Nuclear Energy Density Functionals

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Nuclear Energy Density Functional and Nucleon-Nucleon interaction.

Until now, it has not been possible to construct an interaction that would satisfy three basic conditions:

- Was realistic, i.e. described NN-phases.

- Correctly described the binding energies at the observed nuclear radius.

- Provided a good description of spectroscopy.

Content

1. Hohenberg-Kohn theorem and Kohn-Sham scheme.

2. Nonrelativistic energy density functional
– Skyrme functional.
– Fayans functional.

3.
– Bethe-Weizsäcker formula as the first energy density approach.
– Nuclear energy density functional of A.Bulgac, M.M.Forbes, and S.Jin.

4. Relativistic energy density functional.
– Johnson-Teller-Dürr papers.
– EDF based on the meson exchange model.
– EDF based on chiral EFT.

Consider a system of N interacting particles described by the Hamiltonian

$$\hat{H} \equiv \hat{T} + \hat{v} + \hat{W}$$

Let Ψ be the N-body w.f. and $n(\vec{r})$ the corresponding particle density. Theorem:
–The nongenerate g.s.w.f. is a unique functional of the g.s. density $n_0(\vec{r})$

$$\Psi_0(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N) = \Psi_0[n_0(\vec{r})].$$

As a consequence the g.s. expectation value of any observable is a functional of $n_0(\vec{r})$

$$E_0 \equiv E[n_0(\vec{r})] = \langle \Psi[n_0] | \hat{H} | \Psi[n_0] \rangle$$

There exists functional $F[n]$ such that the energy functional can be written as

$$E[n] = F[n] + \int d^3 r v(\vec{r}) n(\vec{r})$$

The functional $F[n]$ is universal in the sense that for given NN-interaction it does not depend on $v(\vec{r})$
The formal definition of the H-K functional is

$$F[n] = \langle \Psi[n] | \hat{T} | \Psi[n] \rangle + \langle \Psi[n] | \hat{W} | \Psi[n] \rangle$$

The H-K theorem gives no practical guide to the construction of the universal density functional.

The H-K theorem resembles in some respects «Method of contraction description» in statistical physics:

$$t \gg \tau_0 \quad = \quad \frac{r_c}{\bar{v}}$$

$$f_s(x_1, x_2, ..., x_N; t) \quad \rightarrow \quad f_s(x_1, x_2, ..., x_N; f_1(x', t))$$

Functional $f_s(x_1, x_2, ..., x_N; f_1(x', t))$ is universal and do not depend on initial conditions.

$$\mathcal{E} = \int v(\vec{r})n(\vec{r})d\vec{r} + \frac{1}{2}\int\int \frac{n(\vec{r})n(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}d\vec{r}' + T_s[n] + E_{xc}[n],$$

where $E_{xc}[n]$ is by definition the exchange and correlation energy:

$$E_{xc}[n] = \int n[\vec{r}]\varepsilon_{xc}(n(\vec{r}))d\vec{r}.$$

From the stationary properties of $\mathcal{E}$ we obtain the equation:

$$\int \delta n(\vec{r})\{v(\vec{r}) + \int \frac{n(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}' + \frac{\delta T_s[n]}{\delta n(\vec{r})} + \frac{d}{dn}(n\varepsilon_{xc}(n))\}d\vec{r} = 0 \quad (1)$$

subject to the condition

$$\int \delta n(\vec{r})d\vec{r} = 0. \quad (2)$$

The equations (1) and (2) are precisely the same as the one-particle equation:

$$\{-\frac{1}{2}\nabla^2 + [v(n(\vec{r})) + \int \frac{n(\vec{r}')}{|\vec{r}-\vec{r}'|}d\vec{r}' + \frac{d}{dn}(n\varepsilon_{xc}(n))]\}\psi_i(\vec{r}) = \varepsilon_i\psi_i(\vec{r})$$

with $n(\vec{r}) = \sum_{i=1}^{N} |\psi_i(\vec{r})|^2$. The existing theorem makes no statement about the structure of $\varepsilon_{xc}(n)$.

Skyrme functional is constructed as an invariant composed of all possible bilinear terms in the following local densities and currents:

$$\begin{aligned}
\rho_0(\vec{r}) &= \sum_{\sigma,\tau} \rho(\vec{r},\sigma,\tau;\vec{r},\sigma,\tau) \\
\rho_1(\vec{r}) &= \sum_{\sigma,\tau} \rho(\vec{r},\sigma,\tau;\vec{r},\sigma,\tau)\tau \\
\vec{s}_0(\vec{r}) &= \sum_{\sigma,\sigma',\tau} \rho(\vec{r},\sigma,\tau;\vec{r},\sigma',\tau)\vec{\sigma}_{\sigma'\sigma} \\
\vec{s}_1(\vec{r}) &= \sum_{\sigma,\sigma',\tau} \rho(\vec{r},\sigma,\tau;\vec{r},\sigma',\tau)\vec{\sigma}_{\sigma'\sigma}\tau
\end{aligned}$$

$$
\begin{aligned}
\vec{j}_T(\vec{r}) &= \frac{\imath}{2}(\nabla' - \nabla)\rho_T(\vec{r},\vec{r}')|_{\vec{r}=\vec{r}'} - \text{current} \\
\vec{\mathcal{J}}_T(\vec{r}) &= \frac{\imath}{2}(\nabla' - \nabla) \times S_T(\vec{r},\vec{r}')|_{\vec{r}=\vec{r}'} - \text{spin} - \text{current} \quad \text{tensor} \\
\tau_T(\vec{r}) &= \nabla \cdot \nabla' \rho_T(\vec{r},\vec{r}')|_{\vec{r}=\vec{r}'} - \text{kinetic} \quad \text{density} \\
\vec{T}_T(\vec{r}) &= \nabla \cdot \nabla' S_T(\vec{r},\vec{r}')|_{\vec{r}=\vec{r}'} - \text{kinetic} \quad \text{spin} \quad \text{density}
\end{aligned}
$$

The Skyrme functional contains systematically all possible bilinear terms in the local densities and currents up to 2nd order in the derivatives, which are invariant with respect to parity, time-reversal, rotational, translational and isospin transformations.

$$E_{sk} = \sum_{T=0,1} \{C_T^{\rho}\rho_T^2 + C_T^{\Delta\rho}\rho_T\Delta\rho_{\rho_T} + C_T^{\tau}\rho_T\tau_T + C_T^{J}\vec{\mathcal{J}}_T^2$$

$$+C_T^{\Delta J}\rho_T\nabla\cdot\vec{\mathcal{J}} + C_T^{S}\vec{S}_T^2 + C_T^{\Delta S}\vec{s}_T\cdot\Delta\vec{S}_T + C_T^{ST}\vec{S}_T\cdot\vec{T}_T$$

$$+C_T^{\nabla S}(\nabla\cdot S_T)^2 + C_T^{j}\vec{j}_T^2 + C_T^{\nabla j}\vec{S}_T\cdot\nabla\times\vec{j}_T\}$$

In applications the functional is parametrized directly by fitting the coefficients to the ground state data.

$$
\begin{aligned}
\mathcal{E} &= \mathcal{E}_{kin} + \mathcal{E}_v + \mathcal{E}_s + \mathcal{E}_{Coul} + \mathcal{E}_{sl} + \mathcal{E}_{anom}, \\
\mathcal{E}_v &= \frac{2^0}{3_F}\rho_0 \left[a^v_+ \frac{1 - h^v_{1+} x_+}{1 + h^v_{2+} x_+} x^2_+ + a^v_+ \frac{1 - h^v_{1-} x_-}{1 + h^v_{2-} x_-} x^2_- \right], \\
\mathcal{E}_s &= \frac{2^0}{3_F}\rho_0 \frac{a^s_+ r^2_0 (\nabla x_+)^2}{1 + h^s_+ x_+ + h^s_\nabla r^2_0 (\nabla x_+)^2}, \\
x_\pm &= \frac{(\rho_n \pm \rho_p)}{2\rho_0}.
\end{aligned}
$$

Such expressions allow an extrapolation to very high densities.

In 1935 Weizsäcker proposed that an energy density approach could be effective for calculating nuclear binding energy:

$$E = \int F d^3r$$

$$F = \frac{\hbar^2}{32\pi^2 M}\frac{(\nabla\rho)^2}{\rho} + \frac{4\pi\hbar^2}{5M}\left(\frac{3\rho}{8\pi}\right)^{5/3} - f(\rho)$$

Bethe and Bacher in 1936 further developed Weizsäcker's idea and introduced the nuclear mass formula:

$$E(N,Z) = a_v A + a_s A^{2/3} + a_c \frac{Z^2}{A^{1/3}} + a_I \frac{(N-Z)^2}{A}$$

a_v	a_s	a_I	a_c	χ_E
-15.46	16.71	22.84	0.698	3.30 MeV

$$\chi^2_E = \sum \frac{|E^{exp}_{NZ} - E(N,Z)|^2}{N_E}$$

$$N_E = 2375$$

$$
\begin{aligned}
\mathcal{E}[\rho_n,\rho_p] &= \mathcal{E}_{kin}[\rho_n,\rho_p]+\mathcal{E}_C[\rho_n,\rho_p]+\mathcal{E}_{int}[\rho_n,\rho_p] \\
\mathcal{E}_{kin}[\rho_n,\rho_p] &= \sum_{\tau=n,p}\frac{\hbar^2}{2m_\tau}[\frac{1}{9}|\nabla\rho_\tau^{1/2}|^2+\frac{3}{5}(3\pi^2)^{2/3}\rho_\tau^{5/3}]+\ldots \\
\mathcal{E}_{int}[\rho_n,\rho_p] &= (\eta-\frac{1}{2})\sum_{\tau=n,p}\frac{\hbar^2}{2m_\tau}|\nabla\rho_\tau^{1/2}|^2+\sum_{j=0}^{2}\mathcal{E}_j(\rho)\beta^{2j} \\
\mathcal{E}_j(\rho) &= a_j\rho^{5/3}+b_j\rho^2+c_j\rho^{7/3} \\
\rho &= \rho_n+\rho_p, \quad \beta=\frac{(\rho_n-\rho_p)}{(\rho_n+\rho_p)}.
\end{aligned}
$$

The equation that determine equilibrium density of a nucleus is obtained by minimizing

$$
\begin{aligned}
E(N,Z) &= \int d^3r \mathcal{E}[\rho_n,\rho_p] \\
-\eta\frac{\hbar^2}{2m_\tau}\nabla^2\rho_\tau^{1/2} + U_\tau\rho_\tau^{1/2} &= \mu_\tau\rho_\tau^{1/2} \\
U_\tau &= \frac{\partial\mathcal{E}[\rho_n,\rho_p]}{\partial\rho_\tau}
\end{aligned}
$$

η	$\tilde{b}_0$	$\tilde{c}$	$\tilde{a}_1$	$\tilde{b}_1$	χ_E
0.471	-3.15166	2.12378	1.048	-0.610	2.59 MeV

$\tilde{a}_j = a_j\rho_0^{2/3}/\varepsilon_F$, $\tilde{b}_j = b_j\rho_0/\varepsilon_F$, $\tilde{c}_j = c_j\rho_0^{4/3}/\varepsilon_F$

This hydrodynamic theory can be reformulated as

$$\begin{aligned}
\Psi &= \sqrt{\rho}\exp(\frac{\imath}{\tilde{\hbar}}\phi), \quad (\tilde{\hbar}=\eta^{1/2}\hbar) \\
\mathcal{L}(\Psi,\dot{\Psi}) &= \Psi^{+}\left(\tilde{\hbar}\partial_t + \frac{\tilde{\hbar}^2\nabla^2}{2m}\right)\Psi - \mathcal{E}(\rho) \\
\imath\tilde{\hbar}\dot{\Psi} &= -\frac{\tilde{\hbar}^2\nabla^2}{2m}\Psi + \mathcal{E}'(\rho)\Psi
\end{aligned}$$

The paper of M.M.Johnson and E.Teller (1955) was, in fact, the first attempt to construct REDF. The following statements were made:

1. Nuclear interaction is strong. It means that at high energies many mesons can be created, i.e. in NN-collisions several mesons can be in virtual states.

2. In heavy nuclei the average number of mesons is much larger than one. Due to Bose statistics they can be in one and the same state. The wave function of this quantum state corresponds to the nuclear potential.

3. This meson must be scalar.

The next step has been done by H.-P.Dürr. He indicated that Dirac's equation symmetries do possible an introduction of both scalar attractive and vector repulsive potentials. In the stationary limit:

$$H = \vec{\alpha} \cdot \vec{p} + \beta M - \beta S + V_0,$$

where V_0 is a time like component of the vector potential.

Only as few mesons as possible are included.
π: J=0, T=1 and $P = -$
σ: J=0, T=0, P=+
ω: J=1, T=0, $P = -$
ρ: J=1, T=1, $P = -$

Without pions

$$L_{int} = -g_\sigma \bar{\psi}\sigma\psi - g_\omega \bar{\psi}\gamma_\mu \omega^\mu \psi - g_\rho \bar{\psi}\gamma_\mu \vec{\tau}\vec{\rho}^\mu \psi - e\bar{\psi}\gamma_\mu A^\mu \psi$$

The following Dirac equation is derived using this Lagrangian

$$\left(\gamma_\mu(\imath\partial^\mu + V^\mu) + M + S\right)\psi = 0$$

where $S(x) = g_\sigma \sigma(x)$, $V^\mu(x) = g_\omega \omega^\mu(x) + g_\rho \vec{\tau}\vec{\rho}^\mu(x) + eA^\mu(x)$. Since meson masses are large Laplace operator can be neglected in the stationary equations for meson fields, and σ, ω^0 and ρ_3^0 becomes proportional to the corresponding nuclear densities.

For the total energy we obtain

$$E = \int d^3r H(r) = \sum_{i=1}^{A} \int d^3r \psi_i^+(r)(-\imath\vec{\alpha}\cdot\nabla + \beta M)\psi_i(r)$$
$$+\frac{1}{2}\int d^3r \left(m_\sigma^2\sigma^2 - m_\omega^2(\omega^0)^2 - m_\rho^2(\rho_3^0)^2\right)$$
$$+ \int d^3r \left(g_\sigma\rho_s\sigma + g_\omega\rho_v\omega^0 + g_\rho\rho_3\rho_3^0 + e\rho_c A^0\right).$$

Width of σ - meson – 400-700 MeV, $c\tau$ =0.3 fm.

ω - meson - $\hbar/mc = 0.25$ fm.

Relativistic energy density functional based on chiral EFT. N.Finelli, N.Kaiser, D.Vretenar, W.Weise.

In this approach the construction of EDF is based on the following conjectures:

1. The nuclear ground state is characterized by strong scalar and vector fields which have their origin in the in-medium changes of the scalar quark condensate and of the quark density.

2. Pionic fluctuations are superimposed on the condensate background fields.

Relativistic energy density functional based on chiral EFT.

The energy functional is assumed to be decomposed into three terms:

$$F[\rho] = T_{kin}[\rho] + E_H[\rho] + E_{xc}[\rho]$$

E_H is the Hartree energy. We assume that large scalar and vector mean fields, that have their origin in the in-medium changes of the quark condensate, determine E_H.
Pionic fluctuations including one- and two-pion exchange are incorporated in the E_{xc}.

Relativistic energy density functional based on chiral EFT.

The relativistic Lagrangian includes:

isoscalar-scalar (S),

isoscalar-vector (V),

isovector-scalar (TS)

isovector-vector (TV)

and effective four-fermion interaction vertices with density dependent coupling strengths.

Relativistic energy density functional based on chiral EFT.

The ground state energy of the even-even nucleus with A-nucleons is presented as:

$$E_0 = \sum_{k=1}^{A} \varepsilon_k - \frac{1}{2}\int d^3r\{[G_s^{(0)} + G_s^{(\pi)}(\rho)]\rho_s^2 + G_{TS}^{(\pi)}(\rho)\rho_{S3}^2$$
$$+[G_V^{(0)} + G_V^{(\pi)}(\rho)]\rho^2 + G_{TV}^{(\pi)}(\rho)\rho_3^2 + \frac{\partial G_s^{(\pi)}(\rho)}{\partial\rho}\rho_s^2\rho$$
$$+\frac{\partial G_{TS}^{(\pi)}(\rho)}{\partial\rho}\rho_{s3}^2\rho + \frac{\partial G_V^{(\pi)}(\rho)}{\partial\rho}\rho^3 + \frac{\partial G_{TV}^{(\pi)}(\rho)}{\partial\rho}\rho_3^2\rho$$
$$+D_S^{(\pi)}\rho_s\nabla^2\rho_s + e\rho_{ch}A^{(0)}\}$$

where ε_k denotes single particle Kohn-Sham energies.

Relativistic energy density functional based on chiral EFT.

The coupling constants are decomposed as

$$\begin{aligned} G_i(\hat{\rho}) &= G_i^{(0)} + G_i^{(\pi)}(\hat{\rho}), \text{where} \quad i = S, V \\ G_i(\hat{\rho}) &= G_i^{(\pi)}(\hat{\rho}), \text{where} \quad i = TS, TV \end{aligned}$$

The density independent part arise from isoscalar-scalar and -vector background fields, whereas $G_i^{(\pi)}(\hat{\rho})$ are generated by one- and two-pion exchange dynamics.

Relativistic energy density functional based on chiral EFT.

M.A.Shifman, A.I.Vainstein, and V.I.Zakharov

B.L.Ioffe

E.G.Drukarev and E.M.Levin

The following estimates follows from the QCD sum rules:

$$G_S^{(0)} = -\frac{\sigma_N M_N}{m_\pi^2 f_\pi^2}$$

$$G_V^{(0)} = -\frac{4(m_u + m_d) M_N}{m_\pi^2 f_\pi^2}$$

$$\frac{\sigma_N}{m_u + m_d}\rho_s = < \bar{q}q >_p - < \bar{q}q >_0$$

Relativistic energy density functional based on chiral EFT.

The resulting expressions for the density dependent couplings are:

$$
\begin{aligned}
G_s^{(\pi)} &= c_{s1} + c_{s2}\rho^{1/3} + c_{s3}\rho^{2/3} + c_{s4}\rho, \\
G_v^{(\pi)} &= \bar{c}_{v1} + \bar{c}_{v2}\rho^{1/3} + \bar{c}_{v3}\rho^{2/3} + \bar{c}_{v4}\rho, \\
G_{TS}^{(\pi)} &= c_{ts1} + c_{ts2}\rho^{1/3} + c_{ts3}\rho^{2/3} + c_{ts4}\rho, \\
G_{TV}^{(\pi)} &= c_{tv1} + c_{tv2}\rho^{1/3} + c_{tv3}\rho^{2/3} + c_{tv4}\rho,
\end{aligned}
$$

Relativistic energy density functional based on chiral EFT.

The nuclear energy density functional developed above contains at most 7 significant parameters, each clearly related to specific properties of nuclei.

The values of the parameters are adjusted to the properties of nuclear matter, binding energies, charge radii and differences between proton and neutron radii of spherical nuclei.

The resulting optimal parameter set is remarkably close to the anticipated QCD sum rules and ChPT values, with exception of two constants associated with 3-body correlations.

Conclusion

1. The parameters of the NEDF are fitted mainly without reference to any NN-interaction.

2. NEDF is given as expansion in degrees of density and currents (excluding Fayans functional).

3. The changes of the quark condensate and quark density in the presence of the barionic matter are sources of strong scalar (attractive) and vector (repulsive) fields experienced by nucleons in the nucleus. These fields produce Hartree mean field nucleon potential, and are at the origin of the large energy spacings between spin-orbit partner states in nuclei.