Skyrme EDF with 2-, 3- and 4-body terms (and modification of one term that what never explored)

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ESNT Workshop







2-, 3- and 4-body terms in Skyrme EDF

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Problems with he Skyrme EDF

New Skyrme interaction

Regularized Skyrme interaction

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Outline

- Problems and limits of the Standard Skyrme EDF
- Skyrme effective interaction with 2-, 3- and 4-body terms
- Preliminary results
- One term of the Skyrme interaction that was never modified...

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The standard (2-body) Skyrme functional

Effective Skyrme interaction

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

Sometimes complemented with a tensor term

- Possibly complemented with a D-wave term
- Higher order derivative terms ?
- Other density dependent terms ?
- Different interaction in the pairing channel

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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 ⁴⁸Ca



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

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Linear response – Instabilities in infinite nuclear matter

Response of the system to a perturbation given by

$$\begin{split} \mathcal{Q}^{(\alpha)} &= \sum_{a} e^{i\mathbf{q}\cdot\mathbf{r}_{a}} \,\, \Theta_{a}^{(\alpha)},\\ \Theta_{a}^{\rm ss} &= 1_{a}, \quad \Theta_{a}^{\rm vs} = \boldsymbol{\sigma}_{a}, \quad \Theta_{a}^{\rm sv} = \vec{\tau}_{a}, \quad \Theta_{a}^{\rm vv} = \boldsymbol{\sigma}_{a}\vec{\tau}_{a} \end{split}$$

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 a tensor interaction

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Linear response as a tool for diagnosis



 D. Davesne, M. Martini, K.B., J. Meyer, Phys. Rev. C80, 024314 (2009), erratum: Phys. Rev. C 84, 059904(E) (2011).

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Linear response as a tool for diagnosis



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2-. 3- and

4-body terms in Skyrme EDF

Code developed in Lyon can treat

(D. Davesne, A. Pastore, T. Lesinski, M. Martini)

- General two-, three-body Skyrme interaction
- Four-body contact interaction
- Tensor interaction
- D-wave interaction
- Symmetric matter and pure neutron matter
- Interactions or functionals

This code is now used in the fitting procedure.

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"Standard" EDFs, instabilities and Murphy's law



Murphy's law: "Anything that can go wrong will go wrong".

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Effective interaction Vs. Functional

■ Interactions: time even and time odd parts of the functional are entirely determined by the interaction parameters

 \Rightarrow Spin instabilities can not be predicted from infinite homogeneous nuclear matter or spherical nuclei calculations...

Functional: more flexible \Rightarrow "dangerous" terms, *e.g.* $\rho_1 \Delta \rho_1$, $\mathbf{s}_0 \Delta \mathbf{s}_0$, $\mathbf{s}_1 \Delta \mathbf{s}_1$, ... can be separately adjusted or disregarded.

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Mean field and beyond





See: PRC 79, 044318, 044319 and 044320.

- \Rightarrow Three-body interaction ? (*Cf* J. Sadoudi thesis, CEA Saclay)
- \Rightarrow Four-body interaction ?
- \Rightarrow In Hartree, Fock and pairing terms...

¹ in some specific cases only !

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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) shows that

- Stability in infinite nuclear matter and correct reproduction of masses can not be achived with 2- and 3-body terms...
- A 4-body term is required
- What about pairing ?

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Skyrme effective interaction with 2-, 3- and 4-body terms

Two-body effective interaction

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

Complemented it with

$$3 \frac{u_0}{2} \delta_{12} \delta_{13} + \frac{3}{2} \frac{u_1}{u_1} \left(1 + \frac{y_1}{p^{\sigma}} \right) \left[\delta_{12} \delta_{13} \mathbf{k}_{12}^2 + \frac{\mathbf{k}_{12}'^2}{u_1^2} \delta_{12} \delta_{13} \right] + 3 \frac{u_2}{u_2} \left(1 + \frac{y_{21}}{p_{12}'} + \frac{y_{22}}{p_{13}'} \right) \mathbf{k}_{12}' \cdot \delta_{12} \delta_{13} \mathbf{k}_{12} + \frac{u_0}{u_1} \delta_{12} \delta_{13} \delta_{14}$$

And possibly: tensor, D-wave and 3-body spin-orbit...

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Interactions with 2-, 3- and 4-body terms

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

 \rightarrow They generate nicer figures !



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Tentative fit with simplified interaction: SLyMR0

See: Phys. Scr. 2013 014013

■ 3- and 4-body terms reduced to

 $3 u_0 \delta_{12} \delta_{13} + v_0 \delta_{12} \delta_{13} \delta_{14}$

■ 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... 2-, 3- and 4-body terms in Skyrme EDF

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SLyMR0: Results



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Work in progress: SLyMR1 interaction

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



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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 Robin Jodon's presentation.

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Collaboration

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- 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

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• UW: T. Lesinski

A parameter of the Skyrme interaction that was never changed...

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A parameter of the Skyrme interaction that was never changed...

... the range !

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Regularized Skyrme effective interaction

(Work done with J. Dobaczewski and F. Raimondi)

$$v = \tilde{\delta}_{0}(\mathbf{r}_{1}, \mathbf{r}_{2}; \mathbf{r}_{3}, \mathbf{r}_{4}) t_{0} \left(1_{\sigma q} + x_{0} 1_{q} \hat{P}^{\sigma} - y_{0} 1_{\sigma} \hat{P}^{q} - z_{0} \hat{P}^{\sigma} \hat{P}^{q} \right) + \tilde{\delta}_{1}(\mathbf{r}_{1}, \mathbf{r}_{2}; \mathbf{r}_{3}, \mathbf{r}_{4}) t_{1} \left(1_{\sigma q} + x_{1} 1_{q} \hat{P}^{\sigma} - y_{1} 1_{\sigma} \hat{P}^{q} - z_{1} \hat{P}^{\sigma} \hat{P}^{q} \right) + \tilde{\delta}_{2}(\mathbf{r}_{1}, \mathbf{r}_{2}; \mathbf{r}_{3}, \mathbf{r}_{4}) t_{2} \left(1_{\sigma q} + x_{2} 1_{q} \hat{P}^{\sigma} - y_{2} 1_{\sigma} \hat{P}^{q} - z_{2} \hat{P}^{\sigma} \hat{P}^{q} \right)$$

with

$$\begin{split} \tilde{\delta}_{0}(\mathbf{r}_{1},\mathbf{r}_{2};\mathbf{r}_{3},\mathbf{r}_{4}) &= \delta(\mathbf{r}_{1}-\mathbf{r}_{3})\delta(\mathbf{r}_{2}-\mathbf{r}_{4})g_{\mu}(\mathbf{r}_{1}-\mathbf{r}_{2})\\ \tilde{\delta}_{1}(\mathbf{r}_{1},\mathbf{r}_{2};\mathbf{r}_{3},\mathbf{r}_{4}) &= \frac{1}{2}\,\delta(\mathbf{r}_{1}-\mathbf{r}_{3})\delta(\mathbf{r}_{2}-\mathbf{r}_{4})g_{\mu}(\mathbf{r}_{1}-\mathbf{r}_{2})\left[\mathbf{k}_{12}^{*2}+\mathbf{k}_{34}^{2}\right]\\ \tilde{\delta}_{2}(\mathbf{r}_{1},\mathbf{r}_{2};\mathbf{r}_{3},\mathbf{r}_{4}) &= \delta(\mathbf{r}_{1}-\mathbf{r}_{3})\delta(\mathbf{r}_{2}-\mathbf{r}_{4})g_{\mu}(\mathbf{r}_{1}-\mathbf{r}_{2})\,\mathbf{k}_{12}^{*}\cdot\mathbf{k}_{34} \end{split}$$

and

$$g_{\mu}(\mathbf{r}) = \frac{e^{-\frac{r^2}{\mu^2}}}{\left(\mu\sqrt{\pi}\right)}$$

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Preliminary remarks

Two-body effective interaction

- **No** density dependence !
- Simple expression with 12 parameters (plus the spin-orbit term)
- Compact expressions for infinite nuclear matter properties (check the arXiv at the end of this week)
- Relatively simple to implement in a code on harmonic oscillator basis (done in HFODD)
- Is it possible to reproduce the empirical properties of the saturation point ?
- Is it possible to have correct binding energies for nuclei ?

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Functional

For i=0, 1 et 2: four direct and four exchange terms with coupling constants

$$\begin{cases}
A_i^{\rho_0} = \frac{1}{2} t_i \left(1 + \frac{1}{2} x_i - \frac{1}{2} y_i - \frac{1}{4} z_i \right) \\
A_i^{\rho_1} = -\frac{1}{2} t_i \left(\frac{1}{2} y_i + \frac{1}{4} z_i \right) \\
A_i^{s_0} = \frac{1}{2} t_i \left(\frac{1}{2} x_i - \frac{1}{4} z_i \right) \\
A_i^{s_1} = -\frac{1}{8} t_i z_i
\end{cases}$$

and

$$\begin{cases} B_i^{\rho_0} = -\frac{1}{2} t_i \left(\frac{1}{4} + \frac{1}{2} x_i - \frac{1}{2} y_i - z_i \right) \\ B_i^{\rho_1} = -\frac{1}{2} t_i \left(\frac{1}{4} + \frac{1}{2} x_i \right) \\ B_i^{\mathbf{s}_0} = -\frac{1}{2} t_i \left(\frac{1}{4} - \frac{1}{2} y_i \right) \\ B_i^{\mathbf{s}_1} = -\frac{1}{8} t_i \end{cases}$$

 \Rightarrow the 12 time-odd coupling constants can be expressed using the 12 time-even ones

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Adjustment of the parameters

- No spherical code for now...
- **HFODD:** 1 magic nucleus on 10 shells $\simeq 15$ minutes
- Use of infinite nuclear matter to limit the number of free parameters
- Handmade non professional adjustment
- Exact treatment of the Coulomb interaction

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Masses of doubly magic nuclei



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