Nuclear Energy Density Functional Method

How to (safely...) account for correlations in ground and excited states of heavy nuclei?

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Ultimate goals

**Ground state**
Mass, deformation

**Spectroscopy**
Spectroscopy

**Collective modes**
RPA, QRPA, GCM

**Reaction properties**
Fusion, transfer, elastic

**Heavy elements**
Fission, fusion, SHE

**Exotic behaviors**
Drip-lines, halos

**Astrophysics**
r-process, NS, SN

From underlying NN and NNN interactions
Nuclear EDF method: key points

I EDF method addresses both ground and excited states
One single energy functional
Two levels of many-body implementations
• Single reference
• Multi reference

II EDF method addresses both structure and reactions properties
Two different schemes
• Time independent for structure properties
• Time dependent for structure and reaction properties

III EDF method is currently transitioning from empirical to non/less empirical
Energy kernel(s) so far built by analogy with matrix elements of fictitious « H »
• Base-line and insights from strict « H »-based approach
• EDF extends it empirically to grasp additional necessary correlations
Accuracy/predictive power of current empirical EDFs not sufficient/satisfactory
• Need to improve current phenomenology (e.g. M. Stoitsov, M. Kortelainen)
• Constrain EDF kernels from vacuum H and MBPT (e.g. T. Lesinski, B. Gebremariam)
Departure from « H »-based picture is at the origin of potentially serious problems
• Need to better formulate the empirical method
• Work needed to formulate the two-level EDF method from first principles
Single-Reference = « Mean-field »

I Formalism in a nutshell
\[ \mathcal{E}[\rho, \kappa, \kappa^*] = \text{functional of one-body density matrices} \]
\[ \rho_{ji} = \langle \Phi | c_i^+ c_j | \Phi \rangle \quad ; \quad \kappa_{ji} = \langle \Phi | c_i c_j | \Phi \rangle \]
\[ |\Phi\rangle = \text{auxiliary, symmetry-breaking product state (N, Z, J^2, P^2, \Pi)} \]

II Included correlations
- « Bulk » ones into \( \mathcal{E}[\rho, \kappa, \kappa^*] \) (2\textsuperscript{nd} order MBPT in infinite nuclear matter)
- « Static » collective ones through symmetry breaking (\( \rho \) and \( \kappa \))
- Outside the frame of standard HK theorem of DFT

III Applications and observables
- Nuclear equation of state
- Binding energies (different for odd/even nuclei)
- Shell structure \( \varepsilon \) and pairing gaps \( \Delta \) through total energy differences
- Deformation properties and fission barriers
- Charge densities, neutron skin, radii
- Individual and rotational excitations
Standard energy functionals

I Functional form
• Skyrme is quasi-local / Gogny is non-local
• Skyrme’s basic structure is bilinear in the following local densities

\[
\rho_q(\vec{r}) \equiv \sum_\sigma \rho_q(\vec{r}\sigma, \vec{r}\sigma) \quad \text{Matter density}
\]
\[
\tau_q(\vec{r}) \equiv \sum_\sigma \nabla \cdot \nabla' \rho_q(\vec{r}\sigma, \vec{r}'\sigma)|_{\vec{r}=\vec{r}', \sigma} \quad \text{Kinetic density}
\]
\[
\bar{s}_q(\vec{r}) \equiv \sum_{\sigma\sigma'} \rho_q(\vec{r}\sigma, \vec{r}'\sigma) \bar{\sigma}_{\sigma',\sigma} \quad \text{Spin density}
\]
\[
\bar{j}_q(\vec{r}) \equiv \sum_\sigma i/2 (\nabla' - \nabla) \rho_q(\vec{r}\sigma, \vec{r}'\sigma)|_{\vec{r}=\vec{r}', \sigma} \quad \text{Current density}
\]
\[
\bar{\rho}_q(\vec{r}) \equiv \sum_\sigma \kappa_q(\vec{r}\sigma, \vec{r}\bar{\sigma}) \bar{\sigma} \quad \text{Pair density}
\]

II Basic features
• Symmetry rules to build allowed terms
• Simplistic density-dependent couplings at this point
  • \( \mathcal{E}[\rho, \kappa, \kappa^*] = \langle \Phi||H||\Phi\rangle/\langle \Phi|\Phi\rangle \) would tie Cs together/forbid dens.-dep. Cs
• Universal = applicable to all nuclei without local adjustment
• Empirical = no link to NN/NNN + fitted to experimental data
Multi-Reference = « Beyond mean-field »

I Formalism in a nutshell

\[ \mathcal{E}[\rho^{01}, \kappa^{01}, \kappa^{10*}] = \text{functional of one-body transition density matrices} \]

\[ \rho_{ij}^{01} = \frac{\langle \Phi_0 | a_j^+ a_i | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \quad \kappa_{ij}^{01} = \frac{\langle \Phi_0 | a_j a_i | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \]

\{ |\Phi_0\rangle ; |\Phi_1\rangle \} = \text{MR set of auxiliary, symmetry-breaking product states}

II Further correlations included

- « Dynamical » collective ones
- Fluctuations of \( |\Delta]\rangle e^{i\phi} \) of broken symmetries
- M. Bender et al.

III Applications and observables

- All what is calculated in SR
- Vibrational excitations (note: QRPA is a small amplitude limit of MR EDF)
- Rotational bands of transitional nuclei
- LACM and shape coexistence
- E.M. transitions in the lab frame

\[ \mathcal{E}^k = \sum_{\{0,1\} \in \text{MR}} \frac{f_0^k f_1^k}{f_0^k} \mathcal{E}[0, 1] \langle \Phi_0 | \Phi_1 \rangle \frac{\langle \Phi_0 | \Phi_1 \rangle}{\sum_{\{0,1\} \in \text{MR}} f_0^k f_1^k} \]

\[ \mathcal{E}[0, 1] \equiv \mathcal{E}[\rho^{01}, \kappa^{01}, \kappa^{10*}] \]
Some tricky points

I Should SR-EDF be final for gs and MR-EDF left for excited states?
Some practitioners believe so by analogy with DFT

- Symmetry breaking/restoring?
- Intrinsic DFT [J. Messud et al., arXiv:0904.0162]? For all symmetries? Is that convenient?

II Seems difficult in practice to account for dynamical correlations in SR-EDF

III Danger of double counting correlations
Splitting into « bulk/static/dynamical » not based on first principles

- There is no obvious separation of (energy) scales
- EDF built empirically and fitted at the SR level so far

Need to design a non-empirical framework

- On going effort as for building the SR-EDF from NN/NNN + MBPT
- But how does MR-EDF fits in? No first-principle backup so far

IV Unexpected, though very serious, additional difficulties...
Spurious divergencies and steps in PNR calculations

I Given the SR EDF

\[ \mathcal{E}_{SR}[\rho^{00}, \kappa^{00}, \kappa^{00*}] = \sum_{ij} t_{ij} \rho_{ji}^{00} + \frac{1}{2} \sum_{ijkl} \tilde{v}_{ijkl}^{\rho_{ij}} \rho_{ki}^{00} \rho_{lj}^{00} + \frac{1}{4} \sum_{ijkl} \tilde{v}_{ijkl}^{\kappa_{ij}} \kappa_{ij}^{00} \kappa_{kl}^{00} \]

\[ + \frac{1}{6} \sum_{ijklmn} \tilde{v}_{ijklmn}^{\rho_{ijk}} \rho_{li}^{00} \rho_{mj}^{00} \rho_{nk}^{00} + \frac{1}{4} \sum_{ijklmn} \tilde{v}_{ijklmn}^{\kappa_{ijk}} \kappa_{ij}^{00} \kappa_{jk}^{00} \kappa_{mn}^{00} + \ldots \]

II Particle Number Restoration: one particular MR mode

\[ \mathcal{E}^N \equiv \int_0^{2\pi} d\varphi \frac{e^{-i\varphi N}}{2\pi c_N^2} \mathcal{E}_{MR}[\Phi_0, \Phi_\varphi] \langle \Phi_0 | \Phi_\varphi \rangle \]

with the MR set

\[
\left\{
|\Phi_\varphi\rangle \equiv e^{i\varphi \hat{N}} |\Phi_0\rangle ; \varphi \in [0, 2\pi] \\
\mathcal{E}_{MR}[\Phi_0, \Phi_\varphi] \equiv \mathcal{E}_{SR}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0*}]
\right\}
\]

But where does this prescription come from!?

[J. Dobaczewski et al., PRC76 (2007)]

[M. Bender, T. Duguet, IJMP E16 (2007)]
Definition of non-diagonal EDF kernels for MR calculations

\[ \mathcal{E}_H \left( \rho^{00}, \kappa^{00}, \kappa^{00*} \right) \]

- Hamiltonian based

\[ \rho_{ij}^{00} = \frac{\langle \Phi_0 | a_j^+ a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle}, \quad \kappa_{ij}^{00} = \frac{\langle \Phi_0 | a_j a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} \]

\[ \mathcal{E}_{EDF} \left( \rho^{00}, \kappa^{00}, \kappa^{00*} \right) \]

- EDF case

\[ \rho_{ij}^{00} = \frac{\langle \Phi_0 | a_j^+ a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle}, \quad \kappa_{ij}^{00} = \frac{\langle \Phi_0 | a_j a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} \]

\[ \mathcal{E}_{EDF} \left( \rho^{01}, \kappa^{01}, \kappa^{01*} \right) \]

- Generalized Wick Theorem (GWT)

\[ \rho_{ij}^{01} = \frac{\langle \Phi_0 | a_j^+ a_i \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle}, \quad \kappa_{ij}^{01} = \frac{\langle \Phi_0 | a_j a_i \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle}, \ldots \]

\[ \mathcal{E}_{EDF} \left( \rho^{01}, \kappa^{01}, \kappa^{01*} \right) \]

- Standard Wick Theorem (SWT)

\[ \rho_{ij}^{01} = \frac{\langle \Phi_0 | a_j^+ a_i \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle}, \quad \kappa_{ij}^{01} = \frac{\langle \Phi_0 | a_j a_i \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle}, \ldots \]

- [B. Balian, E. Brezin, Nuovo Cimento 64 (1969)]

- Is the GWT-based extension procedure to be questioned in the EDF context?
- If it is so, all MR modes and not only PNR should be compromised
- Is there a safe and motivated alternative?
The problem is indeed not specific to PNR

I Particle number restoration

II Angular momentum restoration

EDF with integer powers $\rho^2$

III Shape mixing

To be studied
Pathologies due to departure from “H”-based picture

(I) [D. Lacroix, T. Duguet, M. Bender, to appear in PRC; arXiv:0809.2041]

I Sources of pathologies

- **Self-Interaction (SR+MR)**
  - Not dramatic a priori
  - Need to be characterized

- **Self-Pairing (SR+MR)**
  - Not dramatic a priori
  - Need to be characterized

- **GWT-motivated procedure within EDF framework (MR only)**
  - Divergences, sharp steps, smooth steps plus kink

II Cure MR EDF kernels first

- Find alternative to GWT
- Identify critical terms
- Remove pathologies in EDF case
Starting point:

\[ |\Phi_0\rangle = C_0 \prod_{\nu} \alpha_{\nu} |0\rangle \]
\[ |\Phi_1\rangle = C_1 \prod_{\nu} \beta_{\nu} |0\rangle \]

\[ \alpha_{\nu}^+ = \sum_{i} (U_{i\nu}^0 a_i^+ + V_{i\nu}^0 a_i) \]
\[ \beta_{\nu}^+ = \sum_{i} (U_{i\nu}^1 a_i^+ + V_{i\nu}^1 a_i) \]

\[ \beta_{\mu}^+ = \sum_{\nu} (A_{\nu\mu} \alpha_{\nu}^+ + B_{\nu\mu} \alpha_{\nu}) \]
\[ A = U_0^+ U_1 + V_0^+ V_1 \]
\[ B = V_0^T U_1 + U_0^T V_1 \]

The Balian-Brezin (Thouless) strategy => GWT

Start from \( |\Phi_1\rangle \propto e^{S(\alpha,\alpha^+)} |\Phi_0\rangle \)
\[ \beta = e^S \alpha e^{-S} \]
valid for \( \langle \Phi_0 | \Phi_1 \rangle \neq 0 \)

Work on the transformation

\[ \frac{\langle \Phi_0 | \hat{H} | \Phi_1 \rangle}{\langle \Phi_0 | \Phi_1 \rangle} = e^H (\rho_0^1, \kappa_0^1, \kappa_1^0) \]

The Bloch-Messiah-Zumino Strategy => SWT

Work directly on A and B

\[ A = D \tilde{A} C \quad B = D^* \tilde{B} C \]

\[ B(p) = \begin{pmatrix} 0 & \tilde{B}_{pp} \\ \tilde{B}_{pp} & 0 \end{pmatrix} \quad \tilde{A}(p) = \begin{pmatrix} \tilde{A}_{pp} & 0 \\ 0 & \tilde{A}_{pp} \end{pmatrix} \]

Simplify the connection (valid if \( \langle \Phi_0 | \Phi_1 \rangle = 0 \))

\[ \tilde{\beta}_{\nu}^+ = \tilde{A}_{\nu\nu} \tilde{\alpha}_{\nu}^+ + \tilde{B}_{\nu\nu} \tilde{\alpha}_{\nu} \]
\[ |\Phi_1\rangle = c_{01} \prod (\tilde{A}_{pp}^* + \tilde{B}_{pp}^* \tilde{\alpha}_p \tilde{\alpha}_p^+) |\Phi_0\rangle \]
Interest of the Bloch-Messiah-Zumino technique
some Theorems made simple/recovered

\[ |\Phi_1\rangle = \tilde{c}_{01} \prod (\tilde{A}_{pp}^* + \tilde{B}_{pp}^* \tilde{a}_p^+ \tilde{a}_p^+) |\Phi_0\rangle \]

Overlaps

\[ \langle \Phi_0 | \Phi_1 \rangle = \tilde{c}_{01} \prod \tilde{A}_{pp}^* = \tilde{c}_{01} \sqrt{\det(\tilde{A}^*)}. \]

(Onishi-Yoshida)

Thouless

\[ |\Phi_1\rangle = \tilde{c}_{01} \prod \tilde{A}_{pp}^* (1 + \tilde{Z}_{pp} \tilde{a}_p^+ \tilde{a}_p^+) |\Phi_0\rangle = N_{01} e^{\sum_p \tilde{Z}_{pp} \tilde{a}_p^+ \tilde{a}_p^+} |\Phi_0\rangle \]

if \( \tilde{A}_{pp}^* \neq 0 \) we define \( \tilde{Z}_{pp} = (\tilde{B}_{pp} \tilde{A}_{pp}^{-1})^* \)

Expectation values through SWT instead of GWT

MR

MR

SR

MR

Thomas Duguet - INT Program on Effective Field Theories and the Many-Body Problem - Seattle, April 2009
Correct GWT-based definition of MR kernels

Strategy: compare SWT to GWT for MR kernel from “H” + extend to EDF

Notations \( \langle \Phi_0 | \Phi_1 \rangle = \bar{A}_{\nu \nu} \langle \Phi_0 | \Phi_1, \nu \rangle = \bar{A}_{\nu \nu} \bar{A}_{\mu \mu} \langle \Phi_0 | \Phi_1, \nu, \mu \rangle \)

with \( \langle \Phi_0 | \Phi_1, \nu \rangle = \langle \Phi_0 | \Phi_1, \bar{\nu} \rangle \) and \( \langle \Phi_0 | \Phi_1, \nu, \mu \rangle = \langle \Phi_0 | \Phi_1, \nu, \bar{\nu} \rangle = 0 \)

\( \langle \Phi_0 | \hat{V}_{12} | \Phi_1 \rangle \) Direct

\begin{align*}
&+ \frac{1}{2} \sum_{\nu \mu i j k l} \hat{V}_{i v}^{0} \hat{V}_{j u}^{0} \hat{V}_{i 0}^{0} \hat{V}_{i 0}^{0} \bar{\nu}_{i j k l}^{0} \langle \Phi_0 | \Phi_1 \rangle \\
&+ \frac{1}{2} \sum_{\nu \mu i j k l} \hat{V}_{i v}^{0} \hat{V}_{j u}^{0} \hat{V}_{l 0}^{0} \hat{U}_{k 0}^{0} \bar{\nu}_{i j k l}^{0} \bar{B}_{p v}^{*} \langle \Phi_0 | \Phi_1, \nu \rangle \\
&+ \frac{1}{2} \sum_{\nu \mu i j k l} \hat{V}_{i v}^{0} \hat{V}_{j u}^{0} \hat{U}_{l 0}^{0} \hat{U}_{k 0}^{0} \bar{\nu}_{i j k l}^{0} \bar{B}_{p v}^{*} \bar{B}_{p v}^{*} \langle \Phi_0 | \Phi_1, \nu, \mu \rangle \\
&+ \frac{1}{4} \sum_{\nu \mu i j k l} \hat{V}_{i v}^{0} \hat{U}_{l 0}^{0} \hat{U}_{i 0}^{0} \hat{U}_{k 0}^{0} \bar{\nu}_{i j k l}^{0} \langle \Phi_0 | \Phi_1 \rangle \\
&+ \frac{1}{4} \sum_{\nu \mu i j k l} \hat{V}_{i v}^{0} \hat{U}_{j 0}^{0} \hat{U}_{l 0}^{0} \hat{U}_{k 0}^{0} \bar{\nu}_{i j k l}^{0} \bar{B}_{p v}^{*} \langle \Phi_0 | \Phi_1, \nu \rangle \\
&+ \frac{1}{4} \sum_{\nu \mu i j k l} \hat{V}_{i v}^{0} \hat{U}_{j 0}^{0} \hat{U}_{i 0}^{0} \hat{U}_{k 0}^{0} \bar{\nu}_{i j k l}^{0} \bar{B}_{p v}^{*} \bar{B}_{p v}^{*} \langle \Phi_0 | \Phi_1, \nu, \mu \rangle \\
&+ \frac{1}{4} \sum_{\nu \mu i j k l} \hat{V}_{i v}^{0} \hat{V}_{j 0}^{0} \hat{U}_{l 0}^{0} \hat{U}_{k 0}^{0} \bar{\nu}_{i j k l}^{0} \bar{B}_{p v}^{*} \bar{B}_{p v}^{*} \langle \Phi_0 | \Phi_1, \nu, \mu \rangle
\end{align*}

Summary of pathologies

\{ \text{SR- self-interaction} \}

\{ \text{MR self-inter/self-pairing} \}

\{ \text{Diverg/step} \}

\{ \text{SR-self-inter/self-pairing} \}

\{ \text{MR self-inter/self-pairing} \}

\{ \text{Diverg/step} \}
Practical regularization procedure

(I) \[ [D. Lacroix, T. Duguet, M. Bender, to appear in PRC; arXiv:0809.2041] \]

I Start from a given SR EDF \( \mathcal{E}_{SR}[\rho^{00}, \kappa^{00}, \kappa^{00}^*] \)
Can only depend on integer powers of the density matrices

II Consider a MR mode
Can be any combination modes allowed by the code

III Given \( \{|\Phi_0\rangle; |\Phi_1\rangle\} \) proceed to BMZ decomposition of Bogoliubov transfo
To be done for each pair of reference states

IV Define \( \mathcal{E}_{MR}[\Phi_0, \Phi_1] = \mathcal{E}_{SR}[\rho^{01}, \kappa^{01}, \kappa^{10}^*] \) and subtract spurious terms
Leaves SR EDF untouched

First application: particle number restoration


I Step III above is trivial in this particular case

II Terms to be removed from \( \mathcal{E}_{MR}[\Phi_0, \Phi_\varphi] \)

\[
\begin{align*}
\rho \rho \text{ term } \quad & \mathcal{E}_{CG}^{\rho \rho}[0, \varphi] = \frac{1}{2} \sum_p \left\{ \tilde{v}_{pppp}^{\rho} + \tilde{v}_{pppp}^{\rho} + \tilde{v}_{pppp}^{\rho} + \tilde{v}_{pppp}^{\rho} \right\} (u_p v_p)^4 \frac{(e^{2i\varphi} - 1)^2}{(u_p^2 + v_p^2 e^{2i\varphi})^2} \\
\kappa \kappa \text{ term } \quad & \mathcal{E}_{CG}^{\kappa \kappa}[0, \varphi] = -\sum_p \tilde{v}_{pppp}^{\kappa \kappa} (u_p v_p)^4 \frac{(e^{2i\varphi} - 1)^2}{(u_p^2 + v_p^2 e^{2i\varphi})^2}
\end{align*}
\]
First application: particle number restoration

- Regularized results are mesh independent
- Regularization most often reduces the gain from PNR
- Correction important at but also away from steps
- Correction of the order of 0.5 to 1.0 MeV
- Small enough for existing calculations to make sense
- Of the order of the required mass accuracy and spectroscopic scale
- In all cases, correction reduces the noise
- Need to study other MR modes
Conclusions

- Specific difficulties to be considered seriously

- Regularization method valid for any MR calculation

- Application to Particle Number Restoration
  (II) Bender et al, First application to PNR, to appear in PRC; arXiv:0809.2045

- Specific case of fractional power of the density: $\rho^\gamma$

- Need to build
  (i) Correctable EDF for MR calculations
  (ii) SI- and SP-free EDF

- Need a constructive frame
Extra material
Addition

I TDDFT accounts for excited states

• Linear response = extended RPA
• Adiabatic approximation $\Leftrightarrow$ Residual interaction $= \frac{\delta^2 E}{\delta^2 \rho}$
• Looks like nuclear RPA but NO feedback onto g.s. energy
• Excitation in odd nuclei include fractionation of strength
Energy Density Functional method: as practitioners use it

**Basic elements**
- Approaches not based on a correlated wave-function
- Energy is postulated to be a functional of one-body density (matrices) $\mathcal{E}[\rho, \kappa, \kappa^*]$
- Symmetry breaking is at the heart of the method
- Two formulations (i) Single-Reference (ii) Multi-Reference

**Pros**
- Use of full single-particle space
- Collective picture but fully quantal
- Universality of the EDF ($A \approx 16$)
- Ground-state description
- Static (smooth) correlations

**Difficulties**
- No universal parametrization
- Empirical ≠ predictive power
- Spectroscopy / odd nuclei
- Dynamical (fluctuating) correlations
- Limited accuracy ($\sigma_{2135}^{\text{mass}} \approx 700$ keV)

- Skyrme = quasi-local / Gogny = non-local
- Parameters adjusted on a set of data (bias on bulk properties so far)
- Good performances for properties of known nuclei
- “Asymptotic freedom” as one jumps into the next major shell
Energy Density Functionals: Implications

The binding energy is a functional of densities and currents
Skyrme EDF: all local densities up to second order in $\sigma$ and derivatives

- Binding and nuclear equation of state
- Shell structure and pairing gaps
- Deformation and fission barriers
- Charge densities, neutron skin, radii
- Individual and rotational excitations

Time-independent multi-reference
- Add dynamical correlations to SR
- Vibrational excitations
- Rotational bands of transitional nuclei
- LACM and shape coexistence
- E.M. transitions

Time-dependent single-reference
- Vibrational excitations
- Reactions

Good performances for known nuclei
"Asymptotic freedom" as one goes away from known data

Empirical = no link to NN/NN

Stable isotopes
- Good performances for known nuclei
- "Asymptotic freedom" as one goes away from known data

Empirical = no link to NN/NN

Couplings adjusted on a restricted set of data
Extrapolated to all other observable and nuclei

SPIRAL2 will help constrain isovector part of EDF
- In the next major shell
- Up to $(N-Z)/A \sim 0.33$

Stable isotopes
- Good performances for known nuclei
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Limitations of current EDFs: one specific example

Shell evolution with N-Z

*Opening and closing of shell gaps not under control*

*Impact the balance between spherical and deformed configurations*

Weakening of N=40 shell gap in neutron-rich Cr isotopes

- Onset of deformation
- Position of $\nu g_{9/2}$ shell at N=40
- Constraints on shell position and evolution

H. Oba, M. Matsuo (2008)
Implementations: limitations

Quantum collective fluctuations in reactions
*Impossibility to account for tunneling in sub-barrier fusion*

Fusion cross section

- Very satisfactory fusion barriers
- Wide range of reaction partners
- Above-threshold cross section
- No adjustment whatsoever

Sub-barrier fusion
- Quantum tunneling
- Time-dependent MR-EDF formalism

Time-dependent SR-EDF calculation

C. Simenel (2007)
Construction of the EDF: Single-Ref.
The "nuclear physics strategy"

Hamiltonian case

$$\hat{H} = \sum_{ij} t_{ij} a_i^+ a_j + \frac{1}{4} \sum_{ijkl} \bar{\nu}_{ijkl} a_i^+ a_j^+ a_l a_k + \cdots$$

Standard Wick Theorem

$$\frac{\langle \Phi_0 | \hat{H} | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} = \sum_{ij} t_{ij} \rho_{ji}^{00} + \frac{1}{2} \sum_{ijkl} \bar{\nu}_{ijkl} \rho_{ki}^{00} \rho_{lj}^{00} + \frac{1}{4} \sum_{ijkl} \bar{\nu}_{ijkl} \kappa_{ij}^{00} \kappa_{kl}^{00}$$

$$\equiv \mathcal{E}^H(\rho^{00}, \kappa^{00}, \kappa^{00*})$$

Breaking the link with the Hamiltonian

- Introduction of new terms $\rho^\gamma$
- Different interactions in ph and pp channels $\bar{\nu}^\rho \neq \bar{\nu}^{\kappa\kappa}$
- Technical issues: coulomb, exchange...

Energy Density Functional case

$$\mathcal{E}_{EDF}(\rho^{00}, \kappa^{00}, \kappa^{00*}) = \sum_{ij} t_{ij} \rho_{ji}^{00} + \frac{1}{2} \sum_{ijkl} \bar{\nu}_{ijkl}^\rho \rho_{ki}^{00} \rho_{lj}^{00} + \frac{1}{4} \sum_{ijkl} \bar{\nu}_{ijkl}^{\kappa\kappa} \kappa_{ij}^{00} \kappa_{kl}^{00}$$

Thomas Duguet - INT Program on Effective Field Theories and the Many-Body Problem - Seattle, April 2009
Particle Number Restoration

(II) Bender et al, First application to PNR, arXiv/0809.2045

Trial state

\[ |\Psi^N\rangle = \int_0^{2\pi} \frac{d\varphi}{2\pi c_N} e^{-i\varphi N} |\Phi\varphi\rangle \quad \text{with} \quad |\Phi\varphi\rangle = e^{i\varphi N} |\Phi_0\rangle \]

EDF calculations

\[ \frac{\langle \Phi_0 | \hat{H} | \Phi\varphi \rangle}{\langle \Phi_0 | \Phi\varphi \rangle} \rightarrow \mathcal{E}[0, \varphi] \]

\[ \mathcal{E}^N \equiv \int_0^{2\pi} \frac{d\varphi}{2\pi c_N^2} e^{-i\varphi N} \mathcal{E}[0, \varphi] \langle \Phi_0 | \Phi\varphi \rangle \]

Connecting states

\[ |\Phi_0\rangle = \prod (u_p + v_p a_p^+ a_p^+) |0\rangle \]

\[ |\Phi\varphi\rangle = \prod (u_p + v_p e^{2i\varphi} a_p^+ a_p^+) |0\rangle \]

\[ |\Phi\varphi\rangle = \tilde{c}_{01} \prod (\tilde{A}_{pp}^* + \tilde{B}_{pp}^* \tilde{\alpha}_p \tilde{\alpha}_p^+) |\Phi_0\rangle \]

with

\[ \tilde{A}_{pp}^* = \tilde{A}_{pp} = e^{-i\varphi} (u_p^2 + v_p^2 e^{2i\varphi}) \]

\[ \tilde{B}_{pp}^* = -\tilde{B}_{pp} = u_p v_p (e^{i\varphi} - e^{-i\varphi}) \]
Correction of spurious contributions

Identify problems and correct MR calculations without modifying current EDF strategy
Limited to integer power of densities (Generalization to k-body interactions)

Valid also for mixing Slater Determinants
Should correct divergences observed in Zdunczuk et al, nucl-th/0610118

Illustration for Particle Number Restoration
Confirm the intuition Bender and Duguet, Int.J. Mod. Phys. E16 (2007)