Developing a Modern Energy Density Functional for Oxygen-28

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Energy Density Functional

What is its importance?
• Nuclear matter
• Exotic nuclei
• Astrophysical phenomena

Problem?
• Need to use existing data to fit EDF for better predictions
Why Oxygen-28?

- The nucleus $^{28}\text{O}$ has magic numbers of nucleons.
- $^{28}\text{O}$ is unbound (not observed).
- $^{28}\text{O}$ has high proton-neutron asymmetry.
- If this phenomena can be understood, it will provide more reliable predictions for unknown nuclear masses outside the valley of nuclear stability.
Mean-Field Theory

• Nucleus is a many-body system with complicated strong two-body interaction
• Obtaining a solution to the many-body Schrodinger equation is very difficult

\[ H = \sum_i -\frac{\hbar^2}{2m_i} \nabla_i^2 + \sum_{i<j} V_{ij} \]

\[ H\Psi_n (1,...,A) = E_n \Psi_n (1,...,A) \]
Mean-Field Theory

In the Mean-Field Approximation, a particle interacts with an average potential produced by all other particles in the system.

Here, we write the Hamiltonian using a central potential $U$ and residual interaction $H_{\text{res}}$

$$H = \sum_i \left[ \frac{\vec{p}_i^2}{2m_i} + U(\vec{r}_i) \right] + H_{\text{res}}$$

$$H_{\text{res}} = \sum_{ij} V_{ij} - \sum_i U(\vec{r}_i)$$
Hartree-Fock Method

The total wave function is written as an antisymmetric product of single particle wave functions. It can be represented using the antisymmetry operator $\hat{A}$ or a Slater Determinant.

$$\Phi = \hat{A} \phi_i(1) \ldots \phi_A(A)$$

$$\Phi = \frac{1}{\sqrt{A!}} \begin{vmatrix}
\phi_1(\vec{r}_1, \sigma_1, \tau_1) & \phi_2(\vec{r}_1, \sigma_1, \tau_1) & \ldots & \phi_A(\vec{r}_1, \sigma_1, \tau_1) \\
\phi_1(\vec{r}_2, \sigma_2, \tau_2) & \phi_2(\vec{r}_2, \sigma_2, \tau_2) & \ldots & \phi_A(\vec{r}_2, \sigma_2, \tau_2) \\
\vdots & \vdots & \ddots & \vdots \\
\phi_1(\vec{r}_A, \sigma_A, \tau_A) & \phi_2(\vec{r}_A, \sigma_A, \tau_A) & \ldots & \phi_A(\vec{r}_A, \sigma_A, \tau_A)
\end{vmatrix}$$
In the spherical symmetry approximation of the nucleus, the single particle wave functions can be separated into their radial, spin, and isospin components.

\[ \phi_i(\vec{r}, \sigma, \tau) = \frac{R_{\alpha_i}(r)}{r} Y_{jlm}(r, \sigma) \chi_{m_z}(\tau) \]

Using the total wave function and the Hamiltonian operator, one can calculate the expectation value of the binding energy

\[ E = \left\langle \Phi \left| \hat{H}_{\text{total}} \right| \Phi \right\rangle = \int H(\vec{r}) d\vec{r} \]

Minimizing \( E \), we obtain the well-known Hartree-Fock equations.
Skyrme Interaction

Two potentials: Coulomb and strong nuclear.

\[ V_{ij}^{\text{Coul}} = -\frac{e^2}{4} \sum_{i,j=1}^{A} \frac{\tau_{ij}^2 + \tau_{ij}}{|\vec{r}_i - \vec{r}_j|} \]

The standard Skyrme-type interaction is given by the following for the strong nuclear:

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

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

\[ i W_0 \vec{k}_{ij} \delta(\vec{r}_i - \vec{r}_j) (\vec{\sigma}_i + \vec{\sigma}_j) \vec{k}_{ij} \]

\[ t_i, x_i, \alpha, W_0 \text{ are 10 Skyrme parameters} \]
The resulting Hartree-Fock equations are:

\[ \frac{\hbar^2}{2m^*_r(r)} \left[ -R^\alpha_r(r) + \frac{l_{\alpha}(l_{\alpha} + 1)}{r^2} R^\alpha_r(r) \right] - \frac{d}{dr} \left( \frac{\hbar^2}{2m^*_r(r)} \right) R^\alpha_r(r) + \]

\[ \left[ U^\tau_r(r) + \frac{1}{r} \frac{d}{dr} \left( \frac{\hbar^2}{2m^*_r(r)} \right) + \frac{j_{\alpha}(j_{\alpha} + 1) - l_{\alpha}(l_{\alpha} + 1) - \frac{3}{4}}{r} W^\tau_r(r) \right] R^\alpha_r(r) \]

\[ = \varepsilon^\alpha_r R^\alpha_r(r) \]

where \( m^*_r(r) \), \( U^\tau_r(r) \), and \( W^\tau_r(r) \) are the effective mass, the potential, and the spin orbit potential. These are given in terms of Skryme parameters and nuclear densities.
Continue with HF-method

1) Initial guess of the single-particle wave functions should start close to the solution.

2) Solve HF equation and iterate to get new set of single-particle wave functions
The Skyrme Interaction KDE0v1 [1]

There exist over 300 Skyrme parameterizations in literature. Recently, 240 Skyrme interaction parameter sets were analyzed for their ability to pass the following constraints from experimental data [2]:

1. Properties of nuclear matter close to saturation density
2. Properties of finite nuclei
3. Observational data on neutron stars

KDE0v1 is the only interaction to pass the test


## Parameters of Skyrme Interactions and Their Nuclear Matter Properties

<table>
<thead>
<tr>
<th>Parameter</th>
<th>KDE0 [1]</th>
<th>KDE0v1 [1]</th>
<th>KDE0v1*</th>
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<tbody>
<tr>
<td>$t_0$ (MeV fm$^3$)</td>
<td>-2526.5110</td>
<td>-2553.0843</td>
<td><strong>-2537.7658</strong></td>
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<tr>
<td>$t_1$ (MeV fm$^5$)</td>
<td>430.9418</td>
<td>411.6963</td>
<td>411.6963</td>
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<td>$t_2$ (MeV fm$^5$)</td>
<td>-398.3775</td>
<td>-419.8712</td>
<td>-419.8712</td>
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<td>$t_3$ (MeV fm$^{3(1+\alpha)}$)</td>
<td>14235.5193</td>
<td>14603.6069</td>
<td><strong>14515.9853</strong></td>
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<td>$x_0$</td>
<td>0.7583</td>
<td>0.6483</td>
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<td>$X_1$</td>
<td>-0.3087</td>
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<td>-0.3472</td>
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<td>$X_2$</td>
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<td>$X_3$</td>
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<td>$W_0$ (MeV fm$^5$)</td>
<td>128.9649</td>
<td>124.4100</td>
<td><strong>158.0007</strong></td>
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<td>$\alpha$</td>
<td>0.1676</td>
<td>0.1673</td>
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### Properties

<table>
<thead>
<tr>
<th>Properties</th>
<th>KDE0 [1]</th>
<th>KDE0v1 [1]</th>
<th>KDE0v1*</th>
</tr>
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<tbody>
<tr>
<td>B/A (MeV)</td>
<td>16.11</td>
<td>16.23</td>
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<td>K (MeV)</td>
<td>228.82</td>
<td>227.54</td>
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<td>$\rho_0$ (fm$^{-3}$)</td>
<td>0.161</td>
<td>0.165</td>
<td>0.163</td>
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<tr>
<td>J (MeV)</td>
<td>33.00</td>
<td>34.58</td>
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<td>L (MeV)</td>
<td>45.22</td>
<td>54.59</td>
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Binding Energy of Neutron 1d3/2 Orbital in $^{28}$O
<table>
<thead>
<tr>
<th>Isotope</th>
<th>Experiment</th>
<th>KDE0v1</th>
<th>%DifExp</th>
<th>KDE0v1*</th>
<th>%DifExp</th>
<th>%DifKDE0v1</th>
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<tbody>
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<td>$^{28}$O</td>
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<td>165.67</td>
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<td>$^{24}$O</td>
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<td>$^{16}$O</td>
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<td>$^{208}$Pb</td>
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<td>$^{90}$Zr</td>
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<td>$^{40}$Ca</td>
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<td>-0.393</td>
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</table>
Conclusions

We have determined a new Skyrme interaction KDE0v1*

• KDE0v1* predicts a lower binding energy for O-28 than that of O-24 which means an unbound O-28, in agreement with experiment.

• KDE0v1* predicts an unbound orbital 1d 3/2 for O-28.

• KDE0v1* yields results within 3.3% of experimental values for the above nuclei. It is not as close as KDE0v1, and lowers all these nuclei’s binding energies with the exception of O-24.

A better fit, by varying all the Skyrme parameters, should be carried out.
Grant PHY-1263281
Special thanks to Shalom Shlomo, Giacomo Bonasera, and Mason Anders for their work and aid in this project’s development.