Group Meeting Slides

Patryk Kozlowski

November 2, 2025

Outline

1. GW

2. Cumulant Expansion

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Introduction

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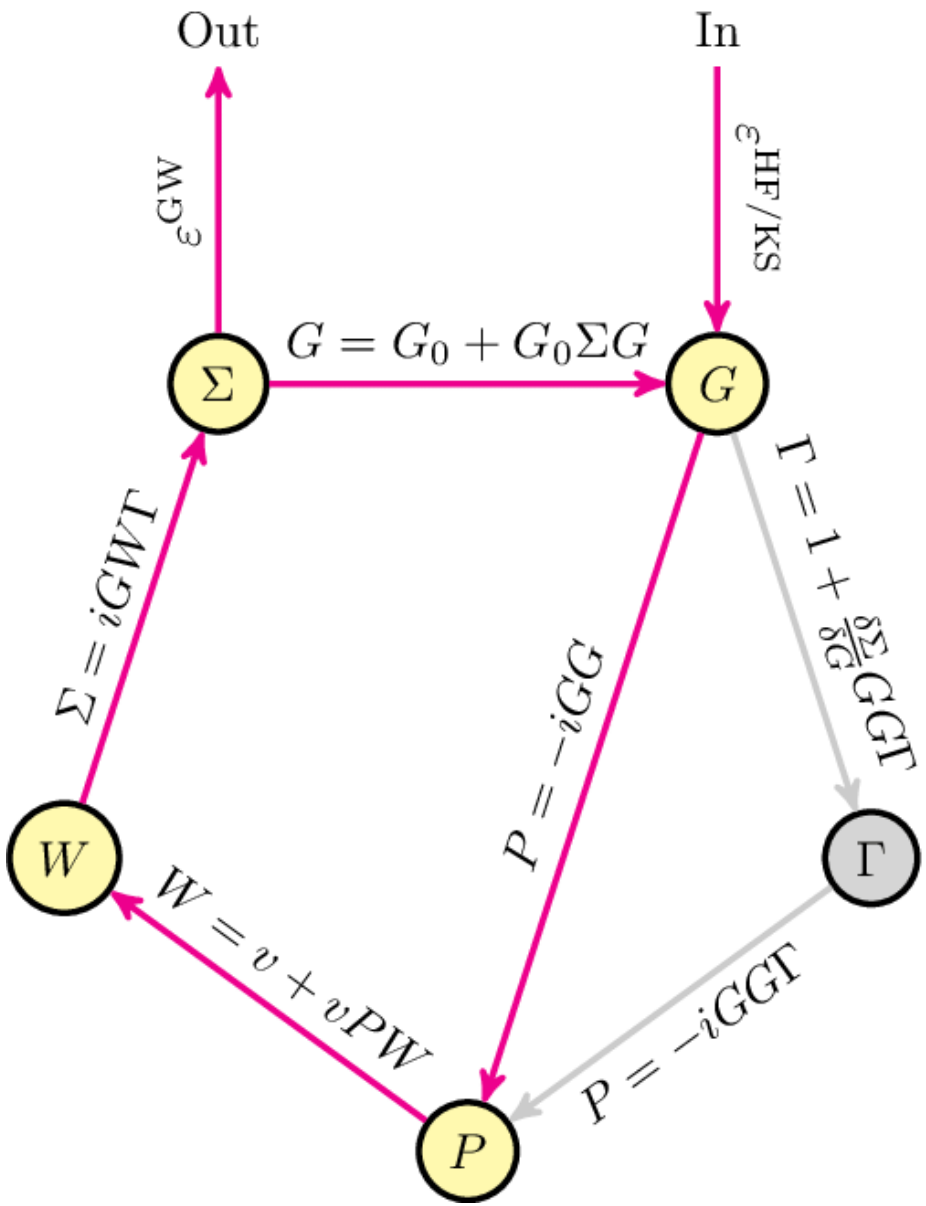
where G is the interacting Green's function, G_0 is the non-interacting Green's function, and Σ is the proper self-energy. The GW approximation for the self-energy is

$$\Sigma = iGW\Gamma \tag{2}$$

$$\approx iGW \tag{3}$$

Hedin's Equations [1]



Frequency Integral [?]

Practically,

$$\Sigma^{GW}(\mathbf{r},\mathbf{r}';\omega) = \frac{i}{2\pi}\int_{-\infty}^{\infty} d\omega' G\left(\mathbf{r},\mathbf{r}';\omega+\omega'\right) W\left(\mathbf{r},\mathbf{r}';\omega'\right) \tag{4}$$

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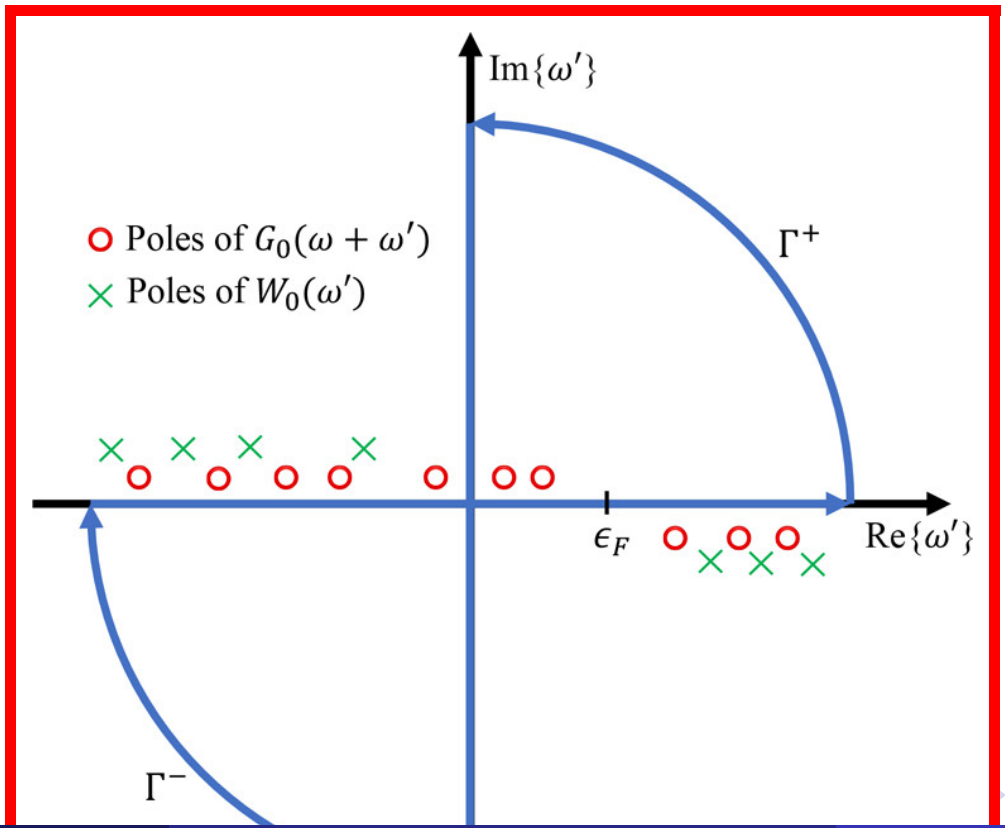

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Contour deformation	$O(N^5)$	Deform the contour to do the integral in a piecewise fashion. Accurate for deep core orbitals.
Frequency-free	$O(N^4)$	Eliminate frequency variable in the convolution, so we are not constrained by the poles.

Solving the quasi-particle (QP) equation

In *GW*, we can compute QP energies by solving:

$$\epsilon_p^{QP} = \epsilon_p^{HF} + \Sigma_{pq}^c(\omega)\delta_{pq} \tag{6}$$

with

$$\Sigma_{pq}^c(\omega) = \sum_{\mu}^{\text{RPA}} \left(\sum_{i}^{\text{occupied}} \frac{w_{pi}^{\mu} w_{iq}^{\mu}}{\omega - (\epsilon_i - \Omega_\mu) + i\eta} + \sum_{a}^{\text{virtual}} \frac{w_{pa}^{\mu} w_{aq}^{\mu}}{\omega - (\epsilon_a + \Omega_\mu) - i\eta} \right) \tag{7}$$

Using Lowdin partitioning we can recast this as a matrix problem

$$\boldsymbol{H}^{GW} = \begin{pmatrix} \boldsymbol{F} & \boldsymbol{W}^{<} & \boldsymbol{W}^{>} \\ \boldsymbol{W}^{<,\dagger} & \boldsymbol{d}^{<} & 0 \\ \boldsymbol{W}^{>,\dagger} & 0 & \boldsymbol{d}^{>} \end{pmatrix} \tag{8}$$

where the QP energies are the eigenvalues of $\boldsymbol{H}^{GW}$.

Moment-conserving GW [?]

1. Devises a Lanczos procedure to iteratively diagonalize equation 8.
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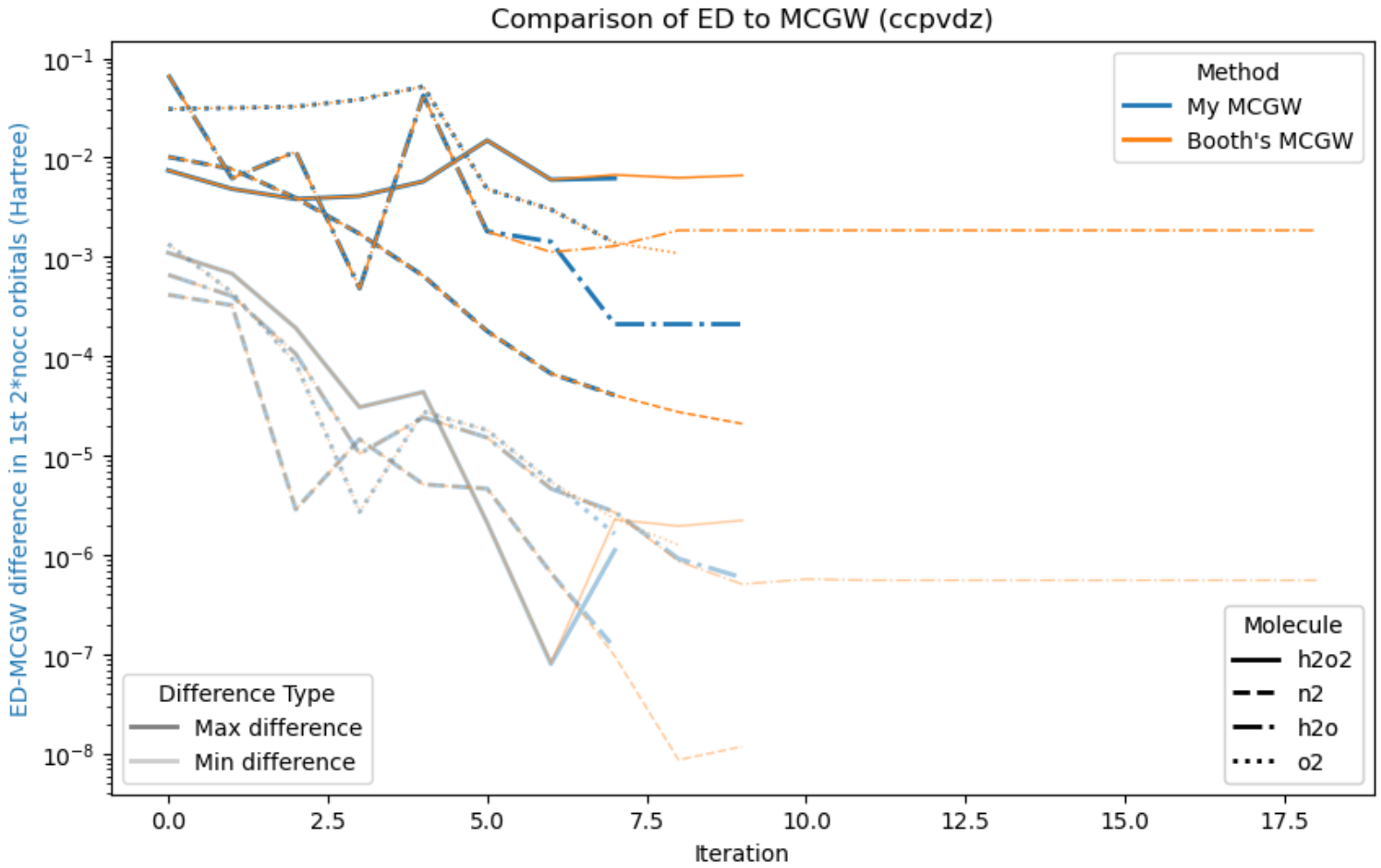

Why?

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1. A Krylov subspace is never explicitly constructed.
2. Therefore, it cannot be reorthogonalized, so there is no guarantee that the Ritz values will converge to the true eigenvalues.

Outline

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2. Cumulant Expansion

How it is derived

The cumulant expansion is a technique used to improve the description of electron correlation effects in many-body systems. It provides a way to go beyond the GW approximation by including higher-order interactions and capturing satellite features in spectral functions.

Analytical self-consistency

The analytical self-consistency condition in the cumulant expansion framework ensures that the Green's function and the self-energy are mutually consistent. This is achieved by iteratively updating the self-energy based on the current Green's function and vice versa.

Current project

Our current project focuses on implementing the cumulant expansion in the context of the GW approximation. We aim to develop a computational framework that can efficiently handle the increased complexity of the self-energy calculations while maintaining the accuracy of the results.

Summary

In summary, the GW approximation and cumulant expansion are powerful tools for studying electronic structures in materials. By incorporating electron correlation effects more accurately, these methods provide deeper insights into the properties of complex systems.

Thank for listening!

References I

[1] Pierre-François Loos, Pina Romaniello, and J. Berger. Green functions and self-consistency: Insights from the spherium model. *Journal of Chemical Theory and Computation*, 14, 03 2018. doi: 10.1021/acs.jctc.8b00260.