Modern Energy Functional for Nuclei and Nuclear Matter

By: Alberto Hinojosa, Tecnológico de Monterrey

REU Cyclotron 2008, Mentor: Dr. Shalom Shlomo

Introduction

1. Important task: Develop a modern EDF with enhanced predictive power for properties of rare nuclei.

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

3. 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.

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

The many-body Hamiltonian is given by

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

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. The many-nucleon (fermion) wave function Φ is approximated by an antisymmetric product of single particle wave functions $\varphi_i(r)$.

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

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

where,

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

The total energy is

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

The Skyrme interaction

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

$$V_{ij}^{NN} = t_0(1+x_0P_{ij}^{\sigma})\delta(\vec{r}_i-\vec{r}_j) + \frac{1}{2}t_1(1+x_1P_{ij}^{\sigma})[\vec{k}_{ij}^2\delta(\vec{r}_i-\vec{r}_j) + \delta(\vec{r}_i-\vec{r}_j)\vec{k}_{ij}^2]$$
$$+t_2(1+x_2P_{ij}^{\sigma})\vec{k}_{ij}\delta(\vec{r}_i-\vec{r}_j)\vec{k}_{ij} + \frac{1}{6}t_3(1+x_3P_{ij}^{\sigma})\rho^{\alpha}\left(\frac{\vec{r}_i+\vec{r}_j}{2}\right)\delta(\vec{r}_i-\vec{r}_j) +$$
$$iW_0\vec{k}_{ij}\delta(\vec{r}_i-\vec{r}_j)(\vec{\sigma}_i+\vec{\sigma}_j)\times\vec{k}_{ij}$$

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

The Hartree-Fock equations

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

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

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

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

And the Skyrme energy density functional is

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

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

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

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

$$\mathcal{H}_{fin} = \frac{1}{32}\left[3t_1(2+x_1)-t_2(2+x_2)\right](\nabla\rho)^2$$
$$-\frac{1}{32}\left[3t_1(2x_1+1)+t_2(2x_2+1)\right]\left[(\vec{\nabla}\rho_p)^2+(\vec{\nabla}\rho_n)^2\right],$$

$$\mathcal{H}_{so} = \frac{W_0}{2}\left[\mathbf{J}\cdot\nabla\rho + \mathbf{J}_p\cdot\nabla\rho_p + \mathbf{J}_n\cdot\nabla\rho_n\right],$$

$$\mathcal{H}_{sg} = -\frac{1}{16}(t_1x_1+t_2x_2)\mathbf{J}^2 + \frac{1}{16}(t_1-t_2)\left[\mathbf{J}_p^2+\mathbf{J}_n^2\right].$$

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

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

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

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

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

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

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

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.

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

- Rms radii for the valence neutron:

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

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

- 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.

The 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, α, W_0 are written in term of B/A, K_{nm}, ρ_{nm},...
2. Define $\vec{v} = \left(B/A, K_{nm}, \rho_{nm}, m^*/m, E_s, J, L, \kappa, G_0', W_0\right)$
3. Calculate χ_{old}^2 for a given set of experimental data and the corresponding HF results (using an initial guess Skyrme parameters).
4. Determine a new set 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
   $$v_r \to v_r + d\eta$$
   + Use this modified vector $\vec{v}$ to generate a new set of Skyrme parameters.
5. Go back to HF and calculate χ_{new}^2.
6. The new set of Skyrme parameters is accepted only if
   $$P(\chi^2) = \exp\left(\frac{\chi_{old}^2 - \chi_{new}^2}{T}\right) > \beta$$
   $$0 < \beta < 1$$
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.

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	-783.982	-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

Charge RMS Radii (fm)

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
^{100}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

Cyclotron Institute
Texas A&M University

National Science Foundation
WHERE DISCOVERIES BEGIN

Grant numbers: PHY-0355200
PHY-463291-00001

Office of Science
U.S. DEPARTMENT OF ENERGY

Grant number: DOE-FG03-93ER40773