Skyrme EDF
for beyond mean-field calculations

K. Bennaceur

Université Claude Bernard Lyon 1,
Institut de Physique Nucléaire de Lyon, CNRS/IN2P3,
F-69622 Villeurbanne cedex, France.

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: $E \neq \langle \hat{T} + \hat{V}_2(\rho_0) \rangle$
- Constaints from beyond mean-field calculations
- Constaints 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*

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

- Sometimes complemented with a tensor term
- Possibly complemented with a D-wave term
- Higher order derivative terms ?
- Other density dependent terms ?

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

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

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

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

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

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

$$\mathcal{H}_{\text{so}} = -\frac{W_0}{2} \left[\rho_0 \boldsymbol{\nabla}\cdot\mathbf{J}_0 + \sum_q \rho_q \boldsymbol{\nabla}\cdot\mathbf{J}_q \right] = \sum_{T=0,1} C_T^{\nabla J} \rho_T \boldsymbol{\nabla}\cdot\mathbf{J}_T$$

$$\mathcal{H}_{\text{sg}} = -\frac{t_1 x_1 + t_2 x_2}{16} \mathbf{J}_0^2 + \frac{t_1 - t_2}{16} \sum_q \mathbf{J}_q^2 = \sum_{T=0,1} C_T^{\mathbf{J}} \mathbf{J}_T^2$$

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

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

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

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

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

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

$$\mathbf{C_0^{\nabla J} \neq 3C_1^{\nabla J} : SLy10}$$

$$\mathcal{H}_{\text{so}} = -\frac{W_0}{2}\left[\rho_0 \boldsymbol{\nabla}\cdot\mathbf{J}_0 + \sum_q \rho_q \boldsymbol{\nabla}\cdot\mathbf{J}_q\right] = \sum_{T=0,1} C_T^{\nabla J}\rho_T \boldsymbol{\nabla}\cdot\mathbf{J}_T$$

$$\mathcal{H}_{\text{sg}} = -\frac{t_1x_1 + t_2x_2}{16}\mathbf{J}_0^2 + \frac{t_1 - t_2}{16}\sum_q \mathbf{J}_q^2 = \cancel{\sum_{T=0,1} C_T^J \mathbf{J}_T^2} \quad \mathbf{: SLy4}$$

From effective interaction to EDF: further simplifications

- Different interaction used in the pairing channel

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

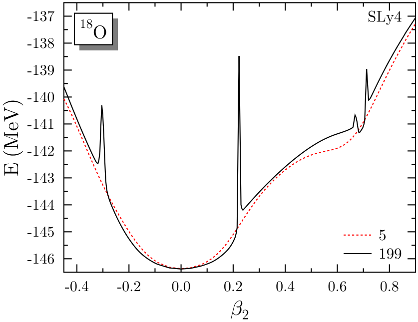
- *Unconvenient* terms sometimes disregarded: $\mathbf{s}_0 \cdot \Delta \mathbf{s}_0\,, \quad \mathbf{s}_1 \cdot \Delta \mathbf{s}_1\,.$

- 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



Poles

and steps

in the projected energy

See: PRC 79, 044318, 044319 and 044320.

⇒ Density dependent term must be droped...

⇒ 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:

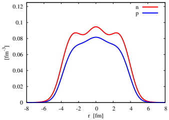
A. Pastore, D. Davesne, K.B., J. Meyer and V. Hellemans,
Phys. Scr. **2013**, 014014.

A. Pastore, K.B., D. Davesne, J. Meyer,
Int. J. of Modern Phys. E Vol. 21, No. 05, 1250040.

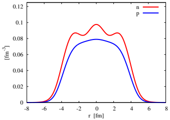
Finite size instabilities in nuclei

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

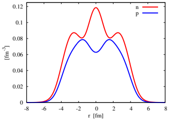
- Example: isospin instability in ^{48}Ca



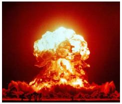
$C_1^{\Delta\rho} = 15$ MeV fm^5
$\sim$ SLy5



25 MeV fm^5



35 MeV fm^5



$\gtrsim 36$ MeV fm^5

T. Lesinski, K.B., T. Duguet, J. Meyer, PRC 74, 044315 (2006).

Linear response – Instabilities in infinite nuclear matter

Response of the system to a perturbation given by

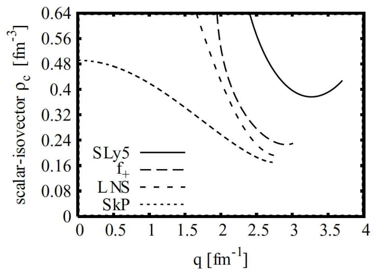
$$\mathcal{Q}^{(\alpha)} = \sum_a e^{i\mathbf{q}\cdot\mathbf{r}_a}\ \Theta_a^{(\alpha)}\,,$$

$$\Theta_a^{\mathrm{ss}} = 1_a,\quad \Theta_a^{\mathrm{vs}} = \boldsymbol{\sigma}_a,\quad \Theta_a^{\mathrm{sv}} = \vec{\tau}_a,\quad \Theta_a^{\mathrm{vv}} = \boldsymbol{\sigma}_a\vec{\tau}_a$$

Response functions are given by

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

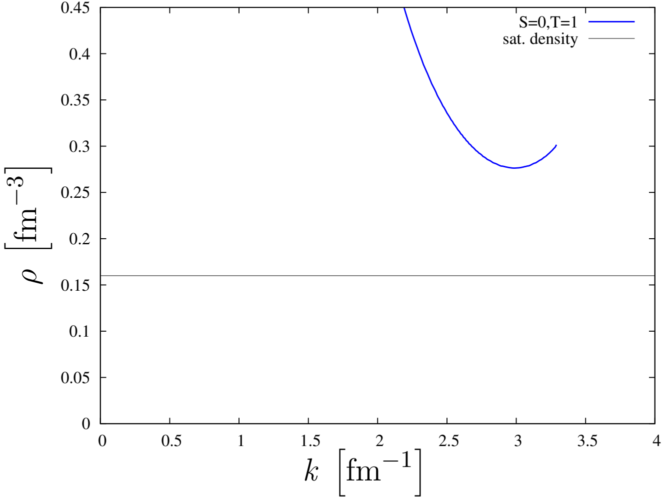
(Cf. C. Garcia–Recio *et al.*, Ann. of Phys. 214 (1992) 293–340)



- 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

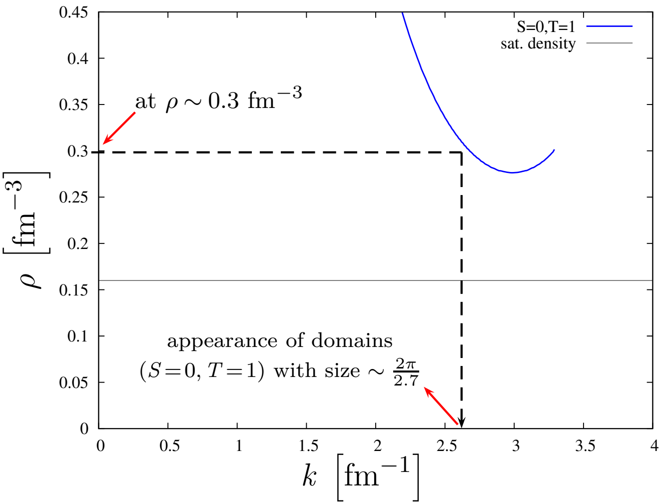
Pole of the response at $E = 0$ $\equiv$ instability



- T. Lesinski, K.B., T. Duguet, J. Meyer, PRC 74, 044315 (2006);
- D. Davesne, M. Martini, K.B., J. Meyer, Phys. Rev. C80, 024314 (2009), **erratum:** Phys. Rev. C 84, 059904(E) (2011).

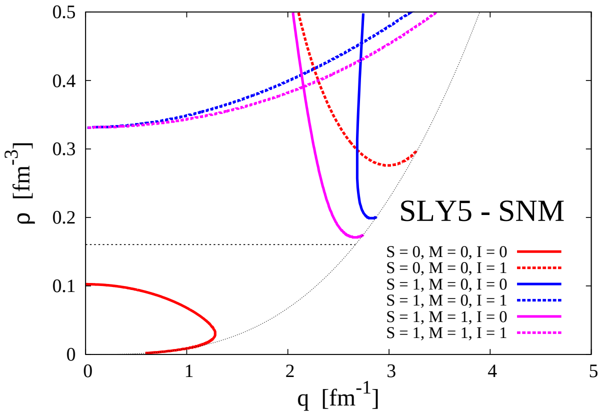
Linear response as a tool for diagnosis

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



- T. Lesinski, K.B., T. Duguet, J. Meyer, PRC 74, 044315 (2006);
- D. Davesne, M. Martini, K.B., J. Meyer, Phys. Rev. C80, 024314 (2009), **erratum:** Phys. Rev. C 84, 059904(E) (2011).

“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 calcualtions

- 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

$$\begin{aligned} V_{\text{eff}} &= t_0 \left(1 + x_0 \hat{P}^\sigma\right) \delta(\mathbf{r}) && \text{local} \\ &+ \tfrac{1}{2} t_1 \left(1 + x_1 \hat{P}^\sigma\right) \left(\mathbf{k}'^2 \delta(\mathbf{r}) + \delta(\mathbf{r}) \mathbf{k}^2\right) && \text{non local} \\ &+ t_2 \left(1 + x_2 \hat{P}^\sigma\right) \mathbf{k}' \cdot \delta(\mathbf{r}) \mathbf{k} && \text{non local} \\ &+ \mathrm{i}\, W_0\, \hat{\boldsymbol{\sigma}} \cdot \left[\mathbf{k}' \times \delta(\mathbf{r}) \mathbf{k}\right] && \text{spin-orbit} \end{aligned}$$

- Complemented it with

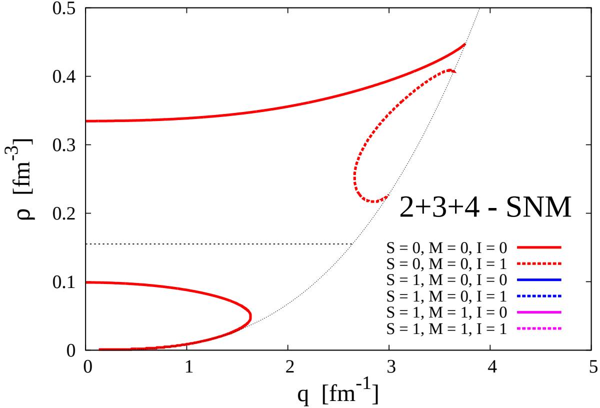
$$\begin{aligned} &3\, u_0\, \delta(\mathbf{r}_{12})\, \delta(\mathbf{r}_{13}) \\ &+\tfrac{3}{2} u_1 \left(1 + y_1 \hat{P}^\sigma\right) \left[\delta(\mathbf{r}_{12})\delta(\mathbf{r}_{13})\, \mathbf{k}_{12}^2 + \mathbf{k}_{12}'^2\, \delta(\mathbf{r}_{12})\delta(\mathbf{r}_{13})\right] \\ &+3\, u_2 \left(1 + y_{21} \hat{P}_{12}^\sigma + y_{22} \hat{P}_{13}^\sigma\right) \mathbf{k}_{12}' \cdot \delta(\mathbf{r}_{12})\delta(\mathbf{r}_{13}) \mathbf{k}_{12} \\ &+ v_0\, \delta(\mathbf{r}_{12})\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{14}) \end{aligned}$$

- 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

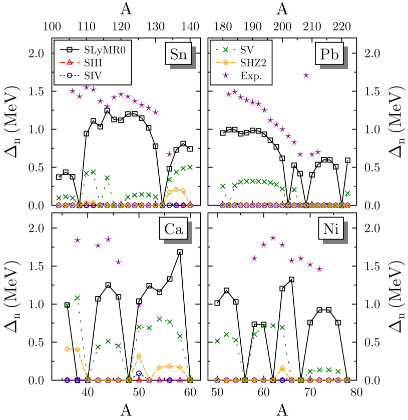
- 3- and 4-body terms reduced to

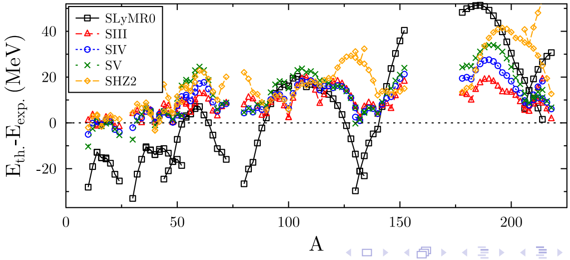
$$3\, u_0\, \delta(\mathbf{r}_{12})\delta(\mathbf{r}_{13}) \;+\; v_0\, \delta(\mathbf{r}_{12})\delta(\mathbf{r}_{13})\delta(\mathbf{r}_{14})$$

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

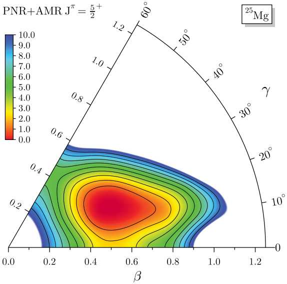
- Allows to test the mean-field and beyond mean-field machinery: Beyond mean-field calculations (B. Bally, M. Bender) in progress...

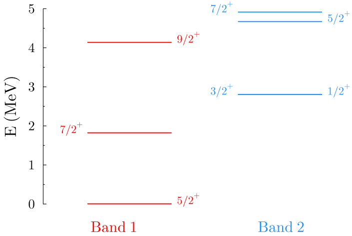
SLyMR0: Results





SLyMR0: Results for ^{25}Mg

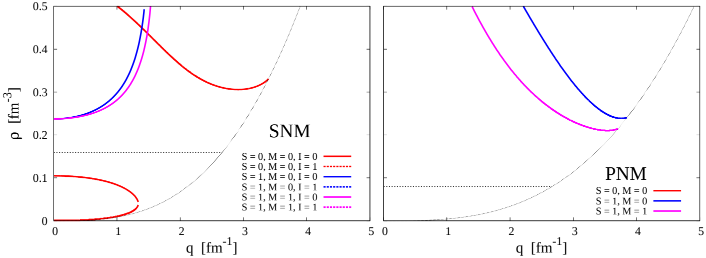




Calculation for odd-even nucleus with blocking and projection on N, Z and J

Work in progress: SLyMR1 interaction

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



$\rho_{\rm sat} = 0.16\ \text{fm}^{-3}$ $E/A = -16.1$ MeV $K_\infty = 315$ MeV $m^*/m = 0.62$

$a_I = 28.8$ MeV $L = 49.7$ MeV $Q = -376$ MeV $\frac{\Delta m*}{m} = 0.29 > 0$

$F_0 = -0.12$ $F'_0 = 0.46$ $G_0 = -0.36$ $G'_0 = 0.26$

$F_1 = -1.14$ $F'_1 = 1.37$ $G_1 = -0.63$ $G'_1 = 0.16$

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 ?
  $\rightarrow$ 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
  $\rightarrow$ 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