State-averaged multideterminantal density functional theory based on ensembles and range separation

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Motivation and strategy

- Linear response TD-DFT, which is a time-dependent single-reference perturbation theory, does not treat quasi-degenerate states adequately.
- This is problematic for describing strongly correlated molecular systems (transition metal and actinide chemistry, avoided crossings, conical intersections, ...).
- For such systems, the standard quantum chemical approach is multi-state multireference perturbation theory (MS-CASPT2, QD-NEVPT2). In contrast to MP2, the zeroth-order wavefunctions are multiconfigurational. They are all described with the same set of orbitals that are optimized by state averaging.
- We want to develop a rigorous and computationally cheaper alternative to these methods by using DFT.
- State averaging can be performed in principle exactly in ensemble DFT (eDFT) for excited states.
- Multiconfigurational wavefunctions can be introduced in standard (ground-state) DFT by means of range separation.
- Therefore range-separated eDFT provides a rigorous framework for merging state-averaged multiconfigurational methods with DFT.

Ensemble DFT

- Variational principle for an equi-ensemble (*Theophilou*): if Ψ and Ψ' are orthonormal then

$$\langle\Psi|\hat{H}|\Psi\rangle + \langle\Psi'|\hat{H}|\Psi'\rangle \geq E_0 + E_1$$

- Generalization: for a given ensemble weight w,

$$(1-w)\langle\Psi|\hat{H}|\Psi\rangle + w\langle\Psi'|\hat{H}|\Psi'\rangle = (1-2w)\underbrace{\langle\Psi|\hat{H}|\Psi\rangle}_{\geq E_0} + w\Big(\underbrace{\langle\Psi|\hat{H}|\Psi\rangle + \langle\Psi'|\hat{H}|\Psi'\rangle}_{\geq E_0 + E_1}\Big)$$

- *Gross-Oliveira-Kohn* (GOK) variational principle:

$$\boxed{\text{for } 0 \leq w \leq 1/2, \qquad (1-w)\langle\Psi|\hat{H}|\Psi\rangle + w\langle\Psi'|\hat{H}|\Psi'\rangle \geq E^w}$$

where E^w is the exact ensemble energy: $E^w = (1-w)E_0 + wE_1 \quad \rightarrow \quad \omega = \dfrac{\mathrm{d}E^w}{\mathrm{d}w} = E_1 - E_0$

- E^w is a functional of the ensemble density $n^w(\mathbf{r}) = (1-w)n_0(\mathbf{r}) + wn_1(\mathbf{r})$

Ensemble DFT

- Trial ensemble density matrix operator: $\hat{\gamma}^w = (1-w)|\Psi\rangle\langle\Psi| + w|\Psi'\rangle\langle\Psi'|$.

- The GOK variational principle can be written in a compact form as $\boxed{E^w \leq \mathrm{Tr}\left[\hat{\gamma}^w \hat{H}\right].}$

- With $\hat{H} = \hat{T} + \hat{W}_{\mathrm{ee}} + \int d\mathbf{r}\, v_{\mathrm{ne}}(\mathbf{r})\hat{n}(\mathbf{r})$ it comes $E^w \leq \mathrm{Tr}\left[\hat{\gamma}^w(\hat{T}+\hat{W}_{\mathrm{ee}})\right] + \int d\mathbf{r}\, v_{\mathrm{ne}}(\mathbf{r}) n_{\hat{\gamma}^w}(\mathbf{r})$

  where the trial ensemble density equals $n_{\hat{\gamma}^w}(\mathbf{r}) = \mathrm{Tr}\left[\hat{\gamma}^w \hat{n}(\mathbf{r})\right] = (1-w)n_{\Psi}(\mathbf{r}) + w n_{\Psi'}(\mathbf{r})$

- Hohenberg–Kohn theorem for ensembles*: $\boxed{E^w = \min_n \left\{ F^w[n] + \int d\mathbf{r}\, v_{\mathrm{ne}}(\mathbf{r}) n(\mathbf{r}) \right\}}$

  where the ensemble Levy–Lieb functional equals

$$F^w[n] = \min_{\hat{\gamma}^w \to n} \left\{ \mathrm{Tr}\left[\hat{\gamma}^w(\hat{T}+\hat{W}_{\mathrm{ee}})\right] \right\}$$

*E. K. U. Gross, L. N. Oliveira, and W. Kohn, Phys. Rev. A 37, 2809 (1988)

Kohn–Sham eDFT

- Kohn–Sham decomposition of the ensemble Levy–Lieb functional: $\boxed{F^w[n] = T_{\rm s}^w[n] + E_{\rm Hxc}^w[n]}$

  where the ensemble non-interacting kinetic energy equals

$$T_{\rm s}^w[n] = \min_{\hat{\gamma}^w \to n} \left\{ {\rm Tr}\left[\hat{\gamma}^w \hat{T}\right] \right\} = {\rm Tr}\left[\hat{\Gamma}_{\rm s}^w[n]\hat{T}\right]$$

  and $\boxed{E_{\rm Hxc}^w[n] = E_{\rm H}[n] + E_{\rm xc}^w[n]}$ with $E_{\rm H}[n] = \frac{1}{2}\int\int d\mathbf{r}d\mathbf{r}' \, \frac{n(\mathbf{r})n(\mathbf{r}')}{\mid \mathbf{r} - \mathbf{r}' \mid}$

- Exact KS-eDFT variational ensemble energy expression:

$$\boxed{E^w = \min_{\hat{\gamma}^w} \left\{ {\rm Tr}\left[\hat{\gamma}^w \hat{T}\right] + E_{\rm Hxc}^w[n_{\hat{\gamma}^w}] + \int d\mathbf{r}\, v_{\rm ne}(\mathbf{r}) n_{\hat{\gamma}^w}(\mathbf{r}) \right\}}$$

*E. K. U. Gross, L. N. Oliveira, and W. Kohn, Phys. Rev. A 37, 2809 (1988)

- The minimizing density matrix operator is a non-interacting one,

$$\hat{\Gamma}_s^w = (1-w)|\Phi_0^{\mathrm{KS},w}\rangle\langle\Phi_0^{\mathrm{KS},w}| + w|\Phi_1^{\mathrm{KS},w}\rangle\langle\Phi_1^{\mathrm{KS},w}|,$$

  which reproduces the exact physical ensemble density $n^w(\mathbf{r})$. It is obtained from the self-consistent KS-eDFT equations

$$\left[\hat{T} + \int d\mathbf{r}\left(v_{\mathrm{ne}}(\mathbf{r}) + \frac{\delta E_{\mathrm{Hxc}}^w\left[n_{\hat{\Gamma}_s^w}\right]}{\delta n(\mathbf{r})}\right)\hat{n}(\mathbf{r})\right]|\Phi_i^{\mathrm{KS},w}\rangle = \mathcal{E}_i^{\mathrm{KS},w}|\Phi_i^{\mathrm{KS},w}\rangle, \qquad i = 0, 1.$$

- According to the Hellmann–Feynman theorem,

$$\boxed{\omega = \frac{\mathrm{d}E^w}{\mathrm{d}w} = \mathcal{E}_1^{\mathrm{KS},w} - \mathcal{E}_0^{\mathrm{KS},w} + \left.\frac{\partial E_{\mathrm{xc}}^w[n]}{\partial w}\right|_{n=n^w}}$$

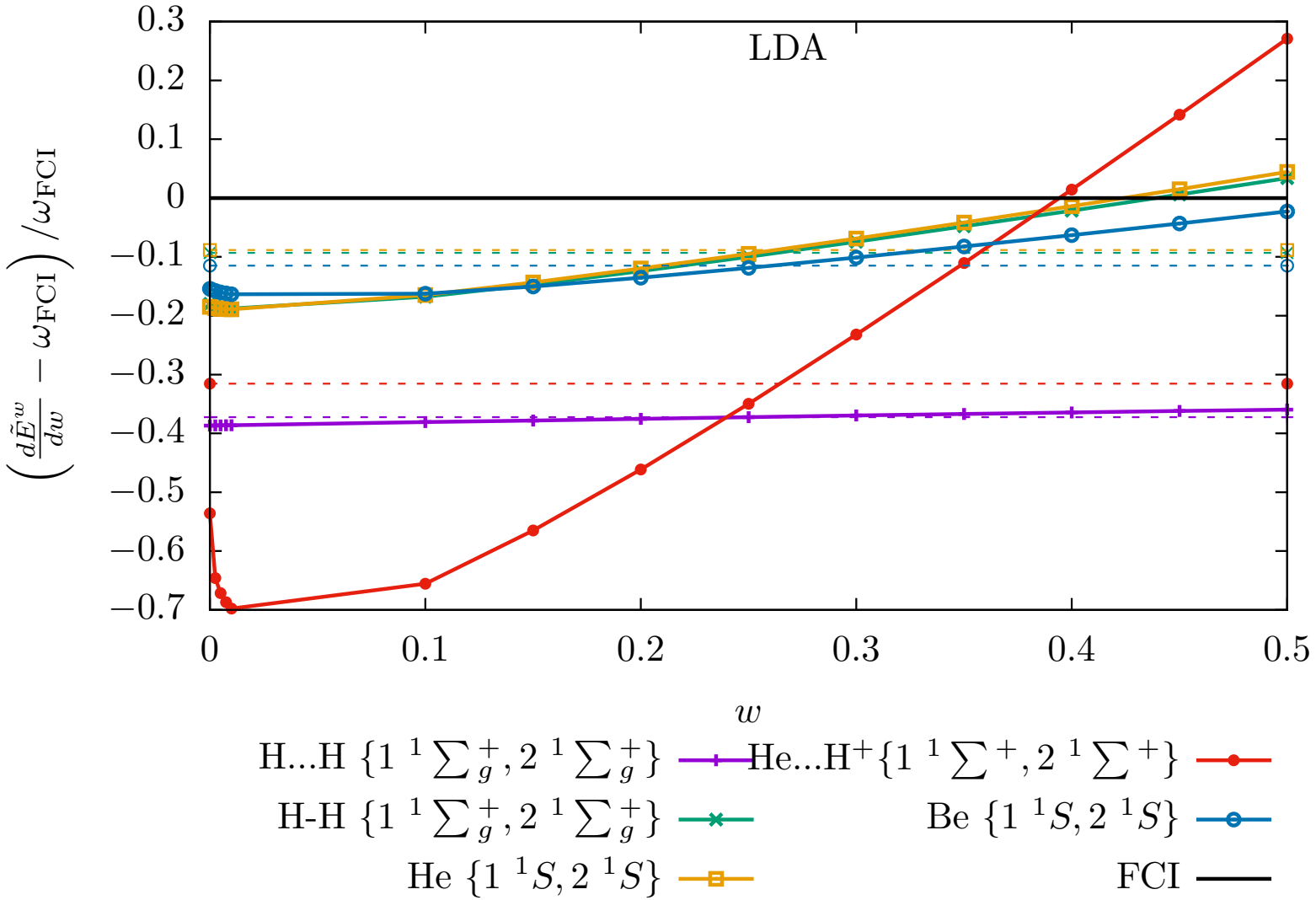
- If the first excitation is a single electron excitation then

$$\omega = \varepsilon_{\mathrm{L}}^w - \varepsilon_{\mathrm{H}}^w + \left.\frac{\partial E_{\mathrm{xc}}^w[n]}{\partial w}\right|_{n=n^w} \xrightarrow[w\to 0]{} \omega = \varepsilon_{\mathrm{L}} - \varepsilon_{\mathrm{H}} + \underbrace{\left.\frac{\partial E_{\mathrm{xc}}^w[n^0]}{\partial w}\right|_{w=0}}$$

Δ_{xc}: derivative discontinuity (DD)*

*M. Levy, *Phys. Rev. A* **52**, R4313 (1995).

Weight-independent density-functional approximation (WIDFA): $E^w_{\rm Hxc}[n] \to E_{\rm Hxc}[n], \quad E^w \to \tilde{E}^w$



Md. M. Alam, S. Knecht, and E. Fromager, Phys. Rev. A 94, 012511 (2016).

Linear interpolation method (LIM)

- In the exact theory: $2(E^{w=1/2} - E_0) = \omega = \dfrac{\mathrm{d}E^w}{\mathrm{d}w}$
- The WIDFA ensemble energy $\tilde{E}^w$ has curvature.
- The WIDFA excitation energy obtained from

$$\boxed{\mathrm{d}\tilde{E}^w/\mathrm{d}w = \tilde{\mathcal{E}}_1^{\mathrm{KS},w} - \tilde{\mathcal{E}}_0^{\mathrm{KS},w}}$$

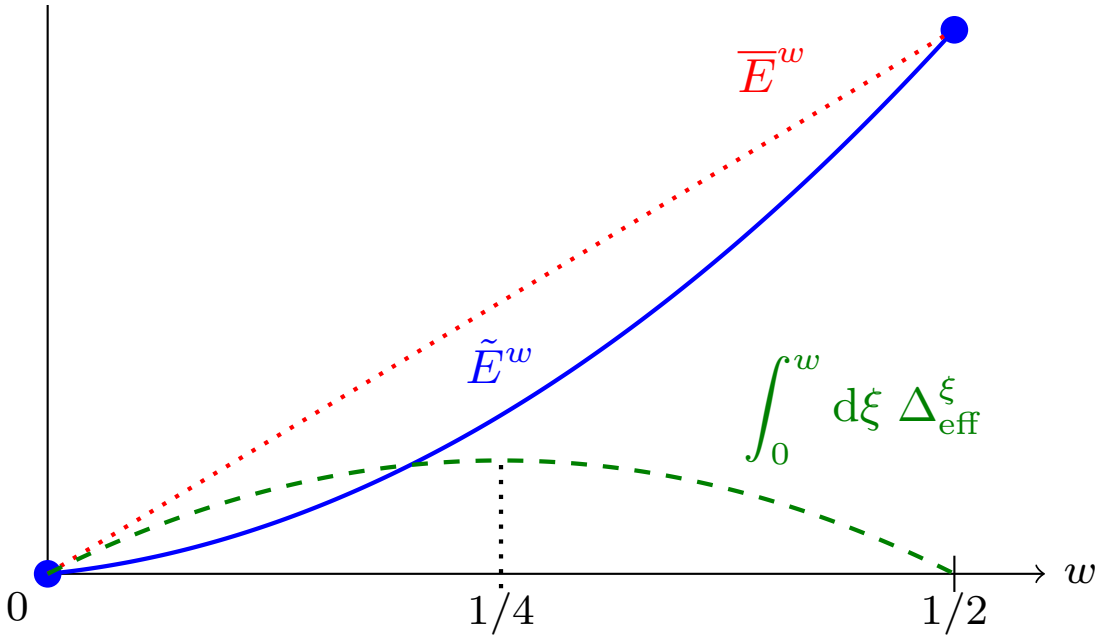
  is weight-dependent (!)

- On the other hand, we have $\boxed{\omega_{\mathrm{LIM}} = 2\left(\tilde{E}^{w=1/2} - E_0\right)}$

that is a well-defined approximate excitation energy, by analogy with the fundamental gap problem *

T. Stein, J. Autschbach, N. Govind, L. Kronik, and R. Baer, *J. Phys. Chem. Lett.* **3**, 3740 (2012).

Linear interpolation method (LIM)

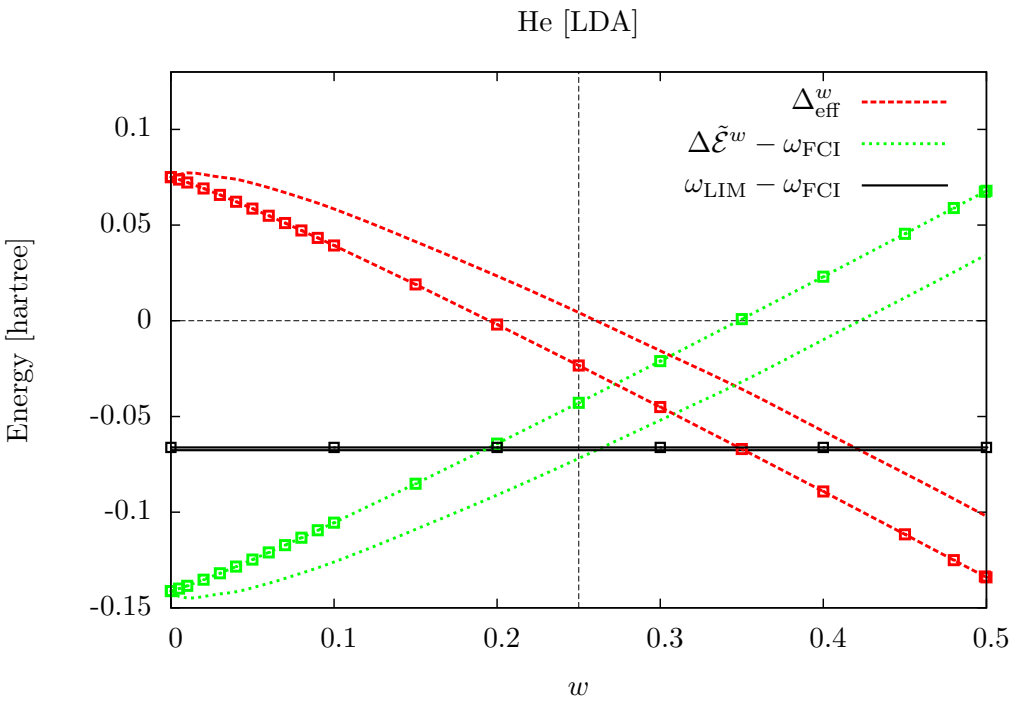


$$\underbrace{E_0 + 2w\big(\tilde{E}^{w=1/2} - E_0\big)}_{\downarrow\ \overline{E}^w} = \tilde{E}^w + \underbrace{\int_0^w \mathrm{d}\xi\ \Delta_{\mathrm{eff}}^{\xi}}_{\downarrow\ \text{curvature correction}} \quad \Rightarrow \quad \underbrace{2(\tilde{E}^{w=1/2} - E_0)}_{\downarrow\ \text{excitation energy}} = \tilde{\varepsilon}_1^{\mathrm{KS},w} - \tilde{\varepsilon}_0^{\mathrm{KS},w} + \underbrace{\Delta_{\mathrm{eff}}^{w}}_{\downarrow\ \text{effective DD}}$$

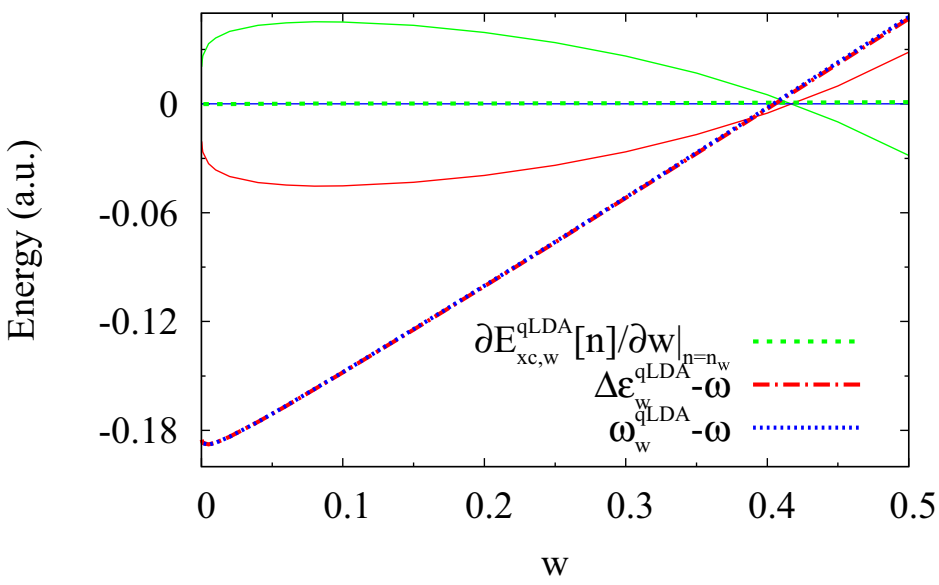
B. Senjean, S. Knecht, H. J. Aa. Jensen, and E. Fromager, *Phys. Rev. A* **92**, 012518 (2015).

Effective DD in He [$1^1S \rightarrow 2^1S$]

□, □ : no self-consistency

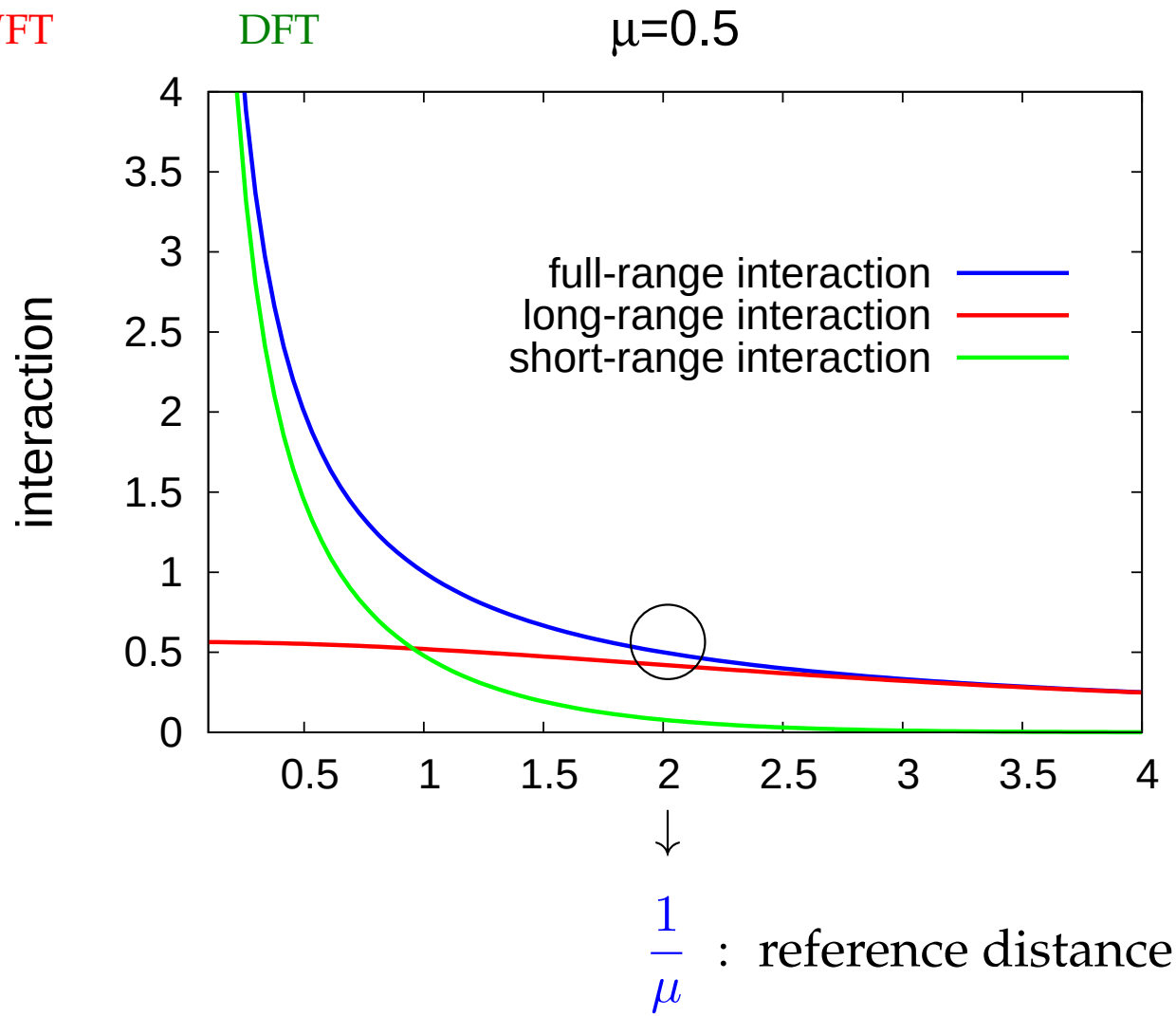


B. Senjean *et al.*, *Phys. Rev. A* **92**, 012518 (2015).



Z-h. Yang *et al.*, *Phys. Rev. A* **90**, 042501 (2014).

$$\frac{1}{r_{12}} = \underbrace{\frac{\mathrm{erf}(\mu r_{12})}{r_{12}}}_{\text{WFT}} + \underbrace{\frac{1-\mathrm{erf}(\mu r_{12})}{r_{12}}}_{\text{DFT}} \qquad \text{where} \qquad \mathrm{erf}(\mu r_{12}) = \frac{2}{\sqrt{\pi}} \int_0^{\mu r_{12}} e^{-t^2}\, dt$$



$\frac{1}{\mu}$: reference distance in a.u.

- Exact range-separated ground-state energy expression (*Savin*):

$$E_0 = \min_{\Psi} \left\{ \langle \Psi | \hat{T} + \hat{W}_{\rm ee}^{\rm lr,\mu} + \hat{V}_{\rm ne} | \Psi \rangle + E_{\rm Hxc}^{\rm sr,\mu}[n_\Psi] \right\}$$

- The minimizing wavefunction Ψ_0^μ is the ground state of a long-range interacting system whose density equals the exact ground-state density n_0.
- Ψ_0^μ fulfils the self-consistent equation

$$\left(\hat{T} + \hat{W}_{\rm ee}^{\rm lr,\mu} + \hat{V}_{\rm ne} + \int d\mathbf{r} \, \frac{\delta E_{\rm Hxc}^{\rm sr,\mu}}{\delta n(\mathbf{r})}[n_{\Psi_0^\mu}] \, \hat{n}(\mathbf{r}) \right) |\Psi_0^\mu\rangle = \mathcal{E}_0^\mu |\Psi_0^\mu\rangle$$

- standard KS-DFT is recovered when $\mu = 0$
- pure WFT is recovered when $\mu \to +\infty$

- Short-range functionals: srLDA, srPBE, ... (*Savin, Toulouse, Gori-Giorgi, Stoll, Goll, Scuseria, ...*)
- Long-range-interacting wave function calculation: HF-srDFT, FCI-srDFT, ...

Range-separated ensemble DFT

- **Range separation** of the ensemble Levy–Lieb functional[a,b]: $\boxed{F^{w}[n] = F^{\mathrm{lr},\mu,w}[n] + E_{\mathrm{Hxc}}^{\mathrm{sr},\mu,w}[n]}$

  where $F^{\mathrm{lr},\mu,w}[n] = \min_{\hat{\gamma}^{w}\to n}\left\{\mathrm{Tr}\left[\hat{\gamma}^{w}(\hat{T}+\hat{W}_{\mathrm{ee}}^{\mathrm{lr},\mu})\right]\right\}.$

- **Exact** range-separated expression for the ensemble energy:

$$E^{w} = (1-w)\langle\Psi_0^{\mu,w}|\hat{T}+\hat{W}_{\mathrm{ee}}^{\mathrm{lr},\mu}+\hat{V}_{\mathrm{ne}}|\Psi_0^{\mu,w}\rangle + w\langle\Psi_1^{\mu,w}|\hat{T}+\hat{W}_{\mathrm{ee}}^{\mathrm{lr},\mu}+\hat{V}_{\mathrm{ne}}|\Psi_1^{\mu,w}\rangle + E_{\mathrm{Hxc}}^{\mathrm{sr},\mu,w}[n^{w}],$$

  where the auxiliary ground- and first-excited-state wavefunctions fulfil the **self-consistent** equations

$$\left(\hat{T}+\hat{W}_{\mathrm{ee}}^{\mathrm{lr},\mu}+\hat{V}_{\mathrm{ne}}+\int \mathrm{d}\mathbf{r}\,\frac{\delta E_{\mathrm{Hxc}}^{\mathrm{sr},\mu,w}[n^{w}]}{\delta n(\mathbf{r})}\hat{n}(\mathbf{r})\right)|\Psi_i^{\mu,w}\rangle = \mathcal{E}_i^{\mu,w}|\Psi_i^{\mu,w}\rangle, \qquad i=0,1$$

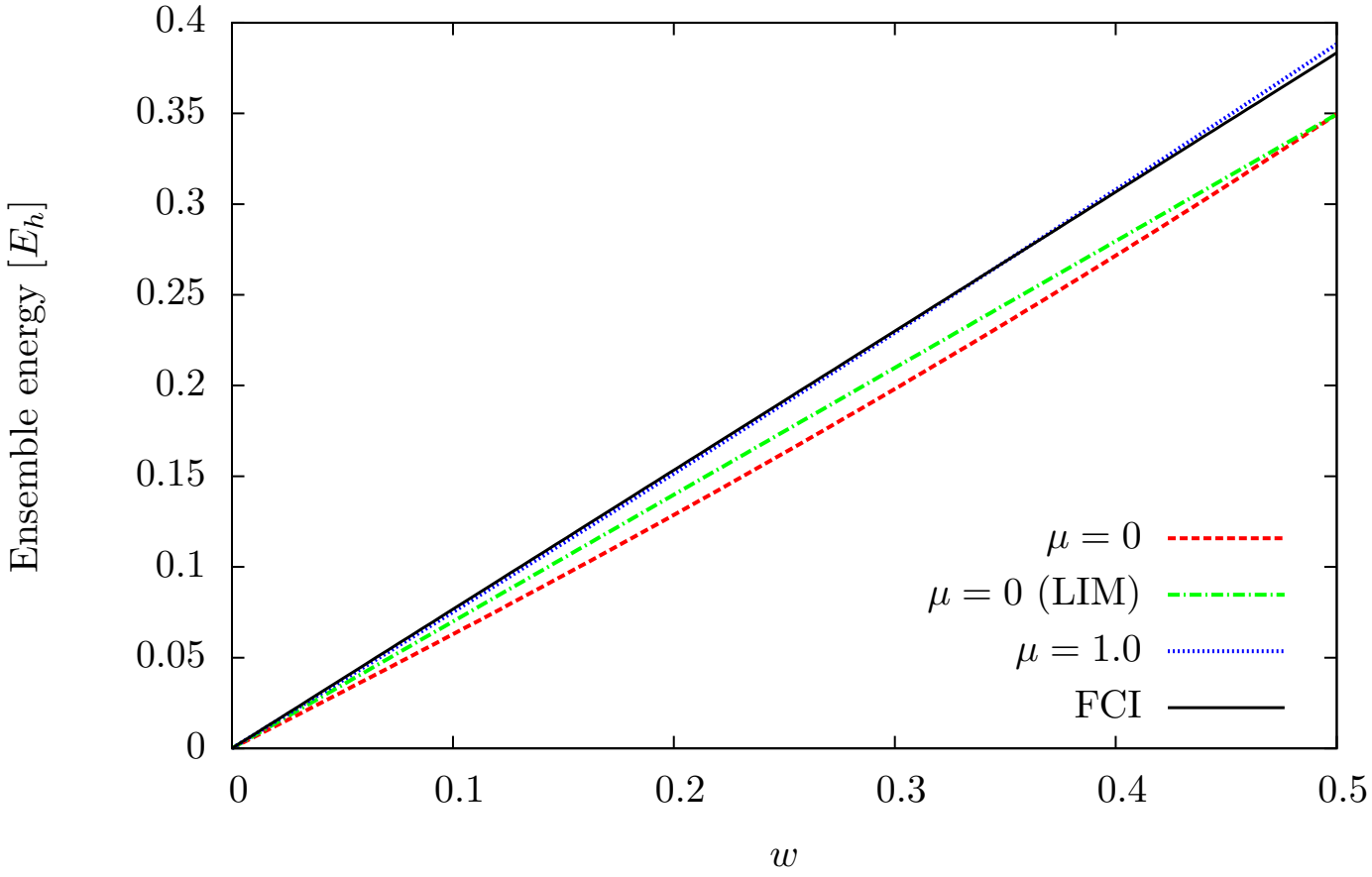
  and reproduce the **exact physical ensemble density** $n^{w}(\mathbf{r}) = (1-w)n_{\Psi_0^{\mu,w}}(\mathbf{r}) + w\,n_{\Psi_1^{\mu,w}}(\mathbf{r}).$

[a] E. Pastorczak, N. I. Gidopoulos, and K. Pernal, Phys. Rev. A 87, 062501 (2013).

[b] O. Franck and E. Fromager, *Mol. Phys.* **112**, 1684 (2014).

He[$1^1S, 2^1S$], srLDA, aug-cc-pVQZ

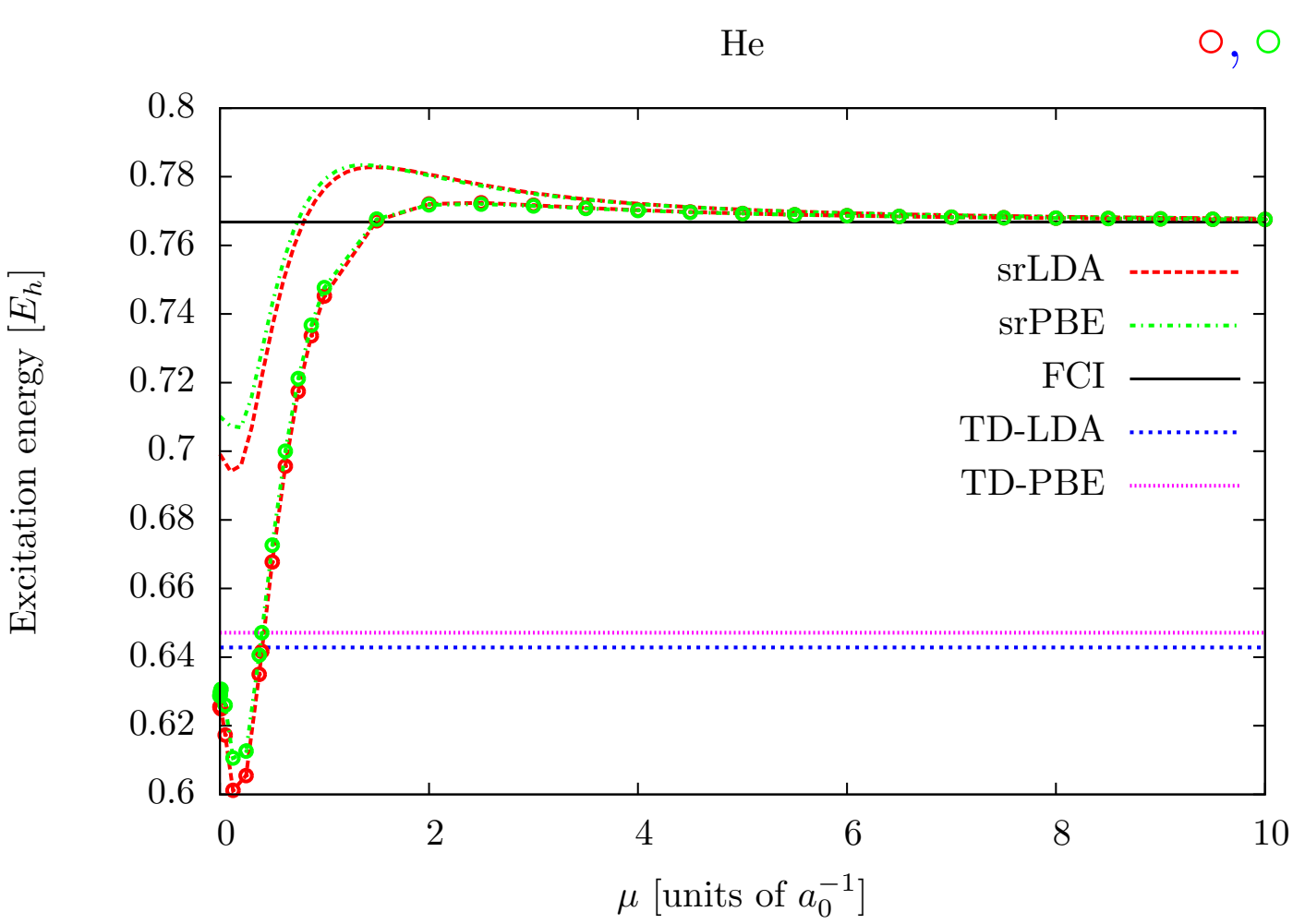
Weight-independent density-functional approximation (WIDFA): $E_{\mathrm{Hxc}}^{\mathrm{sr},\mu,w}[n] \rightarrow E_{\mathrm{Hxc}}^{\mathrm{sr},\mu}[n]$,



B. Senjean, S. Knecht, H. J. Aa. Jensen, and E. Fromager, *Phys. Rev. A* **92**, 012518 (2015).

Excitation energies obtained with LIM and range separation

$1^1S \rightarrow 2^1S$

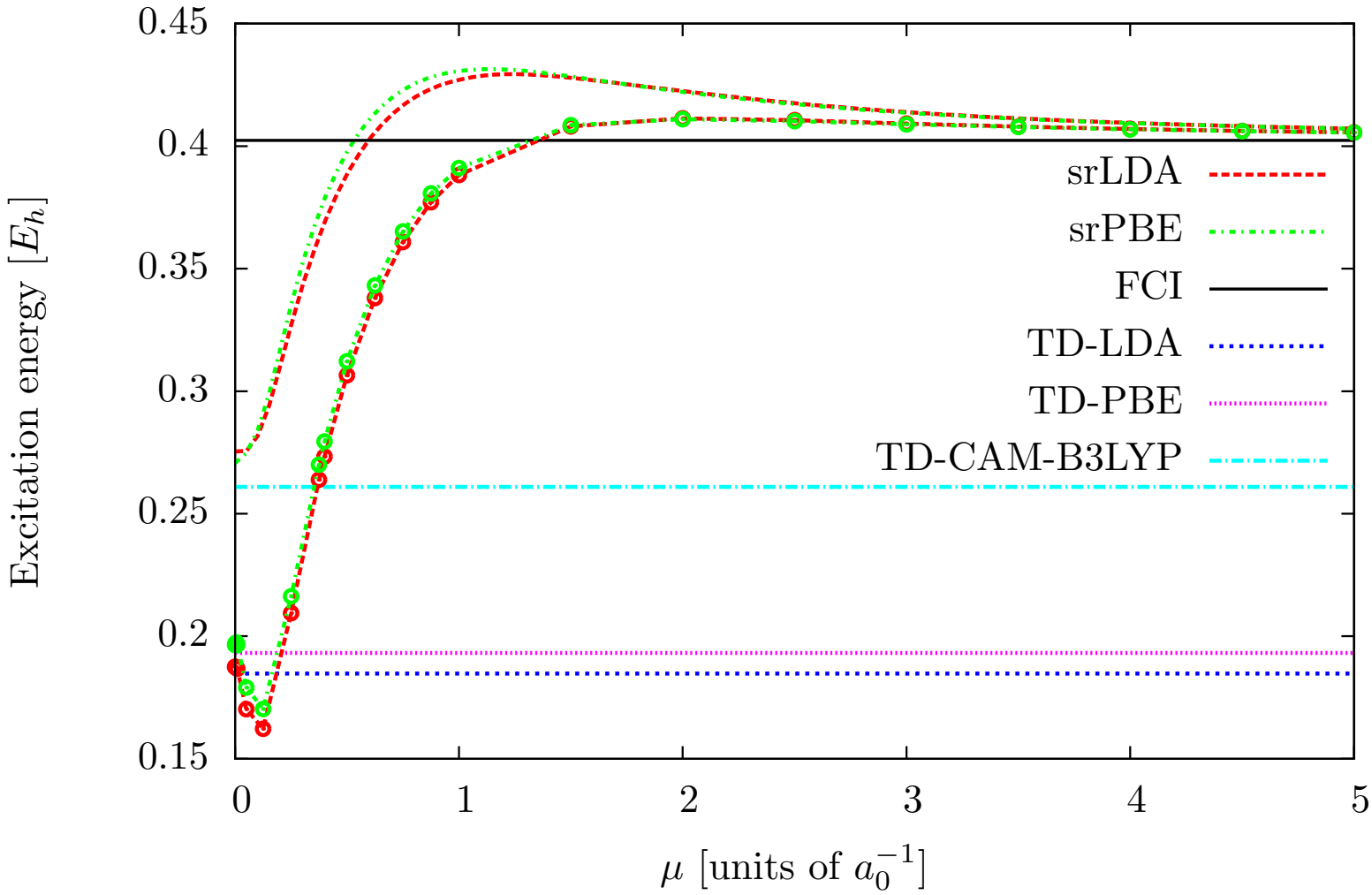


B. Senjean, S. Knecht, H. J. Aa. Jensen, and E. Fromager, *Phys. Rev. A* **92**, 012518 (2015).

$1^1\Sigma^+ \rightarrow 2^1\Sigma^+$

HeH^+ $[R = 8.0a_0]$

$\circ, \circ$: $\mathcal{E}_1^\mu - \mathcal{E}_0^\mu$

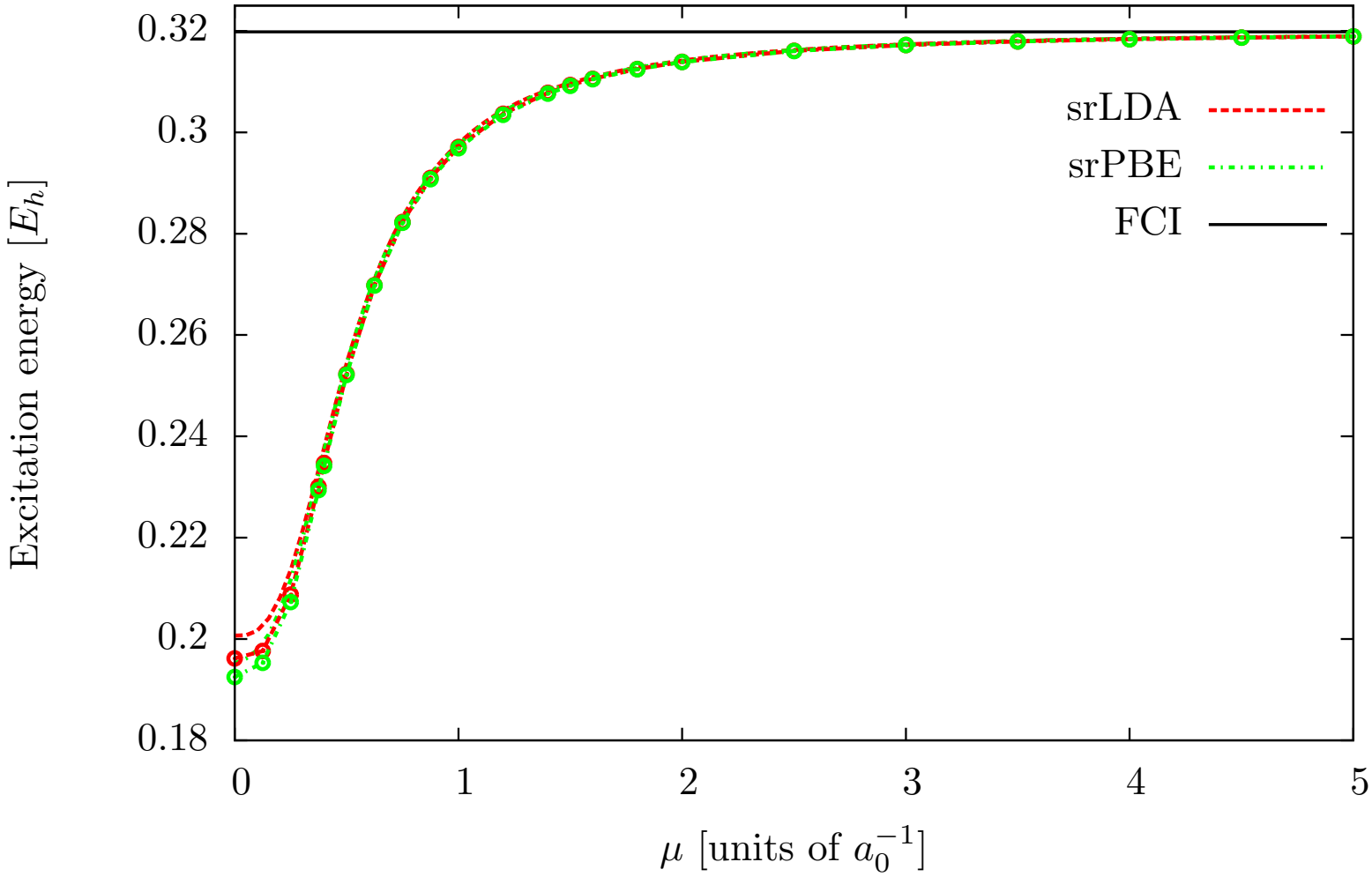


B. Senjean, S. Knecht, H. J. Aa. Jensen, and E. Fromager, *Phys. Rev. A* **92**, 012518 (2015).

$1^1\Sigma_g^+ \rightarrow 2^1\Sigma_g^+$

H_2 $[R = 3.7a_0]$

$\circ, \circ$: $\mathcal{E}_1^\mu - \mathcal{E}_0^\mu$



B. Senjean, S. Knecht, H. J. Aa. Jensen, and E. Fromager, *Phys. Rev. A* **92**, 012518 (2015).

WIDFA, curvature and ghost interaction error

- Where does the curvature of the WIDFA ensemble energy come from ?
- In range-separated eDFT, the short-range Hartree energy is quadratic in w $\Big($unless $n_0(\mathbf{r}) = n_1(\mathbf{r})\Big)$:

$$E_{\rm H}^{\rm sr,\mu}[n^w] = (1-w)^2 E_{\rm H}^{\rm sr,\mu}[n_0] + w^2 E_{\rm H}^{\rm sr,\mu}[n_1] + w(1-w) \int\int d\mathbf{r}d\mathbf{r}' \boxed{n_0(\mathbf{r})n_1(\mathbf{r}')} \frac{{\rm erfc}(\mu|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|}.$$

- In addition, an unphysical short-range **"ghost interaction"** (GI) is introduced.
- This is a well-known problem in KS-eDFT* ($\mu = 0$ limit).
- Both curvature and GI errors are removed in the exact theory by the complementary weight-dependent ensemble short-range xc functional $E_{\rm xc}^{\rm sr,\mu,w}[n]$.
- This is not the case at the WIDFA level since the weight-independent ground-state short-range xc functional is used.

*N. I. Gidopoulos, P. G. Papaconstantinou, and E. K. U. Gross, Phys. Rev. Lett. 88, 033003 (2002).

Exact exchange in range-separated eDFT

- Alternative decomposition of the exact ensemble short-range xc functional:

$$E_{\mathrm{xc}}^{\mathrm{sr},\mu,w}[n] = \underbrace{\mathrm{Tr}\left[\hat{\Gamma}^{\mu,w}[n]\hat{W}_{\mathrm{ee}}^{\mathrm{sr},\mu}\right]}_{\text{explicitly linear in } w} - E_{\mathrm{H}}^{\mathrm{sr},\mu}[n] \quad + \quad E_{\mathrm{c,md}}^{\mathrm{sr},\mu,w}[n]$$

  where $\hat{\Gamma}^{\mu,w}[n]$ is the ensemble long-range interacting density matrix operator with density n (rather than the usual non-interacting KS ensemble density matrix operator), hence the name multideterminantal (md) exact exchange.

- This decomposition leads to the exact energy expression $\boxed{E^{w} = \mathrm{Tr}\left[\hat{\Gamma}^{\mu,w}\hat{H}\right] + E_{\mathrm{c,md}}^{\mathrm{sr},\mu,w}[n_{\hat{\Gamma}^{\mu,w}}]}$

  where $\hat{\Gamma}^{\mu,w}$ reproduces the exact physical ensemble density $n^{w}(\mathbf{r})$.

- In the $\mu = 0$ limit, we obtain an ensemble Hartree–Fock-like energy (calculated with KS-eDFT orbitals) complemented by a density-functional correlation energy.

Md. M. Alam, S. Knecht, and E. Fromager, Phys. Rev. A 94, 012511 (2016).

GI correction in range-separated eDFT: practical calculation

- We use the WIDFA long-range interacting ensemble density matrix operator $\hat{\gamma}^{\mu,w}$, thus avoiding the (more rigorous) use of optimized effective potential (OEP) techniques.

- We use the ground-state LDA[1] for the complementary md correlation functional:

$$E_{\mathrm{c,md}}^{\mathrm{sr},\mu,w}[n] \to E_{\mathrm{c,md}}^{\mathrm{sr},\mu}[n]$$

- Thus we obtain an approximate GI-corrected (GIC) range-separated ensemble energy[2]

$$\tilde{E}_{\mathrm{GIC}}^{\mu,w} = \mathrm{Tr}\left[\hat{\gamma}^{\mu,w}\hat{H}\right] + E_{\mathrm{c,md}}^{\mathrm{sr},\mu}[n_{\hat{\gamma}^{\mu,w}}]$$

- Excitation energies are then computed with the LIM, hence the name GIC-LIM for the method.

[1] S. Paziani, S. Moroni, P. Gori-Giorgi, and G. B. Bachelet, Phys. Rev. B 73, 155111 (2006).

[2] Md. M. Alam, S. Knecht, and E. Fromager, Phys. Rev. A 94, 012511 (2016).

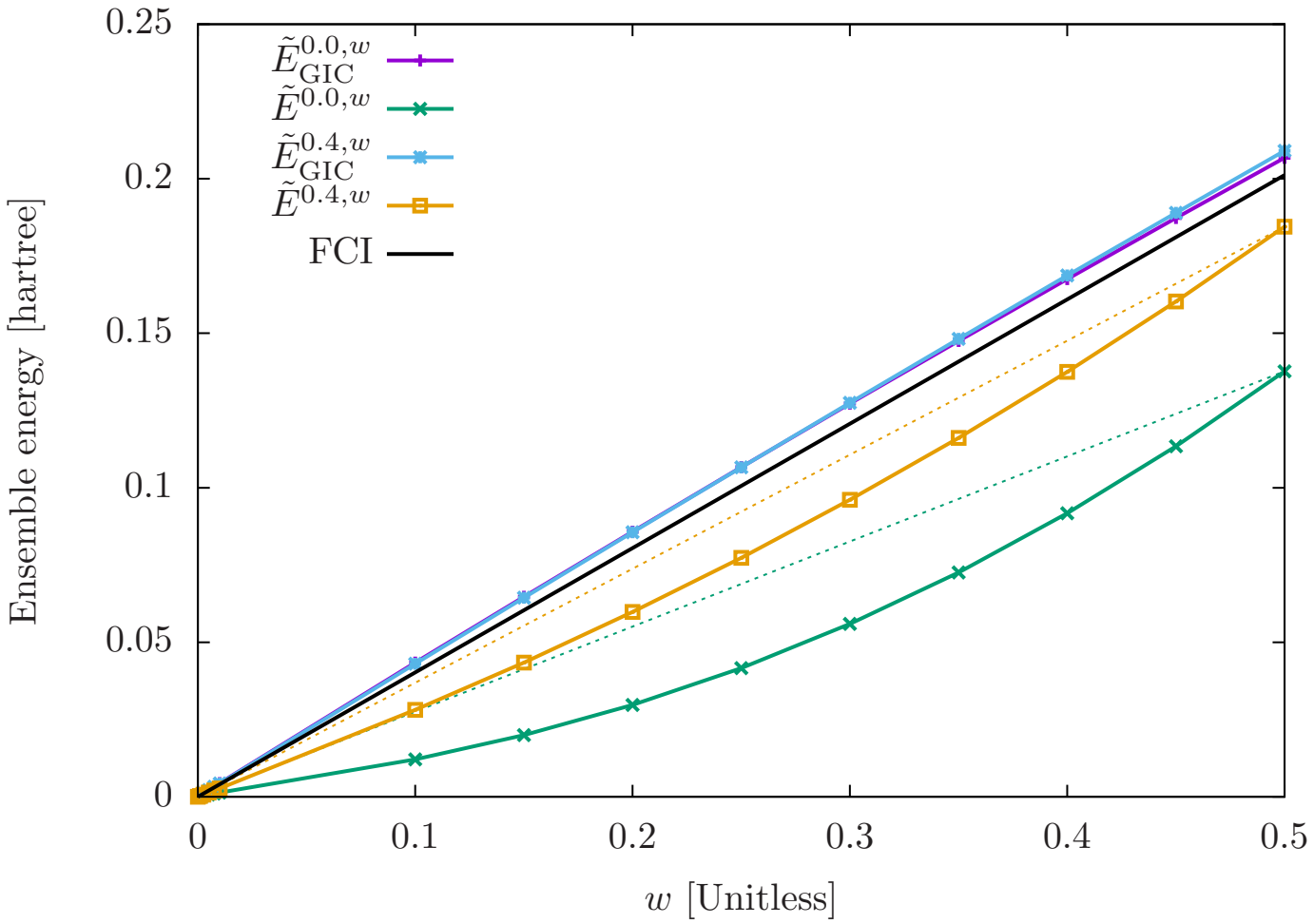


FIG. 2. Weight dependence of the WIDFA and GIC ensemble energies in HeH^+ for $\mu = 0$ and $\mu = 0.4a_0^{-1}$. The FCI and LIM (dashed lines) are also shown. Energies are shifted by their values at $w = 0$ for ease of comparison.

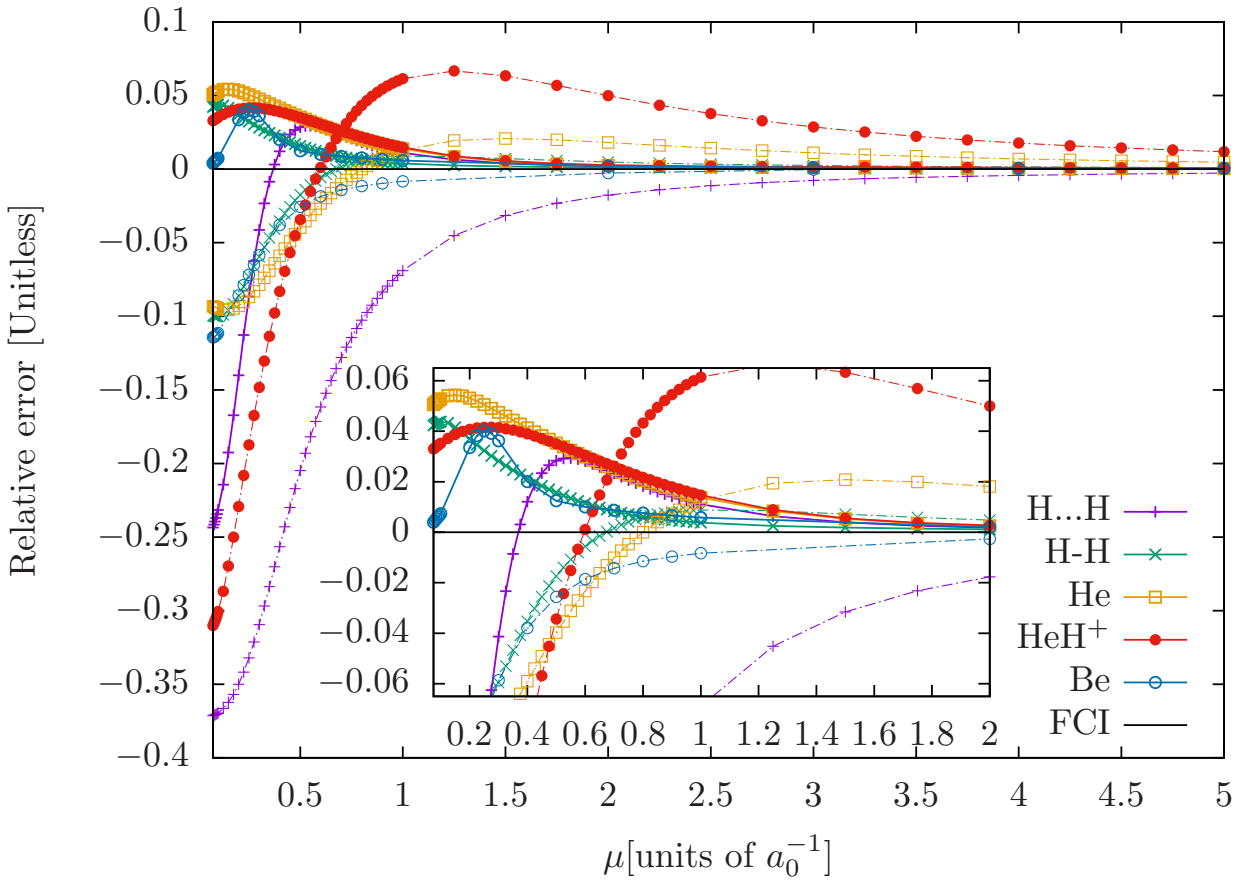


FIG. 3. Relative error with respect to the FCI obtained for the LIM (dash-dotted lines) and GIC-LIM (solid lines) excitation energies when varying μ. Inset: Zoom-in on the range $0 \leqslant \mu \leqslant 2.0 a_0^{-1}$. Excitations in the stretched HeH^+ ($1^1\Sigma^+ \rightarrow 2^1\Sigma^+$) and $H\ldots H$ ($1^1\Sigma_g^+ \rightarrow 2^1\Sigma_g^+$) molecules correspond to a charge transfer and a double excitation, respectively.

Extrapolation technique in range-separated eDFT

- The ground-state range-separated energy $\tilde{E}^{\mu}$ is μ-dependent in practice since approximate short-range xc functionals are used.
- This energy reduces to the exact ground-state energy E_0 when $\mu \to +\infty$.
- Taylor expansion[1] for large μ:

$$\tilde{E}^{\mu} = E_0 + \frac{a}{\mu^2} + \mathcal{O}\left(\frac{1}{\mu^3}\right) \quad \longrightarrow \quad \mu \frac{\partial \tilde{E}^{\mu}}{\partial \mu} = -\frac{2a}{\mu^2} + \mathcal{O}\left(\frac{1}{\mu^3}\right)$$

thus leading to $\tilde{E}^{\mu} + \underbrace{\frac{\mu}{2}\frac{\partial \tilde{E}^{\mu}}{\partial \mu}}_{\text{extrapolation correction}} = E_0 + \mathcal{O}\left(\frac{1}{\mu^3}\right)$

- This extrapolation scheme can be applied to WIDFA range-separated ensemble energies. Its combination with LIM gives extrapolated LIM (ELIM) excitation energies[2].

[1] A. Savin, J. Chem. Phys. 140, 18A509 (2014).

[2] B. Senjean, E. D. Hedegård, M. M. Alam, S. Knecht, and E. Fromager, Mol. Phys. 114, 968 (2016).

Extrapolation technique in range-separated eDFT

- The GIC range-separated ensemble energy $\tilde{E}^{\mu,w}_{\mathrm{GIC}}$ converges faster[1,2] (as $1/\mu^3$) towards the exact ensemble energy E^w when $\mu \to +\infty$.

- Therefore, in this case, the extrapolation scheme reads

$$\underbrace{\tilde{E}^{\mu,w}_{\mathrm{GIC}} + \frac{\mu}{3}\frac{\partial \tilde{E}^{\mu,w}_{\mathrm{GIC}}}{\partial \mu}}_{\text{extrapolated GIC (EGIC) energy}} = E^w + \mathcal{O}\left(\frac{1}{\mu^4}\right)$$

- Combining EGIC with LIM gives EGIC-LIM excitation energies.

[1] Md. M. Alam, S. Knecht, and E. Fromager, Phys. Rev. A 94, 012511 (2016).
[2] Md. M. Alam, S. Knecht, and E. Fromager, to be submitted, (2016).

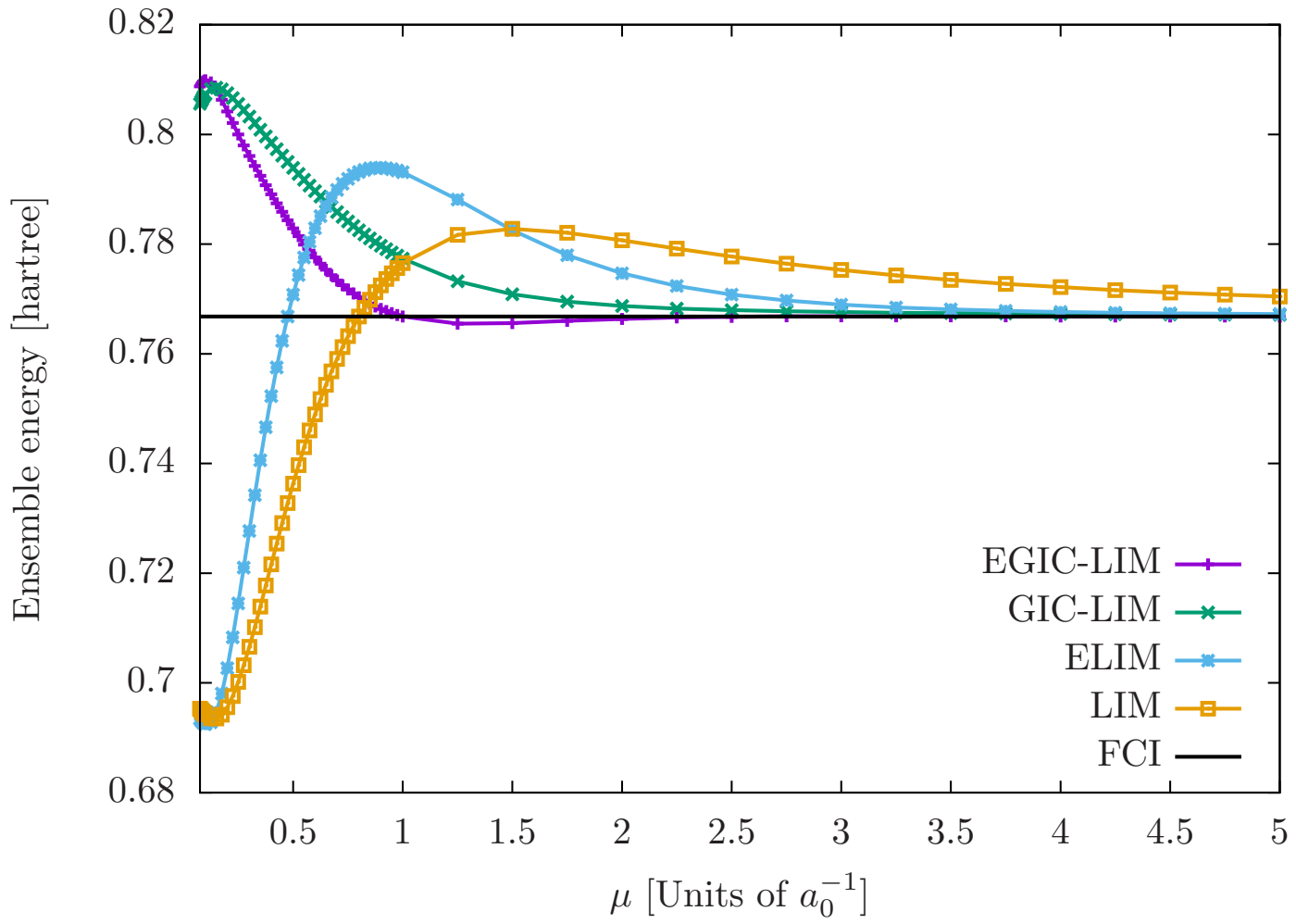


FIG. 6. LIM and GIC-LIM $1^1S \rightarrow 2^1S$ excitation energies obtained in He with and without extrapolation corrections when varying μ. Comparison is made with the FCI. See text for further details.

Conclusions and outlook

- Range-separated eDFT provides a rigorous framework for combining state-averaged multiconfigurational methods with DFT.
- Self-consistent implementation at the long-range FCI level in the DALTON program package.
- Long-term project: use state-averaged CASSCF rather than FCI $\rightarrow$ state-averaged CASDFT method !
- A linear interpolation method (LIM) for computing excitation energies in KS-eDFT has been proposed. The key idea is to use total ensemble energies rather than orbital energies.
- LIM is also applicable to range-separated eDFT.
- A ghost-interaction correction (GIC) has been proposed in the context of range-separated eDFT.
- Very promising results have been obtained when combining GIC with LIM, even at the KS-eDFT level ($\mu = 0$ limit).
- When range separation is used, the accuracy of GIC-LIM can be further improved by means of an extrapolation correction.
- LIM can be extended to higher excitations (linear interpolations between equiensembles up the multiplet of interest)
- We currently apply range-separated eDFT to the modeling of conical intersections.

Collaborators

- Hans Jørgen Aa. Jensen *(Odense, Denmark)*
- Stefan Knecht *(ETH, Zürich, Switzerland)*
- Bruno Senjean *(PhD student, Strasbourg, France)*
- Md. Mehboob Alam *(post-doc, Strasbourg, France)*
- Erik D. Hedegård *(ETH, Zürich, Switzerland)*

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http://quantique.u-strasbg.fr/ISTPC

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GDR Correl: **http://gdrcorelec.ups-tlse.fr**
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