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

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

- Two families of (early) interactions
  - Skyrme zero-range interaction
    \[ \hat{V}_{12} \propto \delta(r_2 - r_1) \]
    depends on gradients, gives a functional of local densities, needs a cut-off.
    → Set of differential equations
  - Gogny (and Brink-Boeker) finite-range interaction
    \[ \hat{V}_{12} \propto e^{-\frac{(r_2 - r_1)^2}{\mu^2}} \]
    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)

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

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

- Finite-range may improve \( K_{\infty} \) but not \( m^*/m \)

- Need for a three-body term

\[ V_{123} = t_3 \delta(r_2 - r_1) \delta(r_3 - r_1). \]

→ improves the effective mass but...
From a three-body term to a density dependent term

- Collapse a spin polarized matter!!

\[ t_3 \delta(r_2 - r_1) \delta(r_3 - r_1) \longrightarrow \frac{1}{6} t_3 \rho_0 \delta(r_2 - r_3). \]

not an interaction anymore.

- Incompressibility much too high!

\[ \frac{1}{6} t_3 \rho_0 \delta(r_2 - r_3) \longrightarrow \frac{1}{6} t_3 \rho_0^\alpha \delta(r_2 - r_3). \]
The standard (2-body) Skyrme functional

- Effective Skyrme interaction

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

- 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 \(\propto \rho_0^\alpha\)

- \(\rho_0^\alpha\) seems to be the key to success:
  - \(\heartsuit\) Incompressibility
  - \(\heartsuit\) Effective mass
  - \(\heartsuit\) 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 constrain the time-odd terms

- Functionals: more flexible
  - Complicated, poorly determined or “dangerous” terms, e.g. $J^2$, $\rho_1 \Delta \rho_1$, $s_0 \Delta s_0$, $s_1 \Delta s_1$, ... 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

- UNEDF$n'$ ($n' = 0, 1, 2$) Phys. Rev. C 82, 024313, C 85, 024304 and C 89, 054314
Beyond mean-field calculations

- Beyond mean field calculations with an EDF

![Graph showing poles and steps in the projected energy](image)

**Poles and steps in the projected energy**

**Expl:** Particle number restoration in constrained calc. for $^{18}\text{O}$

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 $\hat{V} = \hat{V}(\rho^\alpha_0)$ 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 $\hat{V} = \hat{V}(\rho_0)$

■ 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...)

HFB calculations from a regularized pseudo-potential

K. Bennaceur

Introduction
History
Finite-range pseudo-potential
Pairing
Three-body interaction
Conclusion
Finite-range pseudo-potential

- Interaction at NLO

\[
v = \tilde{v}_0(r_1, r_2; r_3, r_4) t_0 \left( 1\sigma_q + x_0 1_q \hat{P}^\sigma - y_0 1_\sigma \hat{P}^q - z_0 \hat{P}^\sigma \hat{P}^q \right) \\
+ \tilde{v}_1(r_1, r_2; r_3, r_4) t_1 \left( 1\sigma_q + x_1 1_q \hat{P}^\sigma - y_1 1_\sigma \hat{P}^q - z_1 \hat{P}^\sigma \hat{P}^q \right) \\
+ \tilde{v}_2(r_1, r_2; r_3, r_4) t_2 \left( 1\sigma_q + x_2 1_q \hat{P}^\sigma - y_2 1_\sigma \hat{P}^q - z_2 \hat{P}^\sigma \hat{P}^q \right)
\]

with

\[
\tilde{v}_0(r_1, r_2; r_3, r_4) = \delta(r_1 - r_3)\delta(r_2 - r_4) g_a(r_1 - r_2)
\]

\[
\tilde{v}_1(r_1, r_2; r_3, r_4) = \delta(r_1 - r_3)\delta(r_2 - r_4) g_a(r_1 - r_2) \frac{1}{2} \left[ k_{12}^* + k_{34}^2 \right]
\]

\[
\tilde{v}_2(r_1, r_2; r_3, r_4) = \delta(r_1 - r_3)\delta(r_2 - r_4) g_a(r_1 - r_2) k_{12}^* \cdot k_{34}
\]

and \[ g_a(r) = \frac{e^{-\frac{r^2}{a^2}}}{\left( a\sqrt{\pi} \right)^3} \]

- Higher order derivatives provide an order-by-order correctible theory

- Complete derivation of the functional up to N^3LO
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

<table>
<thead>
<tr>
<th>$\langle \Delta n \rangle$ [MeV]</th>
<th>$a = 0.8$ fm</th>
<th>$a = 1.0$ fm</th>
<th>D1S</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{tot}$ [MeV]</td>
<td>-379.369</td>
<td>-382.961</td>
<td>-384.186</td>
</tr>
</tbody>
</table>
Three-body interaction

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

- **Finite-range three-body**

  \[
  V_{3N} = C_{3N} \times e^{\frac{\alpha_{3N}^2}{(r_2 - r_1)^2 + (r_3 - r_2)^2 + (r_1 - r_3)^2}}
  \]

  as suggested by A. Zapp, R. Roth, H. Hergert

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

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

  \[
  V_{3N} = t_3 \delta(r_1 - r_2) \delta(r_2 - r_3)
  \]

  ♥ No collapse of polarized matter thanks to the finite-range two-body

  ♠ Not very flexible...

  ♠ Divergence of the energy beyond the HF approximation

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1 unpublished, as far as I know...
Semi-contact three-body interaction (*aka* the Good)

- \( V_{ijk} = \frac{1}{3} \left( V_{ijk} + V_{ikj} + V_{kji} \right) \) with\(^2\)

\[
V_{ijk} = \left( v_0 + v_\sigma \hat{P}\sigma + v_\tau \hat{P}\tau + v_{\sigma\tau} \hat{P}\sigma \hat{P}\tau \right) g_a (r_1 - r_2) \delta \left( r_3 - \frac{r_1 + r_2}{2} \right)
\]

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

\[\begin{align*}
V_{ijk} &= \frac{1}{3} \left( V_{ijk} + V_{ikj} + V_{kji} \right) \\
V_{ijk} &= \left( v_0 + v_\sigma \hat{P}\sigma + v_\tau \hat{P}\tau + v_{\sigma\tau} \hat{P}\sigma \hat{P}\tau \right) g_a (r_1 - r_2) \delta \left( r_3 - \frac{r_1 + r_2}{2} \right)
\end{align*}\]

- 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."


\[\begin{align*}
\end{align*}\]
“Just enough” regularized interaction (aka the not so Ugly)

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

\[ V_{ijk} \equiv u_0 \delta(\mathbf{r}_1 - \mathbf{r}_2) \left( 1 + \hat{P}_{12}^\sigma \right) g_a(\mathbf{r}_2 - \mathbf{r}_3) \]

- which gives in the pairing channel...

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

- 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...