Hartree-Fock approximation in nuclear physics

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1. Introduction

Let's consider system of N particles, which interact by two-body interactions $v_{i,j}$. The Hamiltonian of the system has form

$$H = T + V = \sum_{i=1}^{N} t_i + \frac{1}{2} \sum_{i,j=1, i \neq j}^{N} v_{ij} = \sum_{i=1}^{N} \frac{-\hbar^2}{2m} \vec{\nabla}^2 + \frac{1}{2} \sum_{i,j=1, i \neq j}^{N} v_{i,j}(\vec{r}_i, \vec{r}_j).$$

This Hamiltonian describes the many-body system. The corresponding Schödinger equation is the system of N strongly coupled equations.

Consideration of many nucleons in nuclei cames across on difficulties:

- It is difficult to apply the dynamical equations for each nucleon in nuclei, because the number of nucleon in nuclei is too high.
- It is difficult to apply the statistical equations for nuclei, because the number of nucleon in nuclei is too small for statistical approach.
- The interaction between nucleon is strong, complex and short-range.

Therefore it is necessary to apply the approximate theory.

2. Hartree approximation

Hartree approximation (1927): The state of any single particle of complex many-body system is determined by the self-consistent potential formed by interaction of this particle with all other particles.

Let's propose that

1) Schödinger single-particle equation for each particle has form

$$\frac{-\hbar^2}{2m}\vec{\nabla}^2\psi_i(\vec{r}_i) + V_i(\vec{r}_i)\psi_i(\vec{r}_i) = \varepsilon_i\psi_i(\vec{r}_i),$$

where ψ_i and V_i are wave function and the self-consistent potential for particle i, respectively, and wave functions obey the normalization condition $< \psi_i|\psi_i >= 1$;

2) the wave function of the total system of N particle is determined as

$$\Psi = \psi_1(\vec{r}_1)\psi_2(\vec{r}_2)\psi_3(\vec{r}_3)...\psi_N(\vec{r}_N).$$

Than the total energy of the system is

$$E =< \Psi|H|\Psi >= \sum_{i=1}^{N} < \psi_i|\frac{-\hbar^2}{2m}\left(\frac{d}{d\vec{r}_i}\right)^2|\psi_i > + \frac{1}{2}\sum_{i,j=1,i\neq j}^{N} < \psi_i\psi_j|v_{i,j}(\vec{r}_i,\vec{r}_j)|\psi_i\psi_j > .$$

The wave function can be determined by using the variation principle

$$\delta\left(<\Psi|H|\Psi> - \sum_{i=1}^{N} \varepsilon_i <\psi_i|\psi_i>\right) = 0,$$

where ε_i are the Lagrangian coefficients related to the normalization condition $<\psi_i|\psi_i>= 1$. The variations are performed on the functions ψ_i. Note that

$$\delta <\Psi|H|\Psi> = <\delta\Psi|H|\Psi> + <\Psi|H|\delta\Psi> .$$

$\Psi>$ is the complex function, therefore we can vary real and imaginary part independently, which is equivalent to carry out variation on $|\Psi>$ and $<\Psi|$ independently.

By taking the variation we obtain the Schrödinger equation

$$\frac{-\hbar^2}{2m}\left(\frac{d}{d\vec{r}_i}\right)^2 \psi_i + \sum_{j=1, i\neq j}^{N} <\psi_j|v_{i,j}(\vec{r}_i, \vec{r}_j)|\psi_j> \psi_i - \varepsilon_i\psi_i = 0.$$

The self-consistent potential for particle i is

$$V_i(\vec{r}_i) = \sum_{j=1, i\neq j}^{N} <\psi_j|v_{i,j}(\vec{r}_i, \vec{r}_j)|\psi_j> .$$

3. Hartree-Fock approximation

In 1930 V. A. Fock independently pointed out that the Hartree method did not respect the principle of antisymmetry of the wave function.

It was then shown that a Slater determinant, a determinant of single-particle wave particles first used by Heisenberg and Dirac in 1926, trivially satisfies the antisymmetric property.

Correct wave function of the total system of N fermions is

$$\Psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(\vec{r}_1) & \psi_1(\vec{r}_2) & \psi_1(\vec{r}_3) & ... & \psi_1(\vec{r}_N) \\ \psi_2(\vec{r}_1) & \psi_2(\vec{r}_2) & \psi_2(\vec{r}_3) & ... & \psi_2(\vec{r}_N) \\ \psi_3(\vec{r}_1) & \psi_3(\vec{r}_2) & \psi_3(\vec{r}_3) & ... & \psi_3(\vec{r}_N) \\ ... & ... & ... & ... & ... \\ \psi_N(\vec{r}_1) & \psi_N(\vec{r}_2) & \psi_N(\vec{r}_3) & ... & \psi_N(\vec{r}_N) \end{vmatrix}.$$

Here wave function $\psi_i(\vec{r}_i) = \varphi_i(\vec{r}_i)\xi_i$ contains space $\varphi_i(\vec{r}_i)$ and spin ξ_i parts.

For example, system of two particles

$$\Psi = \frac{1}{\sqrt{2}} \begin{vmatrix} \psi_1(\vec{r}_1) & \psi_1(\vec{r}_2) \\ \psi_2(\vec{r}_1) & \psi_2(\vec{r}_2) \end{vmatrix} = \frac{1}{\sqrt{2}}[\psi_1(\vec{r}_1)\psi_2(\vec{r}_2) - \psi_2(\vec{r}_1)\psi_1(\vec{r}_2)].$$

The antisymmetric property is fulfil $\Psi(\psi_1(\vec{r}_1), \psi_2(\vec{r}_2)) = -\Psi(\psi_2(\vec{r}_2), \psi_1(\vec{r}_1))$ due to anti commutator relation for fermi-particle $\psi_i(\vec{r}_i)\psi_j(\vec{r}_j) + \psi_j(\vec{r}_j)\psi_i(\vec{r}_i) = \delta_{ij}\ \delta(\vec{r}_i - \vec{r}_j)$

The Schrödinger equation for determination of the wave functions and eigenvalue of the single-particle energy ε_i is

$$\frac{-\hbar^2}{2m}\left(\frac{d}{d\vec{r}_i}\right)^2\psi_i(\vec{r}_i)+\frac{1}{2}\sum_{j=1}^{N}\left[\left(\int d^3r_j\ \psi_j^*(\vec{r}_j)v_{i,j}(\vec{r}_i,\vec{r}_j)\psi_j(\vec{r}_j)\right)\psi_i(\vec{r}_i)\right.$$
$$\left.-\int d^3r_j\ \psi_j^*(\vec{r}_j)v_{i,j}(\vec{r}_i,\vec{r}_j)\psi_j(\vec{r}_i)\psi_i(\vec{r}_j)\right]-\varepsilon_i\psi_i(\vec{r}_i)=0.$$

Note that subscript i describes the number of state and the spin state.

We can rewrite this equation in the form

$$\frac{-\hbar^2}{2m}\left(\frac{d}{d\vec{r}_i}\right)^2\psi_i(\vec{r}_i)+V_d(\vec{r}_i)\psi_i(\vec{r}_i)+\int d^3r_j\ V_{ex}(\vec{r}_i,\vec{r}_j)\psi_i(\vec{r}_j)-\varepsilon_i\psi_i(\vec{r}_i)=0,$$

where

$$V_d(\vec{r}_i)=\sum_{j=1}^{N}\int d^3r_j\ \psi_j^*(\vec{r}_j)v_{i,j}(\vec{r}_i,\vec{r}_j)\psi_j(\vec{r}_j)$$

is the direct self-consistent potential and

$$V_{ex}(\vec{r}_i,\vec{r}_j)=-\sum_{j=1}^{N}\psi_j^*(\vec{r}_j)v_{i,j}(\vec{r}_i,\vec{r}_j)\psi_j(\vec{r}_i)$$

is the exchange self-consistent potential.

In the case of finite-range interaction the direct potential $V_d(\vec{r}_i)$ is local, while the exchange potential $V_{ex}(\vec{r}_i, \vec{r}_j)$ is non-local.

If the exchange particle-particle interaction is zero-range, i.e. $v_{i,j}(\vec{r}_i, \vec{r}_j) = v_0\delta(\vec{r}_i - \vec{r}_j)$, than both the exchange potential and Schrödinger equation are local

$$V_{ex}(\vec{r}_i, \vec{r}_j) = -v_0 \sum_{j=1}^{N} \psi_j^*(\vec{r}_j)\delta(\vec{r}_i - \vec{r}_j)\psi_j(\vec{r}_i)$$

and Schrödinger equation has the form

$$\frac{-\hbar^2}{2m}\left(\frac{d}{d\vec{r}_i}\right)^2 \psi_i(\vec{r}_i) + V_d(\vec{r}_i)\psi_i(\vec{r}_i) - v_0\left(\sum_{j=1}^{N} \psi_j^*(\vec{r}_i)\psi_j(\vec{r}_i)\right)\psi_i(\vec{r}_i) - \varepsilon_i\psi_i(\vec{r}_i) = 0,$$

Conclusion: Hartree-Fock is microscopic approach for consideration of many-fermion systems, based on the wave functions and fermion-fermion potential.

4. Skyrme force.

Skyrme-force nucleon-nucleon interaction

$$
\begin{aligned}
v_{\text{Skyrme}}(\vec{r}_1,\vec{r}_2) = {} & t_0(1+x_0P_\sigma)\delta(\vec{r}_1-\vec{r}_2) && \text{central term}\\
& +\frac{1}{2}t_1(1+x_1P_\sigma)[\overleftarrow{\mathbf{P}}^2\ \delta(\vec{r}_1-\vec{r}_2)+\delta(\vec{r}_1-\vec{r}_2)\ \overrightarrow{\mathbf{P}}^2] && \\
& +t_2(1+x_2P_\sigma)\ \overleftarrow{\mathbf{P}}\ \delta(\vec{r}_1-\vec{r}_2)\ \overrightarrow{\mathbf{P}} && \text{non}-\text{local term}\\
& +\frac{1}{6}t_3\rho^\alpha(\frac{\vec{r}_1+\vec{r}_2}{2})(1+x_3P_\sigma)\delta(\vec{r}_1-\vec{r}_2) && \text{density}-\text{dependent term}\\
& +iW_0\left[\overleftarrow{\mathbf{P}}\times\delta(\vec{r}_1-\vec{r}_2)\ \overrightarrow{\mathbf{P}}\right](\vec{\sigma}_1+\vec{\sigma}_2) && \text{spin}-\text{orbit term}
\end{aligned}
$$

where $P_\sigma = \frac{1}{2}(1+\vec{\sigma}_1\vec{\sigma}_2) = \frac{1}{2}\left(1+2(\vec{S}^2-\vec{s}_1^2-\vec{s}_2^2)\right)) = S(S-1)-1 = \begin{cases} 1, & \text{for} S=1 \\ -1, & \text{for} S=0 \end{cases}$,

$\mathbf{P} = \frac{1}{2i}[\vec{\nabla}_1-\vec{\nabla}_2]$,

t_0, t_1, t_2, x_0, x_1, x_2, α and W_0 are parameters of the Skyrme forces.

Skyrme interaction is zero-range!

The energy density functional

$$\mathcal{E}[\rho_p(\vec{r}), \rho_n(\vec{r})] = \frac{\hbar^2}{2m}[\tau_p(\vec{r}) + \tau_n(\vec{r})] + \mathcal{V}(\vec{r}),$$

where m is the nucleon mass, $\tau_p = \sum_{i=1}^{Z} |\vec{\nabla}\psi_\alpha|^2$ and $\tau_n = \sum_{i=1}^{N} |\vec{\nabla}\psi_\alpha|^2$ are the proton and neutron kinetic energies.

The potential energy density functional splits into Skyrme and Coulomb (direct and exchange) parts

$$\mathcal{V}(\vec{r}) = \mathcal{V}_{\text{Skyrme}}(\vec{r}) + \mathcal{V}_{\text{Coul}}(\vec{r}).$$

The Skyrme energy density functional is

$$\mathcal{V}_{\text{Skyrme}}(\vec{r}) = \mathcal{V}_0 + \mathcal{V}_3 + \mathcal{V}_{eff} + \mathcal{V}_{fin} + \mathcal{V}_{so} + \mathcal{V}_{sg},$$

where

$$\mathcal{V}_0 = \frac{t_0}{2}[(1 + \frac{1}{2}x_0)\rho^2 - (x_0 + \frac{1}{2})(\rho_p^2 + \rho_n^2)]$$

is a zero range term,

$$\mathcal{V}_3 = \frac{1}{12}t_3\rho^\alpha[(1 + \frac{1}{2}x_3)\rho^2 - (x_3 + \frac{1}{2})(\rho_p^2 + \rho_n^2)]$$

is the density dependent term (note, for modern parametrizations $\alpha = 1$, or $\frac{1}{3}$ or $\frac{1}{6}$),

$$\mathcal{V}_{eff} = \frac{1}{4}[t_1(1+\frac{1}{2}x_1) + t_2(1+\frac{1}{2}x_2)]\tau\rho + \frac{1}{4}[t_2(x_2+\frac{1}{2}) - t_1(x_1+\frac{1}{2})](\tau_p\rho_p + \tau_n\rho_n)$$

is an effective mass term,

$$\mathcal{V}_{fin} = \frac{1}{16}[3t_1(1+\frac{1}{2}x_1) - t_2(1+\frac{1}{2}x_2)](\nabla\rho)^2 - \frac{1}{16}[3t_1(x_1+\frac{1}{2}) + t_2(x_2+\frac{1}{2})](\nabla\rho_n)^2 + (\nabla\rho_p)^2)$$

is a finite range term,

$$\mathcal{V}_{so} = \frac{1}{2}W_0(\vec{J}\vec{\nabla}\rho + \vec{J}_p\vec{\nabla}\rho_p + \vec{J}_n\vec{\nabla}\rho_n)$$

is a spin-orbit term and

$$\mathcal{V}_{sg} = -\frac{1}{16}(t_1x_1 + t_2x_2)\vec{J}^2 + \frac{1}{16}(t_1 - t_2)(\vec{J}_p^2 + \vec{J}_n^2)$$

is a term due to the tensor coupling with spin and gradient.

The functional employs the usual particle densities $\rho_q = \sum_i n_i|\psi_i|^2$, $\rho = \rho_p + \rho_n$, and the spin-orbit densities $\vec{J}_q = \sum_i \psi_i^+\vec{\sigma} \times \vec{\nabla}\psi_i$, where ψ_i are the single-particle wave functions and q stands for either protons or neutrons.

The Coulomb energy density functional is the sum of direct and exchange terms

$$\mathcal{V}_{\rm Coul}(\vec{r}) = \frac{e^2}{2}\rho_p(\vec{r})\int \frac{\rho_p(\vec{r\prime})}{|\vec{r} - \vec{r\prime}|}d\vec{r\prime} - \frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}(\rho_p(\vec{r}))^{4/3}.$$

The parameters b_i and b'_i are chosen to give the most compact formulation of the energy functional, the corresponding mean-field Hamiltonian, and residual interaction. They are related to the standard Skyrme parameters t_i and x_i by:

$$
\begin{aligned}
b_0 &= t_0(1+\tfrac{1}{2}x_0), \\
b_1 &= \tfrac{1}{4}\left[t_1(1+\tfrac{1}{2}x_1)+t_2(1+\tfrac{1}{2}x_2)\right], \\
b_2 &= \tfrac{1}{8}\left[3t_1(1+\tfrac{1}{2}x_1)-t_2(1+\tfrac{1}{2}x_2)\right], \\
b_3 &= \tfrac{1}{4}t_3(1+\tfrac{1}{2}x_3), \\
b_4 &= \tfrac{1}{2}t_4,
\end{aligned}
$$

$$
\begin{aligned}
b'_0 &= t_0(\tfrac{1}{2}+x_0), \\
b'_1 &= \tfrac{1}{4}\left[t_1(\tfrac{1}{2}+x_1)-t_2(\tfrac{1}{2}+x_2)\right], \\
b'_2 &= \tfrac{1}{8}\left[3t_1(\tfrac{1}{2}+x_1)+t_2(\tfrac{1}{2}+x_2)\right], \\
b'_3 &= \tfrac{1}{4}t_3(\tfrac{1}{2}+x_3),
\end{aligned}
$$

The total binding energy of a nucleus is obtained self-consistently from the energy functional:

$$E = E_{\rm kin} + V_{Sk}(\rho,\tau) + V_{Sk,ls}(\rho,\vec{J}) + V_{\rm Coul}(\rho_p),$$

where

$$\begin{aligned}
E_{\rm kin} &= \int d^3r \frac{\hbar^2}{2m}\tau, \\
E_{Sk} &= \int d^3r \left\{ \frac{b_0}{2}\rho^2 + \frac{b_3}{3}\rho^{\alpha+2} + b_1\rho\tau - \frac{b_2}{2}\rho\Delta\rho \right. \\
&\quad \left. - \sum_q \left(\frac{b_0'}{2}\rho_q^2 + \frac{b_3'}{3}\rho^\alpha\rho_q^2 + b_1'\rho_q\tau_q - \frac{b_2'}{2}\rho_q\Delta\rho_q \right) \right\}, \\
E_{Coul} &= \frac{1}{2}e^2 \int d^3r\, d^3r' \rho_p(\vec{r}) \frac{1}{|\vec{r}-\vec{r}'|}\rho_p(\vec{r}') - \frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{\frac{1}{3}} \int d^3r [\rho_p(\vec{r})]^{\frac{4}{3}},
\end{aligned}$$

and the spin-orbit functional can be written as

$$\begin{aligned}
E_{Sk,ls} = \int d^3r \left\{ -b_4\rho\vec{\nabla}\cdot\vec{J} - b_4'\sum_q \rho_q(\vec{\nabla}\cdot\vec{J}_q) \right. \quad &+ \frac{\theta_{\rm ls}}{12}\left[\left(\frac{3}{2}b_1 + b_2 - b_1' + 6b_2'\right)\vec{J}^2 \right. \\
&\left. \left. - \left(b_1 + 2b_2 - \frac{1}{2}b_1' + 3b_2'\right)\sum_q \vec{J}_q^2 \right] \right\}.
\end{aligned}$$

This spin-orbit functional encompasses two different options, namely, one either ignores the $\vec{J}^2$ contributions ($\theta_{\rm ls}=0$) or takes them into account ($\theta_{\rm ls}=1$). Furthermore, the spin-orbit functional is given in the extended form of which allows a separate adjustment of isoscalar and isovector spin-orbit force. The standard Skyrme forces use the particular combination $b'_4{=}b_4$ which was motivated by the derivation from a two-body zero-range spin-orbit interaction, but these particular settings are not obligatory when taking the viewpoint of an energy-density functional.

$$E_{Sk,ls} = \int d^3r \left\{ -b_4\rho\vec{\nabla}\cdot\vec{J} - b'_4\sum_q \rho_q(\vec{\nabla}\cdot\vec{J}_q) \quad + \frac{\theta_{\rm ls}}{12}\left[\left(\frac{3}{2}b_1+b_2-b'_1+6b'_2\right)\vec{J}^2 \right.\right. \\ \left.\left. - \left(b_1+2b_2-\frac{1}{2}b'_1+3b'_2\right)\sum_q \vec{J}_q^2\right]\right\}.$$

The Skyrme Parametrizations

Parameters of the Skyrme forces.

Force	t_0	t_1	t_2	t_3	x_0	x_1	x_2	x_3
SkM*	-2645.0	410.0	-135.0	15595.0	0.090	0.0	0.0	0.0
SkT6	-1794.2	294.0	-294.0	12817.0	0.392	-0.5	-0.5	0.5
SLy4	-2488.913	486.818	-546.395	13777.0	0.8340	-0.3438	-1.0	1.3540
SkI1	-1913.619	439.809	2697.594	10592.267	-0.954536	-5.782388	-1.287379	-1.561421
SkI3	-1762.88	561.608	-227.090	8106.2	0.3083	-1.1722	-1.0907	1.2926
SkI4	-1855.827	473.829	1006.855	9703.607	0.405082	-2.889148	-1.325150	1.145203
SkP	-2931.70	320.618	-337.409	18708.96	0.29215	0.65318	-0.53732	0.18103
SkO	-2103.653	303.352	791.674	13553.252	-0.210701	-2.810752	-1.461595	-0.429881
SkO’	-2099.419	301.531	154.781	13526.464	-0.029503	-1.325732	-2.323439	-0.147404

Parameters of the Skyrme forces.

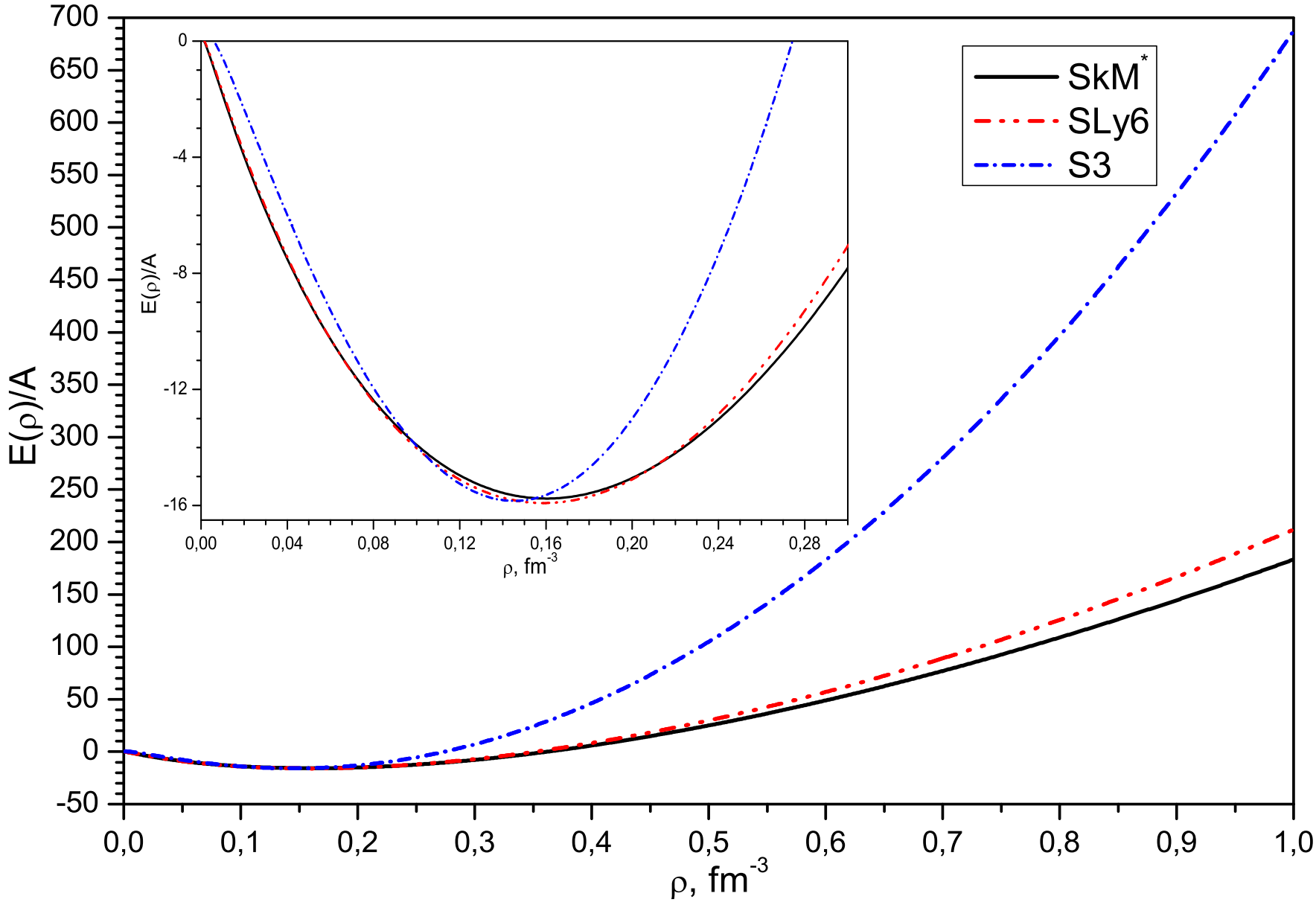
Force	b_4	b'_4	α	$\hbar^2/2m$	$\theta_{\rm ls}$
SkM*	65.0	65.0	1/6	20.7525	0
SkT6	53.5	53.5	1/3	20.750	1
SLy4	61.5	61.5	1/6	20.73553	0
SkI1	62.130	62.130	1/4	20.7525	0
SkI3	94.254	0.0	1/4	20.7525	0
SkI4	183.097	-180.351	1/4	20.7525	0
SkP	50.0	50.0	1/6	20.73	1
SkO	176.578	-198.7490	1/4	20.73553	0
SkO'	143.895	-82.8888	1/4	20.73553	1

Parameters of the new Skyrme forces (various Lyon force)

	SLy4	SLy5	SLy6	SLy7	SkM*
t_0 (MeV fm^3)	-2488.91	-2484.88	-2479.50	-2482.41	-2645.00
t_1 (MeV fm^5)	486.82	483.13	462.18	457.97	410.00
t_2 (Mev fm^5)	-546.39	-549.40	-448.61	-419.85	-135.00
t_3 (Mev fm$^{3+3\alpha}$)	13777.0	13763.0	13673.0	13677.0	15595.0
x_0	0.834	0.778	0.825	0.846	0.09
x_1	-0.344	-0.328	-0.465	-0.511	0.00
x_2	-1.000	-1.000	-1.000	-1.000	0.00
x_3	1.354	1.267	1.355	1.391	0.00
α	1/6	1/6	1/6	1/6	1/6
W_0 (MeV fm^5)	123.0	126.0	122.0	126.0	130.0

Properties of symmetric infinite nuclear matter for the Skyrme effective interactions.

$$\frac{E}{A} = \frac{3\hbar^2}{10m}\left(\frac{3\pi^2}{2}\right)^{2/3}\rho^{2/3} + \frac{3}{8}t_0\rho + \frac{3}{80}[3t_1 + (5+4x_2)t_2]\left(\frac{3\pi^2}{2}\right)^{2/3}\rho^{5/3} + \frac{1}{16}t_3\rho^{\alpha+1}.$$



$$\rho_\infty^{\rm Exp} = 0.16 \pm 0.005 \quad {\rm fm}^{-3}; \qquad K_\infty^{\rm Exp} = 210 \pm 20 \quad {\rm MeV}$$

Force	SLy4	SLy5	SLy6	SLy7	SkM*
ρ_∞ (fm^{-3})	0.160	0.160	0.159	0.158	0.160
k_F (fm^{-1})	1.333	1.334	1.330	1.328	1.334
a_v (MeV)	-15.969	-15.983	-15.920	-15.894	-15.770
K_∞ (MeV)	229.9	229.9	229.8	229.7	216.6
m^*_∞/m	0.70	0.70	0.69	0.69	0.79
a_{sym} (MeV)	32.00	32.03	31.96	31.99	30.03
κ (E1;T = 1)	0.25	0.25	0.25	0.25	0.53
a_{surf} (MeV) (Z/A = 0.5)	18.11	18.04	17.36	17.00	17.38
a_{surf} (MeV) (Z/A = 0.3916)	16.67	16.56	15.98	15.66	16.01

$$\begin{aligned} K_\infty &= 9\rho_0 \left(\frac{d^2 E(\rho)/A}{d\rho^2} \right)_{\rho=\rho_0} \\ &= -\frac{3\hbar^2}{5m} \left(\frac{3\pi^2}{2} \right)^{2/3} \rho_0^{2/3} + \frac{3}{8}[3t_1 + (5+4x_2)t_2] \left(\frac{3\pi^2}{2} \right)^{2/3} \rho^{5/3} + \frac{9}{16}\alpha(\alpha+1)t_3\rho_0^{\alpha+1} \end{aligned}$$

$$\frac{m^*_\infty}{m} = \left(1 + \frac{1}{16}\frac{2m}{\hbar^2}\rho_0[3t_1 + (5+4x_2)t_2]\right)^{-1};$$

$$\left.\frac{m^*}{m}\right|_{\text{isovect}} = \frac{1}{1+\kappa} = 1 + \frac{m}{2\hbar^2}[t_1(1+\frac{x_1}{2}) + t_2(1+\frac{x_2}{2})]$$

$$\begin{aligned} a_{sym} &= \frac{1}{2}\frac{d^2E(\rho)/A}{dI^2} = \frac{1}{3}\frac{\hbar^2}{2m}\left(\frac{3\pi^2}{2}\right)^{2/3}\rho^{2/3} - \frac{1}{4}t_0(x_0+\frac{1}{2})\rho \\ &- \frac{1}{24}\left(\frac{3\pi^2}{2}\right)^{2/3}[3t_1x_1 - (5+4x_2)t_2]\rho^{5/3} - \frac{1}{24}t_3(x_3+\frac{1}{2})\rho^{\alpha+1} \\ I &= \frac{N-Z}{A} \end{aligned}$$

surface energy coefficient
a_s (MeV)
17
18
Force
SkO'
SkO
SkP
Ski4
Ski3
Ski1
SLy4
SkT6
Z_0
SkM*

5. Gogny force.

Finite-range force

$$V(\vec{r}_1,\vec{r}_2) = \sum_{i=1}^{2} e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_i^2}[W_i + B_iP_\sigma - H_iP_\tau - M_iP_\sigma P_\tau]$$
$$+ iW_0(\vec{\sigma}_1+\vec{\sigma}_2)\vec{k}\times\delta(\vec{r}_1-\vec{r}_2)\vec{k} + t_3(1+P_\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho^{1/3}(\frac{1}{2}(\vec{r}_1+\vec{r}_2))$$
$$P_\sigma = \frac{1}{2}(1+\vec{\sigma}_1\vec{\sigma}_2) = \frac{1}{2}\left(1+2(\vec{S}^2-\vec{s}_1^{\,2}-\vec{s}_2^{\,2})\right) = S(S-1)-1 = \begin{cases} 1, & \text{for } S=1 \\ -1, & \text{for } S=0 \end{cases}$$

where

i	μ_i fm	W_i	B_i	H_i	M_i MeV	W_0 MeV fm^5	t_0 MeV fm^4
1	0.7	-402.4	-100	-496.2	-23.56	115	1350
2	1.2	-21.30	-11.77	37.27	-68.81		

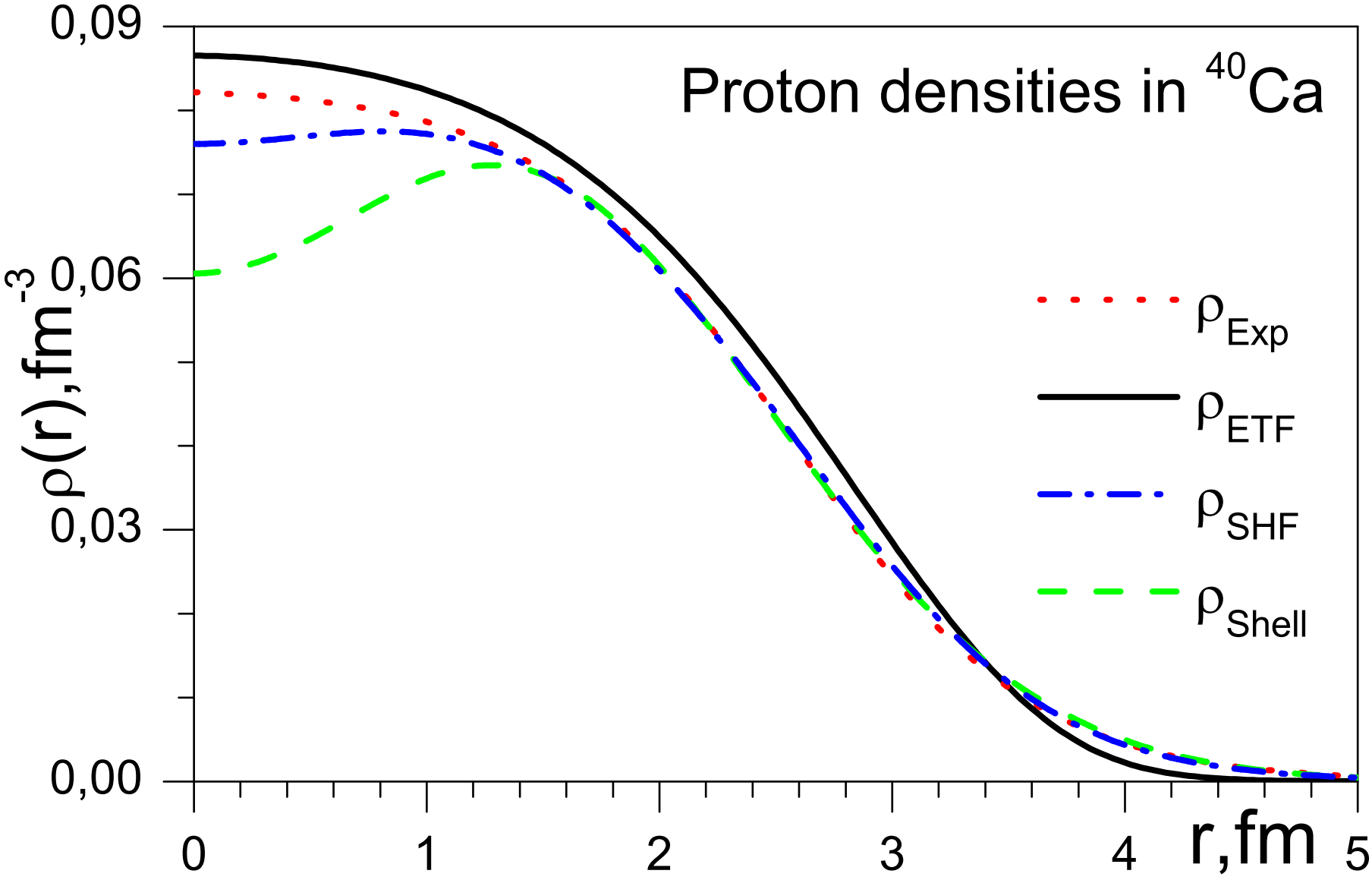
6. Schrödinger equation within HF+Skyrme force model.

Within the Hartree1Fock approximation, these single particle wave functions and their corresponding single particle energies are obtained from the self-consistent equation:

$$\left\{ -\vec{\nabla}\frac{\hbar^2}{2m_q^*(r)}\vec{\nabla} + U_q(\vec{r}) + \delta_{q,prot}U_{\rm Coul}(\vec{r}) - i\vec{W}_q(\vec{r})(\vec{\nabla}\times\sigma) - e_i) \right\}\phi_i^q(\vec{r},s) = 0$$

where $q = protons, neutrons$,

$$\begin{aligned}
\frac{\hbar^2}{2m_q^*(r)} &= \frac{\hbar^2}{2m} + \frac{1}{4}[t_1(1+x_1/2)+t_2(1+x_2/2)]\rho(\vec{r}) - \frac{1}{4}[t_1(1/2+x_1)+t_2(1/2+x_2)]\rho_q(\vec{r}),\\
U_q(\vec{r}) &= t_0[(1+x_0/2)\rho(\vec{r}) - (1/2+x_0)\rho_q(\vec{r})]\\
&+ \frac{1}{12}t_3\left\{(1+x_3/2)(2+\alpha)\rho^{\alpha+1}(\vec{r}) - (x_3+1/2)\left[2\rho^{\alpha}(\vec{r})\rho_q(\vec{r}) + \alpha\rho^{\alpha-1}(\vec{r})(\rho_p^2(\vec{r}) + \rho_n^2(\vec{r}\right.\right.\\
&+ \frac{1}{4}[t_1(1+x_1/2)+t_2(1+x_2/2)]\tau + \frac{1}{4}[t_2(x_2+1/2) - t_1(x_1+1/2)]\tau_q\\
&+ \frac{1}{8}[t_2(1+x_2/2) - 3t_1(1+x_1/2)]\nabla^2\rho(\vec{r}) + \frac{1}{8}[3t_1(x_1+1/2) + t_2(x_2+1/2)]\nabla^2\rho_q(\vec{r})\\
&+ \frac{1}{8}(t_1-t_2)\vec{J}_q - \frac{1}{8}(t_1x_1+t_2x_2)\vec{J},\\
\vec{W}_q(\vec{r}) &= \frac{1}{2}W_0(\vec{\nabla}\rho(\vec{r}) + \vec{\nabla}\rho_q(\vec{r})), \quad U_{\rm Coul}(\vec{r}) = \frac{e^2}{2}\rho_p(\vec{r})\int\frac{\rho_p(\vec{r\prime})}{|\vec{r}-\vec{r\prime}|}d\vec{r\prime} - \frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}(\rho_p(\vec{r}))^{4/}\\
\tau_q(\vec{r}) &= \sum_{i=1,s}^{N_q}\left|\vec{\nabla}\psi_i^q(\vec{r},s)\right|^2, \quad \vec{J}_q(\vec{r}) = \sum_{i=1,s,s'}^{N_q}\psi_i^{q*}(\vec{r},s')\vec{\nabla}\psi_i^q(\vec{r},s)\times\langle s'|\vec{\sigma}|s\rangle.
\end{aligned}$$

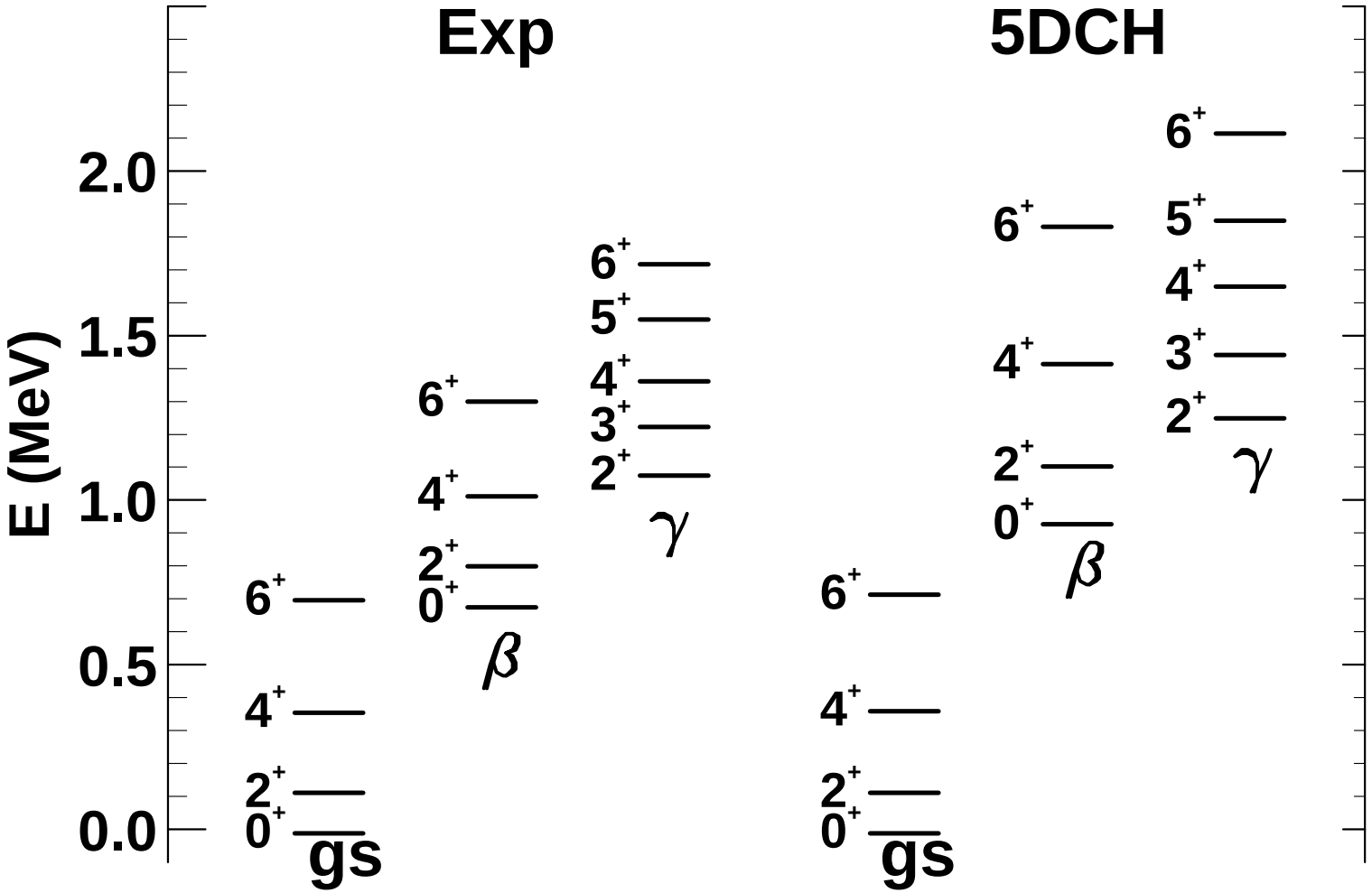


The density distribution, binding energy, root mean square charge radii, single-particle level structure near the Fermi energy are well described in the framework of HF.

Binding energy and RMS charge radii.

Nucleus	Binding energy, MeV		RMS charge radii, fm	
	SkM*	exp	SkM*	exp
^{16}O	131.5	127.6	2.79	2.73
^{40}Ca	347.9	342.1	3.50	3.49
^{48}Ca	428.1	416.0	3.52	3.48
^{56}Ni	495.1	484.0	3.75	3.75
^{90}Zr	796.6	783.9	4.28	4.37
^{140}Ce	1188.0	1172.7	4.88	4.88
^{208}Pb	1652.7	1636.5	5.49	5.50

Levels in ^{152}Sm



7. Numerical solution of Schrödinger equation.

Let's consider for simplicity Schrödinger equation for proton in nucleus with Z protons

$$[-\frac{\hbar^2}{2m}\nabla^2 + V]\Psi = E\Psi$$

where

$$V = V_{\rm Coul}(r) + V_{\rm CR}(r) + iW_{\rm CI}(r) + (V_{\rm SR}(r) + iW_{\rm SR}(r))\hbar^2(\vec{S}\vec{L}),$$

$$V_{\rm Coul}(r) = \begin{cases} \frac{(Z-1)e^2}{r}, & r \geq R_{\rm Coul}, \\ \frac{(Z-1)e^2}{R_{\rm Coul}}\left[\frac{3}{2} - \frac{r^2}{2R^2_{\rm Coul}}\right], & r < R_{\rm Coul}, \end{cases}$$

is the Coulomb energy,

$$V_{\rm CR}(r) = \frac{V_0}{1 + \exp\left((r - R_C)/d_C\right)},$$

$$W_{\rm CR}(r) = \frac{W_0}{1 + \exp\left((r - R_{CW}/d_{CW}\right)},$$

$$V_{\rm LS}(r) = \frac{d}{dr}\frac{V_{\rm SR}}{1 + \exp\left((r - R_{\rm SR})/d_{\rm SR}\right)},$$

$$W_{\rm LS}(r) = \frac{d}{dr}\frac{W_{\rm SR}}{1 + \exp\left((r - R_{\rm SW})/d_{\rm SW}\right)}.$$

are the central real and imaginary potentials, and spin-orbital real and imaginary potentials.

Note that for neutron the Coulomb potential omits and other potentials are the same, but the differences are related to the parameter values.

The total wave function is

$$\Psi = \frac{\psi_{j\ell}(r)}{r} Y_{lm}(\Omega)\xi_s.$$

Separation of the variables appearing in the complete Schödinger equation leads to the usual radial equation for the each value of the orbital and total angular momenta ℓ and j

$$\left\{ -\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - \frac{k^2}{E}[E - (V_{\rm Coul}(r) + V_{\rm CR}(r) + iW_{\rm CI}(r)) \right.$$
$$\left. -(V_{\rm SR}(r) + iW_{\rm SR}(r))\hbar^2(j(j+1) - \ell(\ell+1) - s(s+1))/2] \right\} \psi_{j\ell} = 0$$

where $k = (2mE/\hbar^2)^{1/2}$.

This equation can be written in the form

$$\frac{d^2}{dr^2}\psi(r) = A(r)\psi(r).$$

We introduce the auxiliary function

$$\zeta(r) = \psi(r) - \frac{h^2}{12}A(r)\psi(r),$$

where h is step of finite difference algorithm. For function ζ there is Noumerov (Boris Vasil'evich Noumerov) algorithm based on the finite difference formula for three consecutive points on a mesh with step h,

$$\zeta_{i+1}(r_{i+1}) = \left[2 + \frac{h^2 A_i}{1 - (h^2/12)A_i}\right]\zeta_i(r_i) - \zeta_{i-1}(r_{i-1}).$$

The boundary conditions at $r = 0$ is $\psi(r) = 0$.

Asymptotic at $r \to \infty$ for bound levels $E < 0$ is $\psi(r) \sim \exp\left[-\sqrt{-2mE/\hbar^2}r\right]$.

Asymptotic at $r \to \infty$ for quasi-stationary levels $E > 0$ is

$\psi(r) \sim \sin\left[\sqrt{2mE/\hbar^2}r + \delta_\ell - \ell\pi/2\right]$, where δ_ℓ is scattering phase.

Relativistic mean field equations

The basic Ansatz of the RMF theory is a Lagrangian density where nucleons are described as Dirac particles which interact via the exchange of various mesons. The Lagrangian density considered is written in the form:

$$\begin{aligned}\mathcal{L} &= \bar{\psi}(i\partial\!\!\!/ - M)\psi + \tfrac{1}{2}\partial_\mu\sigma\partial^\mu\sigma - U(\sigma) - \tfrac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \\ &\tfrac{1}{2}m_\omega^2\omega_\mu\omega^\mu - \tfrac{1}{4}\vec{R}_{\mu\nu}\vec{R}^{\mu\nu} + \tfrac{1}{2}m_\rho^2\vec{\rho}_\mu\vec{\rho}^\mu - \tfrac{1}{4}F_{\mu\nu}F^{\mu\nu} \\ &g_\sigma\bar{\psi}\sigma\psi \;-\; g_\omega\bar{\psi}\omega\!\!\!/\psi \;-\; g_\rho\bar{\psi}\vec{\rho}\!\!\!/\vec{\tau}\psi - \; e\bar{\psi}A\!\!\!/\psi\end{aligned} \tag{1}$$

The meson fields included are the isoscalar σ meson, the isoscalar-vector ω meson and the isovector-vector ρ meson. The latter provides the necessary isospin asymmetry.

The arrows in Eq. (1) denote the isovector quantities. The Lagrangian contains also a non-linear scalar self-interaction of the σ meson.

$$U(\sigma) \;= \frac{1}{2}m_\sigma^2\sigma^2 \;+\; \frac{1}{3}g_2\sigma^3 \;+\; \frac{1}{4}g_3\sigma^4 \tag{2}$$

This term is important for appropriate description of surface properties [**?**]. M, m_σ, m_ω and m_ρ are the nucleon-, the σ-, the ω- and the ρ-meson masses respectively, while g_σ, g_ω, g_ρ and $e^2/4\pi = 1/137$ are the corresponding coupling constants for the mesons and the photon. The field tensors of the vector mesons and of the electromagnetic fields take the following form:

$$\Omega^{\mu\nu} = \;\partial^\mu\omega^\nu - \partial^\nu\omega^\mu \tag{3}$$

$$\vec{R}^{\mu\nu} = \partial^{\mu}\vec{\rho}^{\nu} - \partial^{\nu}\vec{\rho}^{\mu} \tag{4}$$

$$F^{\mu\nu} = \partial^{\mu}A^{\nu} - \partial^{\nu}A^{\mu} \tag{5}$$

The variational principle gives the equations of motion. The mean field approximation is introduced at this stage by treating the fields as the c-number or classical fields. This results into a set of coupled equations namely the Dirac equation with potential terms for the nucleons and the Klein-Gordon type equations with sources for the mesons and the photon. For the static case, along with the time reversal invariance and charge conservation the equations get simplified. The resulting equations, known as RMF equations have the following form.

The Dirac equation for the nucleon:

$$\{-i\alpha\nabla + V(\mathbf{r}) + \beta[M + S(\mathbf{r})]\}\psi_i = \varepsilon_i\psi_i, \tag{6}$$

where $V(\mathbf{r})$ represents the *vector* potential:

$$V(\mathbf{r}) = g_{\omega}\omega_0(\mathbf{r}) + g_{\rho}\tau_3\rho_0(\mathbf{r}) + e\frac{1+\tau_3}{2}A_0(\mathbf{r}), \tag{7}$$

and $S(\mathbf{r})$ is the *scalar* potential:

$$S(\mathbf{r}) = g_{\sigma}\sigma(\mathbf{r}) \tag{8}$$

the latter contributes to the effective mass as:

$$M^*(\mathbf{r}) = M + S(\mathbf{r}). \tag{9}$$

The Klein-Gordon equations for the meson and the electromagnetic fields with the nucleon densities as sources:

$$\{-\Delta + m_\sigma^2\}\sigma(\mathbf{r}) = -g_\sigma \rho_s(\mathbf{r}) - g_2\sigma^2(\mathbf{r}) - g_3\sigma^3(\mathbf{r}) \tag{10}$$

$$\{-\Delta + m_\omega^2\}\omega_0(\mathbf{r}) = g_\omega \rho_v(\mathbf{r}) \tag{11}$$

$$\{-\Delta + m_\rho^2\}\rho_0(\mathbf{r}) = g_\rho \rho_3(\mathbf{r}) \tag{12}$$

$$-\Delta A_0(\mathbf{r}) = e\rho_c(\mathbf{r}) \tag{13}$$

The corresponding densities are:

$$\begin{aligned}
\rho_s &= \sum_{i=1}^{A} n_i \bar{\psi}_i \, \psi_i. \\
\rho_v &= \sum_{i=1}^{A} n_i \psi_i^+ \, \psi_i. \\
\rho_3 &= \sum_{p=1}^{Z} n_i \psi_p^+ \, \psi_p \; - \; \sum_{n=1}^{N} n_i \psi_n^+ \, \psi_n. \\
\rho_c &= \sum_{p=1}^{Z} n_i \psi_p^+ \, \psi_p.
\end{aligned} \tag{14}$$

Here the sums are taken over the particle states only. This implies that the contributions from negative-energy states are neglected (*no-sea* approximation), i.e. the vacuum is not polarized. The π meson does not contribute in the present relativistic mean field (Hartree)

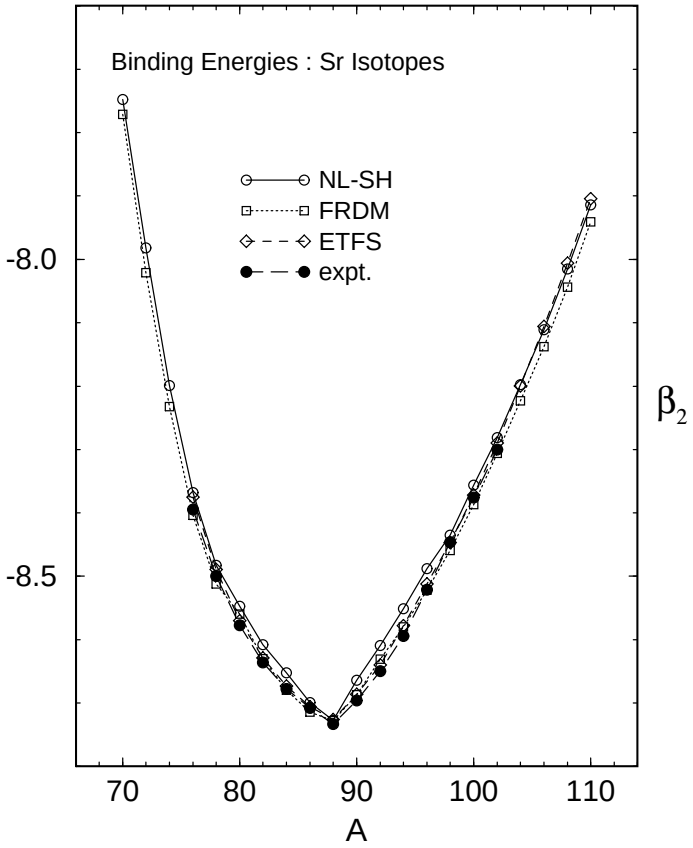
approximation because of its pseudo nature. The occupation number n_i is introduced to account for pairing which is important for open shell nuclei. In the absence of pairing it takes the value one (zero) for the levels below (above) the Fermi surface. In the presence of pairing the partial occupancies (n_i) are obtained in the constant gap approximation (BCS) through the well known expression:

$$n_i = \frac{1}{2}\left(1 - \frac{\varepsilon_i - \lambda}{\sqrt{(\varepsilon_i - \lambda)^2 + \Delta^2}}\right) \tag{15}$$

The ε_i is the single-paricle energy for the state i and chemical potential or Fermi energy λ for protons (neutrons) is obtained from the requirement

$$\sum_i n_i = \text{ the number of protons (Z)or the number of neutrons (N)} \tag{16}$$

The sum is taken over protons (neutrons) states. The gap parameter Δ is calculated from the observed odd-even mass differences.



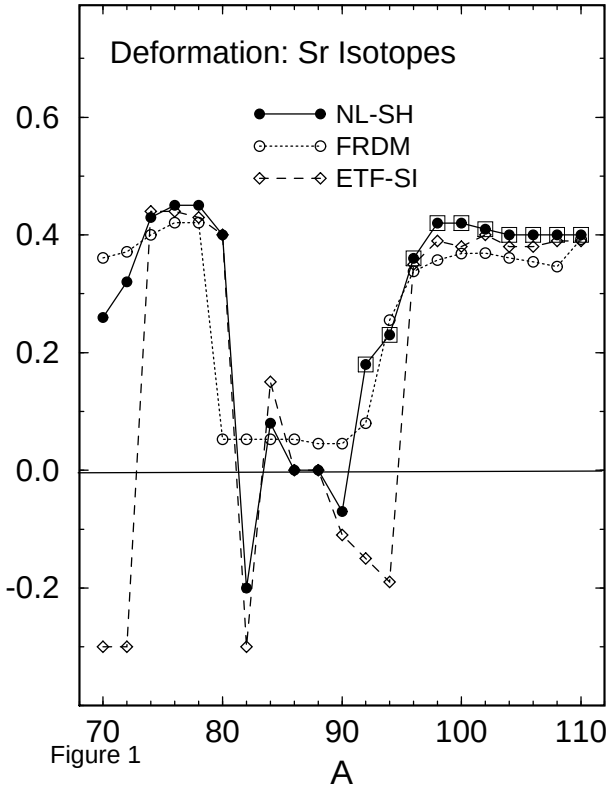


Figure 1

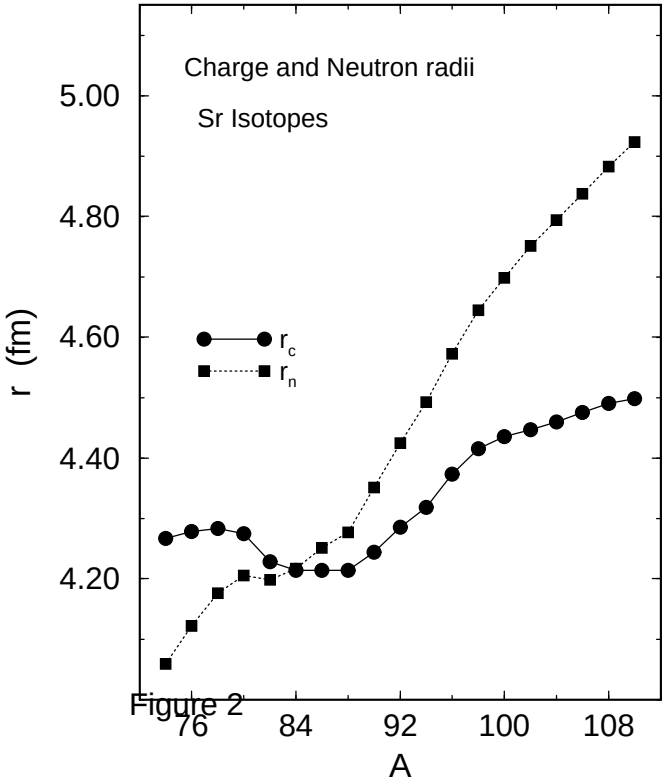


Figure 2

Thanks for your attention!