Multi-reference Energy Density Functional method Constraints from consistency requirements

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Nuclear Physics Workshop, Sept. 22-26, 2010, Kazimierz Dolny, Poland



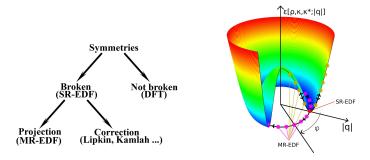


- Introduction
 - Differences between wave-function and EDF methods
- Constraining the MR-EDF method
 - \bullet Basic consistency requirements
 - Unexpected pathologies
 - Regularization method
 - New constraints?
- Perspectives

Talk in one slide

Context

- Two-step nuclear EDF method (i) single-reference (ii) multi-reference
- Built by analogy with wave-function based methods (no existence theorem)
- SR-EDF has both similarities and differences with (standard) DFT
- Strongly relies on spontaneous symmetry breaking (SR) and restoration (MR)



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- Built by analogy with wave-function based methods (no existence theorem)
- SR-EDF has both similarities and differences with (standard) DFT
- Strongly relies on spontaneous symmetry breaking (SR) and restoration (MR)

Take-away message

- MR-EDF tackles long-range fluctuations and accesses collective excitations
- MR-EDF calculations must be constrained through consistency requirements

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Two-level variational wave-function method

1^{st}	level:	HFB	

2^{nd} level: projected HFB + GCM

Trial WF:
$$|\Phi_q\rangle = \prod_{\mu} \beta_{\mu}^q |0\rangle$$

Trial WF:
$$|\Psi\rangle=\sum_q f_q |\Phi_q\rangle=\sum_{|\,q\,|} g_{|\,q\,|} P_X |\Phi_{|\,q\,|}\rangle$$

Sym. break.
$$q = |q|e^{i\varphi} \neq 0$$

Sym. restor. (\sum_{α}) and zero-point fluct. $(\sum_{|\alpha|})$

$$[\mathbf{X},\mathbf{H}] = \mathbf{0} \ \mathbf{for} \ \{\mathbf{X}\} = \{\mathbf{N},\mathbf{Z},\mathbf{P},\mathbf{J^2},\mathbf{J_z},\mathbf{T^2},\mathbf{T_z},\mathcal{T^2}\}$$

Static collective correlations

Dynamical collective correlations

$$E_{|q|}^{1^{\rm st}} = \langle \Phi_q | H | \Phi_q \rangle$$

Standard Wick Theorem

 $\mathbf{E}_{|\mathbf{q}|}^{1^{\mathrm{st}}}$ is a functional of diagonal density matrices ρ^{qq} , κ^{qq} and κ^{qq*}

$$E_X^{2^{\mathrm{nd}}} = \langle \Psi | H | \Psi \rangle = \sum_{\substack{qq'}} f_q^* f_{q'} \langle \Phi_q | H | \Phi_{q'} \rangle$$

Generalized Wick Theorem

$$\langle \Phi_q | H | \Phi_{q'} \rangle = E[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}] \langle \Phi_q | \Phi_{q'} \rangle$$

 $\mathbf{E}_{\mathbf{x}}^{2^{\mathrm{nd}}}$ invokes the SAME functional of (all) transition density matrices $\rho^{qq'}$. $\kappa^{qq'}$ and $\kappa^{q'q*}$

Ingredients of the nuclear EDF method

Two-level energy density functional method

1 st level: single-reference	$2^{ ext{nd}}$ level: multi-reference			
Trial state $ \Phi_q\rangle = \prod_{\mu} \beta_{\mu}^q 0\rangle$	Trial set of states $\{ \Phi_q\rangle\} \neq \Psi\rangle$			
Sym. break. $q = q e^{i\varphi} \neq 0$	Sym. restor. (\sum_{φ}) and zero-point fluct. $(\sum_{ q })$			
$[\mathbf{X},\mathbf{H}] = 0 \ \mathbf{for} \ \{\mathbf{X}\} = \{\mathbf{N},\mathbf{Z},\mathbf{P},\mathbf{J^2},\mathbf{J_z},\mathbf{T^2},\mathbf{T_z},\mathcal{T^2}\}$				
Static collective correlations	Dynamical collective correlations			
$\mathcal{E}_{ q }^{\mathrm{SR}} \equiv \mathcal{E}[\Phi_q; \Phi_q] \neq \langle \Phi_q H \Phi_q \rangle$	$\mathcal{E}_{X}^{\mathrm{MR}} \equiv \sum_{qq'} f_{q}^{*} f_{q'} \mathcal{E}[\Phi_{q}; \Phi_{q'}] \langle \Phi_{q} \Phi_{q'} \rangle \neq \langle \Psi H \Psi \rangle$			
Bulk of correlations resummed into $\mathcal{E}[\Phi_q;\Phi_{q'}] \equiv \mathcal{E}[\rho^{qq'},\kappa^{qq'},\kappa^{q'q*}]$				
$\delta\bigg[\mathcal{E}^{\mathrm{SR}} - \lambda \mathrm{Tr}\{\rho\} - \lambda^{ \mathbf{q} } \mathrm{Tr}\{\rho \mathbf{Q}\}\bigg] = 0$	$\delta\mathcal{E}_{\mathbf{X}}^{\mathrm{MR}}/\delta\mathbf{f}_{\mathbf{q}}^{*}=0$			

Hill-Wheeler-Griffin-like equations

HFB-like equations

Ingredients of the nuclear EDF method

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Relevant questions

- Is the WF→EDF mapping efficient? Is it safe? How is it constrained?
- **②** Is the GWT-inspired mapping $\mathcal{E}[\Phi_q; \Phi_{q'}] \equiv \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}]$ appropriate?

$$\begin{array}{ccc} \mathcal{E}_{|q|}^{\text{on}} \equiv \mathcal{E}[\Phi_q;\Phi_q] \neq \langle \Phi_q | H | \Phi_q \rangle & & & & & \\ \mathcal{E}_X^{\text{nin}} \equiv \sum_{qq'} f_q^* f_{q'} \, \mathcal{E}[\Phi_q;\Phi_{q'}] \, \langle \Phi_q | \Phi_{q'} \rangle \neq \langle \Psi | H | \Psi \rangle \end{array}$$

Bulk of correlations resummed into $\mathcal{E}[\Phi_q; \Phi_{q'}] \equiv \mathcal{E}[\rho^{qq'}, \kappa^{qq'}, \kappa^{q'q*}]$

$$\begin{split} \delta \bigg[\mathcal{E}^{\mathrm{SR}} - \lambda \mathrm{Tr}\{\rho\} - \lambda^{|\mathbf{q}|} \mathrm{Tr}\{\rho \mathbf{Q}\} \bigg] &= \mathbf{0} \\ & \downarrow \\ \mathbf{HFB\text{-like equations}} \end{split}$$

$$\delta \mathcal{E}_{\mathbf{X}}^{\mathrm{MR}}/\delta \mathbf{f}_{\mathbf{q}}^{*} = \mathbf{0}$$

Hill-Wheeler-Griffin-like equations

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Set of constraints from consistency requirements

SR-EDF

[J. Dobaczewski, J. Dudek, APP B27 (1996) 45]

- $\mathcal{E}_{|q|}^{SR}$ must be real and a scalar under all $\mathcal{R}(g) \in \text{symmetry group } \mathcal{G}$
- Example: rules to build local Skyrme EDF to 2^{nd} order in σ_{ν} and ∇

$$\mathcal{E}[\rho,\kappa,\kappa^*] \equiv \int d\vec{r} \, \mathcal{E}[\rho_T(\vec{r}),\tau_T(\vec{r}),J_{T,\mu\nu}(\vec{r}),\vec{s}_T(\vec{r}),\vec{j}_T(\vec{r}),\vec{T}_T(\vec{r}),\vec{F}_T(\vec{r}),\tilde{\rho}_T(\vec{r});\nabla]$$

MR-EDF

[L. Robledo, IJMP E16 (2007) 337; JPG 37 (2010) in press]

- $oldsymbol{\odot} \mathcal{E}_X^{\mathrm{MR}}$ must be real and a scalar under all $\mathcal{R}(g) \in \mathrm{symmetry}$ group \mathcal{G}
- Occupance of MR and SR schemes
 - $\bullet \ \mathcal{E}_X^{\mathrm{MR}} = \mathcal{E}_{|q|}^{\mathrm{SR}} \text{ when } \{|\Phi_q\rangle\} \longrightarrow |\Phi_q\rangle$
 - **9** Chemical potential λ must be recovered from Kamlah expansion of $\mathcal{E}_N^{\mathrm{MR}}$
 - **QRPA** must be recovered through harmonic limit of $\mathcal{E}_X^{\mathrm{MR}}$

Extension to MR kernel must implicate transition densities only

Diagonal SR kernel $\mathcal{E}[\rho^{qq}, \kappa^{qq}, \kappa^{qq^*}]$

GWT-inspired connection (only) viable option?

Off-diagonal MR kernel $\mathcal{E}[
ho^{ ext{qq'}}, \kappa^{ ext{qq'}}, \kappa^{ ext{q'q}*}]$

Set of constraints from consistency requirements

SR-EDF

[J. Dobaczewski, J. Dudek, APP B27 (1996) 45]

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- Example: rules to build local Skyrme EDF to 2^{nd} order in σ_{ν} and ∇

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MR-EDF

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- ullet $\mathcal{E}_X^{\mathrm{MR}}$ must be real and a scalar under all $\mathcal{R}(g) \in \mathrm{symmetry}$ group \mathcal{G}
- Consistency of MR and SR schemes
 - $\mathcal{E}_X^{\mathrm{MR}} = \mathcal{E}_{|q|}^{\mathrm{SR}} \text{ when } \{|\Phi_q\rangle\} \longrightarrow |\Phi_q\rangle$
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Off-diagonal MR kernel $\mathcal{E}[\rho^{\mathbf{q}\mathbf{q}'}, \kappa^{\mathbf{q}\mathbf{q}'}, \kappa^{\mathbf{q}'\mathbf{q}*}]$

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Unexpected pathologies

Particle number restoration (PNR) as an example

- Select appropriate MR set $\{|\Phi_{\varphi}\rangle \equiv e^{i\hat{N}\varphi}|\Phi_{0}\rangle; \varphi \in [0,2\pi]\}$
- $\textbf{ ②} \ \, \text{Define non-diagonal MR kernel } \mathcal{E}[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi_0*}] \langle \Phi_0|\Phi_\varphi\rangle \,\, \text{from SR functional}$
- **3** Expand MR kernel in a Fourier series over U(1) Irreps

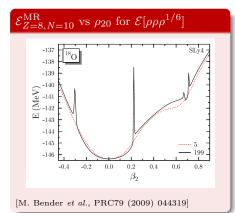
$$\mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi_0*}] \langle \Phi_0 | \Phi_{\varphi} \rangle = \sum_{N \in \mathbb{Z}} c_N^2 \, \mathcal{E}_N^{\mathrm{MR}} \, e^{iN\varphi}$$
$$\langle \Phi_0 | \Phi_{\varphi} \rangle = \sum_{N \in \mathbb{Z}} c_N^2 \, e^{iN\varphi}$$

to obtain real, scalar, particle-number-restored MR energies

$$\mathcal{E}_{N}^{\text{MR}} \equiv \int_{0}^{2\pi} d\varphi \frac{e^{-i\varphi N}}{2\pi c_{N}^{2}} \mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0} *] \langle \Phi_{0} | \Phi_{\varphi} \rangle$$

Compute... so far so good...

Unexpected pathologies

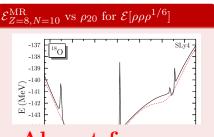


 $\mathcal{E}_{Z=8,N=10}^{\overline{\mathrm{MR}}} \text{ vs } \rho_{20} \text{ for } \mathcal{E}[\rho\rho\rho]$ -131-132-133-140 -134-135 -138 -139- 5 angles -140-141 -0.2 0.0 0.2 0.4 0.6 0.8

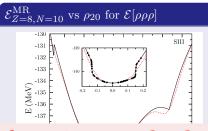
 $[{\rm M.~Bender}~et~al.,~{\rm PRC79}~(2009)~044319]$

- Divergencies and finite steps [J. Dobaczewski et al., PRC76 (2007) 054315]
- $\ \, \textbf{\o} \,$ Non-analyticity of $\mathcal{E}[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi 0\,*}]$ over $\mathbb{C}^*\text{-plane}$ with $e^{i\varphi}\equiv z$
- \bullet $\mathcal{E}_N^{\mathrm{MR}} \neq 0$ for $N \leq 0!!$ [M. Bender, T.D., D. Lacroix, PRC79 (2009) 044319]
- Similar problems for other MR modes, e.g. angular momentum restoration

Unexpected pathologies



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Absent from wave-function method

1-

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



 $[{\rm M.~Bender}~et~al.,~{\rm PRC79}~(2009)~044319]$

- ① Divergencies and finite steps [J. Dobaczewski et al., PRC76 (2007) 054315]
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Regularization method

Origin of the problem and its solution

- Alternative method to define $\mathcal{E}[\Phi_q;\Phi_{q'}]$ that relies on
 - Considering Bogoliubov transformation connecting $|\Phi_q\rangle$ to $|\Phi_{q'}\rangle$
 - Using Bloch-Messiah-Zumino decomposition to reach BCS-like connection

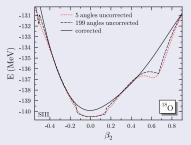
$$|\Phi_{q'}\rangle = \tilde{\mathcal{C}}_{qq'} \prod_{p>0} \left(\bar{A}_{pp}^* + \bar{B}_{p\bar{p}}^* \, \tilde{\alpha}_p^+ \, \tilde{\alpha}_{\bar{p}}^+ \right) |\Phi_q\rangle$$

- **3** Using SWT to compute $\langle \Phi_q | H | \Phi_{q'} \rangle / \langle \Phi_q | \Phi_{q'} \rangle$
- lacktriangle Extending to EDF disconnected from genuine operator H
- $\ \, \textbf{OWT-inspired} \,\, \mathcal{E}[\Phi_q;\Phi_{q'}] \equiv \mathcal{E}[\rho^{qq'},\kappa^{qq'},\kappa^{q'q*}] \,\, \textbf{unsafe in EDF context}$
 - Provides dangerous terms with weights that are zero with SWT
 - Such terms cancel for WF method but not for more general EDF
 - Originates from self interaction and self pairing in the EDF kernel

[D. Lacroix, T. D., M. Bender, PRC 79 (2009) 044318]

Regularized PNR calculations

- $\mathbb{E}_{REG}[\Phi_0; \Phi_{\varphi}] \equiv \mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0 *}] \mathcal{E}_{C}[\langle \Phi_0 | ; | \Phi_{\varphi} \rangle]$
 - lacktriangle Analytical over \mathbb{C}^*
 - $m{\Theta}$ $\mathcal{E}_N^{\mathrm{MR}}$ free from divergencies and steps while $\mathcal{E}_N^{\mathrm{MR}}=0$ for $N\leq 0$



- The correction
 - is crucial at critical points but also away from them
 - \bigcirc depends non-trivially on the quadrupole deformation ρ_{20}
 - is on the MeV scale = mass accuracy/spectroscopic scales

[M. Bender, T. D., D. Lacroix, PRC 79 (2009) 044319]

Regularization method

Regularized PNR calculations

- $\mathbb{E}_{REG}[\Phi_0; \Phi_{\varphi}] \equiv \mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0 *}] \mathcal{E}_{C}[\langle \Phi_0 | ; | \Phi_{\varphi} \rangle]$
 - \bullet Analytical over \mathbb{C}^*
 - \mathcal{E}_{N}^{MR} free from divergencies and steps while $\mathcal{E}_{N}^{MR} = 0$ for N < 0

Mathematical constraints from wave-function belonging to Irrep

- Physics tell us that $\mathcal{E}_N^{\mathrm{MR}} = 0$ for $N \leq 0$ in PNR
- **②** What about expansion coefficients for other symmetry groups $\mathcal{G} = \{R(g)\}$?

$$\mathcal{E}[\rho^{gg'}, \kappa^{gg'}, \kappa^{g'g*}] \langle \Phi_g | \Phi_{g'} \rangle = \sum_{\lambda ab} c_{\lambda a}^* c_{\lambda b} \, \mathcal{E}_{\lambda}^{MR} \, S_{ab}^{\lambda}(g - g')$$
$$\langle \Phi_g | \Phi_{g'} \rangle = \sum_{\lambda ab} c_{\lambda a}^* c_{\lambda b} \, S_{ab}^{\lambda}(g - g')$$

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Angular momentum restoration

Expansion of MR kernel over Irreps of SO(3)

$$\mathcal{E}[\rho^{0\Omega},\kappa^{0\Omega},\kappa^{\Omega\Omega*}] \left<\Phi_0|\Phi_\Omega\right> \quad = \quad \sum_{LMK} c_{LM}^* \, c_{LK} \,\, \mathcal{E}_L^{\mathrm{MR}} \,\, D_{MK}^L(\Omega)$$

Wave-function method

[T. D., J. Sadoudi, JPG 37 (2010) 064009

$$E_L^{\text{MR}} = \frac{1}{2} \int d\vec{R} \, d\vec{r} \, V(r) \, \rho_{LMLM}^{[2]}(\vec{R}, \vec{r}) = \int d\vec{R} \, \sum_{L'=0}^{2L} \mathcal{V}_L^{L'0}(R) \, C_{LML'0}^{LM} \, Y_{L'}^{0}(\hat{R})$$

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

EDF method

■ Properties of $\mathcal{E}[\rho^{0\Omega}, \kappa^{0\Omega}, \kappa^{\Omega 0}]$ needed to verify the above property?

$$\mathcal{E}_{L}^{\text{MR}} = \int d\vec{R} \sum_{L'=0}^{!} \mathcal{E}_{L}^{L'?}(R) Y_{L'}^{?}(\hat{R})$$

■ Unfinished calculation so far

Angular momentum restoration

Expansion of MR kernel over Irreps of SO(3)

$$\mathcal{E}[\rho^{0\Omega},\kappa^{0\Omega},\kappa^{\Omega\Omega}^{*}] \left\langle \Phi_{0} | \Phi_{\Omega} \right\rangle \quad = \quad \sum_{LMK} c_{LM}^{*} \, c_{LK} \, \, \mathcal{E}_{L}^{\text{MR}} \, D_{MK}^{L}(\Omega)$$

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$$\mathcal{E}_{L}^{\mathrm{MR}} = \int d\vec{R} \sum_{L'=0}^{?} \mathcal{E}_{L}^{L'?}(R) Y_{L'}^{?}(\hat{R})$$

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Expansion of MR kernel over Irreps of SO(3)

$$\mathcal{E}[\rho^{0\Omega}, \kappa^{0\Omega}, \kappa^{\Omega 0 *}] \langle \Phi_0 | \Phi_{\Omega} \rangle = \sum_{LMK} c_{LM}^* c_{LK} \; \mathcal{E}_L^{\text{MR}} \; D_{MK}^L(\Omega)$$

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[T. D., J. Sadoudi, JPG 37 (2010) 064009]

$$E_L^{\text{MR}} = \frac{1}{2} \int d\vec{R} \, d\vec{r} \, V(r) \, \rho_{LMLM}^{[2]}(\vec{R}, \vec{r}) = \int d\vec{R} \, \sum_{L'=0}^{2L} \mathcal{V}_L^{L'0}(R) \, C_{LML'0}^{LM} \, Y_{L'}^0(\hat{R})$$

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

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■ Properties of $\mathcal{E}[\rho^{0\Omega}, \kappa^{0\Omega}, \kappa^{\Omega 0}]$ needed to verify the above property?

$$\mathcal{E}_{L}^{\text{MR}} = \int d\vec{R} \sum_{L'=0}^{?} \mathcal{E}_{L}^{L'?}(R) \, \underline{Y_{L'}^?(\hat{R})}$$

■ Unfinished calculation so far

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Perspectives

To be done in the near future

- Build correctable EDF of the form $\mathcal{E}[\rho^n, (\kappa^* \kappa)^m]$
 - [J. Sadoudi, T. D., M. Bender, K. Bennaceur, in progress]
- Perform systematic regularized MR calculations for AMR and $\Delta \rho_{20}$ mixing [J. Sadoudi, M. Bender, T.D., D. Lacroix, in progress]
- Derive constraints on EDF kernel to satisfy AMR mathematical property [J. Sadoudi, T. D., in progress]
- Need a constructive framework for MR-EDF method

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Ingredients of the nuclear EDF method

Non-negligible differences between EDF and WF methods

- $\bullet \text{ Energy } E_{|q|}^{1^{\text{st}}} = \langle \Phi_q | T + V_{\text{skyrme}} | \Phi_q \rangle = E[\rho^{qq}, \kappa^{qq}, \kappa^{qq*}] \langle \Phi_q | \Phi_q \rangle$
- ② Replace $E[\rho^{qq}, \kappa^{qq}, \kappa^{qq*}]$ by $\mathcal{E}[\rho^{qq}, \kappa^{qq}, \kappa^{qq*}]$ to resum correlations

Skyrme average energy

$$\begin{split} E[\rho,\kappa,\kappa^*] &= \sum_{qq'} \int d^3r \left[\frac{C_{qq'}^{\rho\rho}}{c_{qq'}^{\rho}} \rho_q \rho_{q'} + \frac{C_{qq'}^{\rho\Delta\rho}}{c_{qq'}^{\rho}} \rho_q \Delta \rho_{q'} + \frac{C_{qq'}^{\rho\tau}}{c_{qq'}^{\rho}} \left(\rho_q \tau_{q'} - \vec{j}_q \cdot \vec{j}_{q'} \right) \right. \\ &+ C_{qq'}^{ss} \vec{s}_q \cdot \vec{s}_{q'} + C_{qq'}^{s\Delta s} \vec{s}_q \cdot \Delta \vec{s}_{q'} + C_{qq'}^{\rho\nabla J} \left(\rho_q \vec{\nabla} \cdot \vec{J}_{q'} + \vec{j}_q \cdot \vec{\nabla} \times \vec{s}_{q'} \right) \\ &+ C_{qq'}^{\nabla s\nabla s} \left(\nabla \cdot \vec{s}_q \right) (\nabla \cdot \vec{s}_{q'}) + C_{qq'}^{JJ} \left(\sum_{\mu\nu} J_{q,\mu\nu} J_{q',\mu\nu} - \vec{s}_q \cdot \vec{T}_{q'} \right) \\ &+ C^{J\bar{J}} \left(\sum_{\mu} J_{q,\mu\mu} \sum_{\mu} J_{q,\mu\mu} + \sum_{\mu\nu} J_{q,\mu\nu} J_{q,\nu\mu} - 2 \vec{s}_q \cdot \vec{F}_q \right) \right] \\ &+ \sum_{q} \int d^3r \left[C_{qq}^{\tilde{\rho}\tilde{\rho}} |\tilde{\rho}_q|^2 + \dots \right] + \sum_{q} \int d^3r \frac{\hbar^2}{2m} \tau_q \end{split}$$

Ingredients of the nuclear EDF method

Non-negligible differences between EDF and WF methods

- Energy $E_{|q|}^{1^{\text{st}}} = \langle \Phi_q | T + V_{\text{skyrme}} | \Phi_q \rangle = E[\rho^{qq}, \kappa^{qq}, \kappa^{qq*}] \langle \Phi_q | \Phi_q \rangle$
- **2** Replace $E[\rho^{qq}, \kappa^{qq}, \kappa^{qq*}]$ by $\mathcal{E}[\rho^{qq}, \kappa^{qq}, \kappa^{qq*}]$ to resum correlations

Skyrme energy density functional

$$\mathcal{E}[\rho, \kappa, \kappa^*] = \sum_{qq'} \int d^3r \left[C_{qq'}^{\rho\rho} \rho_q \rho_{q'} + C_{qq'}^{\rho\Delta\rho} \rho_q \Delta \rho_{q'} + C_{qq'}^{\rho\tau} \left(\rho_q \tau_{q'} - \vec{j}_q \cdot \vec{j}_{q'} \right) \right.$$

$$\left. + C_{qq'}^{ss} \vec{s}_q \cdot \vec{s}_{q'} + C_{qq'}^{s\Delta s} \vec{s}_q \cdot \Delta \vec{s}_{q'} + C_{qq'}^{\rho\nabla J} \left(\rho_q \vec{\nabla} \cdot \vec{J}_{q'} + \vec{j}_q \cdot \vec{\nabla} \times \vec{s}_{q'} \right) \right.$$

$$\left. + C_{qq'}^{\nabla s\nabla s} \left(\nabla \cdot \vec{s}_q \right) (\nabla \cdot \vec{s}_{q'}) + C_{qq'}^{JJ} \left(\sum_{\mu\nu} J_{q,\mu\nu} J_{q',\mu\nu} - \vec{s}_q \cdot \vec{T}_{q'} \right) \right.$$

$$\left. + C_{qq'}^{J\bar{J}} \left(\sum_{\mu} J_{q,\mu\mu} \sum_{\mu} J_{q,\mu\mu} + \sum_{\mu\nu} J_{q,\mu\nu} J_{q,\nu\mu} - 2 \vec{s}_q \cdot \vec{F}_q \right) \right] \right.$$

$$\left. + \sum_{q} \int d^3r \left[C_{qq}^{\tilde{\rho}\tilde{\rho}} |\tilde{\rho}_q|^2 + \dots \right] + \sum_{q} \int d^3r \frac{\hbar^2}{2m} \tau_q \right.$$

Link with QRPA

QRPA from Time-Dependent SR-EDF calculations

1 Adiabatic-type scheme (omitting anomalous densities κ)

$$A_{minj} = (\epsilon_m - \epsilon_i) \, \delta_{mn} \, \delta_{ij} + \frac{\partial^2 \mathcal{E}[\rho]}{\partial \rho_{im} \partial \rho_{nj}} \quad ; \quad B_{minj} = \frac{\partial^2 \mathcal{E}[\rho]}{\partial \rho_{im} \partial \rho_{jn}}$$

Extensions (e.g. second RPA...) needed to access spreading width

QRPA from Projection+GCM in WF method

QRPA (WF)

$$A_{minj} = (\epsilon_m - \epsilon_i)\delta_{mn}\delta_{ij} + \bar{v}_{mjin}$$
 ; $B_{minj} = \bar{v}_{mnij}$

- QRPA (WF) is recovered from the harmonic limit of GCM (WF)
 [B. Jancovici, D. H. Schiff, NP58 (1964) 678]
 - Use Thouless parameterization $|\Phi_q\rangle = \exp[\sum_{im} z_{mi}^{q*} a_m^{\dagger} a_i] |\Phi_0\rangle$
 - \bigcirc Expand $\langle \Phi_q | H | \Phi_{q'} \rangle / \langle \Phi_q | \Phi_{q'} \rangle$ to second order in $\mathbf{z}^{\mathbf{q}} / \mathbf{z}^{\mathbf{q}'}$
 - \bigcirc Assume gaussian overlap $\langle \Phi_q | \Phi_{q'} \rangle \propto \exp[\text{Tr}(\mathbf{z}^{\mathbf{q}} \mathbf{z}^{\mathbf{q}'\dagger})]$
 - HFB + GCM can tackle large amplitude anharmonic collective motions

Link with QRPA

QRPA from Time-Dependent SR-EDF calculations

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Ground-state correlation energy associated with $X = J^2$

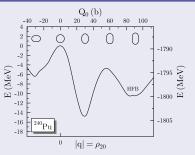
Collective coordinates = "Order parameter"

- |q| = multipole moments of $\rho(\vec{r})$
- $\mathbf{Q} \quad \varphi = \text{Euler angles } (\alpha, \beta, \gamma)$

From static deformation

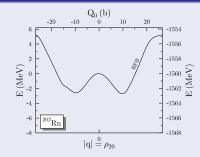
$$\Delta\mathcal{E}_{|q|_{\mathrm{min}}}^{\mathrm{SR}} = \mathrm{Min}_{|q|} \Big\{ \mathcal{E}_{|q|}^{\mathrm{SR}} \Big\} - \mathcal{E}_{0}^{\mathrm{SR}}$$

Well-deformed nucleus for $|q| = \rho_{20}$



[M. Bender, private communication]

Transitional nucleus for $|q| = \rho_{20}$



[M. Bender, private communication]

Ground-state correlation energy associated with $X = J^2$

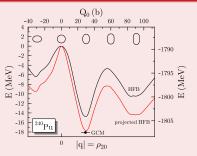
Collective coordinates = "Order parameter"

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- $\mathbf{Q} \quad \varphi = \text{Euler angles } (\alpha, \beta, \gamma)$

From dynamical fluctuations

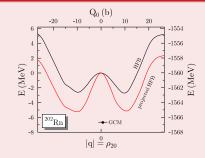
$$\Delta\mathcal{E}_{J=0}^{\mathrm{MR}} = \mathcal{E}_{J=0}^{\mathrm{MR}} - \mathrm{Min}_{|q|} \Big\{ \mathcal{E}_{|q|}^{\mathrm{SR}} \Big\}$$

Stiff nucleus for $|q| = \rho_{20}$



[M. Bender, private communication]

Soft nucleus for $|q| = \rho_{20}$

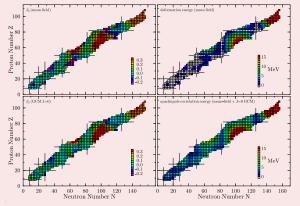


[M. Bender, private communication]

Ground-state correlation energy associated with $X = J^2$

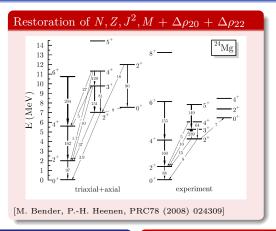
Systematic of quadrupole correlations: $\rho_{20} \neq 0 + J = 0 + \Delta \rho_{20}$

[M. Bender, G.-F. Bertsch, P.-H. Heenen, PRC73 (2006) 034322]



- Operation Deformation In Leavy Deformation Deformation In Leavy Deformation Deformation
- Right balance between open- and closed-shell nuclei from single EDF
- Improve ground-state observables systematically, e.g. $\sigma_{2149}^{\text{mass}} = 800 \text{keV}$

Collective excitations



Energy spectrum

- Vibrational + rotational states
- Nicely aligned with experiment
- Too spread out spectrum

Electromagnetic transitions

- Restoration of (J^2, J_z) essential
- Selection rules recovered
- \blacksquare Good in- and out-band B(E2)