Approximate SCGW: A Unified View

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Full vs approximate SCGW

$$\hat{H}(\mathcal{E}_n)\,|\Psi_n\rangle \equiv \left[\hat{H}_0 + \hat{\Sigma}(\mathcal{E}_n)\right]|\Psi_n\rangle = \mathcal{E}_n\,|\Psi_n\rangle$$

$$\hat{H}_s\,|\psi_\nu\rangle = \epsilon_\nu\,|\psi_\nu\rangle$$

$$|\Psi_n\rangle = \sum_\nu C_{\nu n}\,|\psi_\nu\rangle$$

Full SCGW

$\hat{H}(\mathcal{E}_n) \rightarrow \hat{H}(\mathcal{E}_n) \rightarrow \hat{H}(\mathcal{E}_n)$

$$\sum_\nu \left[H_{\mu\nu}(\mathcal{E}_n) - \mathcal{E}_n\delta_{\mu\nu}\right]C_{\nu n} = 0$$

$$H_{\mu\nu}(\mathcal{E}_n) = \langle\psi_\mu|\,\hat{H}_0\,|\psi_\nu\rangle + \Sigma_{\mu\nu}(\mathcal{E}_n)$$

Approx. SCGW

$\hat{H}(\mathcal{E}_n) \rightarrow \hat{H}_s \rightarrow \hat{H}(\mathcal{E}_n)$

- non-hermiticity ➔ Hermitization of Σ

$$\overline{\Sigma}_{\mu\nu}(\mathcal{E}_n) \equiv \frac{1}{2}\left[\Sigma_{\mu\nu}(\mathcal{E}_n) + \Sigma^*_{\nu\mu}(\mathcal{E}_n)\right]$$

- energy dependence ➔ how to define $\hat{H}_s$?

Different schemes for energy dependence

- Faleev-van Schilfgaarde-Kotani (QSGW) scheme (PRL 2004)

$$\hat{H}_s \rightarrow \overline{H}^{(i)}_{\mu\nu} \equiv \langle\psi_\mu|\,\hat{H}_0\,|\psi_\nu\rangle + \frac{1}{2}\left[\overline{\Sigma}_{\mu\nu}(\epsilon_\mu) + \overline{\Sigma}_{\mu\nu}(\epsilon_\nu)\right]$$

- Shishkin-Marsman-Kresse scheme (PRL, 2007)

$$\left[\hat{H}_0 + \hat{\Sigma}(\tilde{\mathcal{E}}_n) + \hat{\Sigma}'(\tilde{\mathcal{E}}_n)\left(\mathcal{E}_n - \tilde{\mathcal{E}}_n\right)\right]|\Psi_n\rangle = \mathcal{E}_n\,|\Psi_n\rangle$$

$$\sum_\nu H_{\mu\nu}(\tilde{\mathcal{E}}_n)C_{\nu n} = \mathcal{E}_n S_{\mu\nu}(\tilde{\mathcal{E}}_n)C_{\nu n}$$

$$H_{\mu\nu}(\tilde{\mathcal{E}}_n) \equiv \langle\psi_\mu|\,\hat{H}_0 + \Sigma(\tilde{\mathcal{E}}_n) - \tilde{\mathcal{E}}_n\hat{\Sigma}'(\tilde{\mathcal{E}}_n)\,|\psi_\nu\rangle$$

$$S_{\mu\nu}(\tilde{\mathcal{E}}_n) \equiv \delta_{\mu\nu} - \Sigma'_{\mu\nu}(\tilde{\mathcal{E}}_n)$$

➔ use the same regularization (hermiticity, energy dependence) as in QSGW

➔ Equivalent to QSGW at convergence

Different schemes for energy dependence (cont.)

- Static COHSEX (Hedin (1965); Bruneval(2006))

$$\Sigma^{\mathrm{COHSEX}}(\mathbf{x},\mathbf{x}') = \Sigma^{\mathrm{COH}}(\mathbf{x},\mathbf{x}') + \Sigma^{\mathrm{SEX}}(\mathbf{x},\mathbf{x}')$$

$$\Sigma^{\mathrm{COH}}(\mathbf{x},\mathbf{x}') = \frac{1}{2}\delta(\mathbf{x}-\mathbf{x}')\left[W(\mathbf{x},\mathbf{x}';0) - v(\mathbf{r}-\mathbf{r}')\right]$$

$$\Sigma^{\mathrm{SEX}}(\mathbf{x},\mathbf{x}') = -\sum_{n}^{\mathrm{occ}} \psi_n(\mathbf{x})\psi_n^*(\mathbf{x}')W(\mathbf{x},\mathbf{x}';0)$$

- Sakuma-Miyake-Aryasetiawan scheme (PRB 2008)
  - Solve hermitized QP equation with full energy dependence
  - Define effective H_s using QP energies and wave-functions

$$\sum_{\nu}\left[H_{\mu\nu}(\mathcal{E}_n) - \mathcal{E}_n\delta_{\mu\nu}\right]C_{\nu n} = 0$$

$$H_{\mu\nu}(\mathcal{E}_n) = \langle\psi_\mu|\,\hat{H}_0\,|\psi_\nu\rangle + \Sigma_{\mu\nu}(\mathcal{E}_n)$$

$$\hat{H}_s \rightarrow H_{\mathrm{QP}} = \sum_n |\Psi_n\rangle\,\mathcal{E}_n\,\langle\Psi_n|$$