HFB calculations from a regularized pseudo-potential

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Outline

- Brief history of effective interactions
- Constraints *from beyond*
- Finite-range pseudo-potential
- Pairing
- Three-body interactions: The Good, the Bad and the (not so) Ugly

Brief history of nuclear effective interactions

- Effective interactions in non-relativistic approaches

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

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

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

    depends on gradients, gives a functional of local densities, needs a cut-off.
    → Set of **differential** equations

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

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

    gives a functional of the non-local density, no cut-off.
    → Set of **integro-differential** equations

Need for a three-body interaction

- Two-body interactions: very poor properties for the saturation point of infinite nuclear matter (*e.g.* "SV" interaction)

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

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

- Finite-range may improve K_∞ but not m^*/m

- 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...

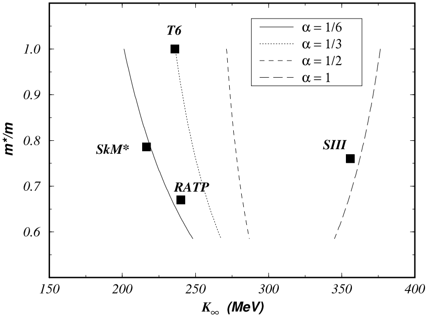
From a three-body term to a density dependent term

- 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*

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

- Sometimes complemented with tensor, D-wave terms, etc.

  T. Lesinski, M. Bender, K.B., T. Duguet, J. Meyer, Phys. Rev. C76, 014312

- Gogny interaction: finite-range + zero-range $\propto \rho_0^\alpha$
- ρ_0^α seems to be the key to succes:
  - Incompressibility
  - Effective mass
  - Stability in spin channels

Effective interaction Vs. Functional

$$E \neq \langle \hat{T} + \hat{V}_{\text{eff}} \rangle$$

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

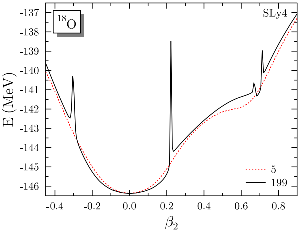
- Functionals: more flexible
  - Complicated, poorly determined or "dangerous" terms, *e.g.* $\mathbb{J}^2$, $\rho_1 \Delta \rho_1$, $\mathbf{s}_0 \Delta \mathbf{s}_0$, $\mathbf{s}_1 \Delta \mathbf{s}_1$, ... can be separately adjusted or disregarded.
  - Simpler interactions can be used in the pairing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

⇒ Very efficient at the mean-field level

- SLyn ($n = 4, 5, 6, 7$),
  Nucl. Phys. **A 627** (1997) 710 and **A 635** (1998) 231
- UNEDFn' ($n' = 0, 1, 2$)
  Phys. Rev. **C 82**, 024313, **C 85**, 024304 and **C 89**, 054314

Beyond mean-field calculations

- Beyond mean field calculations with an EDF



Poles and steps in the projected energy

Expl: Particle number restoration in constrained calc. for ^{18}O

Fig. from M. Bender, PRC 79, 044319

- Poles in the projected energy if $E \neq \langle \hat{T} + \hat{V} \rangle$

  First discussed in M. Anguiano *et al.*, NPA 696 (2001) 467

  Revisited in J. Dobaczewski *et al.*, PRC 76, 054315 (2007)

  and D. Lacroix *et al.*, PRC 79, 044318 (2009)

- Steps in the projected energy if $\hat{V} = \hat{V}(\rho_0^\alpha)$ with $\alpha \notin \mathbb{N}$

  Discussed in T. Duguet *et al.*, PRC 79, 044320 (2009)

Effective interactions for beyond mean-field calculations

- Possible strategies to avoid singularities or to regularized them

  M. Bender *et al.*, PRC 79, 044319 (2009)
  T.R. Rodríguez, J.L. Egido, PRC 81, 064323 (2010)
  G. Hupin *et al.* PRC 84, 014309 (2011)
  W. Satuła, J. Dobaczewski, PRC 90, 054303 (2014)

  G. Salvioni's talk

- But no universal solution as long as $E \neq \langle \hat{T} + \hat{V} \rangle$ or $\hat{V} = \hat{V}(\rho_0)$

  L.M. Robledo, J. Phys. G 37, 064020 (2010)

- One way is to go back to $E = \langle \hat{T} + \hat{V} \rangle$ without density dependent term

  $\rightarrow$ SLyMR0 (and SLyMR1) interaction

- Satisfying properties at the mean-field level ?

- What about Coulomb ? (not a zero-range interaction, for sure...)

Finite-range pseudo-potential

- Interaction at NLO

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

with

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

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

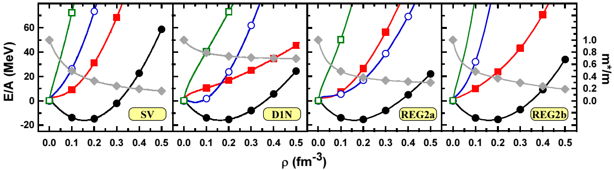
- Higher order derivatives provide an order-by-order correctible theory
  J. Dobaczewski, K.B., F. Raimondi, J. Phys. G 39 (2012) 125103
- Complete derivation of the functional up to N^3LO
  F. Raimondi, K.B., J. Dobaczewski, J. Phys. G 41 (2014) 055112

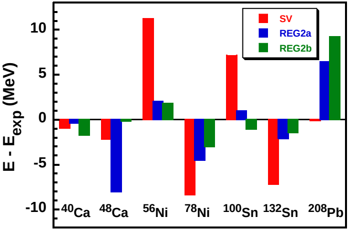
Preliminary results

- Interaction implemented in the HFODD code (no pairing yet)
  - "Handmade" parameters fitting
    (1 spherical doubly magic nucleus $\simeq$ 15 minutes)
  - Two versions of the interactions:

Reg2a:
$t_1 = -t_2$

Reg2b:
$t_1 \neq -t_2$





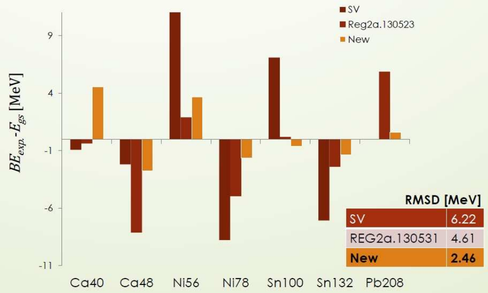
Better than SV, but
not a tremendous achievement

Can we do better ?

How to correct the effective mass ?

Masses of doubly magic nuclei

- Development of a new spherical code
- Allows for more efficient fits

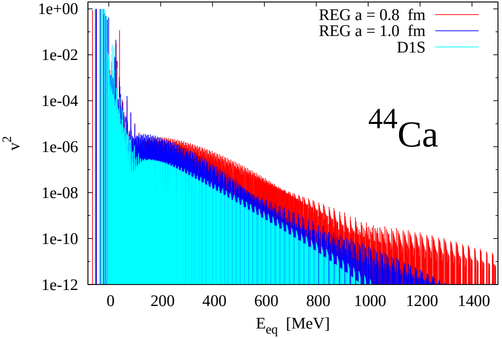


With

$$E/A = -16.2 \text{ MeV}, \quad \rho_{\text{sat}} = 0.16 \text{ fm}^{-3}, \quad K_\infty = 230.5 \text{ MeV},$$
$$m^*/m = 0.41, \quad J = 32.3 \text{ MeV}$$

First results with pairing

- Pairing strength adjusted through 1 matrix element (see Andrea's talk)
- The regularized interaction can give attractive pairing
- Adjustment not trivial...
- Comparison for ^{44}Ca



		$a = 0.8$ fm	$a = 1.0$ fm	D1S
$\langle\Delta_n\rangle$	[MeV]	1.264	1.180	1.104
$E_{\rm p}$	[MeV]	-9.805	-7.874	-7.950
$E_{\rm tot}$	[MeV]	-379.369	-382.961	-384.186

Three-body interaction

m^*/m can only be increased by a term that is beyond two-body...

- Finite-range three-body

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

  as suggested by A. Zapp, R. Roth, H. Hergert[1]

  Neither Goog nor Bad, simply **not** usable in actual codes...

- Zero-range three-body (*aka* the Bad)

$$V_{3\mathrm{N}} = t_3\,\delta(\mathbf{r}_1-\mathbf{r}_2)\,\delta(\mathbf{r}_2-\mathbf{r}_3)$$

  - ♥ No collapse of polarized matter thanks to the finite-range two-body
  - ♠ Not very flexible...
  - ♠ Divergence of the energy beyond the HF approximation

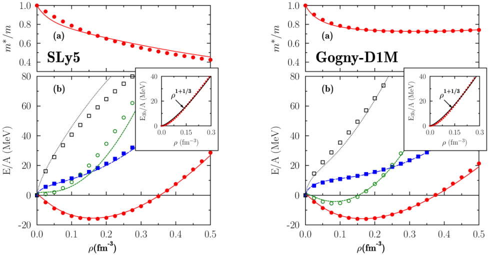
[1] unpublished, as far as I know...

Semi-contact three-body interaction (*aka* the Good)

- $V_{\overline{ijk}} = \frac{1}{3}\left(V_{\overline{ij}k} + V_{\overline{ik}j} + V_{\overline{kj}i}\right)$ with[2]

$$V_{\overline{ij}k} = \left(v_0 + v_\sigma \hat{P}^\sigma + v_\tau \hat{P}^\tau + v_{\sigma\tau} \hat{P}^\sigma \hat{P}^\tau\right) g_a(\mathbf{r}_1 - \mathbf{r}_2)\, \delta\left(\mathbf{r}_3 - \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}\right)$$

- Highly flexible interaction, tested with 2-body part of Skyrme or Gogny



D. Lacroix, K.B. Phys. Rev. C 91, 011302 (R) (2015)

- No divergence of the energy beyond the HF approximation
- Can even generate a surface-peaked effective mass
- But...

"*As a next step, it is now planned to implement this non-local 3-body interaction in codes for finite systems, which presents a formidable technical challenge.*" M. Bender

[2] see J. Sadoudi *et al.*, Phys. Rev. C 88, 064326 for the notations.

"Just enough" regularized interaction (*aka* the not so Ugly)

- We can consider (please suggest a name for it)

$$V_{\overline{ij}k} \equiv u_0\, \delta(\mathbf{r}_1 - \mathbf{r}_2) \left(1 + \hat{P}^\sigma_{12}\right) g_a(\mathbf{r}_2 - \mathbf{r}_3)$$

- which gives in the pairing channel...

$$E_p = u_0 \sum_q \int \mathrm{d}^3 r_1\, \mathrm{d}^3 r_2\, g(\mathbf{r}_1 - \mathbf{r}_2)$$
$$\times \Big\{ \frac{3}{4} \left[\tilde{\rho}^*_q(\mathbf{r}_1, \mathbf{r}_2)\tilde{\rho}_q(\mathbf{r}_2, \mathbf{r}_1) + \tilde{\mathbf{s}}^*_q(\mathbf{r}_1, \mathbf{r}_2) \cdot \tilde{\mathbf{s}}_q(\mathbf{r}_2, \mathbf{r}_1)\right] \rho_{\bar{q}}(\mathbf{r}_1)$$
$$+ \frac{1}{4} \left[\tilde{\rho}^*_q(\mathbf{r}_1, \mathbf{r}_2)\tilde{\mathbf{s}}_q(\mathbf{r}_2, \mathbf{r}_1) + \tilde{\mathbf{s}}^*_q(\mathbf{r}_1, \mathbf{r}_2)\tilde{\rho}_q(\mathbf{r}_2, \mathbf{r}_1)\right] \cdot \mathbf{s}_{\bar{q}}(\mathbf{r}_1) \Big\}$$

- Easy to implement, gives no divergence in HFB calculations (as long as you don't mix protons and neutrons)
- Can be complemented with higher order terms...

Conclusion and roadmap

- We propose a new finite-range pseudo-potential which gives
  - all infinite nuclear matter empirical properties but m^*/m
  - encouraging results for doubly magic nuclei
  - an order-by-order correctible approach
- ph part fully implemented in HFODD (3D code)
- Partially implemented in a new spherical code (local version)
- Better controle of pairing properties and Landau parameters (Andrea's talk)
- The semi-contact three-body interaction may solve the remaining problems...
- Long term goal: use for beyond mean-field calculations...