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Issues in global analysis and optimizations of Skyrme forces

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- X.Y. Xiong, J. C. Pei, W.J. Chen, Phys. Rev. C 93, 024311 (2016)
- Z.W. Zuo, J.C. Pei, X.Y. Xiong, Y. Zhu , arXiv:1709.00802

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.

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

Tensor term

$$\frac{1}{2}T(\boldsymbol{\sigma}_1\cdot\boldsymbol{k}\boldsymbol{\sigma}_2\cdot\boldsymbol{k} - \frac{1}{3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\boldsymbol{k}^2 + \text{conj.})$$
$$\frac{1}{2}U(\boldsymbol{\sigma}_1\cdot\boldsymbol{k}'\boldsymbol{\sigma}_2\cdot\boldsymbol{k} - \frac{1}{3}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\boldsymbol{k}'\cdot\boldsymbol{k} + \text{conj.})$$

$$V(\vec{r}_1,\vec{r}_2) = t_0(1+x_0P_\sigma)\delta(\vec{r}) \qquad \text{central term}$$
$$+\frac{1}{2}t_1(1+x_1P_\sigma)[\vec{P}'^2\delta(\vec{r})+\delta(\vec{r})\vec{P}^2]$$
$$+t_2(1+x_2P_\sigma)\vec{P}'\delta(\vec{r})\vec{P} \qquad \text{non-local terms}$$
$$+iW_0\vec{\sigma}\bullet[\vec{P}'\times\delta(\vec{r})\vec{P}] \qquad \text{spin-orbit term}$$

3-body term in Skyrme force:

Important for saturation properties

$$v_{ijk}^{(3)} = t_3\delta(\vec{r}_i-\vec{r}_j)\delta(\vec{r}_j-\vec{r}_k)$$

$$V_{ijk}^{(3)} \sim V_{ij}^{(2)\prime} = \frac{1}{6}t_3(1+P_\sigma)\delta(\vec{r}_i-\vec{r}_j)\rho\left(\frac{\vec{r}_i+\vec{r}_j}{2}\right)$$

Too large incompressibility

$$\boxed{V_{ijk}^{(3)} \sim V_{ij}^{(2)\prime} = \frac{1}{6}t_3(1+P_\sigma)\delta(\vec{r}_i-\vec{r}_j)\rho(\vec{r})^{\gamma}}$$

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

γ ranges from 1/6 to 1
γ=1/6 in SLy4, SkM*, SkP; 0.25 in SkIx
γ=1/3 in Gogny, Bsk1
UNEDF0=0.32, UNEDF1=0.27

Various Optimizations

- UNEDF Skyrme forces have been extremely optimized using POUNDERS

  M. Kortelainen et al., Phys. Rev. C 82, 024313 (2010).

- Brussel Skyrme forces with phenomenological corrections obtained high precisions

  S. Goriely, et al., Phys. Rev. C 82, 035804 (2010)

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

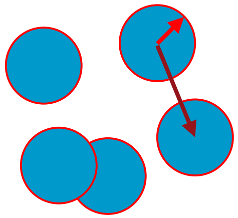
- Other developments: Pionless EFT, density matrix expansion, Pseudopotential Skyrme forces to 6^{th} order, ab initio EDF

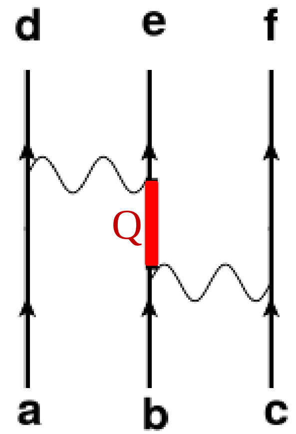
  B. G. Carlsson, et al.,PRC 78, 044326 (2008)
  M. Stoitsov, et al., PRC 82, 054307 (2010)
  M. Grasso, D. Lacroix, and U. van Kolck, Phys. Scr. 91, 063005(2016).
  R. J. Furnstahl, Lecture Notes in Physics, Vol.852, 133(Springer-Verlag, 2012).

Our refitting procedure

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

$$\rho = k_F^3/3\pi^2$$ a=r/d





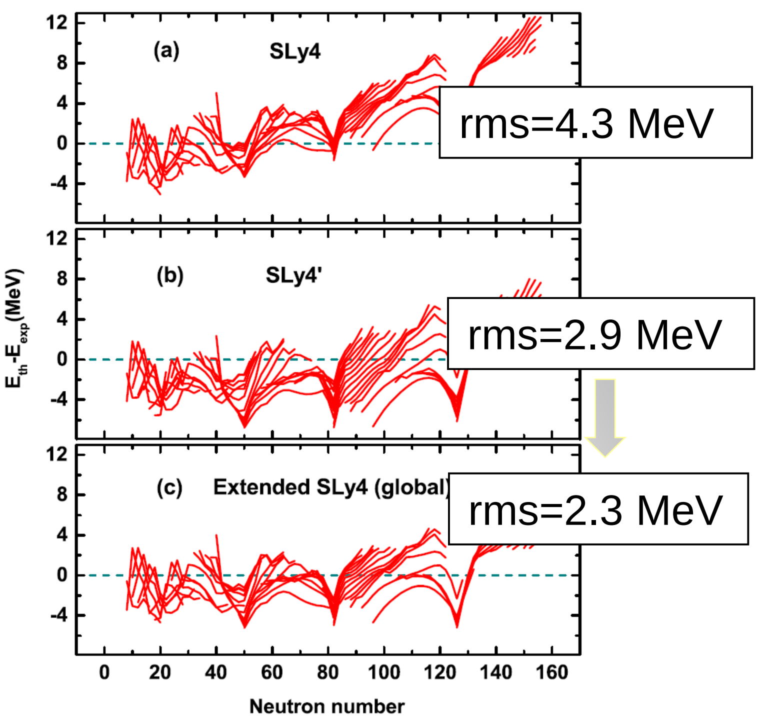
Lee-Yang-Hung, Phys. Rev. 105, 1119 (1957).

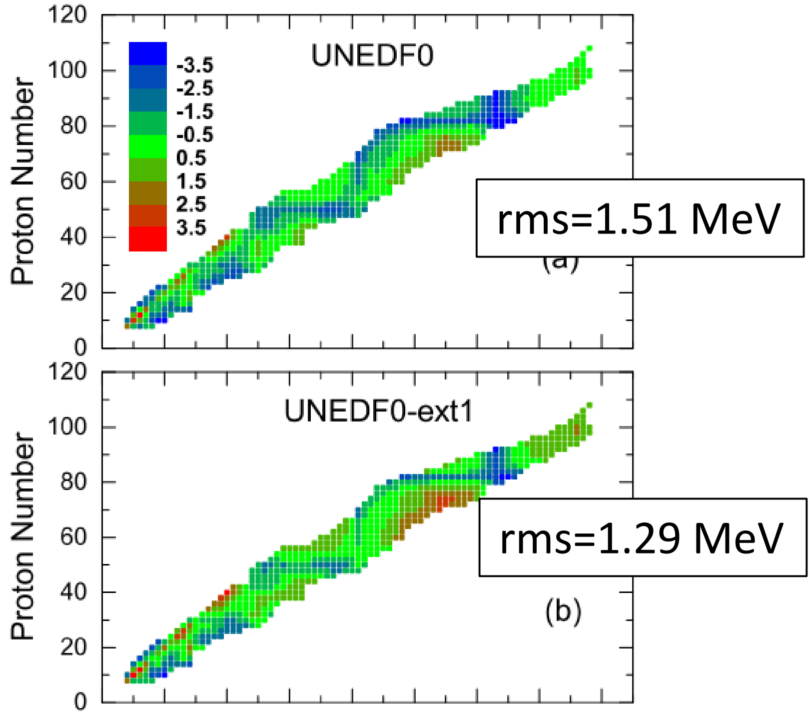
$$v_{ij}^{(2)\prime} = \tfrac{1}{6}t_3(1+x_3P_\sigma)\rho(\mathbf{R})^\gamma\delta(\boldsymbol{r}_i-\boldsymbol{r}_j)$$
$$+\tfrac{1}{6}t_{3E}(1+x_{3E}P_\sigma)\rho(\mathbf{R})^{\gamma+\frac{1}{3}}\delta(\boldsymbol{r}_i-\boldsymbol{r}_j).$$

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

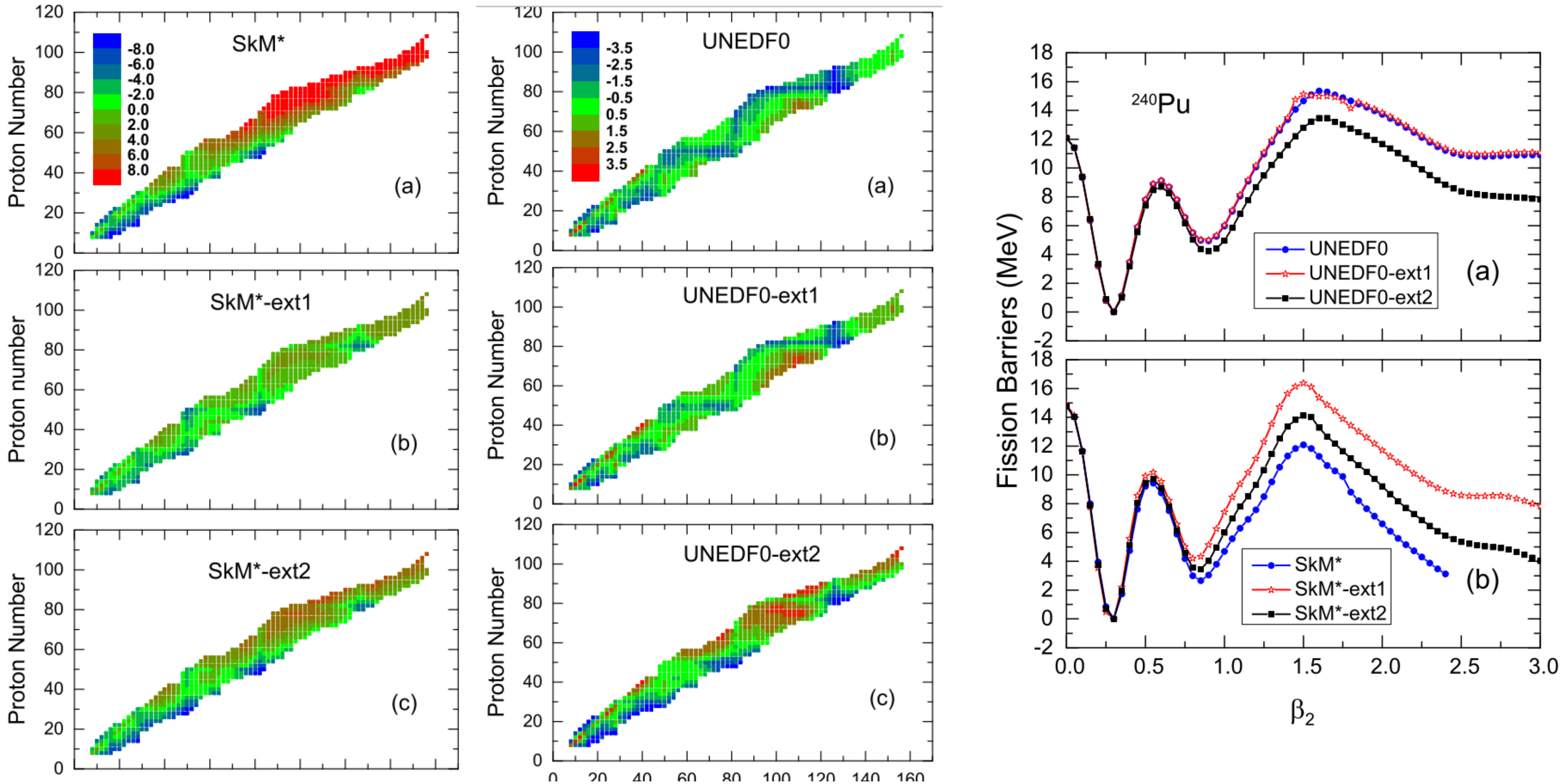
Binding energies





- Calculations of 603 even-even nuclei, reduce the rms by 10~20%
- 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

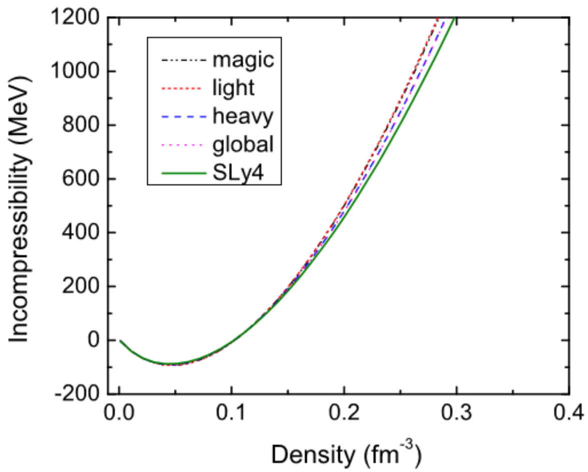
Fission barriers

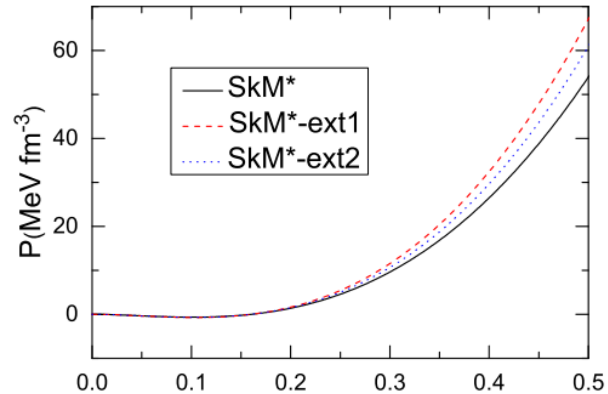


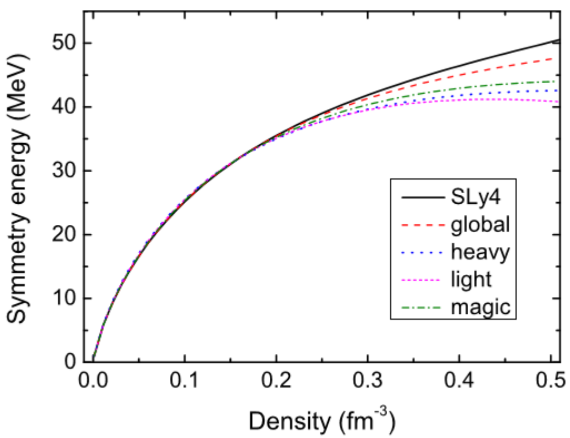
- Parameter sets which are good at binding energies are not good at fission barriers
- Proton-rich heavy nuclei are less binding, neutron-rich medium nuclei are over binding, indicting conflicting isospin dependences

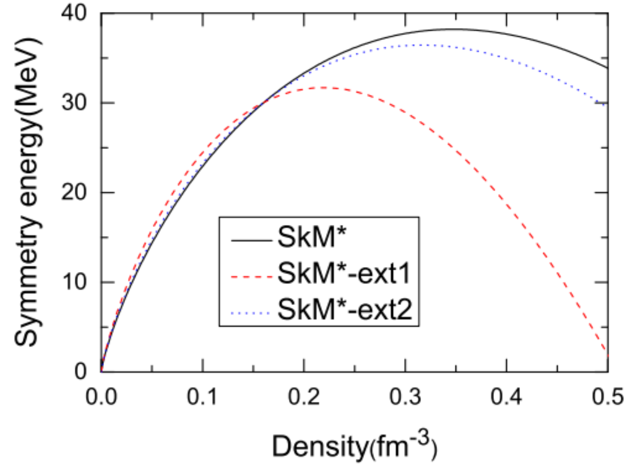
(surface symmetry energy, N. Nikola et al, PRC83, 034305 (2011)

EOS





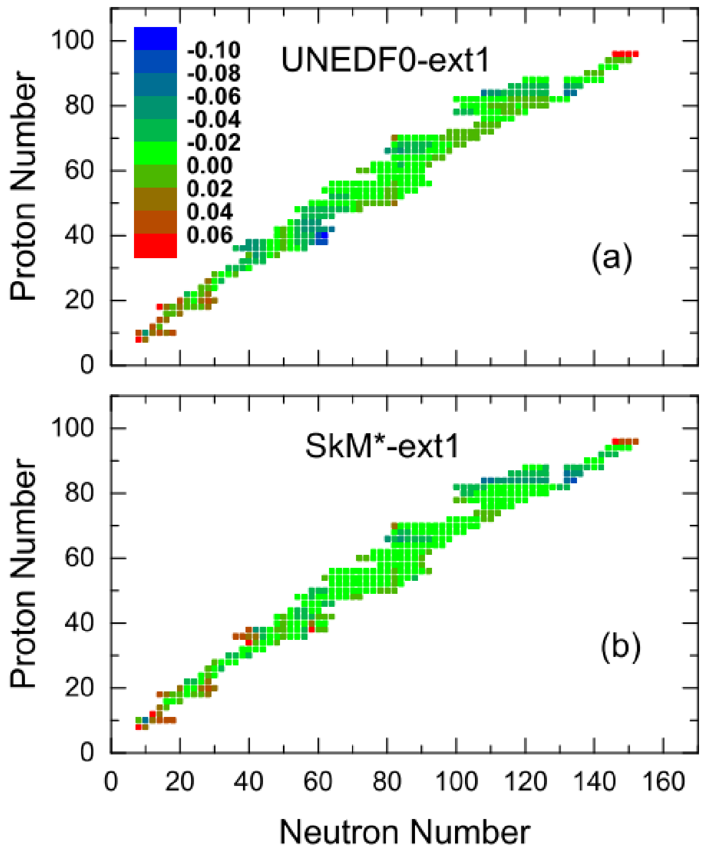




- High-order density dependent term is needed for high-density EOS, neutron stars
- Increase incompressibility and pressure at high densities
- Reduce symmetry energies at high densities

(soft symmetry energy by π^-/π^+ ratio , Z.G.Xiao et al, PRL 102, 062502 (2009).

Charge radii



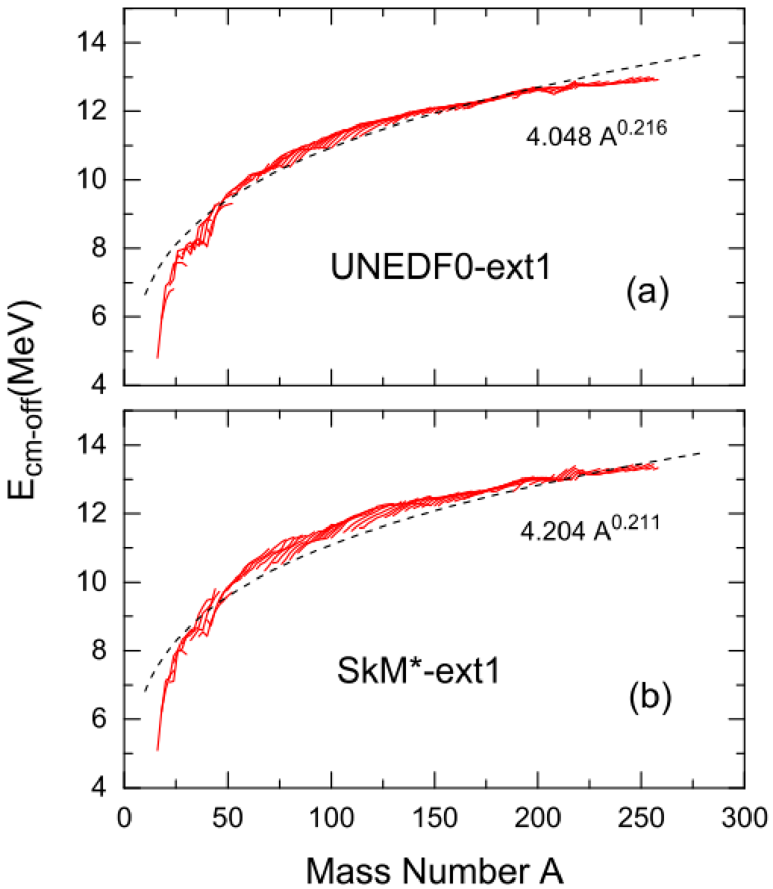
Charge radii of 309 even nuclei
SkM* (rms=0.023 fm) is slightly better than UNEDF0 (rms=0.027 fm)

CoM corrections

The two-body center of mass correction

$$E_{c.m.} = \frac{1}{2mA}\sum_{i=1}^{A}\mathbf{P}_i^2 + \frac{1}{2mA}\sum_{i>j}\mathbf{P}_i\cdot\mathbf{P}_j$$

Important for surface energy and fission barriers, Bender, et al, Eur. Phys. J. A 7, 467 (2000).



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: $-14.92A^{0.046}$

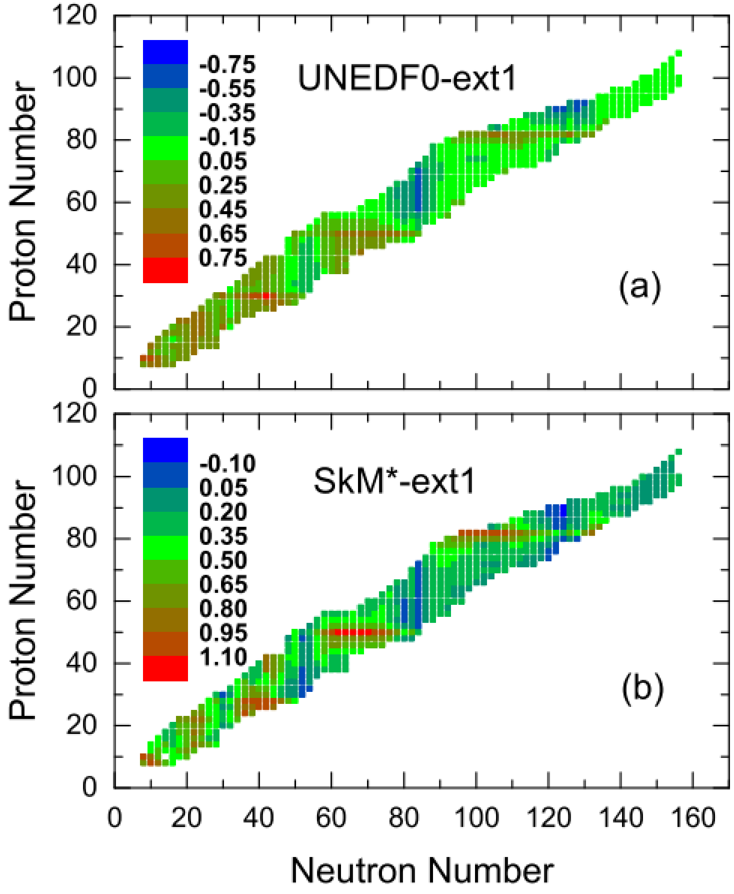
Total CoM: $-18.61A^{-0.213}$

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



$$\Delta E_{LN} = E_{\mathrm{HF-LN}} - E_{\mathrm{HF-BCS}}$$

BCS: rms =1.31

LN: rms=1.29

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

M. Samyn, et al.,
Phys. Rev. C 70, 044309 (2004).

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!