Introduction

Effective interactions / EDF

New Skyrme interaction

Regularized Skyrme interaction

Three-body term

Summary

Density-independent effective interaction for mean-field and beyond mean-field calculations

K. Bennaceur

Université Claude Bernard Lyon 1,
Institut de Physique Nucléaire de Lyon (CNRS/IN2P3),
Department of Physics, University of Jyväskylä.

From nuclear structure to particle transfer reactions and back,
ETC*, November 4-8, 2013

Outline

- “Standard” effective interactions and/or EDFs
- Extented and regularized Skyrme interactions
- Properties in infinite nuclear matter
- Preliminary results for finite nuclei

Effective interactions and EDFs

- Effective interactions and/or effective Energy Density Functionals

$$E = \langle \hat{T} + \hat{V}_{\text{eff}} \rangle = \int \mathcal{E}(\mathbf{r})\, \mathrm{d}^3 r$$

  are the key ingredients for the mean-field and beyond mean-field calculations

- They depend on coupling constants fitted on
  - infinite nuclear matter empirical properties
  - nuclear data (masses, radii, ...)

- Used at the mean-field level: "SR-EDF" (HF, HFB, ...)
- or beyond: RPA or "MR-EDF" (GCM, symmetry restauration)

Introduction
Effective interactions / EDF
New Skyrme interaction
Regularized Skyrme interaction
Three-body term
Summary

A brief history of the effective interactions

Introduction

Effective interactions / EDF

New Skyrme interaction

Regularized Skyrme interaction

Three-body term

Summary

- Effective interactions in non-relativistic approaches

$$\hat{V}_{\text{eff}} \equiv V_{12} + V_{\text{so}} + V_{\text{Coul.}} + V_{\text{T}}$$

- Two families of (early) interactions
  - Skyrme zero-range interaction

    $$V_{12} \propto \text{“}\,\delta(\mathbf{r}_2 - \mathbf{r}_1)\,\text{”}$$

    depends on gradients, gives a functional of local densities, needs a cut-off.

  - Brink-Boeker (and Gogny) finite-range interaction

    $$V_{12} \propto \text{“}\,e^{-\frac{(\mathbf{r}_2 - \mathbf{r}_1)^2}{\mu^2}}\,\text{”}$$

    gives a functional of the non-local density, no cot-off.

Need for a three-body interaction

- Very poor properties for the saturation point of infinite nuclear matter (“SV” interaction)

$$\rho_{\text{sat}} = 0.155 \text{ fm}^{-3}, \quad B = -16.05 \text{ MeV}, \quad K_\infty = 305.7 \text{ MeV},$$

$$m^*/m = 0.38, \quad J = 32.8 \text{ MeV}.$$

- Need for a three-body term

$$V_{123} = t_3\,\delta(\mathbf{r}_2 - \mathbf{r}_1)\,\delta(\mathbf{r}_3 - \mathbf{r}_1).$$

$\rightarrow$ improves the effective mass but...

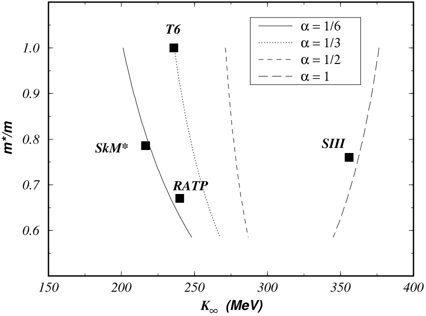
From a three-body term to a density dependent term

- Collapse a spin polarized matter !!

$$t_3\,\delta(\mathbf{r}_2-\mathbf{r}_1)\,\delta(\mathbf{r}_3-\mathbf{r}_1) \quad\longrightarrow\quad \frac{1}{6}\,t_3\,\rho_0\,\delta(\mathbf{r}_2-\mathbf{r}_3)\,.$$

not an interaction anymore.

- Incompressibility much to high !



$$\frac{1}{6}\,t_3\,\rho_0\,\delta(\mathbf{r}_2-\mathbf{r}_3) \quad\longrightarrow\quad \frac{1}{6}\,t_3\,\rho_0^{\alpha}\,\delta(\mathbf{r}_2-\mathbf{r}_3)\,.$$

The standard (2-body) Skyrme functional

- Effective Skyrme *interaction*

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

- Sometimes complemented with tensor, D-wave terms, etc.
- Higher order derivatives ? Other density dependent terms ?
- Different interaction in the pairing channel
- ρ_0^α is the key to succes:
  - $\longrightarrow$ Incompressibility
  - $\longrightarrow$ Effective mass
  - $\longrightarrow$ Stability in the spin channels

Effective interactions Vs. Functionals

- Interactions:
  - time-even, time-odd ans pairing parts of the functional are entirely determined by the interaction parameters
  - Difficult to have satisfying properties in all channels
  - Few observables to constrain the time-odd terms

- Functionals: more flexible
  - Complicated, poorly determined or "dangerous" terms, *e.g.* $\mathbb{J}^2$, $\rho_1\Delta\rho_1$, $\mathbf{s}_0\Delta\mathbf{s}_0$, $\mathbf{s}_1\Delta\mathbf{s}_1$, ... can be separately adjusted or disregarded.
  - Simpler interactions can be used in the pairing channel

$\Rightarrow$ Very efficient at the mean-field level

Introduction

Effective interactions / EDF

New Skyrme interaction

Regularized Skyrme interaction

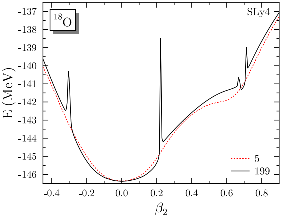
Three-body term

Summary

Beyond mean-field calculations

- Beyond mean field calculations with a Skyrme EDF

(with terms $\propto \rho^{\alpha}, \quad \alpha \notin \mathbb{N}$)



Poles → that can be corrected[1]

and steps in the projected energy → that can not !

... what about coul-ex ?

See:
M. Anguiano *et al.* NPA 696 (2001) 467,
J. Dobaczewski *et al.* PRC 76, 054315 (2007),
PRC 79, 044318, 044319 and 044320,
and L.M. Robledo, J. Phys. G 37, 064020 (2010).

⇒ Need for an interaction (*i.e.* without ρ_0^{α}) for the Hartree, Fock and pairing terms !

⇒ Three-body interaction ? (*Cf* J. Sadoudi thesis, CEA Saclay)

⇒ Four-body interaction ? Something else ?

[1] in some specific cases only !

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

- Two-body effective interaction

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

- Complemented it with

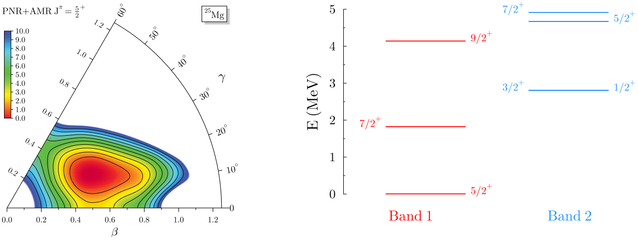
$$
\begin{aligned}
&3 u_0 \, \delta_{12}\delta_{13} \\
&+\frac{3}{2} u_1 \left(1 + y_1 \hat{P}^\sigma\right) \left[\delta_{12}\delta_{13}\mathbf{k}_{12}^2 + \mathbf{k}_{12}'^2 \delta_{12}\delta_{13}\right] \\
&+3 u_2 \left(1 + y_{21} \hat{P}_{12}^\sigma + y_{22} \hat{P}_{13}^\sigma\right) \mathbf{k}_{12}'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

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

First exploratory work: J. Sadoudi *et al.*, Phys. Scr. 2013 014013.

Preliminary results

Odd-even nucleus with symmetry restoration



A primer in nuclear structure !
Calculation based on an interaction (SLyMR0)
One quasi-particle state
Projection on N, Z and J

Calculations by B. Bally and collaborators (CENBG, Bordeaux)

Regularized Skyrme effective interaction

- Interaction ar NLO

$$v = \tilde{v}_0(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)\, t_0 \left(1_{\sigma q} + x_0 1_q \hat{P}^\sigma - y_0 1_\sigma \hat{P}^q - z_0 \hat{P}^\sigma \hat{P}^q\right)$$
$$+ \tilde{v}_1(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)\, t_1 \left(1_{\sigma q} + x_1 1_q \hat{P}^\sigma - y_1 1_\sigma \hat{P}^q - z_1 \hat{P}^\sigma \hat{P}^q\right)$$
$$+ \tilde{v}_2(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4)\, t_2 \left(1_{\sigma q} + x_2 1_q \hat{P}^\sigma - y_2 1_\sigma \hat{P}^q - z_2 \hat{P}^\sigma \hat{P}^q\right)$$

with

$$\tilde{v}_0(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = \delta(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_2-\mathbf{r}_4) g_a(\mathbf{r}_1-\mathbf{r}_2)$$
$$\tilde{v}_1(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = \delta(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_2-\mathbf{r}_4) g_a(\mathbf{r}_1-\mathbf{r}_2)\, \frac{1}{2}\left[\mathbf{k}_{12}^{*2} + \mathbf{k}_{34}^2\right]$$
$$\tilde{v}_2(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_3,\mathbf{r}_4) = \delta(\mathbf{r}_1-\mathbf{r}_3)\delta(\mathbf{r}_2-\mathbf{r}_4) g_a(\mathbf{r}_1-\mathbf{r}_2)\, \mathbf{k}_{12}^{*} \cdot \mathbf{k}_{34}$$

and

$$g_a(\mathbf{r}) = \frac{e^{-\frac{r^2}{a^2}}}{\left(a\sqrt{\pi}\right)^3}$$

- Higher order derivative terms provide an order-by-order correctible theory

See J. Dobaczewski, K.B., F. Raimondi, J. Phys. G **39**, 125103

Preliminary remarks

- For the moment: Standard zero-range spin-orbit interaction
- Two flavors for this interaction
  - $t_2 = -t_1$: "REG2a" interaction → much simpler...
  - $t_2 \neq -t_1$: "REG2b" interaction
- **Two-body** effective interaction
- **No** density dependence !
- Simple expression with 12 parameters (plus the spin-orbit term)
- Compact expressions for infinite nuclear matter properties (*Cf.* `arXiv:1305.7210`)
- 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 ?

Introduction

Effective interactions / EDF

New Skyrme interaction

Regularized Skyrme interaction

Three-body term

Summary

Functional

For $i = 0$, 1 and 2: 4 direct + 4 exch. terms with coupling constants

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

and

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

- 8 independent coupling constants for REG2a, 12 for REG2b
- More degrees of freedom to adjust the different channels than with a zero-range interaction

Introduction

Effective interactions / EDF

New Skyrme interaction

Regularized Skyrme interaction

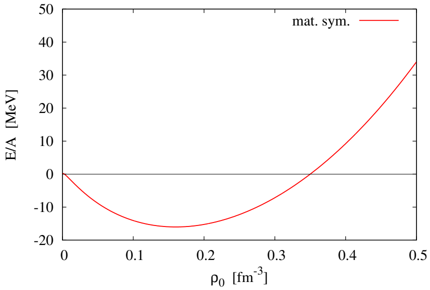
Three-body term

Summary

Adjustment of the parameters

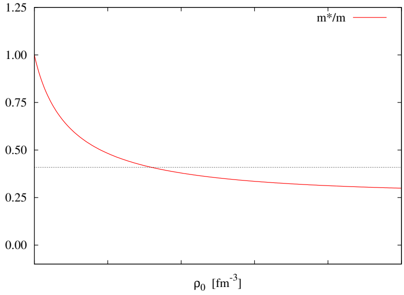
- No spherical code (for now)...
- HFODD: 1 magic nucleus on 10 shells $\simeq$ 15 minutes
- Use of infinite nuclear matter to limit the number of free parameters
- Handmade non professional adjustment (*POUNDerS* on the way)
- Exact treatment of the Coulomb interaction

Infinite nuclear matter (REG2b)



$$a = 0.8 \text{ fm}$$

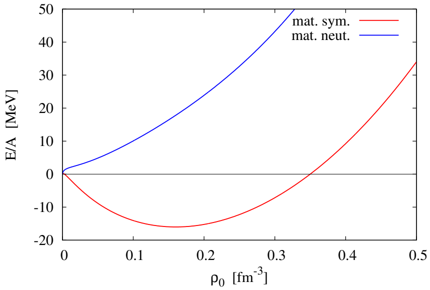
$$\rho_{\text{sat}} = 0.16 \text{ fm}^{-3}$$
$$E/A = -16 \text{ MeV}$$
$$K_\infty = 230 \text{ MeV}$$
$$J$$
$$L$$
$$K_{\text{sym}}$$



$$m^*/m = 0.41 \quad :-($$

masses of doubly magic nuclei

Infinite nuclear matter (REG2b)



$a = 0.8$ fm

$\rho_{\text{sat}} = 0.16\ \text{fm}^{-3}$

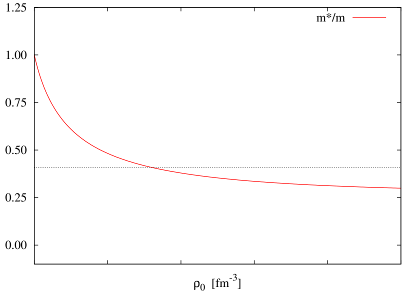
$E/A = -16$ MeV

$K_\infty = 230$ MeV

$J = 32$ MeV

$L = 58$ MeV

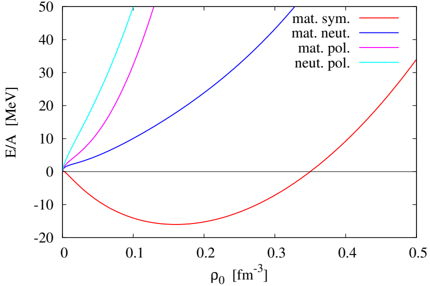
$K_{\text{sym}} = -175$ MeV



$m^*/m = 0.41$:-(

masses of doubly magic nuclei

Infinite nuclear matter (REG2b)



$a = 0.8$ fm

$\rho_{\mathrm{sat}} = 0.16\ \mathrm{fm}^{-3}$

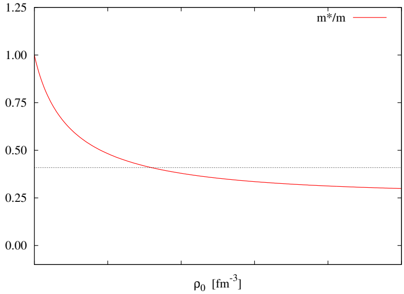
$E/A = -16$ MeV

$K_\infty = 230$ MeV

$J = 32$ MeV

$L = 58$ MeV

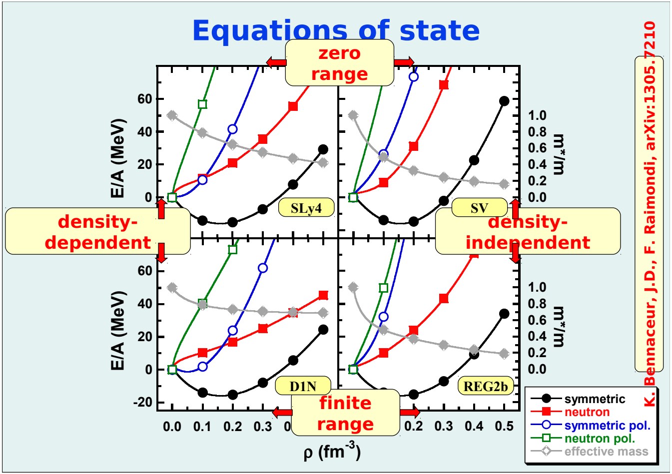
$K_{\mathrm{sym}} = -175$ MeV



$m^*/m = 0.41$:-(

masses of doubly magic nuclei

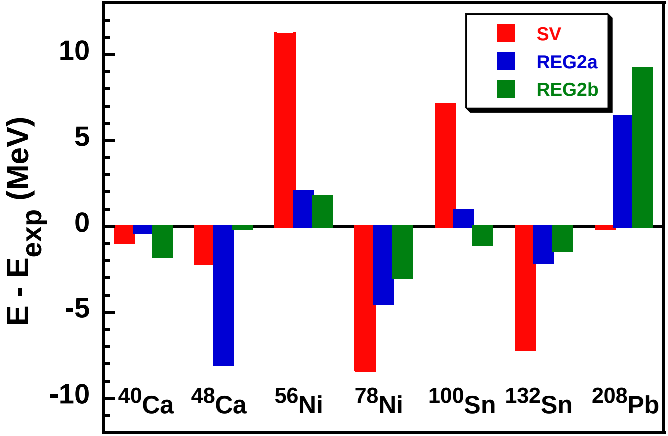
Comparison in infinite nuclear matter



Jacek Dobaczewski

JYVÄSKYLÄN YLIOPISTO

Masses of doubly magic nuclei



Better than SV, not a tremendous achievement.

How to correct the effective mass ?

3-body term

- One can consider a finite range 3-body interaction

$$V_{3N} = C_{3N} \times e^{-\frac{(\mathbf{r}_2-\mathbf{r}_1)^2+(\mathbf{r}_3-\mathbf{r}_2)^2+(\mathbf{r}_1-\mathbf{r}_3)^2}{\alpha_{3N}^2}}$$

  as suggested by A. Zapp, R. Roth, H. Hergert[2]

- Or an easier the handle 3-body zero-range

$$v_3 = t_3\,\delta(\mathbf{r}_2-\mathbf{r}_1)\,\delta(\mathbf{r}_3-\mathbf{r}_1)$$

[2] unpublished, as far as I know...

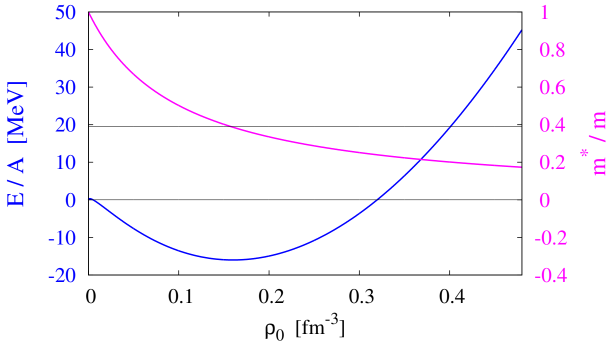
Zero-range 2-body

- Two-body zero-range $\simeq$ SV interaction
- Fixed:

$$\rho_{\rm sat} = 0.16\ {\rm fm}^{-3}, \qquad B = -16\ {\rm MeV}$$

- Calculated:

$$K_\infty = 306\ {\rm MeV}, \qquad Q = -174\ {\rm MeV}, \qquad m^*/m = 0.39$$



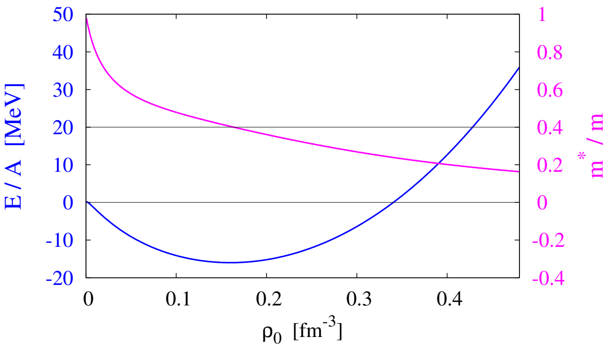
Finite-range 2-body

- Finite-range 2-body ($a = 1$ fm) $\simeq$ Reg2b interaction
- Fixed:

$$\begin{array}{rclcrcl} \rho_{\text{sat}} & = & 0.16\ \text{fm}^{-3}, & & K_\infty & = & 230\ \text{MeV}, \\ B & = & -16\ \text{MeV}, & & Q & = & -174\ \text{MeV} \end{array}$$

- Calculated:

$$m^*/m = 0.40$$



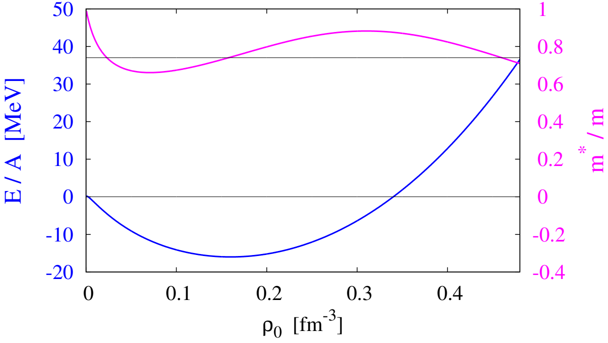
Finite-range 2-body + Zero-range 3-body

- Finite-range 2-body ($a = 1$ fm), $t_3 = 9600$ MeV fm^6 adjusted by hand
- Fixed:

$$\begin{array}{rclcrcl} \rho_{\text{sat}} & = & 0.16\ \text{fm}^{-3}, & & K_\infty & = & 230\ \text{MeV}, \\ B & = & -16\ \text{MeV}, & & Q & = & -174\ \text{MeV} \end{array}$$

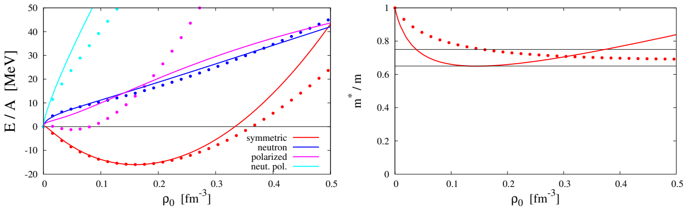
- Calculated:

$$m^*/m = 0.74$$



Finite-range 2-body + Zero-range 3-body

- First exploratory work:
  - "Reg2a" form + Zero-range 3-body
  - parameters adjusted so that masses of doubly magic nuclei are correct within 5 %
- Interaction stable in all channels (comparison with D1N)



$$\rho_{\text{sat}} = 0.16\ \text{fm}^{-3}, \quad B = -16\ \text{MeV}, \quad K_\infty = 265\ \text{MeV}$$
$$m^*/m = 0.65, \quad J = 31.3\ \text{MeV}$$

- Ready for a fit...

Summary

- The final goal of this work is to develop an effective interaction that can be used in mean-field and beyond mean-field calculations
- The 2-body version reproduce correctly the empirical saturation properties of infinite nuclear matter but the effective mass that is too low
- A 3-body contact term seems to solve this problem
- Properties in the pairing channel not studied yet...

Introduction

Effective interactions / EDF

New Skyrme interaction

Regularized Skyrme interaction

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Summary

Work done in collaboration with

- J. Dobaczewski (Univ. of Warsaw / Univ. of Jyväskylä)
- F. Raimondi (TRIUMF)

Thank you...