Why go back to pseudo-potential-based EDF models?

A proposal for novel/safe/improvable parametrizations of off-diagonal EDF kernels

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ESNT workshop on

New developments in nuclear energy density functional models

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Outline

Frame

- Does not follow the historical perspective (see J. P. Ebran)
- Is limited to the non-relativistic/time-independent framework
- Focuses entirely on the formalism
- Uses the Skyrme family of parameterizations for illustration
- Covers the full fledged multi-reference formalism
  - *Not QRPA, collective (e.g. Bohr) Hamiltonian etc that derive from it*

Objectives

- Introduce the complete formalism *as it is used* from a modern perspective
- Underline some formal difficulties faced by traditional parameterizations
- Pave the way for talks focusing on overcoming/bypassing those difficulties
  - Regularization method(s)
  - Pseudo-potential-based *off-diagonal* kernels
    - Effective-mean-field kernels
    - Beyond-effective-mean-field kernels from novel many-body method

Caveats

- Does not relate to all topics/variants
- Other options/angles discussed during the week

Nuclear EDF framework

1. *Reference states and symmetries*
2. *Building off-diagonal energy and norm kernels*
3. *Single-reference implementation*
4. *Multi-reference implementation*

[T. Duguet, LNP 879 (2014) 293]

Reference states and symmetry group

Bogoliubov transformation

$$\beta_\mu^{(g)} = \sum_i U_{i\mu}^{(g)*} a_i + V_{i\mu}^{(g)*} a_i^\dagger$$

$$\beta_\mu^{(g)\dagger} = \sum_i V_{i\mu}^{(g)} a_i + U_{i\mu}^{(g)} a_i^\dagger \ .$$

Bogoliubov state

g = collective label to be defined

$$|\Phi^{(g)}\rangle = \prod_\mu \beta_\mu^{(g)} |0\rangle$$

Product state

$$\beta_\mu^{(g)} |\Phi^{(g)}\rangle \quad = \quad 0 \ \forall \ \mu$$

Vacuum of quasi-particles

Symmetry group of nuclear H

$\mathcal{G} = \{R(\alpha)\}$ ***with*** $[R(\alpha), H] = 0$

$$\alpha \equiv \{\alpha_i \in D_i \, ; \, i = 1, \ldots, r\}$$

Compact Lie group

Infinitesimal generators $\vec{C} = \{C_i ; i = 1, \ldots, r\}$

Lie algebra $[C_i, C_j] = c_{ij}^k C_k$

Casimir operator Λ ***and exponential map for R(α)***

Decomposition over IRREPs

$$f(\alpha) \equiv \sum_{\lambda ab} f_{ab}^\lambda \ S_{ab}^\lambda(\alpha)$$

Orthogonal IRREPs

$$\langle \Psi^{\lambda a} | R(\alpha) | \Psi^{\lambda' b} \rangle \equiv S_{ab}^\lambda(\alpha) \delta_{\lambda\lambda'}$$

$$\int_{\mathcal{G}} dm(\alpha) \, S_{ab}^{\lambda *}(\alpha) \, S_{a'b'}^{\lambda'}(\alpha) = \frac{v_{\mathcal{G}}}{d_\lambda} \, \delta_{\lambda\lambda'} \, \delta_{aa'} \, \delta_{bb'}$$

Reference states

Symmetries of interest

$$\vec{P}, N, Z, J^2, M, \Pi, T^2, T_z, \mathcal{T}$$

$|g| \neq 0$ if symmetry broken

$\mathcal{G}$	$\lvert g \rvert$	$\alpha = \mathrm{Arg}(g)$
$U(1)$	$\lvert\lvert\kappa\rvert\rvert$	φ
$SU(2)$	$\rho_{\lambda\mu}\ (\lambda > 2J)$	α,β,γ

Paired system

Deformed system

Reference states

1) Symmetry unrestricted reference state $|\Phi\rangle$

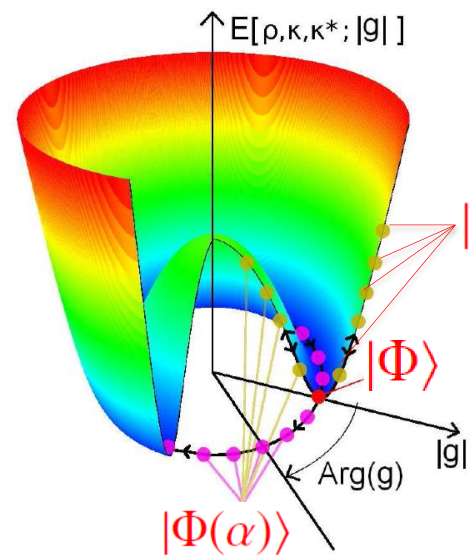
2) Rotated reference state $|\Phi(\alpha)\rangle \equiv R(\alpha)|\Phi\rangle$

3) Deformed reference state $|\Phi(|g|)\rangle \equiv U(|g|)|\Phi\rangle$

➡ ***Non perturbative Thouless transformations***

4) Full set of reference states $|\Phi^g\rangle \equiv |\Phi(|g|,\alpha)\rangle$

➡ ***Order parameter*** $g = \langle\Phi^{(g)}|G|\Phi^{(g)}\rangle \equiv |g|e^{i\alpha}$



Single-reference potential energy surface

Caveats

- g can also gather individual excitations
- Mostly deal with rotation next
- Alternatively focus on U(1) or SU(2)

Off -diagonal energy and norm kernels

Basic input to nuclear EDF method

Norm kernel $N(\alpha',\alpha) \equiv \langle \Phi(\alpha') | \Phi(\alpha) \rangle$ ***Different angles***

Energy kernel $H(\alpha',\alpha) \equiv h(\alpha',\alpha) N(\alpha',\alpha)$ ***with*** $h(\alpha',\alpha) \equiv h[\langle \Phi(\alpha')| ; |\Phi(\alpha)\rangle]$ ***Unknown functional***

Constraints

Independence of the reference frame

1) $h[\langle \Phi(\alpha')| R^\dagger(\alpha'') ; R(\alpha'')|\Phi(\alpha)\rangle] = h[\langle \Phi(\alpha')| ; |\Phi(\alpha)\rangle] \Rightarrow h(\alpha',\alpha) = h(0, \alpha-\alpha')$

2) SR chemical potential from Kamlah expansion of MR-EDF

3) QRPA from harmonic expansion of full-fledged MR-EDF

$\boxed{h(\alpha) \text{ and } N(\alpha)}$

[L.M. Robledo, IJMP E16 (2007) 337]

Working choice

$h(\alpha) \equiv h[\rho^{0\alpha}, \kappa^{0\alpha}, \kappa^{\alpha 0 *}]$ ***Functional of transition density matrices***

$$\rho_{ij}^{\alpha'\alpha} \equiv \frac{\langle \Phi(\alpha')| a_j^\dagger a_i |\Phi(\alpha)\rangle}{\langle \Phi(\alpha')|\Phi(\alpha)\rangle} \; ; \; \kappa_{ij}^{\alpha'\alpha} \equiv \frac{\langle \Phi(\alpha')| a_j a_i |\Phi(\alpha)\rangle}{\langle \Phi(\alpha')|\Phi(\alpha)\rangle} \; ; \; \kappa_{ij}^{\alpha\alpha' *} \equiv \frac{\langle \Phi(\alpha')| a_i^\dagger a_j^\dagger |\Phi(\alpha)\rangle}{\langle \Phi(\alpha')|\Phi(\alpha)\rangle}$$

Toy Skyrme EDF

Set of local densities

No isospin, no gradient correction, no spin-orbit, no tensor

$$\rho^{\alpha'\alpha}(\vec{r}) \equiv \sum_{ij}\sum_{\sigma}\varphi_j^*(\vec{r}\sigma)\varphi_i(\vec{r}\sigma)\rho_{ij}^{\alpha'\alpha}$$

Matter density

$$\tau^{\alpha'\alpha}(\vec{r}) \equiv \sum_{ij}\sum_{\sigma}[\vec{\nabla}\varphi_j^*(\vec{r}\sigma)]\cdot[\vec{\nabla}\varphi_i(\vec{r}\sigma)]\rho_{ij}^{\alpha'\alpha}$$

Kinetic density

$$\vec{s}^{\alpha'\alpha}(\vec{r}) \equiv \sum_{ij}\sum_{\sigma'\sigma}\varphi_j^*(\vec{r}\sigma')\vec{\sigma}_{\sigma'\sigma}\varphi_i(\vec{r}\sigma)\rho_{ij}^{\alpha'\alpha}$$

Spin density

$$\tilde{\rho}^{\alpha'\alpha}(\vec{r}) \equiv \sum_{ij}\sum_{\sigma}\sigma\,\varphi_j(\vec{r}\sigma)\varphi_i(\vec{r}\bar{\sigma})\kappa_{ij}^{\alpha'\alpha}$$

Pairing density

Off-diagonal energy kernel

Couplings to be fitted on data (could further depend on densities)

$$h^{\text{toy}}[\rho^{0\alpha},\kappa^{0\alpha},\kappa^{\alpha 0*}] \equiv \int d\vec{r}\left[\frac{\hbar^2}{2m}\tau^{0\alpha}(\vec{r}) + C^{\rho\rho}\,\rho^{0\alpha}(\vec{r})\rho^{0\alpha}(\vec{r}) + C^{ss}\,\vec{s}^{0\alpha}(\vec{r})\cdot\vec{s}^{0\alpha}(\vec{r}) + C^{\tilde{\rho}\tilde{\rho}}\,\tilde{\rho}^{\alpha 0*}(\vec{r})\tilde{\rho}^{0\alpha}(\vec{r})\right]$$

Quasi local functional

Structure constrained by symmetries (N, Z, J^2, M, T)

[E. Perlinska *et al.*, PRC69 (2004) 014316]

Mean-field pseudo-potential-based EDF kernel

Pseudo-Hamilton operator to be distinguished from

1) **Realistic Hamiltonian**
2) **Density-dependent Hamiltonian**

$$H_{\text{pseudo}} \equiv \sum_{ij} t_{ij} a_i^\dagger a_j + \left(\frac{1}{2!}\right)^2 \sum_{ijkl} \bar{v}^{2N\,\text{pseudo}}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k + \left(\frac{1}{3!}\right)^2 \sum_{ijklmn} \bar{v}^{3N\,\text{pseudo}}_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l + \cdots$$

Off-diagonal effective mean-field energy kernel

Effective-mean-field off-diagonal matrix element

$$h_{\text{pseudo}}[\rho^{0\alpha}, \kappa^{0\alpha}, \kappa^{\alpha 0 *}] \equiv \frac{\langle \Phi | H_{\text{pseudo}} | \Phi(\alpha) \rangle}{\langle \Phi | \Phi(\alpha) \rangle}$$

Off diagonal Wick theorem

$$= \sum_{ij} t_{ij} \rho^{0\alpha}_{ij}$$

$$+ \frac{1}{2} \sum_{ijkl} \bar{v}^{2N\,\text{pseudo}}_{ijkl} \rho^{0\alpha}_{ki} \rho^{0\alpha}_{lj} + \frac{1}{6} \sum_{ijklmn} \bar{v}^{3N\,\text{pseudo}}_{ijklmn} \rho^{0\alpha}_{li} \rho^{0\alpha}_{mj} \rho^{0\alpha}_{nk} + \cdots$$

$$+ \frac{1}{4} \sum_{ijkl} \bar{v}^{2N\,\text{pseudo}}_{ijkl} \kappa^{\alpha 0 *}_{ij} \kappa^{0\alpha}_{kl} + \frac{1}{4} \sum_{ijklmn} \bar{v}^{3N\,\text{pseudo}}_{ijklmn} \kappa^{\alpha 0 *}_{ij} \kappa^{0\alpha}_{lm} \rho^{0\alpha}_{nk} + \cdots$$

Same matrix elements

Fully antisymmetrized matrix elements

Pseudo-potential-based toy Skyrme EDF kernel

Toy Skyrme pseudo-potential operator

$$v_{\text{toy}}^{2N\,\text{pseudo}} \equiv t_0\,(1 - P_\sigma)\,\delta(\vec{r}_1 - \vec{r}_2)$$

Spin-exchange operator

Off-diagonal effective mean-field energy kernel

$$h_{\text{pseudo}}^{\text{toy}}[\rho^{0\alpha}, \kappa^{0\alpha}, \kappa^{\alpha 0 *}] \equiv \frac{\langle \Phi | H_{\text{pseudo}}^{\text{toy}} | \Phi(\alpha) \rangle}{\langle \Phi | \Phi(\alpha) \rangle}$$

Formally identical to $h^{\text{toy}}[\rho^{0\alpha}, \kappa^{0\alpha}, \kappa^{\alpha 0 *}]$

$$= \int d\vec{r} \left[\frac{\hbar^2}{2m} \tau^{0\alpha}(\vec{r}) + A^{\rho\rho}\, \rho^{0\alpha}(\vec{r})\, \rho^{0\alpha}(\vec{r}) + A^{ss}\, \vec{s}^{\,0\alpha}(\vec{r}) \cdot \vec{s}^{\,0\alpha}(\vec{r}) + A^{\tilde{\rho}\tilde{\rho}}\, \tilde{\rho}^{\alpha 0 *}(\vec{r})\, \tilde{\rho}^{0\alpha}(\vec{r}) \right]$$

Fingerprints of Pauli principle encoded in operator-based kernel

BUT

$$\boxed{\begin{aligned} A^{\rho\rho} &= -A^{ss} = \frac{t_0}{2} \\ A^{\rho\rho} &= +A^{\tilde{\rho}\tilde{\rho}} = \frac{t_0}{2} \end{aligned}}$$

Interrelations among couplings

Pauli principle violated in $h^{\text{toy}}[\rho^{0\alpha}, \kappa^{0\alpha}, \kappa^{\alpha 0 *}]$

Free fit of the three couplings

Pauli principle and self-interaction/-pairing

Local densities

$$f^{0\alpha}(\vec r) \equiv \sum_{ij} W^{f}_{ji}(\vec r)\,\rho^{0\alpha}_{ij}$$

$$\tilde f^{0\alpha}(\vec r) \equiv \sum_{ij} W^{\tilde f}_{ji}(\vec r)\,\kappa^{0\alpha}_{ij}$$

$$W^{\rho}_{ji}(\vec r) = \sum_{\sigma} \varphi^{*}_{j}(\vec r\sigma)\,\varphi_{i}(\vec r\sigma)$$

$$\vec W^{\vec s}_{ji}(\vec r) = \sum_{\sigma'\sigma} \varphi^{*}_{j}(\vec r\sigma')\,\vec\sigma_{\sigma'\sigma}\,\varphi_{i}(\vec r\sigma)$$

$$W^{\tilde\rho}_{ji}(\vec r) = \sum_{\sigma} \sigma\,\varphi_{j}(\vec r\sigma)\,\varphi_{i}(\vec r\bar\sigma)$$

Toy polynomial EDF kernel

$$h^{\mathrm{toy}}[\rho^{0\alpha},\kappa^{0\alpha},\kappa^{\alpha 0*}] = \sum_{ij} t_{ij}\,\rho^{0\alpha}_{ij} + \frac{1}{2}\sum_{ijkl} \bar v^{2N\,\mathrm{toy}\,\rho\rho}_{ijkl}\,\rho^{0\alpha}_{ki}\,\rho^{0\alpha}_{lj} + \frac{1}{4}\sum_{ijkl} \bar v^{2N\,\mathrm{toy}\,\kappa\kappa}_{ijkl}\,\kappa^{\alpha 0*}_{ij}\,\kappa^{0\alpha}_{kl}$$

with

$$\bar v^{2N\,\mathrm{toy}\,\rho\rho}_{ijkl} \equiv 2\int d\vec r\left[B^{\rho\rho}\,W^{\rho}_{ik}(\vec r)\,W^{\rho}_{jl}(\vec r) + B^{ss}\,\vec W^{\vec s}_{ik}(\vec r)\cdot\vec W^{\vec s}_{jl}(\vec r)\right]$$

$$\bar v^{2N\,\mathrm{toy}\,\kappa\kappa}_{ijkl} \equiv 4\int d\vec r\,B^{\tilde\rho\tilde\rho}\,W^{\tilde\rho *}_{ij}(\vec r)\,W^{\tilde\rho}_{kl}(\vec r)$$

General	*Pseudo-potential based*
$B^{ff'} \equiv C^{ff'}$	$B^{ff'} \equiv A^{ff'}$
$\bar v^{2N\,\mathrm{toy}\rho\rho}_{ijkk} \neq 0$ $\bar v^{2N\,\mathrm{toy}\rho\rho}_{ijkl} \neq \bar v^{2N\,\mathrm{toy}\kappa\kappa}_{ijkl}$	$\bar v^{2N\,\mathrm{toy}\rho\rho}_{ijkk} = 0$ $\bar v^{2N\,\mathrm{toy}\rho\rho}_{ijkl} = \bar v^{2N\,\mathrm{toy}\kappa\kappa}_{ijkl}$

Spurious self interaction

Spurious self pairing

[M. Bender, T. Duguet, D. Lacroix, PRC79 (2009) 044319]

Single reference implementation

Minimization $E^{SR}_{|g|} \equiv \mathrm{Min}_{\{|\Phi^{(g)}\rangle\}}\left\{\mathcal{E}_{|g|}\right\}$ **for a fixed g**

where

Independent of α = Arg(g)

$$\mathcal{E}_{|g|} \equiv \underbrace{h(g,g)}_{\text{Diagonal part of EDF kernel}} - \lambda_n\left[N - \langle\Phi^{(g)}|N|\Phi^{(g)}\rangle\right] - \lambda_p\left[Z - \langle\Phi^{(g)}|Z|\Phi^{(g)}\rangle\right] - \lambda_{|g|}\left[|g| - |\langle\Phi^{(g)}|G|\Phi^{(g)}\rangle|\right]$$

Diagonal part of EDF kernel

Equation of motion

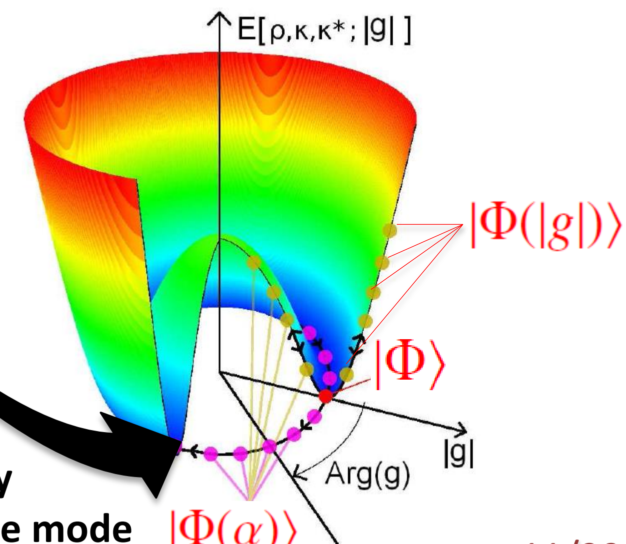
Bogoliubov-De-Gennes equation

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -h^*+\lambda \end{pmatrix}^{(g)} \begin{pmatrix} U \\ V \end{pmatrix}^{(g)}_{\mu} = E^{|g|}_{\mu} \begin{pmatrix} U \\ V \end{pmatrix}^{(g)}_{\mu}$$

One-body fields **govern**

$$h^{(g)} - \lambda \equiv \frac{\delta \mathcal{E}_{NZ|g|}}{\delta \rho^{gg*}}$$ ***Effective one-body motion***

$$\Delta^{(g)} \equiv \frac{\delta \mathcal{E}_{NZ|g|}}{\delta \kappa^{gg*}}$$ ***Effective pair correlations***



Broken symmetry
Pseudo Goldstone mode

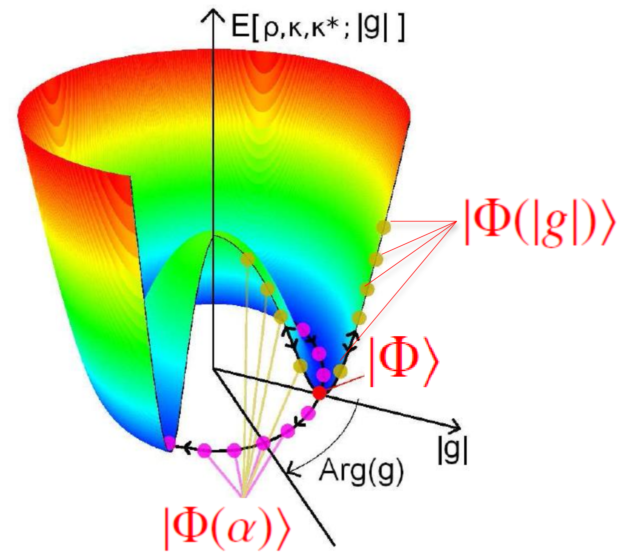
Multi reference implementation – ex: SU(2)

Quantum fluctuations in finite systems

Finite inertia **with respect to |g|**
- ***Shape fluctuations***
- ***Vibrational excitations***

with respect to α = Arg(g)
- ***Symmetry restoration***
- ***Rotational excitations***

Objectives of the MR EDF method



MR-EDF method – ex: AMR

Euler angles

IRREPs: Wigner D functions

Expansion of off-diagonal energy and norm kernels over IRREPs

$$\begin{cases} N(\Omega) \equiv \sum_{JMK} N^J_{MK}\, \mathcal{D}^J_{MK}(\Omega) \\ h(\Omega)\, N(\Omega) \equiv \sum_{JMK} E^J_{MK}\, N^J_{MK}\, \mathcal{D}^J_{MK}(\Omega) \end{cases}$$

Sum rules

$$1 = \sum_{JM} N^J_{MM}$$

$$E^{SR} = \sum_{JM} E^J_{MM}\, N^J_{MM}$$

AMR energy

$$E^J \equiv \frac{\sum_{MK} f^{J*}_M f^J_K \int_{SU(2)} d\Omega\, D^{J*}_{MK}(\Omega)\, h(\Omega)\, N(\Omega)}{\sum_{MK} f^{J*}_M f^J_K \int_{SU(2)} d\Omega\, D^{J*}_{MK}(\Omega)\, N(\Omega)} = \frac{\sum_{MK} f^{J*}_M f^J_K\, E^J_{MK}\, N^J_{MK}}{\sum_{MK} f^{J*}_M f^J_K\, N^J_{MK}}$$

From Hill-Wheeler equation

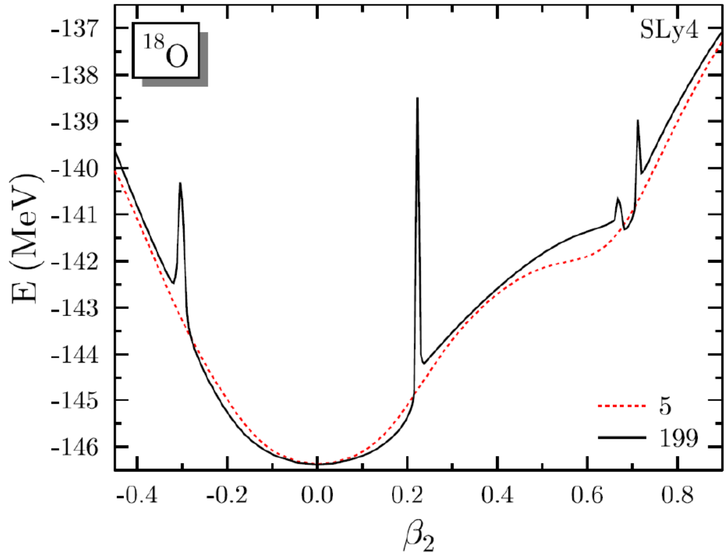
Well formulated without projected state!

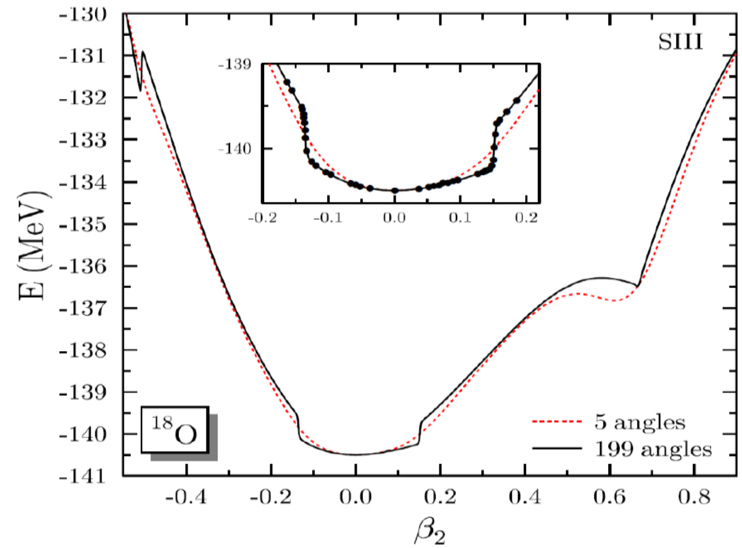
Pathologies in MR-EDF calculations

1. *Illustrations and origin*
2. *Overcoming these pathologies?*

Pathologies in multi-reference EDF calculations

$$h[\rho^{0\phi},\kappa^{0\phi},\kappa^{\phi 0*}] \propto \qquad \rho^{0\phi}\rho^{0\phi}\underline{(\rho^{0\phi})^{\gamma}} + \kappa^{\phi 0*}\kappa^{0\phi} \qquad \rho^{0\phi}\rho^{0\phi} + \kappa^{\phi 0*}\kappa^{0\phi}$$





PNR energy

$$E^A = \frac{\int_0^{2\pi} d\phi\, e^{-iA\phi}\, h(\phi)\, N(\phi)}{\int_0^{2\pi} d\phi\, e^{-iA\phi}\, N(\phi)}$$

Sum rules

$$1 = \sum_{A>0} N^A \qquad E^{SR} = \sum_{A>0} E^A N^A$$

Detailed analysis

1. Spurious divergencies and steps
2. *$E^A\, N^A \neq 0$* for *$A \leq 0$* !
3. True for 99% of modern EDF parameterizations
4. Relate to non-analytical character of *$h(\phi)\, N(\phi)$* over C-plane
5. Originate from self-interaction and self-pairing in *$h(\phi)$*
6. Common to all MR modes

[J. Dobaczewski et al., PRC76 (2007) 054315]
[D. Lacroix, T. Duguet, M. Bender, PRC79 (2009) 044318]
[M. Bender, T. Duguet, D. Lacroix, PRC79 (2009) 044319]
[T. Duguet *et al*., PRC79 (2009) 044320]

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Possible paths for future developments

Regularization methods

1) Early proposition **[D. Lacroix, T. Duguet, M. Bender, PRC79 (2009) 044318]**
- ***Rooted in the removal of self-interaction and self-pairing contaminations***
- ***Solves problem for PNR alone***
- ***Only applies to polynomial functionals (1% of existing parametrizations)***
- ***Does not work as soon as one mixes PNR with any other MR mode (e.g. AMR, GCM…)***
- ***Involded numerical implementation***

No talk this week

2) Recent proposition **[W. Satula, J. Dobaczewski, arXiv:1407.0857]**
- ***Empirical method***
- ***Solves problem for any MR mode***
- ***Only applies to polynomial functionals (1% of existing parametrizations)***
- ***Simple numerical implementation***

Jacek's talk

Pseudo-potential based approaches

Safe by construction but challenging to reach good enough phenomenology

1. **Effective mean-field kernel from**
    1. **Finite-range pseudo-potential (Jacek's talk)**
    2. **Augmented Skyrme-like pseudo-potential (Michael's and Karim's talks)**
2. **Effective beyond-mean-field off-diagonal energy and norm kernels from MBPT (now)**

[T. Duguet, arXiv:1406.7183]

Many-body perturbation theory of off-diagonal energy and norm kernels

~~Symmetry-restored coupled-cluster theory~~

Angular-momentum-restored coupled-cluster formalism

[T. Duguet, J. Phys. G: Nucl. Part. Phys (2014), in print; arXiv:1406.7183]

Particle-number-restored Bogoliubov coupled-cluster formalism

[T. Duguet, in preparation (2014)]

Set up (SU(2) for today)

Nuclear Hamiltonian

$$H = \sum_{\alpha\beta} t_{\alpha\beta}\, c^\dagger_\alpha c_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta}\, c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma$$

1. **Ab initio context = realistic nuclear hamiltonian**
2. **Present context = preferred pseudo potential**

Same symmetries

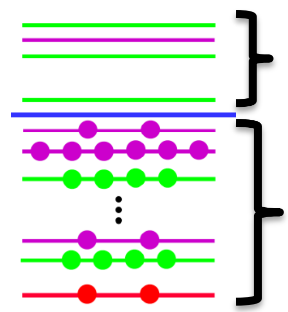
Eigen-states of H are eigen-states of (J^2,J_z)

$[H, R(\Omega)] = 0$ **leads to** $H|\Psi^{JM}_\mu\rangle = E^J_\mu |\Psi^{JM}_\mu\rangle$

Reference Slater determinant

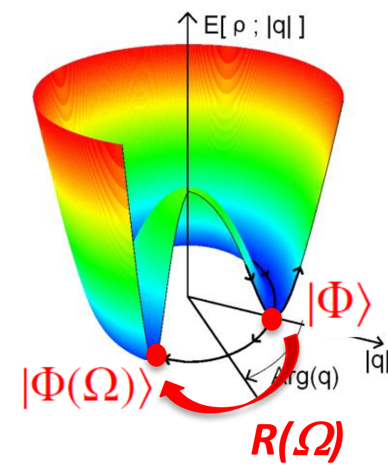
$$|\Phi\rangle \equiv \prod_{i=1}^{N} a^\dagger_i |0\rangle$$

1. **Deformed**
2. **Closed shell**



Particle states a,b,c…

Hole states i,j,k…



Rotated state

$$|\Phi(\Omega)\rangle = \prod_{i=1}^{N} a^\dagger_{\bar{i}} |0\rangle$$

with $a^\dagger_{\bar{\alpha}} = \sum_\beta R_{\beta\alpha}(\Omega) a^\dagger_\beta$ **and** $R_{\alpha\beta}(\Omega) \equiv \langle\alpha|R(\Omega)|\beta\rangle$

$\langle\Phi|\Phi(\Omega)\rangle = \det M(\Omega)$ **where** $M_{\alpha\beta}(\Omega) \equiv R_{\alpha\beta}(\Omega)\delta_{\alpha i}\delta_{\beta j}$

Master equations (1)

Evolution operator $\mathcal{U}(\tau) \equiv e^{-\tau H}$

Time-evolved state $|\Psi(\tau)\rangle \equiv \mathcal{U}(\tau)|\Phi\rangle$ **satisfying** $H\,|\Psi(\tau)\rangle = -\partial_\tau|\Psi(\tau)\rangle$

Exact off-diagonal kernels

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

Dynamical equation

$$H(\tau,\Omega) = -\partial_\tau N(\tau,\Omega)$$

Ground state and energy

$$\lim_{\tau\to\infty} |\Psi(\infty)\rangle = |\Psi_0^{J_0}\rangle \qquad \mathcal{H}(\infty,\Omega) = E_0^{J_0}\,\mathcal{N}(\infty,\Omega)$$

-True for all Ω

-Usual sym. unrest. MB schemes ($\Omega = 0$)

Expand un-rotated energy kernel $\mathcal{H}(\infty,0) = E_0^{J_0}$

Reduced kernels

$$\mathcal{O}(\tau,\Omega) \equiv O(\tau,\Omega)/N(\tau,0)$$

$\mathcal{N}(\tau,0) = 1$ **Intermediate normalization**

Master equations (2)

Expansion of rotated kernels over IRREPs of SU(2)

$$N(\infty,\Omega) = e^{-\tau E_0^{J_0}} \sum_{MK} \langle \Phi | \Psi_0^{J_0 M} \rangle \langle \Psi_0^{J_0 K} | \Phi \rangle D^{J_0}_{MK}(\Omega)$$

$$H(\infty,\Omega) = e^{-\tau E_0^{J_0}} E_0^{J_0} \sum_{MK} \langle \Phi | \Psi_0^{J_0 M} \rangle \langle \Psi_0^{J_0 K} | \Phi \rangle D^{J_0}_{MK}(\Omega)$$

Time propagation selects the proper IRREP

Straight ratio

$$\mathcal{H}(\infty,\Omega) = E_0^{J_0} \, \mathcal{N}(\infty,\Omega)$$

Truncating kernels expanded around symmetry-breaking reference $|\Phi\rangle$

$$N_{\text{approx}}(\infty,\Omega) \equiv \sum_J \sum_{MK} \mathcal{N}^J_{MK} \, D^J_{MK}(\Omega)$$

$$H_{\text{approx}}(\infty,\Omega) \equiv \sum_J \sum_{MK} \mathcal{E}^J_{MK} \, \mathcal{N}^J_{MK} \, D^J_{MK}(\Omega)$$

IRREPs still mixed as τ -> ∞

<=>

The good symmetry is lost

Extract good IRREP

Orthogonality of IRREPs

Symmetry-restored energy

$$E_0^{J_0} = \frac{\sum_{MK} f_M^{J_0 *} f_K^{J_0} \int_{SU(2)} d\Omega \, D^{J_0 *}_{MK}(\Omega) \, \mathcal{H}(\infty,\Omega)}{\sum_{MK} f_M^{J_0 *} f_K^{J_0} \int_{SU(2)} d\Omega \, D^{J_0 *}_{MK}(\Omega) \, \mathcal{N}(\infty,\Omega)}$$

Superfluous in exact limit but not after truncation

Diagonal kernels $D^J_{MK}(0) = \delta_{MK}$

$$N_{\text{approx}}(\infty,0) \equiv \sum_J \sum_M \mathcal{N}^J_{MM} \otimes$$

$$H_{\text{approx}}(\infty,0) \equiv \sum_J \sum_M \mathcal{E}^J_{MM} \, \mathcal{N}^J_{MM} \otimes$$

No fingerprint of mixing left to be used

Benefit of inserting rotation operator in kernels!

Many-body perturbation theory (1)

Symmetry-breaking unperturbed system

$H \equiv H_0 + H_1$ **where** $H_0 \equiv T + U = \sum_\alpha e_\alpha a^\dagger_\alpha a_\alpha$ **Such that** $[H_0, R(\Omega)] \neq 0$ **and** $[H_1, R(\Omega)] \neq 0$

$$\left.\begin{array}{l} H_0\,|\Phi\rangle = \varepsilon_0\,|\Phi\rangle \\ H_0\,|\Phi^{ab\ldots}_{ij\ldots}\rangle = (\varepsilon_0 + \varepsilon^{ab\ldots}_{ij\ldots})\,|\Phi^{ab\ldots}_{ij\ldots}\rangle \end{array}\right\} \text{ with } \left\{\begin{array}{l} \varepsilon_0 = \sum_{i=1}^{N} e_i \\ \varepsilon^{ab\ldots}_{ij\ldots} = e_a + e_b + \ldots - e_i - e_j - \ldots \end{array}\right.$$

Off diagonal unperturbed one-body density matrix

Ω-dependent part couples p and h spaces

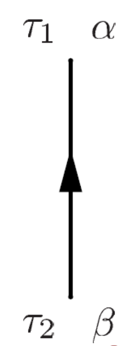
$$\rho_{\alpha\beta}(\Omega) \equiv \frac{\langle\Phi|a^\dagger_\beta a_\alpha|\Phi(\Omega)\rangle}{\langle\Phi|\Phi(\Omega)\rangle} \longrightarrow \rho(\Omega) = \begin{pmatrix} 1^{hh} & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ R(\Omega)M^{-1}(\Omega) & 0 \end{pmatrix} \equiv \rho(0) + \rho^{ph}(\Omega)$$

Defined earlier as $\rho^{0\Omega}_{\alpha\beta}$

Density matrix of sym. unrest. reference state

Off-diagonal unperturbed propagator = basic contraction for Wick Theorem

$$G^0_{\alpha\beta}(\tau_1, \tau_2; \Omega) \equiv \frac{\langle\Phi|T[a_\alpha(\tau_1)a^\dagger_\beta(\tau_2)]|\Phi(\Omega)\rangle}{\langle\Phi|\Phi(\Omega)\rangle} = G^0_{\alpha\alpha}(\tau_1 - \tau_2)\delta_{\alpha\beta} + G^{ph}_{\alpha\beta}(\tau_1, \tau_2)\rho^{ph}_{\alpha\beta}(\Omega)$$



Many-body perturbation theory (2)

Rotated norm kernel

Evolution operator $\mathcal{U}(\tau)$

Off diagonal Wick theorem
[R. Balian. E. Brezin, NC 64, 37 (1969)]

$$N(\tau,\Omega) = \langle\Phi|\underbrace{e^{-\tau H_0}\, T e^{-\int_0^\tau d\tau_1 H_1(\tau_1)}}_{\mathcal{U}(\tau)}|\Phi(\Omega)\rangle = e^{-\tau\varepsilon_0 + n(\tau,\Omega)}\,\langle\Phi|\Phi(\Omega)\rangle$$

Size extensive

where $n(\tau,\Omega) \equiv \sum_{k=1}^{\infty} n^{(k)}(\tau,\Omega)$ = connected vacuum-to-vacuum diagrams

Rotated energy kernel

Factorization valid for any operator kernel $O(\tau,\Omega)$

$$H(\tau,\Omega) = \langle\Phi|e^{-\tau H_0}\, T e^{-\int_0^\tau d\tau_1 H_1(\tau_1)}(T+V)|\Phi(\Omega)\rangle = h(\tau,\Omega)\,N(\tau,\Omega)$$

Ab initio formulation of h(Ω)!

where $h(\tau,\Omega) \equiv t(\tau,\Omega) + v(\tau,\Omega) \equiv \sum_{n=0}^{\infty}\left[t^{(n)}(\tau,\Omega) + v^{(n)}(\tau,\Omega)\right]$

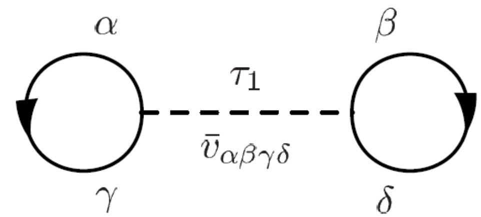
and $o(\tau,\Omega)$ = connected vacuum-to-vacuum diagrams *linked* to O

Size extensive

Many-body perturbation theory (3)

Connected norm diagrams – Example at first order

$$n_V^{(1)}(\tau,\Omega) = -\frac{1}{2}\sum_{\alpha\beta\gamma\delta}\int_0^\tau d\tau_1\, \bar{v}_{\alpha\beta\gamma\delta}\, G^0_{\gamma\alpha}(\tau_1,\tau_1;\Omega)\, G^0_{\delta\beta}(\tau_1,\tau_1;\Omega)$$



$$= -\frac{\tau}{2}\sum_{ij}\bar{v}_{ijij} \Big\} \quad n_V^{(1)}(\tau,0)$$ ***= standard diagonal MBPT contribution***

$$-\sum_{ija}\frac{\bar{v}_{ijaj}}{e_a-e_i}\rho^{ph}_{ai}(\Omega)\left(1-e^{-\tau(e_a-e_i)}\right)$$

$$-\frac{1}{2}\sum_{ijab}\frac{\bar{v}_{ijab}}{e_a+e_b-e_i-e_j}\left(1-e^{-\tau(e_a+e_b-e_i-e_j)}\right)\rho^{ph}_{ai}(\Omega)\rho^{ph}_{bj}(\Omega)$$

Genuinely Ω-dependent part

Large τ limit

$$n(\tau,0) \underset{\tau\to\infty}{\longrightarrow} -\tau\Delta E_0^{J_0} + \ln\left[\sum_M |\langle\Phi|\Psi_0^{J_0 M}\rangle|^2\right]$$

$$n(\tau,\Omega) - n(\tau,0) \underset{\tau\to\infty}{\longrightarrow} \aleph(\Omega)$$

$$\mathcal{N}(\infty,\Omega) = e^{\aleph(\Omega)}\langle\Phi|\Phi(\Omega)\rangle$$

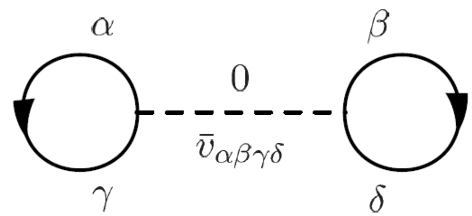
$$\equiv \mathcal{N}(\Omega)$$

Goldstone linked-cluster based on UHF
->nice but not what we are after!

$$\Delta E_0^{J_0} = \langle\Phi|H_1\sum_{k=1}^{\infty}\left(\frac{1}{\varepsilon_0 - H_0}H_1\right)^{k-1}|\Phi\rangle_c$$

Many-body perturbation theory (3)

Connected/linked potential energy diagrams – example at zero order



$$v^{(0)}(\tau,\Omega) = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \bar{v}_{\alpha\beta\gamma\delta}\, G^{0}_{\gamma\alpha}(0,0;\Omega)\, G^{0}_{\delta\beta}(0,0;\Omega)$$

$$= +\frac{1}{2}\sum_{ij} \bar{v}_{ijij} \Big\} \quad v^{(0)}(\tau,0)$$ *= standard diagonal MBPT contribution*

$$+\sum_{ijc} \bar{v}_{ijcj}\, \rho^{ph}_{ci}(\Omega)$$

$$+\frac{1}{2}\sum_{ijab} \bar{v}_{ijab}\, \rho^{ph}_{ai}(\Omega)\, \rho^{ph}_{bj}(\Omega)$$

Genuinely Ω-dependent part

One recognizes

$$\frac{\langle \Phi | V^{2\mathrm{N}} | \Phi(\Omega)\rangle}{\langle \Phi | \Phi(\Omega)\rangle}$$

Signals the symmetry breaking

Large τ limit $\quad h(\tau,\Omega) \underset{\tau\to\infty}{\longrightarrow} h(\Omega) \Big\} \quad \mathcal{H}(\infty,\Omega) = h(\Omega)\,\mathcal{N}(\Omega)$

In the exact limit $\quad \dfrac{\partial}{\partial\Omega} h(\Omega) = 0$

After truncation $\quad \dfrac{\partial}{\partial\Omega} h(\Omega) \neq 0$

Many-body perturbation theory (4)

Direct MBPT expansion $\mathcal{N}(\tau,\Omega) = e^{-\tau\varepsilon_0 + n(\tau,\Omega)} \langle \Phi | \Phi(\Omega) \rangle$ *does not ensure the symmetry restoration*

Solution to this key problem comes from

- **Coupled ODEs satisfied by Wigner D functions** [D. A. Varshalovich *et al.*, *Quantum Theory of Angular Momentum*, 1988]
- **Expansion of** $J_i(\tau,\Omega)$ **over Wigner D functions**
- **Factorization of connected kernels** $j_i(\tau,\Omega)$

Initial condition

$$\mathcal{N}(\tau,0) = 1$$

Coupled ODEs

$$\begin{aligned}
\frac{\partial}{\partial\alpha}\mathcal{N}(\tau,\Omega) + \frac{i}{\hbar} j_z(\tau,\Omega)\,\mathcal{N}(\tau,\Omega) &= 0 \\
\frac{\partial}{\partial\beta}\mathcal{N}(\tau,\Omega) - \frac{i}{\hbar}\Big[\sin\alpha\, j_x(\tau,\Omega) - \cos\alpha\, j_y(\tau,\Omega)\Big]\mathcal{N}(\tau,\Omega) &= 0 \\
\frac{\partial}{\partial\gamma}\mathcal{N}(\tau,\Omega) + \frac{i}{\hbar}\Big[\sin\beta\cos\alpha\, j_x(\tau,\Omega) + \sin\beta\sin\alpha\, j_y(\tau,\Omega) + \cos\beta\, j_z(\tau,\Omega)\Big]\mathcal{N}(\tau,\Omega) &= 0
\end{aligned}$$

This rational ensures that the symmetry is exactly restored at any truncation order of $j_i(\tau,\Omega)$

$$\frac{\int_{SU(2)} d\Omega\, D^{J*}_{MK}(\Omega)\, \mathcal{J}_z(\tau,\Omega)}{\int_{SU(2)} d\Omega\, D^{J*}_{MK}(\Omega)\, \mathcal{N}(\tau,\Omega)} = M\hbar$$

$$\boxed{\frac{\sum_{MK} f^{J*}_M f^J_K \int_{D_{SU(2)}} d\Omega\, D^{J*}_{MK}(\Omega)\, \mathcal{J}^2(\tau,\Omega)}{\sum_{MK} f^{J*}_M f^J_K \int_{D_{SU(2)}} d\Omega\, D^{J*}_{MK}(\Omega)\, \mathcal{N}(\tau,\Omega)} = J(J+1)\hbar^2}$$

Note: Extends to any order a known result of projected HF

e.g. [K. Enami et al., PRC59 (1999) 135]

Many-body perturbation theory (5)

Algebraic expressions become cumbersome beyond lowest order

Very much compacted by using *transformed* kinetic and potential energy operators

Bi-orthogonal system

$$
\begin{aligned}
|\tilde{\alpha}\rangle &\equiv D(\Omega)|\alpha\rangle \\
\langle\tilde{\alpha}| &\equiv \langle\alpha|D^{-1}(\Omega)
\end{aligned}
$$

$$D(\Omega) \equiv 1 + \rho^{ph}(\Omega)$$

Ex: for a generic two-body operator

$$\tilde{O}(\Omega) \equiv \left(\frac{1}{n!}\right)^2 \sum_{\alpha\ldots\beta\gamma\ldots\delta} O_{\tilde{\alpha}\ldots\tilde{\beta}\tilde{\gamma}\ldots\tilde{\delta}}(\Omega)\, a^\dagger_\alpha \ldots a^\dagger_\beta a_\delta \ldots a_\gamma$$

Example at lowest order (in the τ infinity limit)

$$
\begin{aligned}
t^{(0)}(\Omega) &= \sum_i t_{ii} + \sum_{ia} t_{ia}\, \rho^{ph}_{ai}(\Omega) \\
&= \sum_i t_{\tilde{i}\tilde{i}}(\Omega) \\
v^{(0)}(\Omega) &= \frac{1}{2}\sum_{ij} \bar{v}_{ijij} + \frac{1}{2}\sum_{ijc} \bar{v}_{ijcj}\, \rho^{ph}_{ci}(\Omega) + \frac{1}{2}\sum_{ijd} \bar{v}_{ijid}\, \rho^{ph}_{dj}(\Omega) + \frac{1}{2}\sum_{ijab} \bar{v}_{ijab}\, \rho^{ph}_{ai}(\Omega)\, \rho^{ph}_{bj}(\Omega) \\
&= \frac{1}{2}\sum_{ij} \bar{v}_{\tilde{i}\tilde{j}\tilde{i}\tilde{j}}(\Omega)
\end{aligned}
$$

GWT → SWT

$$\frac{\langle\Phi|H|\Phi(\Omega)\rangle}{\langle\Phi|\Phi(\Omega)\rangle} = \langle\Phi|\tilde{H}(\Omega)|\Phi\rangle$$

Cases of interest

Symmetry-restored energy

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

Standard MBPT recovered at $\Omega = 0$ or if $|\Phi\rangle$ does not break the symmetry

$$E_0^J = h(0)$$

Projected Hartree-Fock is recovered at lowest order

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

$$j_k^{(0)}(\Omega) = \frac{\langle \Phi | J_k | \Phi(\Omega) \rangle}{\langle \Phi | \Phi(\Omega) \rangle} = \sum_i (j_k)_{i\tilde{i}}(\Omega)$$

ODEs

$$N^{(0)}(\Omega) = \langle \Phi | \Phi(\Omega) \rangle = \det M(\Omega)$$

Basis for standard pseudo-potential-based MR-EDF method with effective mean-field kernels

$$E_0^{J(0)} = \frac{\langle \Phi_0^{JM} | H | \Phi_0^{JM} \rangle}{\langle \Phi_0^{JM} | \Phi_0^{JM} \rangle}$$

where

$$|\Phi_0^{JM}\rangle \equiv \sum_K f_K^J P_{MK}^J |\Phi\rangle$$

$$P_{MK}^J \equiv \frac{2J+1}{16\pi^2} \int_{D_{SU(2)}} d\Omega \, D_{MK}^{J*}(\Omega) \, R(\Omega)$$

Cases of interest

SWT

Beginning of an exponential

$$o^{(0+1)}(\Omega) = \langle\Phi|\Big[1 + \underbrace{\mathcal{T}_1^{\dagger(1)}(\Omega) + \mathcal{T}_2^{\dagger(1)}(\Omega)}\Big]\tilde{O}(\Omega)|\Phi\rangle_c$$

Symmetry-restored theory at first order

$$t^{(0+1)}(\Omega) = \sum_i t_{\tilde{i}\tilde{i}}(\Omega) + \sum_{ia} \mathcal{T}_{ia}^{\dagger(1)}(\Omega)\, t_{\tilde{a}\tilde{i}}(\Omega)$$

$$v^{(0+1)}(\Omega) = \frac{1}{2}\sum_{ij} \bar{v}_{\tilde{i}\tilde{j}\tilde{i}\tilde{j}}(\Omega) + \sum_{ija} \mathcal{T}_{ia}^{\dagger(1)}(\Omega)\, \bar{v}_{\tilde{a}\tilde{j}\tilde{i}\tilde{j}}(\Omega) + \frac{1}{4}\sum_{ijab} \mathcal{T}_{ijab}^{\dagger(1)}(\Omega)\, \bar{v}_{\tilde{a}\tilde{b}\tilde{i}\tilde{j}}(\Omega)$$

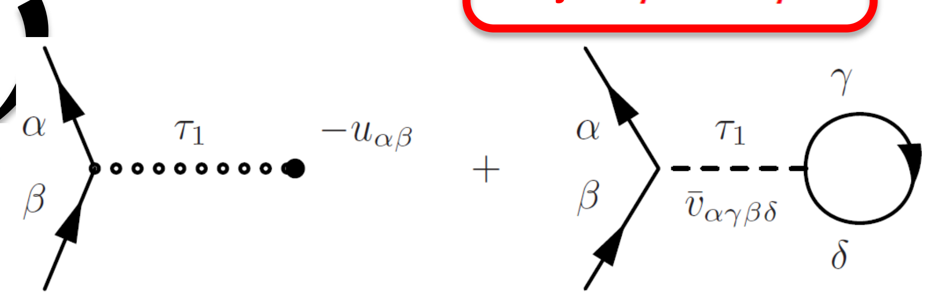
$$j_k^{(0+1)}(\Omega) = \sum_i (j_k)_{\tilde{i}\tilde{i}}(\Omega) + \sum_{ia} \mathcal{T}_{ia}^{\dagger(1)}(\Omega)\, (j_k)_{\tilde{a}\tilde{i}}(\Omega)$$

$$N^{(0+1)}(\Omega) = \aleph^{(1)}(\Omega)\langle\Phi|\Phi(\Omega)\rangle$$

Rich functional

Not just $\rho^{00} \rightarrow \rho^{0\Omega}$

$$\mathcal{T}_{\alpha\beta}^{\dagger(1)}(\Omega) =$$



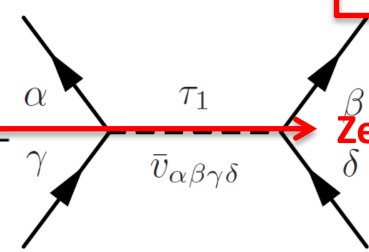
First-order off-diagonal CCSD amplitudes

$$\mathcal{T}_{ia}^{\dagger(1)}(\Omega) = -\frac{1}{e_\beta - e_\alpha}\underbrace{\Big[\sum_j \bar{v}_{ijaj} - u_{ia}\Big]} - \sum_{jb}\frac{\bar{v}_{ijab}}{\boxed{e_a + e_b - e_i - e_j}}\rho_{bj}^{ph}(\Omega)$$

Energy dependence

$$\mathcal{T}_{ijab}^{\dagger(1)}(\Omega) = -\frac{\bar{v}_{ijab}}{e_a + e_b - e_i - e_j}$$

$$\mathcal{T}_{\alpha\beta\gamma\delta}^{\dagger(1)}(\Omega) =$$



Zero for HF reference state

Proposal: new safe SR- and MR-EDF approach

Pseudo-potential-based off-diagonal kernels at first order in MBPT

$$h^{(0+1)}(\Omega) \equiv h^{(0+1)}[\rho^{0\Omega};\{e_\alpha\}]$$

$$j_k^{(0+1)}(\Omega) \equiv j_k^{(0+1)}[\rho^{0\Omega};\{e_\alpha\}]$$

$$\mathcal{N}^{(0+1)}(\Omega) \equiv \aleph^{(1)}[\rho^{0\Omega};\{e_\alpha\}]\langle\Phi|\Phi(\Omega)\rangle$$

ODEs

$$\mathcal{N}^{(0+1)}(0) = 1$$

Key features

1) Richer pseudo-potential-based kernels
2) Any pseudo-potential (need REG for ZR)
3) MBPT sequence, i.e. improvable
4) Modified energy AND norm kernels
5) Density matrix AND energy dependent

SR-EDF implementation

1. Effective HF problem

Employ $h^{(0)}[\rho^{00}]$ → $\rho^{00},\{e_\alpha\}$ → $E^{SR} \equiv h^{(0+1)}[\rho^{00};\{e_\alpha\}]$

Mean-field diagonal energy kernel — *HF reference state* — *Full diagonal energy kernel in HF basis*

2. Compute the energy

MR-EDF implementation

Solve ODEs from $j_k^{(0+1)}(\Omega)$

$$E^J \equiv \frac{\sum_{MK} f_M^{J*} f_K^J \int_{SU(2)} d\Omega\, D_{MK}^{J*}(\Omega)\, h^{(0+1)}(\Omega)\, \mathcal{N}^{(0+1)}(\Omega)}{\sum_{MK} f_M^{J*} f_K^J \int_{SU(2)} d\Omega\, D_{MK}^{J*}(\Omega)\, \mathcal{N}^{(0+1)}(\Omega)}$$

+ Hill-Wheeler equation

Full off-diagonal energy and norm kernels in bi-orthogonal bases

Already formulated for HFB reference states and PNR

Microscopic theoretical approaches

Ab-initio **many-body theories**

- Based on *elementary* interactions
- *Complete* and disjointed error estimate

Examples

- FY, HH, NCSM, GFMC, LEFT
- SCGF, IMSRG, CC…

Limited reach
Controlled extrapolations

Test fundamental interactions
Do not focus on accuracy at first

Interesting potential cross-feeding in the next ten years

Extended reach
Uncontrolled extrapolations

Do not probe fundamental interactions
Aims at high accuracy around known data

Effective **many-body theories**

- Based on *effective* interactions
- *Partial* and composite error estimate

Examples

- EDF, conventional CI, SMMC…