Modern Energy Functional for Nuclei and Nuclear Matter

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Introduction

- Important task: Develop a modern Energy Density Functional (EDF) with enhanced predictive power for properties of rare nuclei.

- We start from EDF obtained from Skyrme N-N interaction.

- The effective Skyrme interaction has been used in mean-field models for several decades and many different parameterizations of the interaction have been realized to reproduce nuclear masses, radii and other data of nuclei. Since more experimental data has become available, we are able to fit our results to a broader collection of nuclei at and far from the stability line.

The many-body problem

- In order to determine the properties of a nucleus it is necessary to solve the time-independent Schrödinger equation.

$$H\Psi_n(1,\ldots,A) = E_n\Psi_n(1,\ldots,A)$$

- The many-body Hamiltonian is given by

$$H = \sum_i -\frac{\hbar^2}{2m_i}\vec{\nabla}_i^2 + \sum_{i\langle j} V_{ij}$$

- Unfortunately, it is difficult to obtain a solution to the many-body equation.

The Hartree-Fock Method

- Hartree-Fock (HF) is a method for obtaining an approximate solution to the many body problem in Quantum Mechanics.
- It uses the mean field approximation, where each particle interacts with an average potential produced by its interaction with all other particles.
- Effects due to correlated motion of many nucleons are not accounted for by the HF approximation.

Slater determinants

- In HF the many-nucleon (fermion) wave function Φ is approximated by an antisymmetric product of single particle wave functions $\varphi_i(r)$.
- This wave function Φ can be written as a Slater determinant, which guarantees an antisymmetric wave function of the *A* nucleons system.

$$\Phi = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_1(\vec{r}_1,\sigma_1,\tau_1) & \phi_2(\vec{r}_1,\sigma_1,\tau_1) & \dots & \phi_A(\vec{r}_1,\sigma_1,\tau_1) \\ \phi_1(\vec{r}_2,\sigma_2,\tau_2) & \phi_2(\vec{r}_2,\sigma_2,\tau_2) & \dots & \phi_A(\vec{r}_2,\sigma_2,\tau_2) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_1(\vec{r}_A,\sigma_A,\tau_A) & \phi_2(\vec{r}_A,\sigma_A,\tau_A) & \dots & \phi_A(\vec{r}_A,\sigma_A,\tau_A) \end{vmatrix}$$

The Hartree Fock Equation

- The HF equation is derived using Variational Calculus, by minimizing the Energy Functional.

$$E = \left\langle \Phi \middle| \hat{H}_{total} \middle| \Phi \right\rangle$$

- The total Hamiltonian of the nucleus is

$$\hat{H}_{total} = T + V = \sum_{i=1}^{A} \frac{p_i^2}{2m_i} + \sum_{i\langle j=1} V\left(\vec{r}_i, \vec{r}_j\right)$$

where,

$$V(\vec{r}_i, \vec{r}_j) = V_{ij}^{NN} + V_{ij}^{Coul}.$$

- The total energy is

$$E = \left\langle \Phi \middle| \hat{H}_{total} \middle| \Phi \right\rangle = -\frac{\hbar^2}{2m} \sum_{i=1}^{A} \int \phi_{\alpha_i}^*(\vec{r}) \Delta \phi_{\alpha_i}(\vec{r}) d\vec{r}$$

$$+ \sum_{i\langle j}^{A} \int \phi_{\alpha_i}^*(\vec{r}) \phi_{\alpha_j}^*(\vec{r}\,') V(\vec{r}, \vec{r}\,') \phi_{\alpha_i}(\vec{r}) \phi_{\alpha_j}(\vec{r}\,') d\vec{r} d\vec{r}\,'$$

$$- \sum_{i\langle j}^{A} \int \phi_{\alpha_i}^*(\vec{r}) \phi_{\alpha_j}^*(\vec{r}\,') V(\vec{r}, \vec{r}\,') \phi_{\alpha_i}(\vec{r}\,') \phi_{\alpha_j}(\vec{r}) d\vec{r} d\vec{r}\,'$$

Skyrme interaction

- To model the nuclear force V^{NN}, the Skyrme effective nucleon-nucleon interaction is used.

$$V_{ij}^{NN} = t_0(1 + x_0\ P_{ij}^{\ \sigma})\delta(\vec{r}_i - \vec{r}_j) + \frac{1}{2}t_1(1 + x_1 P_{ij}^{\ \sigma})[\overleftarrow{k}_{ij}^2\delta(\vec{r}_i - \vec{r}_j) + \delta(\vec{r}_i - \vec{r}_j)\vec{k}_{ij}^2]$$

$$+ t_2(1 + x_2 P_{ij}^{\ \sigma})\overleftarrow{k}_{ij}\delta(\vec{r}_i - \vec{r}_j)\vec{k}_{ij} + \frac{1}{6}t_3(1 + x_3 P_{ij}^{\ \sigma})\rho^{\alpha}\left(\frac{\vec{r}_i + \vec{r}_j}{2}\right)\delta(\vec{r}_i - \vec{r}_j) +$$

$$iW_0\overleftarrow{k}_{ij}\delta(\vec{r}_i - \vec{r}_j)(\vec{\sigma}_i + \vec{\sigma}_j) \times \vec{k}_{ij}.$$

where, P_{ij}^{σ} is the spin exchange operator, $\vec{k}_{ij} = -i(\vec{\nabla}_i - \vec{\nabla}_j)/2$ and $\overleftarrow{k}_{ij} = -i(\overleftarrow{\nabla}_i - \overleftarrow{\nabla}_j)/2$, where the right and left arrows indicate that the momentum operators act on the right and on the left, respectively.

t_i, x_i, α, W_0 are the Skyrme parameters, which need to be determined.

The total energy is then given by

$$E = \left\langle \Phi \middle| \hat{H}_{total} \middle| \Phi \right\rangle = \left\langle \Phi \middle| T + V_{Coulomb} + V_{12} \middle| \Phi \right\rangle = \int H(\vec{r}) d\vec{r},$$

where the energy density functional $H(\vec{r})$ is

$$H(\vec{r}) = H_{Kinetic}(\vec{r}) + H_{Coulomb}(\vec{r}) + H_{Skyrme}(\vec{r})$$

$$H_{Kinetic}(\vec{r}) = \frac{\hbar^2}{2m_p}\tau_p(\vec{r}) + \frac{\hbar^2}{2m_n}\tau_n(\vec{r})$$

$$H_{Coulomb}(\vec{r}) = \frac{e^2}{2}\left[\rho_{ch}(\vec{r})\int \frac{\rho_{ch}(\vec{r}\,')}{\left|\vec{r}-\vec{r}\,'\right|} d\vec{r}\,' - \int \frac{\left|\rho_{ch}(\vec{r},\vec{r}\,')\right|^2}{\left|\vec{r}-\vec{r}\,'\right|} d\vec{r}\,'\right]$$

And the Skyrme energy density functional is

$$H_{Skyrme}(\vec{r}) = H_0 + H_3 + H_{eff} + H_{fin} + H_{so} + H_{sg}$$

$$\mathcal{H}_0 = \frac{1}{4} t_0 \left[(2 + x_0)\rho^2 - (2x_0 + 1)(\rho_p^2 + \rho_n^2) \right],$$

$$\mathcal{H}_3 = \frac{1}{24} t_3 \rho^\alpha \left[(2 + x_3)\rho^2 - (2x_3 + 1)(\rho_p^2 + \rho_n^2) \right],$$

$$\mathcal{H}_{\text{eff}} = \frac{1}{8} \left[t_1(2 + x_1) + t_2(2 + x_2) \right] \tau\rho + \frac{1}{8} \left[t_2(2x_2 + 1) - t_1(2x_1 + 1) \right] (\tau_p \rho_p + \tau_n \rho_n),$$

$$\begin{aligned}
\mathcal{H}_{\text{fin}} &= \frac{1}{32} \left[3t_1(2 + x_1) - t_2(2 + x_2) \right] (\nabla\rho)^2 \\
&\quad - \frac{1}{32} \left[3t_1(2x_1 + 1) + t_2(2x_2 + 1) \right] \left[(\vec{\nabla}\rho_p)^2 + (\vec{\nabla}\rho_n)^2 \right], \\
\mathcal{H}_{\text{so}} &= \frac{W_0}{2} \left[\mathbf{J} \cdot \nabla\rho + \mathbf{J}_p \cdot \nabla\rho_p + \mathbf{J}_n \cdot \nabla\rho_n \right], \\
\mathcal{H}_{\text{sg}} &= -\frac{1}{16}(t_1 x_1 + t_2 x_2)\mathbf{J}^2 + \frac{1}{16}(t_1 - t_2) \left[\mathbf{J}_p^2 + \mathbf{J}_n^2 \right].
\end{aligned}$$

$$\rho(\vec{r}) = \sum_{\tau} \rho_{\tau}(\vec{r}) \qquad \rho_{\tau}(\vec{r}) = \sum_{i=1}^{A} \sum_{\sigma} \phi_i^*(\vec{r},\sigma,\tau)\phi_i(\vec{r},\sigma,\tau)$$

$$\tau(\vec{r}) = \sum_{\tau} \tau_{\tau}(\vec{r}) \qquad \tau_{\tau}(\vec{r}) = \sum_{i=1}^{A} \sum_{\sigma} \left|\vec{\nabla}\phi_i(\vec{r},\sigma,\tau)\right|^2$$

$$\vec{J}(\vec{r}) = \sum_{\tau} \vec{J}_{\tau}(\vec{r}) \qquad \vec{J}_{\tau}(\vec{r}) = -i\sum_{i=1}^{A} \sum_{\sigma,\sigma'} \phi_i^*(\vec{r},\sigma,\tau)\left[\vec{\nabla}\phi_i(\vec{r},\sigma',\tau)\times\left\langle\sigma\left|\vec{\sigma}\right|\sigma'\right\rangle\right]$$

$$\rho_{ch}(\vec{r},\vec{r}') = \sum_{i,\sigma,\sigma'} \phi_i^*(\vec{r},\sigma,\frac{1}{2})\phi_i(\vec{r}',\sigma',\frac{1}{2})$$

Now we apply the variation principle to derive the Hartree-Fock equations. We minimize

$$E = \left\langle \Phi \left| \hat{H}_{total} \right| \Phi \right\rangle$$

$$\frac{\delta}{\delta\rho_{\sigma,\tau}}\left[E - \sum_i \varepsilon_i \int \rho_{\sigma,\tau} d\vec{r}\right] = \frac{\delta E}{\delta\rho_{\sigma,\tau}} - \frac{\delta\left[\sum_i \varepsilon_i \int \rho_{\sigma,\tau} d\vec{r}\right]}{\delta\rho_{\sigma,\tau}} = 0$$

where

$$\delta E = \sum_{\sigma,\tau} \int \left[\frac{\hbar^2}{2m_\tau^*(\vec{r})} \delta\tau_{\sigma\tau}(\vec{r}) + U_\tau(\vec{r}) \delta\rho_{\sigma\tau}(\vec{r}) + \vec{W}_\tau(\vec{r}) \delta\vec{J}_{\sigma\tau}(\vec{r}) \right] d\vec{r}$$

$$\delta\rho_{\sigma\tau} = \sum_{i,\sigma'} \phi_i(\vec{r},\sigma',\tau) \delta\phi_i^*(\vec{r},\sigma',\tau)$$

$$\delta\tau_{\sigma\tau}(\vec{r}) = \sum_{i,\sigma'} \vec{\nabla}\phi_i(\vec{r},\sigma',\tau) \vec{\nabla}\delta\phi_i^*(\vec{r},\sigma',\tau)$$

$$\delta\vec{J}_{\sigma\tau}(\vec{r}) = -i \sum_{i,\sigma',\sigma''} \delta\phi_i^*(\vec{r},\sigma',\tau) \left[\vec{\nabla}\phi_i(r,\sigma'',\tau) \times \left\langle \sigma' \middle| \vec{\sigma} \middle| \sigma'' \right\rangle \right]$$

Hartree-Fock Equations

After carrying out the minimization of energy, we obtain the HF equations:

$$\frac{\hbar^2}{2m_\tau^*(r)}\left[-R_\alpha''(r)+\frac{l_\alpha(l_\alpha+1)}{r^2}R_\alpha(r)\right]-\frac{d}{dr}\left(\frac{\hbar^2}{2m_\tau^*(r)}\right)R_\alpha'(r)$$

$$+\left[U_\tau(r)+\frac{1}{r}\frac{d}{dr}\left(\frac{\hbar^2}{2m_\tau^*(r)}\right)+\frac{\left[j_\alpha(j_\alpha+1)-l_\alpha(l_\alpha+1)-\frac{3}{4}\right]}{r}W_\tau(r)\right]R_\alpha(r)$$

$$=\varepsilon_\alpha R_\alpha(r)$$

where $m_\tau^*(r)$, $U_\tau(r)$, and $W_\tau(r)$ are the effective mass, the potential and the spin orbit potential. They are given in terms of the Skyrme parameters and the nuclear densities.

Definitions

$$\frac{\hbar^2}{2m_\tau^*(\vec{r})} = \frac{\hbar^2}{2m_\tau} + \frac{1}{4}\left[t_1(1+\frac{1}{2}x_1) + t_2(1+\frac{1}{2}x_2)\right]\rho(\vec{r}) - \frac{1}{4}\left[t_1(\frac{1}{2}+x_1) - t_2(\frac{1}{2}+x_2)\right]\rho_\tau(\vec{r})$$

$$U_\tau(\vec{r}) = t_0(1+\frac{1}{2}x_0)\rho(\vec{r}) - t_0(\frac{1}{2}+x_0)\rho_\tau(\vec{r}) + \frac{1}{4}\left[t_1(1+\frac{1}{2}x_1) + t_2(1+\frac{1}{2}x_2)\right]\tau(\vec{r})$$

$$-\frac{1}{4}\left[t_1(\frac{1}{2}+x_1) - t_2(\frac{1}{2}+x_2)\right]\tau_\tau(\vec{r}) + \frac{\alpha+2}{12}t_3(1+\frac{1}{2}x_3)\rho^{\alpha+1}(\vec{r})$$

$$-\frac{\sigma}{12}t_3(\frac{1}{2}+x_3)\rho^{\alpha-1}(\vec{r})\left(\rho_\tau^2(\vec{r}) + \rho_{-\tau}^2(\vec{r})\right) - \frac{1}{6}t_3(\frac{1}{2}+x_3)\rho^\alpha(\vec{r})\rho_\tau$$

$$-\frac{1}{8}\left[3t_1(1+\frac{1}{2}x_1) - t_2(1+\frac{1}{2}x_2)\right]\nabla^2\rho(\vec{r}) + \frac{1}{8}\left[3t_1(\frac{1}{2}+x_1) + t_2(\frac{1}{2}+x_2)\right]\nabla^2\rho_\tau(\vec{r})$$

$$-\frac{1}{2}W_0\left[\nabla\vec{J}(\vec{r}) + \nabla\vec{J}_\tau(\vec{r})\right] + \delta_{\tau,\frac{1}{2}}e^2\int d\vec{r}\,'\frac{\rho_{ch.}(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|},$$

$$W_\tau(\vec{r}) = \frac{1}{2}W_0\left[\nabla\vec{\rho}(\vec{r}) + \nabla\vec{\rho}_\tau(\vec{r})\right] + \frac{1}{8}(t_1 - t_2)\vec{J}_\tau(\vec{r}) - \frac{1}{8}[t_1x_1 - t_2x_2]\vec{J}(\vec{r})$$

Fitted data

- The binding energies for 14 nuclei ranging from normal to the exotic (proton or neutron) ones: ^{16}O, **^{24}O**, **^{34}Si**, ^{40}Ca, ^{48}Ca, **^{48}Ni**, ^{56}Ni, ^{68}Ni, ^{78}Ni, ^{88}Sr, ^{90}Zr, **^{100}Sn**, ^{132}Sn, and ^{208}Pb.

- Charge rms radii for 7 nuclei: ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, **^{88}Sr**, ^{90}Zr, ^{208}Pb.

- **The spin-orbit splittings for 2*p* proton and neutron orbits for ^{56}Ni**

$$\varepsilon(2p_{1/2}) - \varepsilon(2p_{3/2}) = 1.88 \text{ MeV (neutron)}$$
$$\varepsilon(2p_{1/2}) - \varepsilon(2p_{3/2}) = 1.83 \text{ MeV (proton).}$$

- **Rms radii for the valence neutron:**

in the $1d_{5/2}$ orbit for ^{17}O $\quad r_n(1d_{5/2}) = 3.36\, fm$

in the $1f_{7/2}$ orbit for ^{41}Ca $\quad r_n(1f_{7/2}) = 3.99\, fm$

- **The breathing mode energy for 4 nuclei: ^{90}Zr (17.81 MeV), ^{116}Sn (15.9 MeV), ^{144}Sm (15.25 MeV), and ^{208}Pb (14.18 MeV).**

Note: Bold face indicates data taken in our fit for the first time.

Simulated annealing method (SAM)

The SAM is a method for optimization problems of large scale, in particular, where a desired global extremum is hidden among many local extrema.

We use the SAM to determine the values of the Skyrme parameters by searching the global minimum for the chi-square function

$$\chi^2 = \frac{1}{N_d - N_p} \sum_{i=1}^{N_d} \left(\frac{M_i^{\exp} - M_i^{th}}{\sigma_i} \right)^2$$

N_d is the number of experimental data points.

N_p is the number of parameters to be fitted.

$M_i^{\exp}$ and M_i^{th} are the experimental and the corresponding theoretical values of the physical quantities.

σ_i is the adopted uncertainty.

Implementing the SAM to search the global minimum of χ^2 function:

1. $t_i,\ x_i,\ \alpha,\ W_0$ are written in terms of $B/A,\quad K_{nm},\quad \rho_{nm},\ldots$

2. Define $\vec{v}(B/A, K_{nm}, \rho_{nm}, m^*/m, E_s, J, L, \kappa, G_0^{'}, W_0)$

3. Calculate χ^2_{old} for a given set of experimental data and the corresponding HF results (using an <u>initial guess</u> Skyrme parameters).

4. Determine a <u>new set</u> of Skyrme parameters by the following steps:

   + Use a random number to select a component v_r of vector $\vec{v}$

   + Use another random number η to get a new value of v_r

$$v_r \rightarrow v_r + d\eta$$

   + Use this modified vector $\vec{v}$ to generate a new set of Skyrme parameters.

5. Go back to HF and calculate χ^2_{new}

6. The new set of Skyrme parameters is accepted only if

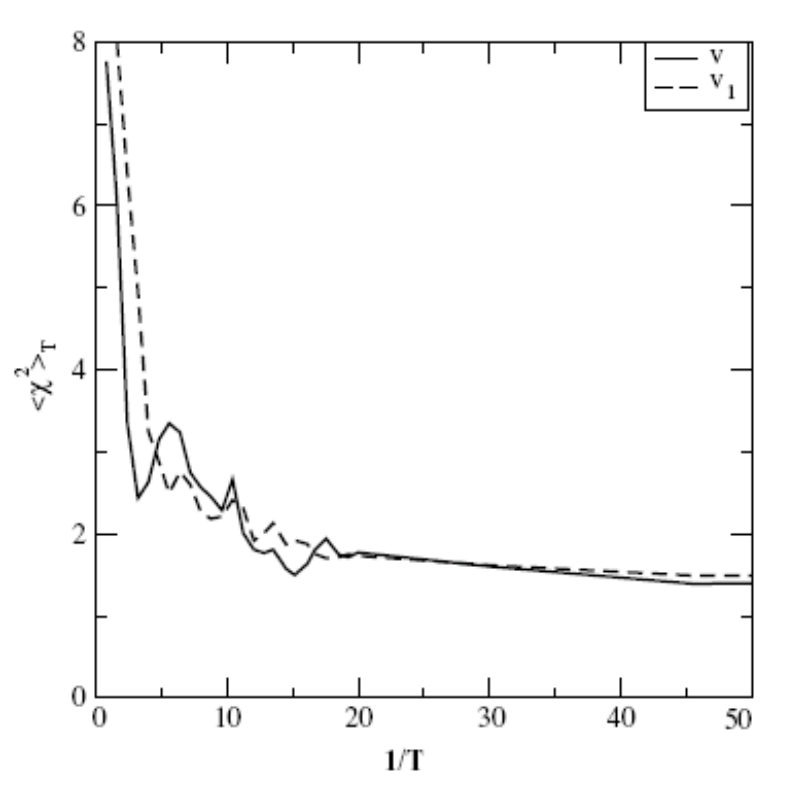
$$P(\chi^2) = \exp\left(\frac{\chi^2_{old} - \chi^2_{new}}{T}\right) > \beta$$

$$0 < \beta < 1$$

7. Starting with an initial value of $T = T_i$, we repeat steps 4 - 6 for a large number of loops.

8. Reduce the parameter T as $T = \frac{T_i}{k}$ and repeat steps 1 - 7

9. Keep doing this way until hopefully reaching global minimum of χ^2



Variation of the average value of $\langle \chi^2 \rangle_T$ as a function of the inverse of the control parameter T for the KDE0 interaction for the two different choices of the starting parameter.

Results

Skyrme Parameters

Parameter	KDE0 (HF)	KDEX(HF+CORR)
t_0 (MeV fm^3)	-2526.51 (140.63)	-1419.83 (14.68)
t_1 (MeV fm^5)	430.94 (16.67)	309.14 (8.79)
t_2 (MeV fm^5)	-398.38 (27.31)	-172.96 (3.92)
t_3 (MeV fm$^{3(1+\alpha)}$)	14235.5 (680.73)	10465.4 (133.29)
x_0	0.7583 (0.0655)	0.14741 (0.00437)
x_1	-0.3087 (0.0165)	-0.08527 (0.0046)
x_2	-0.9495 (0.0179)	-0.6144 (0.0159)
x_3	1.1445 (0.0882)	0.02197 (0.00106)
W_0 (MeV fm^5)	128.96 (3.33)	98.90 (2.27)
α	0.1676 (0.0163)	0.4989 (0.0103)

Binding Energies (MeV)

		$\Delta B = B^{exp} - B^{th}$	
Nuclei	B^{exp}	KDE0	KDEX
^{16}O	-127.620	0.394	3.202
^{24}O	-168.384	-0.581	4.582
^{34}Si	-283.427	-0.656	2.868
^{40}Ca	-342.050	0.005	0.699
^{48}Ca	-415.990	0.188	2.529
^{48}Ni	-347.136	-1.437	4.946
^{56}Ni	-483.991	1.091	1.853
^{68}Ni	-590.408	0.169	1.532
^{78}Ni	-641.940	-0.252	2.597
^{88}Sr	-768.468	0.826	2.985
^{90}Zr	-783.892	-0.127	0.913
^{100}Sn	-824.800	-3.664	0.180
^{132}Sn	-1102.850	-0.422	1.752
^{208}Pb	-1636.430	0.945	-5.584

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Charge RMS Radii (fm)

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Nuclei	Experiment	KDE0	KDEX
^{16}O	2.73	2.771	2.713
^{40}Ca	3.49	3.490	3.456
^{48}Ca	3.48	3.501	3.485
^{56}Ni	3.75	3.768	3.848
^{88}Sr	4.219	4.221	4.213
^{90}Zr	4.258	4.266	4.261
^{132}Sn	4.709	4.710	4.717
^{208}Pb	5.500	5.489	5.499

Single-particle Energies for ^{40}Ca (MeV)

Orbits	Exp	KDE0	KDEX
Protons			
$1s^{1/2}$	-50 ±11	-39.40	-35.972
$1p^{3/2}$		-26.95	-25.253
$1p^{1/2}$	-34 ±6	-22.93	-22.21
$1d^{5/2}$		-14.49	-13.787
$2s^{1/2}$	-10.9	-9.48	-8.3158
$1d^{3/2}$	-8.3	-7.59	-8.7067
$1f^{7/2}$	-1.4	-2.38	-2.0307
Neutrons			
$1s^{1/2}$		-47.77	-44.042
$1p^{3/2}$		-34.90	-33.074
$1p^{1/2}$		-30.78	-29.958
$1d^{5/2}$		-22.08	-21.344
$2s^{1/2}$	-18.1	-17.00	-15.724
$1d^{3/2}$	-15.6	-14.97	-16.197
$1f^{7/2}$	-8.32	-9.60	-9.2673
$2p^{3/2}$	-6.2	-4.98	-4.3458

Conclusions

- We developed a new Skyrme interaction.
- Uses correlation-effect corrected data.
- Better reproduces ^{16}O and ^{208}Pb charge rms radii.
- Charge rms radius for ^{16}O incompatible with monopole energies in our model.
- Possible improvements:
  - More work on optimization.
  - Different sets of data.

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