Restoring symmetries within the multi-reference nuclear EDF method

Formal aspects, difficulties, regularized calculations and remaining problems

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Outline

1. Question of present interest
2. Multi-reference energy density functional method
   - Elements of formalism and difficulties
   - Regularization method and remaining problems
3. Conclusions

Outline

Question of present interest

Handling symmetries within an energy density functional method

- H characterized by a symmetry group $\mathcal{G}$ [e.g. $\vec{P}_{\text{cm}}$, (J,M), (N,Z), $\Pi\ldots$]
- H and $|\Psi_n^{X_{\mathcal{G}}}\rangle$ are not manipulated explicitly

Density Functional Theory

- Symmetry dilemma is an issue
- Methods have been developed to deal with it, e.g.
  1. Symmetrized DFT [A. Görling, PRA 47 (1993) 2783]
  2. Symmetry-constrained DFT [H. Fertig, W. Kohn, PRA 62 (2000) 052511]
  3. Ensemble DFT [E. K. U. Gross, L. N. Oliveira, W. Kohn, PRA 37 (1988) 2809]

Nuclear Energy Density Functional method

1. Symmetries are first broken on purpose to grasp collective correlations
2. Restoration of symmetries historically *inspired* from projection techniques
   - Can it be properly formulated without any reference to H and $|\Psi_n^{X_{\mathcal{G}}}\rangle$?
   - Does it perform well?

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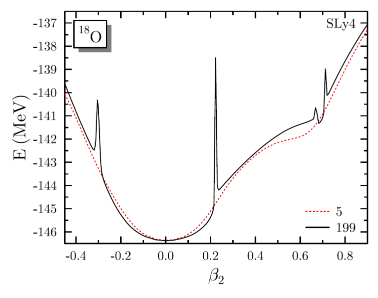
The problem that has led us to go back to the roots

Potential energy as a function of axial quadrupole deformation (β_2)

1. Includes the restoration of good N and Z
2. Employs two functionals having different analytic structures

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

$E[\rho,\kappa,\kappa^*] \propto A\rho + B\rho\rho\rho^{1/6} + C\rho\kappa^*\kappa$



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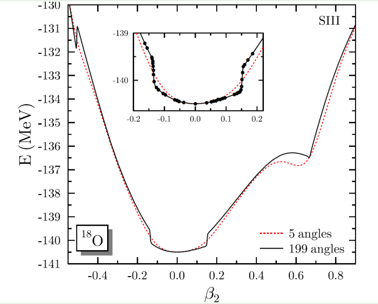

How profound is the problem?

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The overall method in a nutshell

Symmetry group

1. $\mathcal{G} \equiv \left\{R(\alpha)\ ;\ \alpha \in D_{\mathcal{G}}\right\}$ with volume $v_{\mathcal{G}}$
   e.g. Lie groups $U(1)$ $[N,Z]$ and $SO(3)$ $[J,M]$
2. Irreps $S^{\lambda}_{ab}(\alpha) \equiv \langle \Phi^{\lambda a}|R(\alpha)|\Phi^{\lambda b}\rangle$ of dim. d_λ

Building blocks

1. Symmetry-breaking Bogoliubov states $|\Phi^{(g)}\rangle$
2. Labelled by order parameter $g \equiv |g|\, e^{i\alpha}$
3. Off-diagonal norm and energy kernels

$$N[g',g] \equiv \langle \Phi^{(g')}|\Phi^{(g)}\rangle$$
$$E[g',g] \equiv E[\rho^{g'g}, \kappa^{g'g}, \kappa^{gg'\,*}]$$

is a functional of transition density matrices

$$\rho^{g'g}_{ij} \equiv \frac{\langle \Phi^{(g')}|a^\dagger_j a_i|\Phi^{(g)}\rangle}{\langle \Phi^{(g')}|\Phi^{(g)}\rangle} \quad ; \quad \kappa^{g'g}_{ij} \equiv \frac{\langle \Phi^{(g')}|a_j a_i|\Phi^{(g)}\rangle}{\langle \Phi^{(g')}|\Phi^{(g)}\rangle}$$

which re-sums bulk correlations

4. Empirical param. (Gogny, Skyrme,...)

Two successive levels of implementation

1. Single-reference (SR) [looks like DFT]
   - E^{SR}_0 invokes $E[g,g]$ only
   - Broken symmetries $(N,Z,J,M\ldots)$
   - Bulk prop. + limited spectro.
2. Multi-reference (MR)
   - E^{MR}_k invokes full $E[g',g]$
   - Sym. rest. + coll. fluct.
   - G.S. correlations + spectro.
   - Approx: QRPA, Bohr Hamilt.

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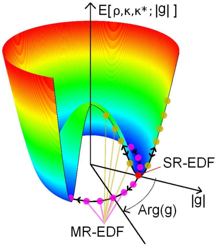


The symmetry restoration in more details

Symmetry-restored energies (diagonal in $|g|$)

1. Expand off-diagonal kernels over Irreps

$$N[0,\alpha] \equiv \sum_{\lambda ab} \mathcal{N}^{\lambda}_{ab}\, S^{\lambda}_{ab}(\alpha)$$

$$E[0,\alpha]\, N[0,\alpha] \equiv \sum_{\lambda ab} \mathcal{E}^{\lambda}_{ab}\, \mathcal{N}^{\lambda}_{ab}\, S^{\lambda}_{ab}(\alpha)$$

2. Extract coefficients for the targeted Irrep

$$\mathcal{N}^{\lambda}_{ab} = \frac{d_\lambda}{v_{\mathcal{G}}} \int_{D_{\mathcal{G}}} dm(\alpha) S^{\lambda *}_{ab}(\alpha)\, N[0,\alpha]$$

$$\mathcal{E}^{\lambda}_{ab}\, \mathcal{N}^{\lambda}_{ab} = \frac{d_\lambda}{v_{\mathcal{G}}} \int_{D_{\mathcal{G}}} dm(\alpha) S^{\lambda *}_{ab}(\alpha)\, E[0,\alpha]\, N[0,\alpha] \,.$$

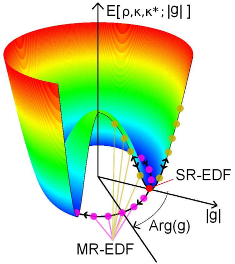
3. Mix over components spanning the targeted Irrep

$$E^{MR}_{\lambda k} \equiv \text{Min}_{f^{\lambda k *}_{a}} \left\{ \frac{\sum_{a,b} f^{\lambda k *}_{a}\, f^{\lambda k}_{b}\, \mathcal{E}^{\lambda}_{ab}\, \mathcal{N}^{\lambda}_{ab}}{\sum_{a,b} f^{\lambda k *}_{a}\, f^{\lambda k}_{b}\, \mathcal{N}^{\lambda}_{ab}} \right\} .$$

Sum rules at each $|g|$ from $S^{\lambda}_{ab}(0) = \delta_{ab}$

$$1 = \sum_{\lambda} d_\lambda\, \mathcal{N}^{\lambda}_{aa}$$

$$E^{SR}_{0} = \sum_{\lambda} d_\lambda\, \mathcal{E}^{\lambda}_{aa}\, \mathcal{N}^{\lambda}_{aa}$$



Symmetry restoration formulated without any reference to H and $|\Psi^{\lambda a}_{k}\rangle$

[T. Duguet, J. Sadoudi, J. Phys. G: Nucl. Part. Phys. 37 (2010) 064009]

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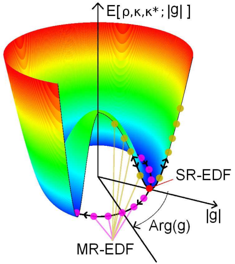

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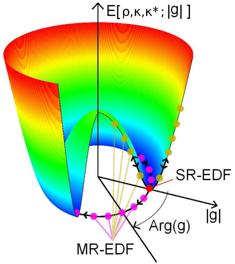

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Example

Particle number restoration (PNR) (at fixed $|g|$)

1. $U(1)$ group $\left\{R(\varphi) = e^{iN\varphi} \; ; \; \varphi \in [0, 2\pi]\right\}$
2. Fourier decomposition of kernels on Irreps

$$N[0,\varphi] \equiv \sum_{\mathrm{N}\in\mathbb{Z}} \mathcal{N}_{\mathrm{N}} \, e^{i\mathrm{N}\varphi}$$

$$E[0,\varphi] \, N[0,\varphi] \equiv \sum_{\mathrm{N}\in\mathbb{Z}} \mathcal{E}_{\mathrm{N}} \, \mathcal{N}_{\mathrm{N}} \, e^{i\mathrm{N}\varphi}$$

3. Particle-number-restored energies

$$\mathcal{N}_{\mathrm{N}} = \frac{1}{2\pi} \int_0^{2\pi} d\varphi \, e^{-i\mathrm{N}\varphi} \, N[0,\varphi]$$

$$\mathcal{E}_{\mathrm{N}} = \frac{\mathcal{N}_{\mathrm{N}}^{-1}}{2\pi} \int_0^{2\pi} d\varphi \, e^{-i\mathrm{N}\varphi} \, E[0,\varphi] \, N[0,\varphi]$$

No reference made to a projected state

4. Sum rules at each $|g|$

$$E_0^{\mathrm{SR}} \equiv \sum_{\mathrm{N}\in\mathbb{Z}} \mathcal{E}_{\mathrm{N}} \, \mathcal{N}_{\mathrm{N}}$$

Functional form of kernel $E[g', g]$

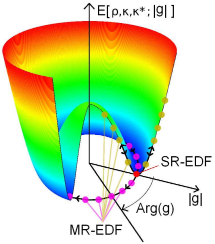
Following properties are mandatory

1. $\mathcal{E}_k^{\mathrm{MR}}$ real and scalar under $R(\alpha) \in \mathcal{G}$
2. μ^{SR} recovered through Kamlah
3. QRPA recovered as harmonic limit

Choice $E[g', g] \equiv E[\rho^{g'g}, \kappa^{g'g}, \kappa^{gg'*}]$

1. Satisfies all the above
2. Consistent with $E_{\mathcal{H}}[g', g] = \frac{\langle \Phi^{(g')} | \mathcal{H} | \Phi^{(g)} \rangle}{\langle \Phi^{(g')} | \Phi^{(g)} \rangle}$

[L. M. Robledo, JPG 37 (2010) 064020]



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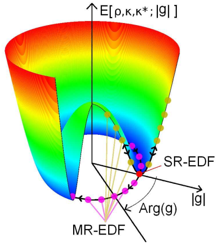

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Is that sufficient?

1. Satisfies all the above
2. Consistent with $E_{\mathcal{H}}[g', g] = \frac{\langle \Phi^{(g')} | \mathcal{H} | \Phi^{(g)} \rangle}{\langle \Phi^{(g')} | \Phi^{(g)} \rangle}$

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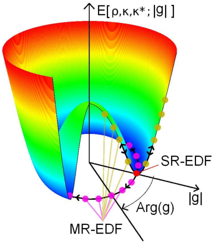
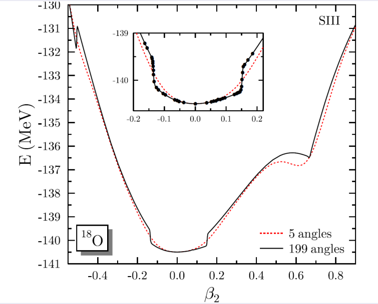


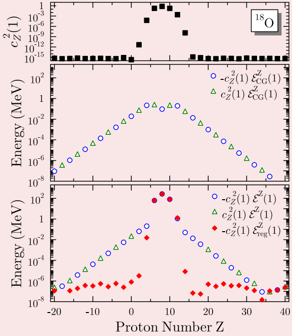
Divergences and steps in PNR calculations

$\mathcal{E}_{N,Z}$ for $E[\rho,\kappa,\kappa^*] \propto A\rho + B\rho\rho + C\kappa^*\kappa$



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

$\mathcal{N}_Z$ and $\mathcal{E}_Z\,\mathcal{N}_Z$ versus Z at fixed β_2



1. Divergencies and finite steps in PNR calculations [J. Dobaczewski *et al.*, PRC76 (2007) 054315]
2. Correspondingly $\mathcal{E}_N\,\mathcal{N}_N \neq 0$ for $N \leq 0$ [M. Bender, T. Duguet, D. Lacroix, PRC79 (2009) 044319]
3. Relate to non-analytic character of $E[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi 0\,*}]N[0,\varphi]$ over $\mathbb{C}^*$-plane with $e^{i\varphi} \equiv z$
4. Due to self-interaction/pairing in $E[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi 0\,*}]$ [M. Bender, T. Duguet, D. Lacroix, PRC79 (2009) 044319]
5. Similar problems for other MR modes, e.g. angular momentum restoration

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Towards sound Multi-Reference EDF calculations

Regularization method

[D. Lacroix, T. Duguet, M. Bender, PRC79 (2009) 044318]

$\mathcal{H}$-based kernel *in a specific basis*

$$E^{\mathrm{GWT}}_{\mathcal{H}}[\rho^{g'g},\kappa^{g'g},\kappa^{gg'*}] \equiv E^{\mathrm{SWT}}_{\mathcal{H}}[g',g] + E^{\mathrm{C}}[g',g]$$

✔ $E^{\mathrm{C}}[g',g] = 0$ for $\mathcal{H}$-based kernel

✘ $\neq 0$ and non-analytic otherwise

Regularized energy kernel

$$E_{\mathrm{REG}}[g',g] \equiv E[\rho^{g'g},\kappa^{g'g},\kappa^{gg'*}] - E^{\mathrm{C}}[g',g]$$

The method is originally designed

- For any MR mixing, i.e. any $|g|$ and α
- For polynomial kernels only

[T. Duguet *et al.*, PRC79 (2009) 044320]

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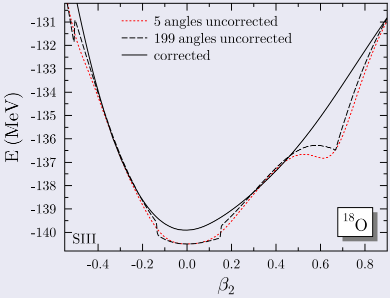
[T. Duguet *et al.*, PRC79 (2009) 044320]

Regularized $\mathcal{E}_{\mathrm{N,Z}}$ for $E \propto A\rho + B\rho\rho + C\kappa^*\kappa$



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

Regularized results

- ✔ are free from steps and divergences
- are modified *away* from them
- ✔ are independent of the discretization
- are modified by about 1 MeV
- ✔ provide $\mathcal{E}_{\mathrm{N}}\,\mathcal{N}_{\mathrm{N}} = 0$ for $\mathrm{N} \leq 0$

Towards sound Multi-Reference EDF calculations

Regularization method

[D. Lacroix, T. Duguet, M. Bender, PRC79 (2009) 044318]

$\mathcal{H}$-based kernel *in a specific basis*

$$E^{\mathrm{GWT}}_{\mathcal{H}}[\rho^{g'g},\kappa^{g'g},\kappa^{gg'*}] \equiv E^{\mathrm{SWT}}_{\mathcal{H}}[g',g] + E^{\mathrm{C}}[g',g]$$

✔ $E^{\mathrm{C}}[g',g] = 0$ for $\mathcal{H}$-based kernel

✘ $\neq 0$ and non-analytic otherwise

Regularized energy kernel

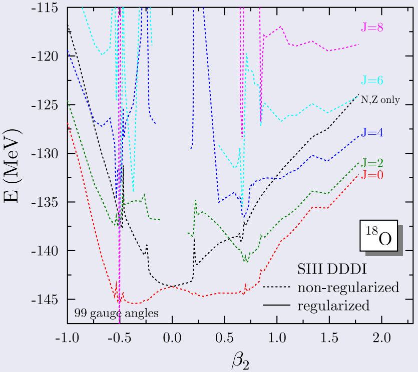
$$E_{\mathrm{REG}}[g',g] \equiv E[\rho^{g'g},\kappa^{g'g},\kappa^{gg'*}] - E^{\mathrm{C}}[g',g]$$

The method is originally designed

- For any MR mixing, i.e. any $|g|$ and α
- For polynomial kernels only

[T. Duguet *et al.*, PRC79 (2009) 044320]

Unregularized $\mathcal{E}_{\mathrm{N,Z,J}}$ for $E \propto A\rho + B\rho\rho + C\rho\kappa^*\kappa$



[M. Bender *et al.*, unpublished]

Unregularized results

- ✘ display steps and divergences
- ✘ strongly depend on the discretization
- ✘ provide $\mathcal{E}_{\mathrm{N,Z,J}}\,\mathcal{N}_{\mathrm{N,Z,J}} \neq 0$ for $\mathrm{N,Z} \leq 0$

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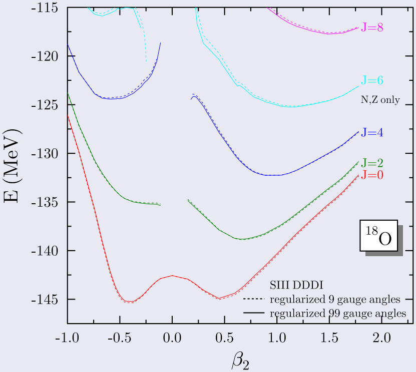

[M. Bender *et al.*, unpublished]

Regularized results

- ✔ are free from steps and divergences
- ✘ slowly depend on the discretization
- ✘ provide $\mathcal{E}_{\mathrm{N,Z,J}}\,\mathcal{N}_{\mathrm{N,Z,J}} \neq 0$ for $\mathrm{N,Z} \leq 0$

Towards sound Multi-Reference EDF calculations

Regularization method

[D. Lacroix, T. Duguet, M. Bender, PRC79 (2009) 044318]

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The method is originally designed

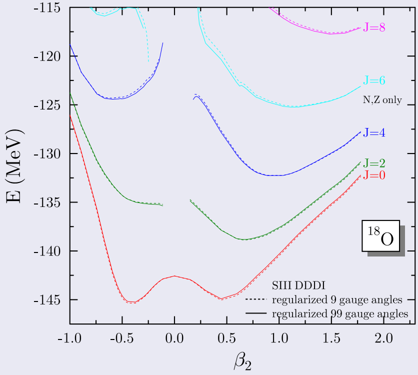
- For any MR mixing, i.e. any $|g|$ and α
- For polynomial kernels only

[T. Duguet *et al.*, PRC79 (2009) 044320]

Alternative route ahead [J. Sadoudi *et al.*, unpublished]

- Rely strictly on $\mathcal{H}$-based kernel
- Challenge to obtain good phenomenology
- New kernel under construction

Regularized $\mathcal{E}_{\rm N,Z,J}$ for $E \propto A\rho + B\rho\rho + C\rho\kappa^*\kappa$



[M. Bender *et al.*, unpublished]

Regularized results

- are free from steps and divergences
- slowly depend on the discretization
- provide $\mathcal{E}_{\rm N,Z,J}\, \mathcal{N}_{\rm N,Z,J} \neq 0$ for $\rm N,Z \leq 0$

Outline

Summary and perspectives

Multi-reference nuclear energy density functional formalism

- Mathematically well formulated without any reference to H and $|\Psi_n^{X_{\mathcal{G}}}\rangle$
- Physical constraints need to be added that are not easy to formulate
- New regularization method
  1. Improves the situation dramatically
  2. Is not free from all problems

Way(s) out?

1. Employ approximations (QRPA, Bohr Hamiltonian...) that "bypass" the problem
2. Rely strictly on $\mathcal{H}$-based kernel, i.e. work within effective projected HFB method
3. Design off-diagonal energy kernel from appropriate ab-initio method
   - Symmetry-restored unrestricted MBPT [T. Duguet, G. Ripka, unpublished]
   - Leads to and angle-dependent/orbital-dependent energy kernel
4. Else? E.g. see talk by T. Lesinski (Friday)

Symmetry dilemma in DFT

What about symmetries in DFT?

- Symmetry group $\mathcal{G}$ of H and lowest eigenstate $|\Psi_i^{PJMN\dots}\rangle$ of given irrep
  1. $\rho_\sigma(\vec{r})$ is not a scalar of $\mathcal{G}$ (except for $\hat{N}$)
  2. $v_{KS}^{\sigma}(\vec{r})$ is not a scalar of $\mathcal{G}$
  3. $\{\varphi_\alpha\}$ do not carry quantum numbers $l, j, m \dots$
  4. Kohn-Sham state $|\Phi_i\rangle$ is not an eigenstate of $\hat{\vec{P}}$, $\hat{J}^2 \dots$

Crucial points about symmetries

- At the minimum of E $\rho_\sigma(\vec{r})$ must reflect quantum numbers of $|\Psi_i^{PJMN\dots}\rangle$
  - Symmetry breaking is outside the frame of Hohenberg-Kohn theorem
- Kohn-Sham state $|\Phi_i\rangle$ should not carry quantum numbers of $|\Psi_i^{PJMN\dots}\rangle$
  - How to maintain the symmetry content of $\rho_\sigma(\vec{r})$ through the iterations?

Solution to symmetry dilemma

Symmetrized DFT

- Keep $|\Phi_i^{PJMN\dots}\rangle$ with same quantum numbers as eigenstate
- HK theorem + KS scheme in terms of the scalar part of the density
- A. Görling, PRA 47 (1993) 2783

Symmetry-constrained DFT

- Focus on symmetries of $\rho_\sigma(\vec{r})$ rather than of $|\Phi_i\rangle$
- Use non-scalar $v_\sigma^{KS}(\vec{r})$ + constrained minimization on $\rho_\sigma(\vec{r})$
- H. Fertig, W. Kohn, PRA 62 (2000) 052511

Ensemble DFT

- Symmetry-preserving statistical density operator built from $|\Phi_i\rangle$
- HK theorem + KS scheme based on scalar ensemble density
- E. K. U. Gross, L. N. Oliveira, W. Kohn, PRA 37 (1988) 2809