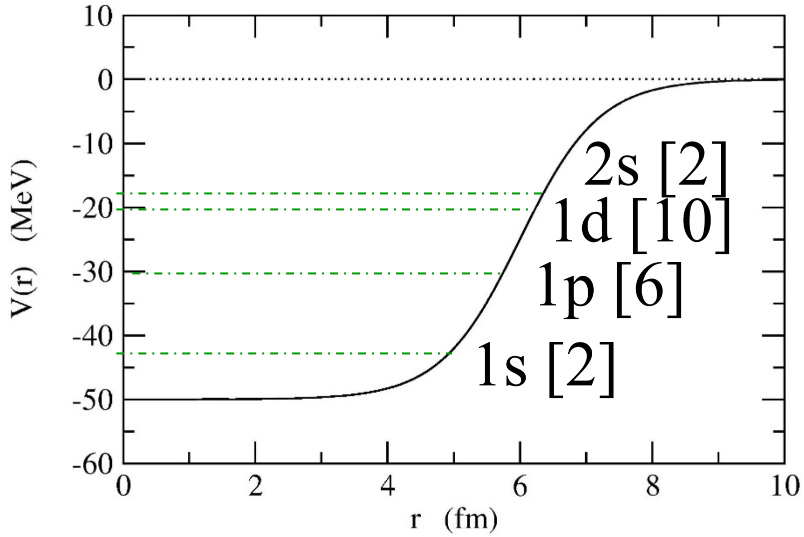
Extra binding for N or Z = 2, 8, 20, 28, 50, 82, 126 (magic numbers)

An interpretation: independent particle motion in a potential well

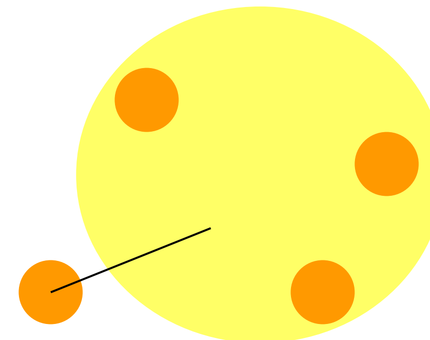


+ spin-orbit interaction

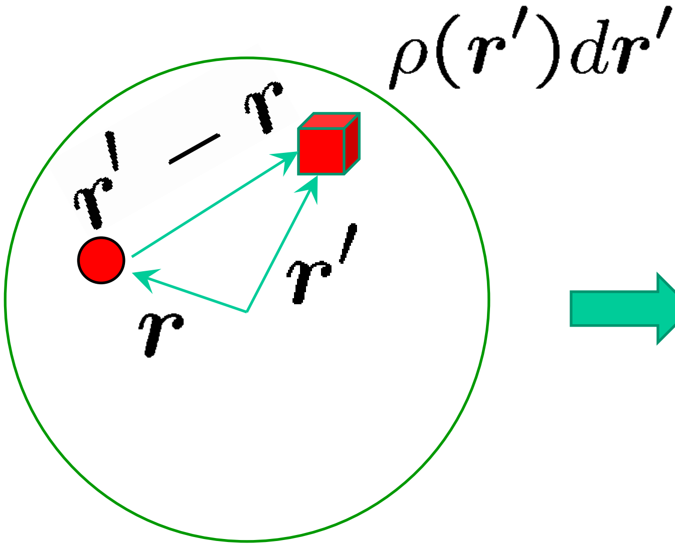
how to construct the potential well?

Mean-field (Hartree-Fock) Theory

平均場



interaction for a nucleon inside a nucleus:



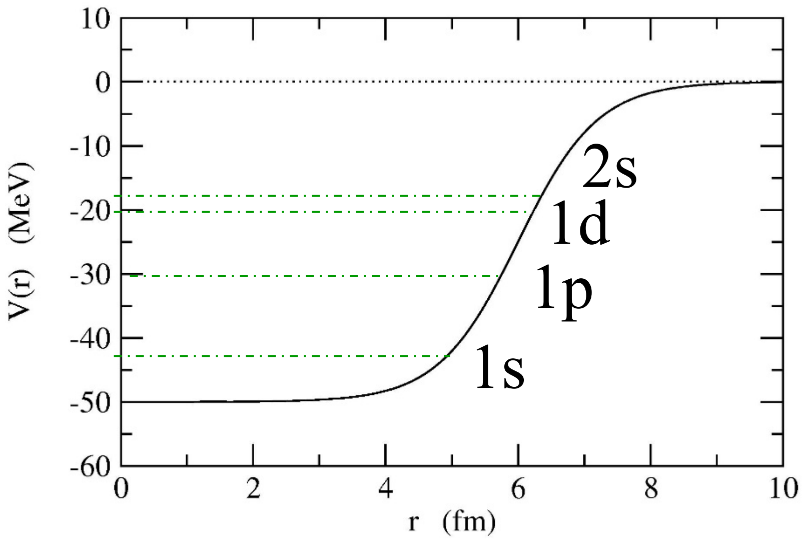
$$v(\boldsymbol{r}' - \boldsymbol{r}) \cdot \underline{\rho(\boldsymbol{r}')d\boldsymbol{r}'}$$

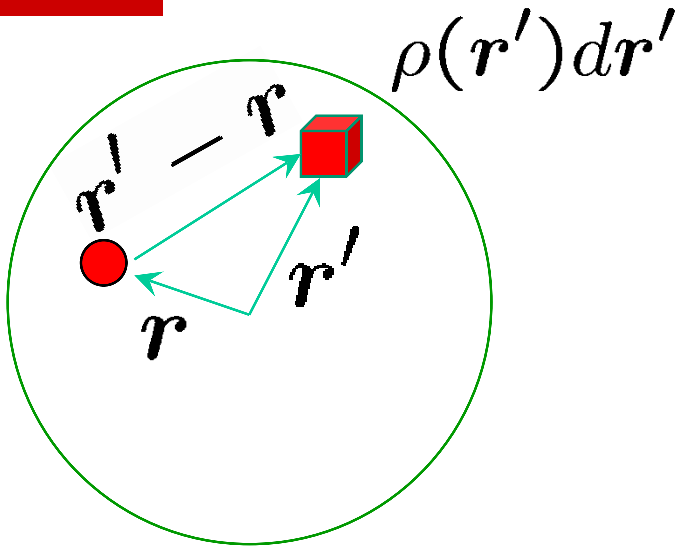
the number of nucleon at *r*'

naively speaking,

$$V(\boldsymbol{r}) \sim \int v(\boldsymbol{r} - \boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

Mean-field (Hartree-Fock) Theory





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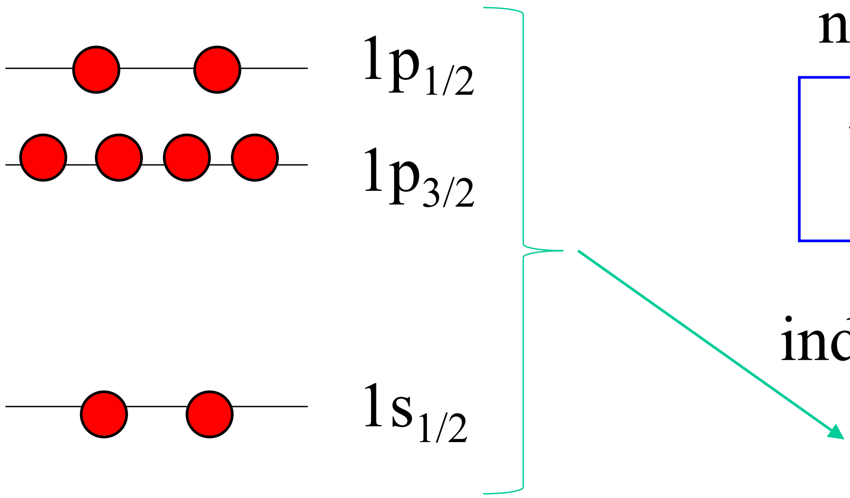
$$V(\boldsymbol{r}) \sim \int v(\boldsymbol{r} - \boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$



shell model

independent motion

$$\rho(\boldsymbol{r}) = \sum_i |\psi_i(\boldsymbol{r})|^2$$

Mean-field (Hartree-Fock) Theory

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

the potential depends on the solutions

⟶ self-consistent solutions

Iteration: $\{\psi_i\} \rightarrow \rho \rightarrow V \rightarrow \{\psi_i\} \rightarrow \cdots$

Mean-field (Hartree-Fock) Theory

$$
\begin{aligned}
0 &= \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}) - \epsilon_i\right]\psi_i(\boldsymbol{r}) \\
&= \left[-\frac{\hbar^2}{2m}\nabla^2 + \int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right)d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r})
\end{aligned}
$$

the potential depends on the solutions

→ self-consistent solutions

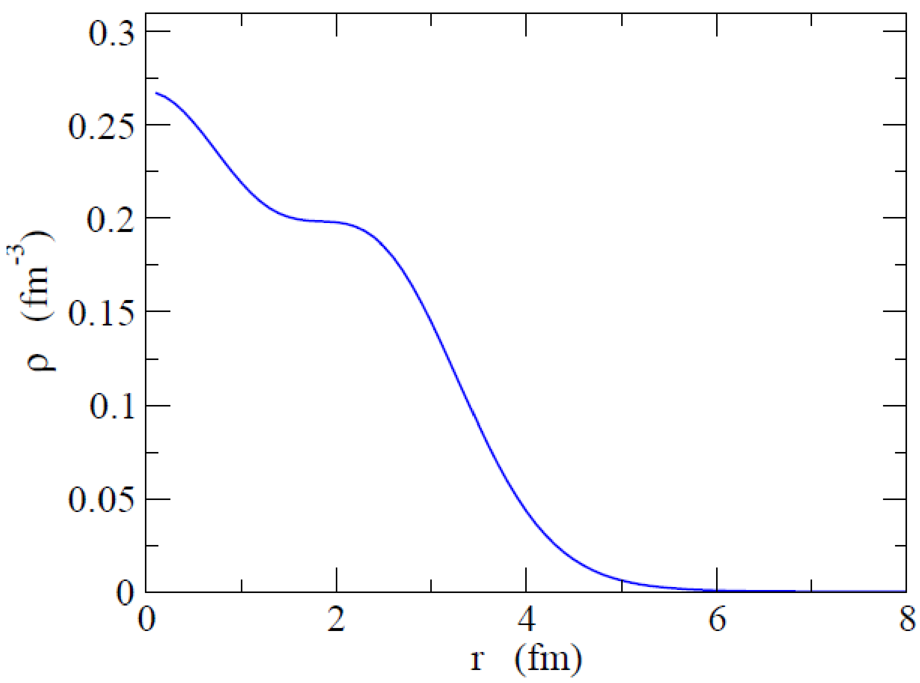
Iteration: $\{\psi_i\} \to \rho \to V \to \{\psi_i\} \to \cdots$

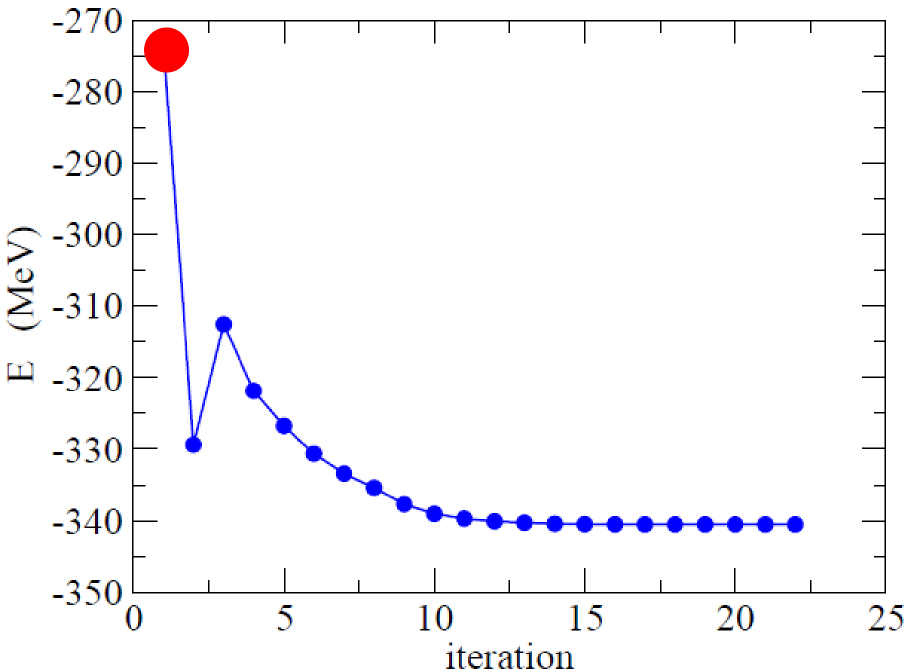
$$
\rho(\boldsymbol{r}) = \sum_i |\psi_i(\boldsymbol{r})|^2, \quad V(\boldsymbol{r}) \sim \int v(\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'
$$

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

"self-consistent solutions"

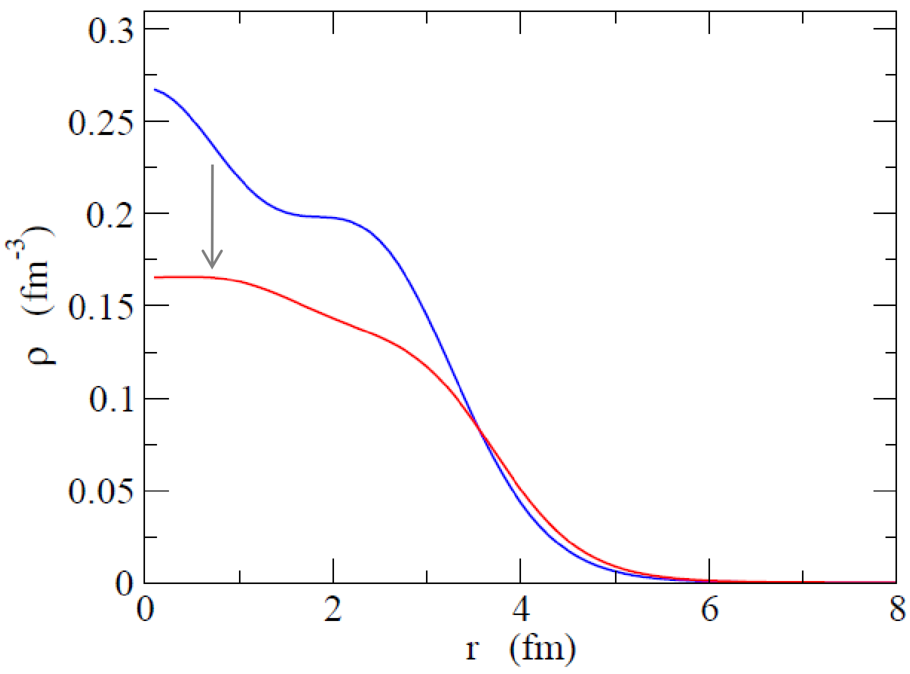
Skyrme-Hartree-Fock calculations for ^{40}Ca

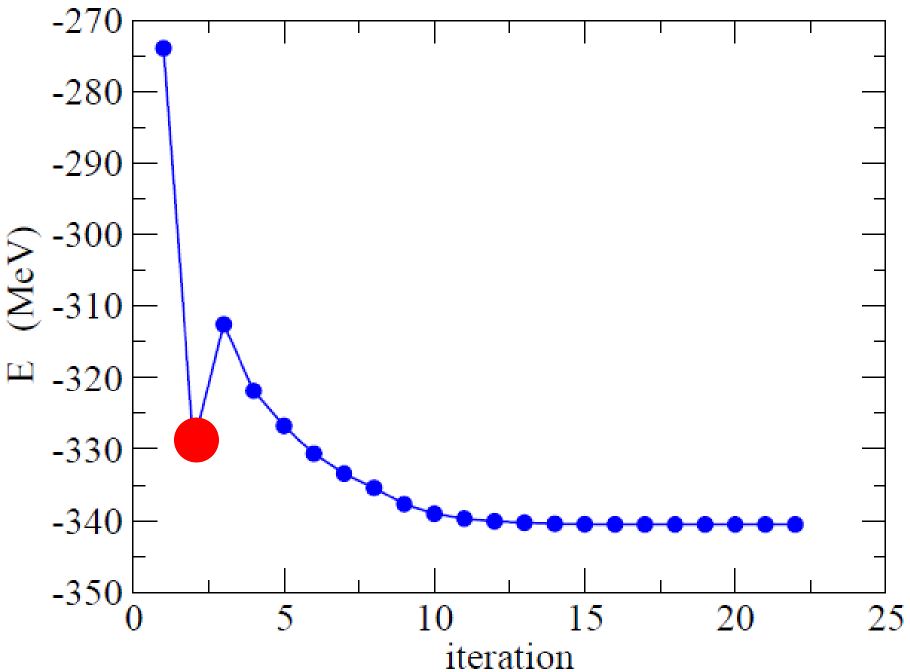




optimize the density by taking into account the nucleon-nucleon interaction

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





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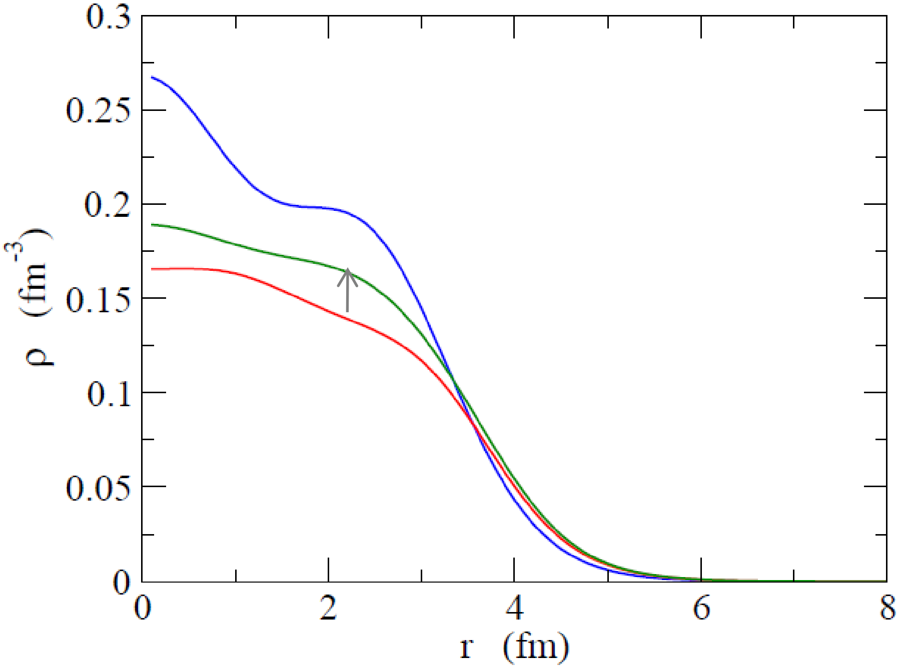
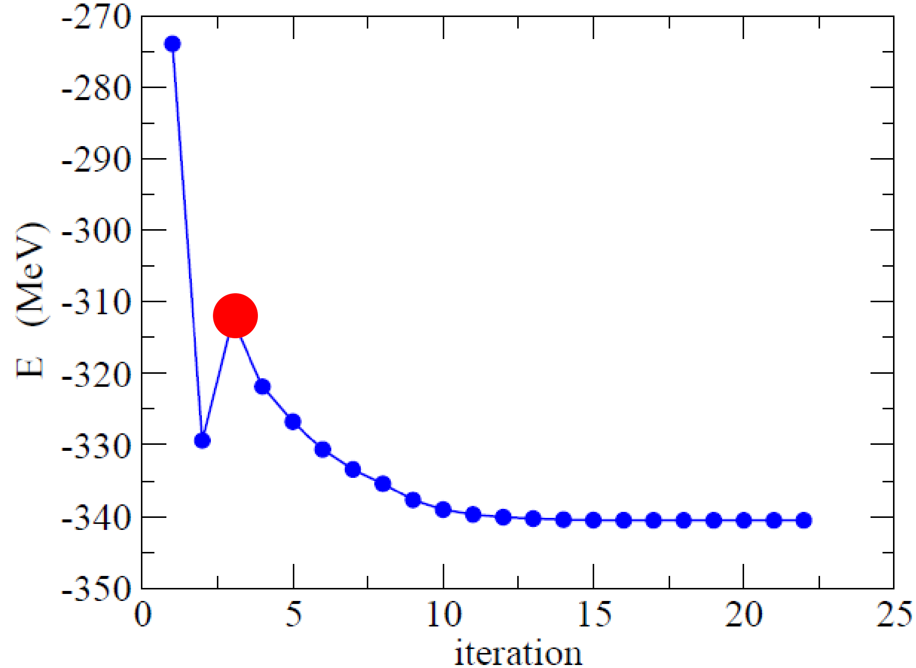
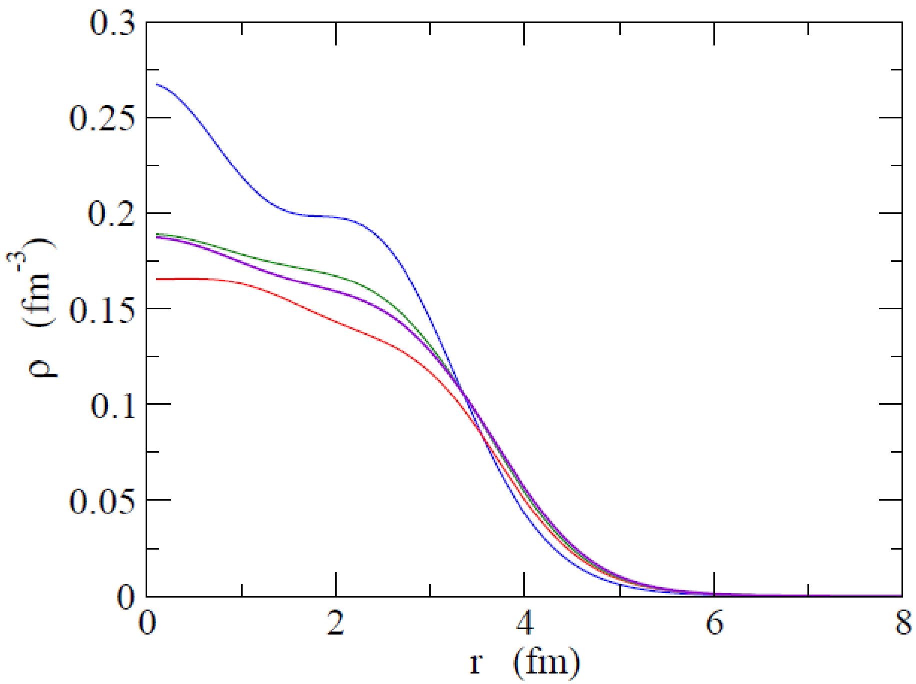
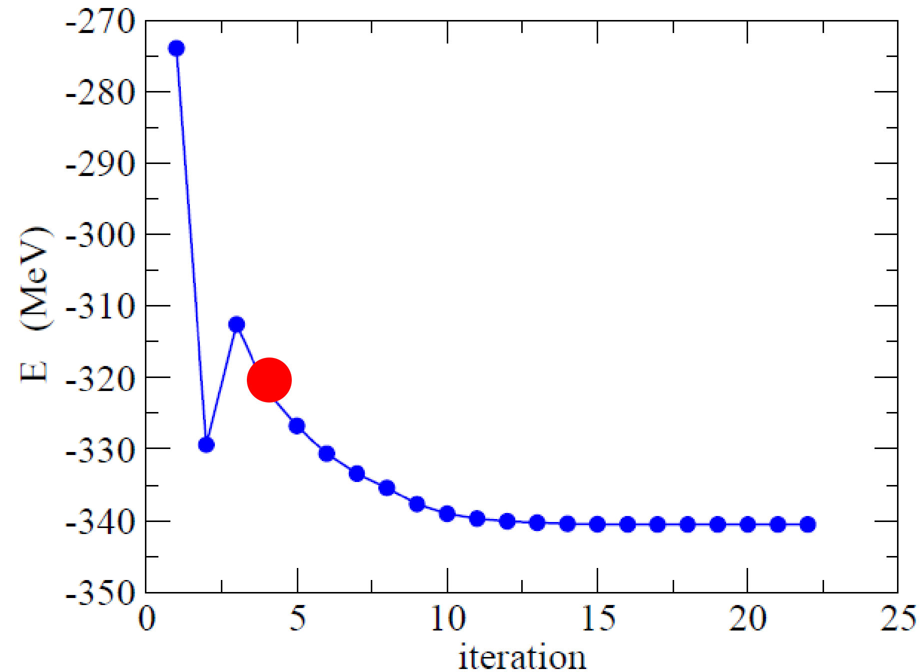




optimize the density by taking into account the nucleon-nucleon interaction

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





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

→ 密度を少しずつ変えながらエネルギーを最適化している

Variational Principle (Rayleigh-Ritz method)

optimization $\longleftrightarrow$ variational principle

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

Variational Principle (Rayleigh-Ritz method)

optimization $\longleftrightarrow$ variational principle

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

$$|\Psi\rangle = \sum_n C_n |\phi_n\rangle$$

$$\longrightarrow \quad \mathrm{lhs} = \frac{\sum_n C_n^2 E_n}{\sum_n C_n^2} \geq E_0$$

H : many-body Hamiltonian

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \cdots) = \psi_1(\boldsymbol{r}_1) \cdot \psi_2(\boldsymbol{r}_2) \cdot \psi_3(\boldsymbol{r}_3) \cdots$$

$\longleftarrow$ many-body wave function for independent particles

Variational Principle (Rayleigh-Ritz method)

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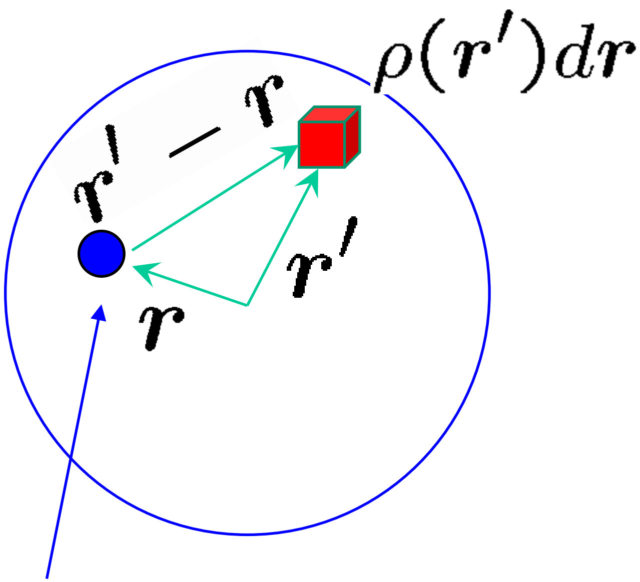
$\longleftarrow$ many-body wave function for independent particles

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \int v(\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r}) = 0$$

change gradually the single-particle potential so that the total energy becomes minimum

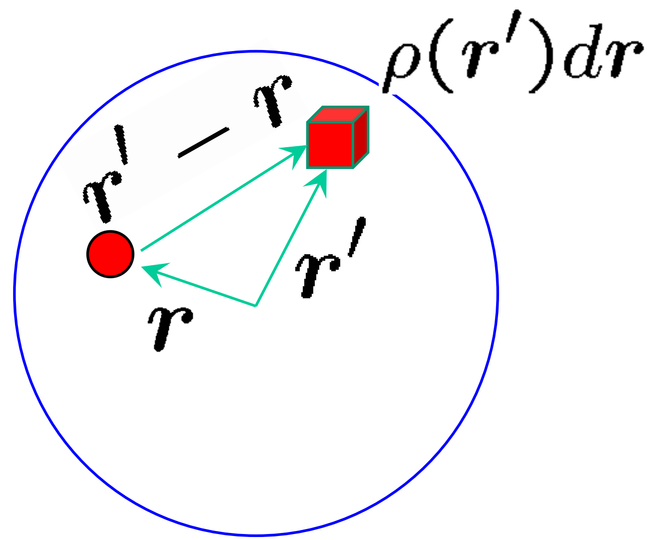
Mean-field (Hartree-Fock) Theory

<u>electro-static potential</u>



test charge

<u>nucleus</u>

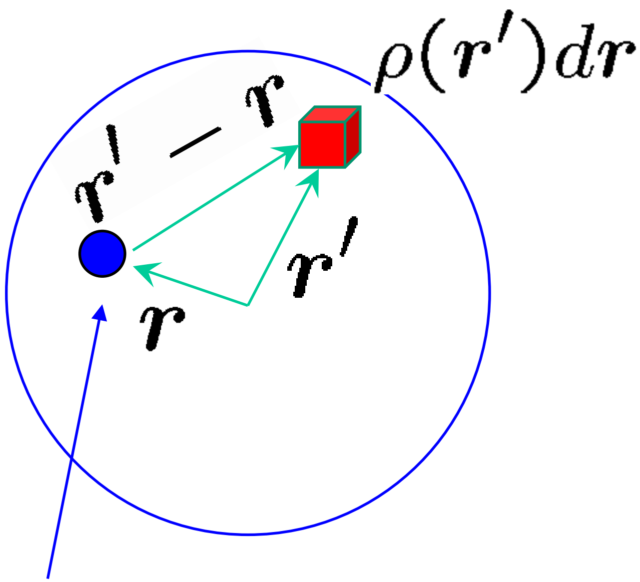


interaction between identical particles

$$V(\boldsymbol{r}) \sim \int v(\boldsymbol{r}-\boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

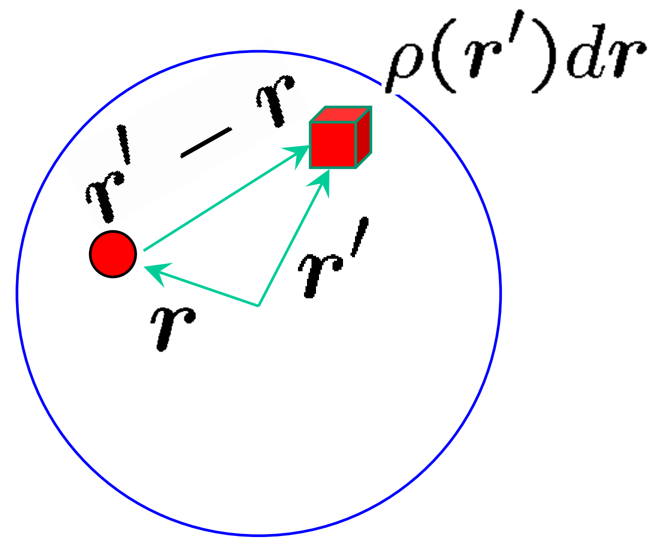
Mean-field (Hartree-Fock) Theory

electro-static potential



test charge

nucleus



interaction between identical particles
$\longrightarrow$ needs anti-symmetrization

$$V(\boldsymbol{r}) \sim \int v(\boldsymbol{r} - \boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}'$$

anti-symmetrization

nucleon: fermion

$$\Psi(x_1, x_2, x_3 \cdots) = -\Psi(x_2, x_1, x_3 \cdots)$$

$$\psi_1(x_1)\psi_2(x_2) \rightarrow$$

anti-symmetrization

nucleon: fermion

$$\Psi(x_1, x_2, x_3 \cdots) = -\Psi(x_2, x_1, x_3 \cdots)$$

$$\psi_1(x_1)\psi_2(x_2) \to \frac{1}{\sqrt{2}}[\psi_1(x_1)\psi_2(x_2) - \psi_2(x_1)\psi_1(x_2)]$$

Slater determinat

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

$$\psi_j^*(\boldsymbol{r}')\psi_j(\boldsymbol{r}')\psi_i(\boldsymbol{r}) \to \psi_j^*(\boldsymbol{r}')\psi_i(\boldsymbol{r}')\psi_j(\boldsymbol{r})$$

anti-symmetrization

nucleon: fermion

$$\Psi(x_1, x_2, x_3 \cdots) = -\Psi(x_2, x_1, x_3 \cdots)$$

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

$$\psi_j^*(\boldsymbol{r}')\psi_j(\boldsymbol{r}')\psi_i(\boldsymbol{r}) \to \psi_j^*(\boldsymbol{r}')\psi_i(\boldsymbol{r}')\psi_j(\boldsymbol{r})$$

$$\to \left[-\frac{\hbar^2}{2m}\nabla^2 + \int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right) d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r})$$

$$-\int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j \psi_j^*(\boldsymbol{r}')\psi_i(\boldsymbol{r}')\right) d\boldsymbol{r}'\psi_j(\boldsymbol{r})$$

exchange term

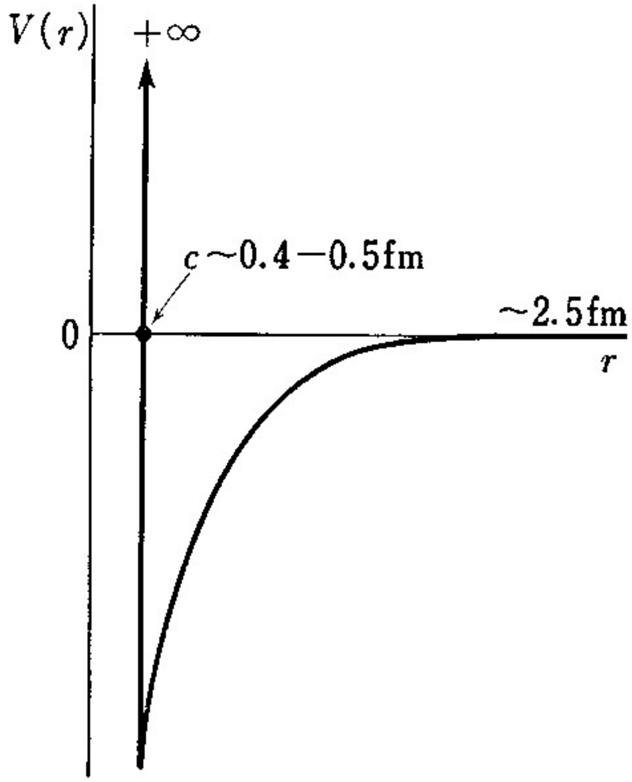
Hartree-Fock theory

anti-symmetrization

$$
\begin{aligned}
0 &= \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right) d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r}) \\
&\to \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + \int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right) d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r}) \\
&\quad - \int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j \psi_j^*(\boldsymbol{r}')\psi_i(\boldsymbol{r}')\right) d\boldsymbol{r}'\psi_j(\boldsymbol{r}) \\
&= \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(\boldsymbol{r}) - \epsilon_i\right]\psi_i(\boldsymbol{r}) + \int d\boldsymbol{r}' V_{\mathsf{NL}}(\boldsymbol{r},\boldsymbol{r}')\psi_i(\boldsymbol{r}')
\end{aligned}
$$

non-local potential

Bare nucleon-nucleon interaction



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

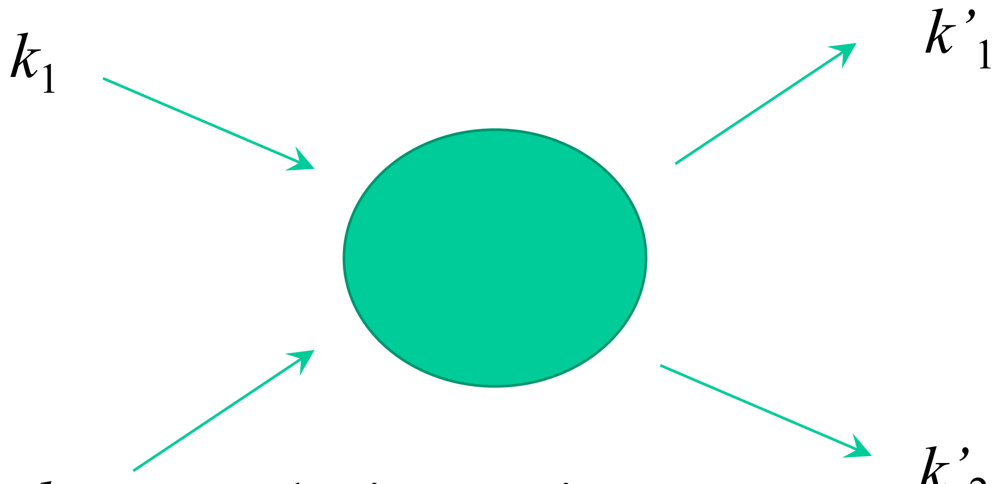
cf. magic numbers

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

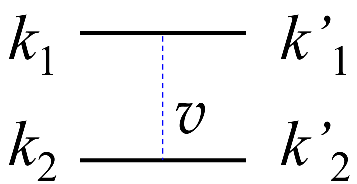
↑

Bruckner's G-matrix

➢ two-body (multiple) scattering *in vacuum*

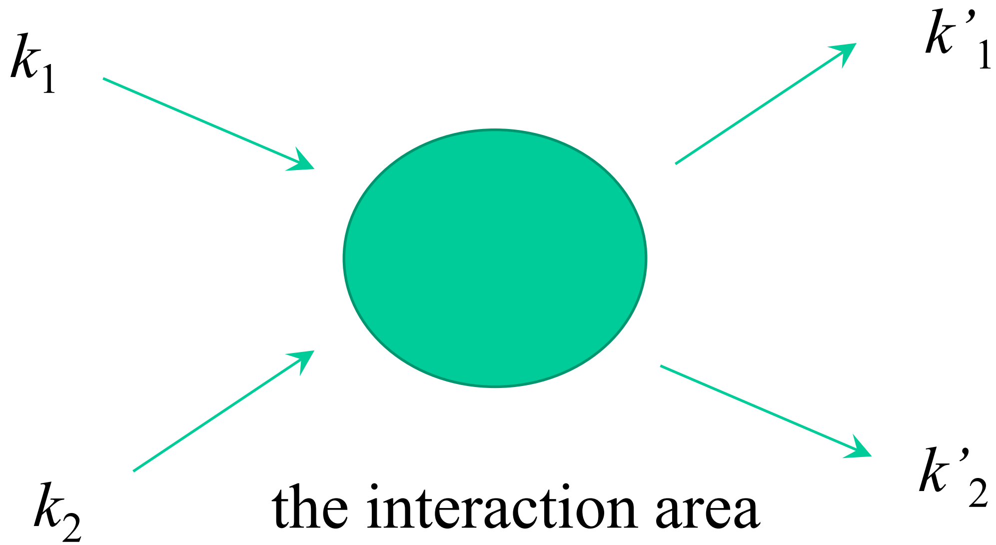


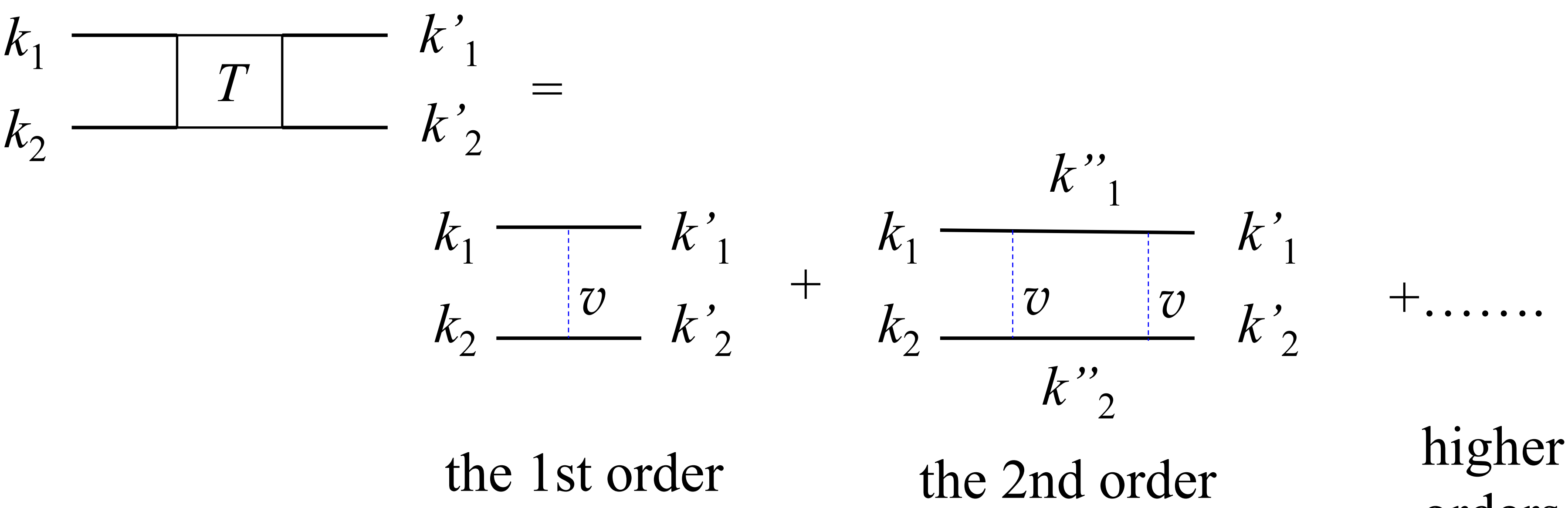
the interaction area



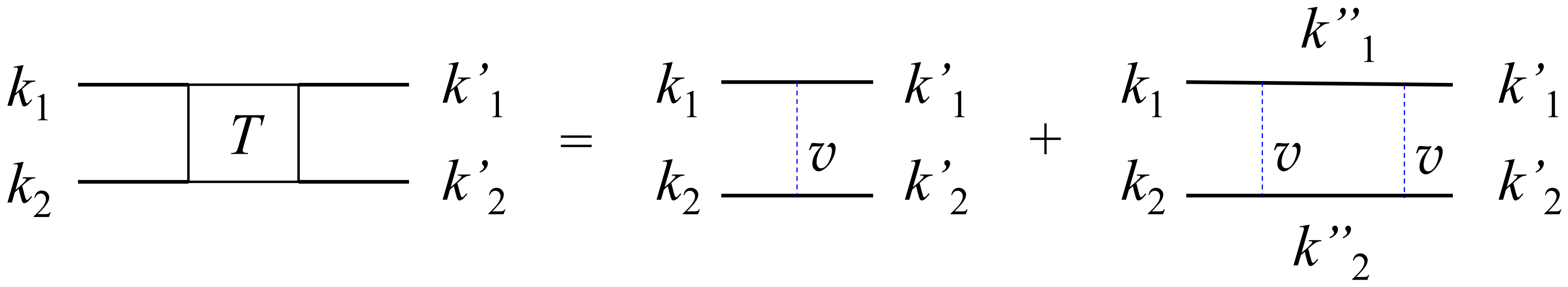
the 1st order

➢ two-body (multiple) scattering *in vacuum*





➢ two-body (multiple) scattering *in vacuum*



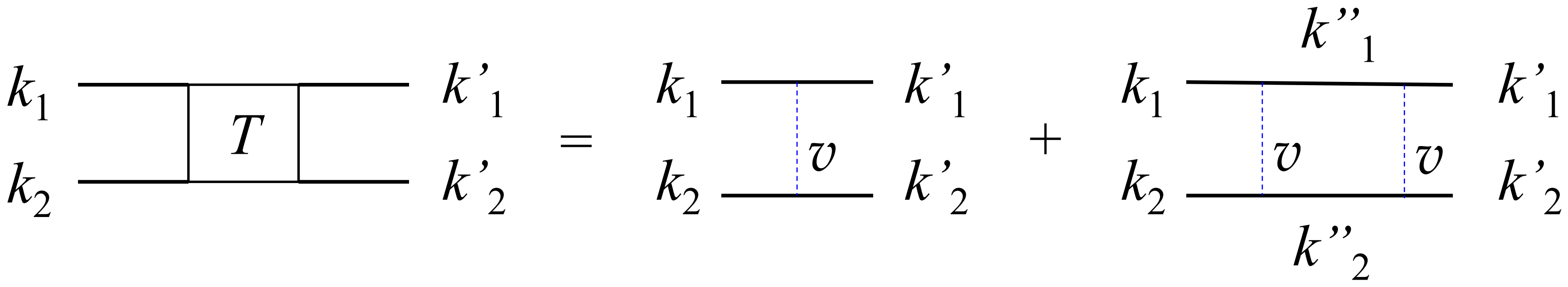
+.......

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V - E\right)\psi = 0$$

Lippmann-Schwinger equation

$$T = v + v\frac{1}{E - H_0}T$$

➢ two-body (multiple) scattering *in vacuum*



+.......

Lippmann-Schwinger equation

$$T = v + v\frac{1}{E - H_0}T$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V - E\right)\psi = 0$$

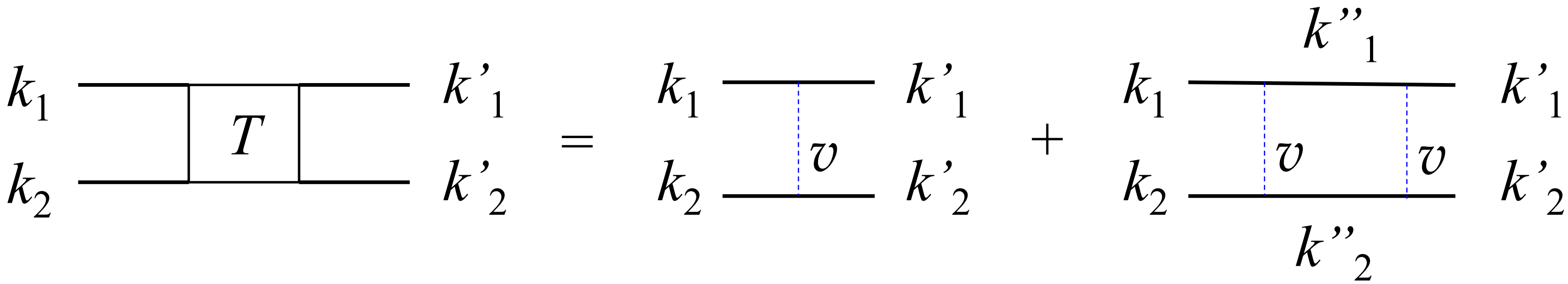
⇨ $$\left(-\frac{\hbar^2}{2m}\nabla^2 - E\right)\psi = -V\psi$$

⇨ $$\psi = \phi - \frac{1}{H_0 - E}V\psi \qquad H_0 = -\frac{\hbar^2}{2m}\nabla^2, \quad (H_0 - E)\phi = 0$$

⇨ $$V\psi = V\phi - V\frac{1}{H_0 - E}V\psi$$

⇨ $(V\psi = T\phi)$ $$T = V - V\frac{1}{H_0 - E}T$$

➢ two-body (multiple) scattering *in vacuum*



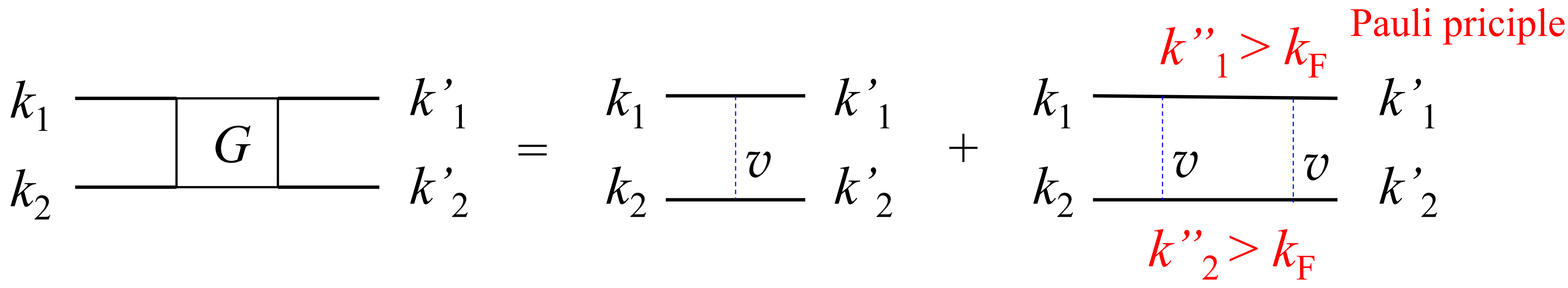
+…….

Lippmann-Schwinger equation

$$T = v + v\frac{1}{E - H_0}T$$

核内における核子間相互作用（媒質効果）

- two-body (multiple) scattering *in medium*



+…….

Bethe-Goldstone equation

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

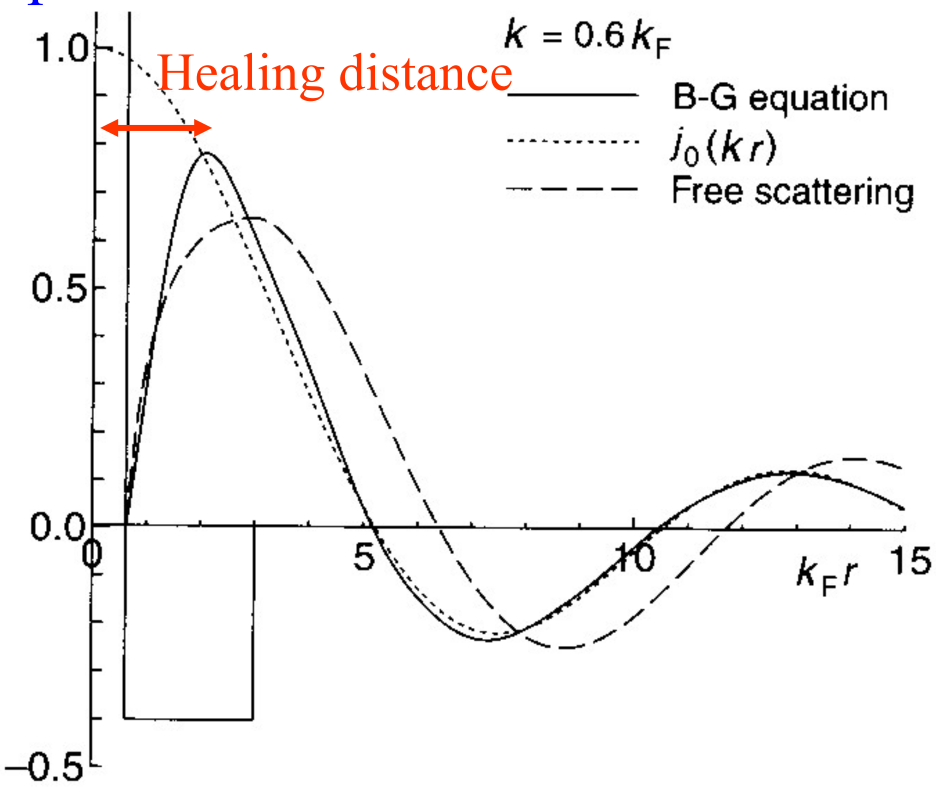
*scattering: suppressed
because intermediate states have to have
$k > k_F$ → independent particle picture

◆Hard core

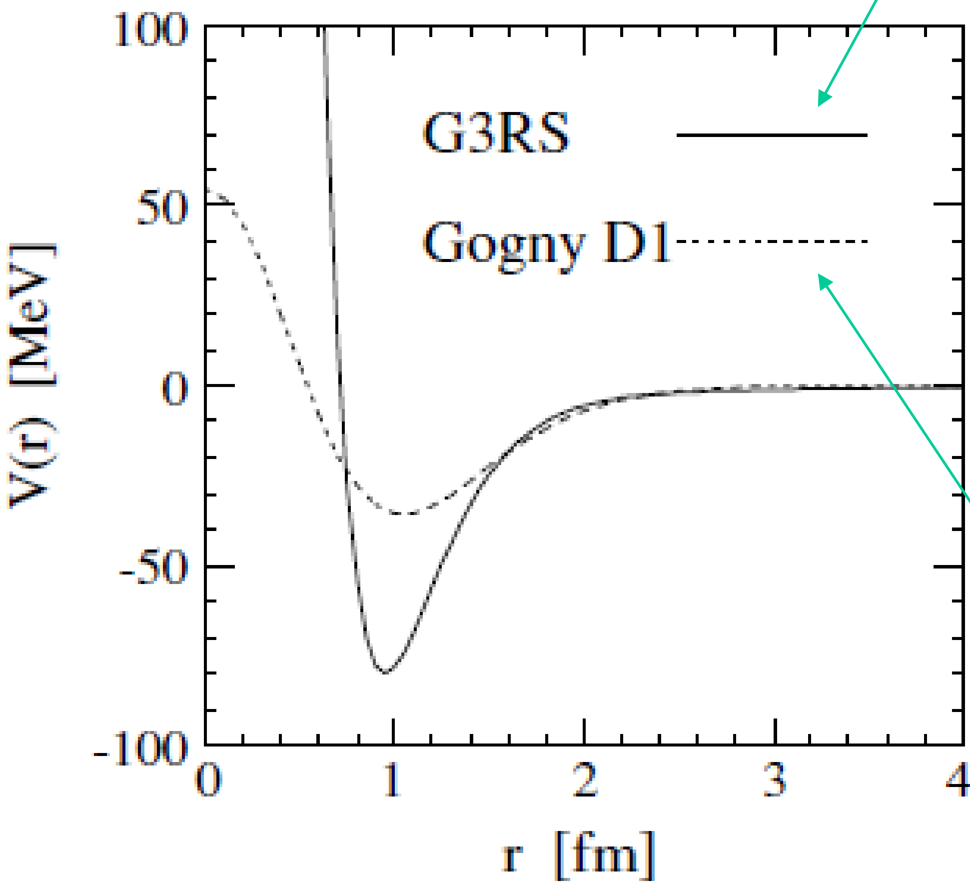
$$G = v + v\frac{Q_F}{E - H_0}G \quad \Longleftrightarrow \quad G = \frac{v}{1 - v\,\frac{Q_F}{E-H_0}}$$

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

◆Independent particle motion



→ use G instead of v in mean-field calculations bare interaction



effective
interaction

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

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

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

if x_i=0, t_1=t_2=0:

$$v(\boldsymbol{r},\boldsymbol{r}') = \underbrace{t_0\delta(\boldsymbol{r}-\boldsymbol{r}')}_{\text{short-range attraction}} + \underbrace{\frac{1}{6}t_3\delta(\boldsymbol{r}-\boldsymbol{r}')\rho^\alpha(\boldsymbol{r})}_{\text{repulsion to avoid collapse}}$$

short-range attraction

repulsion to avoid collapse

$$+\underbrace{iW_0(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot\boldsymbol{k}\times\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k}}_{\text{spin-orbit interaction}}$$

spin-orbit interaction

Skyrme interaction density dependent zero-range interaction

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

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

(note) finite range effect $\Longleftrightarrow$ 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 interaction   density dependent zero-range interaction

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

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

the exchange potential ⟶ local

$$
\begin{aligned}
0 \;=\;& \left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2+\int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j|\psi_j(\boldsymbol{r}')|^2\right)d\boldsymbol{r}'-\epsilon_i\right]\psi_i(\boldsymbol{r}) \\
&-\int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j\psi_j^*(\boldsymbol{r}')\psi_i(\boldsymbol{r}')\right)d\boldsymbol{r}'\psi_j(\boldsymbol{r})
\end{aligned}
$$

Skyrme interactions: 10 adjustable parameters

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

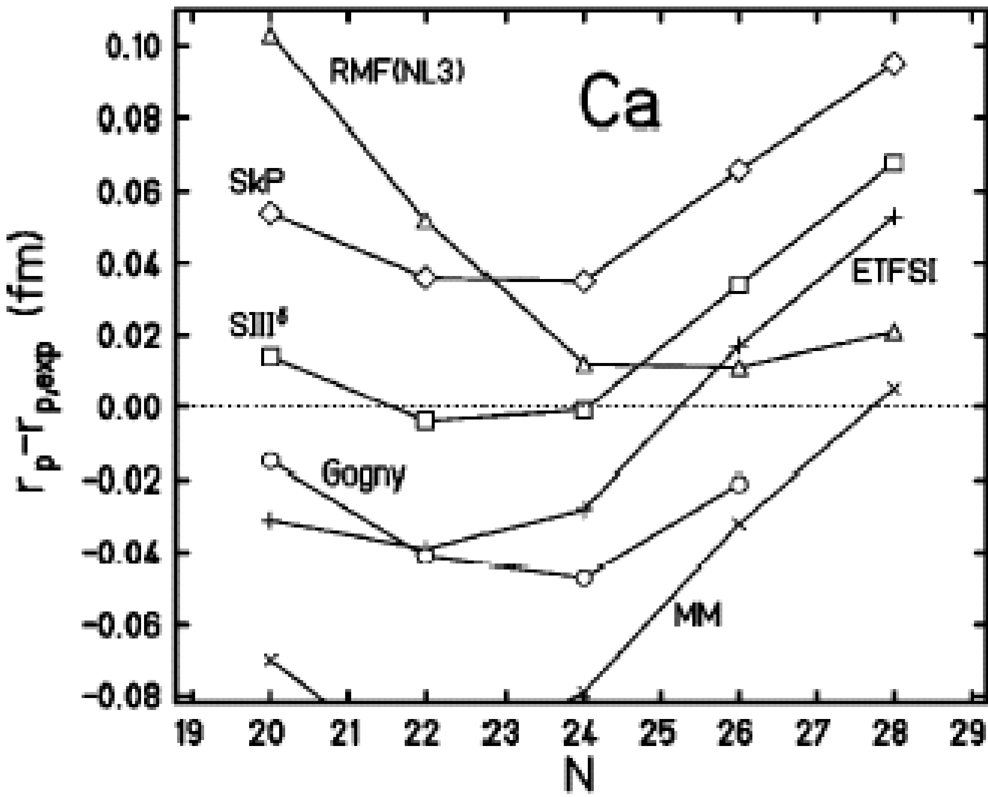
A fitting strategy:

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

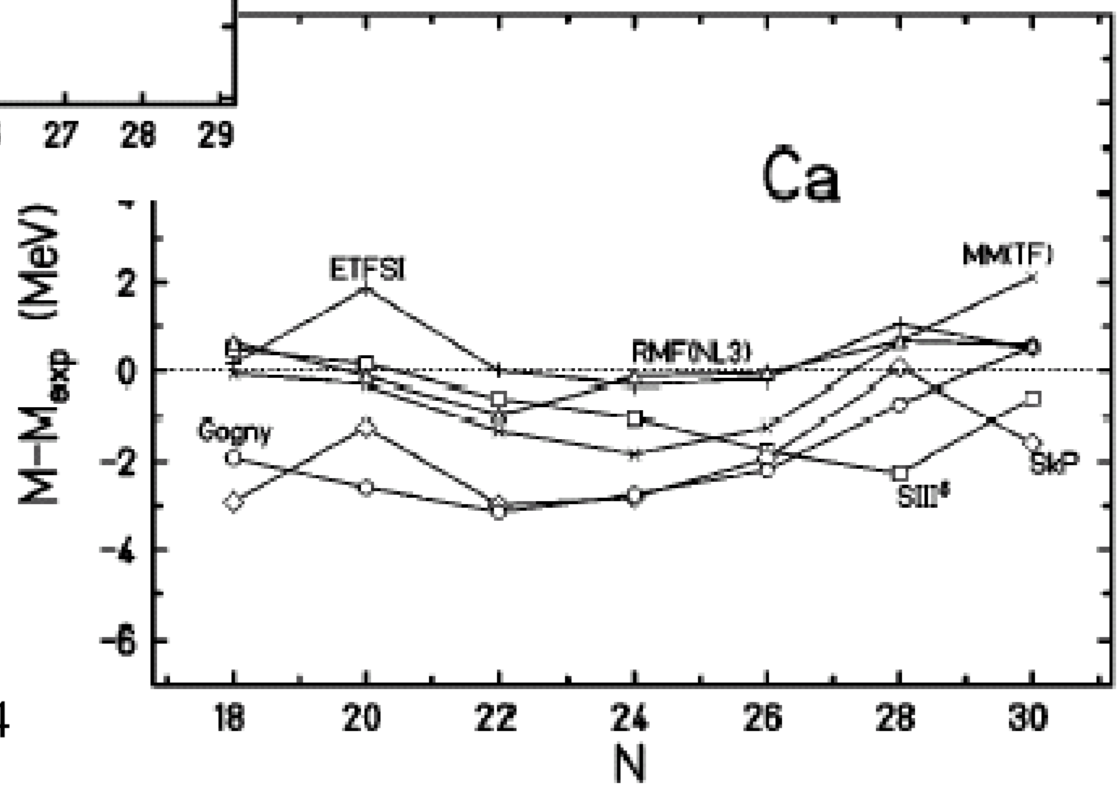
Infinite nuclear matter: E/A, ρ_{eq} ,….

Parameter sets:

SIII, SkM*, SGII, SLy4,…….

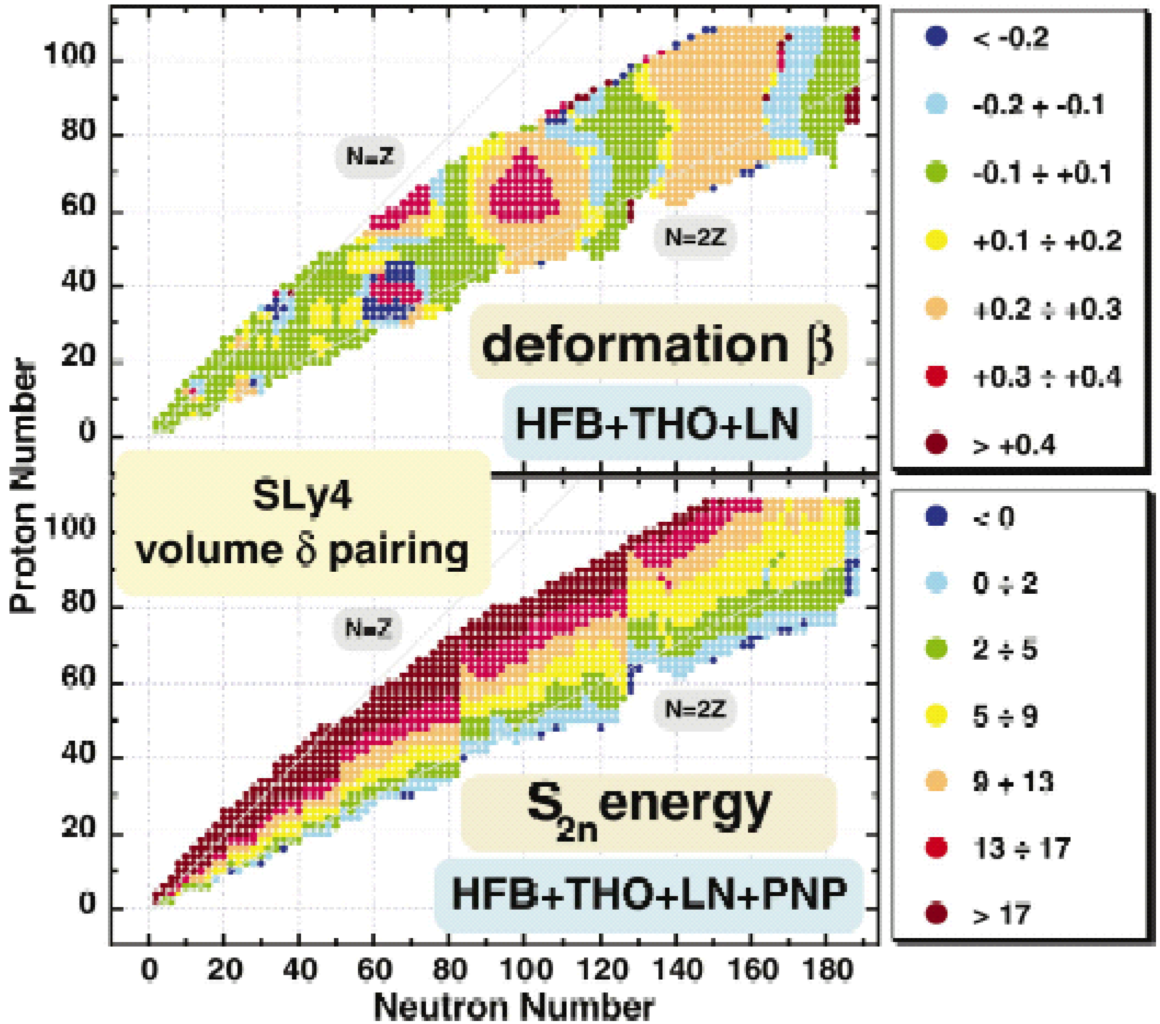


Examples of HF calculations for masses and radii



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

deformation and two-neutron separation energy



M.V. Stoitsov et al., PRC68('03)054312

Density Functional Theory

With Skyrme interaction:

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

Energy functional in terms of local densities

⇕

Close analog to the Density Functional Theory (DFT)

密度汎関数法

Density Functional Theory

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

i) Hohenberg-Kohn Theorem

$H=H_0+V_{ext}$

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

Density: the basic variable
（密度が分かれば原理的に全て分かる）

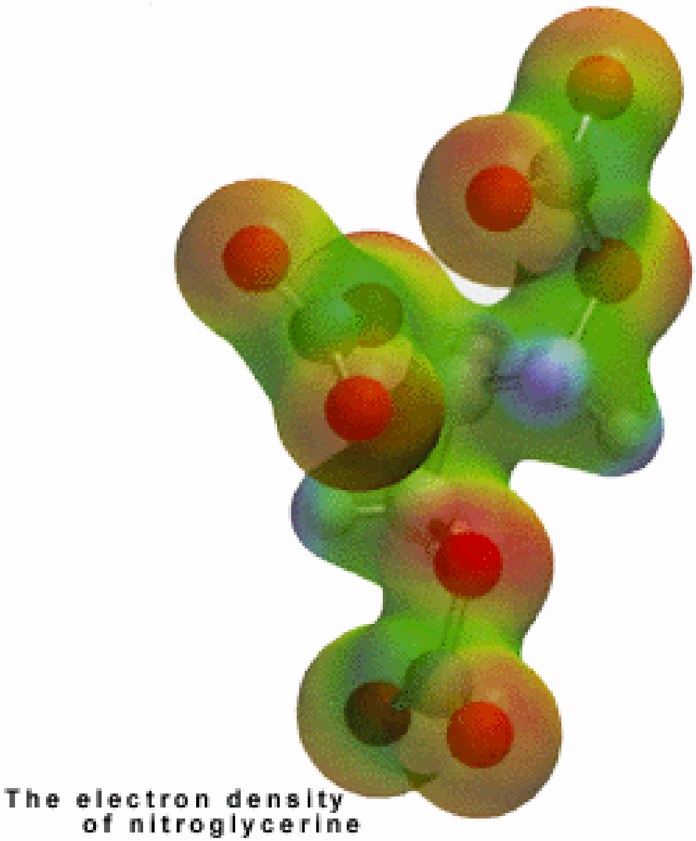
ii) Hohenberg-Kohn variational principle

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

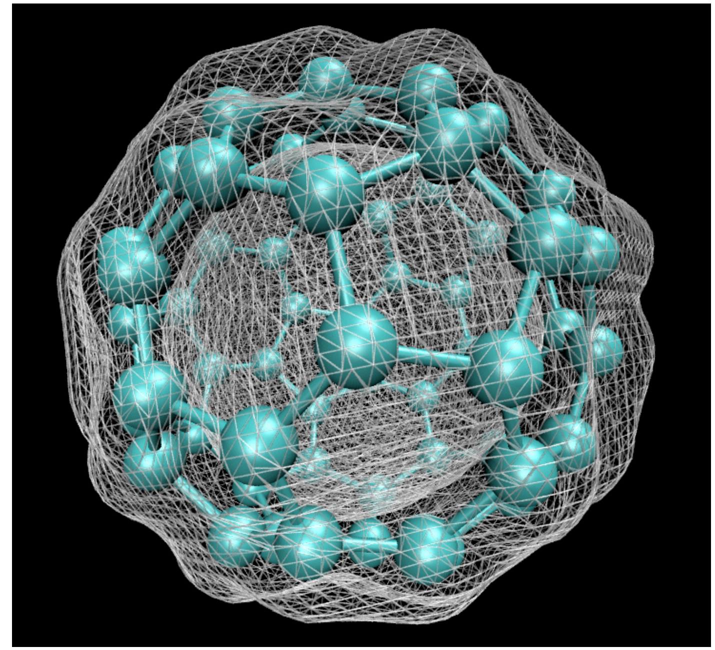
$$\Longrightarrow E[\rho] \geq E_{gs}$$

うまい方法で $E[\rho]$ を作れれば、それを使って多体計算が簡単に行える。

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



ニトログリセリンの電子密度
（Nobelprize.org より）



C_{60} の電子密度
（Wikipedia より）