Iterative CI wavefunction optimization using a similarity-transformed Hamiltonian and VMC

Abdallah Ammar[1], Emmanuel Giner[2] & Anthony Scemama[1]

[1]LCPQ, IRSAMC, UPS/CNRS, Toulouse, France

[2]LCT, Sorbonne Université/CNRS, Paris, France

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CI wavefunction

➙ Configuration Interaction (CI) wavefunction: linear combination of Slater determinants $\{D_I\}$ constructed from sets of orthonormal spin orbitals

$$\Phi(\mathbf{r}_1, \cdots, \mathbf{r}_N) = \sum_{I=1}^{N_{\text{det}}} C_I \, D_I(\mathbf{r}_1, \cdots, \mathbf{r}_N)$$

➙ For large basis sets, full CI computation is not realizable. We improve the truncated wavefunction by adding a Jastrow factor:

$$\Psi(\mathbf{r}_1, \cdots, \mathbf{r}_N) = \underbrace{\sum_{I=1}^{N_{\text{det}}} C_I \, D_I(\mathbf{r}_1, \cdots, \mathbf{r}_N)}_{\Phi(\mathbf{r}_1, \cdots, \mathbf{r}_N)} \exp[J]$$

➙ goal: optimize the determinantal part $\{C_I\}$ in the presence of Jastrow factor for large N_{det}

Generalized eigenvalue problem

➙ The best CI coefficients can be obtained by minimizing the energy. This leads to a generalized matrix eigenvalue equation:

$$\mathbf{H}\,\mathbf{C} = \mathbf{E}\,\mathbf{S}\,\mathbf{C} \qquad \text{where} \quad \begin{cases} \mathbf{H}_{IK} = \left\langle D_I \, \exp\left[J\right] \middle| \widehat{H} \middle| D_K \, \exp\left[J\right] \right\rangle \\ \mathbf{S}_{IK} = \left\langle D_I \, \exp\left[J\right] \middle| D_K \, \exp\left[J\right] \right\rangle \end{cases}$$

- Variational problem (**H** is symmetric & **S** is positive semidefinite)
- $3N$-dimensional integrals

➥ Quantum Monte Carlo methods

Generalized eigenvalue problem

➙ Variational Monte Carlo (VMC)

$$\begin{cases} \mathbf{H}_{IK} \approx \left\langle \dfrac{D_I\, e^J}{\Psi} \dfrac{\widehat{H}\,(D_K\, e^J)}{\Psi} \right\rangle_{\Psi^2} \\ \mathbf{S}_{IK} \approx \left\langle \dfrac{D_I\, e^J}{\Psi} \dfrac{D_K\, e^J}{\Psi} \right\rangle_{\Psi^2} \end{cases}$$

$$\langle X \rangle_{\Psi^2} = \frac{1}{N_{\text{config}}} \sum_{m=1}^{N_{\text{config}}} X(\underbrace{\mathbf{R}_m}_{\text{drawn with } \Psi^2})$$

- large matrices to sample $\sim N_{\text{det}}^2$
- statistical noise

➥ impractical/poor optimization for large N_{det}

Transcorrelated formalism

➙ A symmetric pair correlation factor τ is incorporated in the Hamiltonian

$$\widehat{H}_{\mathrm{TC}} \equiv e^{-\hat{\tau}}\, \widehat{H}\, e^{\hat{\tau}}$$

➙ The similarity-transformed Hamiltonian $\widehat{H}_{\mathrm{TC}}$ and $\widehat{H}$ share the same spectra:

$$\widehat{H}\,\Psi = E\,\Psi \iff \boxed{\widehat{H}_{\mathrm{TC}}\,\Phi = E\,\Phi} \qquad \text{where} \begin{cases} \Psi \equiv \Phi\, e^{\tau} \\ \Phi = \displaystyle\sum_{i=1}^{\infty} \phi_i \end{cases}$$

➙ For a two-body correlation factor, the effective TC Hamiltonian:

$$\begin{aligned} \widehat{H}_{\mathrm{TC}} &= \widehat{H} + \left[\widehat{H}, \hat{\tau}\right] + \frac{1}{2}\left[\left[\widehat{H}, \hat{\tau}\right], \hat{\tau}\right] \\ &= \widehat{H} + \underbrace{\widehat{K}_{12}}_{\text{non-Hermitian 2-body}} + \underbrace{\widehat{L}_{123}}_{\text{3-body}} \end{aligned}$$

Transcorrelated formalism

➙ Advantages:

- N-body integrals ➔ 3-body integrals
- The Coulomb singularity $1/r_{ij}$ can be explicitly removed ➔ improve convergence
- Post-Hartree-Fock (CI, CC, ...) methods can be combined with TC approach

➙ Numerical difficulties:

- **three-body** term
- The TC Hamiltonian is **non-Hermitian**

➙ We propose an iterative scheme to overcome these difficulties

Diagonal dressing

We start with a CI WF $\Phi^{(0)} = \sum_{I=1}^{N_{\text{det}}} C_I^{(0)} D_I$, and a fixed Jastrow factor $\exp[\tau]$

➙ **Goal**: optimize the coefficients by solving the TC eigen-problem in the $\{D_I\}$ basis:

$$\widehat{H}_{\text{TC}} \Phi = E_{\text{TC}} \Phi \Rightarrow \sum_{K=1}^{N_{\text{det}}} \left\langle D_I \middle| \widehat{H}_{\text{TC}} - \widehat{H} + \widehat{H} \middle| D_K \right\rangle C_K^{(i)} = E_{\text{TC}} C_I^{(i)}$$

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$$\sum_{K \neq I} \mathbf{H}_{IK} C_K^{(i)} + \left(\mathbf{H}_{II} + \underbrace{\boxed{\frac{1}{C_I^{(i-1)}} \left\langle D_I \middle| \widehat{H}_{\text{TC}} - \widehat{H} \middle| \Phi^{(i-1)} \right\rangle}}_{\textbf{dressing elements}} \right) C_I^{(i)} \approx E_{\text{TC}} C_I^{(i)}$$

$$\begin{pmatrix} x & & \\ & \ddots & \\ & & x \end{pmatrix}$$

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➥ We have to build the diagonal dressing matrix $\mathbf{\Delta}^{(i-1)}$:

$$\mathbf{\Delta}_{IK}^{(i-1)} = \begin{cases} \dfrac{1}{C_I^{(i-1)}} \left\langle D_I \middle| \widehat{H}_{\text{TC}} - \widehat{H} \middle| \Phi^{(i-1)} \right\rangle & \text{if } I = K \\ 0 & \text{otherwise} \end{cases}$$

Column dressing

➥ It is more stable to dress with the elements

$$\Gamma_{IL}^{(i-1)} = \frac{1}{C_L^{(i-1)}} \left\langle D_I \middle| \widehat{H}_{\mathrm{TC}} - \widehat{H} \middle| \Phi^{(i-1)} \right\rangle$$

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where L corresponds to the largest coefficients $C_L^{(i-1)}$

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➥ The dressing matrix $\mathbf{\Delta}^{(i-1)}$ is chosen to be **symmetric** by construction:

$$\mathbf{\Delta}_{LI}^{(i-1)} = \mathbf{\Delta}_{IL}^{(i-1)} = \Gamma_{IL}^{(i-1)}$$
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➙ An extra term is introduced in the diagonal element to cancel the double counting:

$$\mathbf{\Delta}_{LL}^{(i-1)} = 2\,\Gamma_{LL}^{(i-1)} - \frac{1}{C_L^{(i-1)}} \sum_{K=1}^{N_{\mathrm{det}}} \Gamma_{KL}^{(i-1)} C_K^{(i-1)}$$

Iterative dressing algorithm

① choose a CI WF: $\Phi^{(0)} = \sum_{I=1}^{N_{\text{det}}} C_I^{(0)} D_I$ & a Jastrow factor $\exp(\tau)$

② **with VMC**, evaluate:

- the dressing elements $\left\langle D_I \middle| \widehat{H}_{\text{TC}} - \widehat{H} \middle| \Phi^{(i-1)} \right\rangle$
- the **variational** energy $E^{(i-1)} = \dfrac{\left\langle \Phi^{(i-1)} e^{\tau} \middle| \widehat{H} \middle| e^{\tau} \Phi^{(i-1)} \right\rangle}{\left\langle \Phi^{(i-1)} e^{\tau} \middle| e^{\tau} \Phi^{(i-1)} \right\rangle}$

③ dress the Hamiltonian matrix $\mathbf{H}$ with the symmetric matrix $\mathbf{\Delta}^{(i-1)}$

④ apply Davidson to obtain the new ground state $\Phi^{(i)}$ and $E_{\text{TC}}^{(i)}$

⑤ go back to ②

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- all steps are deterministic except ②
- the TC energy E_{TC} is not variational. *per contra* the VMC energy E is

Iterative dressing algorithm: advantages

- ➙ after few iterations ($\sim 2-4$), we converge to the solution
- ➙ we need to sample only N_{det} elements instead of N_{det}^2
- ➙ handle the **non-Hermiticity** of the TC eigenproblem thanks to the **symmetric dressing**
- ➙ VMC calculation allows to handle **three-body integrals** and evaluate a **variational energy** (instead of the TC energy)
- ➙ reduced statistical errors:

$$\begin{aligned}\left\langle D_I \left| \widehat{H}_{\text{TC}} - \widehat{H} \right| D_K \right\rangle &= \left\langle D_I e^{-\tau} \left| \widehat{T} + \widehat{V} \right| e^{\tau} D_K \right\rangle - \left\langle D_I \left| \widehat{T} + \widehat{V} \right| D_K \right\rangle \\ &= \left\langle D_I e^{-\tau} \left| \widehat{T} \right| e^{\tau} D_K \right\rangle - \left\langle D_I \left| \widehat{T} \right| D_K \right\rangle\end{aligned}$$

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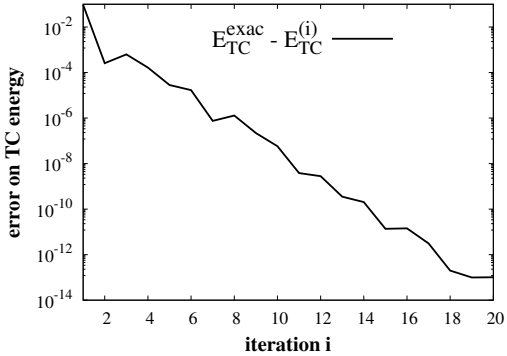
Proof of concept

➙ Jastrow inspired by Range-Separated DFT[1]: $\tau_\mu = \sum_{i<j} \left[\frac{r_{ij}\left(1-\mathrm{erf}\left(\mu r_{ij}\right)\right)}{2} - \frac{\exp\left[-\left(\mu r_{ij}\right)^2\right]}{2\sqrt{\pi}\mu} \right]$

Benchmark: `Be (cc-pcvdz)`

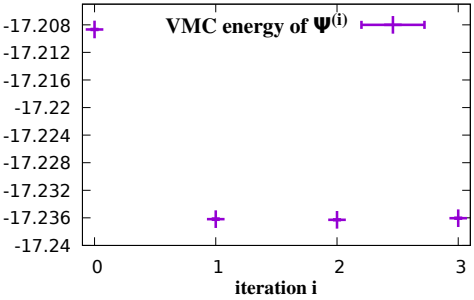


[1] *Emmanuel Giner, J. Chem. Phys.*, **154**, 2021

Application: H_2O (cc-pvdz_ecp_bfd): $N_{\text{det}} \sim 71\,000$

➥ A simple Jastrow factor $\tau = \sum_{i<j}^{N} \frac{a\, r_{ij}}{1 + b\, r_{ij}} - \sum_{A=1}^{M} \sum_{i=1}^{N} \left(\frac{\alpha_A\, r_{iA}}{1 + \alpha_A\, r_{iA}} \right)^2$

CI energy: $E_\Phi = -17.16096$ (no-Jastrow)



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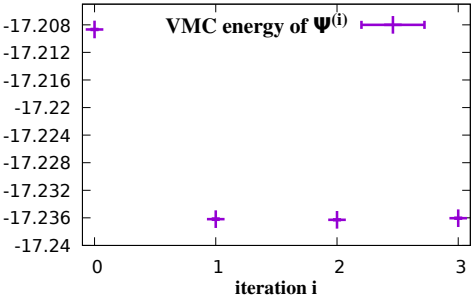

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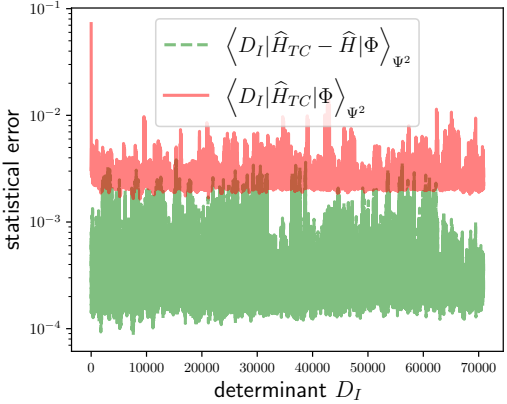

$\langle \text{error} \rangle \approx 8\, \langle \text{error} \rangle$

Modified dressing elements

➙ For an arbitrary choice of Jastrow factor (arbitrary $\widehat{H}_{\mathrm{TC}}$), we have:

$$\begin{aligned}\left\langle D_I \middle| \widehat{H}_{\mathrm{TC}} \middle| D_J \right\rangle &= \left\langle D_I \middle| \widehat{H}_{\mathrm{TC}} - \widehat{H}_\mu + \widehat{H}_\mu - \widehat{H} + \widehat{H} \middle| D_J \right\rangle \\ &= \underbrace{\left\langle D_I \middle| \widehat{H} \middle| D_J \right\rangle}_{\text{matrix to be dressed}} + \underbrace{\left\langle D_I \middle| \widehat{H}_\mu - \widehat{H} \middle| D_J \right\rangle}_{\sim \text{analyitc elements}} + \underbrace{\left\langle D_I \middle| \widehat{H}_{\mathrm{TC}} - \widehat{H}_\mu \middle| D_J \right\rangle}_{\text{VMC elements}}\end{aligned}$$

➙ New dressing elements:

$$\left\langle D_I \middle| \widehat{H}_{\mathrm{TC}} - \widehat{H} \middle| \Phi \right\rangle \rightarrow \boxed{\left\langle D_I \middle| \widehat{H}_{\mathrm{TC}} - \widehat{H}_\mu \middle| \Phi \right\rangle} + \left\langle D_I \middle| \widehat{H}_\mu - \widehat{H} \middle| \Phi \right\rangle$$

➙ Local energies with Jastrow factor are more correlated:

$$\left| \frac{\widehat{H}_{\mathrm{TC}}\,\Phi}{\Phi} - \frac{\widehat{H}_\mu\,\Phi}{\Phi} \right| < \left| \frac{\widehat{H}_{\mathrm{TC}}\,\Phi}{\Phi} - \frac{\widehat{H}\,\Phi}{\Phi} \right| \quad \Rightarrow \textbf{reduced statistical errors}$$

illustration: Be (cc-pcvdz)

- $\tau_{\mathrm{TC}} = \sum_{i<j} \frac{a\, r_{ij}}{1 + b\, r_{ij}} - \sum_{A,i} \left(\frac{\alpha_A\, r_{iA}}{1 + \alpha_A\, r_{iA}} \right)^2$
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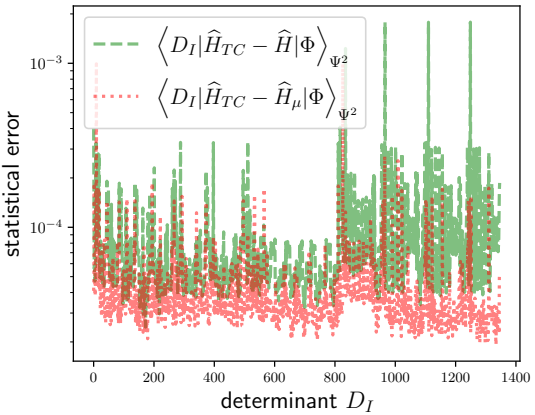
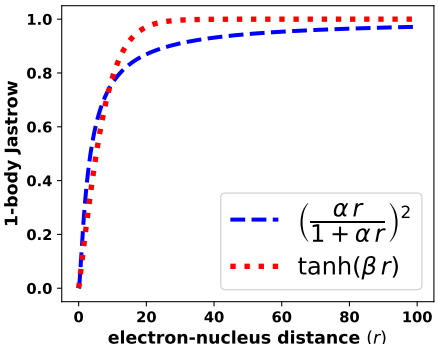


$\langle \text{error} \rangle \approx 2 \, \langle \text{error} \rangle$

1-body Jastrow

➙ we add a 1-body Jastrow to avoid unfavorable effect of the two-body Jastrow factor τ_μ that changes the charge density:

$$\tau_{mu} \rightarrow \tau_{mu} - \sum_{A,i} \tanh\left(\beta_A \, r_{iA}\right)$$



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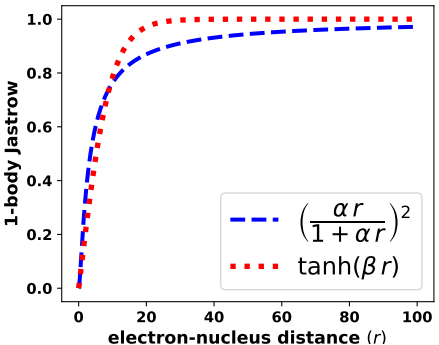

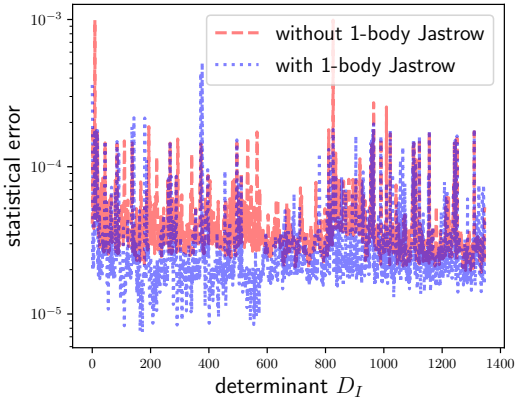

$\langle \text{error} \rangle \approx 1.3\ \langle \text{error} \rangle$

Conclusion

➙ iterative symmetric dressing within TC approach:

- number of elements to sample in VMC: $N_{\text{det}}^2 \rightarrow N_{\text{det}}$
- addresses the **non-Hermiticity** of the TC Hamiltonian & **three-body** terms
- fast convergence ($\sim 2-3$ iterations)

➙ employ $\widehat{H}_\mu$ in the dressing elements calculation allows to reduce the statistical noise

- we can improve the results by adding 1-body term to τ_μ

➙ ongoing work:

- application for larger CI expansion ($N_{\text{det}} \sim 10^6 - 10^7$)
- develop a compact representation for dressing vector

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Thank you for your attention