Falling into the Black Hole of Vertex Corrections

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What's New in Green's Function Methods?

Recent developments in GW and BSE

- GW for resonances
- Analytic nuclear gradients for GW and BSE
- Non-Dyson GW schemes: Decoupling the IP and EA sectors
- Fully self-consistent GW (scGW) with Hartree-Fock-Bogoliubov (HFB) reference

Beyond GW: vertex corrections

- Vertex corrections via extended coupled cluster (ECC)
- Introducing the singles into GW: direct-ring (dr) ECCSD
- Algebraic-diagrammatic construction (ADC) of $G3W2$
- Parquet formalism

Collaborators

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(Postdoc)

Fábris
Kossoski
(Toulouse)

Johannes
Tölle
(Hamburg)

The *GW* Approximation in a Single Slide

quasiparticle energies

$$\left.\begin{aligned} \left[\boldsymbol{f} + \Sigma^{GW}(\omega = \epsilon_\nu^{GW})\right]\psi_\nu^{GW} &= \epsilon_\nu^{GW}\psi_\nu^{GW} \\ \Sigma^{GW}(\omega) &= \left(\boldsymbol{U}^{\text{2h1p}}\right)^\dagger \cdot \left(\omega - \boldsymbol{K}^{\text{2h1p}}\right)^{-1} \cdot \boldsymbol{U}^{\text{2h1p}} \\ &\quad + \left(\boldsymbol{U}^{\text{2p1h}}\right)^\dagger \cdot \left(\omega - \boldsymbol{K}^{\text{2p1h}}\right)^{-1} \cdot \boldsymbol{U}^{\text{2p1h}} \end{aligned}\right\} \underset{\text{upfolding}}{\overset{\text{downfolding}}{\leftrightharpoons}} \left\{\begin{aligned} \boldsymbol{H}\Psi_\nu^{GW} &= \boxed{\epsilon_\nu^{GW}}\,\Psi_\nu^{GW} \\ \boldsymbol{H} &= \begin{pmatrix} \boldsymbol{f} & \left(\boldsymbol{U}^{\text{2h1p}}\right)^\dagger & \left(\boldsymbol{U}^{\text{2p1h}}\right)^\dagger \\ \boldsymbol{U}^{\text{2h1p}} & \boldsymbol{K}^{\text{2h1p}} & \boldsymbol{0} \\ \boldsymbol{U}^{\text{2p1h}} & \boldsymbol{0} & \boldsymbol{K}^{\text{2p1h}} \end{pmatrix} \end{aligned}\right.$$

RPA excitation energies

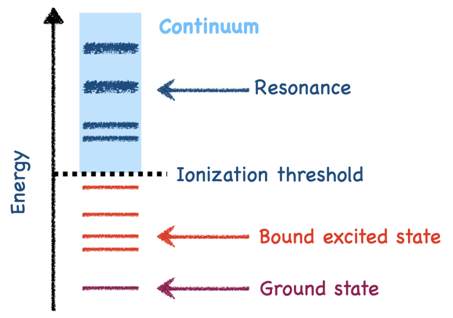
$$\begin{aligned} \left(\boldsymbol{K}^{\text{2h1p}}\right)_{i\nu,j\mu} &= \left(\epsilon_i - \boxed{\Omega_\nu}\right)\delta_{ij}\delta_{\nu\mu} \\ \left(\boldsymbol{K}^{\text{2p1h}}\right)_{a\nu,b\mu} &= \left(\boxed{\epsilon_a} + \Omega_\nu\right)\delta_{ab}\delta_{\nu\mu} \end{aligned} \qquad \begin{aligned} \left(\boldsymbol{U}^{\text{2h1p}}\right)_{i\nu,q} &= M_{qi,\nu} \\ \left(\boldsymbol{U}_1^{\text{2p1h}}\right)_{a\nu,q} &= \boxed{M_{aq,\nu}} \end{aligned}$$

mean-field energies

screened integrals

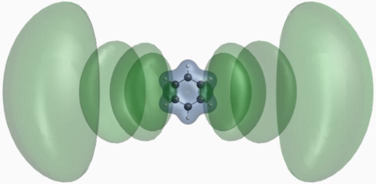
Bintrim & Berkelbach, JCP 154 (2021) 041101; Monino & Loos, JCP 156 (2022) 231101

Electronic Resonances



Jagau, Bravaya & Krylov, Annu. Rev. Phys. Chem. 68 (2017) 525

Complex Absorbing Potential (CAP)



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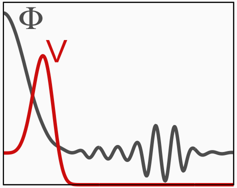

Riss & Meyer, JPB 26 (1993) 4503

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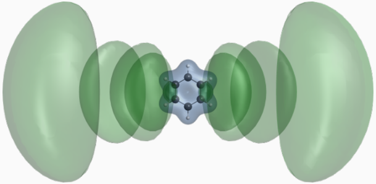
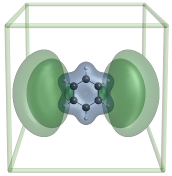
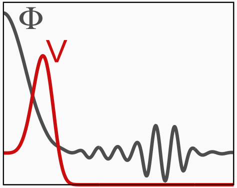




$H = T + V$

$H(\eta) = T + V - i\eta W$



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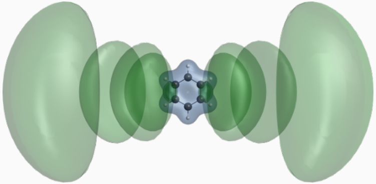

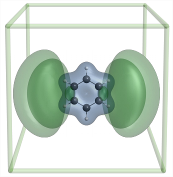

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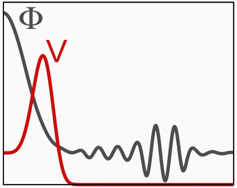

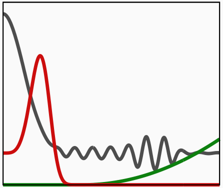

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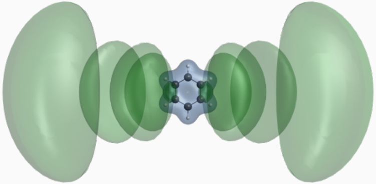

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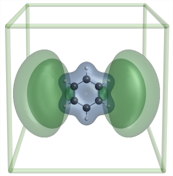

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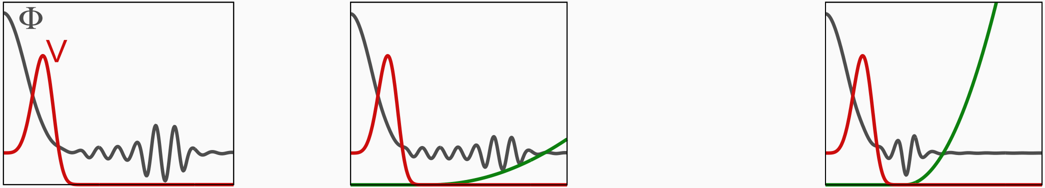

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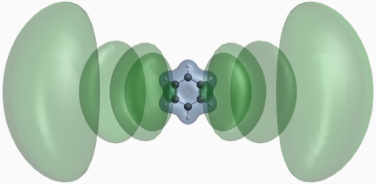

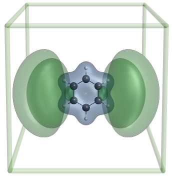

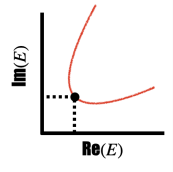

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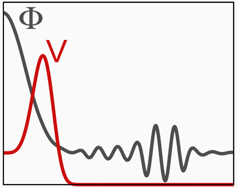

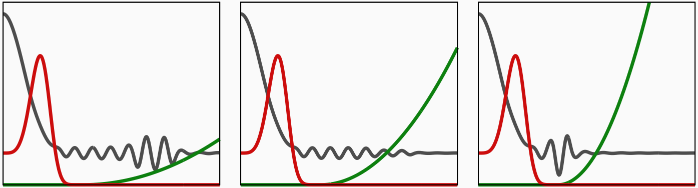

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π Shape Resonance

Complex-valued energy

$$\overset{\text{CAP Hamiltonian}}{\hat{H}(\eta)} = \hat{T} + \hat{V} - i\eta \overset{\text{Absorbing potential}}{\hat{W}} \quad (\eta > 0) \qquad \overset{\text{Energy}}{E} = \underset{\text{Resonance position}}{E_R} - i \overset{\text{Resonance width}}{\Gamma}/2$$

NB: Γ^{-1} is proportional to the resonance lifetime

$N_2{}^-$/aug-cc-pVTZ+3s3p3d

Method	E_R (eV)	Γ (eV)
Experiment	2.316	0.414
CAP-qs*GW*[1]	2.565	0.460
CAP-EA-EOM-CCSD[2]	2.487	0.417
CAP-CIPSI [3]	2.449(1)	0.391(3)

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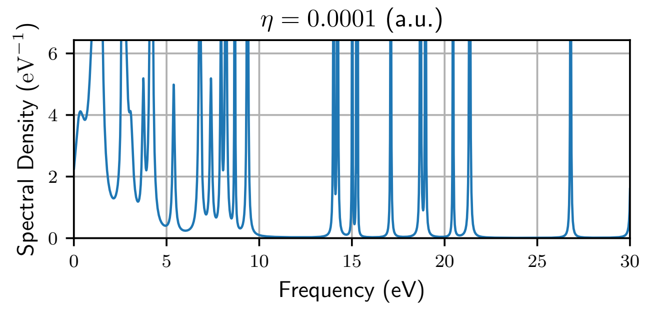
[1] Burth et al. JCTC 21 (2025) 11463

[2] Zuev et al. JCP 141 (2014) 024102

[3] Damour et al. JPCL 15 (2024) 8296

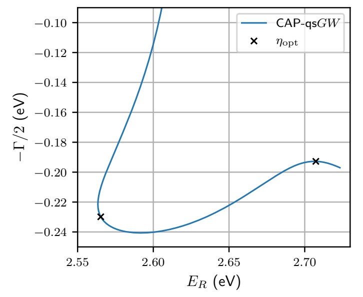
Spectral Function of N_2



Burth, Kossoski & Loos, JCTC 21 (2025) 11463

Spectral function

$$A(\omega) = \frac{1}{\pi}\,\mathrm{Im}\,|G(\omega)|$$



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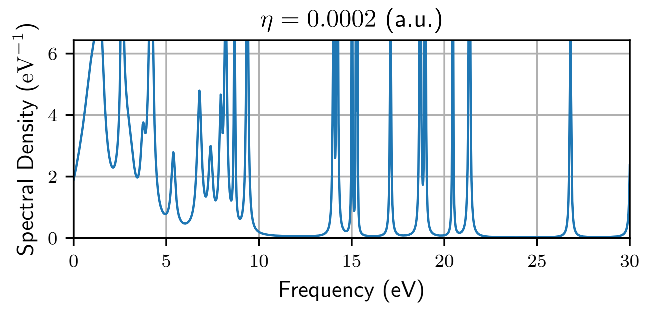

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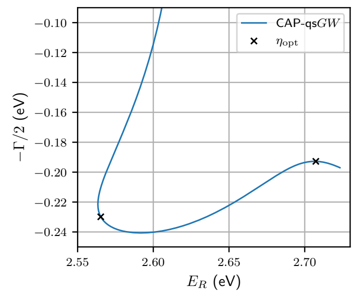

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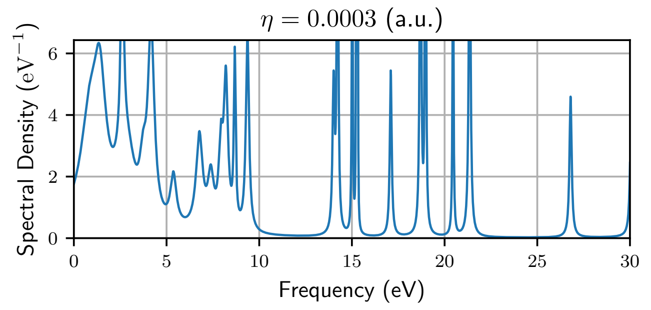

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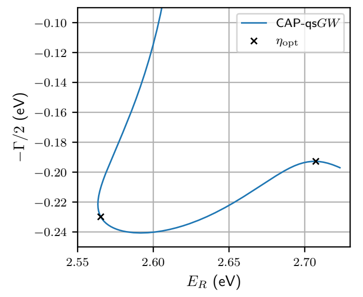

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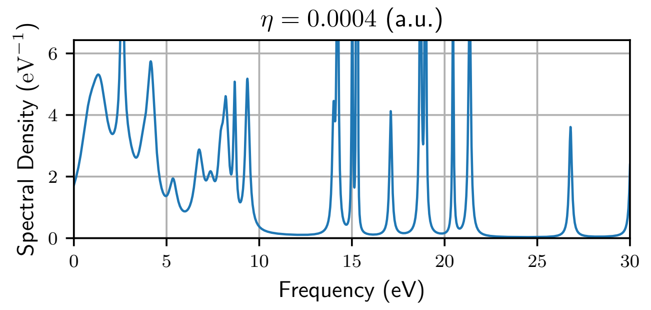

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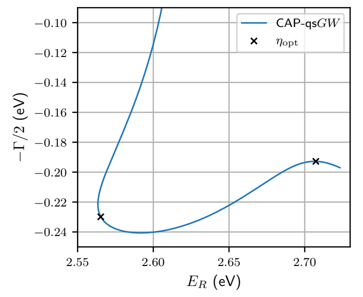

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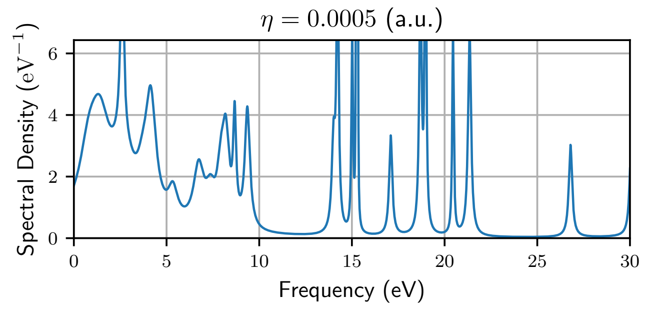

$\eta = 0.0005$ (a.u.)

Burth, Kossoski & Loos, JCTC 21 (2025) 11463

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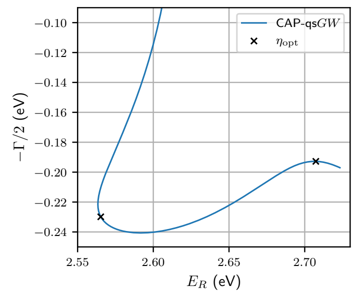

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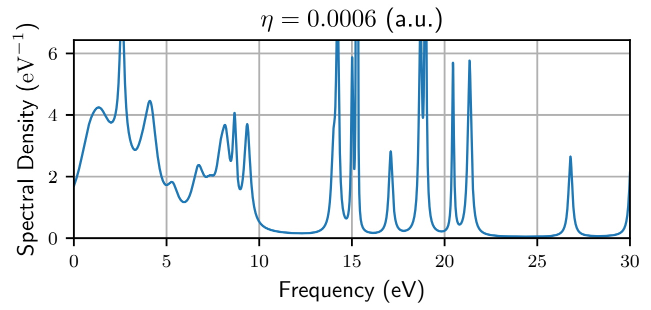

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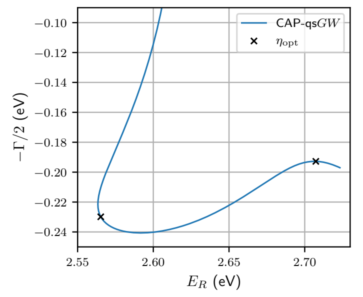

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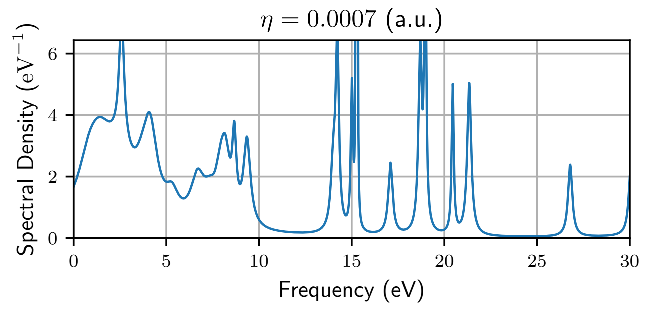

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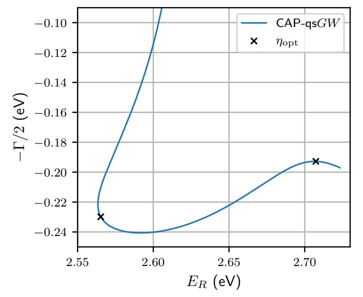

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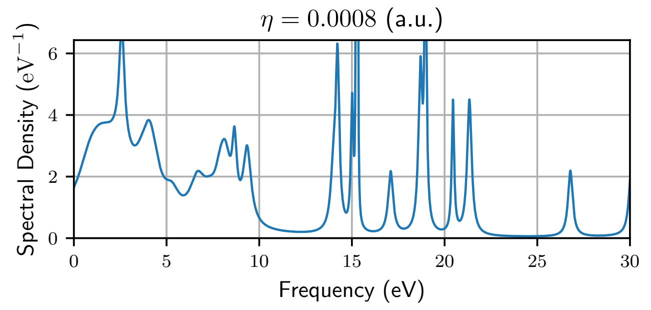

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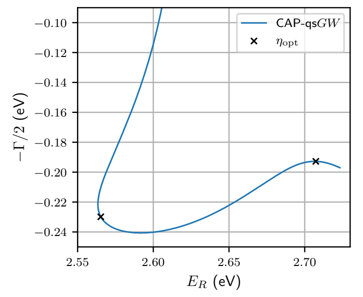

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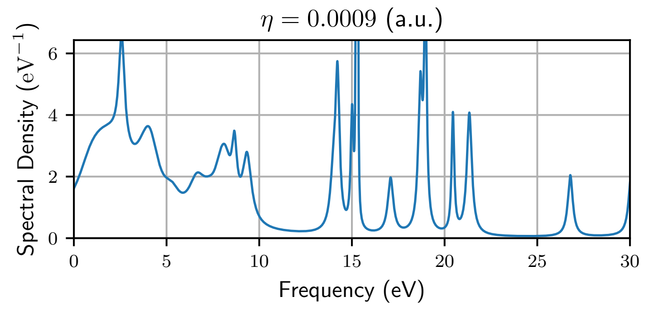

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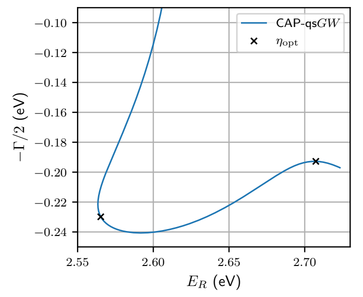

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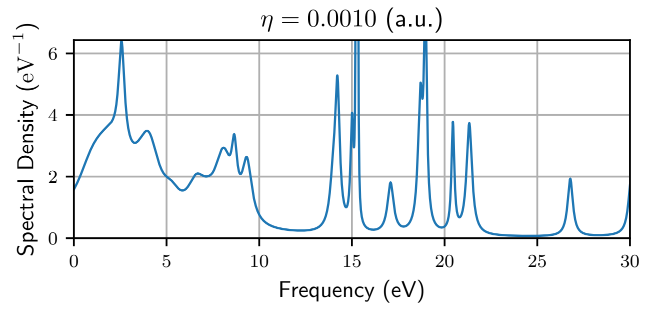

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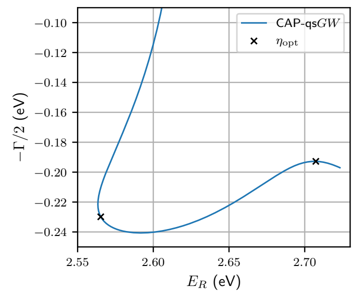

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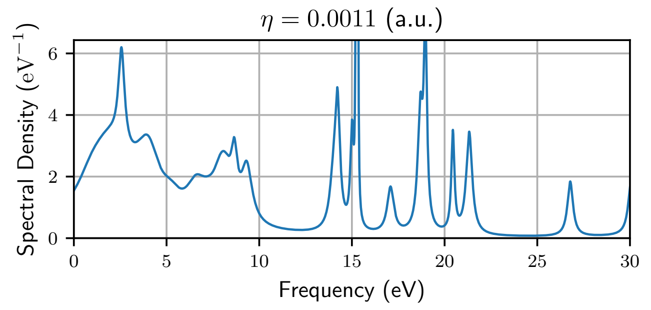

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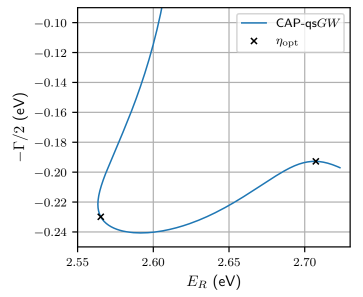

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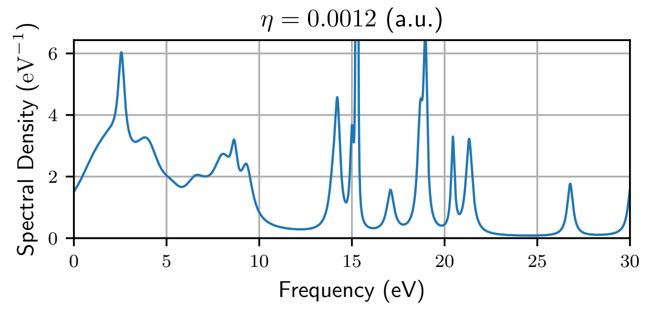

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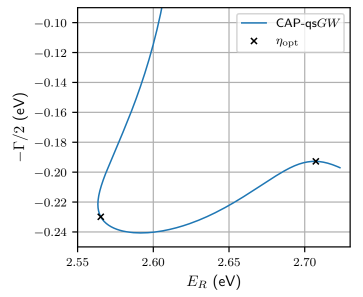

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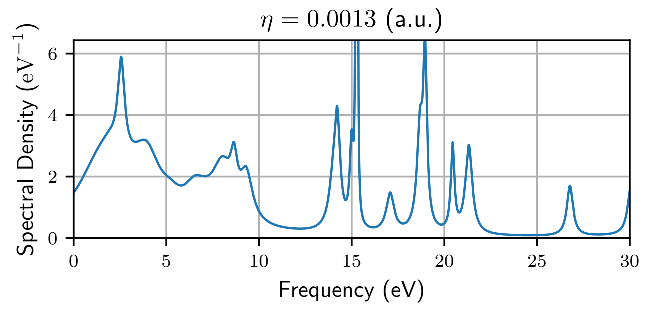

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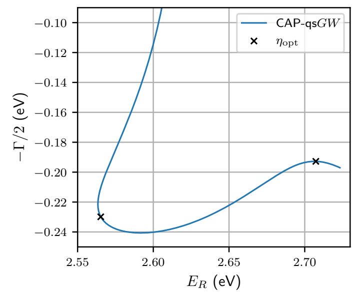

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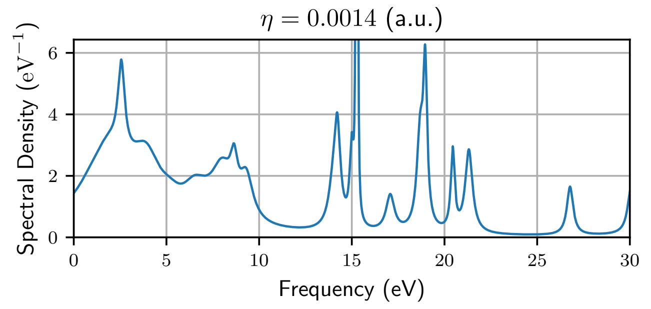

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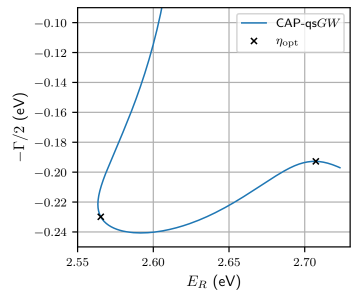

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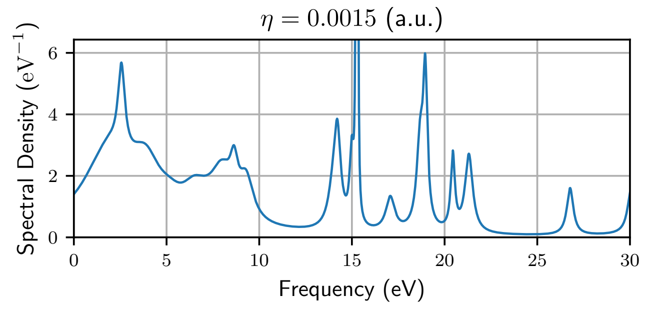

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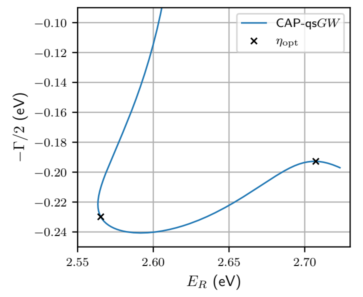

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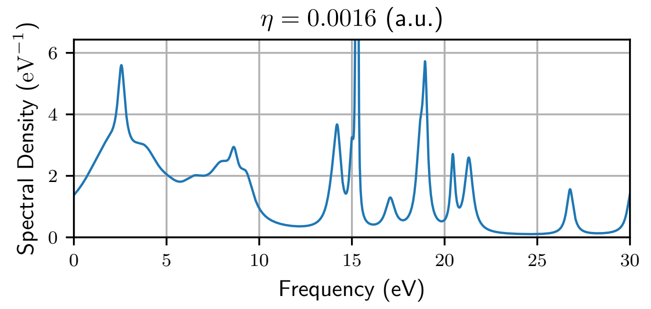

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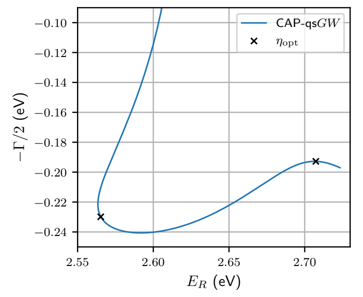


GW for Resonances

Take-home messages

- *GW* interfaced with pyOpenCAP ⇒ CAP-*GW*
  https://github.com/gayverjr/opencap

- Self-consistency is crucial ⇒ quasiparticle self-consistent *GW* (qs*GW*)

- qs*GW* performed with SRG regularization
  Marie & Loos, JCTC 19 (2023) 3943
  Monino & Loos, JCP 156 (2022) 231101

- SRG-qs*GW* is similar in spirit to κ-OOMP2
  Lee & Head-Gordon JCTC 14 (2018) 520
  Shee et al. JPCL 12 (2021) 12084

Analytic Nuclear Gradients for *GW* and Bethe-Salpeter Equation (BSE)

Following the unitary CC (UCC) formalism

- *GW* is IP+EA-EOM-drUCCD
  Tölle & Chan, JCP 158 (2023) 124123

- Derivatives obtained thanks to the formal connection with UCC
  Tölle, JPCL 16 (2025) 3672
  Tölle, Kitsaras & Loos, JPCL 16 (2025) 11134

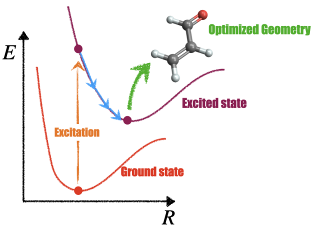
Following the extended CC (ECC) formalism

- *GW* is also IP+EA-EOM-drECCD
  Tölle et al. JCTC (in press) arXiv:2602.10887

- Derivatives obtained thanks to the formal connection with ECC
  Kitsaras, Tölle & Loos, JCP 164 (2026) 044122

- No truncation of commutators but more Lagrange multipliers

$$\bar{H}^{\text{UCC}} = e^{\hat{T}^\dagger} e^{-\hat{T}} \hat{H} e^{\hat{T}} e^{-\hat{T}^\dagger}$$



$$\bar{H}^{\text{ECC}} = e^{\hat{Z}} e^{-\hat{T}} \hat{H} e^{\hat{T}} e^{-\hat{Z}}$$

What's Next?

Future developments

- Dynamical BSE (i.e., BSE with a dynamical kernel) is finally getting some traction
  Loos & Blase, JCP 153 (2020) 114120
  Bintrim & Berkelbach, JCP 156 (2022) 044114
  Wen, Harsha & Zgid, arXiv:2604.22187

$$\begin{pmatrix} \boldsymbol{A}(\omega = \Omega_\nu^N) & \boldsymbol{B} \\ -\boldsymbol{B} & -\boldsymbol{A}(\omega = \Omega_\nu^N) \end{pmatrix} \begin{pmatrix} \boldsymbol{X}_\nu \\ \boldsymbol{Y}_\nu \end{pmatrix} = \Omega_\nu^N \begin{pmatrix} \boldsymbol{X}_\nu \\ \boldsymbol{Y}_\nu \end{pmatrix}$$

- Dynamical BSE (beyond TDA) gradient underway via the UCC route

- Static BSE gradients and non-adiabatic couplings via the ECC route

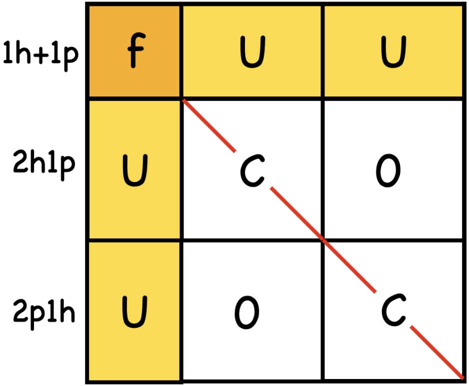
- We want to do non-adiabatic MD with BSE@*GW*

Non-Dyson GW Scheme

What's the idea?

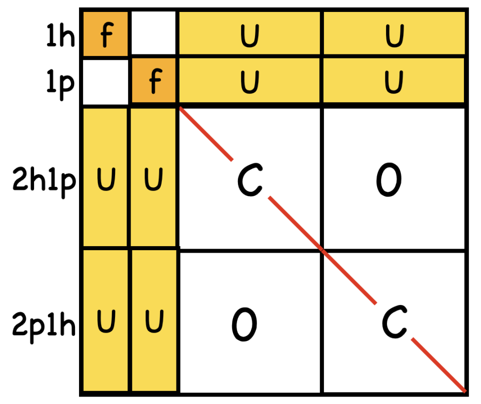
- The idea is to decouple IP and EA sectors: valence IPs/EAs become lowest eigenvalues
- Seminal ideas from Schirmer and coworkers in the ADC context
  Trofimov & Schirmer, JCP 123 (2005) 144115
  Schirmer, Lecture Notes in Chemistry, Vol. 94, Springer
- Previous results were not encouraging
  Bintrim & Berkelbach, JCP 154 (2021) 041101
  Tölle & Chan, JCP 158 (2023) 124123
- We recently found that it's not that bad after all...
  Loos & Tölle, arXiv:2604.08350

Non-Dyson *GW* Scheme: How Does it Work?



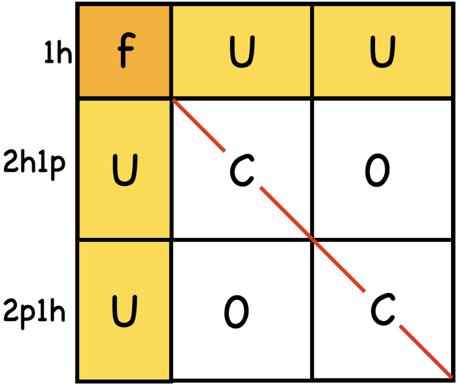
1h+1p	f	U	U
2h1p	U	C	0
2p1h	U	0	C

Non-Dyson GW Scheme: How Does it Work?



1h	f		U	U
1p		f	U	U
2h1p	U	U	C	0
2p1h	U	U	0	C

Non-Dyson *GW* Scheme: How Does it Work?



1h	f	U	U
2h1p	U	C	0
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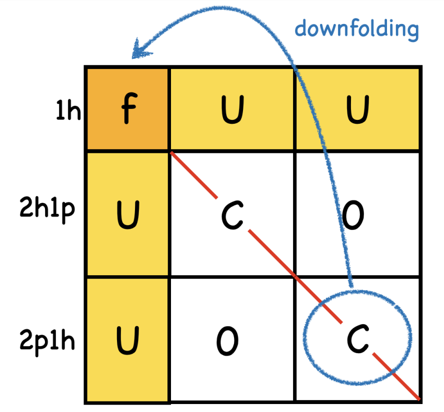
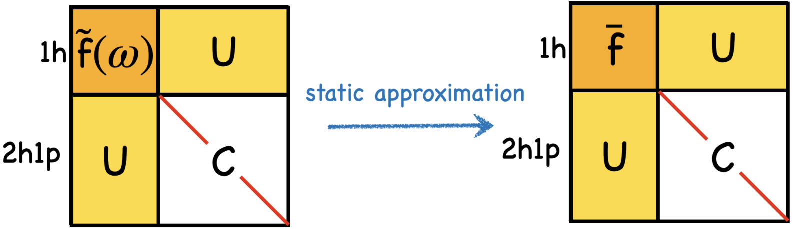
Non-Dyson GW Scheme: How Does it Work?



$$\begin{array}{c|ccc} \text{1h} & f & U & U \\ \text{2h1p} & U & C & 0 \\ \text{2p1h} & U & 0 & C \end{array}$$

Non-Dyson *GW* Scheme: How Does it Work?

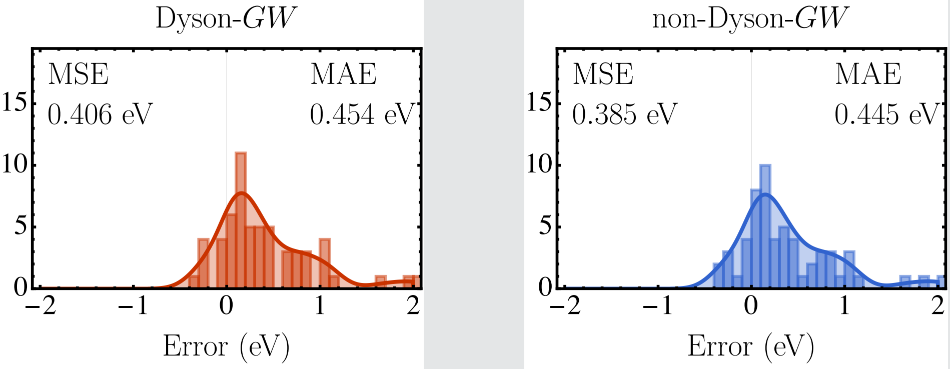


$$\tilde{f}(\omega) = f + \Sigma^{2p1h}(\omega)$$

$$\bar{f} = f + \bar{\Sigma}^{2p1h}$$

Dyson vs Non-Dyson for *GW*

Inner- and outer-valence IPs (aug-cc-pVTZ) for 23 small molecules (FCI reference)



Marie & Loos, JCTC 20 (2024) 4751

Non-Dyson *GW* Schemes

Take-home messages

- Non-Dyson-*GW* systematically reproduces Dyson-*GW*
  Loos & Tölle, arXiv:2604.08350

- Even better for core IPs: justify the cumulant Green's function ansatz
  McClain et al. PRB 93 (2016) 235139
  Loos, Marie & Ammar, Faraday Discuss. 254 (2024) 240

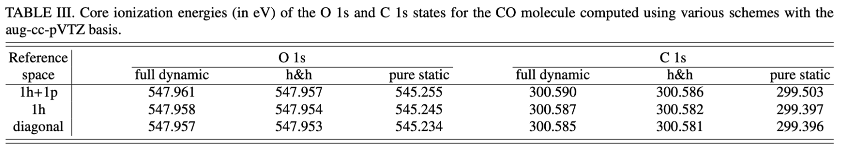


TABLE III. Core ionization energies (in eV) of the O 1s and C 1s states for the CO molecule computed using various schemes with the aug-cc-pVTZ basis.

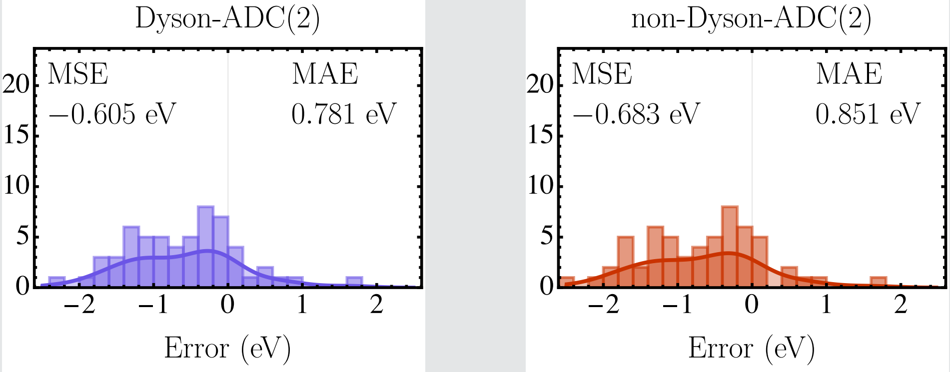
Reference space	O 1s			C 1s		
	full dynamic	h&h	pure static	full dynamic	h&h	pure static
1h+1p	547.961	547.957	545.255	300.590	300.586	299.503
1h	547.958	547.954	545.245	300.587	300.582	299.397
diagonal	547.957	547.953	545.234	300.585	300.581	299.396

- Other hybrid schemes might require regularization

- Is it also true for ADC?

Dyson vs Non-Dyson for ADC(2)

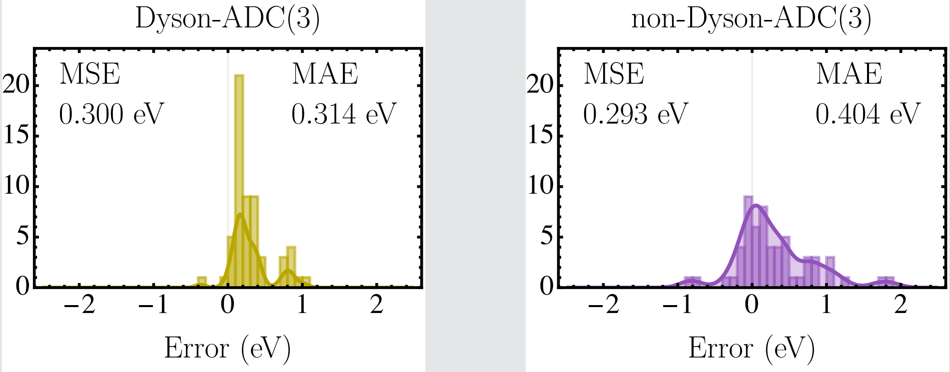
Inner- and outer-valence IPs (aug-cc-pVDZ) for 23 small molecules (FCI reference)



Marie, Tölle & Loos, arXiv:2606.04285

Dyson vs Non-Dyson for ADC(3)

Inner- and outer-valence IPs (aug-cc-pVDZ) for 23 small molecules (FCI reference)



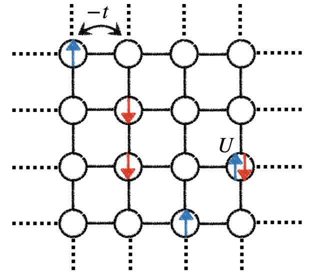
Marie, Tölle & Loos, arXiv:2606.04285

sc*GW*@HFB

GW based on a Hartree-Fock-Bogoliubov (HBF) reference

- Based on our recent work on anomalous propagators (Gorkov propagator)
  Marie et al. PRB 110 (2024) 115155; JCP 162 (2025) 134105
- sc*GW*@HFB for small Hubbard lattices ($U < 0$) where HFB solutions can be found
  Rodriguez-Mayorga, Tölle & Loos, in preparation
  Abraham, Harsha & Zgid, JCTC 20 (2024) 4579
- sc*GW*@HFB looks very bad (probably due to lack of exchange)
- Vertex corrections look promising

$$\boldsymbol{G} = \begin{pmatrix} G^{\text{he}} & G^{\text{hh}} \\ G^{\text{ee}} & G^{\text{eh}} \end{pmatrix} \quad \Rightarrow \quad \chi_0 = -\mathrm{i}\Big[G^{\text{he}} G^{\text{eh}} - G^{\text{hh}} G^{\text{ee}}\Big]$$

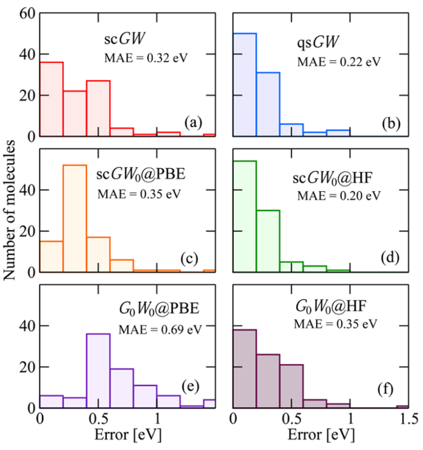


Vertex Corrections

Improving upon *GW* is hard...

Motivations To Go Beyond *GW*

- *GW* is good for principal IPs (e.g., $GW100$), especially if one tunes the starting point
  Caruso et al. JCTC 12 (2016) 5076
- *GW* is getting worse for inner-valence IPs
  Marie & Loos, JCTC 20 (2024) 4751
- It is terrible for core IPs if one does not tune the starting point:
  G_0W_0@PBEh$(\alpha = 0.45)$ or evGW_0@PBE
  Golze et al. JPCL 11 (2020) 1840
  Vo & Berkelbach, arXiv:2508.00168
- Tuning of the starting point is basically element/row dependent:
  $\alpha = 0.45$ for 2nd-row elements and $\alpha = 0.70$ for 3rd-row elements
  Marie, Burth & Loos, arXiv:2604.05920



Motivations To Go Beyond GW

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  Marie & Loos, JCTC 20 (2024) 4751
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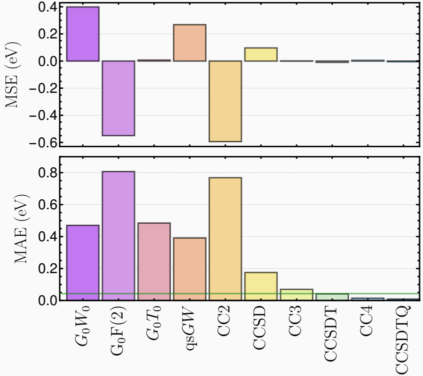


Motivations To Go Beyond *GW*

Core IPs (in eV) of CO in aug-cc-pCVTZ

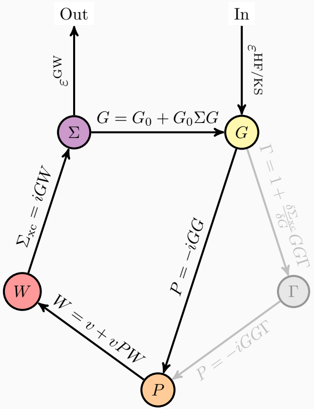
	G_0W_0@HF	evGW@HF	qsGW	IP-EOM-CCSD	G_0W_0@PBEh(α)	**FCI**
C*O	301.69	300.42	298.97	297.66	296.14	**296.26**
CO*	548.88	545.99	545.45	544.26	541.76	**542.47**

Marie, Burth & Loos, arXiv:2604.05920

What do we want?

- We want a scheme weakly sensitive to the starting point
- We want a systematically improvable theory

Hedin's Square



Hedin, Phys. Rev. 139 (1965) A796

The *GW* Approximation

$$\underbrace{G(12)}_{\text{Green's function}} = G_0(12) + \int G_0(13)\Sigma(34)G(42)\,\mathrm{d}(34)$$

$$\underbrace{\Gamma(123)}_{\text{vertex}} = \delta(12)\delta(13)$$

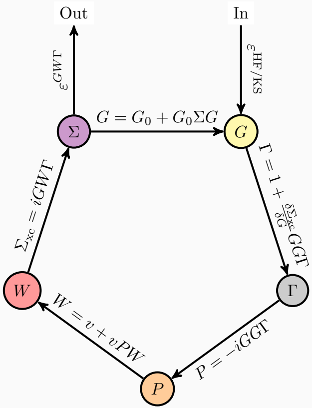
$$\underbrace{P(12)}_{\text{polarizability}} = -\mathrm{i}G(12)G(21)$$

$$\underbrace{W(12)}_{\text{screening}} = v(12) + \int v(13)P(34)W(42)\,\mathrm{d}(34)$$

$$\underbrace{\Sigma_{\text{xc}}(12)}_{\text{self-energy}} = \mathrm{i}G(12)W(12)$$

Golze et al. Front. Chem. 7 (2019) 377; Marie et al. Adv. Quantum Chem. 90 (2024) 157

Hedin's Pentagon



Hedin, Phys. Rev. 139 (1965) A796

Beyond *GW*

$$\underbrace{G(12)}_{\text{Green's function}} = G_0(12) + \int G_0(13)\Sigma(34)G(42)\,\mathrm{d}(34)$$

$$\underbrace{\Gamma(123)}_{\text{vertex}} = \delta(12)\delta(13) + \int \frac{\delta\Sigma_{\mathrm{xc}}(12)}{\delta G(45)} G(46)G(75)\Gamma(673)\,\mathrm{d}(4567)$$

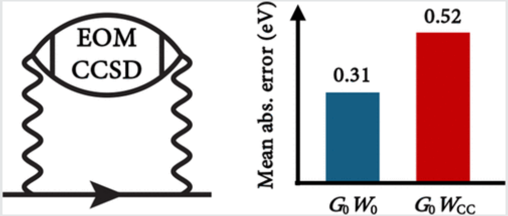
$$\underbrace{P(12)}_{\text{polarizability}} = -\mathrm{i}\int G(13)\,\underset{\uparrow\ \text{inner-vertex correction}}{\Gamma(342)}\,G(41)d(34)$$

$$\underbrace{W(12)}_{\text{screening}} = v(12) + \int v(13)P(34)W(42)\,\mathrm{d}(34)$$

$$\underbrace{\Sigma_{\mathrm{xc}}(12)}_{\text{self-energy}} = \mathrm{i}\int G(14)W(13)\,\underset{\uparrow\ \text{outer-vertex correction}}{\Gamma(423)}\,\mathrm{d}(34)$$

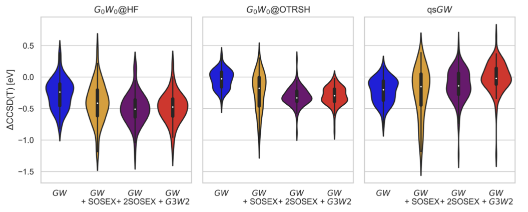
Why Do Vertex Corrections Have a Bad Reputation?

Correcting P alone does not improve IPs



Lewis & Berkelbach, JCTC 15 (2019) 2925

Correcting Σ alone does not improve IPs



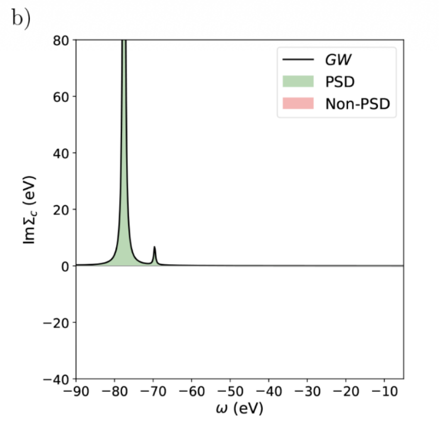
Bruneval & Forster, JCTC 24 (2024) 3218

Take-home messages

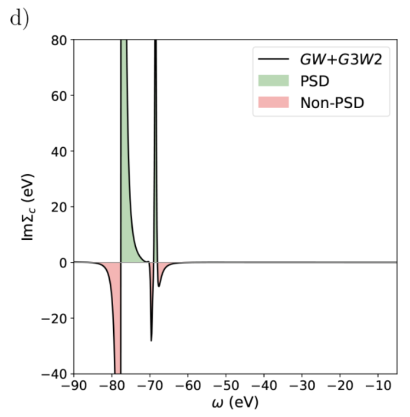
- Inner- and outer-vertex corrections should be treated on equal footing
  Forster & Bruneval, JPCL 15 (2024) 12526
- Are Hedin's equations actually suitable for vertex corrections?

Is the $G3W2$ Self-Energy Positive Semi-Definite (PSD)?

GW self-energy of Ne



$G3W2$ self-energy of Ne



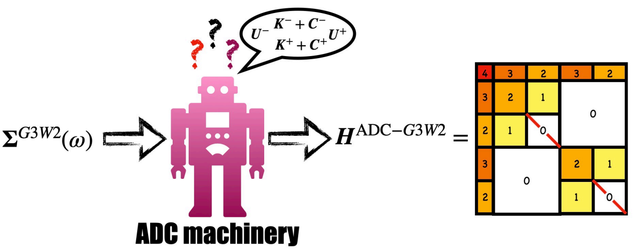
Bruneval, Forster & Pavlyukh, JCTC 21 (2025) 10223

$G3W2$ Made Positive Semi-Definite

The $G3W2$ self-energy

$$\Sigma^{G3W2}(\omega) = \mathrm{i}G \cdot W + \mathrm{i}^2 G \cdot W \cdot G \cdot W \cdot G$$

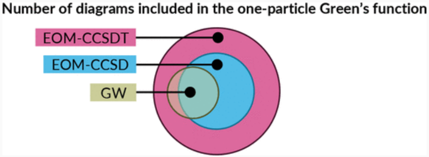
ADC version of $G3W2$



Marie, Tölle & Loos, arXiv:2606.04285

Formal Connections Between *GW* And CC

- *GW* does not resum diagrams the same way as EOM-CC!
  Lange & Berkelbach, JCTC 14 (2018) 4224



$$\bar{H}^{\text{TCC}} = (1 + \hat{Z})e^{-\hat{T}}\hat{H}e^{\hat{T}}$$

- We show that *GW* can be written as two coupled Ricatti equations
  Quintero-Monsebaiz et al. JCP 157 (2022) 231102

- Tölle and Chan found a formal equivalence between IP+EA-EOM-drUCCD and *GW*
  Tölle & Chan, JCP 158 (2023) 124123

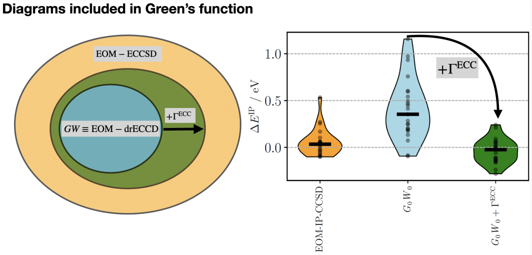
- Recently, we showed that *GW* is also equivalent to IP+EA-EOM-drECCD
  Tölle et al. JCTC (in press) arXiv:2602.10887

ECC-Based Vertex Corrections

- ECCD is, in general, costly but the *GW* electron-boson Hamiltonian is quadratic!
  Tölle & Chan, JCP 158 (2023) 124123

$$\hat{H}_{\text{eB}} = \underbrace{\sum_{pq} f_{pq}\hat{a}_p^\dagger \hat{a}_q}_{\text{electron}} + \underbrace{\sum_{\mu\nu} A_{\mu\nu} b_\mu^\dagger b_\nu + \frac{1}{2}\sum_{\mu\nu} B_{\mu\nu}\left(b_\mu^\dagger b_\nu^\dagger + b_\mu b_\nu\right)}_{\text{boson}} + \underbrace{\sum_{pq\nu} V_{pq,\nu}\hat{a}_p^\dagger\hat{a}_q\left(b_\nu^\dagger + b_\nu\right)}_{\text{electron-boson}}$$

- Thus, it remains N^6, like quadratic CCD.
  van Voorhis & Head-Gordon, CPL 330 (2000) 585
- We found that the static self-energy and exchange-like (SOSEX-type) terms super important


Diagrams included in Green's function

Introducing The Singles Into *GW*

The rationale

- *GW* is IP+EA-EOM-drECCD
- *GW* is very sensitive to the starting orbital
- Can we include the single excitations to at least alleviate this?
- Yes! It gives IP+EA-EOM-drECCSD
- Do we get more orbital relaxation?

Core IPs (in eV) of CO in aug-cc-pCVTZ

	G_0W_0@HF	G_0W_0+S@HF	ΔdrECCD	ΔdrECCSD	IP-EOM-CCSD	**FCI**
C*O	301.69	300.74	298.02	297.66	297.66	**296.26**
CO*	548.88	548.57	542.97	542.96	544.26	**542.47**

Kitsaras, Burth & Loos, in preparation

Parquet Theory

Schwinger-Dyson relationship

$$G^{-1}(11') = G_0^{-1}(11') - \Sigma(11')$$

$$\Sigma(11') = -\mathrm{i}v(12;3'2')\,G_2(3'2';32)\,G^{-1}(31')$$

Bickers, in Theoretical Methods for Strongly Correlated Electrons (2004) 237

Two-body vertex

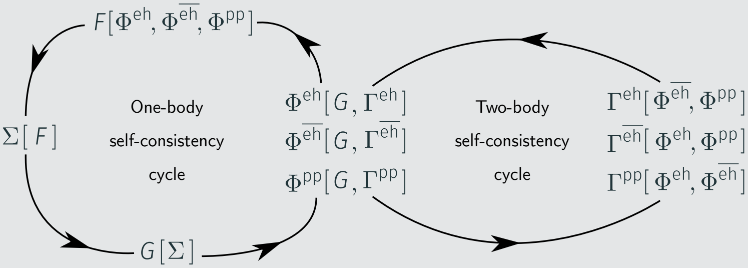
$$G_2(12;34) = G(13)G(24) - G(14)G(23) - G(11')G(3'3)\,\overset{\text{Full two-body vertex}}{F}\,(1'2';3'4')G(4'4)G(22')$$

Parquet decomposition

$$F(12;34) = \underset{\text{Irreducible vertex}}{\Lambda(12;34)} + \underbrace{\Phi^{\text{eh}}(12;34) + \Phi^{\overline{\text{eh}}}(12;34) + \Phi^{\text{pp}}(12;34)}_{\text{can be computed with Bethe-Salpeter equations}}$$

Parquet Algorithm

Self-consistent algorithm



$F[\Phi^{\text{eh}}, \Phi^{\overline{\text{eh}}}, \Phi^{\text{pp}}]$

$\Sigma[F]$

One-body
self-consistency
cycle

$G[\Sigma]$

$\Phi^{\text{eh}}[G, \Gamma^{\text{eh}}]$

$\Phi^{\overline{\text{eh}}}[G, \Gamma^{\overline{\text{eh}}}]$

$\Phi^{\text{pp}}[G, \Gamma^{\text{pp}}]$

Two-body
self-consistency
cycle

$\Gamma^{\text{eh}}[\Phi^{\overline{\text{eh}}}, \Phi^{\text{pp}}]$

$\Gamma^{\overline{\text{eh}}}[\Phi^{\text{eh}}, \Phi^{\text{pp}}]$

$\Gamma^{\text{pp}}[\Phi^{\text{eh}}, \Phi^{\overline{\text{eh}}}]$

Approximations

- Parquet approximation $\Lambda = -\mathrm{i}\bar{\nu}$
- One-shot approximation
- Static kernel approximation for Γ
- Hardcore regularization

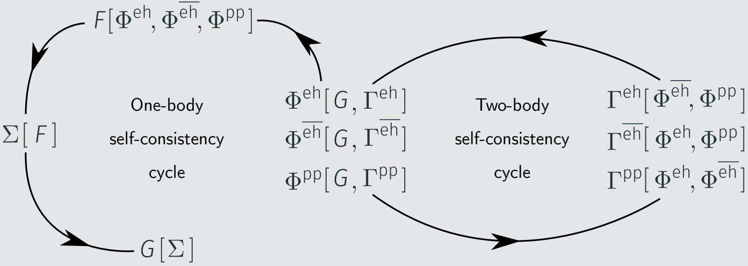
Preliminary statistics on 20 IPs in the aug-cc-pVTZ basis set

Method	osPA	G_0W_0	G_0T_0
MAE	0.29	0.37	0.34

Marie & Loos, JCP 163 (2025) 194115

Parquet Algorithm

Self-consistent algorithm



$F[\Phi^{\text{eh}}, \Phi^{\overline{\text{eh}}}, \Phi^{\text{pp}}]$

$\Sigma[F]$

One-body self-consistency cycle

$G[\Sigma]$

$\Phi^{\text{eh}}[G, \Gamma^{\text{eh}}]$

$\Phi^{\overline{\text{eh}}}[G, \Gamma^{\overline{\text{eh}}}]$

$\Phi^{\text{pp}}[G, \Gamma^{\text{pp}}]$

Two-body self-consistency cycle

$\Gamma^{\text{eh}}[\Phi^{\overline{\text{eh}}}, \Phi^{\text{pp}}]$

$\Gamma^{\overline{\text{eh}}}[\Phi^{\text{eh}}, \Phi^{\text{pp}}]$

$\Gamma^{\text{pp}}[\Phi^{\text{eh}}, \Phi^{\overline{\text{eh}}}]$

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Marie & Loos, JCP 163 (2025) 194115

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- Collaborators: Johannes Tölle, Hugh Burton, Pina Romaniello & Xavier Blase

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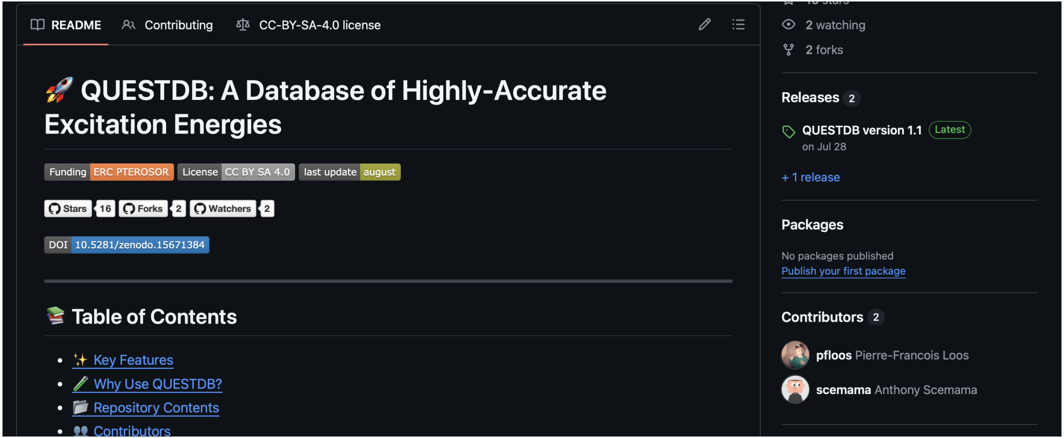
QUEST Database



🚀 QUESTDB: A Database of Highly-Accurate Excitation Energies

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on Jul 28

+ 1 release

Packages

No packages published
Publish your first package

Contributors 2

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https://github.com/pfloos/QUESTDB

Loos, Boggio-Pasqua, Blondel, Lipparini & Jacquemin, JCTC 21 (2025) 8010