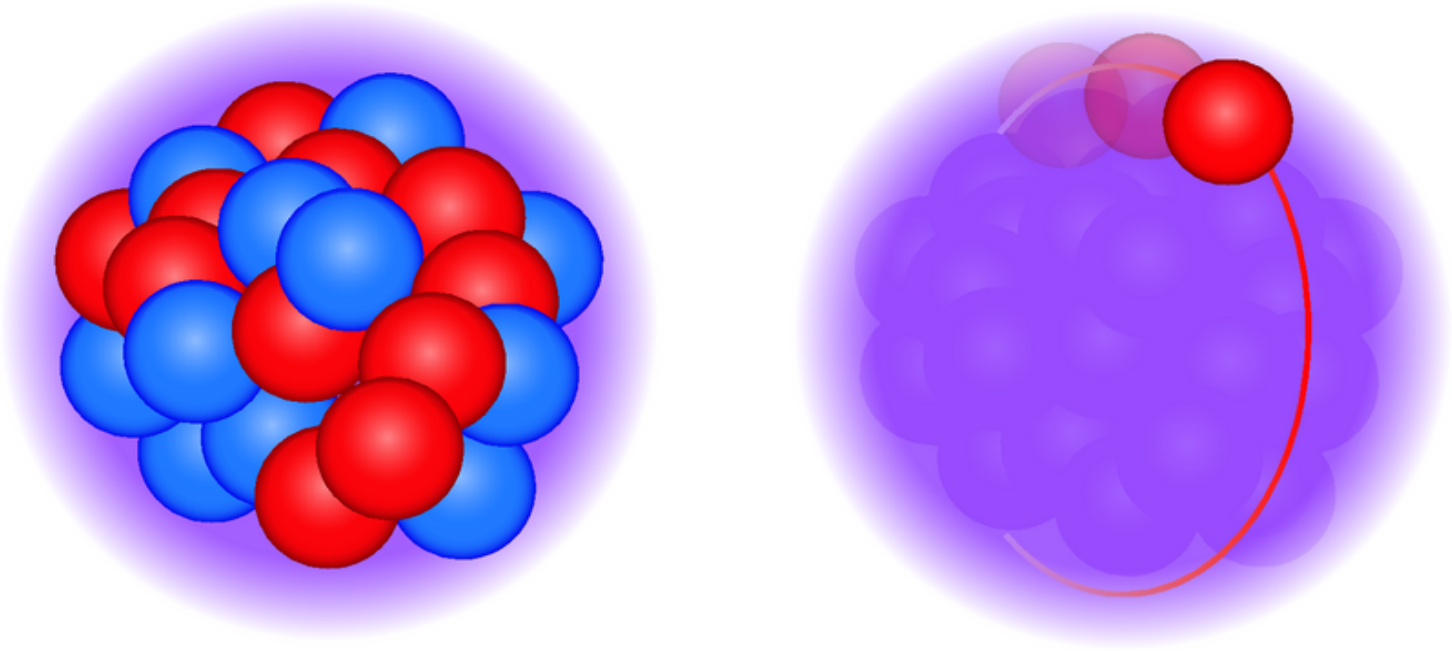
Mean-field concept

(Ref: Isotope Science Facility at Michigan State University, MSUCL-1345, p. 41, Nov. 2006)



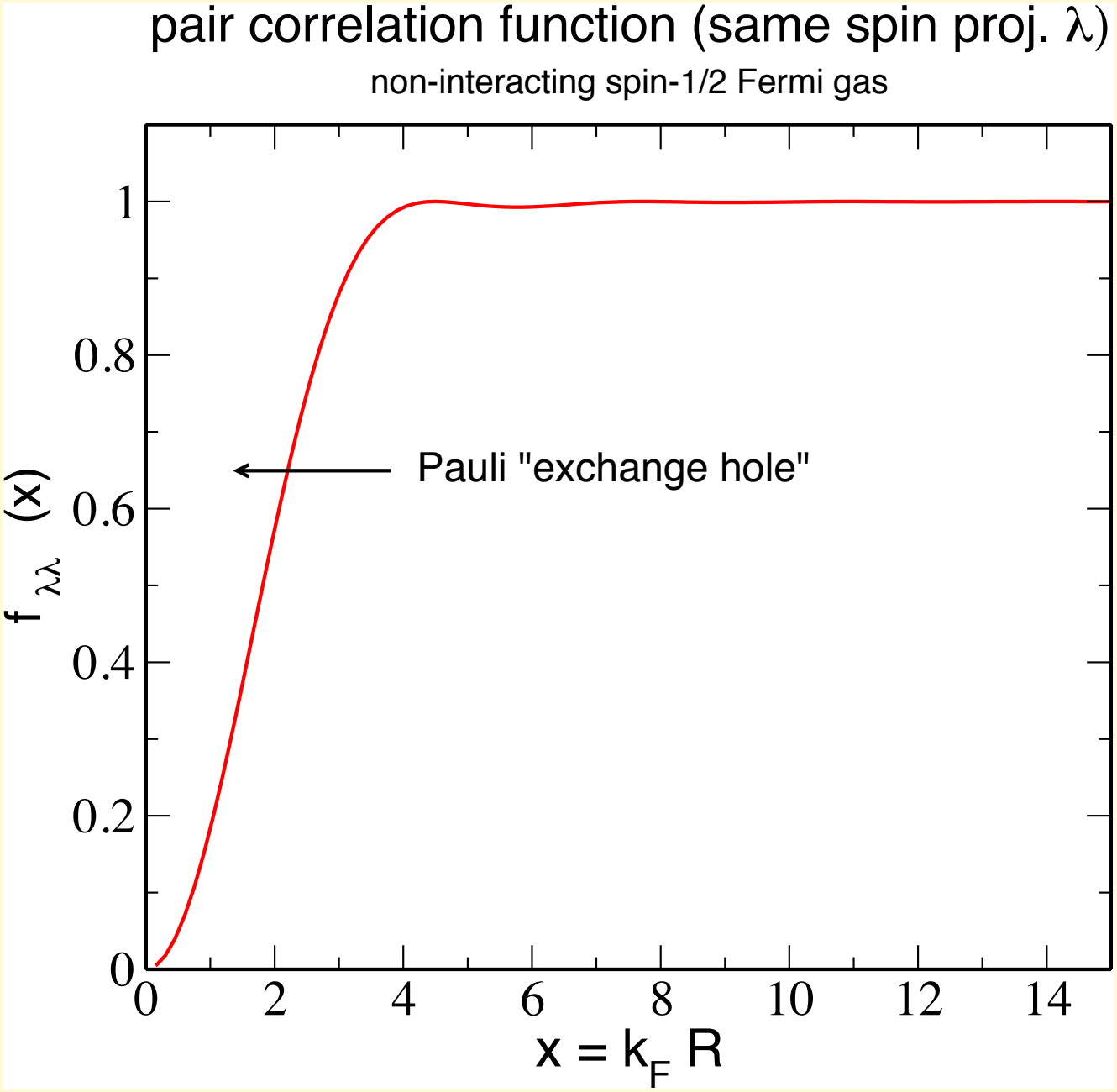
Static Hartree-Fock (HF) theory

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 $V_{NN}(^1S_0) = -2.5$ MeV (at R=0.8 fm it has a value of -100 MeV !)



Fermi momentum

$$p_F = \hbar k_F$$

$$k_F = 1.36\, fm^{-1}$$

Nuclear many-particle Hamiltonian and ground state binding energy

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

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

$$+ \frac{1}{6} \sum_{i,j,k,l,m,n=1}^{\infty} \langle ijk|V^{(3)}|lmn\rangle \hat{c}_i^{\dagger} \hat{c}_j^{\dagger} \hat{c}_k^{\dagger} \hat{c}_n \hat{c}_m \hat{c}_l$$

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

$$\langle \Phi_{g.s.} | \hat{T}^{(1)} + \hat{V}_{Coul}^{(2)} + \hat{V}_{nucl}^{(2)} + \hat{V}_{nucl}^{(3)} | \Phi_{g.s.} \rangle$$

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 phenomeno-logical 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):

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

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

$$\rho_{ji} = < \Phi_0^{HF} | \hat{c}_i^{+} \hat{c}_j | \Phi_0^{HF} >$$

HF one-body density

$$E_0(\rho) = < \Phi_0^{HF} | H | \Phi_0^{HF} >$$

HF energy density functional

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

Variational principle

Lagrange multiplier

condition for single Slater determinant

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

mean field Hamiltonian
(in energy representation)

$$[h,\rho] = 0 \Rightarrow$$

$$h|\phi_i\rangle = \varepsilon_i |\phi_i\rangle$$

$$\rho|\phi_i\rangle = n_i|\phi_i\rangle$$

Hartree-Fock equations

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)

$$V_F\left(\vec{r},\vec{r}'\right) = -V^{(2)}\left(\vec{r},\vec{r}'\right)\rho\left(\vec{r},\vec{r}'\right)$$

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

$$\rho(\vec{r},\vec{r}') = \sum_{i=1}^{F} \varphi_i^*\left(\vec{r}'\right)\varphi_i\left(\vec{r}\right)$$

The self-consistent Hartree-Fock equations: illustration for simple 2-body N-N interaction

Ref: Ring & Schuck, chapter 5

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

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

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 1st order approximation, start e.g. from shell-model wave functions to compute density / density matrix. The HF equations then generate new 2nd 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 (≈ 4000 MeV) at r ≈ 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

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

Pauli blocking

free N-N interaction

single-particle energies

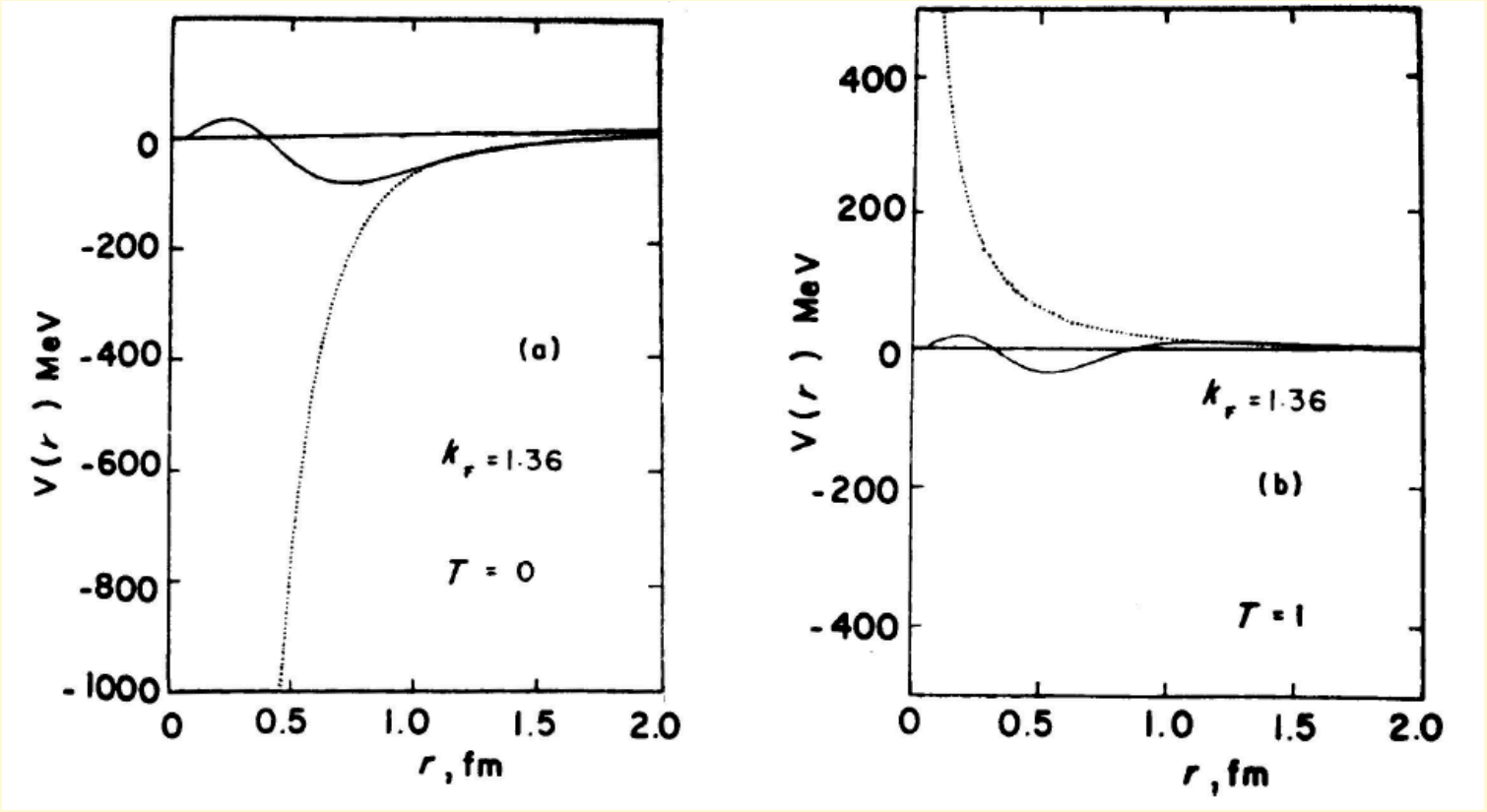
G-matrix = effective interaction

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

Ref: Sprung and Banerjee, Nucl. Phys. A168, 273 (1971)

solid line: "effective" interaction in nuclear matter, from Bethe-Goldstone eq.
dotted line: free N-N interaction



Comments on effective N-N interaction

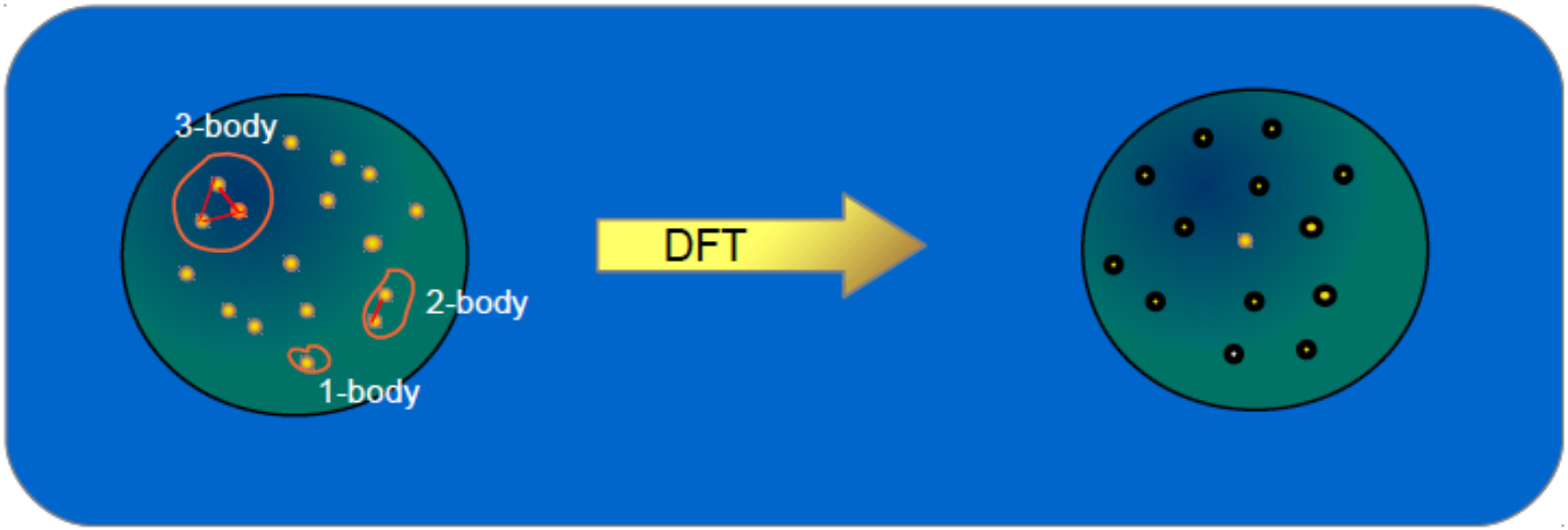
From the numerical results depicted in the last slide we conclude:

- 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)



ab-initio

$$\langle \Psi | H | \Psi \rangle = E$$

Mean-field - EDF

$$\Psi \rightarrow \Phi_{Slater}$$

$$H \rightarrow H_{eff}$$

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

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

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

EDF in NP more complicated

$$v = v_{NN-eff} \rightarrow DFT\,(Hartee - Fock)$$

$$v \neq v_{NN-eff} \rightarrow DFT\,(Kohn - Sham)$$

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:

$$\vec{p} = \hbar\vec{k} = \hbar(\vec{k_1} - \vec{k_2}) \qquad \vec{p'} = \hbar\vec{k'} = \hbar(\vec{k'_1} - \vec{k'_2})$$

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

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

Use inverse Fourier transform: constants → delta function, momenta → 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

$$\hat{k} = \frac{1}{2i}(\nabla_1 - \nabla_2) \qquad \hat{k}' = -\frac{1}{2i}(\nabla_1 - \nabla_2)$$

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

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

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

momentum dependence simulates finite range

$$+it_4(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\left[\hat{k'}\times\delta(\vec{r})\hat{k}\right]$$

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

$$E^{HF}_{g.s.} =< \Phi^{HF}_0 | H | \Phi^{HF}_0 >=$$
$$< \Phi^{HF}_0 | T^{(1)} + V^{(2)}_C + V^{(2)}_{Sk} + V^{(3)}_{Sk} | \Phi^{HF}_0 >$$

$$E^{HF}_{g.s.} = \int d^3r \; \mathcal{H}(\vec{r})$$ total energy density

$$\mathcal{H}(\vec{r}) = \mathcal{H}_{kin}(\tau(\vec{r})) + \mathcal{H}_C(\rho_p(\vec{r})) + \mathcal{H}_{Sk}(\vec{r})$$

$$\mathcal{H}_{kin}(\tau(\vec{r})) = \frac{\hbar^2}{2m}\tau(\vec{r})$$

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

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

exchange term
(Slater approximation)

energy density functional for Skyrme N-N interaction

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

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

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

$$
\begin{aligned}
H_S(\boldsymbol{r}) \;=\; & \frac{\hbar^2}{2\mathrm{m}}\tau+\frac{1}{2}t_0\left(1+\frac{1}{2}x_0\right)\rho^2-\frac{1}{2}t_0\left(\frac{1}{2}+x_0\right)\left[\rho_p^2+\rho_n^2\right]+\frac{1}{4}\left[t_1\left(1+\frac{1}{2}x_1\right)+t_2\left(1+\frac{1}{2}x_2\right)\right](\rho\tau-\boldsymbol{j}^2)\\
&-\frac{1}{4}\left[t_1\left(\frac{1}{2}+x_1\right)-t_2\left(\frac{1}{2}+x_2\right)\right](\rho_p\tau_p+\rho_n\tau_n-\boldsymbol{j}_p^2-\boldsymbol{j}_n^2)-\frac{1}{16}\left[3t_1\left(1+\frac{1}{2}x_1\right)-t_2\left(1+\frac{1}{2}x_2\right)\right]\rho\nabla^2\rho\\
&+\frac{1}{16}\left[3t_1\left(\frac{1}{2}+x_1\right)+t_2\left(\frac{1}{2}+x_2\right)\right](\rho_p\nabla^2\rho_p+\rho_n\nabla^2\rho_n)\\
&+\frac{1}{12}t_3\left[\rho^{\alpha+2}\left(1+\frac{1}{2}x_3\right)-\rho^{\alpha}\left(\rho_p^2+\rho_n^2\right)\left(x_3+\frac{1}{2}\right)\right]\\
&+\frac{1}{4}t_0x_0\boldsymbol{s}^2-\frac{1}{4}t_0(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2)+\frac{1}{24}\rho^{\alpha}t_3x_3\boldsymbol{s}^2-\frac{1}{24}t_3\rho^{\alpha}(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2)\\
&+\frac{1}{32}(t_2+3t_1)\sum_q \boldsymbol{s}_q\cdot\nabla^2\boldsymbol{s}_q-\frac{1}{32}(t_2x_2-3t_1x_1)\boldsymbol{s}\cdot\nabla^2\boldsymbol{s}\\
&+\frac{1}{8}(t_1x_1+t_2x_2)(\boldsymbol{s}\cdot\boldsymbol{T}-\boldsymbol{J}_{\mu\nu}^2)+\frac{1}{8}(t_2-t_1)\sum_q(\boldsymbol{s}_q\cdot\boldsymbol{T}_q-\boldsymbol{J}_{q\mu\nu}^2)\\
&-\frac{t_4}{2}\sum_{qq'}(1+\delta_{qq'})[\boldsymbol{s}_q\cdot\nabla\times\boldsymbol{j}_{q'}+\rho_q\boldsymbol{\nabla}_{\mu\nu}\cdot\boldsymbol{J}_{\mu\nu}]
\end{aligned}
$$

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

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