Mean-field concept

(Ref: Isotope Science Facility at Michigan State University, MSUCL-1345, p. 41, Nov. 2006)
Fundamental puzzle: The nucleons interact strongly. How is it possible for them to move independently in a mean field potential?

Answer: Pauli correlations! Pauli’s spin-statistic theorem requires nucleons with $s=1/2$ to be fermions, i.e. the many-body wave function must be totally anti-symmetric under particle exchange. This anti-symmetry produces a pair correlation function which keeps the nucleons apart (see plot next slide).

Consequently, the average distance between nucleons in a nucleus is about 2.4 fm (see textbook by Ring & Schuck, p.1).

At large distances, the N-N interaction potential is relatively weak: at $R = 2.4$ fm we find $V_{NN}(^{1}S_0) = -2.5$ MeV (at $R=0.8$ fm it has a value of -100 MeV !)
pair correlation function (same spin proj. $\lambda$)

non-interacting spin-1/2 Fermi gas

Pauli "exchange hole"

Fermi momentum

\[ p_F = \hbar k_F \]

\[ k_F = 1.36 \text{ fm}^{-1} \]
Nuclear many-particle Hamiltonian and ground state binding energy

Creation operators for nucleon states: $\hat{c}^\dagger_i$

$$\hat{H} = \sum_{i, j=1}^{\infty} \langle i | t | j \rangle \hat{c}^\dagger_i \hat{c}_j + \frac{1}{2} \sum_{i, j, k, l=1}^{\infty} \langle ij | V^{(2)} | kl \rangle \hat{c}^\dagger_i \hat{c}^\dagger_j \hat{c}_k \hat{c}_l$$

$$+ \frac{1}{6} \sum_{i, j, k, l, m, n=1}^{\infty} \langle ijk | V^{(3)} | lmn \rangle \hat{c}^\dagger_i \hat{c}^\dagger_j \hat{c}^\dagger_k \hat{c}^\dagger_l \hat{c}_m \hat{c}_n$$

$$E_{g.s.} = \langle \Phi_{g.s.} | \hat{H} | \Phi_{g.s.} \rangle =$$

$$= \langle \Phi_{g.s.} | \hat{T}^{(1)} + \hat{V}_{\text{Coul}}^{(2)} + \hat{V}_{\text{nucl}}^{(2)} + \hat{V}_{\text{nucl}}^{(3)} | \Phi_{g.s.} \rangle$$
Hartree-Fock (HF) mean-field theory of nuclei: general remarks

HF is a microscopic theory of nuclear ground state properties.

Excited states (collective and non-collective) are described by the Random Phase Approximation (RPA) which is based on HF theory (see slides in section 4.7a).

Main approximation of HF theory:
For simplicity, the many-body ground state wave function is assumed to be a single Slater determinant, i.e. an anti-symmetrized product of single-particle wave functions.

Use variational principle to determine the “best possible” set of single-particle wave functions for the given nuclear many-body Hamiltonian (→ Hartree-Fock differential equations).
Hartree-Fock (HF) mean-field theory of nuclei: general remarks

HF formalism generates a (non-existent) one-body “mean field” potential from the given 2-body and 3-body N-N interaction. Protons and neutrons move independently in this mean field. HF thus provides a theoretical justification for the phenomenological shell models!

NOTE:
HF theory does not include pairing forces, which are included in the Hartree-Fock-Bogoliubov (HFB) theory, see section 4.6a.
Variational principle (minimize energy functional)

References: Shankar, QM, p. 429    Ring & Schuck, chapter 5

Solving the many-body Schroedinger equation

\[
(H - E) |\Psi\rangle = 0
\]

is equivalent to a variational principle (minimize energy functional):

\[
\delta E[\Psi] = 0 \quad E[\Psi] = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}
\]

Useful for determining the many-body ground state because one can prove that for any arbitrary state vector the energy functional yields an upper bound for the exact ground state energy:

\[
E[\Psi] \geq E_0
\]

In the Hartree-Fock approximation, one restricts the trial state vectors to the subspace of single Slater determinants.
Derivation of HF theory from variational principle

Ref: Blaizot and Ripka, Quantum Theory of Finite Systems, p.177-180

\[ \rho_{ji} = \langle \Phi_0^{HF} | \hat{c}_i \hat{c}_j | \Phi_0^{HF} \rangle \]

HF one-body density

\[ E_0(\rho) = \langle \Phi_0^{HF} | H | \Phi_0^{HF} \rangle \]

HF energy density functional

\[ \delta \left[ E_0(\rho) - \text{tr}\left\{ \Lambda (\rho^2 - \rho) \right\} \right] = 0 \]

Variational principle

Lagrange multiplier

condition for single Slater determinant

\[ h_{ij} = \frac{\partial E_0}{\partial \rho_{ji}} = \langle i | T | j \rangle + \sum_{k,l=1}^{\infty} \langle ik | V^{(2)} | jl \rangle \rho_{lk} + \ldots \]

mean field Hamiltonian (in energy representation)

\[ [h, \rho] = 0 \implies h | \phi_i \rangle = \varepsilon_i | \phi_i \rangle \]

Hartree-Fock equations

\[ \rho | \phi_i \rangle = n_i | \phi_i \rangle \]
The Hartree mean field: 
illustration for simple 2-body N-N interaction
Ref: Ring & Schuck, chapter 5

Assume, for simplicity that 2-body N-N interaction is local, depends only on 
position; no momentum-, spin-, or isospin dependence:

\[ V^{(2)}(\vec{r},\vec{r}') \]

The HF formalism generates, from the given 2-body N-N interaction, 
a (non-existent) 1-body mean field potential in which the nucleons 
move independently. The mean field describes the effect of the 2-
body interactions “on average”.

“Hartree” potential = local mean field (“direct term”)

\[ V_H^{(1)}(\vec{r}) = \int d^3r' V^{(2)}(\vec{r},\vec{r}') \rho(\vec{r}') \]

with the ground state density of nucleus given by

\[ \rho(\vec{r}) = \sum_{i=1}^{F} |\varphi_i(\vec{r})|^2 \]
The Fock exchange potential:
illustration for simple 2-body N-N interaction
Ref: Ring & Schuck, chapter 5

In addition, HF theory generates a (generally non-local) “Fock” potential ("exchange term" due to anti-symmetric product wave functions)

\[ V_F(\vec{r},\vec{r}') = -V(2)(\vec{r},\vec{r}')\rho(\vec{r},\vec{r}') \]

with the ground state density matrix (generalization of nuclear density)

\[ \rho(\vec{r},\vec{r}') = \sum_{i=1}^{F} \varphi_i(\vec{r}')\varphi_i^*(\vec{r}) \]
The self-consistent Hartree-Fock equations: illustration for simple 2-body N-N interaction

Ref: Ring & Schuck, chapter 5

\[
\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{H}^{(1)}(\vec{r})\right] \varphi_i(\vec{r}) + \int d^3r'd V_F(\vec{r}, \vec{r}') \varphi_i(\vec{r}') = \varepsilon_i \varphi_i(\vec{r})
\]

\(i = 1, \ldots, A\)

The HF equations represent a set of A coupled differential equations which determine the single-particle wave functions “self-consistently” from the given 2-body N-N effective interaction.

The Hartree / Fock potentials depend, via density / density matrix, on the single-particle wave functions of all A nucleons. This makes the DEs non-linear!

Need iterative solution: In 1\textsuperscript{st} order approximation, start e.g. from shell-model wave functions to compute density / density matrix. The HF equations then generate new 2\textsuperscript{nd} order wave functions, …
Need for “effective” N-N interaction (in nuclear medium)

Computational reason:
N-N potentials exhibit, for some reaction channels, a strongly repulsive core ($\approx 4000$ MeV) at $r \approx 0.5$ fm. Potential becomes very large, wave function becomes very small. This is numerically unstable.

Many-body physics reasons:
For free N-N scattering, almost all quantum states are unoccupied; in a heavy nucleus, however, many quantum states are occupied and thus “Pauli-blocked” (scattering into these states is forbidden).

For free N-N scattering, the energy of the N-N pair is conserved, by for N-N scattering in nuclear medium the energy of N-N pair is not conserved (energy transfer to other nucleons).
Derive effective interaction (Brückner G-matrix) from Bethe-Goldstone equation

Ref: Ring & Schuck, chapter 4.3.1

$G$-matrix = effective interaction
free N-N interaction

$< ab | G^E | cd > = < ab | \bar{V} | cd > + \frac{1}{2} \sum_{m,n>\varepsilon_F} < ab | \bar{V} | mn > \frac{1}{E - \varepsilon_m - \varepsilon_n + i\eta} < mn | G^E | cd >$

Pauli blocking free N-N interaction single-particle energies G-matrix = effective interaction

This equation must be solved iteratively; not too hard for infinite nuclear medium ("nuclear matter") but fairly difficult for finite nuclei!
Example: tensor components of Reid soft-core N-N interaction

solid line: “effective” interaction in nuclear matter, from Bethe-Goldstone eq.
dotted line: free N-N interaction
Comments on effective N-N interaction

From the numerical results depicted in the last slide we conclude:

• At distances $r > 1.0$ fm, the free N-N interaction and the effective interaction are identical!

• At distances $r < 1.0$ fm, however, the free N-N interaction may become extremely large (almost singular) while the corresponding effective N-N interaction is finite everywhere! This is primarily due to “Pauli blocking”.

• Therefore, the effective interaction is a better starting point for numerical calculations, in particular for mean-field theories (HF, HFB) of heavy nuclei.
Nuclear Mean Field or Energy Density Functional (EDF)

\[ E = \langle \Phi | H_{\text{eff}} | \Phi \rangle = \int d^3r \left\{ H(\rho, \tau, j, s, T, J_{\mu\nu}; r) + H_{\text{Coulomb}}(\rho_p) \right\} \]

**Single-(one-) particle density etc. in terms of s.p. states**

\[ \rho_q(r) = \sum_{i=1}^{A} \sum_{\sigma} \varphi_i^*(r, \sigma, q) \varphi_i(r, \sigma, q) \]

EDF in NP more complicated

- \( v = v_{NN-eff} \rightarrow DFT (\text{Hartee} - \text{Fock}) \)
- \( v \neq v_{NN-eff} \rightarrow DFT (\text{Kohn} - \text{Sham}) \)

ab-initio

\[ \langle \Psi | H | \Psi \rangle = E \]

Mean-field - EDF

\[ \Psi \rightarrow \Phi_{\text{Slater}} \]

\[ H \rightarrow H_{\text{eff}} \]
Phenomenological effective N-N interactions: “Skyrme” interaction

Basic idea of Skyrme (1956): for low-energy nuclear physics, consider potential in momentum space; expand $V$ in powers of momenta:

$$\vec{p} = \hbar \vec{k} = \hbar (\vec{k}_1 - \vec{k}_2) \quad \quad \vec{p'} = \hbar \vec{k}' = \hbar (\vec{k}_1' - \vec{k}_2')$$

$$\langle \vec{k} | v^{(2)} | \vec{k}' \rangle = C_1 + C_2 \left( \vec{k}^2 + \vec{k}'^2 \right) + C_3 \vec{k}' \cdot \vec{k} + \ldots$$

Note: no linear momentum terms which violate time-reversal inv.

Use inverse Fourier transform: constants $\rightarrow$ delta function, momenta $\rightarrow$ gradients:

$$v^{(2)} (\vec{r}) = V_0 \delta (\vec{r}) + V_1 \left[ \delta (\vec{r}) \hat{k}^2 + \hat{k}'^2 \delta (\vec{r}) \right] + V_2 \hat{k}' \cdot \delta (\vec{r}) \hat{k}$$
Skyrme interaction

with relative distance vector \( \vec{r} = (\vec{r}_1 - \vec{r}_2) \)

and with relative momentum operators

\[
\hat{k} = \frac{1}{2i}(\nabla_1 - \nabla_2) \quad \hat{k}' = -\frac{1}{2i}(\nabla_1 - \nabla_2)
\]

Generalize Skyrme interaction: introduce spin-exchange operator

\[
\hat{P}_\sigma = \frac{1}{2}(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2)
\]

\[v_{Sk} = v_{Sk}^{(2)} + v_{Sk}^{(3)}\]

\[v_{Sk}^{(2)} = t_0 \left(1 + x_0 \hat{P}_\sigma\right) \delta(\vec{r})\] zero-range interaction with spin-exchange
Skyrme interaction

\[ \frac{1}{2} t_1 \left( 1 + x_1 \hat{P}_\sigma \right) \left[ \delta(\vec{r}) \hat{k}^2 + \hat{k}'^2 \delta(\vec{r}) \right] \]

\[ + t_2 \left( 1 + x_2 \hat{P}_\sigma \right) \hat{k}' \cdot \delta(\vec{r}) \hat{k} \]

\[ + i t_4 (\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \left[ \hat{k}' \times \delta(\vec{r}) \hat{k} \right] \]

momentum dependence simulates finite range

spin-orbit term

three-body term (original) \( v_{Sk}^{(3)} = t_3 \delta(\vec{r}_1 - \vec{r}_2) \delta(\vec{r}_2 - \vec{r}_3) \)

For spin-saturated even-even nuclei, it is equivalent to density-dependent 2-body interaction:

\[ v_{Sk}^{(3)} \rightarrow v^{(2)}(\rho) = \frac{t_3}{6} (1 + x_3 \hat{P}_\sigma) [\rho(\vec{R})]^\alpha \delta(\vec{r}) \]

with \( \vec{R} = \frac{1}{2} (\vec{r}_1 + \vec{r}_2) \)
Skyrme interaction

Determine 10 parameters

\[ x_0, x_1, x_2, x_3, t_0, t_1, t_2, t_3, t_4, \alpha \]

by least-square fit to binding energies and radii of known nuclei.
Nuclear energy density functional (Skyrme Hartree-Fock)

Calculate binding energy in nuclear ground state

\[
E_{g.s.}^{HF} = \langle \Phi_0^{HF} | H | \Phi_0^{HF} \rangle = \\
\langle \Phi_0^{HF} | T^{(1)} + V_C^{(2)} + V_{Sk}^{(2)} + V_{Sk}^{(3)} | \Phi_0^{HF} \rangle
\]

\[
E_{g.s.}^{HF} = \int d^3r \ H(\bar{r}) \quad \text{total energy density}
\]

\[
H(\bar{r}) = H_{kin}(\tau(\bar{r})) + H_C(\rho_p(\bar{r})) + H_{sk}(\bar{r})
\]

\[
H_{kin}(\tau(\bar{r})) = \frac{\hbar^2}{2m} \tau(\bar{r})
\]
The energy density functional for the Skyrme N-N interaction, $H_C(\vec{r})$, is given by:

$$H_C(\vec{r}) = \frac{e^2}{2} \int d^3 r' \rho_p(\vec{r}') \frac{1}{|\vec{r} - \vec{r}'|} \rho_p(\vec{r}')$$

and the exchange term (Slater approximation) is:

$$-\frac{3}{4} e^2 \left( \frac{3}{\pi} \right)^{1/3} [\rho_p(\vec{r})]^{4/3}$$

This represents the energy density functional for the Skyrme N-N interaction.

$$H_{Sk}(\vec{r}) \equiv H_{Sk} \left( \rho(\vec{r}), \tau(\vec{r}), \vec{j}(\vec{r}), \vec{s}(\vec{r}), \vec{T}(\vec{r}), J_{\mu\nu}(\vec{r}) \right)$$

$H$ depends on various particle/spin densities and currents, which are defined in the next slide.
Densities and currents in EDF

particle density \((q = p / n)\)

\[
\rho_q(\vec{r}) = \sum_{\sigma = \uparrow \downarrow} \sum_{i=1}^{F} |\phi_i(\vec{r}, \sigma, q)|^2
\]

particle current density

\[
\vec{j}_q(\vec{r}) = \frac{\hbar}{2mi} \sum_{\sigma = \uparrow \downarrow} \sum_{i=1}^{F} [\phi_i^*(\vec{r}, \sigma, q) \nabla \phi_i(\vec{r}, \sigma, q) + \text{c.c.}]
\]

spin density

\[
\vec{s}_q(\vec{r}) = \sum_{(\sigma, \sigma') = \uparrow \downarrow} \sum_{i=1}^{F} \phi_i^*(\vec{r}, \sigma, q) \phi_i(\vec{r}, \sigma', q) <\sigma |\vec{\sigma}| \sigma' >
\]

In addition:
- particle kinetic energy density
- spin kinetic energy density
- spin-current tensor \(J_{\mu\nu}\) (contains spin-orbit density)
Nuclear Energy Density Functional

\[ H_s(r) = \frac{\hbar^2}{2m} \tau + \frac{1}{2} t_0 \left( 1 + \frac{1}{2} x_0 \right) \rho^2 - \frac{1}{2} t_0 \left( \frac{1}{2} + x_0 \right) \rho_p^2 + \frac{1}{4} t_0 \left( 1 + \frac{1}{2} x_1 \right) + t_2 \left( 1 + \frac{1}{2} x_2 \right) \left( \rho \tau - j^2 \right) \]

\[ \frac{1}{4} \left[ t_1 \left( \frac{1}{2} + x_1 \right) - t_2 \left( \frac{1}{2} + x_2 \right) \right] \left( \rho_p \tau_p + \rho_n \tau_n - j_p^2 - j_n^2 \right) - \frac{1}{16} \left[ 3t_1 \left( 1 + \frac{1}{2} x_1 \right) - t_2 \left( 1 + \frac{1}{2} x_2 \right) \right] \rho \nabla^2 \rho \]

\[ + \frac{1}{16} \left[ 3t_1 \left( 1 + \frac{1}{2} x_1 \right) + t_2 \left( 1 + \frac{1}{2} x_2 \right) \right] \left( \rho_p \nabla^2 \rho_p + \rho_n \nabla^2 \rho_n \right) \]

\[ + \frac{1}{12} t_3 \rho^2 \left( 1 + \frac{1}{2} x_3 \right) - \rho^2 \left( \rho_p^2 + \rho_n^2 \right) \left( x_3 + \frac{1}{2} \right) \]

\[ + \frac{1}{4} t_0 x_0 s^2 - \frac{1}{4} t_0 (s_n^2 + s_p^2) + \frac{1}{24} \rho x_3 s^2 - \frac{1}{24} t_3 \rho \left( s_n^2 + s_p^2 \right) \]

\[ + \frac{1}{32} \left( t_2 + 3t_1 \right) \sum_q s_q \cdot \nabla^2 s_q - \frac{1}{32} (t_2 x_2 - 3 t_1 x_1) s \cdot \nabla^2 s \]

\[ + \frac{1}{8} (t_1 x_1 + t_2 x_2) (s \cdot T - J^2) + \frac{1}{8} (t_2 - t_1) \sum_q (s_q \cdot T_q - J^2) \]

\[ - \frac{t_4}{2} \sum_{qq'} (1 + \delta_{qq'}) \left[ s_q \cdot \nabla \times j_q + \rho_q \nabla \mu \cdot J_{\mu \nu} \right] \]

\( (s,j,T) \) time-odd, vanish for static HF calculations of even-even nuclei
non-zero for dynamic calculations, odd mass nuclei, cranking etc.

Time-odd terms come in pairs!
Total is TR invariant