Issues in global analysis and optimizations of Skyrme forces

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The Skyrme forces

Skyrme interaction (1956) is a very low-momentum phenomenological effective potential with a 2-body part to the 2nd-order and a 3-body part.

\[ V = \sum_{i<j} v(i, j) + \sum_{i<j<k} v(i, j, k) \]

**central term**
\[ V(\vec{r}_1, \vec{r}_2) = t_0 (1 + x_0 P_\sigma) \delta(\vec{r}) \]

**Tensor term**
\[ \frac{1}{2} T(\sigma_1 \cdot k \sigma_2 \cdot k - \frac{1}{3} \sigma_1 \cdot \sigma_2 k^2 + \text{conj.}) \]
\[ \frac{1}{2} U(\sigma_1 \cdot k' \sigma_2 \cdot k - \frac{1}{3} \sigma_1 \cdot \sigma_2 k' \cdot k + \text{conj.}) \]

**3-body term in Skyrme force:**

Important for saturation properties
\[ v_{ijk}^{(3)} = t_3 \delta(\vec{r}_i - \vec{r}_j) \delta(\vec{r}_j - \vec{r}_k) \]

\[ v_{ijk}^{(3)} \sim v_{ij}^{(2)} = \frac{1}{6} t_3 (1 + P_\sigma) \delta(\vec{r}_i - \vec{r}_j) \rho(\frac{\vec{r}_i + \vec{r}_j}{2}) \]

Too large incompressibility

\[ v_{ijk}^{(3)} \sim v_{ij}^{(2)}, \quad \frac{1}{6} t_3 (1 + P_\sigma) \delta(\vec{r}_i - \vec{r}_j) \rho(\vec{r})^\gamma \]

**Usually a fractional power density dependency is introduced to simulate 3-body and many body forces;** the power dependency is an open question.

\[ \gamma \text{ ranges from } 1/6 \text{ to } 1 \]
\[ \gamma = 1/6 \text{ in } \text{SLy4, SkM*, SkP}; \ 0.25 \text{ in Sklx} \]
\[ \gamma = 1/3 \text{ in Gogny, Bsk1} \]
\[ \text{UNEDF0}=0.32, \text{ UNEDF1}=0.27 \]
Various Optimizations

- UNEDF Skyrme forces have been extremely optimized using POUNDERS

- Brussel Skyrme forces with phenomenological corrections obtained high precisions

- Various extensions of Skyrme forces: additional momentum dependences or density dependencies

- Other developments: Pionless EFT, density matrix expansion, Pseudopotential Skyrme forces to 6th order, ab initio EDF

  M. Stoitsov, et al., PRC 82, 054307 (2010)
Our refitting procedure

\[
\varepsilon = \frac{3\hbar^2}{10m} (3\pi^2)^{2/3} \rho^{5/3} + \frac{\hbar^2 \pi a}{m} \rho^2 + \frac{2\hbar^2 a^2 3^{4/3} \pi^{2/3}}{35m} (11 - 2 \ln 2) \rho^{7/3} \\
+ 0.78 \frac{\hbar^2 a^3 3^{5/3} \pi^{10/3}}{2m} \rho^{8/3}
\]

\[\rho = k_F^3 / 3\pi^2 \quad a = r/d\]


\[
\psi_{ij}^{(2)} = \frac{1}{6} t_3 \left( 1 + x_3 P_\sigma \right) \rho(R)^\nu \delta(r_i - r_j) \\
+ \frac{1}{6} t_3E \left( 1 + x_3E P_\sigma \right) \rho(R)^{\nu+\frac{1}{3}} \delta(r_i - r_j).
\]

With an additional higher-order density dependent terms

- Only refit the momentum independent parameters: t0, t3, t3E, leading regularization terms for saturation properties
- Induced three body and many-body forces are huge in the soft Skyrme force, and a single term may not be sufficient for various systems from dilute halos to high density neutron stars
- Using simulated annealing method, fitting binding energies of 50 nuclei and charge radii of 8 spherical nuclei
**Binding energies**

- Calculations of 603 even-even nuclei, reduce the rms by 10\textasciitilde20\%.
- In light nuclei, binding energies of $N=Z$ nuclei are underestimated (M. Stoitsov, et al. PRL 98, 132502 (2007)).
- In heavy nuclei, the shell effects are overestimated.
Fission barriers

- Parameter sets which are good at binding energies are not good at fission barriers
- Proton-rich heavy nuclei are less binding, neutron-rich medium nuclei are over binding, indicting conflicting isospin dependences
  (surface symmetry energy, N. Nikola et al, PRC83, 034305 (2011))
High-order density dependent term is needed for high-density EOS, neutron stars
• Increase incompressibility and pressure at high densities
• Reduce symmetry energies at high densities
(soft symmetry energy by $\pi^-/\pi^+$ ratio, Z.G.Xiao et al, PRL 102, 062502 (2009).
Charge radii of 309 even nuclei SkM* (rms=0.023 fm) is slightly better than UNEDF0 (rms=0.027 fm)
The two-body center of mass correction

\[ E_{c.m.} = \frac{1}{2mA} \sum_{i=1}^{A} p_i^2 + \frac{1}{2mA} \sum_{i>j} p_i \cdot p_j \]


Two-body CoM: 4.05A^{0.21}  
One-body CoM: -14.58A^{0.047}  
Total CoM: -18.33A^{-0.208}

Two-body CoM: 4.20A^{0.21}  
One-body CoM: -14.92A^{0.046}  
Total CoM: -18.61A^{-0.213}

The two-body com corrections is close to the surface curvature energy A^{1/3}

The usually missing two-body part has different mass dependence, beyond one-body cm optimizations.
Lipkin-Nogami corrections

- Approximate restoration of the particle number conservation

\[ |\Delta E_{LN} = E_{HF-LN} - E_{HF-BCS}| \]

BCS: rms = 1.31
LN: rms = 1.29

- LN corrections show shell effects
- Lipkin-Nogami doesn’t improve the global binding energies significantly


Angular momentum projection has not been considered presently
Perspectives

- To develop a high-precision nuclear energy density functional for general purposes is a challenge.
- The high-order term can improve the descriptions of binding energies by 10~20%; impact high-density EOS.
- Various corrections or restorations, local fluctuations should be systematically studied.
- Skyrme Hartree-Fock ≠ DFT.
- Consider include Bayesian methods and advanced optimizations.

Thank you for your attention!