A similarity renormalization group approach to Green's function methods

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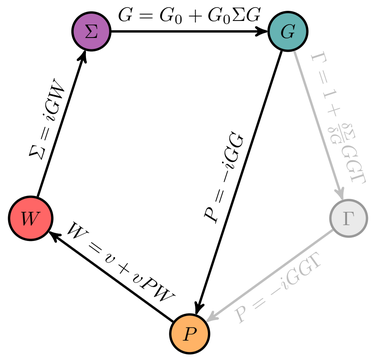
Dynamic *GW*



$$\left[\underbrace{\boldsymbol{F}}_{\text{Fock matrix}} + \underbrace{\boldsymbol{\Sigma}^{GW}(\omega = \epsilon_p^{GW})}_{\text{dynamic self-energy}}\right]\psi_p^{GW} = \epsilon_p^{GW}\psi_p^{GW}$$

$$\Sigma_{pq}^{GW}(\omega) = \sum_{i\nu}\frac{W_{pi}^{\nu}W_{qi}^{\nu}}{\omega - \epsilon_i^{GW} + \Omega_\nu - i\eta} + \sum_{a\nu}\frac{W_{pa}^{\nu}W_{qa}^{\nu}}{\omega - \epsilon_a^{GW} - \Omega_\nu + i\eta}$$

L. Hedin, Phys. Rev. 139, A796 (1965); R. M. Martin, L. Reining, and D. M. Ceperley, (Cambridge University Press, 2016)

Static *GW*

1h & 1p conf.	$\boldsymbol{F}$	$\boldsymbol{W}^{\text{2h1p}}$	$\boldsymbol{W}^{\text{2p1h}}$
2h1p conf.	$\boldsymbol{W}^{\text{2h1p}}$	$\boldsymbol{C}^{\text{2h1p}}$	$\boldsymbol{0}$
2p1h conf.	$\boldsymbol{W}^{\text{2p1h}}$	$\boldsymbol{0}$	$\boldsymbol{C}^{\text{2p1h}}$

internal space $\boldsymbol{P}$ (1h & 1p conf.); external space $\boldsymbol{Q}$ (2h1p conf., 2p1h conf.)

S. J. Bintrim and T. C. Berkelbach, J. Chem. Phys. 154, 041101 (2021).

Similarity Renormalization Group (SRG)

- SRG flow equation

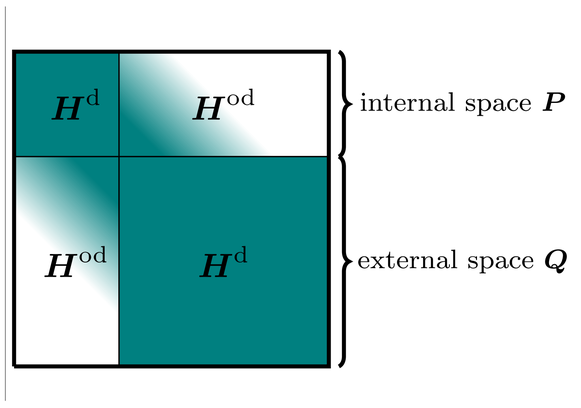
$$\frac{\mathrm{d}\boldsymbol{H}(s)}{\mathrm{d}s} = [\boldsymbol{\eta}(s), \boldsymbol{H}(s)] \quad (1)$$

- Similarity-transformed Hamiltonian

$$\boldsymbol{H}(s) = \boldsymbol{U}(s)\,\boldsymbol{H}\,\boldsymbol{U}^{\dagger}(s) \quad (2)$$

- Wegner generator

$$\boldsymbol{\eta}^{\mathrm{W}}(s) = \left[\boldsymbol{H}^{\mathrm{d}}(s), \boldsymbol{H}^{\mathrm{od}}(s)\right] \quad (3)$$



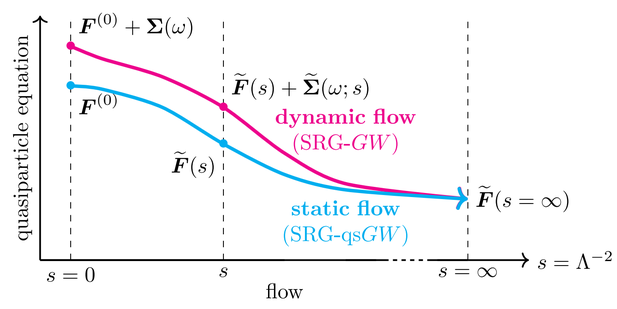
F. Wegner, Ann. Phys. 3, 77 (1994)
S. D. Głazek and K. G. Wilson, Phys. Rev. D 48, 5863 (1993)

SRG-*GW*

$$\widetilde{\boldsymbol{F}}_{pq}(s) = \delta_{pq}\epsilon_p^{\mathrm{HF}} + \sum_{r\nu}\frac{\Delta_{pr}^{\nu} + \Delta_{qr}^{\nu}}{(\Delta_{pr}^{\nu})^2 + (\Delta_{qr}^{\nu})^2}W_{pr}^{\nu}W_{qr}^{\nu}\left[1 - e^{-((\Delta_{pr}^{\nu})^2 + (\Delta_{qr}^{\nu})^2)s}\right]$$

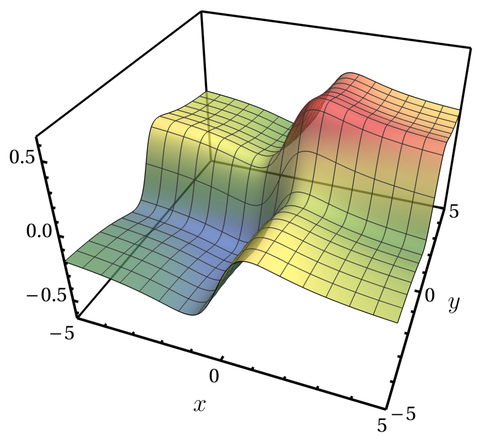
$$\Delta_{pr}^{\nu} = \epsilon_p^{GW} - \epsilon_r^{GW} \pm \Omega_\nu$$

$$\widetilde{\Sigma}_{pq}^{\text{SRG-}GW} = \sum_{i\nu}\frac{e^{-(\Delta_{pi}^{\nu})^2 s}W_{pi}^{\nu}W_{qi}^{\nu}e^{-(\Delta_{qi}^{\nu})^2 s}}{\omega - \epsilon_i^{GW} + \Omega_\nu} + \sum_{a\nu}\frac{e^{-(\Delta_{pa}^{\nu})^2 s}W_{pa}^{\nu}W_{qa}^{\nu}e^{-(\Delta_{qa}^{\nu})^2 s}}{\omega - \epsilon_a^{GW} - \Omega_\nu}$$



Functional form of the qs*GW* and SRG-qs*GW*

$$f^{\text{qs}GW}(x, y; \eta) = \frac{1}{2}\left(\frac{x}{x^2 + \eta^2} + \frac{y}{y^2 + \eta^2}\right)$$



- qs*GW* self-energy:

$$\boldsymbol{\Sigma}_{pq}^{\text{qs}GW}(\eta) = \sum_{r\nu}\frac{1}{2}\left(\frac{\Delta_{pr}^{\nu}}{(\Delta_{pr}^{\nu})^2 + \eta^2} + \frac{\Delta_{qr}^{\nu}}{(\Delta_{qr}^{\nu})^2 + \eta^2}\right)W_{pr}^{\nu}W_{qr}^{\nu}$$

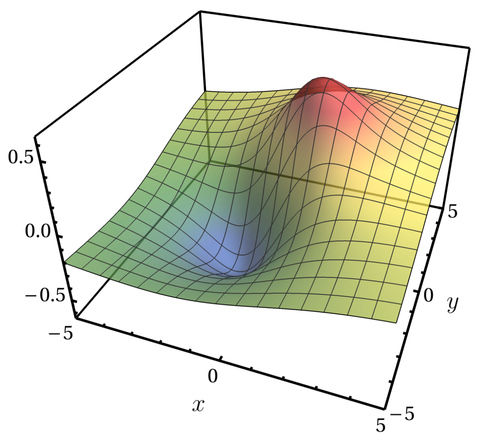
S. V. Faleev, M. van Schilfgaarde, and T. Kotani, Phys. Rev. Lett. 93, 126406 (2004)

- SRG-qs*GW* self-energy:

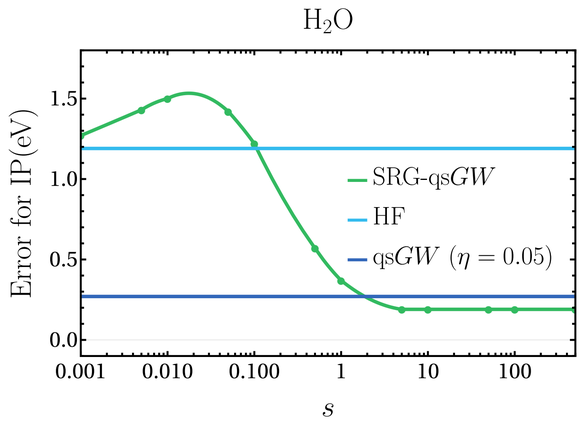
$$\boldsymbol{\Sigma}_{pq}^{\text{SRG-qs}GW}(s) = \sum_{r\nu}\frac{\Delta_{pr}^{\nu} + \Delta_{qr}^{\nu}}{(\Delta_{pr}^{\nu})^2 + (\Delta_{qr}^{\nu})^2}W_{pr}^{\nu}W_{qr}^{\nu}\left[1 - e^{-((\Delta_{pr}^{\nu})^2 + (\Delta_{qr}^{\nu})^2)s}\right]$$

A. Marie and P.-F. Loos, arXiv:2303.05984 (2023)

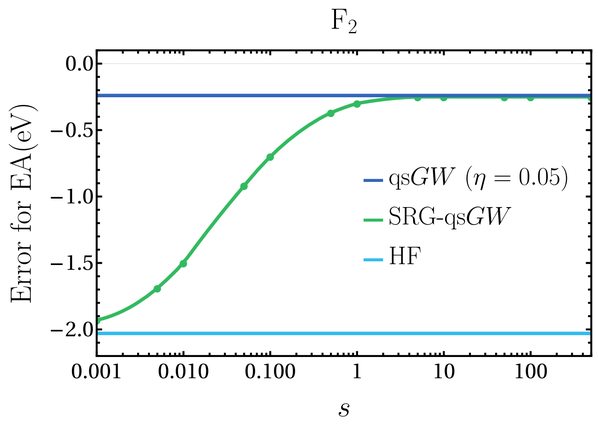
$$f^{\text{SRG-qs}GW}(x, y; \eta) = \frac{x + y}{x^2 + y^2}\left[1 - e^{-(x^2 + y^2)/(2\eta^2)}\right]$$



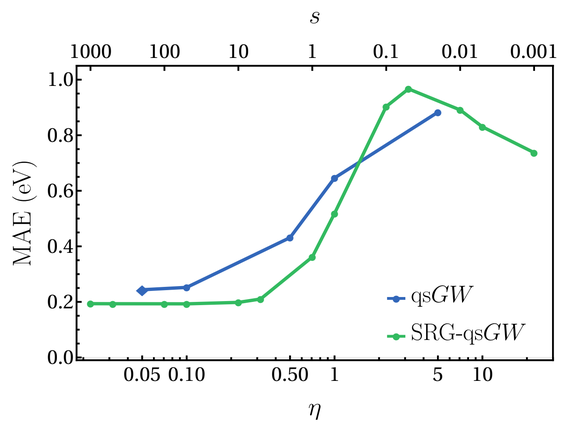
IP flow parameter dependence



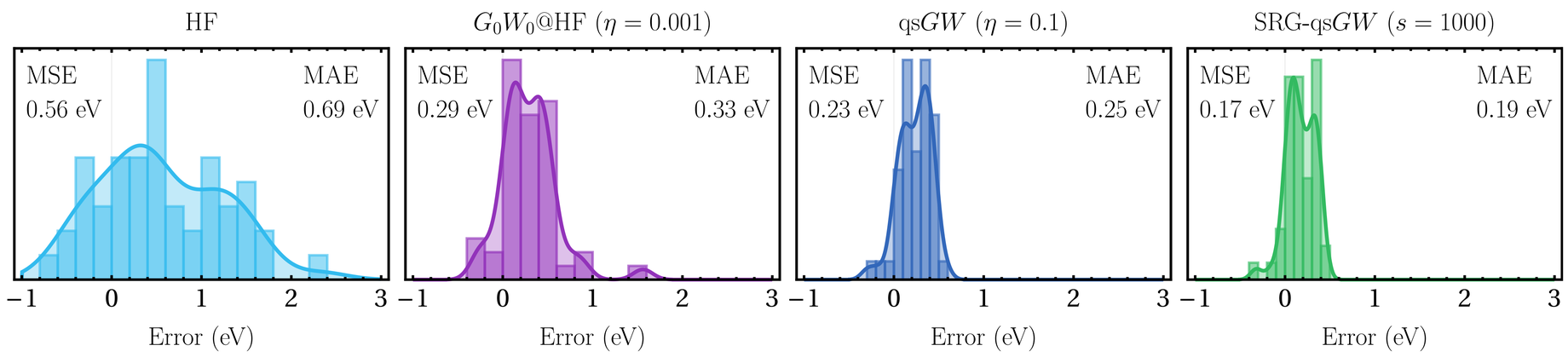
EA flow parameter dependence



MAE flow parameter dependence



*GW*50 statistics



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