Mean-field (Hartree-Fock) Theory

\[ V(r) \sim \int v(r, r') \rho(r') \, dr' \]

Naively speaking,

\[ \rho(r) = \sum_i |\psi_i(r)|^2 \]

Independent motion

Shell model

\( l_{p_{1/2}} \)

\( l_{p_{3/2}} \)

\( l_{s_{1/2}} \)
Mean-field (Hartree-Fock) Theory

naively speaking,

\[ V(r) \sim \int v(r, r') \rho(r') dr' \]

\[ \rho(r) = \sum_i |\psi_i(r)|^2 \]

\[ 0 = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) - \epsilon_i \right] \psi_i(r) \]

\[ = \left[ -\frac{\hbar^2}{2m} \nabla^2 + \int v(r, r') \left( \sum_j |\psi_j(r')|^2 \right) dr' - \epsilon_i \right] \psi_i(r) \]

the potential depends on the solutions
Mean-field (Hartree-Fock) Theory

\[ 0 = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) - \epsilon_i \right] \psi_i(r) \]
\[ = \left[ -\frac{\hbar^2}{2m} \nabla^2 + \int v(r, r') \left( \sum_j |\psi_j(r')|^2 \right) d\mathbf{r}' - \epsilon_i \right] \psi_i(r) \]

the potential depends on the solutions

\[ \text{self-consistent solutions} \]

Iteration: \( \{\psi_i\} \rightarrow \rho \rightarrow V \rightarrow \{\psi_i\} \rightarrow \ldots \)

repeat until the first and the last wave functions are the same.

“self-consistent mean-field theory”
Skyrme-Hartree-Fock calculations for $^{40}\text{Ca}$

optimize the density by taking into account the nucleon-nucleon interaction
Skyrme-Hartree-Fock calculations for $^{40}$Ca

optimize the density by taking into account the nucleon-nucleon interaction
optimize the density by taking into account the nucleon-nucleon interaction
Skyrme-Hartree-Fock calculations for $^{40}$Ca

optimize the density by taking into account the nucleon-nucleon interaction

optimized density (and shape) can be determined automatically
Variational Principle (Rayleigh-Ritz method)

Optimization $\longleftrightarrow$ variational principle

\[
\frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \geq E_{\text{g.s.}}
\]

$H$: many-body Hamiltonian

$\Psi(r_1, r_2, \cdots) = \psi_1(r_1) \cdot \psi_2(r_2) \cdot \psi_3(r_3) \cdots$

← many-body wave function for independent particles

\[
-\frac{\hbar^2}{2m} \nabla^2 + \int \nu(r, r') \rho(r') \, dr' - \epsilon_i \psi_i(r) = 0
\]

change gradually the single-particle potential so that the total energy becomes minimum
Mean-field (Hartree-Fock) Theory

electro-static potential

test charge

interaction between identical particles
→ needs anti-symmetrization

$$V(r) \sim \int v(r, r') \rho(r') dr'$$
anti-symmetrization

nucleon: fermion

\[ \Psi(r_1, r_2, r_3 \cdots) = -\Psi(r_2, r_1, r_3 \cdots) \]

\[ \psi_1(r_1)\psi_2(r_2) \rightarrow [\psi_1(r_1)\psi_2(r_2) - \psi_2(r_1)\psi_1(r_2)] \]

Slater determinant

\[ 0 = \left[ -\frac{\hbar^2}{2m} \nabla^2 + \int v(r, r') \left( \sum_j |\psi_j(r')|^2 \right) dr' - \epsilon_i \right] \psi_i(r) \]

\[ \rightarrow \left[ -\frac{\hbar^2}{2m} \nabla^2 + \int v(r, r') \left( \sum_j |\psi_j(r')|^2 \right) dr' - \epsilon_i \right] \psi_i(r) \]

\[ -\int v(r, r') \left( \sum_j \psi^*_j(r')\psi_i(r') \right) dr'\psi_j(r) \]

exchange term

Hartree-Fock theory
\[0 = \left[ -\frac{\hbar^2}{2m} \nabla^2 + \int v(r, r') \left( \sum_j |\psi_j(r')|^2 \right) dr' - \epsilon_i \right] \psi_i(r)

\rightarrow \left[ -\frac{\hbar^2}{2m} \nabla^2 + \int v(r, r') \left( \sum_j |\psi_j(r')|^2 \right) dr' - \epsilon_i \right] \psi_i(r)

- \int v(r, r') \left( \sum_j \psi_j^*(r') \psi_i(r') \right) dr' \psi_j(r)

= \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) - \epsilon_i \right] \psi_i(r) + \int dr' V_{NL}(r, r') \psi_i(r')

\text{non-local potential}
Hartree-Fock Method and Symmetries

\[
H = -\sum_{i=1}^{A} \frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} \sum_{i,j} v(r_i, r_j) \quad \text{2body } \rightarrow \text{1 body approximation}
\]

\[
= \sum_{i=1}^{A} \left( -\frac{\hbar^2}{2m} \nabla_i^2 + V_{HF}(i) \right) + \frac{1}{2} \sum_{i,j} v(r_i, r_j) - \sum_i V_{HF}(i)
\]

\[ h_{HF} \quad V_{\text{res}} \]

Slater determinant

\[
\psi_{HF}(1, 2, \cdots, A) = \mathcal{A}[\psi_1(1)\psi_2(2)\cdots\psi_A(A)]
\]

Eigen-state of \( h_{HF} \), but not of \( H \)

\[ \psi_{HF} : \text{does not necessarily possess the symmetries that } H \text{ has.} \]

“Symmetry-broken solution”
“Spontaneous Symmetry Broken”
\( \Psi_{HF} \): does not necessarily possess the symmetries that \( H \) has.

**Typical Examples**

- **Translational symmetry:** always broken in nuclear systems

\[
H = -\sum_{i=1}^{A} \frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} \sum_{i,j} v(r_i - r_j) \rightarrow \sum_{i=1}^{A} \left( -\frac{\hbar^2}{2m} \nabla_i^2 + V_{HF}(r_i) \right)
\]

(cf.) atoms

nucleus in the center

translational symmetry: broken from the begining

- **Rotational symmetry**

*Deformed solution*
Symmetry Breaking

Advantage: a large part of many-body correlation can be taken into account without losing the independent particle picture.

an intuitive and transparent view of the nuclear deformation

Disadvantage: a need to restore the symmetry (in principle) to compute experimental observables
Constrained Hartree-Fock method

minimize \( H' = H - \lambda \hat{Q}_{20} \) with a Slater determinant wave function

\[ \hat{Q}_{20} = \sum_i r_i^2 Y_{20}(\vec{r}_i) : \text{quadrupole operator} \]

\( \lambda \) : Lagrange multiplier, to be determined

so that \( \langle \hat{Q}_{20} \rangle = Q \propto R^2 \beta \)

\[ \rightarrow E(\beta) : \text{potential energy curve} \]

\( E(\beta, \gamma) : \text{potential energy surface} \)
RMF calculations for deformed hypernuclei

Hypernuclei: nucleus + Lambda particle

Effect of a Λ particle on nuclear shapes?

Relativistic Mean-field model

Λσ and Λω couplings
Ne isotopes

Si isotopes

Myaing Thi Win and K. Hagino, PRC78(‘08)054311
Bare nucleon-nucleon interaction:

Existence of short range repulsive core

Diagram showing the potential $V(r)$ as a function of distance $r$, with $c \sim 0.4-0.5\text{fm}$ and $\sim 2.5\text{fm}$. The potential approaches $+\infty$ at the origin.
Bare nucleon-nucleon interaction

Phase shift for p-p scattering

(V.G.J. Stoks et al., PRC48(’93)792)
Phase shift:

Radial wave function

\[ \psi_l(r) = \frac{u_l(r)}{r} Y_{lm}(\hat{r}) \]

Asymptotic form:

\[ u_l(r) \to \sin(kr - l\pi/2 + \delta_l) \quad (r \to \infty) \]
Phase shift: $+\text{ve} \rightarrow -\text{ve}$ at high energies

Existence of short range repulsive core
Bruckner’s G-matrix  Nucleon-nucleon interaction \( \textit{in medium} \)

Nucleon-nucleon interaction with a hard core

\[ \text{HF method: does not work} \]

\[ \text{Matrix elements: diverge} \]

…..but the HF picture seems to work in nuclear systems

\textbf{Solution:} a nucleon-nucleon interaction \( \textit{in medium} \) (effective interaction) rather than a bare interaction

\[ \text{Bruckner’s G-matrix} \]
two-body (multiple) scattering in vacuum

\[
\begin{align*}
T_{k_1 k_2} &= T_{k'_1 k'_2} = T_{k_1 k'_1} T_{k_2 k'_2} \\
&= k_1 + \nu \left( k_2 + \nu \right) + \nu \left( k'_1 + \nu \right) + \nu \left( k'_2 + \nu \right)
\end{align*}
\]

Lippmann-Schwinger equation

\[
T = \nu + \frac{1}{E - H_0} T
\]

two-body (multiple) scattering in medium

\[
G_{k_1 k_2} = G_{k'_1 k'_2} = G_{k_1 k'_1} G_{k_2 k'_2} = G_{k_1 k'_1} G_{k_2 k'_2} + G_{k_1 k'_2} G_{k_2 k'_1}
\]

Bethe-Goldstone equation

\[
G = \nu + \nu \frac{Q_F}{E - H_0} G
\]

*scattering: suppressed because intermediate states have to have
\[k > k_F \rightarrow \text{independent particle picture}\]
Hard core

\[ G = v + v \frac{Q_F}{E - H_0} G \]

Even if \( v \) tends to infinity, \( G \) may stay finite.

Independent particle motion

![Graph showing healing distance and scattering](image)

Use \( G \) instead of \( v \) in mean-field calculations.
M. Matsuo, Phys. Rev. C73(‘06)044309
Phenomenological effective interactions

G-matrix

- ab initio
- but, cumbersome to compute (especially for finite nuclei)
- qualitatively good, but quantitatively not successful

HF calculations with a phenomenological effective interaction

Philosophy: take the functional form of $G$, but determine the parameters phenomenologically

- Skyrme interaction (non-rel., zero range)
- Gogny interaction (non-rel., finite range)
- Relativistic mean-field model (relativistic, “meson exchanges”)
Skyrme interaction density dependent zero-range interaction

\[ v(r, r') = t_0(1 + x_0 \hat{P}_\sigma)\delta(r - r') \]
\[ + \frac{1}{2} t_1(1 + x_1 \hat{P}_\sigma)(k^2 \delta(r - r') + \delta(r - r')k^2) \]
\[ + t_2(1 + x_2 \hat{P}_\sigma)k\delta(r - r')k \]
\[ + \frac{1}{6} t_3(1 + x_3 \hat{P}_\sigma)\delta(r - r')\rho^\alpha((r_1 + r_2)/2) \]
\[ + iW_0(\sigma_1 + \sigma_2)k \times \delta(r - r')k \]

the exchange potential \[ k = (\nabla_1 - \nabla_2)/2i \]

(note) finite range effect \[ \iff \] momentum dependence

\[ \langle p|V|p'\rangle = \frac{1}{(2\pi\hbar)^3} \int dr \, e^{-i(p - p') \cdot r/\hbar} V(r) \]
\[ \sim V_0 + V_1(p^2 + p'^2) + V_2pp' + \cdots \]
\[ \to V_0\delta(r) + V_1(\hat{p}^2\delta(r) + \delta(r)\hat{p}^2) + V_2\hat{p}\delta(r)\hat{p} \]
Skyrme interactions: 10 adjustable parameters

\[ v(r, r') = t_0 (1 + x_0 \hat{P}_\sigma) \delta(r - r') \]
\[ + \frac{1}{2} t_1 (1 + x_1 \hat{P}_\sigma)(k^2 \delta(r - r') + \delta(r - r')k^2) \]
\[ + t_2 (1 + x_2 \hat{P}_\sigma)k \delta(r - r')k \]
\[ + \frac{1}{6} t_3 (1 + x_3 \hat{P}_\sigma) \delta(r - r') \rho^\alpha ((r_1 + r_2)/2) \]
\[ + iw_0 (\sigma_1 + \sigma_2)k \times \delta(r - r')k \]

A fitting strategy:

B.E. and \( r_{rms} \): \(^{16}\text{O}, \text{^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{208}Pb, \ldots..} \)

Infinite nuclear matter: \( E/A, \rho_{eq}, \ldots. \)

Parameter sets:

SIII, SkM*, SGII, SLy4, \ldots..
\[ -\frac{\hbar^2}{2m} \nabla^2 \psi_i(r) + \int v(r, r') \rho_{\text{HF}}(r') dr' \psi_i(r) \]
\[ -\int \rho_{\text{HF}}(r, r') v(r, r') \psi_i(r') dr' = \epsilon_i \psi_i(r) \]

**Iteration**

\( V_{\text{HF}} \): depends on \( \psi_i \)  \quad \text{non-linear problem}

**Iteration:** \( \{\psi_i\} \rightarrow \rho_{\text{HF}} \rightarrow V_{\text{HF}} \rightarrow \{\psi_i\} \rightarrow \cdots \)

\(^{208}\text{Pb} \quad \text{(Skirme Hartree-Fock with SKM^∗)}\)

![Graphs showing density and potential](image)
Examples of HF calculations for masses and radii

Z. Patyk et al.,
PRC59(’99)704
deformation and two-neutron separation energy