Proposal for an *ab initio-driven* nuclear EDF

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The future of multireference Density Functional Theory

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Motivation

✪ **Ab initio approaches**

➟ Considerable progress over last few years, still limited applicability

➟ New techniques available

- Symmetry breaking [Somà *et al.* 2011, Hergert *et al.* 2013, Signoracci *et al.* 2014]
- Symmetry restoration [Duguet 2015, Duguet & Signoracci *in preparation*]

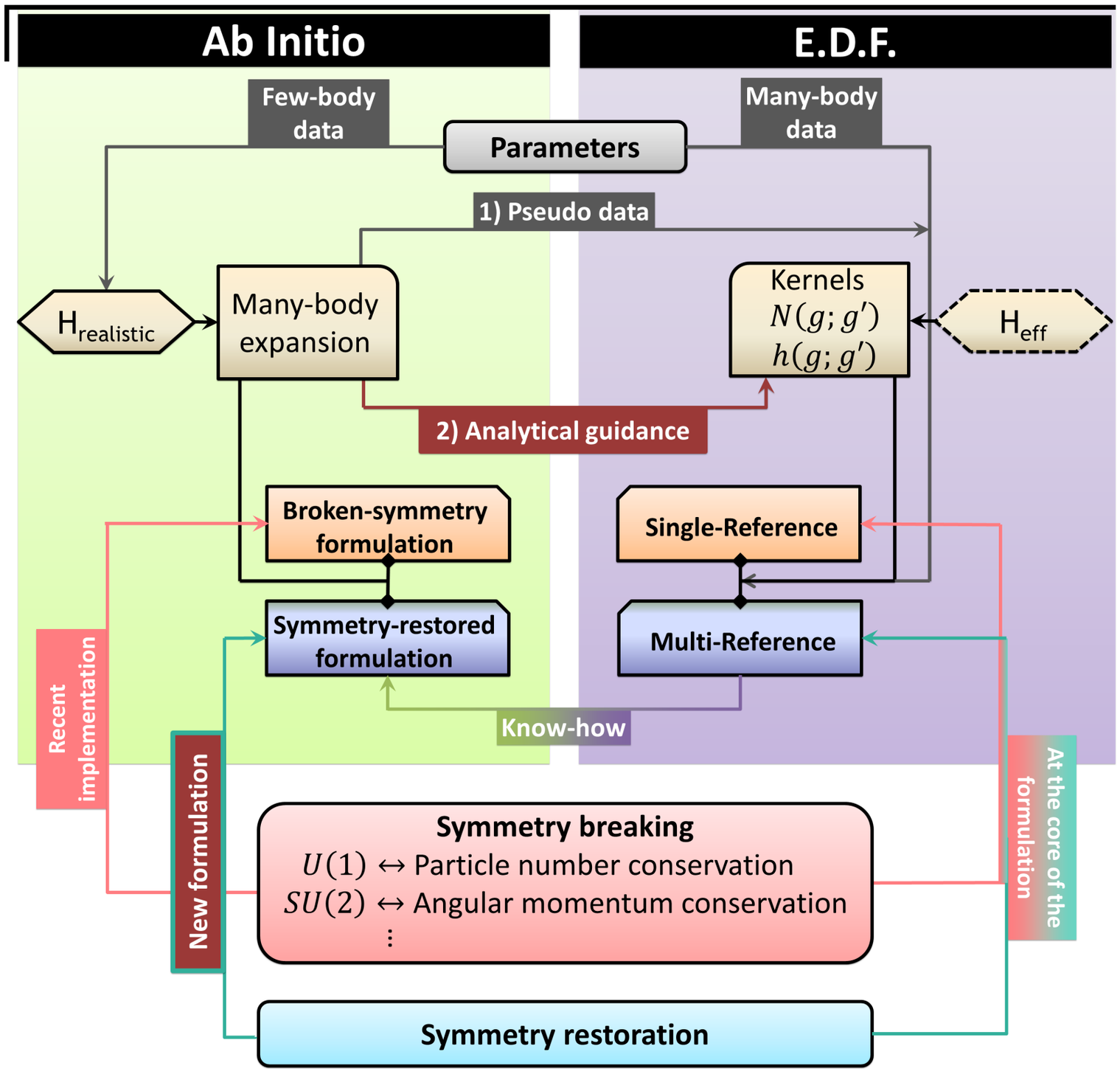
✪ **Nuclear Energy Density Functionals**

➟ Extended reach, SR & MR codes with fantastic potential

➟ However empirical parameterisations plagued with critical pathologies in MR

Can ab initio techniques help in developing safe/correlated/improvable EDFs?

Ab initio vs EDF approaches



Beyond classic MR schemes

✪ **Possible routes**

➠ Regularisation schemes

➠ Stick to pseudopotentials

➠ Work at SR level only?

➠ ....

✪ **This proposal**

1) Effective Hamiltonian based method

2) Use ab initio techniques to systematically enrich EDF kernels with correlations

3) Newly developed symmetry broken/restored MBPT allows for SR/MR implementation

[T. Duguet, J. Phys. G 42 025107 (2015)]

MBPT of off-diagonal kernels

✪ Symmetry group

➟ Consider here the group associated to rotations

$$SU(2) \equiv \{R(\Omega),\, \Omega \in D_{SU(2)}\}$$

$$R(\Omega) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\alpha J_z}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\beta J_y}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\gamma J_z}$$

➟ Matrix elements of the IRREPS of SU(2) are given by the Wigner functions

$$\left\langle \Psi_{\mu}^{JM} \right|\, R(\Omega) \left| \Psi_{\mu'}^{J'K} \right\rangle \equiv \delta_{\mu\mu'}\delta_{JJ'}D^{J}_{MK}(\Omega)$$

➟ Consider a reference state that mixes several IRREPS $|\Phi\rangle$

rotated reference state

$$|\Phi(\Omega)\rangle \equiv R(\Omega)|\Phi\rangle$$

MBPT of off-diagonal kernels

✪ **Exact (fully correlated) off-diagonal kernels**

➟ Introduce time-evolution operator $\mathscr{U}(\tau) \equiv e^{-\tau H_{\rm eff}}$

$$|\Psi(\tau)\rangle \equiv \mathscr{U}(\tau)|\Phi(0)\rangle \longrightarrow H_{\rm eff}\,|\Psi(\tau)\rangle = -\partial_\tau |\Psi(\tau)\rangle$$

and kernels

$$\begin{aligned} N(\tau,\Omega) &\equiv \langle\Psi(\tau)|\mathbb{1}|\Phi(\Omega)\rangle \\ H(\tau,\Omega) &\equiv \langle\Psi(\tau)|H_{\rm eff}|\Phi(\Omega)\rangle \\ J_i(\tau,\Omega) &\equiv \langle\Psi(\tau)|J_i|\Phi(\Omega)\rangle \\ J^2(\tau,\Omega) &\equiv \langle\Psi(\tau)|J^2|\Phi(\Omega)\rangle \end{aligned}$$

$$\Longrightarrow \qquad \mathscr{O}(\tau,\Omega) \equiv \frac{O(\tau,\Omega)}{N(\tau,0)}$$

reduced kernels

MBPT of off-diagonal kernels

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$\Longrightarrow \quad \mathscr{O}(\tau,\Omega) \equiv \dfrac{O(\tau,\Omega)}{N(\tau,0)}$

reduced kernels

evolve to $\tau \to \infty$

$$E_0^J = \frac{\sum_{K'K} f^{J*}_{K'} f^J_K \int_{D_{SU(2)}} d\Omega\, D^{J*}_{K'K}(\Omega)\,\mathscr{H}(\Omega)}{\sum_{K'K} f^{J*}_{K'} f^J_K \int_{D_{SU(2)}} d\Omega\, D^{J*}_{K'K}(\Omega)\,\mathscr{N}(\Omega)}$$

All this is exact… how to expand these kernels around some reference state?

MBPT of off-diagonal kernels

✪ **Reference state**

➟ One starts with splitting $H_{\text{eff}} \equiv H_0 + H_1$ where $H_0 \equiv T + U$ and $H_1 \equiv V^{\text{eff}} - U$

➟ E.g. Hartree-Fock $U \equiv \sum_{\alpha\beta} u_{\alpha\beta} c^\dagger_\alpha c_\beta$ where $u^{\text{HF}}_{\alpha\beta} = \sum_{\gamma\delta} \bar{v}^{\text{eff}}_{\alpha\gamma\beta\delta} \rho^{00}_{\delta\gamma}$

$$H_0 |\Phi(0)\rangle = \varepsilon_0 |\Phi(0)\rangle$$

$$\varepsilon_0 = \sum_{i=1}^{A} (e_i - \mu)$$

MBPT of off-diagonal kernels

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$$H_0 |\Phi(0)\rangle = \varepsilon_0 |\Phi(0)\rangle$$

$$\varepsilon_0 = \sum_{i=1}^{A} (e_i - \mu)$$

✪ **Off-diagonal one-body density matrix**

$$\rho^{0\Omega} = \begin{pmatrix} \mathbb{1}^{hh} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ R(\Omega) M^{-1}(\Omega) & 0 \end{pmatrix} \equiv \rho^{00} + \wp^{0\Omega}$$

vanishes for for Ω=0

with

$$R_{\alpha\beta}(\Omega) \equiv \langle \alpha | R(\Omega) | \beta \rangle$$

$$M_{ij}(\Omega) = R \text{ for hole states}$$

$$\rho^{0\Omega}_{\alpha\beta} \equiv n_\alpha\, \delta_{\alpha\beta} + (1 - n_\alpha)\, n_\beta\, \wp^{0\Omega}_{\alpha\beta}$$

MBPT of off-diagonal kernels

✪ **First-order expansion of the energy kernel**

➟ Expand the evolution operator in powers of H_1

$$\mathscr{U}(\tau) = e^{-\tau H_0}\,\mathrm{T}e^{-\int_0^\tau dt H_1(t)} \qquad \text{where} \qquad H_1(\tau) \equiv e^{\tau H_0} H_1 e^{-\tau H_0}$$

and the perturbation series for any operator can be derived $\Longrightarrow$ **diagrammatic techniques**

MBPT of off-diagonal kernels

✪ **First-order expansion of the energy kernel**

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and the perturbation series for any operator can be derived ⟹ **diagrammatic techniques**

➟ One first proves that any operator factorises as $O(\Omega) \equiv o(\Omega) N(\Omega)$

contains all **connected** diagrams **linked** to O

$$H(\Omega) \equiv h(\Omega) N(\Omega)$$

MBPT of off-diagonal kernels

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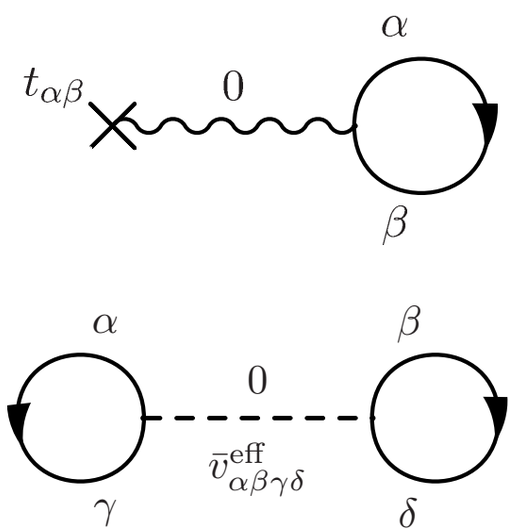
➟ First-order MBPT diagrams give



$$\begin{aligned} h^{(1)}(\Omega) &= \frac{\langle \Phi(0)|H_{\text{eff}}|\Phi(\Omega)\rangle}{\langle \Phi(0)|\Phi(\Omega)\rangle} \\ &= \sum_i t_{ii} + \sum_{ia} t_{ia}\,\wp^{0\Omega}_{ai} \\ &+ \frac{1}{2}\sum_{ij} \bar{v}^{\text{eff}}_{ijij} + \sum_{ijc} \bar{v}^{\text{eff}}_{ijcj}\,\wp^{0\Omega}_{ci} \\ &+ \frac{1}{2}\sum_{ijab} \bar{v}^{\text{eff}}_{ijab}\,\wp^{0\Omega}_{ai}\,\wp^{0\Omega}_{bj} \end{aligned}$$

MBPT of off-diagonal kernels

✪ Bi-orthogonal basis

➟ Introducing the so-called bi-orthogonal basis

$$B(\Omega) \equiv \mathbb{1} + \wp^{0\Omega}$$
$$|\tilde{i}\rangle = |i\rangle + \sum_{kc} |c\rangle R_{ck}(\Omega) M^{-1}_{ki}(\Omega)$$
$$|\tilde{a}\rangle = |a\rangle$$

$$B^{-1}(\Omega) \equiv \mathbb{1} - \wp^{0\Omega}$$
$$\langle\tilde{j}| = \langle j|$$
$$\langle\tilde{b}| = \langle b| - \sum_{kl} R_{bk}(\Omega) M^{-1}_{kl}(\Omega) \langle l|$$

It is possible to write the first-order expansion in a **compact form**

$$h^{(1)}(\Omega) = \frac{\langle\Phi(0)|H_{\text{eff}}|\Phi(\Omega)\rangle}{\langle\Phi(0)|\Phi(\Omega)\rangle}$$
$$= \sum_i t_{ii} + \sum_{ia} t_{ia} \wp^{0\Omega}_{ai}$$
$$+ \frac{1}{2}\sum_{ij} \bar{v}^{\text{eff}}_{ijij} + \sum_{ijc} \bar{v}^{\text{eff}}_{ijcj} \wp^{0\Omega}_{ci}$$
$$+ \frac{1}{2}\sum_{ijab} \bar{v}^{\text{eff}}_{ijab} \wp^{0\Omega}_{ai} \wp^{0\Omega}_{bj}$$

$$h^{(1)}(\Omega) = \sum_i t_{\tilde{i}i}(\Omega) + \frac{1}{2}\sum_{ij} \bar{v}^{\text{eff}}_{\tilde{i}\tilde{j}\tilde{i}\tilde{j}}(\Omega)$$
$$= \langle\Phi(0)|\tilde{H}_{\text{eff}}(\Omega)|\Phi(0)\rangle$$

transformed operator

MBPT of off-diagonal kernels

➟ In fact, one can always reduce the analytical expansion (for any operator) of the **off-diagonal** kernel to the one of the **diagonal** kernel but with the **rotated operator**

➟ E.g. at second order

$$
\begin{aligned}
o^{(2)}(\Omega) &= \frac{\langle \Phi(0)| \left[1 + \mathscr{T}_1^{\dagger\,(2)}(\Omega) + \mathscr{T}_2^{\dagger\,(2)}(\Omega) \right] O |\Phi(\Omega)\rangle_c}{\langle \Phi(0)|\Phi(\Omega)\rangle} \\
&= \langle \Phi(0)| \left[1 + \mathscr{T}_1^{\dagger\,(2)}(\Omega) + \mathscr{T}_2^{\dagger\,(2)}(\Omega) \right] \tilde{O}(\Omega) |\Phi(0)\rangle_c
\end{aligned}
$$

with cluster amplitudes defined as

One-body

$$
\begin{aligned}
\mathscr{T}_{ia}^{\dagger\,(2)}(\Omega) \equiv & -\frac{1}{e_a - e_i} \left[\sum_j \bar{v}^{\text{eff}}_{ijaj} - u_{ia} \right] \\
& - \sum_{jb} \frac{\bar{v}^{\text{eff}}_{ijab}}{e_a + e_b - e_i - e_j} \wp^{0\Omega}_{bj}
\end{aligned}
$$

Two-body

$$
\mathscr{T}_{ijab}^{\dagger\,(2)}(\Omega) \equiv -\frac{\bar{v}^{\text{eff}}_{ijab}}{e_a + e_b - e_i - e_j}
$$

MBPT of off-diagonal kernels

✪ Second-order expansion of the energy kernel

$$
\begin{aligned}
h^{(2)}(\Omega) = & \sum_{i} t_{\tilde{i}\tilde{i}}(\Omega) + \sum_{ia} \mathscr{T}^{\dagger(2)}_{ia}(\Omega)\, t_{\tilde{a}\tilde{i}}(\Omega) \\
& + \frac{1}{2} \sum_{ij} \bar{v}^{\mathrm{eff}}_{\tilde{i}\tilde{j}\tilde{i}\tilde{j}}(\Omega) + \sum_{ija} \mathscr{T}^{\dagger(2)}_{ia}(\Omega)\, \bar{v}^{\mathrm{eff}}_{\tilde{a}\tilde{j}\tilde{i}\tilde{j}}(\Omega) \\
& + \frac{1}{4} \sum_{ijab} \mathscr{T}^{\dagger(2)}_{ijab}(\Omega)\, \bar{v}^{\mathrm{eff}}_{\tilde{a}\tilde{b}\tilde{i}\tilde{j}}(\Omega)
\end{aligned}
$$

➟ Standard MBPT(2) codes can be employed

➟ There exist techniques to reduce computational cost from $\mathbf{N_b^5}$ to $\mathbf{N_b^3 \times N_h}$

[see e.g. Khorosmkaia & Khoromskij 2014]

➟ Reduces to standard MBPT(2) for Ω=0

MBPT of off-diagonal kernels

✪ Expansion of the norm kernel

$$E_0^J = \frac{\sum_{MK} f_M^{J*}\ f_K^J \int_{D_{SU(2)}} \mathrm{d}\Omega\ \ D_{MK}^{J*}(\Omega)\ \ h(\Omega)\ \ \mathcal{N}(\Omega)}{\sum_{MK} f_M^{J*}\ f_K^J \int_{D_{SU(2)}} \mathrm{d}\Omega\ \ D_{MK}^{J*}(\Omega)\ \ \mathcal{N}(\Omega)}$$

➟ The norm kernel has to be computed consistently with the energy kernel

➟ **Argument**: require that applying the restoration scheme to the Casimir and infinitesimal generator of the group one gets the expected values ***at each order of truncation***

↓

In the case of SU(2) $\boldsymbol{J^2 \Longrightarrow J(J+1)\,\hbar}$ and $\boldsymbol{J_z \Longrightarrow M\,\hbar}$

➟ This leads to a set of three coupled ordinary differential equations $\mathcal{N}$ has to satisfy

MBPT of off-diagonal kernels

✪ ODEs for the norm kernel

$$\frac{\partial}{\partial\alpha}\mathcal{N}(\Omega) = -\frac{i}{\hbar}\, j_z(\Omega)\,\mathcal{N}(\Omega)$$

$$\frac{\partial}{\partial\beta}\left(\sin\beta\frac{\partial}{\partial\beta}\right)\mathcal{N}(\Omega)$$
$$+\frac{1}{\sin^2\beta}\left(\frac{\partial^2}{\partial\alpha^2}+\frac{\partial^2}{\partial\gamma^2}\right)\mathcal{N}(\Omega)$$
$$-2\frac{\cos\beta}{\sin^2\beta}\frac{\partial^2}{\partial\alpha\partial\gamma}\mathcal{N}(\Omega) = -\frac{1}{\hbar^2}j^2(\Omega)\mathcal{N}(\Omega)$$

$$\frac{\partial}{\partial\gamma}\mathcal{N}(\Omega) = -\frac{i}{\hbar}\sin\beta\,\cos\alpha\, j_x(\Omega)\,\mathcal{N}(\Omega)$$
$$-\frac{i}{\hbar}\sin\beta\,\sin\alpha\, j_y(\Omega)\,\mathcal{N}(\Omega)$$
$$-\frac{i}{\hbar}\cos\beta\, j_z(\Omega)\,\mathcal{N}(\Omega)$$

MBPT of off-diagonal kernels

✪ **ODEs for the norm kernel**

➟ At a given order n one has to compute $\mathbf{j_x}^{(n)}$, $\mathbf{j_y}^{(n)}$, $\mathbf{j_z}^{(n)}$ and $\mathbf{j}^{2\,(n)}$

e.g. at 2nd order $\quad j_k^{(2)}(\Omega) = \sum_i (j_k)_{\tilde{\imath}\bar{\imath}}(\Omega) + \sum_{ia} \mathscr{T}_{ia}^{\dagger(2)}(\Omega)\,(j_k)_{\tilde{a}\tilde{\imath}}(\Omega)$

and determine the norm from the ODEs

MBPT of off-diagonal kernels

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and determine the norm from the ODEs

➟ The resulting norm can be written as

$$\mathscr{N}^{(2)}(\Omega) \equiv \aleph^{(2)}(\Omega)\,\langle\Phi(0)|\Phi(\Omega)\rangle$$

↓

at first order $\quad \aleph^{(1)}(\Omega) = 1$

(cf. ODEs fulfilled by the plain overlap, i.e. uncorrelated norm kernel)

Conclusive remarks

- ✪ The present formalism consistently treats **non-dynamical** and **dynamical** correlations
  - ➟ Non-dynamical correlations through MR mixing
  - ➟ Dynamical correlations through expansion of kernels in terms of *ph* excitations
  - ➟ In addition, one can enrich H_{eff} with higher-body operators
- ✪ When augmenting the content of the kernels and/or H_{eff}, parameters of H_{eff} must be **re-optimised** fully
- ✪ Consistent treatment of energy and norm kernels is crucial
- ✪ All other operators can be treated on the same footing
- ✪ First obvious step is MBPT(2), but other many-body expansions can be envisioned
  - ➟ Optimise balance between complexity of many-body expansion and that of the effective Hamiltonian
- ✪ The formalism allows to perform safe MR calculations, however it does not guarantee it
  - ➟ Incautious many-body truncations might still induce self-interactions/self-pairing
  - ➟ Further study of which are the **safe truncations** is needed

Appendix

Working scheme for the ab initio-based EDF

A Reference state

(a) Solve, e.g., symmetry-unrestricted Hartree-Fock equations in terms of H_{eff} in the basis of interest to obtain the (deformed) reference state $|\Phi(0)\rangle$. This amounts to using

$$h^{(1)}(0) = h^{(1)}[\rho^{00}],$$

as an input diagonal functional. We denote by $N_b = N_h + N_p$ the dimension of the one-body Hilbert space, where N_h denotes the number of occupied states of $|\Phi(0)\rangle$ and N_p the number of unoccupied states.

(b) Store single-particle energies $\{e_\alpha\}$ and wave-functions $\{\varphi_\alpha\}$.

B Single-reference calculations

(a) Build the diagonal one-body density matrix ρ^{00} along with the matrix elements of T, V_{eff}, J_k and any other observable O in the eigenbasis $\{\varphi_\alpha\}$ of H_0.

(b) Compute from it the diagonal energy kernel at the chosen order n

$$E_{\text{SR}} \equiv h^{(n)}(0) = h^{(n)}[\rho^{00}; \{e_\alpha\}].$$

Proceed similarly for all the other observables O of interest, i.e. compute

$$O_{\text{SR}} \equiv o^{(n)}(0) = o^{(n)}[\rho^{00}; \{e_\alpha\}].$$

Working scheme for the ab initio-based EDF

C Multi-reference calculations

(a) Discretize the intervals of integration over the three Euler angles $\Omega \equiv (\alpha, \beta, \gamma)$.

(b) For each combination of Euler angles

i. Build the $N_b \times N_b$ matrix $R_{\alpha\beta}(\Omega) \equiv \langle \alpha | R(\Omega) | \beta \rangle$ and its $N_h \times N_h$ reduction $M_{ij}(\Omega)$ to the subspace of hole states of $|\Phi(0)\rangle$. Compute the inverse $M^{-1}(\Omega)$.

ii. Build the $N_p \times N_h$ rectangular matrix

$$\wp_{ai}^{0\Omega}(\Omega) \equiv \sum_{i=1}^{N_h} R_{aj}(\Omega) M_{ji}^{-1}(\Omega) \,.$$

iii. Build the bi-orthogonal bases according to Eqs. 61 and 63.

iv. Transform the matrix elements of $T, V_{\rm eff}, J_k$ and any other observable O of interest into the bi-orthogonal system to generate the matrix elements of $\tilde{T}(\Omega)$, $\tilde{V}_{\rm eff}(\Omega)$, $\tilde{J}_k(\Omega)$ and $\tilde{O}(\Omega)$, respectively.

v. Compute and store the off-diagonal linked/connected kernels at the chosen order n

$$\begin{aligned} h^{(n)}(\Omega) &= h^{(n)}[\rho^{0\Omega}; \{e_\alpha\}] \,, \\ o^{(n)}(\Omega) &= o^{(n)}[\rho^{0\Omega}; \{e_\alpha\}] \,, \\ j^{(n)}_{k=x,y,z}(\Omega) &= j^{(n)}_{k=x,y,z}[\rho^{0\Omega}; \{e_\alpha\}] \,. \end{aligned}$$

(c) Using $j^{(n)}_{k=x,y,z}(\Omega)$ for the discretized values of the Euler angles, along with the initial condition $\mathscr{N}^{(n)}(0) = 1$, integrate the three coupled ODEs (Eq. 70) to obtain

$$\mathscr{N}^{(n)}(\Omega) \equiv \aleph^{(n)}[\rho^{0\Omega}; \{e_\alpha\}] \, \langle \Phi(0) | \Phi(\Omega) \rangle \,.$$

for each combination of the Euler angles.

(d) Solve the Hill-Wheeler-Griffin equation to obtain the weights f^J_K (Eq. 27).

(e) Calculate the energy of the yrast states through

$$E^J_{\rm MR} = \frac{\sum_{K'K} f^{J*}_{K'} f^J_K \int_{D_{SU(2)}} d\Omega \, D^{J*}_{K'K}(\Omega) \, h^{(n)}(\Omega) \, \mathscr{N}^{(n)}(\Omega)}{\sum_{K'K} f^{J*}_{K'} f^J_K \int_{D_{SU(2)}} d\Omega \, D^{J*}_{K'K}(\Omega) \, \mathscr{N}^{(n)}(\Omega)} \,.$$

Proceed similarly to compute other observables O of interest[18].

Working scheme for the ab initio-based EDF