A similarity renormalization group approach to Green's function methods

Antoine Marie and Pierre-François Loos

Laboratoire de Chimie et Physique Quantiques (UMR 5626), Université de Toulouse, CNRS, UPS, France

loos@irsamc.ups-tlse.fr

The family of Green's function methods based on the GW approximation has gained popularity in the electronic structure theory thanks to its accuracy in weakly correlated systems combined with its cost-effectiveness. Despite this, self-consistent versions still pose challenges in terms of convergence. A recent study has linked these convergence issues to the intruder-state problem [2]. In this talk, we present a perturbative analysis of the similarity renormalization group (SRG) approach performed on Green's function methods [1]. The SRG formalism enables us to derive, from first principles, the expression of a naturally static and Hermitian form of the self-energy that can be employed in quasiparticle self-consistent GW (qsGW) calculations. The resulting SRG-based regularized self-energy significantly accelerates the convergence of qsGW calculations, slightly improves the overall accuracy, and is straightforward to implement in existing code.

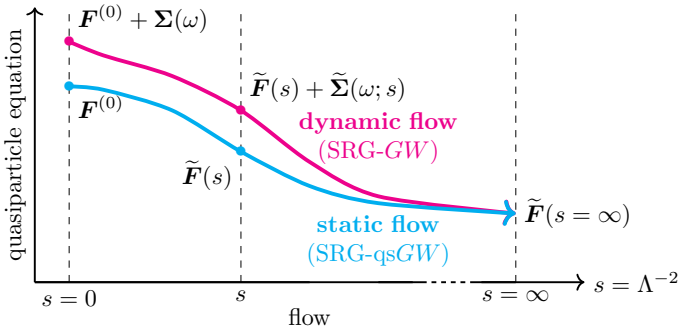

Figure 1: Schematic evolution of the quasiparticle equation as a function of the flow parameter s in the case of the dynamic SRG-GW flow (magenta) and the static SRG-qsGW flow (cyan).

[1] Antoine Marie and Pierre-François Loos. *A similarity renormalization group approach to Green's function methods*. 2023. arXiv: 2303.05984 [physics.chem-ph].

[2] Enzo Monino and Pierre-François Loos. "Unphysical discontinuities, intruder states and regularization in GW methods". In: *J. Chem. Phys.* 156.23 (2022), p. 231101. DOI: 10.1063/5.0089317.