Hartree-Fock Theory

Variational Principle

(Rayleigh-Ritz method)

$$\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \geq E_{\mathrm{g.s.}}$$

(note)

$$|\Psi\rangle = \sum_n C_n |\phi_n\rangle \quad \Rightarrow \quad \mathrm{lhs} = \frac{\sum_n C_n^2 E_n}{\sum_n C_n^2} \geq E_0$$

(note)

$$\frac{\delta}{\delta \Psi^*} \left(\langle \Psi | H | \Psi \rangle - E \langle \Psi | \Psi \rangle \right) = 0$$

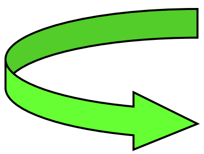
⇒ Schrodinger equation: $H|\Psi\rangle = E|\Psi\rangle$

Example: find an approximate solution for AHV

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 + \beta x^4$$

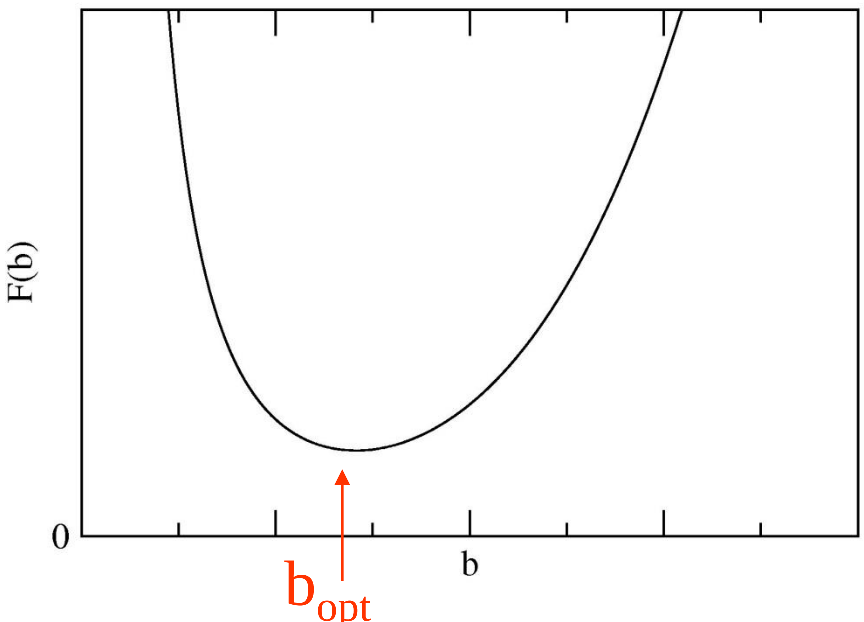
Trial wave function:

$$\Psi(x) = (\pi b^2)^{-1/4}\,\mathrm{exp}(-x^2/2b^2)$$



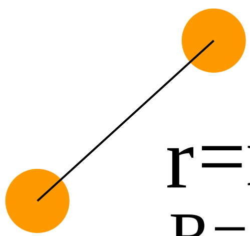
(note) if $\beta = 0, \quad b = \sqrt{\hbar/m\omega}$

$$\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\hbar^2}{4mb^2} + \frac{m\omega^2 b^2}{4} + \frac{3\beta b^4}{4} \equiv F(b)$$



Mean-Field Approximation

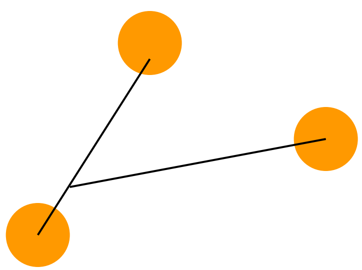
2 body problem



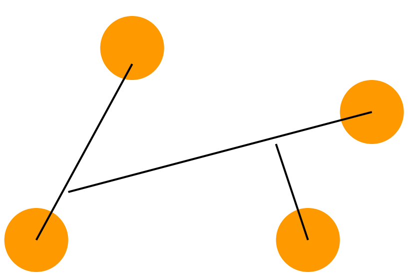
$r = r_1 - r_2$

$R = (m_1 r_1 + m_2 r_2)/(m_1 + m_2)$

3 body problem



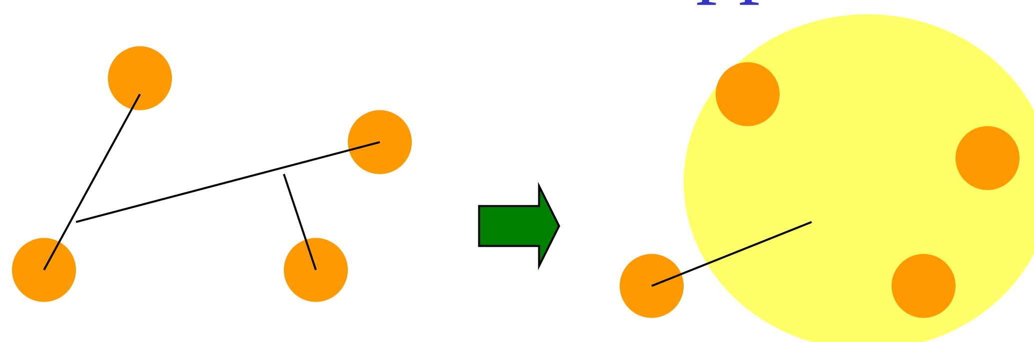
4 body problem



N body problem: necessitates an approximate method

↓

Mean Field Approach

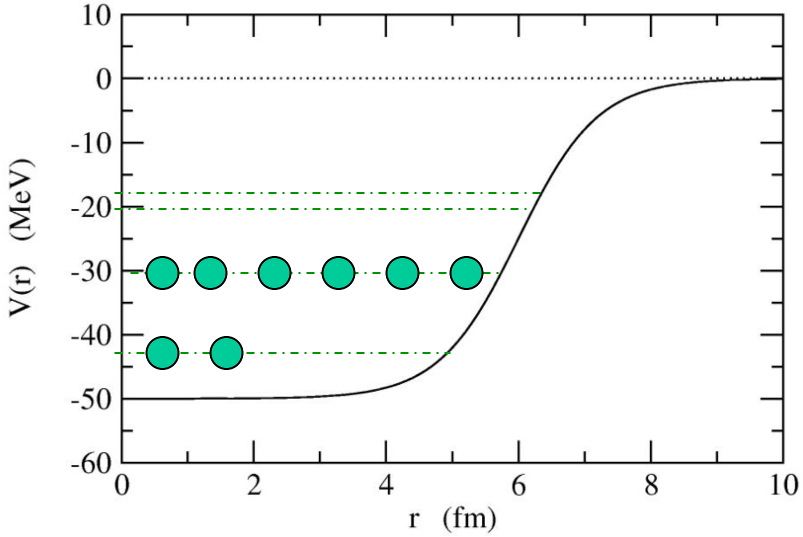


treat the interaction with other particles on average

→ independent particle motion in an *effective one-body potential*

⇧ Variational principle

Hartree-Fock Method



independent particle motion
in a potential well

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

$$= \frac{1}{\sqrt{A!}}\begin{vmatrix} \psi_1(1) & \psi_2(1) & \cdots & \psi_A(1) \\ \psi_1(2) & \psi_2(2) & \cdots & \psi_A(2) \\ \vdots & & & \\ \psi_1(A) & \psi_2(A) & \cdots & \psi_A(A) \end{vmatrix}$$

Slater determinant: antisymmetrization due to the Pauli principle

(note)

$$\Psi(1,2) = (\psi_1(1)\psi_2(2) - \psi_1(2)\psi_2(1))/\sqrt{2}$$

many-body Hamiltonian: $$H = -\sum_{i=1}^{A} \frac{\hbar^2}{2m} \boldsymbol{\nabla}_i^2 + \frac{1}{2} \sum_{i,j}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j)$$

$$\begin{aligned} \langle \Psi | H | \Psi \rangle &= -\frac{\hbar^2}{2m} \sum_{i=1}^{A} \int \psi_i^*(\boldsymbol{r}) \boldsymbol{\nabla}^2 \psi_i(\boldsymbol{r})\, d\boldsymbol{r} \\ &+ \frac{1}{2} \sum_{i,j}^{A} \int \psi_i^*(\boldsymbol{r}) \psi_j^*(\boldsymbol{r}') v(\boldsymbol{r}, \boldsymbol{r}') \psi_i(\boldsymbol{r}) \psi_j(\boldsymbol{r}')\, d\boldsymbol{r} d\boldsymbol{r}' \\ &- \frac{1}{2} \sum_{i,j}^{A} \int \psi_i^*(\boldsymbol{r}) \psi_j^*(\boldsymbol{r}') v(\boldsymbol{r}, \boldsymbol{r}') \psi_i(\boldsymbol{r}') \psi_j(\boldsymbol{r})\, d\boldsymbol{r} d\boldsymbol{r}' \end{aligned}$$

Variation with respect to ψ_i^*

Hartree-Fock equation:

$$\begin{aligned} -\frac{\hbar^2}{2m} \boldsymbol{\nabla}^2 \psi_i(\boldsymbol{r}) &+ \sum_j \int \psi_j^*(\boldsymbol{r}') v(\boldsymbol{r}, \boldsymbol{r}') \psi_j(\boldsymbol{r}') \psi_i(\boldsymbol{r})\, d\boldsymbol{r}' \\ &- \sum_j \int \psi_j^*(\boldsymbol{r}') v(\boldsymbol{r}, \boldsymbol{r}') \psi_j(\boldsymbol{r}) \psi_i(\boldsymbol{r}')\, d\boldsymbol{r}' = \epsilon_i \psi_i(\boldsymbol{r}) \end{aligned}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi_i(\boldsymbol{r}) + \sum_j \int \psi_j^*(\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\psi_j(\boldsymbol{r}')\psi_i(\boldsymbol{r})\,d\boldsymbol{r}'$$
$$-\sum_j \int \psi_j^*(\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\psi_j(\boldsymbol{r})\psi_i(\boldsymbol{r}')\,d\boldsymbol{r}' = \epsilon_i\psi_i(\boldsymbol{r})$$

$\Leftrightarrow$

$$-\frac{\hbar^2}{2m}\nabla^2\psi_i(\boldsymbol{r}) + \int v(\boldsymbol{r},\boldsymbol{r}')\rho_{\mathsf{HF}}(\boldsymbol{r}')d\boldsymbol{r}'\psi_i(\boldsymbol{r})$$
$$-\int \rho_{\mathsf{HF}}(\boldsymbol{r},\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\psi_i(\boldsymbol{r}')\,d\boldsymbol{r}' = \epsilon_i\,\psi_i(\boldsymbol{r})$$

Density matrix:

$$\rho_{\mathsf{HF}}(\boldsymbol{r},\boldsymbol{r}') = \sum_i \psi_i^*(\boldsymbol{r}')\psi_i(\boldsymbol{r})$$
$$\rho_{\mathsf{HF}}(\boldsymbol{r}) = \sum_i \psi_i^*(\boldsymbol{r})\psi_i(\boldsymbol{r}) = \rho_{\mathsf{HF}}(\boldsymbol{r},\boldsymbol{r})$$

(note)

$$\hat{\rho}_{\mathsf{HF}} = \sum_i |\psi_i\rangle\langle\psi_i| \to \hat{\rho}^2_{\mathsf{HF}} = \hat{\rho}_{\mathsf{HF}}$$

Remarks

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi_i(\boldsymbol{r}) + \int v(\boldsymbol{r},\boldsymbol{r}')\rho_{\mathsf{HF}}(\boldsymbol{r}')d\boldsymbol{r}'\psi_i(\boldsymbol{r}) - \int \rho_{\mathsf{HF}}(\boldsymbol{r},\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\psi_i(\boldsymbol{r}')\,d\boldsymbol{r}' = \epsilon_i\,\psi_i(\boldsymbol{r})$$

1. Single-particle Hamiltonian:

$$\hat{h} = \hat{T} + \hat{V}_H + \hat{V}_F$$

$$V_H(\boldsymbol{r}) = \int v(\boldsymbol{r},\boldsymbol{r}')\rho_{\mathsf{HF}}(\boldsymbol{r}')d\boldsymbol{r}'$$

Direct (Hartree) term

$$\hat{V}_F(\boldsymbol{r},\boldsymbol{r}') = -\rho_{\mathsf{HF}}(\boldsymbol{r},\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')$$

Exchange (Fock) term
[non-local pot.]

2. Iteration

V_{HF}: depends on ψ_i $\longleftarrow$ non-linear problem

Iteration: $\{\psi_i\} \to \rho_{\mathsf{HF}} \to V_{\mathsf{HF}} \to \{\psi_i\} \to \cdots$

3. Total energy

(here, we use the Hatree approximation for simplicity, but the same argument holds also for the HF approximation.)

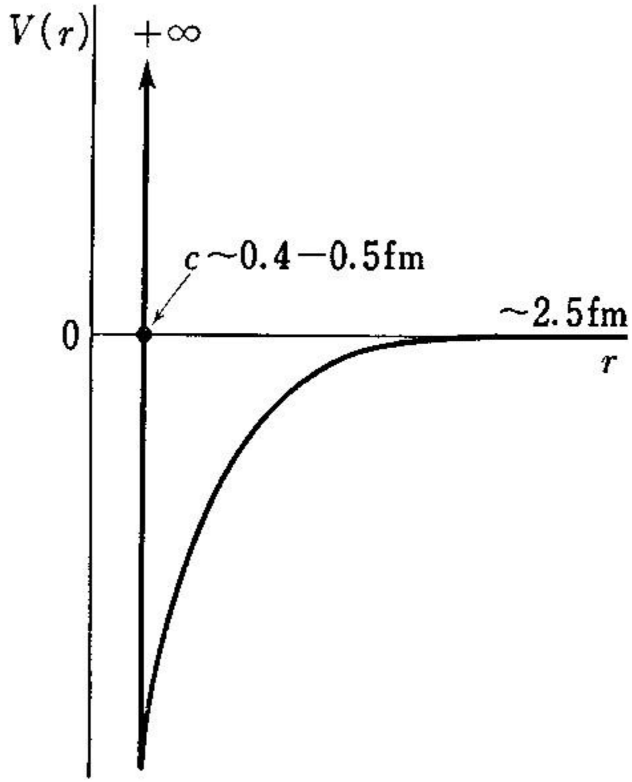
Hartree equation:

$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi_i(\boldsymbol{r})+\int v(\boldsymbol{r},\boldsymbol{r}')\rho_{\mathsf{HF}}(\boldsymbol{r}')d\boldsymbol{r}'\psi_i(\boldsymbol{r})=\epsilon_i\,\psi_i(\boldsymbol{r})$$

$$\begin{aligned}\langle\Psi|H|\Psi\rangle &= -\frac{\hbar^2}{2m}\sum_{i=1}^{A}\int\,\psi_i^*(\boldsymbol{r})\boldsymbol{\nabla}^2\psi_i(\boldsymbol{r})\,d\boldsymbol{r}\\ &\quad+\frac{1}{2}\sum_{i,j}^{A}\int\,\psi_i^*(\boldsymbol{r})\psi_j^*(\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\psi_i(\boldsymbol{r})\psi_j(\boldsymbol{r}')\,d\boldsymbol{r}d\boldsymbol{r}'\\ &= \frac{1}{2}\left(E_{\mathsf{kin}}+\sum_i\epsilon_i\right)\end{aligned}$$

$$E_{\mathsf{kin}}=-\frac{\hbar^2}{2m}\sum_{i=1}^{A}\int\,\psi_i^*(\boldsymbol{r})\boldsymbol{\nabla}^2\psi_i(\boldsymbol{r})\,d\boldsymbol{r}$$

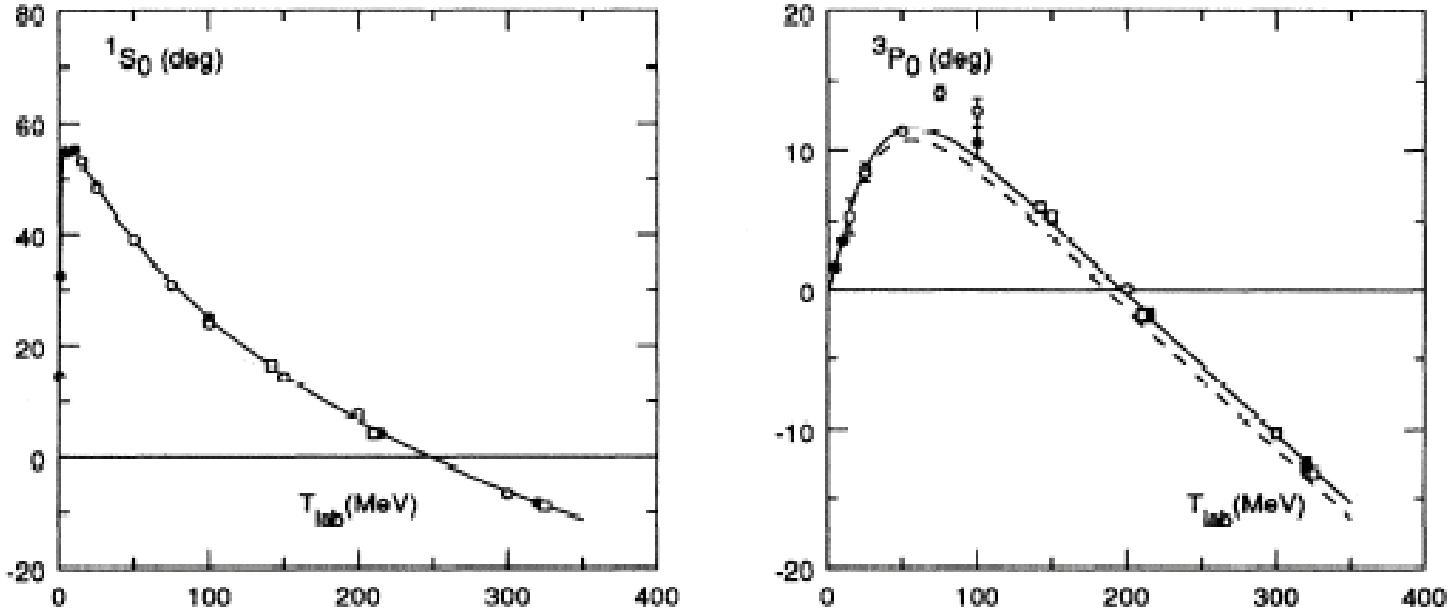
Bare nucleon-nucleon interaction



Existence of short range
repulsive core

Bare nucleon-nucleon interaction

Phase shift for p-p scattering



(V.G.J. Stoks et al., PRC48('93)792)

Phase shift:

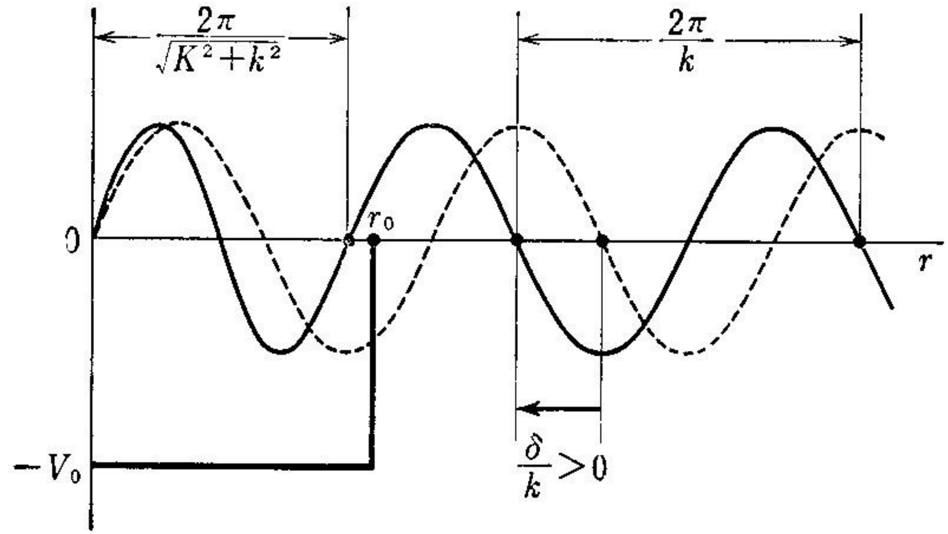
Radial wave function

$$\Psi_l(\boldsymbol{r}) = \frac{u_l(r)}{r} Y_{lm}(\hat{\boldsymbol{r}})$$

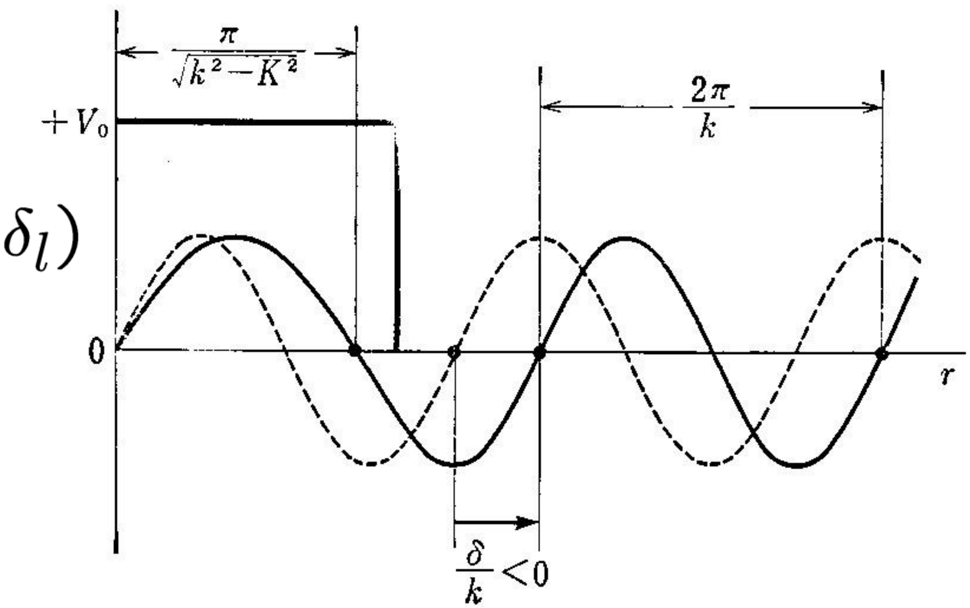
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E\right] u_l(r) = 0$$

Asymptotic form:

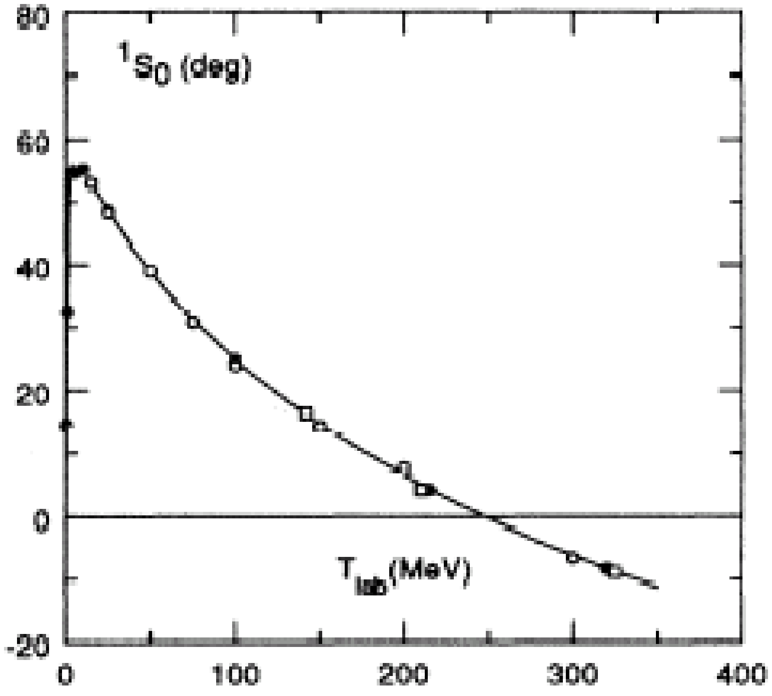
$$u_l(r) \;\rightarrow\; \sin(kr - l\pi/2 + \delta_l) \quad (r \rightarrow \infty)$$

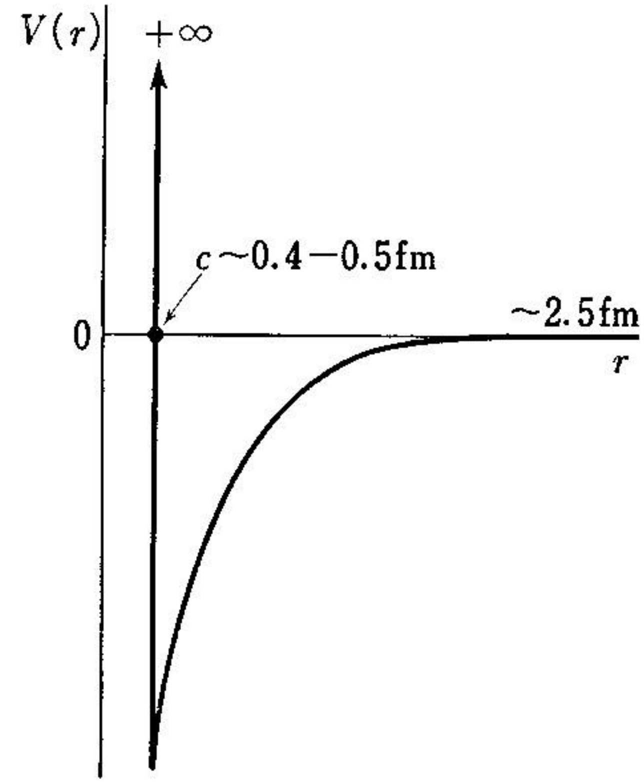


（a） 引 力



（b） 斥 力





Phase shift: +ve ⟶ -ve
at high energies

Existence of short range repulsive core

Bruckner's G-matrix

Nucleon-nucleon interaction *in medium*

Nucleon-nucleon interaction with a hard core

⇨ HF method: does not work

← Matrix elements: diverge

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

Solution: a nucleon-nucleon interaction *in medium* (effective interaction) rather than a bare interaction

⇧

Bruckner's G-matrix

(note) Lippmann-Schwinger equation

$$\left[-\frac{\hbar}{2m}\nabla^2 + V - E\right]\Psi = 0 \qquad \text{or} \qquad \left[-\frac{\hbar}{2m}\nabla^2 - E\right]\Psi = -V\Psi$$

$$\Psi = \Phi - \frac{1}{-\hbar^2\nabla^2/2m - E - i\eta}V\Psi$$

define $T\Phi = V\Psi$ (T-matrix)

$$T\Phi = V\Phi - V\frac{1}{-\hbar^2\nabla^2/2m - E - i\eta}T\Phi$$

For a two-particle system in the momentum representation:

$$|\Phi\rangle = |\boldsymbol{k}_1\boldsymbol{k}_2\rangle$$

$$T_{\boldsymbol{k}_1'\boldsymbol{k}_2',\boldsymbol{k}_1\boldsymbol{k}_2}(E) = v_{\boldsymbol{k}_1'\boldsymbol{k}_2',\boldsymbol{k}_1\boldsymbol{k}_2} + \frac{1}{2}\sum_{\boldsymbol{p}_1,\boldsymbol{p}_2} v_{\boldsymbol{k}_1'\boldsymbol{k}_2',\boldsymbol{p}_1\boldsymbol{p}_2}\frac{1}{E - p_1^2/2m - p_2^2/2m + i\eta}T_{\boldsymbol{p}_1\boldsymbol{p}_2,\boldsymbol{k}_1\boldsymbol{k}_2}(E)$$

$$T\Phi = V\Phi - V\frac{1}{-\hbar^2\nabla^2/2m - E - i\eta}T\Phi$$

For a two-particle system in the momentum representation:

$$T_{\boldsymbol{k}_1'\boldsymbol{k}_2',\boldsymbol{k}_1\boldsymbol{k}_2}(E) = v_{\boldsymbol{k}_1'\boldsymbol{k}_2',\boldsymbol{k}_1\boldsymbol{k}_2} + \frac{1}{2}\sum_{\boldsymbol{p}_1,\boldsymbol{p}_2} v_{\boldsymbol{k}_1'\boldsymbol{k}_2',\boldsymbol{p}_1\boldsymbol{p}_2}\frac{1}{E - p_1^2/2m - p_2^2/2m + i\eta}T_{\boldsymbol{p}_1\boldsymbol{p}_2,\boldsymbol{k}_1\boldsymbol{k}_2}(E)$$

Analogous equation in nuclear medium

$$G_{\boldsymbol{k}_1'\boldsymbol{k}_2',\boldsymbol{k}_1\boldsymbol{k}_2}(E) = v_{\boldsymbol{k}_1'\boldsymbol{k}_2',\boldsymbol{k}_1\boldsymbol{k}_2} + \frac{1}{2}\sum_{\boldsymbol{p}_1,\boldsymbol{p}_2>p_F} v_{\boldsymbol{k}_1'\boldsymbol{k}_2',\boldsymbol{p}_1\boldsymbol{p}_2}\frac{1}{E - p_1^2/2m - p_2^2/2m + i\eta}G_{\boldsymbol{p}_1\boldsymbol{p}_2,\boldsymbol{k}_1\boldsymbol{k}_2}(E)$$

(Bethe-Goldstone equation)

in the operator form: $G = v + v\frac{Q_F}{E - H_0}G$ (G-matrix)

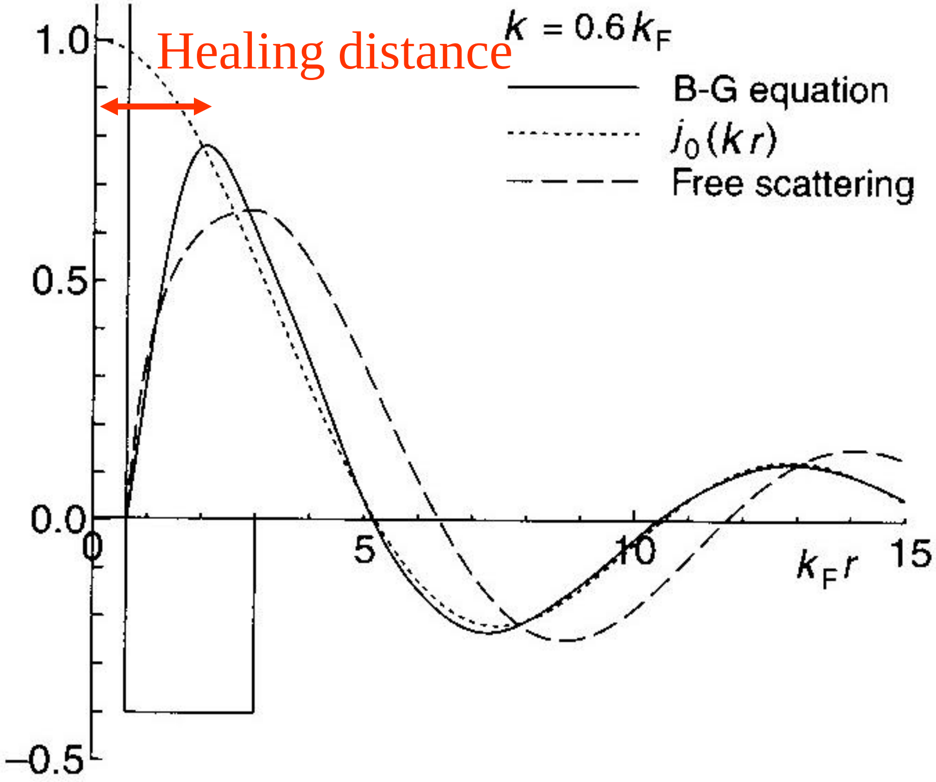
Use G instead of v in HF calculations

◆Hard core

$$G = v + v\frac{Q_F}{E - H_0}G \quad \Longleftrightarrow \quad G = \frac{v}{1 - vQ_F/(E - H_0)}$$

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

◆Independent particle motion



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

$$
\begin{aligned}
v(\boldsymbol{r},\boldsymbol{r}') &= t_0(1+x_0\widehat{P}_\sigma)\delta(\boldsymbol{r}-\boldsymbol{r}') \\
&+\frac{1}{2}t_1(1+x_1\widehat{P}_\sigma)(\boldsymbol{k}^2\delta(\boldsymbol{r}-\boldsymbol{r}')+\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k}^2) \\
&+t_2(1+x_2\widehat{P}_\sigma)\boldsymbol{k}\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k} \\
&+\frac{1}{6}t_3(1+x_3\widehat{P}_\sigma)\delta(\boldsymbol{r}-\boldsymbol{r}')\rho^\alpha((\boldsymbol{r}_1+\boldsymbol{r}_2)/2) \\
&+iW_0(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\boldsymbol{k}\times\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k}
\end{aligned}
$$

$$\boldsymbol{k}=(\boldsymbol{\nabla}_1-\boldsymbol{\nabla}_2)/2i$$

(note) finite range effect ⟺ momentum dependence

$$
\begin{aligned}
\langle\boldsymbol{p}|V|\boldsymbol{p}'\rangle &= \frac{1}{(2\pi\hbar)^3}\int d\boldsymbol{r}\,e^{-i(\boldsymbol{p}-\boldsymbol{p}')\cdot\boldsymbol{r}/\hbar}V(\boldsymbol{r}) \\
&\sim V_0+V_1(\boldsymbol{p}^2+\boldsymbol{p}'^2)+V_2\boldsymbol{p}\boldsymbol{p}'+\cdots \\
&\to V_0\delta(\boldsymbol{r})+V_1(\hat{\boldsymbol{p}}^2\delta(\boldsymbol{r})+\delta(\boldsymbol{r})\hat{\boldsymbol{p}}^2)+V_2\,\hat{\boldsymbol{p}}\delta(\boldsymbol{r})\hat{\boldsymbol{p}}
\end{aligned}
$$

Skyrme interactions: 10 adjustable parameters

$$
\begin{aligned}
v(\boldsymbol{r},\boldsymbol{r}') \;=\; & t_0(1+x_0\widehat{P}_\sigma)\delta(\boldsymbol{r}-\boldsymbol{r}') \\
& +\frac{1}{2}t_1(1+x_1\widehat{P}_\sigma)(\boldsymbol{k}^2\delta(\boldsymbol{r}-\boldsymbol{r}')+\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k}^2) \\
& +t_2(1+x_2\widehat{P}_\sigma)\boldsymbol{k}\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k} \\
& \frac{1}{6}t_3(1+x_3\widehat{P}_\sigma)\delta(\boldsymbol{r}-\boldsymbol{r}')\rho^\alpha((\boldsymbol{r}_1+\boldsymbol{r}_2)/2) \\
& +iW_0(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\boldsymbol{k}\times\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k}
\end{aligned}
$$

A fitting strategy:

B.E. and r_{rms}: ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{208}Pb,…..

Infinite nuclear matter: E/A, ρ_{eq} ,….

Parameter sets:

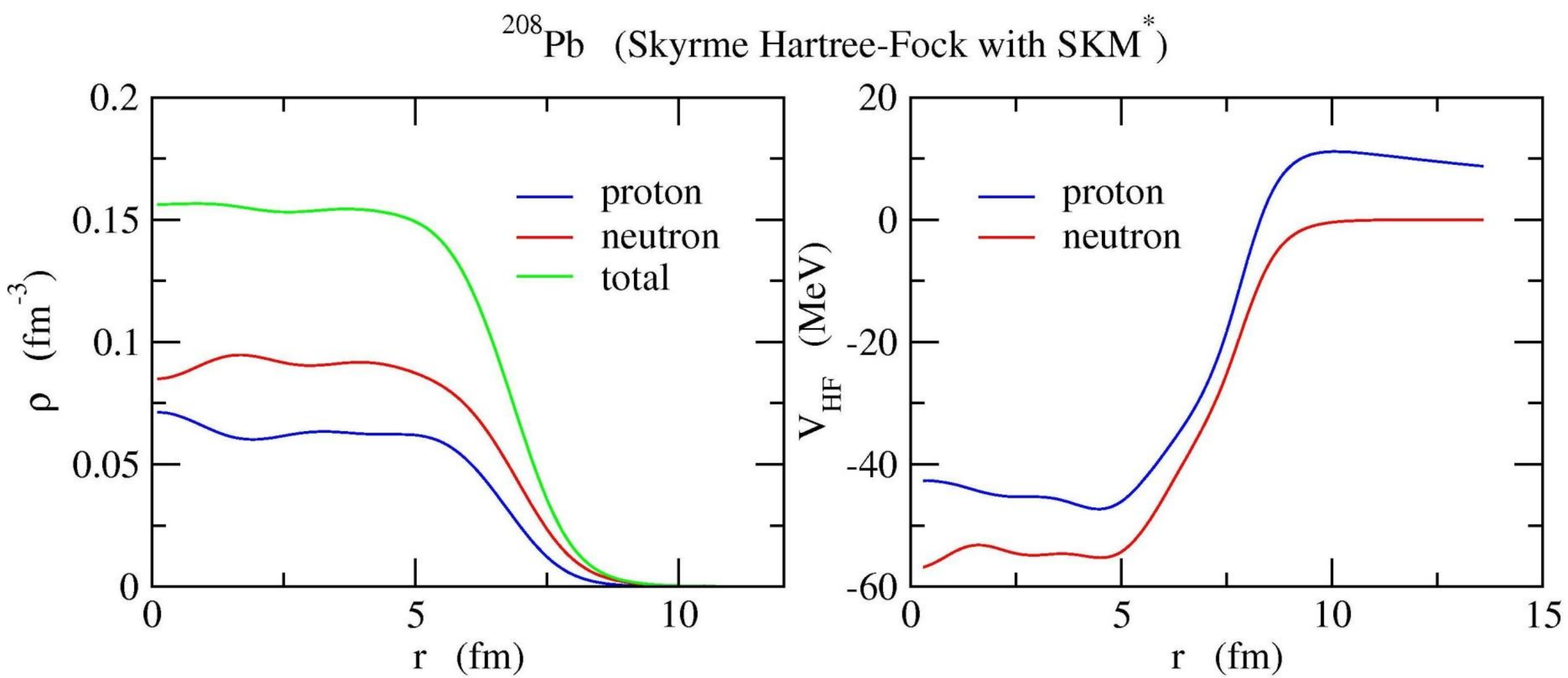
SIII, SkM*, SGII, SLy4,…….

$$-\frac{\hbar^2}{2m}\nabla^2\psi_i(\boldsymbol{r}) + \int v(\boldsymbol{r},\boldsymbol{r}')\rho_{\mathsf{HF}}(\boldsymbol{r}')d\boldsymbol{r}'\psi_i(\boldsymbol{r}) - \int \rho_{\mathsf{HF}}(\boldsymbol{r},\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\psi_i(\boldsymbol{r}')\,d\boldsymbol{r}' = \epsilon_i\,\psi_i(\boldsymbol{r})$$

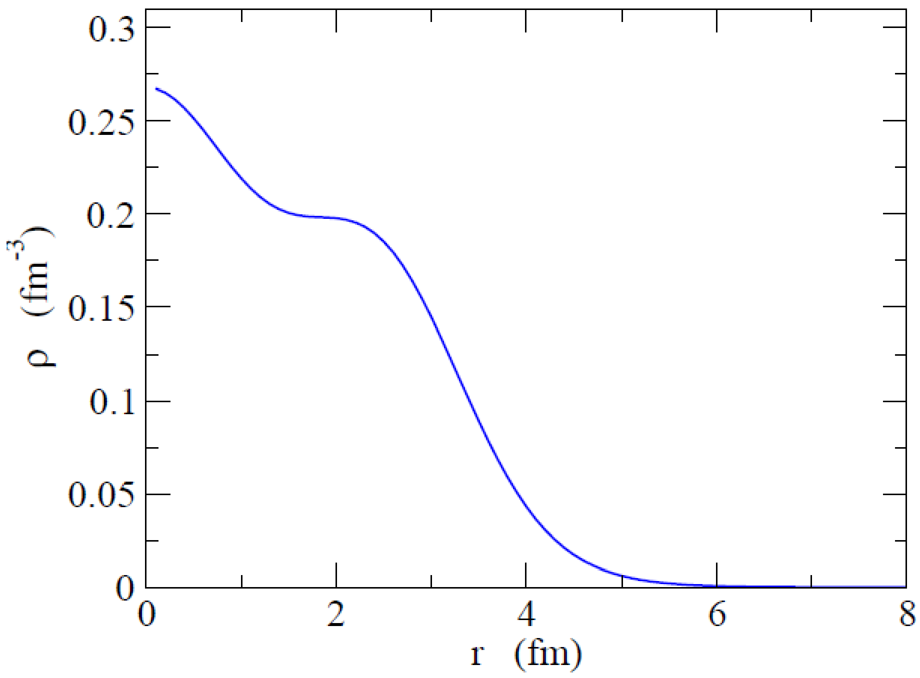
Iteration

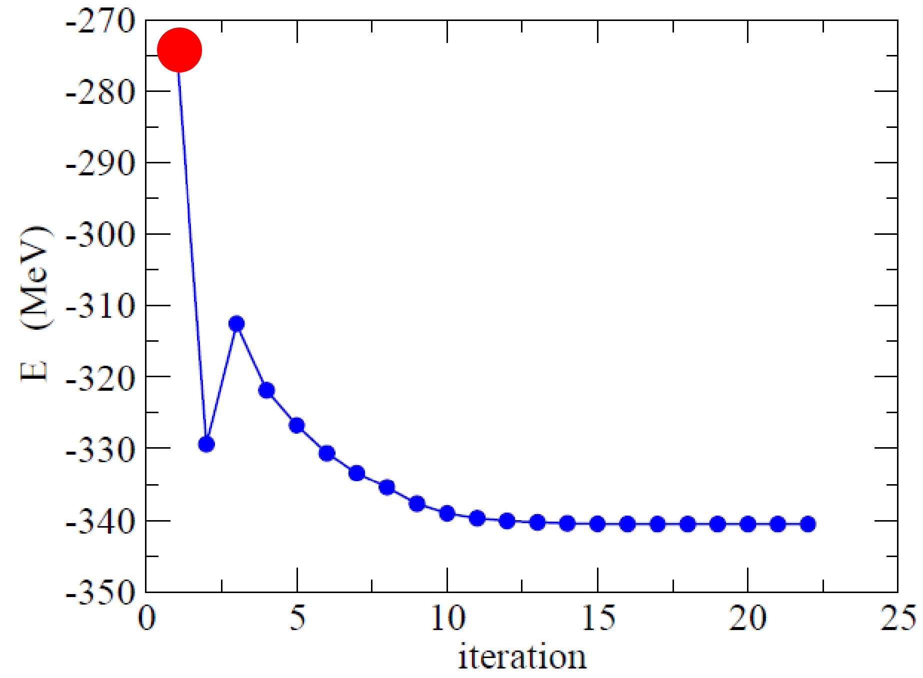
V_{HF}: depends on ψ_i ⟵ non-linear problem

Iteration: $\{\psi_i\} \rightarrow \rho_{\mathsf{HF}} \rightarrow V_{\mathsf{HF}} \rightarrow \{\psi_i\} \rightarrow \cdots$



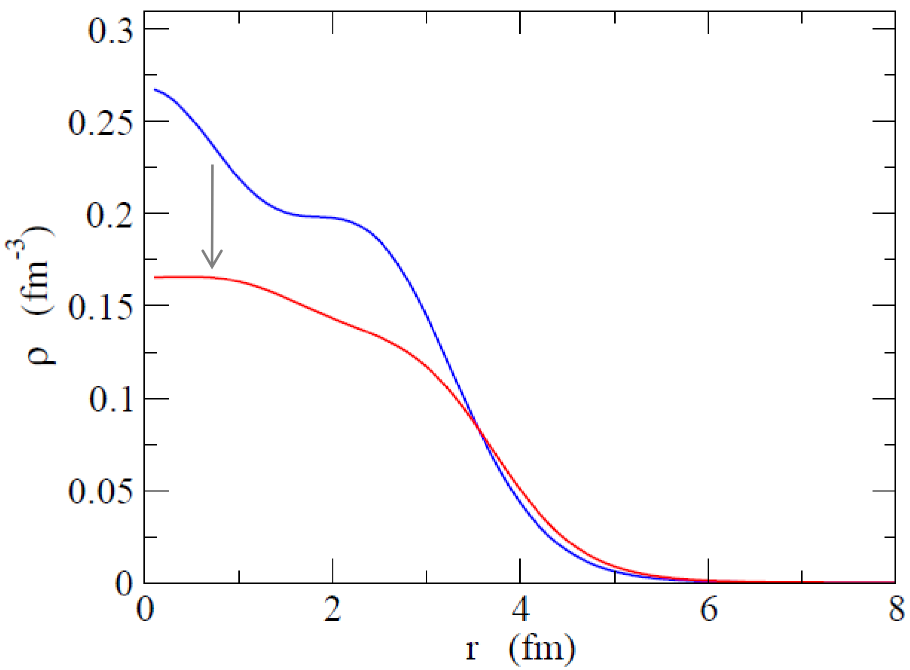
Skyrme-Hartree-Fock calculations for ^{40}Ca

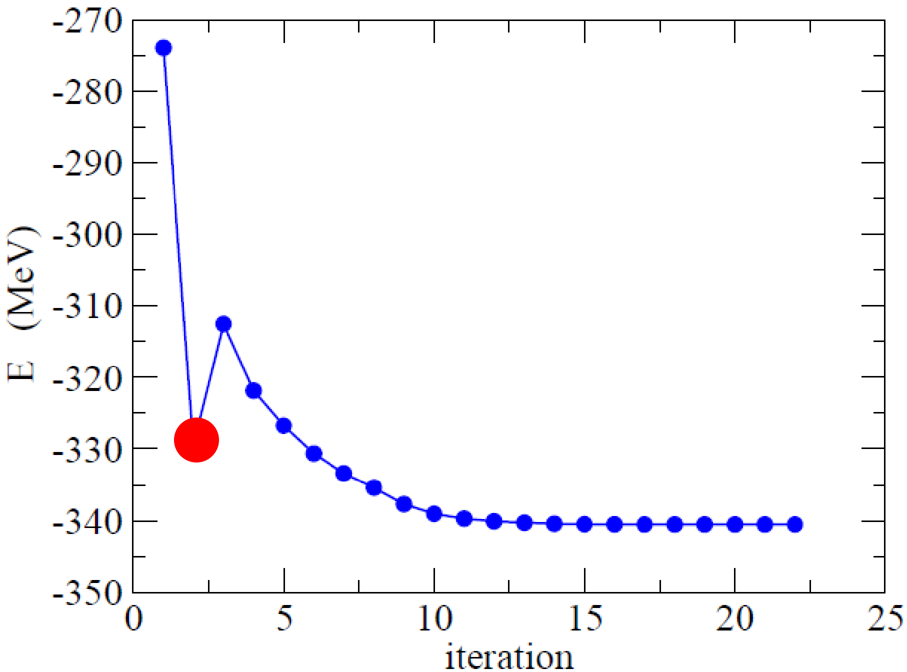




optimize the density by taking into account the nucleon-nucleon interaction

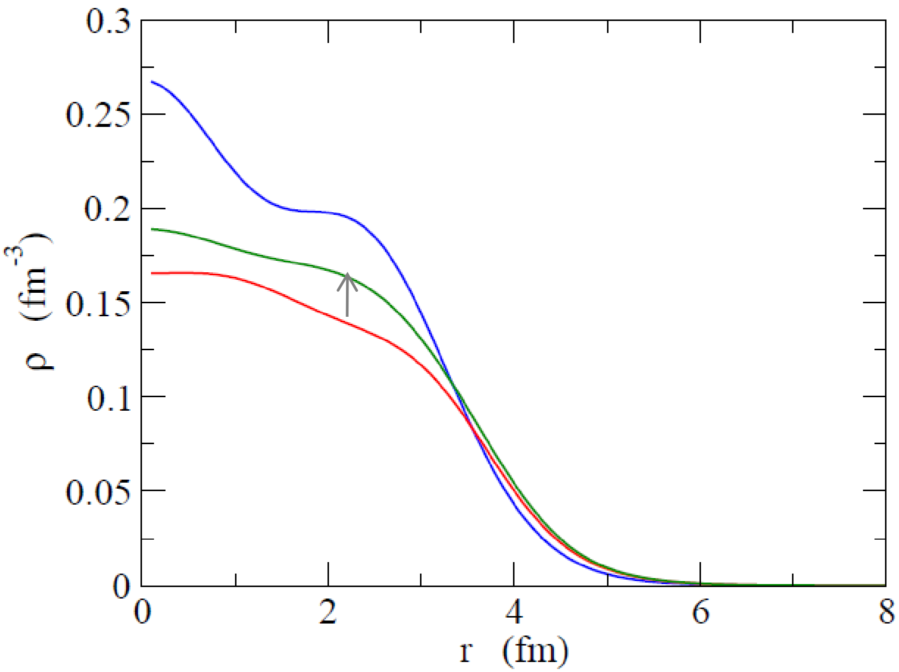
Skyrme-Hartree-Fock calculations for ^{40}Ca

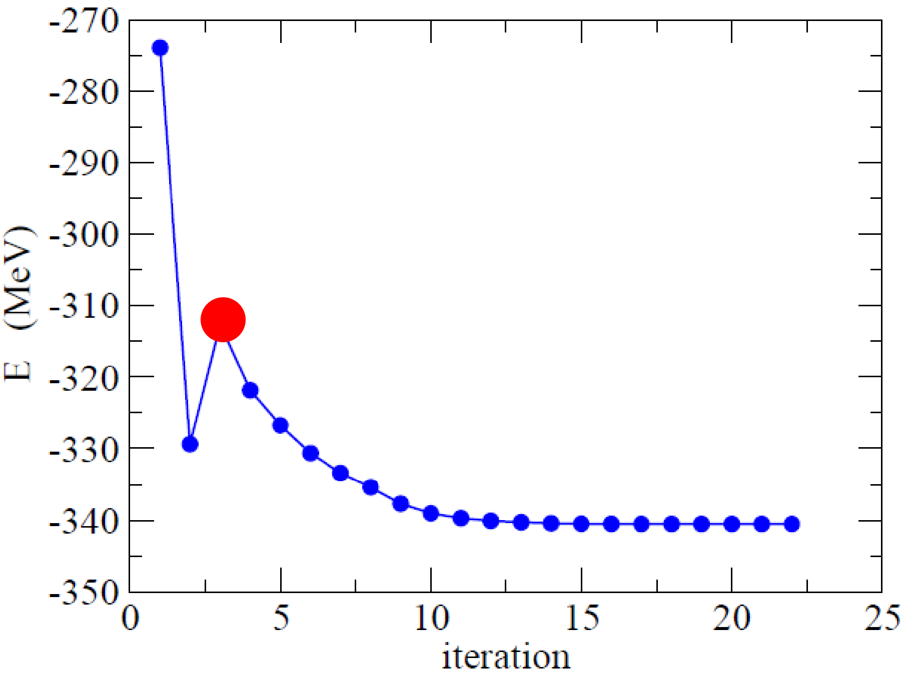




optimize the density by taking into account the nucleon-nucleon interaction

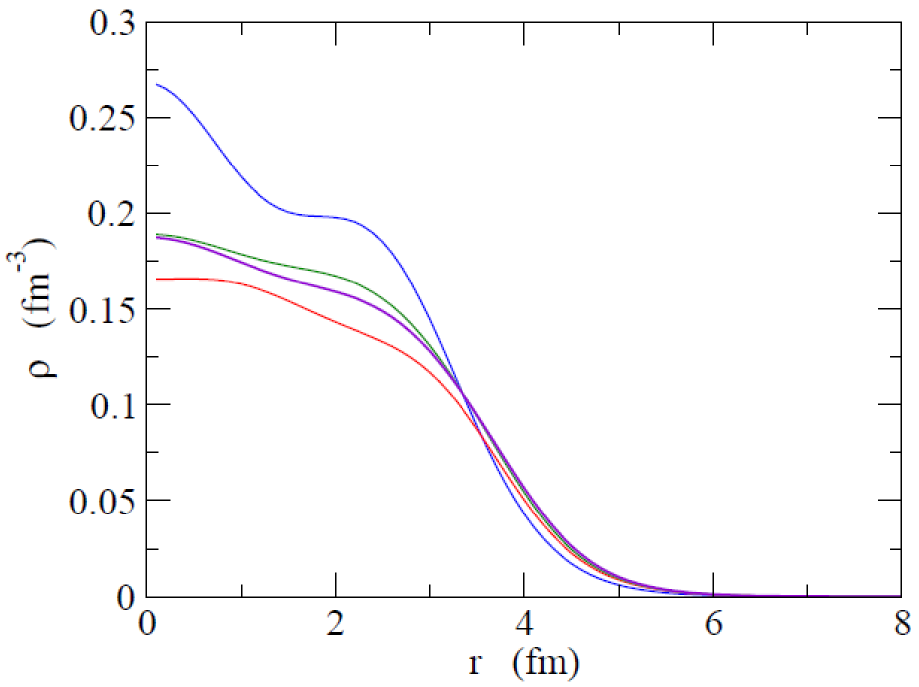
Skyrme-Hartree-Fock calculations for ^{40}Ca

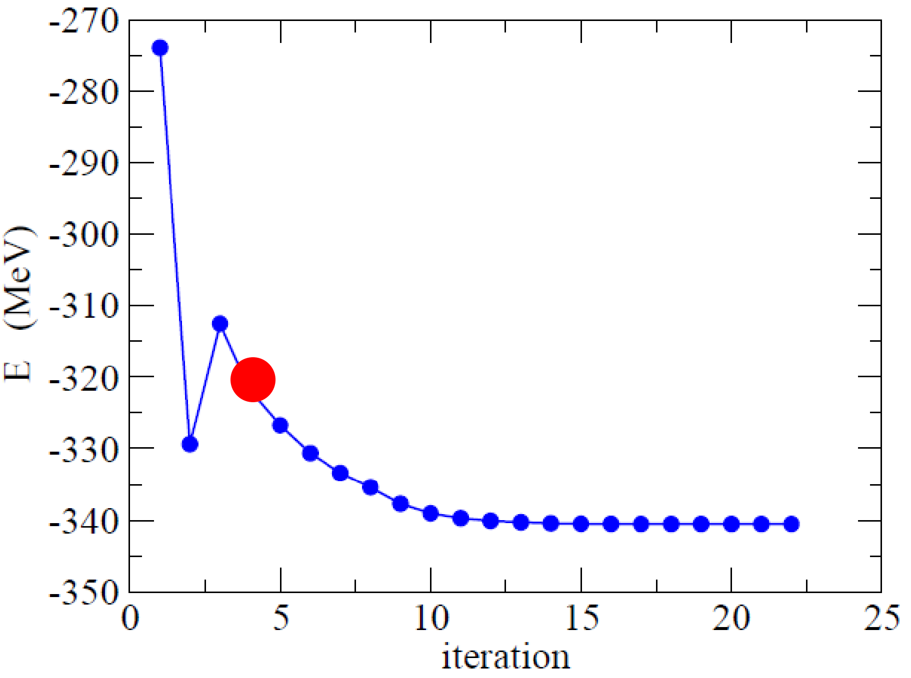




optimize the density by taking into account the nucleon-nucleon interaction

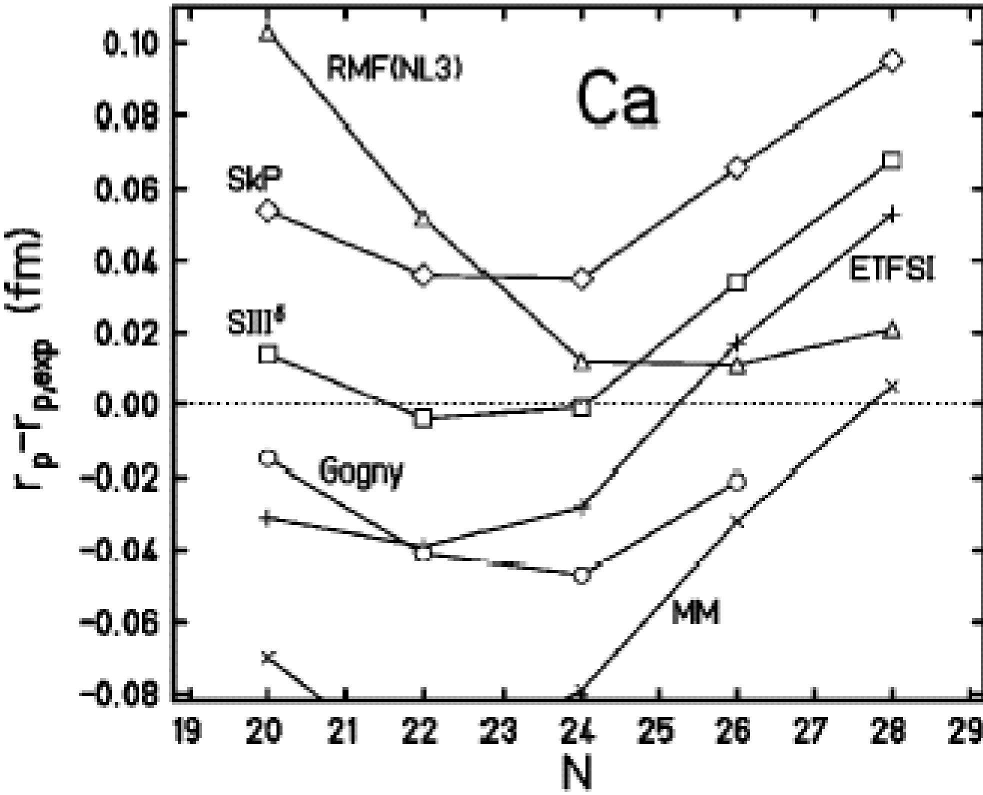
Skyrme-Hartree-Fock calculations for ^{40}Ca



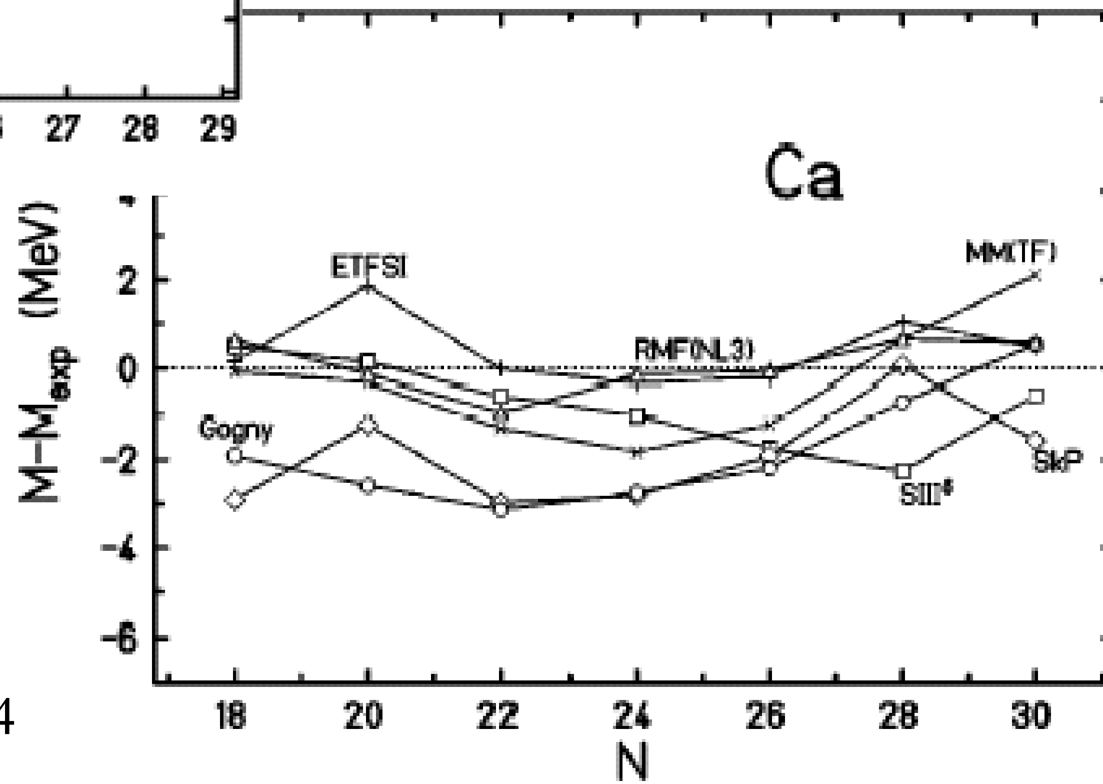


optimize the density by taking into account the nucleon-nucleon interaction

→ optimized density (and shape) can be determined automatically



Examples of HF calculations for masses and radii



Z. Patyk et al., PRC59('99)704

Density Functional Theory

With Skyrme interaction:

$$
\begin{aligned}
\langle \Psi | H | \Psi \rangle &= E[\rho, \tau, J] \\
&= \int d\boldsymbol{r} \left(\frac{\hbar^2}{2m}\tau + \frac{1}{2}t_0(1 + \frac{1}{2}x_0)\rho^2 \right. \\
&\qquad \left. -\frac{1}{2}t_0(x_0 + \frac{1}{2})\sum_q \rho_q^2 \cdots \right)
\end{aligned}
$$

Energy functional in terms of local densities

⇕

Close analog to the Density Functional Theory (DFT)

Density Functional Theory

Ref. W. Kohn, Nobel Lecture (RMP 71('99) 1253)

i) Hohenberg-Kohn Theorem

$H = H_0 + V_{ext}$

$$Lemma: \quad \rho(\boldsymbol{r}) \rightarrow V_{\text{ext}}(\boldsymbol{r})$$ (unique)

→ Density: the basic variable

ii) Hohenberg-Kohn variational principle

$$\left.\begin{aligned} \rho(\boldsymbol{r}) &= \langle\Psi|\sum_i \delta(\boldsymbol{r}-\boldsymbol{r}_i)|\Psi\rangle \\ E[\rho] &= \langle\Psi|H|\Psi\rangle \end{aligned}\right\} \Rightarrow E[\rho] \geq E_{gs}$$

→ The existence of a functional $E[\rho]$, which gives the exact g.s. energy for a given g.s. density

(note) $E[\rho] = E_{\text{HF}}[\rho] + E_{\text{corr}}[\rho]$

→ a part of the correlation effect is included in the Skyrme functional through the value of the parameters

Proof of the Hohenberg-Kohn theorem

Assume that there exist two external potentials, V_1 and V_2, which give the same g.s. density ρ (with different g.s. wave functions, Ψ_1 and Ψ_2)

$$\begin{aligned} E_1 &= \langle \Psi_1 | H_1 | \Psi_1 \rangle \\ &= \int V_1(\boldsymbol{r}) \rho(\boldsymbol{r}) d\boldsymbol{r} + \langle \Psi_1 | T + U | \Psi_1 \rangle \end{aligned}$$

$$\begin{aligned} E_2 &= \langle \Psi_2 | H_2 | \Psi_2 \rangle \\ &= \int V_2(\boldsymbol{r}) \rho(\boldsymbol{r}) d\boldsymbol{r} + \langle \Psi_2 | T + U | \Psi_2 \rangle \end{aligned}$$

(note)

$$\begin{aligned} E_1 &< \langle \Psi_2 | H_1 | \Psi_2 \rangle \\ &= E_2 + \int (V_1(\boldsymbol{r}) - V_2(\boldsymbol{r})) \rho(\boldsymbol{r}) d\boldsymbol{r} \\ E_2 &< E_1 + \int (V_2(\boldsymbol{r}) - V_1(\boldsymbol{r})) \rho(\boldsymbol{r}) d\boldsymbol{r} \end{aligned}$$

? $\rightarrow$ $E_1 + E_2 < E_1 + E_2$

iii) Kohn-Sham Equation

Set $$\rho(\boldsymbol{r}) = \sum_{i=1}^{N} |\phi_i(\boldsymbol{r})|^2$$

Kohn-Sham equation

$$\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \frac{\delta E}{\delta \rho} - \epsilon_i\right)\phi_i(\boldsymbol{r}) = 0$$

(note) $$E[\rho] = E_{\mathrm{HF}}[\rho] + E_{\mathrm{corr}}[\rho]$$

→ KS: extension of HF