n^0 + \sum_{m', m' \neq m} (U_{mm'} - J_{mm'}) n^0$$

$n^0 = \frac{1}{2(2l+1)} \sum_{m,\sigma} n_{m\sigma}$ is the average occupancy

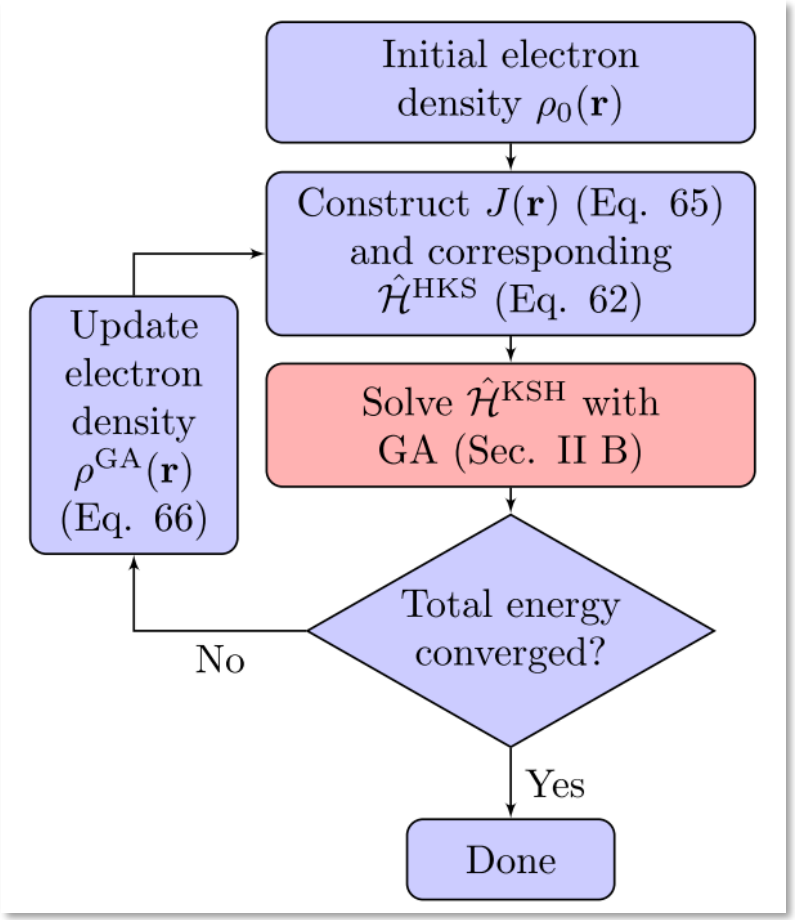
- Nominal DC

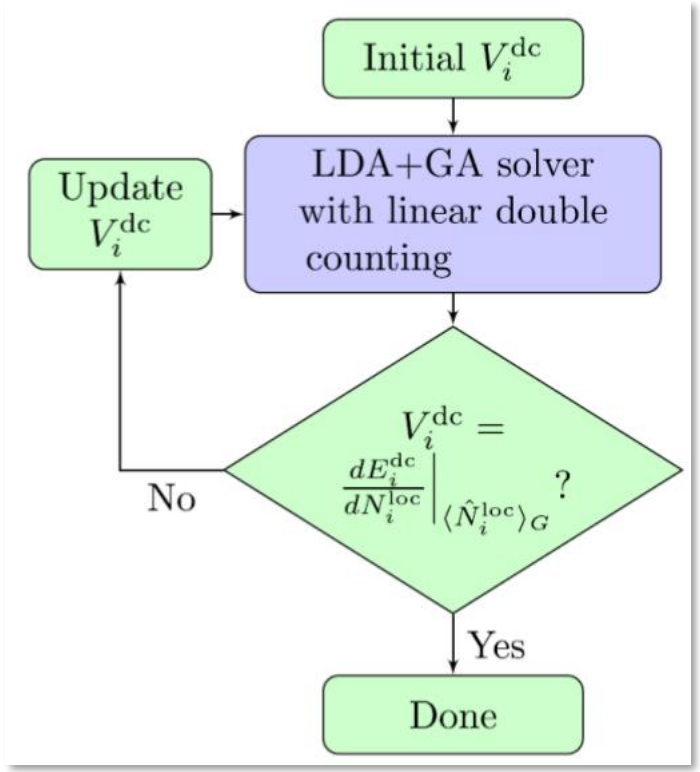
$$\mu_{dc}^{FLL} = U(N_{\text{imp}} - 1/2) + J(N_{\text{imp}}^{\sigma} - 1/2),$$

- "Exact" DC

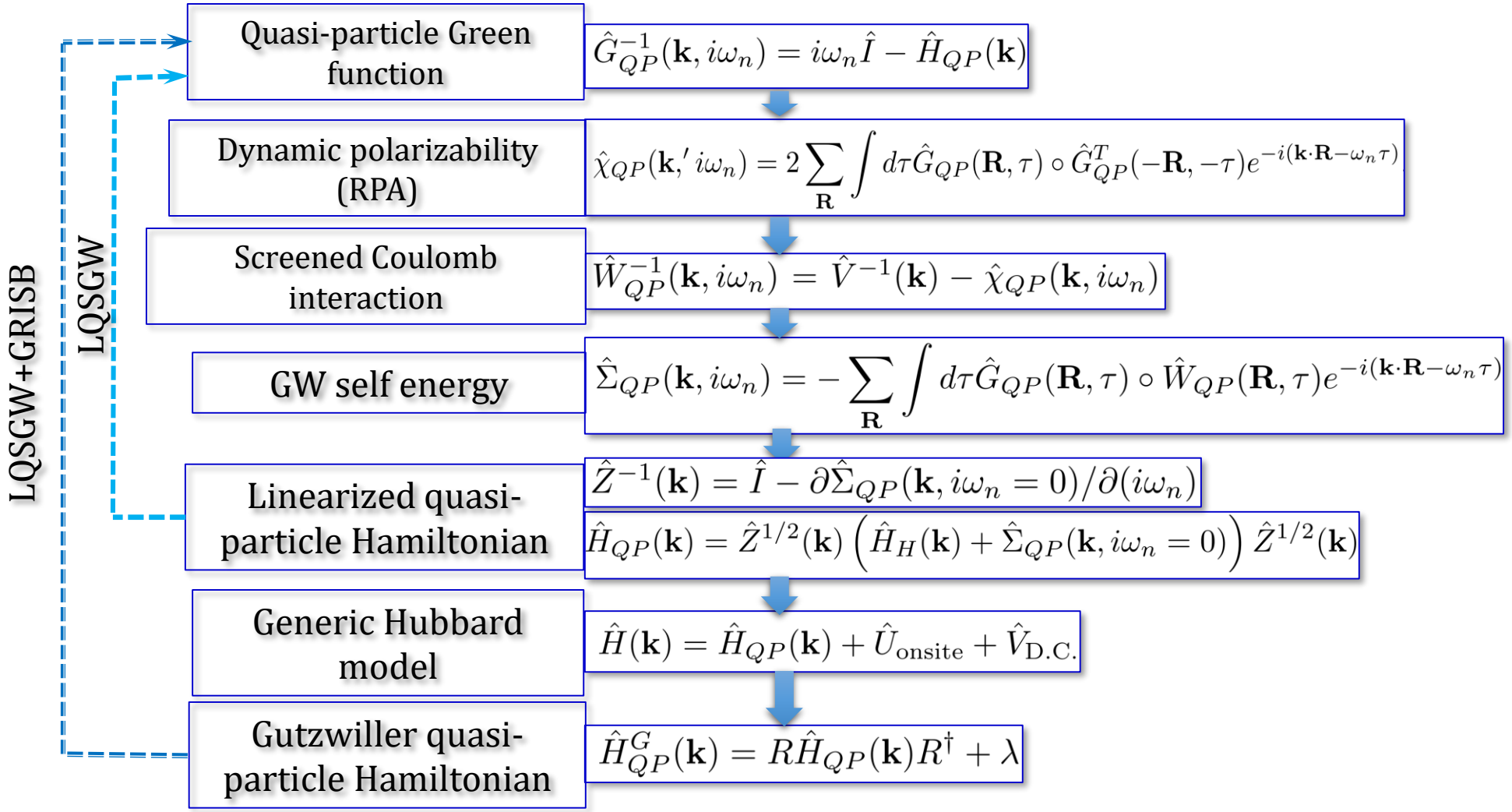
- M. T. Czyżyk and G. A. Sawatzky. Phys. Rev. B **49**, 14211 (1995)
- Kristjan Haule. Phys. Rev. Lett. **115**, 196403 (2015)

Flow chart: DFT+GRISB

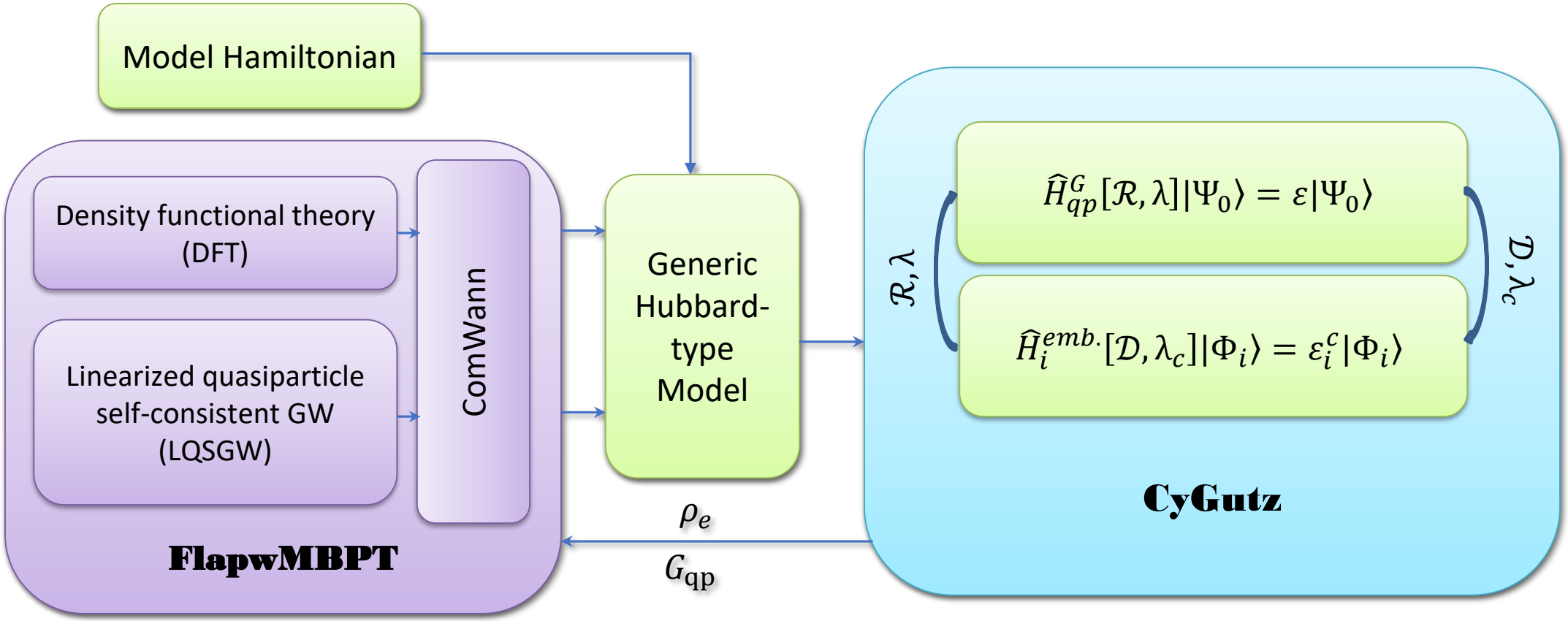




Flow chart: LQSGW+GRISB



ComRISB code structure



Examples:

https://comrisb-tutorial.readthedocs.io/en/latest/

- Single-band Bethe lattice
  - GRISB calculations with increasing *U*
  - GRISB Mott gap revealed by scanning chemical potential
- Checkboard lattice
  - GRISB calculation in PM state
  - GRISB calculation in AFM state
  - Hartree-Fock calculation in AFM state
  - Hartree-Fock calculation in PM state
  - Final Comparison
- ComRISB calculation of Fe
  - DFT-LDA calculation of Fe
  - DFT+GRISB calculation of PM Fe with zero interaction
  - DFT+GRISB calculation of PM Fe
  - DFT+GRISB calculation of FM Fe with screened interaction
- LQSGW+GRISB calculation of FeSe
  - LQSGW calculation of FeSe
  - LQSGW+GRISB calculation of FeSe

Thank You!