Bethe-Salpeter equation for the particle-particle propagator

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Definition

$$1 = (\mathbf{r}_1, \sigma_1, t_1)$$

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

N-**electron ground-state**

Field operators

Electron-hole channel

Electron-hole pair propagation

$$t_2, t_{2'} > t_1, t_{1'} \qquad G_2(12;1'2') = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{T}\left[\hat{\psi}(2)\hat{\psi}^\dagger(2')\right] \hat{T}\left[\hat{\psi}(1)\hat{\psi}^\dagger(1')\right] \middle| \Psi_0^N \right\rangle$$

Electron-hole channel

Electron-hole pair propagation

$$t_2, t_{2'} > t_1, t_{1'} \qquad G_2(12;1'2') = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{T}\left[\hat{\psi}(2)\hat{\psi}^\dagger(2')\right] \hat{T}\left[\hat{\psi}(1)\hat{\psi}^\dagger(1')\right] \middle| \Psi_0^N \right\rangle$$

Electron-hole correlation function

$$-L(12;1'2') = G_2(12;1'2') - G(11')G(22')$$

Electron-hole channel

Electron-hole pair propagation

$$t_2, t_{2'} > t_1, t_{1'} \qquad G_2(12;1'2') = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{T}\left[\hat{\psi}(2)\hat{\psi}^\dagger(2')\right] \hat{T}\left[\hat{\psi}(1)\hat{\psi}^\dagger(1')\right] \middle| \Psi_0^N \right\rangle$$

Electron-hole correlation function

$$-L(12;1'2') = G_2(12;1'2') - G(11')G(22')$$

Electron-hole propagator

$$L(\mathbf{x}_1\mathbf{x}_2;\mathbf{x}_{1'}\mathbf{x}_{2'};t_1-t_2) = \lim_{t_2\to t_{2'},t_1\to t_{1'}} L(12;1'2')$$

$$x_{1'} = (\mathbf{r}_{1'}, \sigma_{1'})$$

Electron-hole channel

Electron-hole pair propagation

$$t_2, t_{2'} > t_1, t_{1'} \qquad G_2(12;1'2') = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{T}\left[\hat{\psi}(2)\hat{\psi}^\dagger(2')\right]\hat{T}\left[\hat{\psi}(1)\hat{\psi}^\dagger(1')\right] \middle| \Psi_0^N \right\rangle$$

Electron-hole correlation function

$$-L(12;1'2') = G_2(12;1'2') - G(11')G(22')$$

Lehman representation

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

Particle-particle channel

Electron-electron pair propagation

$$t_1, t_2 > t_{1'}, t_{2'} \qquad G_2(12;1'2') = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{T}\left[\hat{\psi}(1)\hat{\psi}(2)\right] \hat{T}\left[\hat{\psi}^\dagger(1')\hat{\psi}^\dagger(2')\right] \middle| \Psi_0^N \right\rangle$$

Hole-hole pair propagation

$$t_{1'}, t_{2'} > t_1, t_2 \qquad G_2(12;1'2') = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{T}\left[\hat{\psi}^\dagger(1')\hat{\psi}^\dagger(2')\right] \hat{T}\left[\hat{\psi}(1)\hat{\psi}(2)\right] \middle| \Psi_0^N \right\rangle$$

Particle-particle channel

Electron-electron pair propagation

$$t_1, t_2 > t_{1'}, t_{2'} \qquad G_2(12;1'2') = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{T}\left[\hat{\psi}(1)\hat{\psi}(2)\right] \hat{T}\left[\hat{\psi}^\dagger(1')\hat{\psi}^\dagger(2')\right] \middle| \Psi_0^N \right\rangle$$

Particle-particle correlation function

$$2K(12;1'2') = G_2(12;1'2')$$

Particle-particle channel

Electron-electron pair propagation

$$t_1, t_2 > t_{1'}, t_{2'} \qquad G_2(12;1'2') = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{T}\left[\hat{\psi}(1)\hat{\psi}(2)\right]\hat{T}\left[\hat{\psi}^\dagger(1')\hat{\psi}^\dagger(2')\right] \middle| \Psi_0^N \right\rangle$$

Particle-particle correlation function

$$2K(12;1'2') = G_2(12;1'2')$$

Particle-particle propagator

$$K(\mathbf{x}_1\mathbf{x}_2;\mathbf{x}_{1'}\mathbf{x}_{2'};t_1 - t_{1'}) = \lim_{t_2 \to t_1, t_{2'} \to t_{1'}} K(12;1'2')$$

Particle-particle channel

Electron-electron pair propagation

$$t_1, t_2 > t_{1'}, t_{2'} \qquad G_2(12;1'2') = (-\mathrm{i})^2 \left\langle \Psi_0^N \middle| \hat{T}\left[\hat{\psi}(1)\hat{\psi}(2)\right]\hat{T}\left[\hat{\psi}^\dagger(1')\hat{\psi}^\dagger(2')\right] \middle| \Psi_0^N \right\rangle$$

Particle-particle correlation function

$$2K(12;1'2') = G_2(12;1'2')$$

Lehman representation

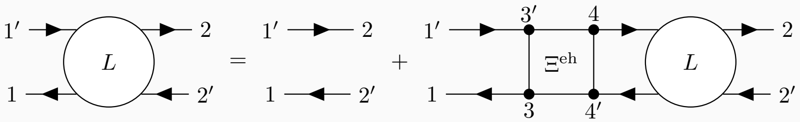
$$K(\mathbf{x}_1\mathbf{x}_2;\mathbf{x}_{1'}\mathbf{x}_{2'};\omega) = \sum_\nu \frac{L_\nu^{N+2}(\mathbf{x}_1\mathbf{x}_2)R_\nu^{N+2}(\mathbf{x}'_1\mathbf{x}'_2)}{\omega - \underbrace{(E_\nu^{N+2} - E_0^N)}_{\text{Double electron affinities}} + \mathrm{i}\eta} - \sum_\nu \frac{L_\nu^{N-2}(\mathbf{x}'_1\mathbf{x}'_2)R_\nu^{N-2}(\mathbf{x}_1\mathbf{x}_2)}{\omega - \underbrace{(E_0^N - E_\nu^{N-2})}_{\text{Double ionization potentials}} - \mathrm{i}\eta}$$

Electron-hole channel

Electron-hole Bethe-Salpeter equation

$$L(12;1'2') = \underbrace{L_0(12;1'2')}_{\text{Independent particle propagator}} + \int \mathrm{d}(3456)\, L_0(14;1'3)\, \underbrace{\Xi^{\text{eh}}(36;45)}_{\text{eh kernel}}\, L(52;62')$$

where $$L_0(12;1'2') = G(12')G(21') \qquad \Xi^{\text{eh}}(12;34) = \left.\frac{\delta\Sigma(13)}{\delta G(42)}\right|_{U=0}$$



Electron-hole channel

Eigenvalue problem

$$\begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{B}^\dagger & \boldsymbol{A} \end{pmatrix} \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix} = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix}$$

$$A_{ia,jb} = (\epsilon_a - \epsilon_i)\delta_{ab}\delta_{ij} + \Xi^{\text{eh}}_{ia,jb}(\omega = 0)$$
$$B_{ia,bj} = \Xi^{\text{eh}}_{ia,bj}(\omega = 0)$$

Approximate kernels

RPA kernel

$$\Xi^{\text{eh},RPA}(12;1'2') = \mathrm{i}\,\frac{\delta\Sigma_{\mathsf{H}}(11')}{\delta G(2'2)}\bigg|_{U=0} = \frac{\delta\left[G(3'3)v(13;1'3')\right]}{\delta G(2'2)}\bigg|_{U=0} = v(12;1'2')$$

Approximate kernels

RPA kernel

$$\Xi^{\text{eh},RPA}(12;1'2') = \mathrm{i}\, \frac{\delta\Sigma_{\text{H}}(11')}{\delta G(2'2)}\bigg|_{U=0} = \frac{\delta\left[G(3'3)v(13;1'3')\right]}{\delta G(2'2)}\bigg|_{U=0} = v(12;1'2')$$

GW kernel

$$\begin{aligned}\Xi^{\text{eh},GW}(12;1'2') = \mathrm{i}\, \frac{\delta\Sigma_{\text{Hxc}}^{GW}(11')}{\delta G(2'2)}\bigg|_{U=0} &= v(12;1'2') - \frac{\delta\left[G(33')W(11';33')\right]}{\delta G(2'2)}\bigg|_{U=0} \\ &= v(12;1'2') - W(11';2'2) - G(33')\,\frac{\delta W(11';33')}{\delta G(2'2)}\bigg|_{U=0}\end{aligned}$$

Electron-hole channel

Eigenvalue problem

$$\begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{B}^\dagger & \boldsymbol{A} \end{pmatrix} \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix} = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix}$$

$$A_{ia,jb} = (\epsilon_a - \epsilon_i)\delta_{ab}\delta_{ij} + \Xi^{\text{eh}}_{ia,jb}(\omega = 0)$$
$$B_{ia,bj} = \Xi^{\text{eh}}_{ia,bj}(\omega = 0)$$

Kernels

$$\Xi^{\text{eh,RPA}}_{ia,jb} = \langle ib|aj \rangle \qquad \Xi^{\text{eh},GW}_{ia,jb} = \langle ib|aj \rangle - W_{ibja}(\omega = 0)$$

- Second-order kernel
- T-matrix kernel
- ...

Usual linear response

Schwinger relation

$$-G_2(12;1'2') + G(11')G(22') = \left.\frac{\delta G(11';[U])}{\delta\, U^{\text{eh}}(2'2)}\right|_{U=0} = L(12;1'2')$$

External potential

External potential

$$\hat{\mathcal{U}}(t_1) = \int \mathrm{d}(\mathbf{x}_1 \mathbf{x}_{1'} t_1')\, \hat{\psi}^\dagger(\mathbf{x}_1) U^{\text{eh}}(11') \hat{\psi}(\mathbf{x}_{1'})$$

Pairing field linear response

Another external potential ...

$$\hat{\mathcal{U}}(t_1) = \frac{1}{2}\left(\int \mathrm{d}(\mathbf{x}_1\mathbf{x}_{1'}t_1')\,\hat{\psi}(\mathbf{x}_1)U^{\mathrm{hh}}(11')\hat{\psi}(\mathbf{x}_{1'}) + \int \mathrm{d}(\mathbf{x}_1\mathrm{d}\mathbf{x}_{1'}t_1')\;\underbrace{\hat{\psi}^\dagger(\mathbf{x}_{1'})\;U^{\mathrm{ee}}(11')\;\hat{\psi}^\dagger(\mathbf{x}_{1'})}_{\text{Non-number conserving}}\right)$$

Pairing field linear response

Another external potential ...

$$\hat{\mathcal{U}}(t_1) = \frac{1}{2}\left(\int \mathrm{d}(\mathbf{x}_1\mathbf{x}_{1'}t_1')\,\hat{\psi}(\mathbf{x}_1)U^{\mathrm{hh}}(11')\hat{\psi}(\mathbf{x}_{1'}) + \int \mathrm{d}(\mathbf{x}_1\mathrm{d}\mathbf{x}_{1'}t_1')\;\underbrace{\hat{\psi}^\dagger(\mathbf{x}_{1'})\;U^{\mathrm{ee}}(11')\;\hat{\psi}^\dagger(\mathbf{x}_{1'})}_{\text{Non-number conserving}}\right)$$

...leading to an alternative Schwinger relation

$$\frac{1}{2}\left(G_2(12;1'2';[U]) - G^{\mathrm{hh}}(12;[U])G^{\mathrm{ee}}(2'1';[U])\right)\Big|_{U=0} = \frac{\delta G^{\mathrm{ee}}(2'1';[U])}{\delta U^{\mathrm{hh}}(12)}\Big|_{U=0} = K(12;1'2')$$

Description of a non-number conserving Hamiltonian

Anomalous propagators

$$G^{\mathrm{hh}}(11';[U]) = (-\mathrm{i}) \langle \Psi_0 | \hat{T} \left[\hat{\psi}(1)\hat{\psi}(1') \right] | \Psi_0 \rangle \quad G^{\mathrm{ee}}(11';[U]) = (-\mathrm{i}) \langle \Psi_0 | \hat{T} \left[\hat{\psi}^\dagger(1)\hat{\psi}^\dagger(1') \right] | \Psi_0 \rangle$$

Nambu formalism and the Gorkov propagator

$$\boldsymbol{G}(11') = (-i) \langle \Psi_0 | \hat{T} \left[\begin{pmatrix} \hat{\psi}(1)\hat{\psi}^\dagger(1') & \hat{\psi}(1)\hat{\psi}(1') \\ \hat{\psi}^\dagger(1)\hat{\psi}^\dagger(1') & \hat{\psi}^\dagger(1)\hat{\psi}(1') \end{pmatrix} \right] | \Psi_0 \rangle = \begin{pmatrix} G^{\mathrm{he}}(11') & G^{\mathrm{hh}}(11') \\ G^{\mathrm{ee}}(11') & G^{\mathrm{eh}}(11') \end{pmatrix}.$$

Gorkov-Dyson equation

$$\boldsymbol{G}^{-1}(11') = \boldsymbol{G}_0^{-1}(11') - \begin{pmatrix} \Sigma^{\mathrm{he}}(11') & \Sigma^{\mathrm{hh}}(11') + U^{\mathrm{ee}}(11') \\ \Sigma^{\mathrm{ee}}(11') + U^{\mathrm{hh}}(11') & \Sigma^{\mathrm{eh}}(11') \end{pmatrix}$$

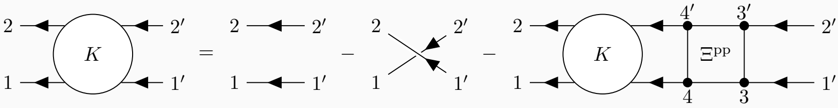
Particle-particle channel

Particle-particle Bethe-Salpeter equation

$$K(12;1'2') = K_0(12;1'2') - \int \mathrm{d}(3456)\, K(12;56)\, \Xi^{\mathrm{pp}}(56;34)\, K_0(34;1'2')$$

Independent particle propagator **pp kernel**

where $$K_0(12;1'2') = \frac{1}{2}[G(11')G(22') - G(21')G(12')] \qquad \Xi^{\mathrm{pp}}(56;34) = \left.\frac{\delta\Sigma^{\mathrm{ee}}(34)}{\delta G^{\mathrm{ee}}(56)}\right|_{U=0}$$



Particle-particle channel

Eigenvalue problem

$$\begin{pmatrix} \boldsymbol{C} & \boldsymbol{B} \\ \boldsymbol{B}^\dagger & \boldsymbol{D} \end{pmatrix} \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix} = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix}$$

$$\begin{aligned} C_{ab,cd}^{\text{RPA}} &= (\epsilon_a + \epsilon_b)\delta_{ac}\delta_{bd} + \Xi_{ab,cd}^{\text{pp}}(\omega = 0) \\ B_{ab,ij}^{\text{RPA}} &= \Xi_{ab,ij}^{\text{pp}}(\omega = 0) \\ D_{ij,kl}^{\text{RPA}} &= -(\epsilon_i + \epsilon_j)\delta_{ik}\delta_{jl} + \Xi_{ij,kl}^{\text{pp}}(\omega = 0) \end{aligned}$$

Approximate kernels

RPA kernel

$$\Xi^{\mathrm{pp},RPA}(12;1'2') = \mathrm{i}\, \left.\frac{\delta\Sigma_{\mathrm{B}}^{\mathrm{ee}}(22')}{\delta G^{\mathrm{ee}}(11')}\right|_{U=0} = \frac{1}{2}\, \left.\frac{\delta\left[G^{\mathrm{ee}}(33')[v(33';22') - v(3'3;22')]\right]}{\delta G^{\mathrm{ee}}(11')}\right|_{U=0}$$

$$= \frac{1}{2}[v(11';22') - v(1'1;22')]$$

Approximate kernels

RPA kernel

$$\Xi^{\text{pp},RPA}(12;1'2') = \mathrm{i} \left. \frac{\delta \Sigma_{\text{B}}^{\text{ee}}(22')}{\delta G^{\text{ee}}(11')} \right|_{U=0} = \frac{1}{2} \left. \frac{\delta \left[G^{\text{ee}}(33')[v(33';22') - v(3'3;22')] \right]}{\delta G^{\text{ee}}(11')} \right|_{U=0}$$
$$= \frac{1}{2}[v(11';22') - v(1'1;22')]$$

pp GW kernel

$$\Xi^{\text{pp},GW}(11';22') = \mathrm{i} \left. \frac{\delta \Sigma_{\text{Bxc}}^{\text{ee},GW}(22')}{\delta G^{\text{ee}}(11')} \right|_{U=0} = \frac{1}{2} \left. \frac{\delta \left[G^{\text{ee}}(33')[W(33';22') - W(3'3;22')] \right]}{\delta G^{\text{ee}}(11')} \right|_{U=0}$$
$$= \frac{1}{2}[W(11';22') - W(1'1;22')]$$

Particle-particle channel

Eigenvalue problem

$$\begin{pmatrix} \boldsymbol{C} & \boldsymbol{B} \\ \boldsymbol{B}^\dagger & \boldsymbol{D} \end{pmatrix} \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix} = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix}$$

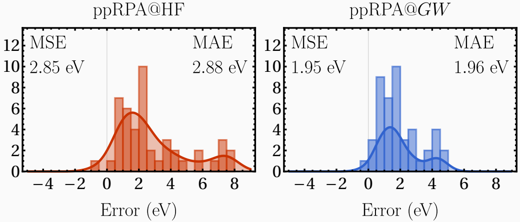
$$\begin{aligned} C^{\text{RPA}}_{ab,cd} &= (\epsilon_a + \epsilon_b)\delta_{ac}\delta_{bd} + \Xi^{\text{pp}}_{ab,cd}(\omega = 0) \\ B^{\text{RPA}}_{ab,ij} &= \Xi^{\text{pp}}_{ab,ij}(\omega = 0) \\ D^{\text{RPA}}_{ij,kl} &= -(\epsilon_i + \epsilon_j)\delta_{ik}\delta_{jl} + \Xi^{\text{pp}}_{ij,kl}(\omega = 0) \end{aligned}$$

Kernels

$$\Xi^{\text{pp,RPA}}_{ij,kl} = \langle ij||kl\rangle \qquad \Xi^{\text{pp},GW}_{ij,kl} = W_{ijkl}(\omega = 0) - W_{ijlk}(\omega = 0)$$

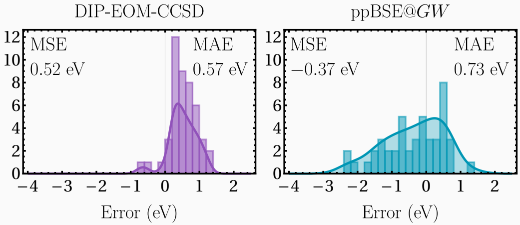
- Second-order kernel
- T-matrix kernel
- ...

Error distribution (w.r.t. FCI) for 46 DIP of 23 small molecules in the aug-cc-pVTZ basis set



Valence double ionization potentials

Error distribution (w.r.t. FCI) for 46 DIP of 23 small molecules in the aug-cc-pVTZ basis set



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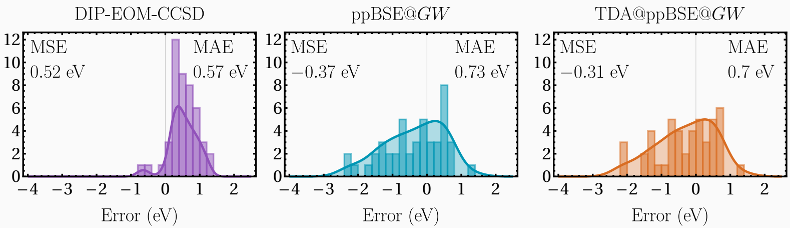

Tamm-Dancoff approximation

$$\begin{pmatrix} \boldsymbol{C} & \boldsymbol{B} \\ \boldsymbol{B}^\dagger & \boldsymbol{D} \end{pmatrix} \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix} = \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{pmatrix} \quad \rightarrow \quad \begin{aligned} \boldsymbol{C}\boldsymbol{X} &= \omega \boldsymbol{X} \\ \boldsymbol{D}\boldsymbol{Y} &= -\omega \boldsymbol{Y} \end{aligned}$$

Dynamical perturbative correction

Static eigenvalue problem

$$\boldsymbol{D}^{(0)} \boldsymbol{Y}_n^{(0)} = -\Omega_n^{(0)} \boldsymbol{Y}_n^{(0)}$$

Partitioning

$$\boldsymbol{D}(\omega) = \boldsymbol{D}^{(0)} + \boldsymbol{D}^{(1)}(\omega)$$

Perturbative correction

$$\Omega_n^{(1)} = (\boldsymbol{Y}_n^{(0)})^\dagger \cdot \boldsymbol{D}^{(1)}(-\Omega_n^{(0)}) \cdot \boldsymbol{Y}_n^{(0)}$$

Sangalli *et al.* J. Chem. Phys. 158 034115 (2011)

Valence double ionization potentials

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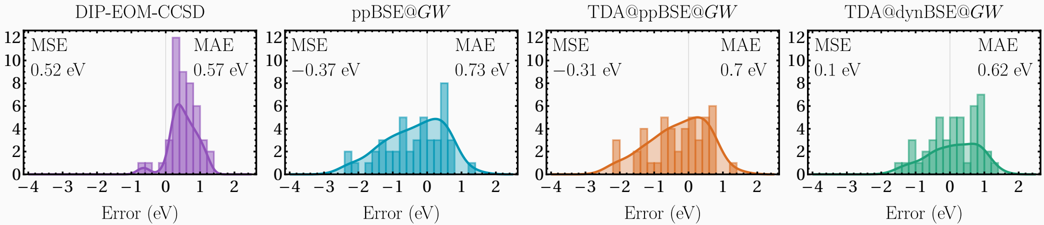
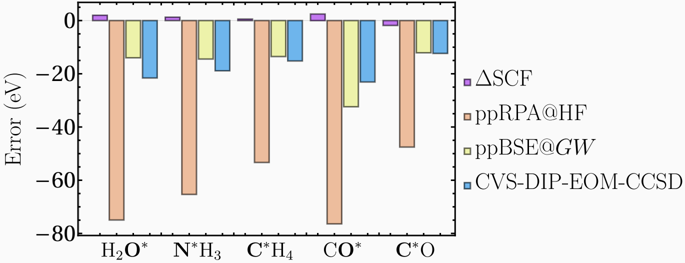


Error with respect to CVS-FCI in the aug-cc-pCVTZ basis set



Conclusion and open questions

Conclusions

- Simple expression for the kernel of the particle-particle channel
- ppBSE brings quantitative improvements for double ionization
- More details in J. Chem. Phys. 162, 134105 (2025)

Questions?

Particle-particle Bethe-Salpeter equation

Derivation

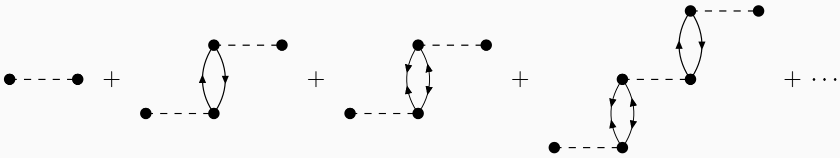
$$
\begin{aligned}
K(12;1'2') &= \left.\frac{\delta G^{\mathrm{ee}}(2'1')}{\delta U^{\mathrm{hh}}(12)}\right|_{U=0} \\
&= G(32') \left.\frac{\delta (G^{-1})^{\mathrm{ee}}(33')}{\delta U^{\mathrm{hh}}(12)}\right|_{U=0} G(3'1') \\
&= -G(32') \left.\frac{\delta U^{\mathrm{hh}}(33')}{\delta U^{\mathrm{hh}}(12)}\right|_{U=0} G(3'1') - G(32') \left.\frac{\delta \Sigma^{\mathrm{ee}}(33')}{\delta U^{\mathrm{hh}}(12)}\right|_{U=0} G(3'1') \\
&= K_0(12;1'2') - \left.\frac{\delta G^{\mathrm{ee}}(44')}{\delta U^{\mathrm{hh}}(12)}\right|_{U=0} \left.\frac{\delta \Sigma^{\mathrm{ee}}(33')}{\delta G^{\mathrm{ee}}(44')}\right|_{U=0} G(3'1')G(32')
\end{aligned}
$$

Gorkov *GW*

Self-energy

$$\boldsymbol{\Sigma}(11') = \mathrm{i}\int \mathrm{d}(33') \begin{pmatrix} W(13';31')G^{\mathrm{he}}(33') & -W(13';31')G^{\mathrm{hh}}(33') \\ -W(31';13')G^{\mathrm{ee}}(33') & W(31';13')G^{\mathrm{eh}}(33') \end{pmatrix}$$

Screened interaction



Valence double ionization potentials

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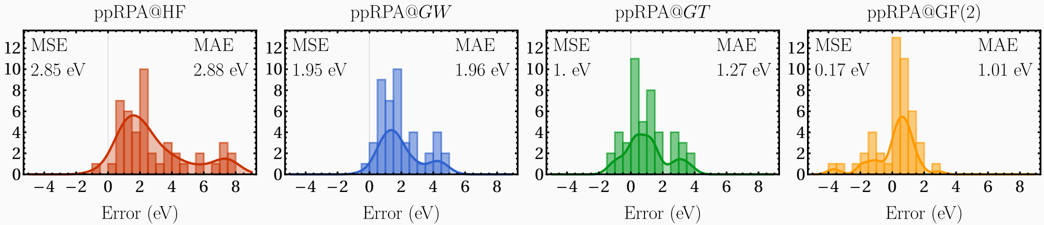

Alternative kernels

Error distribution (w.r.t. FCI) for 46 DIP of 23 small molecules in the aug-cc-pVTZ basis set