Dispersion energies from the random-phase approximation with range separation

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Range-separated DFT

**Extension of Kohn-Sham scheme to multideterminant wavefunction**

\[
E_{\text{exact}} = \min_{\Psi} \left\{ \langle \Psi | \hat{T} + \hat{V}_{ne} + \hat{W}_{ee}^{lr} | \Psi \rangle + E_{Hxc}^{sr}[n\Psi] \right\}
\]

- \( \hat{W}_{ee}^{lr} = \sum_{i<j} \frac{\text{erf}(\mu r_{ij})}{r_{ij}} \): long-range electron-electron interaction
- \( E_{Hxc}^{sr}[n] \): short-range density functional
- Multideterminant wave function: \( \Psi^{lr} = \sum_i c_i \Phi_i \)
- Parameter \( \mu \) controls separation into lr/sr
Range-separated DFT

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- Multideterminant wave function: \( \Psi^{\text{lr}} = \sum_i c_i \Phi_i \)
- Parameter \( \mu \) controls separation into \( \text{lr/sr} \)
- **In practice: approximations** for \( \Psi^{\text{lr}} \) and \( E_{\text{Hxc}}^{\text{sr}}[n] \)
### Range-separated DFT

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- **In practice:** approximations for \( \Psi^{lr} \) and \( E_{\text{Hxc}}^{sr}[n] \)
  - srLDA
  - srPBE
  - etc...
Range-separated DFT

Extension of Kohn-Sham scheme to multideterminant wavefunction

$$E_{\text{exact}} = \min_{\Psi} \left\{ \langle \Psi | \hat{T} + \hat{V}_{ne} + \hat{W}_{ee}^{\text{lr}} | \Psi \rangle + E_{\text{Hxc}}^{\text{sr}}[n_{\Psi}] \right\}$$

- $\hat{W}_{ee}^{\text{lr}} = \sum_{i<j} \frac{\text{erf}(\mu r_{ij})}{r_{ij}}$: long-range electron-electron interaction
- $E_{\text{Hxc}}^{\text{sr}}[n]$: short-range density functional
- Multideterminant wave function: $\Psi^{\text{lr}} = \sum c_i \Phi_i$
- Parameter $\mu$ controls separation into lr/sr

In practice: approximations for $\Psi^{\text{lr}}$ and $E_{\text{Hxc}}^{\text{sr}}[n]$:

- lrHF
- lrMP2
- lrRPA
- lrCC
- vdW

srLDA
srPBE
etc...
1. Short-range density functionals
2. Long-range MP2
3. Long-range RPA from ACFDT
4. Long-range RPA from ring CCD
1. Short-range density functionals

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Short-range exchange energy: LDA

\[ E_{x,LDA}^{sr,\mu}[n] = \int n(r) \varepsilon_{x,\text{unif}}^{sr,\mu}(n(r)) \, dr \]
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Short-range exchange energy: LDA

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\]

For Be atom:

LDA accurate for a short-range interaction
Short-range exchange energy: LDA

\[ E_{x,LDA}^{sr,\mu}[n] = \int n(r) \varepsilon_{x,\text{unif}}^{sr,\mu}(n(r)) \, dr \]

For Be atom:

\[ E_{x}^{sr,\mu} \]

Asymptotic expansion for \( \mu \to \infty \):

\[ E_{x}^{sr,\mu} = -\frac{A_1}{\mu^2} \int n(r)^2 \, dr + \frac{A_2}{\mu^4} \int n(r) \left( \frac{\left| \nabla n(r) \right|^2}{2n(r)} + 4\tau(r) \right) \, dr + \cdots \]
Short-range correlation energy: LDA

\[ E_{c,LDA}^{sr,\mu}[n] = \int n(r) \left[ \varepsilon_{c,\text{unif}}(n(r)) - \varepsilon_{c,\text{unif}}^{lr,\mu}(n(r)) \right] dr \]
Short-range correlation energy: LDA

\[ E_{c, \text{LDA}}^{sr, \mu}[n] = \int n(r) \left[ \epsilon_{c, \text{unif}}(n(r)) - \epsilon_{c, \text{unif}}^{lr, \mu}(n(r)) \right] dr \]

For Be atom:

\[ E_c^{sr, \mu} \text{ (a.u.)} \]

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Short-range correlation energy: LDA

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For Be atom:

Asymptotic expansion for \( \mu \to \infty \):

\[ E_{c}^{sr, \mu} = \frac{B_1}{\mu^2} \int n_{2,c}(r, r) dr + \frac{B_2}{\mu^3} \int n_2(r, r) dr + \cdots \]
Short-range exchange energy: GGA

Short-range GGA functional of Heyd, Scuseria and Ernzerhof (2003) based on the PBE exchange hole:

\[ \varepsilon_{x,\text{GGA}}^{sr,\mu}(n) = \frac{1}{2} \int n_{x,PBE}(n, |\nabla n|, r_{12}) \omega_{ee}^{sr,\mu}(r_{12}) dr_{12} \]

For Be atom:

\[ E_x^{sr,\mu}(\text{a.u.}) \]

\[ \mu (\text{a.u.}) \]

\[ 0 \]

\[ -2.5 \]

\[ -2 \]

\[ -1.5 \]

\[ -1 \]

\[ -0.5 \]

\[ 0 \]

\[ 1 \]

\[ 2 \]

\[ 3 \]

\[ 4 \]

\[ 5 \]

\[ 6 \]

GGA describes well a longer range of interaction
Short-range correlation energy: GGA

Interpolation between PBE at $\mu = 0$ and expansion of LDA for $\mu \to \infty$:

$$\varepsilon_{c,\text{GGA}}^{\text{sr},\mu}(n, |\nabla n|) = \frac{\varepsilon_{c,\text{PBE}}(n, |\nabla n|)}{1 + d_1(n)\mu + d_2(n)\mu^2}$$

For Be atom:

$\varepsilon_{c,\text{GGA}}^{\text{sr},\mu}$ (a.u.)

$E_{c,\text{GGA}}^{\text{sr},\mu}$ (a.u.)

$\mu$ (a.u.)

$\mu$ (a.u.)

$\Rightarrow$ GGA describes well a longer range of interaction
1. Short-range density functionals
2. Long-range MP2
3. Long-range RPA from ACFDT
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Single-determinant reference

Restriction to single-determinant wave functions $\Phi$

$\mapsto$ range-separated hybrid (RSH):

$$E_{RSH} = \min_{\Phi} \left\{ \langle \Phi | \hat{T} + \hat{V}_{ne} + \hat{W}_{ee} | \Phi \rangle + E_{Hxc}^{sr}[n_\Phi] \right\}$$
Single-determinant reference

Restriction to single-determinant wave functions $\Phi$

$\implies$ range-separated hybrid (RSH):

$$E_{\text{RSH}} = \min_{\Phi} \left\{ \langle \Phi | \hat{T} + \hat{V}_{ne} + \hat{W}_{\text{ee}} | \Phi \rangle + E_{\text{sr}}^{\text{Hxc}} [n_{\Phi}] \right\}$$

The minimizing determinant $\Phi_0$ is given by

$$\left( \hat{T} + \hat{V}_{ne} + \hat{V}_{\text{Hx, HF}}^{\text{lr}} + \hat{V}_{\text{Hxc}}^{\text{sr}} \right) |\Phi_0\rangle = \mathcal{E}_0 |\Phi_0\rangle$$
Single-determinant reference

Restriction to single-determinant wave functions $\Phi$

$\Rightarrow$ range-separated hybrid (RSH):

$$E_{RSH} = \min_{\Phi} \left\{ \langle \Phi | \hat{T} + \hat{V}_{ne} + \hat{W}_{ee} | \Phi \rangle + E_{sr}^{Hxc}[n_{\Phi}] \right\}$$

The minimizing determinant $\Phi_0$ is given by

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So the RSH energy is

$$E_{RSH} = \langle \Phi_0 | \hat{T} + \hat{V}_{ne} | \Phi_0 \rangle + E_H + E_{x,HF}^{Ir} + E_{xc}^{sr}$$

This is a hybrid DFT with HF exchange at long range (similar to the LC scheme)
RSH reference contains no dispersion

Example: Ar$_2$ with aug-cc-pV5Z basis, $\mu = 0.5$ bohr$^{-1}$:
Long-range perturbation theory

All what is missing is the long-range correlation energy

\[ E_{\text{exact}} = E_{\text{RSH}} + E_{\text{lr}} \]
Long-range perturbation theory

All what is missing is the **long-range correlation energy**

\[ E_{\text{exact}} = E_{\text{RSH}} + E_{\text{lr}}^{c} \]

**Adiabatic connection** from RSH reference to exact energy:

\[
E^{\lambda} = \min_{\Psi} \left\{ \langle \Psi | \hat{T} + \hat{V}_{\text{ne}} + \hat{V}_{\text{Hx,HF}}^{\text{lr}} + \lambda \hat{W}^{\text{lr}} | \Psi \rangle + E_{\text{Hxc}}^{\text{sr}}[n_{\Psi}] \right\}
\]

with the long-range perturbation operator \( \hat{W}^{\text{lr}} = \hat{W}^{\text{lr}}_{\text{ee}} - \hat{V}_{\text{Hx,HF}}^{\text{lr}} \)
All what is missing is the long-range correlation energy

$$E_{\text{exact}} = E_{\text{RSH}} + E^{\text{lr}}_c$$

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$$E^\lambda = \min_{\Psi} \left\{ \langle \Psi | \hat{T} + \hat{V}_{\text{ne}} + \hat{V}^{\text{lr}}_{\text{Hx,HF}} + \lambda \hat{W}^{\text{lr}} | \Psi \rangle + E^{\text{sr}}_{\text{Hxc}}[n_{\Psi}] \right\}$$

with the long-range perturbation operator $\hat{W}^{\text{lr}} = \hat{W}_{\text{ee}}^{\text{lr}} - \hat{V}^{\text{lr}}_{\text{Hx,HF}}$

Note: the density is NOT constant on this adiabatic connection
All what is missing is the long-range correlation energy

\[ E_{\text{exact}} = E_{\text{RSH}} + E_{\text{lr}}^c \]

**Adiabatic connection** from RSH reference to exact energy:

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with the long-range perturbation operator \( \hat{W}^{\text{lr}} = \hat{W}_{\text{ee}}^{\text{lr}} - \hat{V}_{\text{Hx, HF}}^{\text{lr}} \)

Note: the density is NOT constant on this adiabatic connection

- Zeroth + first orders: \( E^{(0)} + E^{(1)} = E_{\text{RSH}} \)
- Second order: \( E^{(2)} = \langle \Phi_0 | \hat{W}^{\text{lr}} | \Psi^{\text{lr}, (1)} \rangle = E_{\text{RSH}}^{\text{lr}, \text{MP2}} \)
Convergence of binding energy with basis size: Ar$_2$

aug-cc-pVnZ basis, CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional:

IrMP2 has a fast convergence with basis size.
Interaction energy curve of Ne$_2$

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22 weakly-interacting molecular systems from water dimer to DNA base pairs (CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional):
Equilibrium interaction energies of S22 set

22 weakly-interacting molecular systems from water dimer to DNA base pairs (CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional):

![Graph showing the percentage of error on interaction energy for different systems in the S22 set. The graph is divided into sections for H bonded, dispersion, and dispersion + multipoles, with data points for MP2 aVTZ and MP2 aVQZ functional Representations.]
Equilibrium interaction energies of S22 set

22 weakly-interacting molecular systems from water dimer to DNA base pairs (CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional):

$\Rightarrow$ IrMP2 is very similar to standard MP2
Equilibrium interaction energies of S22 set

22 weakly-interacting molecular systems from water dimer to DNA base pairs (CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional):

$\implies$ lrMP2 is very similar to standard MP2
1. Short-range density functionals

2. Long-range MP2

3. Long-range RPA from ACFDT

4. Long-range RPA from ring CCD
Long-range RPA from ACFDT

**Adiabatic connection** from RSH reference to exact energy:

\[
E^{lr}_c = \int_0^1 d\lambda \left\{ \langle \Psi^{lr}_\lambda | \hat{W}^{lr} | \Psi^{lr}_\lambda \rangle - \langle \Phi_0 | \hat{W}^{lr} | \Phi_0 \rangle \right\}
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\[ = \int_0^1 d\lambda \frac{1}{2} \sum_{ia, jb} \langle ab | jj \rangle^{lr} (P^{lr}_{c, \lambda})_{ia,jb} \]
Adiabatic connection from RSH reference to exact energy:

\[ E_{c}^{lr} = \int_{0}^{1} d\lambda \left\{ \langle \Psi_{\lambda}^{lr} | \hat{W}^{lr} | \Psi_{\lambda}^{lr} \rangle - \langle \Phi_{0} | \hat{W}^{lr} | \Phi_{0} \rangle \right\} \]

\[ = \int_{0}^{1} d\lambda \frac{1}{2} \sum_{ia,jb} \langle ab|ij\rangle^{lr}(P_{c,\lambda})_{ia,jb} \]

\( P_{c,\lambda}^{lr} \) from fluctuation-dissipation theorem

\[ P_{c,\lambda}^{lr} = -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \left[ \chi_{\lambda}^{lr}(\omega) - \chi_{0}(\omega) \right] e^{i\omega 0^{+}} \]
Adiabatic connection from RSH reference to exact energy:

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Long-range response function \(\chi_{\lambda}^{lr}(\omega)\) is given by

\[
\chi_{\lambda}^{lr}(\omega)^{-1} = \chi_0(\omega)^{-1} - f_{Hxc,\lambda}^{lr}(\omega)
\]
Long-range RPA from ACFDT

Adiabatic connection from RSH reference to exact energy:

\[
E_{lr}^c = \int_0^1 d\lambda \left\{ \langle \Psi_\lambda^l r | \hat{W}^l r | \Psi_\lambda^l r \rangle - \langle \Phi_0 | \hat{W}^l r | \Phi_0 \rangle \right\}
\]

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= \int_0^1 d\lambda \frac{1}{2} \sum_{ia,jb} \langle ab|ij \rangle^l r (P_{c,\lambda}^l r)_{ia,jb}
\]

\[P_{c,\lambda}^l r \text{ from fluctuation-dissipation theorem}\]

\[
P_{c,\lambda}^l r = - \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \left[ \chi_{\lambda}^l r(\omega) - \chi_0(\omega) \right] e^{i\omega 0^+}
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\]

Two variants:

- direct RPA (dRPA): \(f_{Hxc,\lambda}^l r(\omega) \approx \lambda f_{H}^l r\)
- RPA with HF exchange (RPAX): \(f_{Hxc,\lambda}^l r(\omega) \approx \lambda f_{H}^l r + \lambda f_{x,HF}^l r\)
Convergence of binding energy with basis size: $\text{Ar}_2$

aug-cc-pV$n$Z basis, CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional:

$\Rightarrow$ lrRPA has a fast convergence with basis size
Interaction energy curve of Ne$_2$

aug-cc-pV5Z basis, CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional:
Interaction energy curve of $\text{Ar}_2$

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Equilibrium interaction energies of S22 set

22 weakly-interacting molecular systems from water dimer to DNA base pairs (CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional):

![Graph showing the percentage of error on interaction energy for different systems in the S22 set. The graph distinguishes between H bonded, dispersion, and dispersion + multipoles interactions. The red squares represent dRPA (PBE) aVTZ.](image)
Equilibrium interaction energies of S22 set

22 weakly-interacting molecular systems from water dimer to DNA base pairs (CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional):

![Graph showing the percentage of error on interaction energy for different systems in the S22 set, comparing dRPA (PBE) aVTZ and dRPA (PBE) aVQZ methods. The graph is divided into categories: H bonded, dispersion, and dispersion + multipoles.](image_url)
Equilibrium interaction energies of S22 set

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![Graph showing % of error on interaction energy for different methods and systems in S22 set.](image-url)
Equilibrium interaction energies of S22 set

22 weakly-interacting molecular systems from water dimer to DNA base pairs (CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional):

$\rightarrow$ lrRPAx gives the smallest mean absolute error ($\sim 8\%$)
1. Short-range density functionals  
2. Long-range MP2  
3. Long-range RPA from ACFDT  
4. Long-range RPA from ring CCD
Long-range RPA from ring coupled cluster doubles (rCCD)

- dRPA can be formulated as a *direct* rCCD (without exchange):

\[
E_{c,dRPA}^{lr} = \int_0^1 d\lambda \frac{1}{2} \sum_{ia,jb} \langle ab|ij \rangle^{lr} (P_{c,\lambda}^{lr})_{ia,jb}
\]

\[
= \frac{1}{2} \sum_{ia,jb} \langle ab|ij \rangle^{lr} (T_{drCCD}^{lr})_{ia,jb} \quad \text{Scuseria et al. 08}
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Scuseria et al. 08

\[
= \text{Diagram 1} + \text{Diagram 2} + \cdots
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\]

Scuseria *et al.* 08

\[
= \begin{array}{c}
\begin{array}{c}
\quad
\end{array}
\end{array}
+ \begin{array}{c}
\begin{array}{c}
\quad
\end{array}
\end{array}
+ \cdots
\]

- dRPA + second-order screened exchange (SOSEX) 

Grüneis *et al.* 09
Paier *et al.* 10

\[
E_{c,dRPA+SOSEX}^{lr} = \frac{1}{2} \sum_{ia,jb} \langle ab||ij\rangle^l r (T_{drCCD}^{lr})_{ia,jb}
\]
Long-range RPA from ring coupled cluster doubles (rCCD)

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- dRPA + second-order screened exchange (SOSEX) Gr"uneis et al. 09 Paier et al. 10

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Interaction energy curve of $\text{Ar}_2$

aug-cc-pV5Z basis, CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional:
Equilibrium interaction energies of S22 set

22 weakly-interacting molecular systems from water dimer to DNA base pairs (aVDZ, CP corrected, $\mu = 0.5 \text{ bohr}^{-1}$, srPBE functional):

$\rightarrow$ SOSEX does not improve on dRPA for weak interactions
Long-range RPA from ring CCD with exchange (rCCDx)

- With \textit{antisymmetrized} integrals: RPAx variant of McLachlan-Ball 1964 (equivalent to TDHF plasmon formula)

\[ E_{c,RPAx-II}^{lr} = \frac{1}{4} \sum_{ia,jb} \langle ab||ij\rangle^{lr} \left( T_{rCCDx}^{lr}\right)_{ia,jb} \]
Long-range RPA from ring CCD with exchange (rCCDx)

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\]

- With *non-antisymmetrized* integrals, RPAX variant of Szabo-Ostlund 1977

\[
E_{c,\text{RPAX-SO2}}^{lr} = \frac{1}{2} \sum_{ia,jb} \langle ab | ij \rangle^{lr} \left( T_{rCCDx}^{lr} \right)_{ia,jb}
\]
Long-range RPA from ring CCD with exchange (rCCDx)

- With *antisymmetrized* integrals: RPAX variant of McLachlan-Ball 1964 (equivalent to TDHF plasmon formula)

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\]

- With *non-antisymmetrized* integrals, RPAX variant of Szabo-Ostlund 1977

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E_{c,\text{RPAX-SO2}}^{lr} = \frac{1}{2} \sum_{ia,jb} \langle ab|ij\rangle^{lr} (T_{r\text{CCDx}}^{lr})_{ia,jb}
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Interaction energy curve of Ne$_2$

aug-cc-pV5Z basis, CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional:
Interaction energy curve of $\text{Ar}_2$

aug-cc-pV5Z basis, CP corrected, $\mu = 0.5 \text{ bohr}^{-1}$, srPBE functional:
Equilibrium interaction energies of S22 set

22 weakly-interacting molecular systems from water dimer to DNA base pairs (aVDZ, CP corrected, $\mu = 0.5 \text{ bohr}^{-1}$, srPBE functional):

$\Rightarrow$ IrRPAX-SO2 gives a mean absolute error of $\sim 4\%$
Equilibrium interaction energies of S22 set

22 weakly-interacting molecular systems from water dimer to DNA base pairs (aVDZ, CP corrected, $\mu = 0.5$ bohr$^{-1}$, srPBE functional):

$$\implies \text{IrRPAX-SO2 gives a mean absolute error of } \sim 4\%$$
Spin-adapted RPA for closed-shell systems

The variants based on drCCD only need spin-singlet excitations:

\[
E_{c,\text{dRPA}} = \frac{1}{2} \text{tr} \left[ ^1K^1T_{\text{drCCD}} \right]
\]

with \(^1K_{ia,jb} = 2\langle ab|ij\rangle\)
Spin-adapted RPA for closed-shell systems

The variants based on drCCD only need spin-singlet excitations:

**dRPA**

\[ E_{c,d\text{RPA}} = \frac{1}{2} \text{tr} \left[ {^1K} {^1T}_{\text{drCCD}} \right] \]

with \( {^1K}_{ia,jb} = 2 \langle ab|ij \rangle \)

**dRPA+SOSEX**

\[ E_{c,d\text{RPA+SOSEX}} = \frac{1}{2} \text{tr} \left[ {^1B} {^1T}_{\text{drCCD}} \right] \]

with \( {^1B}_{ia,jb} = 2 \langle ab|ij \rangle - \langle ab|ji \rangle \)
Spin-adapted RPA for closed-shell systems

The variants based on rCCDx may also need spin-triplet excitations:

\[ E_{c,\text{RPAx-II}} = \frac{1}{4} \text{tr} \left[ 1B^1T_{r\text{CCDx}} + 3B^3T_{r\text{CCDx}} \right] \]

with \(3B_{ia,jb} = -\langle ab|ji\rangle\)
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The variants based on rCCDx may also need spin-triplet excitations:

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\[
E_{c,\text{RPAX-II}} = \frac{1}{4} \text{tr} \left[ B_1^1 T_{\text{rCCDx}} + B_3^3 T_{\text{rCCDx}} \right]
\]

with \( B_{ia,jb} = -\langle ab|ji \rangle \)

**RPAX-SO2**

\[
E_{c,\text{RPAX-SO2}} = \frac{1}{2} \text{tr} \left[ K_1^1 T_{\text{rCCDx}} \right]
\]

**RPAX-SO1**

\[
E_{c,\text{RPAX-SO1}} = \frac{1}{2} \text{tr} \left[ B \left( T_{\text{rCCDx}}^1 - B_3^3 T_{\text{rCCDx}} \right) \right]
\]
Equilibrium interaction energies of S22 set

22 weakly-interacting molecular systems from water dimer to DNA base pairs (aVDZ, CP corrected, $\mu = 0.5 \text{ bohr}^{-1}$, srPBE functional):

$\rightarrow$ irRPAX-SO1 and irRPAX-SO2 give almost identical results
### Computational cost

<table>
<thead>
<tr>
<th>Method</th>
<th>Algorithm</th>
<th>Complexity</th>
</tr>
</thead>
<tbody>
<tr>
<td>dRPA</td>
<td>straightforward</td>
<td>$N^6$</td>
</tr>
<tr>
<td></td>
<td>algorithm with RI</td>
<td>$N^4$</td>
</tr>
<tr>
<td>dRPA + SOSEX</td>
<td>algorithm with RI</td>
<td>$N^5$</td>
</tr>
<tr>
<td>RPAX variants</td>
<td>straightforward</td>
<td>$N^6 (N_\sigma^3 N_\nu^3)$</td>
</tr>
<tr>
<td>CCD</td>
<td>$N^6 (N_\sigma^2 N_\nu^4)$</td>
<td></td>
</tr>
</tbody>
</table>
Summary

<table>
<thead>
<tr>
<th>long-range RPA + short-range DFT</th>
</tr>
</thead>
<tbody>
<tr>
<td>seems well suited for van der Waals interactions</td>
</tr>
<tr>
<td>has a fast basis convergence</td>
</tr>
<tr>
<td>several variants with exchange: RPAX-SO2 seems the best</td>
</tr>
<tr>
<td>warning: RPAX can have instabilities</td>
</tr>
<tr>
<td>can RPAX be made fast?</td>
</tr>
</tbody>
</table>

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Toulouse, Zhu, Ángyán, Savin, PRA 82, 032502 (2010)
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Web page: www.lct.jussieu.fr/pagesperso/toulouse/