Green's Function Methods for Quantum Chemistry

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https://pfloos.github.io/WEB_LOOS

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Electronic Schrödinger Equation

Wave Function Theory

Hamiltonian Energy

$$\hat{H}\,\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N) = E\,\Psi(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N)$$

Wave function

kinetic external potential

$$\hat{H} = \hat{T} + \hat{W}_{\text{ee}} + \hat{V}_{\text{ext}} \quad \Rightarrow \quad \boxed{E = E_T + E_W + E_V}$$

electron repulsion

Reduced Quantities

Density Functional Theory

$$N \int \cdots \int \Psi^*(\boldsymbol{r}, \ldots, \boldsymbol{r}_N)\Psi(\boldsymbol{r}, \ldots, \boldsymbol{r}_N)\mathrm{d}\boldsymbol{r}_2 \cdots \mathrm{d}\boldsymbol{r}_N = \overbrace{n(\boldsymbol{r})}^{\text{electron density}}$$

Wave Function Theory (WFT) $\rightsquigarrow$ Density Functional Theory (DFT)

$$E = \underset{✗}{E_T} + \underset{✗}{E_W} + \underset{✓}{E_V}$$

Hohenberg & Kohn, Phys. Rev. 1964 (B864) 136

(Less) Reduced Quantities

Density Matrix Functional Theory

$$N \int \cdots \int \Psi^*(\boldsymbol{r}, \ldots, \boldsymbol{r}_N)\Psi(\boldsymbol{r}', \ldots, \boldsymbol{r}_N)\mathrm{d}\boldsymbol{r}_2 \cdots \mathrm{d}\boldsymbol{r}_N = \underbrace{n_1(\boldsymbol{r}, \boldsymbol{r}')}_{\text{1st-order reduced density matrix}}$$

Wave Function Theory (WFT) $\rightsquigarrow$ Reduced Density Matrix Functional Theory (RDMF)

$$E = \underset{\checkmark}{E_T} + \underset{\times}{E_W} + \underset{\checkmark}{E_V}$$

Gilbert, Phys. Rev. B 12 (1975) 2111

(Even Less) Reduced Quantities

Density Matrix Functional Theory (2nd order)

2nd-order reduced density matrix

$$\frac{N(N-1)}{2}\int\cdots\int\Psi^*(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N)\mathrm{d}\boldsymbol{r}_3\cdots\mathrm{d}\boldsymbol{r}_N = \boxed{n_2(\boldsymbol{r}_1,\boldsymbol{r}_2)}$$

$$E = \underset{\checkmark}{E_T} + \underset{\checkmark}{E_W} + \underset{\checkmark}{E_V}$$

$$E = -\frac{1}{2}\int \nabla^2_{\boldsymbol{r}} n_1(\boldsymbol{r},\boldsymbol{r}')\Big|_{\boldsymbol{r}'=\boldsymbol{r}}\mathrm{d}\boldsymbol{r} + \int\int\frac{n_2(\boldsymbol{r}_1,\boldsymbol{r}_2)}{r_{12}}\mathrm{d}\boldsymbol{r}_1\mathrm{d}\boldsymbol{r}_2 + \int v(\boldsymbol{r})n(\boldsymbol{r})\mathrm{d}\boldsymbol{r}$$

One-Body Green's Function: The Sweet Spot?

One-Body Propagator in the Time Domain

$$\overset{\text{one-body Green's function}}{G(\boldsymbol{r},\boldsymbol{r}';t-t')} = -\mathrm{i}\,\left\langle \Psi_0^N \right| \overset{\text{time-ordering}}{\hat{T}} \Big[\underbrace{\hat{\psi}(\boldsymbol{r}t)\;\hat{\psi}^\dagger(\boldsymbol{r}'t')}_{\text{Field operators}} \Big] \overset{N\text{-electron ground state}}{\left| \Psi_0^N \right\rangle}$$

$$G(\boldsymbol{r},\boldsymbol{r}';t-t') = \begin{cases} -\mathrm{i}\,\langle \Psi_0^N | \hat{\psi}(\boldsymbol{r}t)\hat{\psi}^\dagger(\boldsymbol{r}'t') | \Psi_0^N \rangle & \text{for} \quad t > t' \\ +\mathrm{i}\,\langle \Psi_0^N | \hat{\psi}^\dagger(\boldsymbol{r}'t')\hat{\psi}(\boldsymbol{r}t) | \Psi_0^N \rangle & \text{for} \quad t' < t \end{cases}$$

- $\langle \Psi_0^N | \hat{\psi}(\boldsymbol{r}t)\hat{\psi}^\dagger(\boldsymbol{r}'t') | \Psi_0^N \rangle$ measures the propagation of an electron (electron branch)
- $\langle \Psi_0^N | \hat{\psi}^\dagger(\boldsymbol{r}'t')\hat{\psi}(\boldsymbol{r}t) | \Psi_0^N \rangle$ measures the propagation of a hole (hole branch)

Martin, Reining & Ceperley, *"Interacting Electrons"*

Links With Other Reduced Quantities

Link to RDMFT & DFT

$$n_1(\boldsymbol{r}, \boldsymbol{r}') = -\mathrm{i} \lim_{t' \to t} G(\boldsymbol{r}, \boldsymbol{r}'; t - t') \qquad n(\boldsymbol{r}) = -\mathrm{i} \lim_{t' \to t} \lim_{\boldsymbol{r}' \to \boldsymbol{r}} G(\boldsymbol{r}, \boldsymbol{r}'; t - t')$$

Galitskii-Migdal Energy Functional

$$\begin{aligned} E &= \frac{\mathrm{i}}{2} \int \mathrm{d}\boldsymbol{r} \lim_{t' \to t} \lim_{\boldsymbol{r}' \to \boldsymbol{r}} \nabla^2_{\boldsymbol{r}} G(\boldsymbol{r}, \boldsymbol{r}'; t - t') + \frac{1}{2} \int \mathrm{d}\boldsymbol{r} \lim_{t' \to t} \lim_{\boldsymbol{r}' \to \boldsymbol{r}} \left[\frac{\partial}{\partial t} + \mathrm{i}\hat{h}(\boldsymbol{r}) \right] G(\boldsymbol{r}, \boldsymbol{r}', t - t') + E_V \\ &= \frac{1}{2} \int \mathrm{d}\boldsymbol{r} \lim_{t' \to t} \lim_{\boldsymbol{r}' \to \boldsymbol{r}} \left[\frac{\partial}{\partial t} - \mathrm{i}\hat{h}(\boldsymbol{r}) \right] G(\boldsymbol{r}, \boldsymbol{r}'; t - t') \end{aligned}$$

Wave Function Theory (WFT) $\rightsquigarrow$ Green's Function Functional Theory (GFFT) ?!

Galitskii & Migdal, JETP 7 (1958) 96

Lehmann Representation

One-Body Propagator in the Frequency Domain

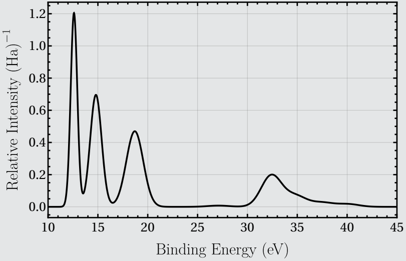
$$G(\mathbf{r},\mathbf{r}';\omega) = \sum_\nu \frac{\mathcal{I}_\nu(\mathbf{r})\mathcal{I}_\nu^*(\mathbf{r}')}{\omega - \underbrace{(E_0^N - E_\nu^{N-1})}_{\nu\text{th ionization potential (IP)}} - i\eta} + \sum_\nu \frac{\mathcal{A}_\nu(\mathbf{r})\mathcal{A}_\nu^*(\mathbf{r}')}{\omega - \underbrace{(E_\nu^{N+1} - E_0^N)}_{\nu\text{th electron affinity (EA)}} + i\eta}$$

Spectral function

$$\boxed{A(\omega) = \frac{1}{\pi}\int d\mathbf{r}\,d\mathbf{r}' \left|\mathrm{Im}\, G(\mathbf{r},\mathbf{r}';\omega)\right|}$$

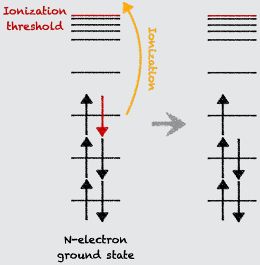
Marie & Loos, JCTC 20 (2024) 4751

Photoemission spectrum of water

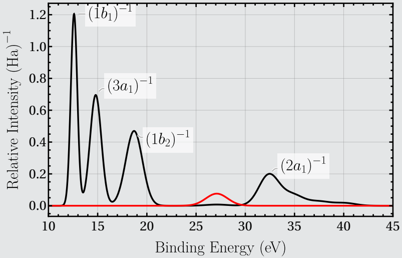


Photoemission Spectroscopy

Single ionization (quasiparticle)

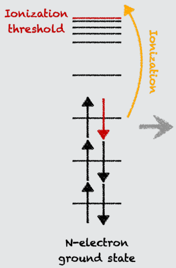


Experimental spectrum of water

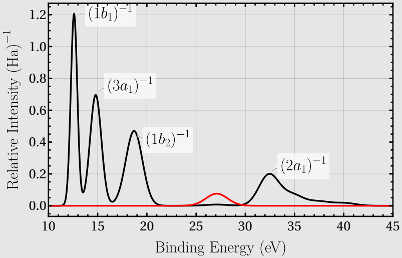


Photoemission Spectroscopy

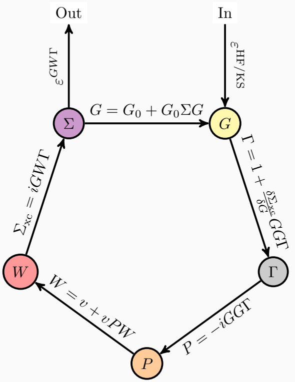
Shake-up transition (satellite)



Experimental spectrum of water



Hedin’s Pentagon



Hedin, Phys. Rev. 139 (1965) A796

Hedin’s Equations

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

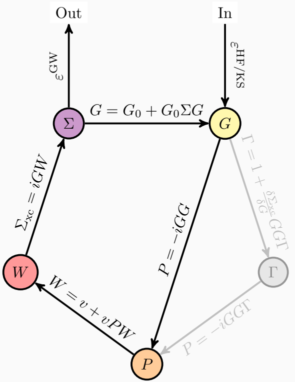
$$\underbrace{\Gamma(123)}_{\text{vertex}} = \delta(12)\delta(13) + \int \frac{\delta \Sigma_{\mathrm{xc}}(12)}{\delta G(45)} G(46)G(75)\Gamma(673)d(4567)$$

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

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

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

Hedin's Square



Hedin, Phys. Rev. 139 (1965) A796

The GW Approximation

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

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

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

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

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

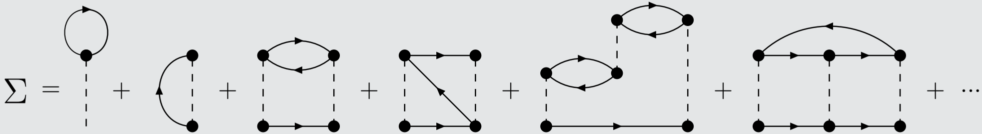
Golze et al. Front. Chem. 7 (2019) 377; Marie et al. Adv. Quantum Chem. 90 (2024) 157

Self-Energy

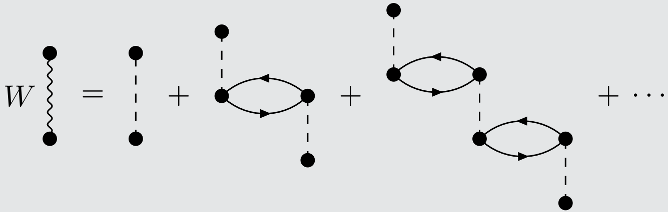
Self-Energy as a Function of the Bare Coulomb Operator

$$\Sigma(11') = \underbrace{-i\bar{v}(12;1'2')G(2'2)}_{\text{first-order terms}} + \underbrace{\frac{1}{2}\bar{v}(12;3'2')G(3'3)G(4'2)G(2'4)\bar{v}(34;1'4')}_{\text{second-order terms}} + \dots$$

Diagrammatic Representation

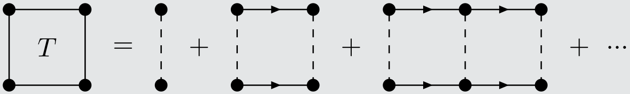


GW Approximation



Hedin, Phys. Rev. 139 (1965) A796

pp *T*-matrix Approximation



Marie, Romaniello & Loos, PRB 110 (2024) 115155

How to Compute G?

The Dyson Equation

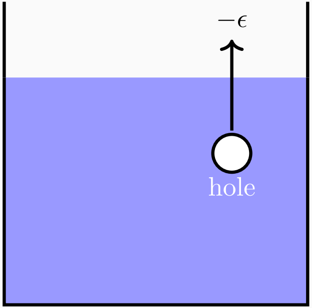
$$\underbrace{G(11')}_{\text{one-body Green's function}} = \overbrace{G_0(11')}^{\text{mean-field propagator}} + \int \mathrm{d}(22')\, G_0(12)\, \underbrace{\Sigma(22')}_{\text{self-energy}}\, G(2'1')$$

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

Quasi-Particle Equation

$$\Big[\underbrace{\boldsymbol{H}_0}_{\text{mean-field Hamiltonian}} + \overbrace{\boldsymbol{\Sigma}}^{\text{self-energy}}(\omega = \epsilon_p)\Big]\, \psi_p(\boldsymbol{x}) = \underbrace{\epsilon_p}_{\text{poles of the Green's function}}\, \overbrace{\psi_p(\boldsymbol{x})}^{\text{Dyson orbitals}},$$

Quasiparticle Concept

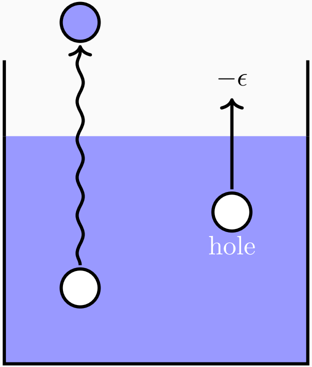


electron removal

- Link to electron-boson Hamiltonian:
  Langreth, PRB 1 (1970) 471
  Hedin, JPCM 11 (1999) R489

- Link to coupled-cluster theory:
  Lange & Berkelbach, JCTC 14 (2018) 4224
  Quintero-Monsebaiz et al. JCP 157 (2022) 231102
  Tolle & Chan, JCP 158 (2023) 124123

Quasiparticle Concept



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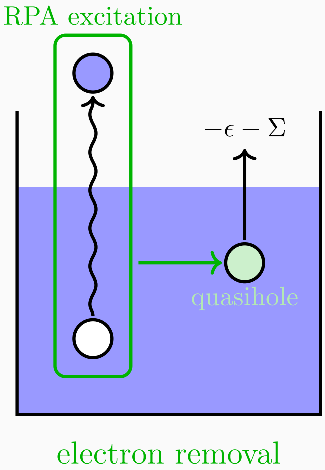
Quasiparticle Concept



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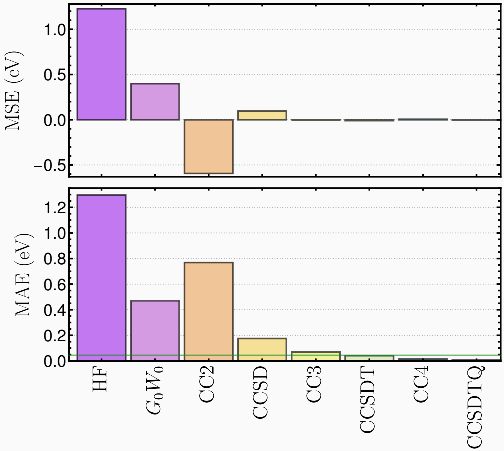
  Tolle & Chan, JCP 158 (2023) 124123

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



Computational cost

- HF $\mathcal{O}(K^4)$
- G_0W_0 $\mathcal{O}(K^6)$ $\rightarrow \mathcal{O}(K^4)$
- IP-EOM-CC2 $\mathcal{O}(K^5)$
- IP-EOM-CCSD $\mathcal{O}(K^6)$
- IP-EOM-CCSDT $\mathcal{O}(K^8)$

Some issues:

- Highly starting point dependent!
- Systematic improvable?

Marie & Loos, JCTC 20 (2024) 4751

Propagation Can be Longer Than Expected

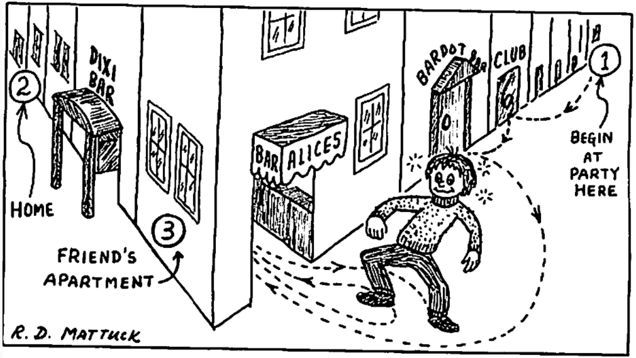


Fig. 1.1 *Propagation of Drunken Man*

(Reproduced with the kind permission of *The Encyclopedia of Physics*)

Mattuck, *"A Guide to Feynman Diagrams in the Many-Body Problem"*

Two-Body Green's Function

Two-Body Propagator in the Time Domain

two-body Green's function

$$\boxed{G_2(12;1'2')} = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{T}\left[\hat{\psi}(2)\hat{\psi}^\dagger(2')\hat{\psi}(1)\hat{\psi}^\dagger(1')\right] \middle| \Psi_0^N \right\rangle$$

Propagation of electron-hole pairs ($t_{1'} > t_1$ and $t_{2'} > t_2$)

$$\boxed{G_2^{\text{eh}}(12;1'2')} = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{\psi}^\dagger(1')\hat{\psi}(1)\hat{\psi}^\dagger(2')\hat{\psi}(2) + \hat{\psi}^\dagger(2')\hat{\psi}(2)\hat{\psi}^\dagger(1')\hat{\psi}(1) \middle| \Psi_0^N \right\rangle$$

Propagation of electron-electron and hole-hole pairs ($t_{1'} > t_{2'}$ and $t_1 > t_2$)

$$\boxed{G_2^{\text{ee}}(12;1'2')} = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{\psi}(1)\hat{\psi}(2)\hat{\psi}^\dagger(1')\hat{\psi}^\dagger(2') \middle| \Psi_0^N \right\rangle$$

$$\boxed{G_2^{\text{hh}}(12;1'2')} = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{\psi}^\dagger(1')\hat{\psi}^\dagger(2')\hat{\psi}(1)\hat{\psi}(2) \middle| \Psi_0^N \right\rangle$$

The Electron-Hole Channel

Electron-Hole Correlation Function

$$\overbrace{L(12;1'2')}^{\text{eh correlation function}} = -G_2(12;1'2') + G(11')G(22')$$

$$L(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_{1'}\mathbf{r}_{2'};\omega) = \sum_{\nu>0} \frac{L_\nu^N(\mathbf{r}_2\mathbf{r}_{2'})R_\nu^N(\mathbf{r}_1\mathbf{r}_{1'})}{\omega - (E_\nu^N - E_0^N - i\eta)} - \sum_{\nu>0} \frac{L_\nu^N(\mathbf{r}_2\mathbf{r}_{2'})R_\nu^N(\mathbf{r}_1\mathbf{r}_{1'})}{\omega - (E_0^N - E_\nu^N + i\eta)}$$

νth (de)excitation energy

Electron-Hole Bethe-Salpeter Equation (eh-BSE)

$$L(12;1'2') = \underbrace{L_0(12;1'2')}_{G(12')G(21')} + \int d(33'44')\, L_0(13';1'3)\, \Xi^{\text{eh}}(34';3'4)\, L(42;4'2')$$

eh kernel

Strinati, Riv. Nuovo Cimento 11 (1988) 1; Blase et al. JPCL 11 (2020) 7371

Electron-Hole Effective Interaction Kernel

Effective Interaction Kernel

$$\Xi^{\text{eh}}(12;1'2') = \frac{\delta\Sigma(11')}{\delta G(2'2)} \qquad \underbrace{\boxed{\Sigma_{\text{xc}}}}_{\text{exchange-correlation}} = \mathrm{i}GW \quad \Rightarrow \quad \frac{\delta\Sigma_{\text{xc}}}{\delta G} = \mathrm{i}\frac{\delta G}{\delta G}W + \mathrm{i}G\underbrace{\frac{\delta W}{\delta G}}_{=0} = \mathrm{i}W$$

Casida Equations for eh-BSE

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

If no correlation, $W_{ij,ab} = \langle ib|ja\rangle$, then
eh-BSE becomes RPAx (or TDHF)!

Matrix Elements With Static Screening

$$A_{ia,jb} = \overbrace{(\epsilon_a^{GW} - \epsilon_i^{GW})}^{\text{quasiparticle energies}} \delta_{ij}\delta_{ab} + \underbrace{\langle ib|aj\rangle}_{\text{Hartree}} - \underbrace{W_{ij,ab}}_{\text{exchange-correlation}}$$

$$B_{ia,jb} = \langle ij|ab\rangle - W_{ib,aj}$$

The Particle-Particle Channel

Particle-Particle Correlation Function

$$\underbrace{K(12;1'2')}_{\text{pp correlation function}} = -G_2(12;1'2') + \underbrace{G^{\text{hh}}(12)G^{\text{ee}}(2'1')}_{\text{anomalous propagators}}$$

$$K(\mathbf{r}_1\mathbf{r}_2;\mathbf{r}_{1'}\mathbf{r}_{2'};\omega) = \sum_\nu \frac{L_\nu^{N+2}(\mathbf{r}_1\mathbf{r}_2)R_\nu^{N+2}(\mathbf{r}'_1\mathbf{r}'_2)}{\omega - (\underbrace{E_\nu^{N+2} - E_0^N}_{\nu\text{th double EA (DEA)}} - \mathrm{i}\eta)} - \sum_\nu \frac{L_\nu^{N-2}(\mathbf{r}'_1\mathbf{r}'_2)R_\nu^{N-2}(\mathbf{r}_1\mathbf{r}_2)}{\omega - (\underbrace{E_0^N - E_\nu^{N-2}}_{\nu\text{th double IP (DIP)}} + \mathrm{i}\eta)}$$

Particle-Particle Bethe-Salpeter Equation (pp-BSE)

$$K(12;1'2') = \underbrace{K_0(12;1'2')}_{\frac{1}{2}[G(21')G(12')-G(11')G(22')]} - \int d(33'44')K(12;44')\underbrace{\Xi^{\text{pp}}(44';33')}_{\text{pp kernel}}K_0(33';1'2')$$

Marie, Romaniello, Loos, PRB 110 (2024) 115155; Marie et al. JCP 162 (2025) 134105

Particle-Particle Effective Interaction Kernel

Effective Interaction Kernel

$$\Xi^{\mathrm{pp}}(11';22') = \frac{\delta\Sigma^{\mathrm{ee}}(22')}{\delta G^{\mathrm{ee}}(11')}\bigg|_{U=0} \qquad \underbrace{\boxed{\Sigma^{GW}_{\mathrm{Bc}}}}_{\text{Bogoliubov-correlation}} = -\mathrm{i}G^{\mathrm{ee}}W \quad \Rightarrow \quad \mathrm{i}\frac{\delta\Sigma^{GW}_{\mathrm{Bc}}(11')}{\delta G^{\mathrm{ee}}(22')} = \frac{1}{2}[W(11';22') - W(11';2'2)]$$

Casida Equations for pp-BSE

$$\begin{pmatrix} \boldsymbol{C} & \boldsymbol{B} \\ -\boldsymbol{B}^{\dagger} & -\boldsymbol{D} \end{pmatrix} \begin{pmatrix} \boldsymbol{X}_{\nu} \\ \boldsymbol{Y}_{\nu} \end{pmatrix} = \Omega_{\nu}^{N\pm 2} \begin{pmatrix} \boldsymbol{X}_{\nu} \\ \boldsymbol{Y}_{\nu} \end{pmatrix}$$

If no correlation, $W_{pq,rs} = \langle ps|qr\rangle$, then pp-BSE becomes pp-RPA!

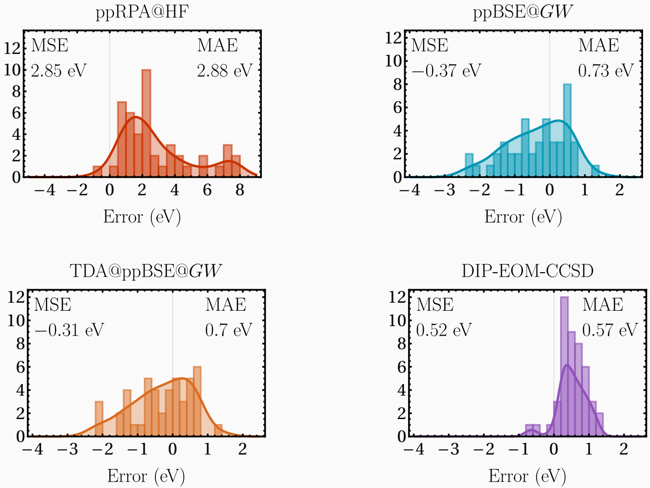
Matrix Elements With Static Screening

$$C_{ab,cd} = \overbrace{(\epsilon_a^{GW} + \epsilon_b^{GW})}^{\text{quasiparticle energies}} \delta_{ac}\delta_{bd} + \underbrace{W_{ac,bd} - W_{ad,bc}}_{\text{Bogoliubov-correlation}}$$

$$B_{ab,ij} = W_{ai,bj} - W_{aj,bi}$$

$$D_{ij,kl} = -(\epsilon_i^{GW} + \epsilon_j^{GW})\delta_{ik}\delta_{jl} + W_{ik,jl} - W_{il,jk}$$

Singlet and Triplet DIPs (aug-cc-pVTZ) for 23 small molecules (FCI reference)



Marie & Loos, JCTC 20 (2024) 4751; Marie et al. JCP 162 (2025) 134105

Parquet Theory [Marie & Loos, arxiv:2509.03253]

Schwinger-Dyson Relationship

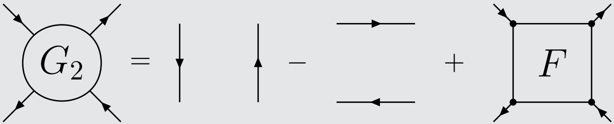
$$G^{-1}(11') = G_0^{-1}(11') - \Sigma(11')$$

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

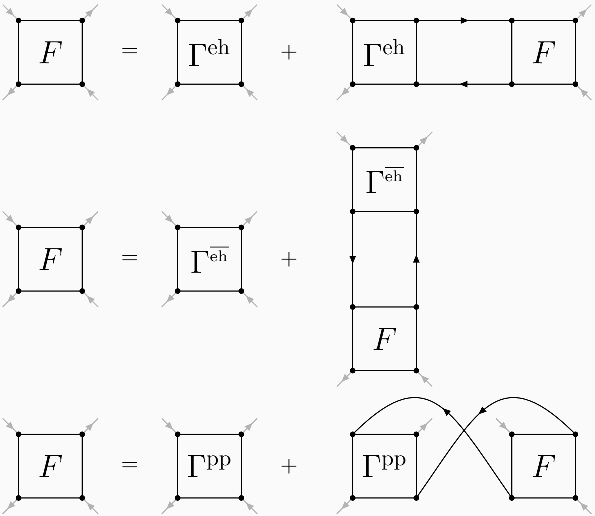
Two-body Vertex

Full two-body vertex

$$G_2(12;34) = G(13)G(24) - G(14)G(23) - G(11')G(3'3)\,\boxed{F}\,(1'2';3'4')G(4'4)G(22')$$



Parquet theory aims at computing F, hence G_2, through Dyson equations


F = Γ^{eh} + Γ^{eh} F
F = $\Gamma^{\overline{\mathrm{eh}}}$ + $\Gamma^{\overline{\mathrm{eh}}}$ F
F = Γ^{pp} + Γ^{pp} F

Two-body Vertex

Parquet Decomposition

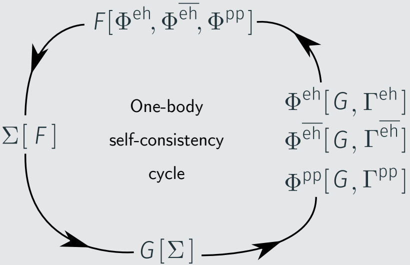
$$F(12;34) = \underbrace{\Lambda(12;34)}_{\text{Irreducible vertex}} + \underbrace{\Phi^{\mathrm{eh}}(12;34) + \Phi^{\overline{\mathrm{eh}}}(12;34) + \Phi^{\mathrm{pp}}(12;34)}_{\text{can be computed with Bethe-Salpeter equations}}$$

Proper way to account for different correlation channels in the self-energy without double counting!

De Dominicis & Martin, J. Math. Phys. 5 (1964) 14; ibid 5 (1964) 31
Bickers, *"Self-consistent many-body theory for condensed matter systems"* in Theoretical Methods for Strongly Correlated Electrons (2004) 237

Parquet Algorithm

Self-Consistent Algorithm



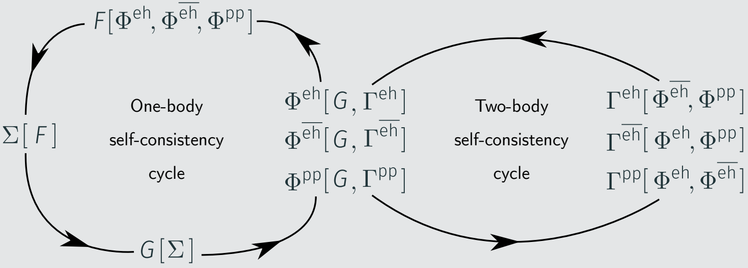
Approximations

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

One-shot parquet approximation (osPA)

Full two-body self-consistency, single one-body iteration in the diagonal approximation

Self-Consistent Algorithm



Approximations

- Parquet approximation $\Lambda = -i\bar{v}$
- One-shot approximation
- Static kernel approximation for Γ

One-shot parquet approximation (osPA)

Full two-body self-consistency, single one-body iteration in the diagonal approximation

Parquet Algorithm

Self-Consistent Algorithm

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

$\Sigma[F]$

One-body
self-consistency
cycle

$G[\Sigma]$

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

Two-body
self-consistency
cycle

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

Approximations

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One-shot parquet approximation (osPA)

Full two-body self-consistency, single one-body iteration in the diagonal approximation

Preliminary Results on Principal IPs

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, arxiv:2509.03253

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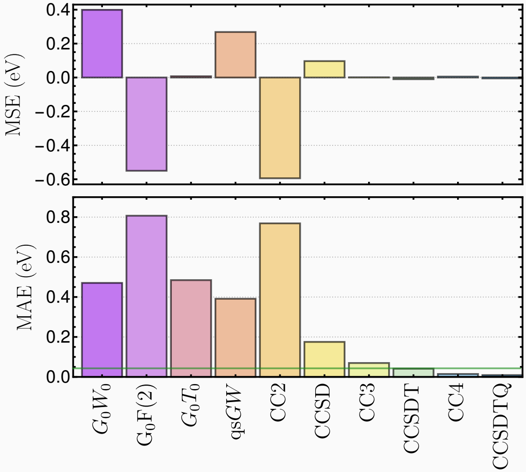
https://pfloos.github.io/WEB_LOOS

https://lcpq.github.io/PTEROSOR

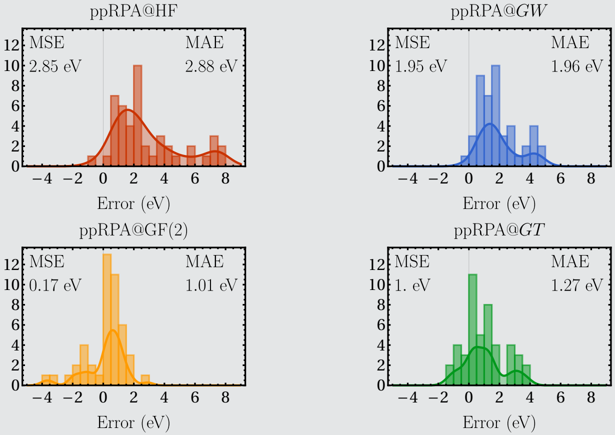
Inner- and Outer-valence IPs (aug-cc-pVTZ) for 23 small molecules (FCI reference)



Marie & Loos, JCTC 20 (2024) 4751

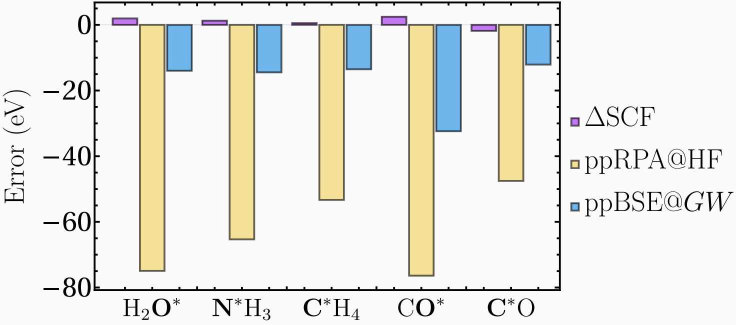
Singlet and Triplet DIPs (aug-cc-pVTZ) for 23 small molecules (FCI reference)

Effect of the Quasiparticle Energies



Marie & Loos, JCTC 20 (2024) 4751; Marie et al. JCP 162 (2025) 134105

(Single-Site) Double Core Holes (aug-cc-pCVTZ & CVS-FCI reference)



Cederbaum et al. JCP 85 (1986) 6513; Marie et al. JCP 162 (2025) 134105

Parquet Algorithm