Breaking and restoring symmetries within the energy density functional

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Outline

1. Introduction
   - Breaking symmetries
2. Wave-function methods
   - Symmetry unrestricted Hartree-Fock
   - Projection methods
3. Energy Density Functional methods
   - Ingredients of the EDF method
4. Pathologies
   - Particle number restoration
   - Angular momentum restoration
5. Conclusion

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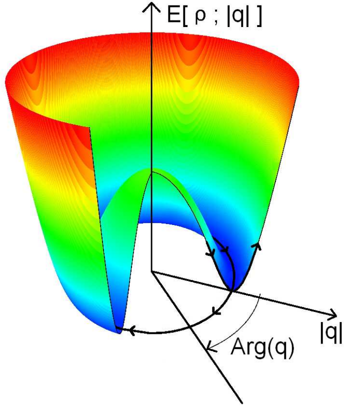
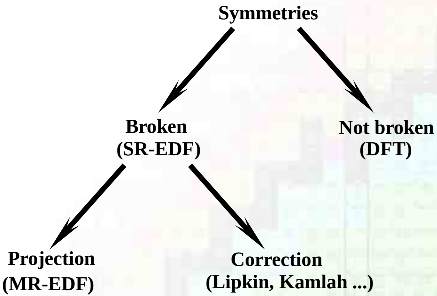
Context

1. Two-step nuclear EDF method (i) single-reference (ii) multi-reference
2. Built by analogy with wave-function based methods
3. SR-EDF has both similarities and differences with DFT
4. Strongly relies on spontaneous symmetry breaking and restoration





Outline

Symmetry unrestricted Hartree-Fock-Bogoliubov

Hartree-Fock-Bogoliubov approximation

1. Approx. of indep. QP w.f. $|\Psi^N\rangle \simeq |\Phi\rangle = \prod_i \beta_i|0\rangle$, U_{ji}, V_{ji} are to be determined
2. HFB Energy : $E^{HFB} = \frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} \Rightarrow$ SWT $\Rightarrow E^{HFB} = E[\rho,\kappa,\kappa^*]$
3. Variational principle : $\delta\Big(E[\rho,\kappa,\kappa^*] + \text{constraints}\Big) = 0$ gives HFB equations

Hamiltonian, QP operators and densities

- QP annihilation operator : $\beta_i = \sum_j U^*_{ij} a_j + V^*_{ij} a^\dagger_j$
- Hamiltonian (in "2nd quantization") : $H = \sum_{ij} t_{ij}\, c^\dagger_i c_j + \frac{1}{2}\sum_{ijkl} \bar{v}_{ijkl}\, c^\dagger_i c^\dagger_j c_k c_l$
- Normal and anormal density matrices are defined as

$$\rho_{ij} = \frac{\langle\Phi|c^\dagger_j c_i|\Phi\rangle}{\langle\Phi|\Phi\rangle} \quad , \quad \kappa_{ij} = \frac{\langle\Phi|c_j c_i|\Phi\rangle}{\langle\Phi|\Phi\rangle}$$

Symmetry unrestricted Hartree-Fock-Bogoliubov

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Symmetry breaking context

- Symmetries S of the Hamiltonian $\rightarrow [H, S] = 0$
- Densities (wave-function) are allowed to break symmetries to minimize the energy
  - Static collective correlation
- Symmetries broken example : translational, rotational, particule number invariance
- Symmetries need to be restored thanks to projection method
  - Dynamical collective correlation

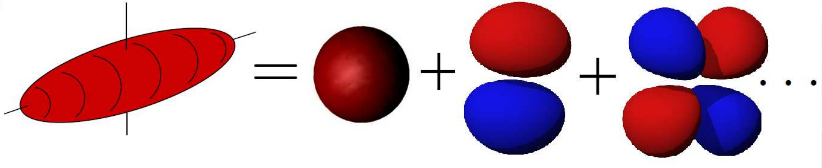
Breaking symmetries in mean field methods

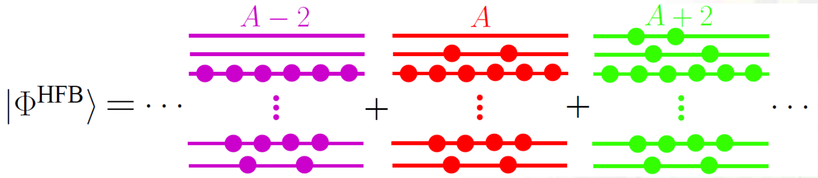
Rotation invariance

- Angular correlations
- Quadrupole component
- Rotational band

Particle number invariance

- Pairing correlations
- S-wave attraction
- Gap, OEMS, moment of inertia, ...





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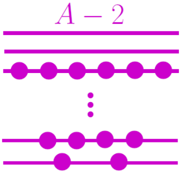
$$|\Psi^{L=0M}\rangle =$$

$$|\Psi^{A\text{-}2}\rangle =$$



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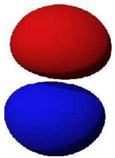
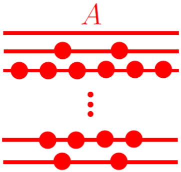
$$|\Psi^{L=1M}\rangle =$$



$$|\Psi^{A}\rangle =$$



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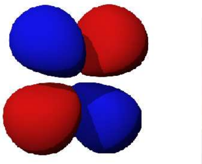
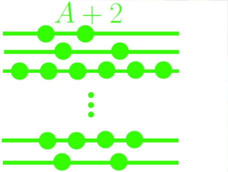
$$|\Psi^{L=2M}\rangle =$$



$$|\Psi^{A+2}\rangle =$$



Projection method

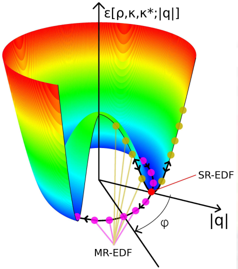
General case

1. Symmetry breaking state $|\Phi\rangle = \sum_{\lambda a} c_{\lambda a} |\Psi_a^\lambda\rangle$
2. Projected state/energy is obtained thanks to

$$|\Psi_a^\lambda\rangle = \frac{1}{c_{\lambda b}} \frac{d_\lambda}{v_\mathcal{G}} \int_\mathcal{G} dm(g) S_{ab}^{\lambda *}(g) R(g) |\Phi\rangle$$

$$E^\lambda = \frac{1}{c_{\lambda b}^* c_{\lambda a}} \frac{d_\lambda}{v_\mathcal{G}} \int_\mathcal{G} dm(g) S_{ab}^{\lambda *}(g) \langle\Phi| H R(g) |\Phi\rangle$$

3. Can be proved using
   - $\langle\Psi_a^\lambda| R(g) |\Psi_b^{\lambda'}\rangle = S_{ab}^\lambda(g)\delta_{\lambda\lambda'}$
   - $\int_\mathcal{G} dm(g) S_{ab}^{\lambda *}(g) S_{a'b'}^{\lambda'}(g) = \frac{v_\mathcal{G}}{d_\lambda}\delta_{\lambda\lambda'}\delta_{aa'}\delta_{bb'}$



- Using Generalized Wick Theorem : $\langle\Phi^0|H|\Phi^g\rangle = E[\rho^{0g}, \kappa^{0g}, \kappa^{g0*}]\langle\Phi^0|\Phi^g\rangle$
- $E[\rho^{0g}, \kappa^{0g}, \kappa^{g0*}]$ is the same functional but of transition density matrices

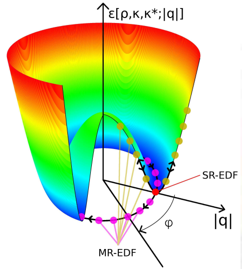
Projection method

Particle-number restoration

1. Symmetry breaking state $|\Phi\rangle = \sum_N c_N |\Psi^N\rangle$
2. Projected state/energy is obtained thanks to

$$|\Psi^A\rangle = \frac{1}{c_A}\frac{1}{2\pi}\int d\varphi e^{iA\varphi} e^{i\hat{N}\varphi}|\Phi\rangle$$
$$E^A = \frac{1}{c_A^* c_A}\frac{1}{2\pi}\int d\varphi\, e^{-iA\varphi}\langle\Phi|H e^{i\hat{N}\varphi}|\Phi\rangle$$

3. Can be proved using
   - $\langle\Psi^A|e^{i\hat{N}\varphi}|\Psi^{A'}\rangle = e^{iA\varphi}\delta_{AA'}$
   - $\int d\varphi e^{-iA\varphi} e^{iA'\varphi} = 2\pi\delta_{AA'}$



- Using Generalized Wick Theorem : $\langle\Phi^0|H|\Phi^\varphi\rangle = E[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi 0*}]\langle\Phi^0|\Phi^\varphi\rangle$
- $E[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi 0*}]$ is the same functional but of transition density matrices

Projection method

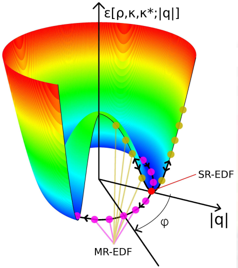
Angular-momentum restoration

1. Symmetry breaking state $|\Phi\rangle = \sum_{lm} c_{lm}|\Psi^l_m\rangle$
2. Projected state/energy is obtained thanks to

$$|\Psi^l_m\rangle = \frac{1}{c_{lk}}\frac{2l+1}{8\pi^2}\int d\Omega D^{l*}_{mk}(\Omega)R(\Omega)|\Phi\rangle$$

$$E^l = \frac{1}{c^*_{lk}c_{lm}}\frac{2l+1}{8\pi^2}\int d\Omega D^{l*}_{mk}(\Omega)\langle\Phi|HR(\Omega)|\Phi\rangle$$

3. Can be proved using
   - $\langle\Psi^l_m|R(\Omega)|\Psi^{l'}_k\rangle = D^l_{mk}(\Omega)\delta_{ll'}$
   - $\int d\Omega D^{l*}_{mk}(\Omega)D^{l'}_{m'k'}(\Omega) = \frac{8\pi^2}{2l+1}\delta_{ll'}\delta_{mm'}\delta_{kk'}$



- Using Generalized Wick Theorem : $\langle\Phi^0|H|\Phi^\Omega\rangle = E[\rho^{0\Omega},\kappa^{0\Omega},\kappa^{\Omega 0*}]\langle\Phi^0|\Phi^\Omega\rangle$
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Ingredients of the EDF method

Two-level variational wave-function method

1^{st} level: HFB	2^{nd} level: projected HFB
Trial WF : $\lvert\Phi_0\rangle = \prod_\mu \beta_\mu \lvert 0\rangle$ Sym. break. $q = \lvert q\rvert e^{ig} \neq 0$	Trial WF: $\lvert\Psi_a^\lambda\rangle = \frac{1}{c_{\lambda b}} \frac{d_\lambda}{v_{\mathcal{G}}} \int_{\mathcal{G}} dm(g) S_{ab}^{\lambda *}(g) R(g) \lvert\Phi_0\rangle$ Sym. restor.
$E_{\lvert q\rvert}^{1^{\mathrm{st}}} = \langle\Phi_0\lvert H\rvert\Phi_0\rangle$ $\Downarrow$ Standard Wick Theorem $\Downarrow$ $\langle\Phi_0\lvert H\rvert\Phi_0\rangle = E[\rho, \kappa, \kappa^*]$	$E_\lambda^{2^{\mathrm{nd}}} = \langle\Phi_0\lvert H\rvert\Psi_a^\lambda\rangle = \frac{1}{c_{\lambda b}^* c_{\lambda a}} \frac{d_\lambda}{v_{\mathcal{G}}} \int_{\mathcal{G}} dm(g) S_{ab}^{\lambda *}(g) \langle\Phi_0\lvert H\rvert\Phi_g\rangle$ $\Downarrow$ Generalized Wick Theorem $\Downarrow$ $\langle\Phi_0\lvert H\rvert\Phi_g\rangle = E[\rho^{0g}, \kappa^{0g}, \kappa^{g0\,*}]\,\langle\Phi_0\lvert\Phi_g\rangle$

Ingredients of the EDF method

Two-level energy density functional method

1^{st} **level: single-reference**	2^{nd} **level: multi-reference**
Trial state $\vert\Phi_0\rangle = \prod_\mu \beta_\mu \vert 0\rangle$	Trial **set of states** $\{\vert\Phi_g\rangle \equiv R(g)\vert\Phi_0\rangle; g \in v_{\mathcal{G}}\} \neq \vert\Psi_a^\lambda\rangle$
Sym. break. $q = \vert q\vert e^{i\varphi} \neq 0$	Sym. restor.
$\mathcal{E}_{\vert q\vert}^{\text{SR}} \equiv \mathcal{E}[\rho, \kappa, \kappa^*]$	$\mathcal{E}^\lambda \equiv \frac{1}{c_{\lambda b}^* c_{\lambda a}} \frac{d_\lambda}{v_{\mathcal{G}}} \int_{\mathcal{G}} dm(g) S_{ab}^{\lambda *}(g) \mathcal{E}[\rho^{0g}, \kappa^{0g}, \kappa^{g0\,*}] \langle\Phi_0\vert\Phi_g\rangle$ $\mathcal{E}^\lambda \neq \langle\Phi_0\vert H\vert\Psi_a^\lambda\rangle$

Bulk of correlations resummed into $\mathcal{E}[\rho^{0g}, \kappa^{0g}, \kappa^{g0\,*}]$

Ingredients of the EDF method

Two-level energy density functional method

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Trial state $\|\Phi_0\rangle = \prod_\mu \beta_\mu \|0\rangle$	Trial **set of states** $\{\|\Phi_g\rangle \equiv R(g)\|\Phi_0\rangle; g \in v_{\mathcal{G}}\} \neq \|\Psi_a^\lambda\rangle$
	$\mathcal{E}^\lambda \neq \langle\Phi_0\|H\|\Psi_a^\lambda\rangle$

Relevant questions

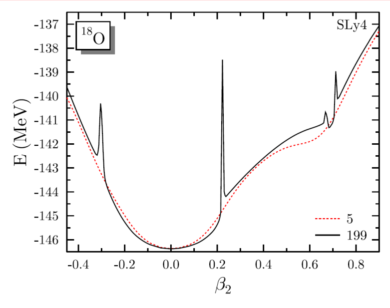
1. Is the WF→EDF mapping efficient? Is it safe? How is it constrained?
2. Is the GWT-inspired mapping $\mathcal{E}[\rho^{0g}, \kappa^{0g}, \kappa^{g0\,*}]$ appropriate?

Bulk of correlations resummed into $\mathcal{E}[\rho^{0g}, \kappa^{0g}, \kappa^{g0\,*}]$

Outline

Particle number restoration pathologies

$\mathcal{E}^{MR}_{Z=8,N=10}$ vs ρ_{20} for $\mathcal{E}[\rho\rho\rho^{1/6}]$



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

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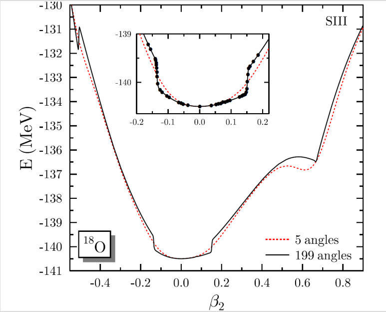

[M. Bender, T. Duguet, D. Lacroix, PRC79 (2009) 044319]

1. Divergencies and finite steps [J. Dobaczewski *et al.*, PRC76 (2007) 054315]
2. GWT-inspired $\mathcal{E}[\rho^{0g}, \kappa^{0g}, \kappa^{g0\,*}]$ unsafe in EDF context
3. Originates from self interaction and self pairing in the EDF kernel

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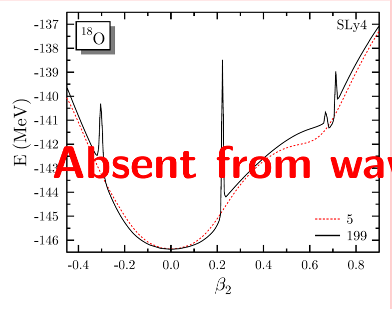

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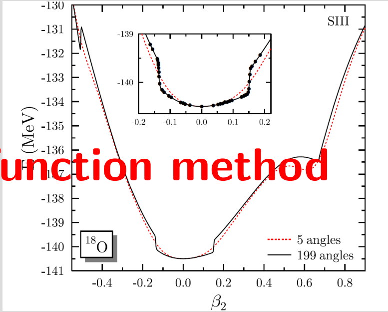

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Absent from wave-function method

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2. GWT-inspired $\mathcal{E}[\rho^{0g}, \kappa^{0g}, \kappa^{g0\,*}]$ unsafe in EDF context
3. Originates from self interaction and self pairing in the EDF kernel

Particle number restoration pathologies

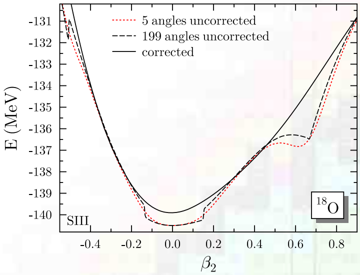
- The Fourier decomposition of MR kernel on $U(1)$ Irreps reads

$$\mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0\,*}]\,\langle \Phi_0 | \Phi_\varphi \rangle \quad = \quad \sum_{A \in \mathbb{Z}} c_A^2 \; \mathcal{E}_A^{MR} \; e^{iA\varphi}$$

- $\mathcal{E}_A^{MR} \neq 0$ for $A \leq 0$!! [M. Bender, T. Duguet, D. Lacroix, PRC79 (2009) 044319]

Regularized PNR calculations

1. $\mathcal{E}_{REG} \equiv \mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0\,*}] - \mathcal{E}_C[\langle \Phi_0 |; | \Phi_\varphi \rangle]$
2. $\mathcal{E}_A^{MR}$ is free from divergencies/steps
3. $\mathcal{E}_A^{MR} = 0$ for $A \leq 0$
4. Depends on the quadrupole deformation
5. Crucial at critical points and *away* from them
6. On the MeV scale = mass accuracy



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Regularized PNR calculations

Fourier coefficients

Can we find math. properties from w.f. methods that may not be respected by EDFs ?

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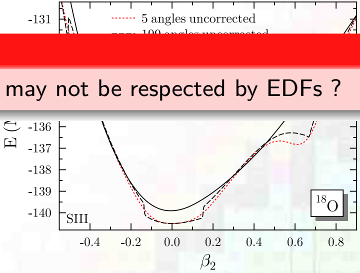

[M. Bender *et al.* PRC79 (2009) 044319]

Angular momentum restoration

- The "Fourier" decomposition of MR kernel on $SO(3)$ Irreps reads

$$\mathcal{E}[\rho^{0\Omega}, \kappa^{0\Omega}, \kappa^{\Omega 0\,*}]\,\langle\Phi_0|\Phi_\Omega\rangle \quad = \quad \sum_{lmk} c^*_{lm} c_{lk}\; D^l_{mk}(\Omega)\; \mathcal{E}^l$$

Wave-function methods : angular-momentum-restored energy

- After "tedious but straightforward calculations"

$$E^l \quad = \quad \frac{1}{2}\int d\vec{R}d\vec{r}\, V(r)\, \rho^{[2]}_{lmlm}(\vec{R},\vec{r}) = \int d\vec{R} \sum_{l'=0}^{2l} \mathcal{V}^{l'0}_l(R)\;\; C^{lm}_{lml'0} Y^0_{l'}(\hat{R})$$

- Mathematical property of the angular-momentum-restored density energy

EDF methods : angular-momentum-restored MR energy

- After "tedious but ... calculation"

$$\mathcal{E}^l \quad = \quad \int d\vec{R} \sum_{l'=0}^{??} \mathcal{E}^{l'??}_l(R)\; Y^{??}_{l'}(\hat{R})$$

T. Duguet, J. Sadoudi : arXiv:1001.0673v2

Outline

Conclusions

Constraints on EDF

- Open up new path towards constraining MR-EDF calculations [T. Duguet, J. Sadoudi : arXiv:1001.0673v2]
- Find constrains for a bilinear Skyrme like EDF
- Find constrains for a general Skyrme like EDF