Exploring density-matrix expansions for local chiral interactions

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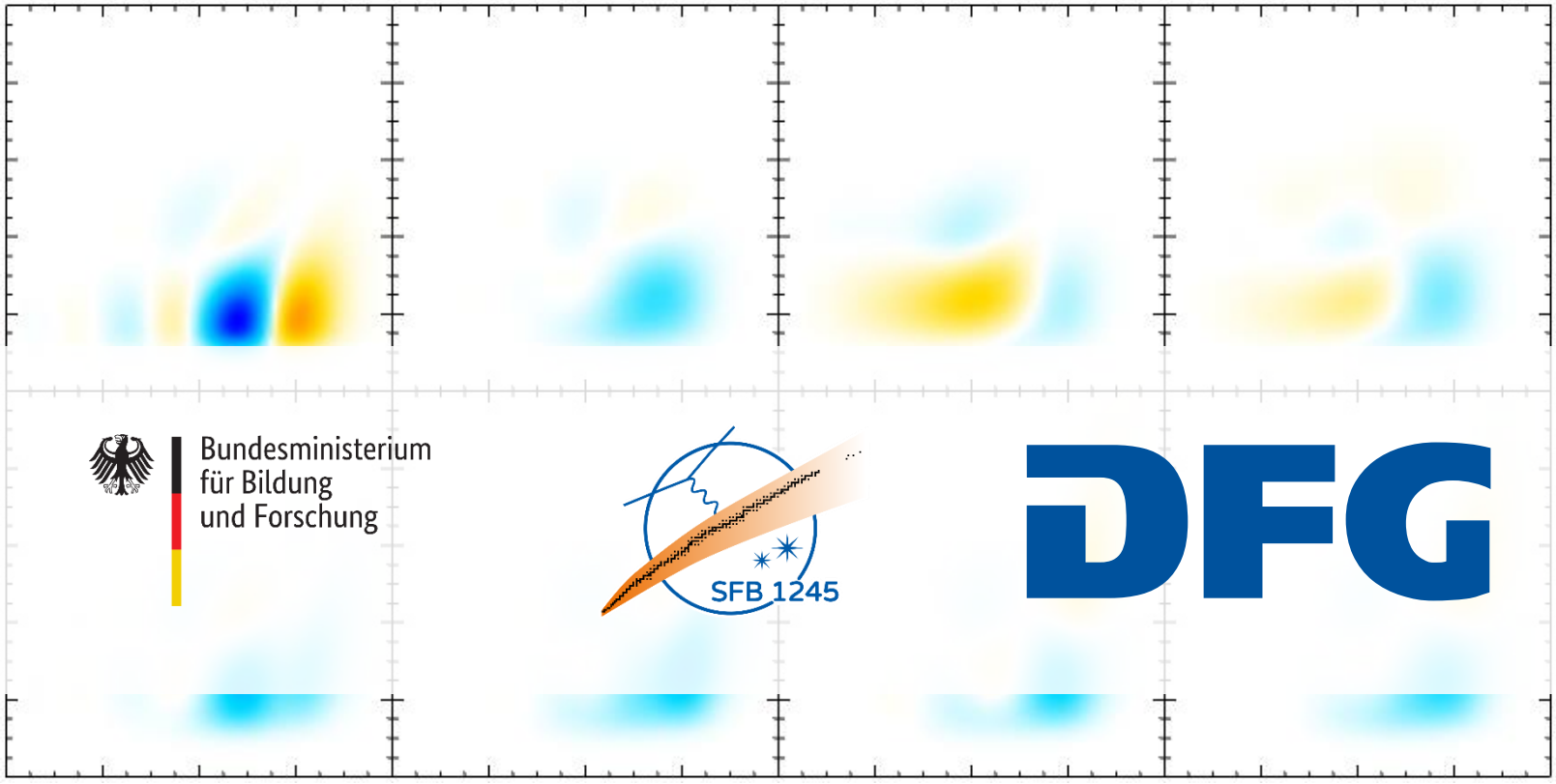

Motivation

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Energy-density functionals (EDFs) allow for consistent description of nuclei across entire nuclear chart

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Standard (Skyrme) EDFs may have reached accuracy limit

$\Longrightarrow$ More complicated functional forms needed (?) McDonnell et al., PRL **114**, 122501 (2015) Zhang et al., PRC **98**, 064306 (2018)

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Employing density-matrix expansion (DME)

$\Longrightarrow$ Incorporate exchange contributions from long-range chiral forces explicitly in EDF (parameter-free)

$\Longrightarrow$ Semi-phenomenological Skyrme-like EDF with coupling functions instead of coupling constants Navarro Pérez et al., PRC 97, 054304 (2018)

Motivation

Root-mean square deviations between experimental binding energies and predictions from different EDFs for ~620 nuclei:

	EDF	rms deviation [MeV]
Skyrme	UNEDF2	1.98
Skyrme + PSA-DME	+ NN @ LO	1.99
	+ NN @ N^2LO	1.57
	+ NN+Δ @ N^2LO	1.26
	+ NN+Δ+3N @ N^2LO	1.72

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Systematics not understood $\Longrightarrow$ Revisit DME implementation
$\Longrightarrow$ Is further EDF improvement possible by altering the DME choice?

Density-matrix expansions

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DMEs for scalar parts of one-body density matrix (OBDM) of time-reversal invariant systems

$$\rho\left(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\right) \approx \sum_{n=0}^{n_{\max}} r^n \Pi_n(k(\mathbf{R})r)\mathcal{P}_n(\mathbf{R})$$

$\Longrightarrow$ Series in non-locality r

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$\mathcal{P}_n(\mathbf{R})$ are different local densities, e.g.,

$$\rho(\mathbf{R}) = \sum_i |\phi_i(\mathbf{R})|^2, \qquad \tau(\mathbf{R}) = \sum_i |\boldsymbol{\nabla}\phi_i(\mathbf{R})|^2$$

Density-matrix expansions

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Example DME variant: PSA-DME

Gebremariam et al., PRC 82, 014305 (2010)
Gebremariam et al., NPA 851, 17 (2011)

$$\Pi_0(x)=\frac{3j_1(x)}{x}, \qquad \Pi_2(x)=\frac{3j_1(x)}{x},$$

$$k(\mathbf{R})=k_{\mathrm{F}}(\mathbf{R})=\left[3\pi^2\rho(\mathbf{R})\right]^{1/3}$$

Comparison of density-matrix expansions

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Consider 11 closed-shell nuclei with densities from SLy4 EDF calculation

Chabanat et al., NPA 635, 231 (1998),
Erratum: NPA 643, 441 (1998)

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Scalar-isoscalar exchange energy due to regulated Yukawa interaction

(non-self-consistent tests)

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$$W_0^{\mathrm{ex}} = -\frac{9}{8}\int \mathrm{d}\mathbf{R}\,\mathrm{d}\mathbf{r}\;\underbrace{\rho_0\left(\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\right)^2}\,V(r)$$

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DME variant

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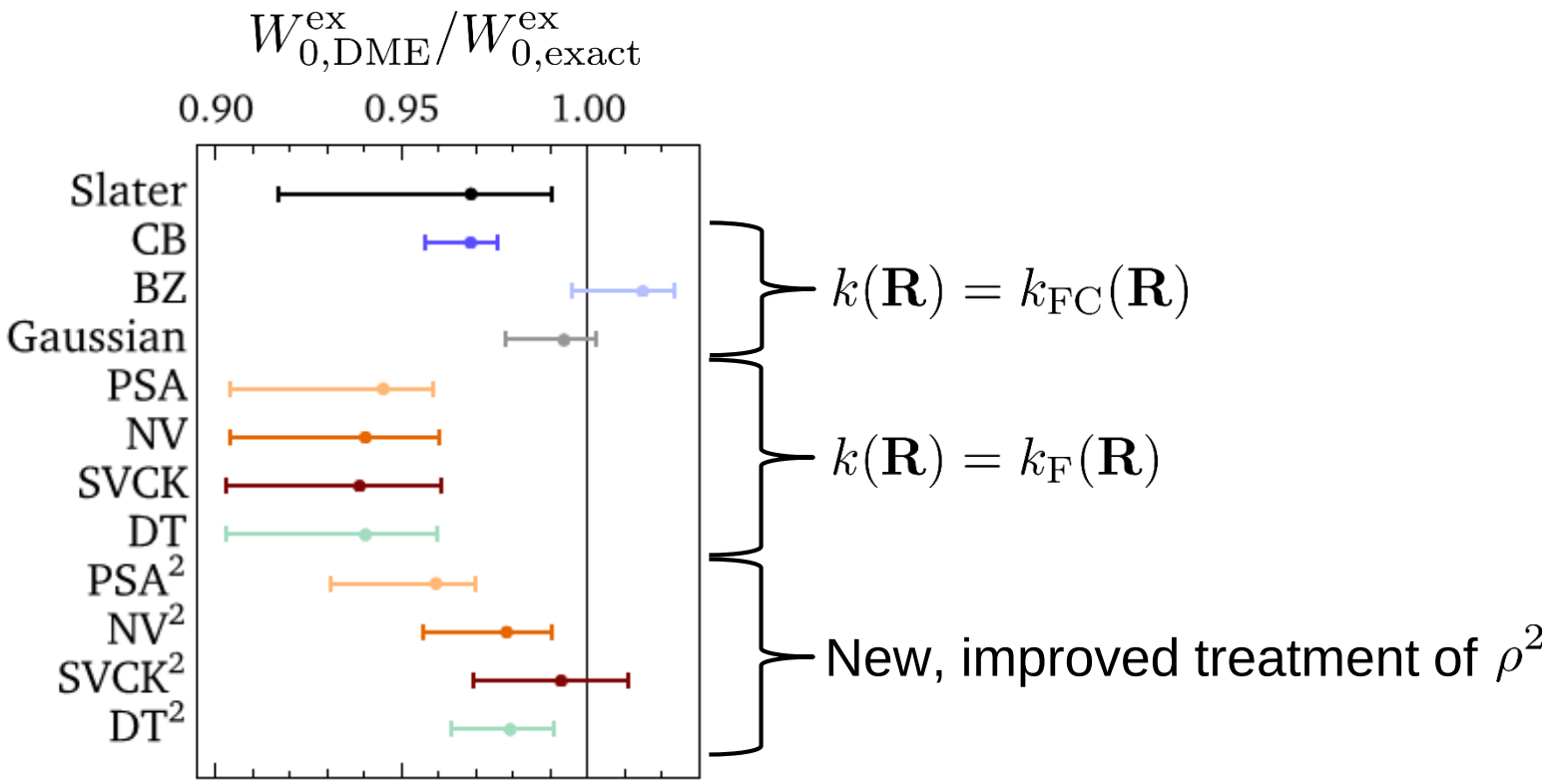

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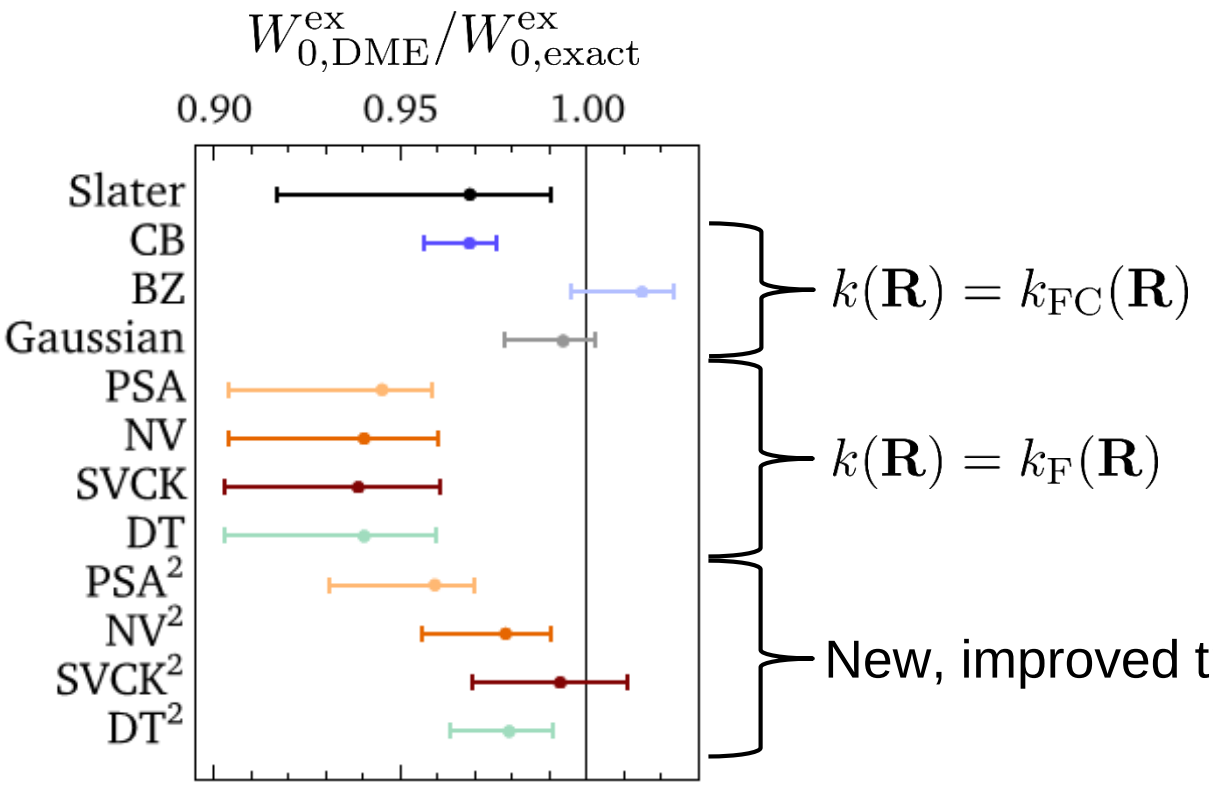
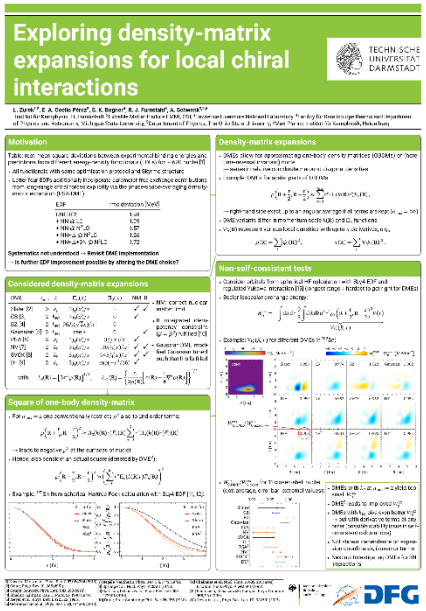
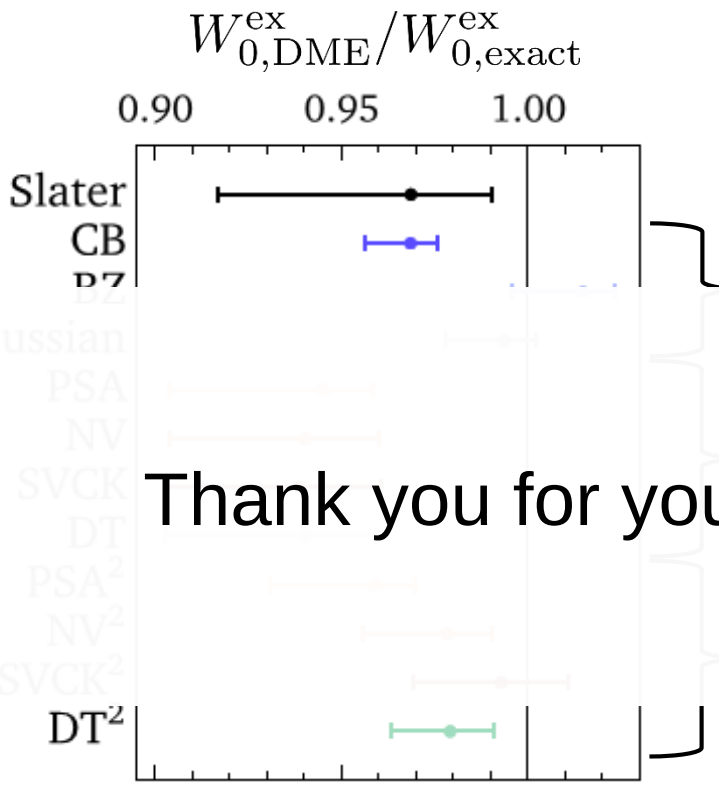


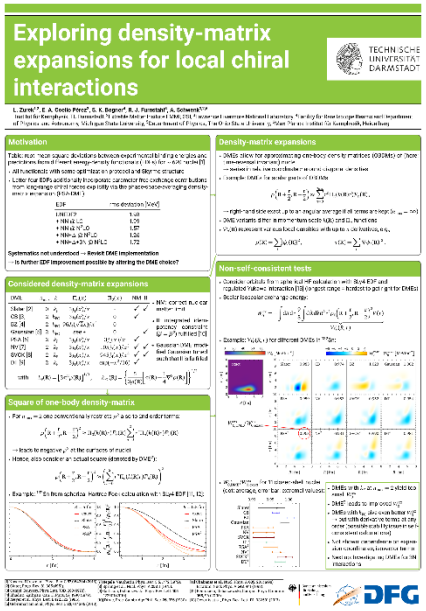


More details and results at poster

Next up: Investigating DMEs for 3N interactions

Comparison of density-matrix expansions





Thank you for your attention

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