Skyrme EDF for beyond mean-field calculations

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THEXO Workshop, ECT*, July 2013
Outline

- Skyrme mean-field and beyond mean-field calculations for masses and excitations
- Standard effective Skyrme interaction: $E = \langle \hat{T} + \hat{V}_2(\rho_0) \rangle$
- Standard effective EDF: $E \neq \langle \hat{T} + \hat{V}_2(\rho_0) \rangle$
- Constraints from beyond mean-field calculations
- Constraints from mean-field calculations
- New Skyrme effective interaction: $E = \langle \hat{T} + \hat{V}_2 + \hat{V}_3 + \hat{V}_4 \rangle$
Microscopic calculation of contributions of some correlations on ground states energies

- Mean-field approximation relies on a very simple wave function for the ground state of the system.

- Some beyond mean-field effects might be absorbed in an effective way by refitting the coupling constants of the EDF or by using schematic corrections.

- Some ground state correlations can be microscopically calculated by going beyond the mean-field approximation by
  - the mechanism of symmetry breaking and restauration
  - the mixing of states along collective coordinates (GCM)

See M. Bender, G.F. Bertsch and P.-H. Heenen, PRC 73, 034322:
- How large are these correlation energies?
- How much do they fluctuate?
The standard (2-body) Skyrme *interaction*

- **Effective Skyrme *interaction***

\[
V_{\text{eff}}(\mathbf{r}) = t_0 \left( 1 + x_0 \hat{P}^\sigma \right) \delta(\mathbf{r}) \quad \text{local}
\]
\[
+ \frac{1}{2} t_1 \left( 1 + x_1 \hat{P}^\sigma \right) \left[ k'^2 \delta(\mathbf{r}) + \delta(\mathbf{r}) \mathbf{k}^2 \right] \quad \text{non local}
\]
\[
+ t_2 \left( 1 + x_2 \hat{P}^\sigma \right) \mathbf{k}' \cdot \delta(\mathbf{r}) \mathbf{k} \quad \text{non local}
\]
\[
+ \frac{1}{6} t_3 \left( 1 + x_3 \hat{P}^\sigma \right) \rho_0^\alpha \delta(\mathbf{r}) \quad \text{density dep.}
\]
\[
+ i W_0 \, \hat{\sigma} \cdot \left[ \mathbf{k}' \times \delta(\mathbf{r}) \mathbf{k} \right] \quad \text{spin-orbit}
\]

- Sometimes complemented with a tensor term
- Possibly complemented with a D-wave term
- Higher order derivative terms?
- Other density dependent terms?
Skyrme EDF for beyond MF

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Introduction

Skyrme EDFs

New constraints

New Skyrme interaction

From effective interaction to EDF (« \( \hat{T} \) even » part)

\[
\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{\text{eff}} + \mathcal{H}_{\text{fin}} + \mathcal{H}_{\text{so}} + \mathcal{H}_{\text{sg}} + \mathcal{H}_{\text{coul}}
\]

\[
\mathcal{H}_0 = \frac{1}{4} t_0 \left( (2 + x_0) \rho_0^2 - (2x_0 + 1) \sum_q \rho_q^2 \right)
\]

\[
\mathcal{H}_3 = \frac{1}{24} t_3 \rho_0^\alpha \left( (2 + x_3) \rho_0^2 - (2x_3 + 1) \sum_q \rho_q^2 \right)
\]

\[
\mathcal{H}_{\text{eff}} = \frac{1}{8} \left[ t_1 (2 + x_1) + t_2 (2 + x_2) \right] \tau_0 \rho_0
\]

\[
+ \frac{1}{8} \left[ t_2 (2x_2 + 1) - t_1 (2x_1 + 1) \right] \sum_q \tau_q \rho_q
\]

\[
\mathcal{H}_{\text{fin}} = \frac{1}{32} \left[ t_2 (2 + x_2) - 3 t_1 (2 + x_1) \right] \rho_0 \Delta \rho_0
\]

\[
+ \frac{1}{32} \left[ 3 t_1 (2x_1 + 1) + t_2 (2x_2 + 1) \right] \sum_q \rho_q \Delta \rho_q
\]

\[
\mathcal{H}_{\text{so}} = -\frac{W_0}{2} \left[ \rho_0 \nabla \cdot \mathbf{J}_0 + \sum_q \rho_q \nabla \cdot \mathbf{J}_q \right]
\]

\[
\mathcal{H}_{\text{sg}} = -\frac{t_1 x_1 + t_2 x_2}{16} \mathbf{J}_0^2 + \frac{t_1 - t_2}{16} \sum_q \mathbf{J}_q^2
\]
From effective interaction to EDF (« $\hat{T}$ even » part)

$$
\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{\text{eff}} + \mathcal{H}_{\text{fin}} + \mathcal{H}_{\text{so}} + \mathcal{H}_{\text{sg}} + \mathcal{H}_{\text{coul}}
$$

$$
\mathcal{H}_0 = \frac{1}{4} t_0 \left[ (2 + x_0) \rho_0^2 - (2x_0 + 1) \sum_q \rho_q^2 \right] = \sum_{T=0,1} C_T [\rho_0] \rho_T^2
$$

$$
\mathcal{H}_3 = \frac{1}{24} t_3 \rho_0^\alpha \left[ (2 + x_3) \rho_0^2 - (2x_3 + 1) \sum_q \rho_q^2 \right] = \sum_{T=0,1} C_T^T \tau_T \rho_T
$$

$$
\mathcal{H}_{\text{eff}} = \frac{1}{8} \left[ t_1 (2 + x_1) + t_2 (2 + x_2) \right] \tau_0 \rho_0 + \frac{1}{8} \left[ t_2 (2x_2 + 1) - t_1 (2x_1 + 1) \right] \sum_q \tau_q \rho_q = \sum_{T=0,1} C_T^\Delta \rho_T \Delta \rho_T
$$

$$
\mathcal{H}_{\text{fin}} = \frac{1}{32} \left[ t_2 (2 + x_2) - 3 t_1 (2 + x_1) \right] \rho_0 \Delta \rho_0 + \frac{1}{32} \left[ 3 t_1 (2x_1 + 1) + t_2 (2x_2 + 1) \right] \sum_q \rho_q \Delta \rho_q = \sum_{T=0,1} C_T^{\nabla J} \rho_T \nabla \cdot J_T
$$

$$
\mathcal{H}_{\text{so}} = - \frac{W_0}{2} \left[ \rho_0 \nabla \cdot J_0 + \sum_q \rho_q \nabla \cdot J_q \right] = \sum_{T=0,1} C_T^{\nabla J} \rho_T \nabla \cdot J_T
$$

$$
\mathcal{H}_{\text{sg}} = - \frac{t_1 x_1 + t_2 x_2}{16} J_0^2 + \frac{t_1 - t_2}{16} \sum_q J_q^2 = \sum_{T=0,1} C_T^{J^2} \rho_T : \text{SLy4}
$$
From effective interaction to EDF: further simplifications

- Different interaction used in the pairing channel

\[ V_p(r) = V_0 \left[ 1 - \left( \frac{\rho_0(r)}{\rho_{sat}} \right)^{\alpha'} \right] \delta(r) \]

- **Unconvenient** terms sometimes disregarded: \( s_0 \cdot \Delta s_0, \ s_1 \cdot \Delta s_1 \).

- Fit of the parameters on infinite nuclear matter properties on (ground state) properties of (doubly magic) nuclei
  - Good results for ground state properties of even-even nuclei (but how good is good ?)
  - Encouraging constrained HF and beyond mean-field results

- Several annoying technical questions
  - Coupling constants of the time odd part of the functional
  - Calculations sometimes do not converge for some functional
  - How to deal with the density dependent terms in beyond mean-field calculations?
Mean field and beyond

- Beyond mean field calculations with a Skyrme EDF

See: PRC 79, 044318, 044319 and 044320.

⇒ Density dependent term must be dropped...
⇒ Three-body interaction ?
⇒ Four-body interaction ?
⇒ In Hartree, Fock and pairing terms...
New strong constraints on the EDF

The EDF must be derived from an interaction: \( E = \langle \hat{T} + \hat{V} \rangle \)

- No density dependence
- All terms kept in the functional (Hartree, Fock and pairing)
- Must give attractive pairing

But that’s not all:

- First, mean-field calculations must give converged results

See:

Finite size instabilities in nuclei

- Instabilities often experienced with the skyrme functionals
  - Ferromagnetic instabilities: (spin polarization) $n \uparrow, p \uparrow$
  - Isospin instabilities: neutron-proton **segregation**
  - Both: $n \uparrow, p \downarrow$

- Example: isospin instability in $^{48}$Ca

\[ C_1^{\Delta \rho} = 15 \text{ MeV fm}^5 \]
\[ \sim \text{SLy5} \]
\[ 25 \text{ MeV fm}^5 \]
\[ 35 \text{ MeV fm}^5 \]
\[ \gtrsim 36 \text{ MeV fm}^5 \]

Linear response – Instabilities in infinite nuclear matter

Response of the system to a perturbation given by

$$Q^{(\alpha)} = \sum_a e^{i \mathbf{q} \cdot \mathbf{r}_a} \Theta^{(\alpha)}_a,$$

$$\Theta^s_s = 1_a, \quad \Theta^v_s = \sigma_a, \quad \Theta^s_v = \mathbf{\tau}_a, \quad \Theta^v_v = \sigma_a \mathbf{\tau}_a$$

Response functions are given by

$$\chi^{(\alpha)}(\omega, \mathbf{q}) = \frac{1}{\Omega} \sum_n |\langle n | Q^{(\alpha)} | 0 \rangle|^2 \left( \frac{1}{\omega - E_{n0} + i\eta} - \frac{1}{\omega + E_{n0} - i\eta} \right)$$


- Predicts instabilities in finite size systems
- Easy to implement
- Negligible computation time
- Might be crucial with tensor, 3- or 4-body terms
Linear response as a tool for diagnosis

Pole of the response at $E = 0 \equiv$ instability

- $T. \text{Lesinski, K.B.}, T. \text{Duguet, J. Meyer, PRC 74, 044315 (2006)}$;
Linear response as a tool for diagnosis

Pole of the response at $E = 0$ \(\equiv\) instability

at $\rho \sim 0.3 \text{ fm}^{-3}$

appearance of domains $(S=0, T=1)$ with size $\sim \frac{2\pi}{2.7}$

- T. Lesinski, K.B., T. Duguet, J. Meyer, PRC 74, 044315 (2006);
“Standard” EDFs, instabilities and Murphy’s law

Murphy’s law: “Anything that can go wrong will go wrong”.

Instabilities are very difficult to detect with a code working on an harmonic oscillator basis.
New Skyrme effective interaction for mean-field and beyond mean-field calculations

- We need
  - An interaction (no density dependence)
  - That can be used in all channels (attractive pairing)
  - Stable in all spin/isospin channel

- Previous work (thesis of J. Sadoudi):
  - Finite size instability can be avoided and correct reproduction of masses can be achieved with 2- and 3-body terms
  - A 4-body might help
  - Properties in the pairing channel not considered at that time.
Skyrme effective interaction with 2-, 3- and 4-body terms

(Cf J. Sadoudi thesis, CEA Saclay)

- Two-body effective interaction

\[
V_{\text{eff}} = t_0 \left(1 + x_0 \hat{P}^\sigma\right) \delta(\mathbf{r}) \quad \text{local}
\]
\[
+ \frac{1}{2} t_1 \left(1 + x_1 \hat{P}^\sigma\right) \left(k'^2 \delta(\mathbf{r}) + \delta(\mathbf{r}) k^2\right) \quad \text{non local}
\]
\[
+ t_2 \left(1 + x_2 \hat{P}^\sigma\right) k' \cdot \delta(\mathbf{r}) k \quad \text{non local}
\]
\[
+ i W_0 \mathbf{\hat{\sigma}} \cdot \left[k' \times \delta(\mathbf{r}) k\right] \quad \text{spin-orbit}
\]

- Complemented it with

\[
3 u_0 \delta(\mathbf{r}_{12}) \delta(\mathbf{r}_{13})
\]
\[
+ \frac{3}{2} u_1 \left(1 + y_1 \hat{P}^\sigma\right) \left[\delta(\mathbf{r}_{12}) \delta(\mathbf{r}_{13}) k_{12}^2 + k'_{12}^2 \delta(\mathbf{r}_{12}) \delta(\mathbf{r}_{13})\right]
\]
\[
+ 3 u_2 \left(1 + y_{21} \hat{P}^\sigma \right) k'_{12} \cdot \delta(\mathbf{r}_{12}) \delta(\mathbf{r}_{13}) k_{12}
\]
\[
+ v_0 \delta(\mathbf{r}_{12}) \delta(\mathbf{r}_{13}) \delta(\mathbf{r}_{14})
\]

- And possibly: tensor, D-wave and 3-body spin-orbit...
Interactions with 2-, 3- and 4-body terms

Stability: How do the 3- and 4-body terms change the picture?

→ They generate nicer figures!

No hint in the Landau parameters!
Tentative fit with simplified interaction: SLyMR0

See: Phys. Scr. 2013 014013
J. Sadoudi, M. Bender, K.B., D. Davesne, R. Jodon, T. Duguet

- 3- and 4-body terms reduced to

\[ 3u_0 \delta(r_{12})\delta(r_{13}) + v_0 \delta(r_{12})\delta(r_{13})\delta(r_{14}) \]

- Infinite nuclear matter properties
  - \( \rho_{\text{sat}} = 0.152 \text{ fm}^{-3} \),
  - \( E/A = -15.04 \text{ MeV} \),
  - \( K_\infty = 264.2 \text{ MeV} \),
  - \( m^*/m = 0.47 \),
  - \( J = 23 \text{ MeV} \).

- Allows to test the mean-field and beyond mean-field machinery:
  Beyond mean-field calculations (B. Bally, M. Bender) in progress...
SLyMR0: Results

Skyrme EDFs
New constraints
New Skyrme interaction
SLyMR0: Results for $^{25}$Mg

Calculation for odd-even nucleus with blocking and projection on N, Z and J
Work in progress: SLyMR1 interaction

- Interaction with 2-, 3- and 4-body terms
- Used both in the $ph$ and $pp$ channels
- Perfectly stable!
- Incompressibility too high for the moment

\[
\begin{align*}
\rho_{\text{sat}} &= 0.16 \text{ fm}^{-3} \\
a_I &= 28.8 \text{ MeV} \\
F_0 &= -0.12 \\
F_1 &= -1.14 \\
F'_0 &= 0.46 \\
F'_1 &= 1.37 \\
E/A &= -16.1 \text{ MeV} \\
L &= 49.7 \text{ MeV} \\
K_\infty &= 315 \text{ MeV} \\
Q &= -376 \text{ MeV} \\
\frac{\Delta m^*}{m} &= 0.29 > 0 \\
m^*/m &= 0.62 \\
G_0 &= -0.36 \\
G_1 &= -0.63 \\
G'_0 &= 0.26 \\
G'_1 &= 0.16
\end{align*}
\]
Properties of SLyMR1

- Attractive pairing but too weak...
  
  Pairing is built from all terms of the interaction, where the attraction comes from? What can be tuned to enhance it?

- What about surface properties?
  
  How the 2- and 3-body gradient terms act on the surface?
  → Constraint on surface energy will be added

- Four-body term: is it really needed?
  
  Life is complicated and the four-body term may have driven us to a bad region of parameters
  → Attempt to make a fit without the 4-body term.
Collaboration

- **IPN Lyon**: K. Bennaceur, D. Davesne, R. Jodon, J. Meyer
- **CENBG**: B. Avez, B. Bally, M. Bender, J. Sadoudi
- **IRFU**: T. Duguet
- **ULB**: V. Heelemans, P.H. Heenen, A. Pastore, M. Martini
- **UW**: T. Lesinski