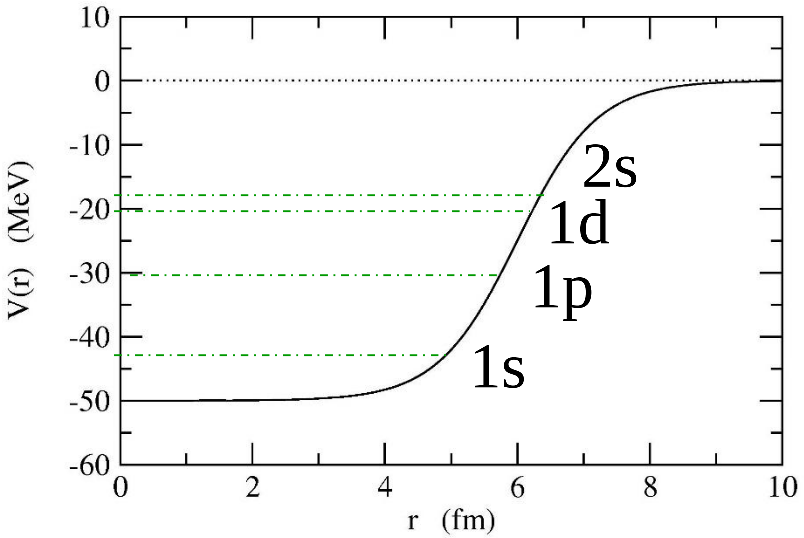
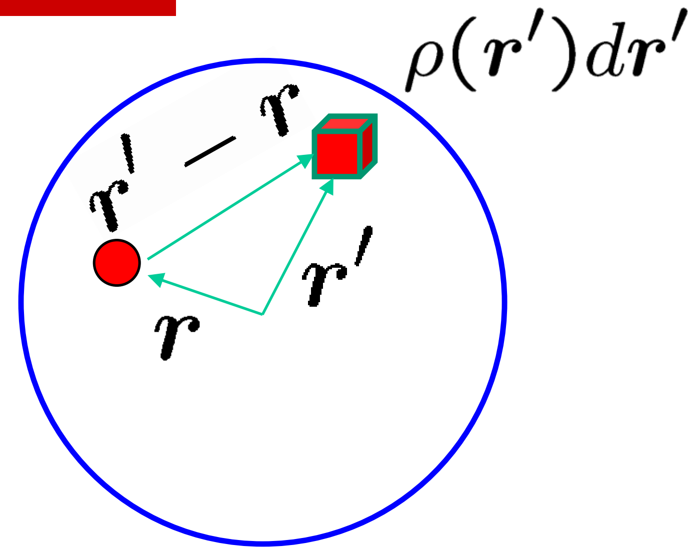
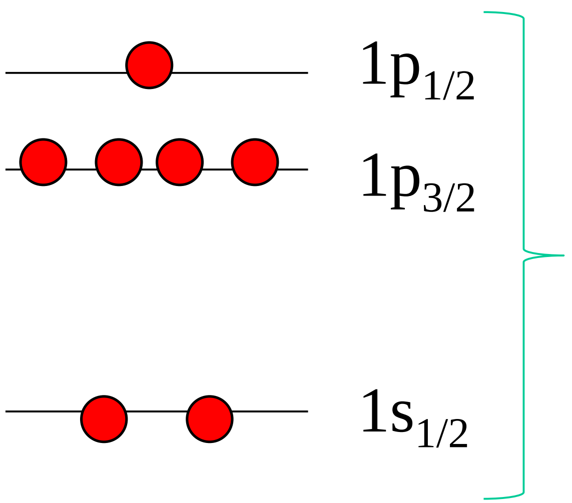
Mean-field (Hartree-Fock) Theory







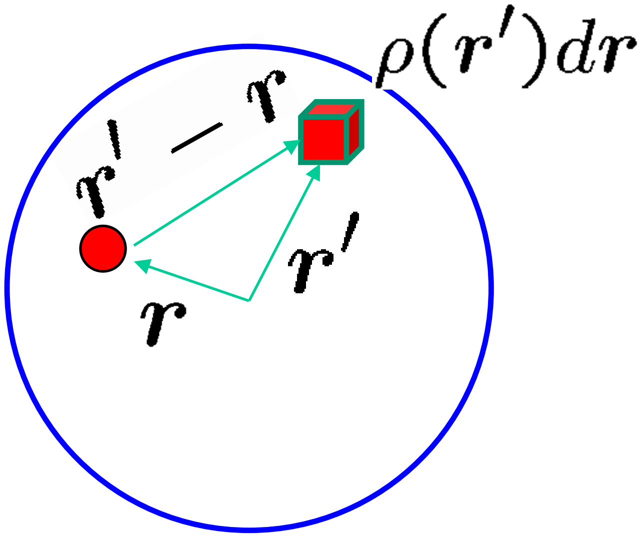
shell model

naively speaking,

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

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

Mean-field (Hartree-Fock) Theory



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

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

the potential depends on the solutions

Mean-field (Hartree-Fock) Theory

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the potential depends on the solutions

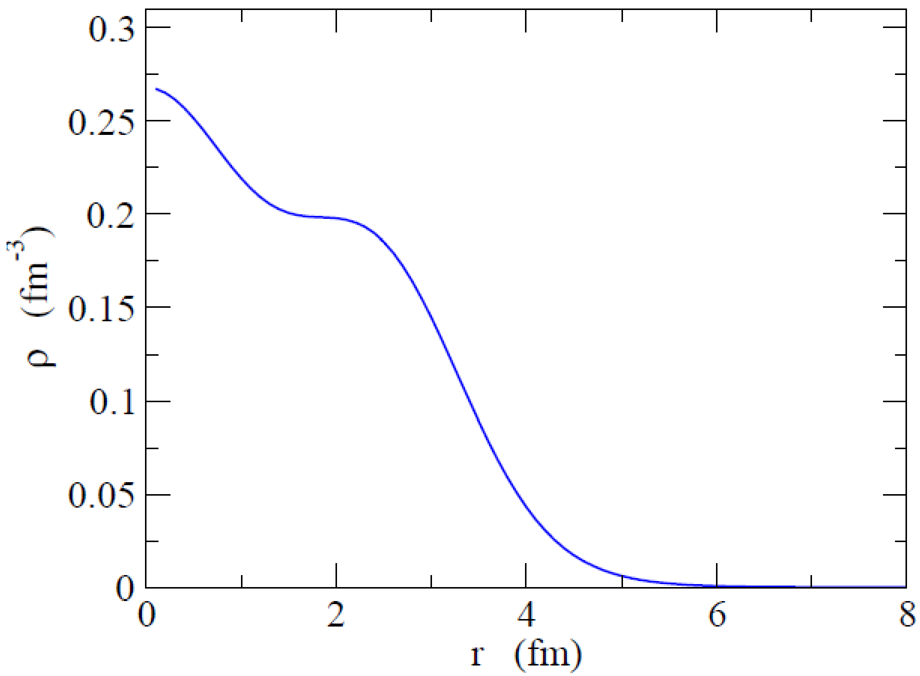
$\longrightarrow$ self-consistent solutions

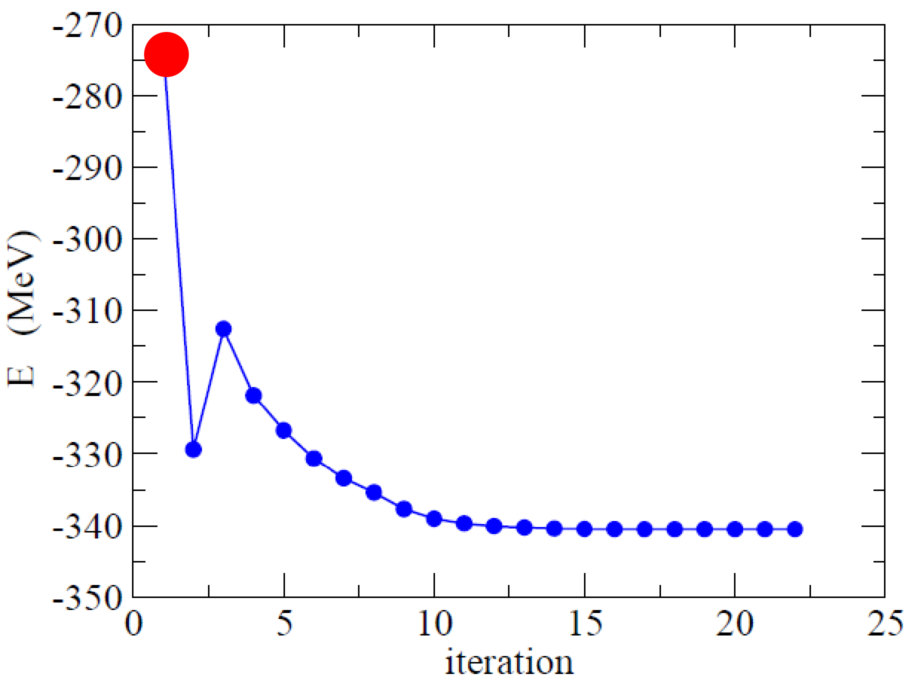
Iteration: $\{\psi_i\} \to \rho \to V \to \{\psi_i\} \to \cdots$

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

"self-consistent mean-field theory"

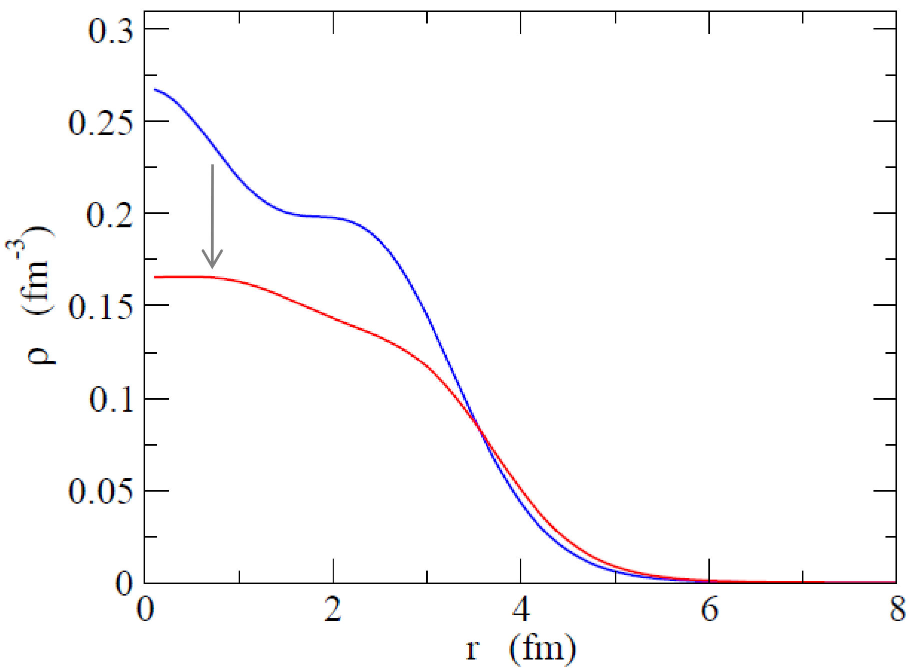
Skyrme-Hartree-Fock calculations for ^{40}Ca

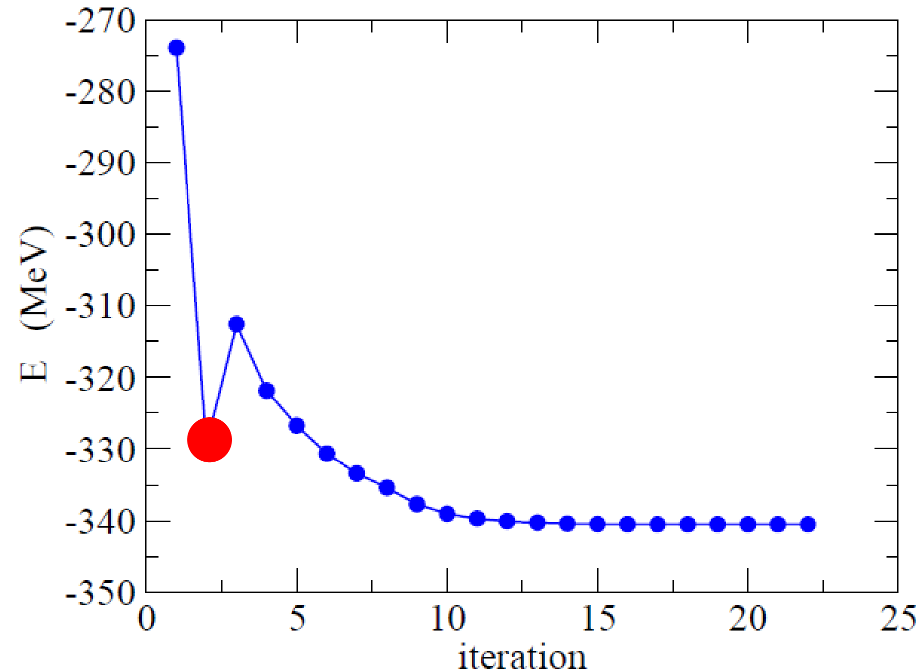




optimize the density by taking into account the nucleon-nucleon interaction

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





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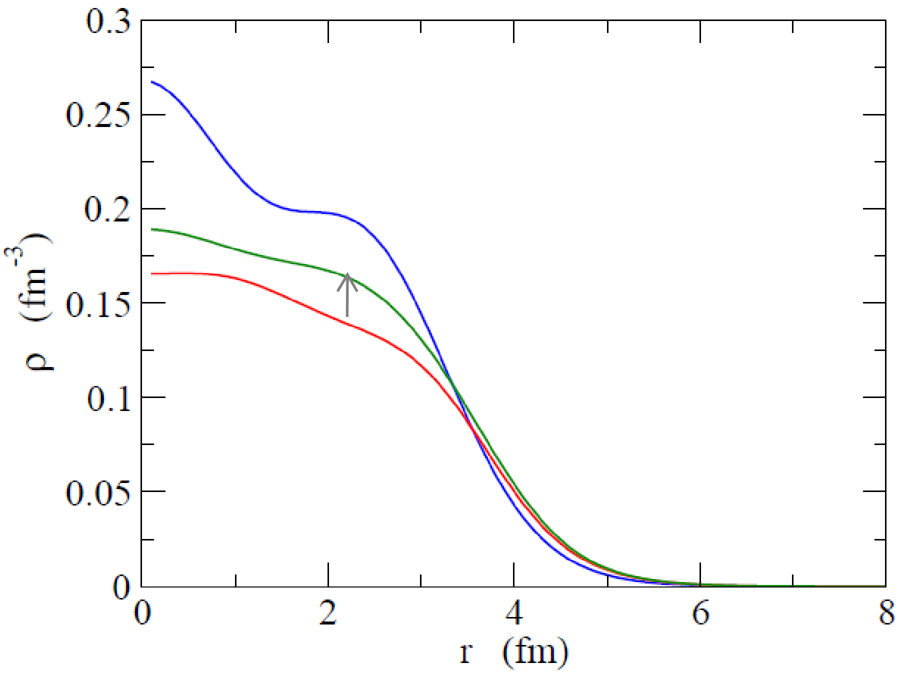
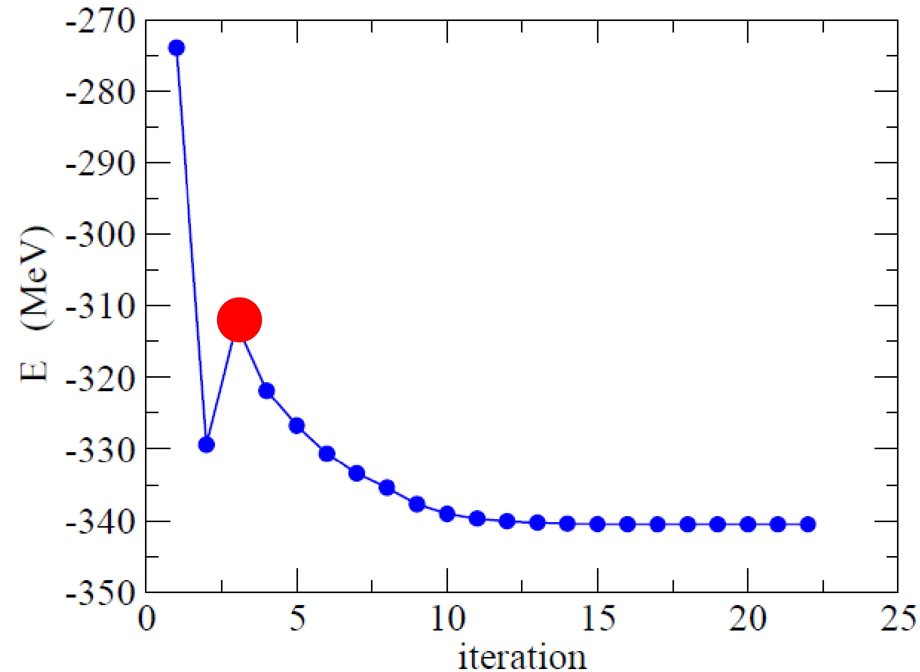
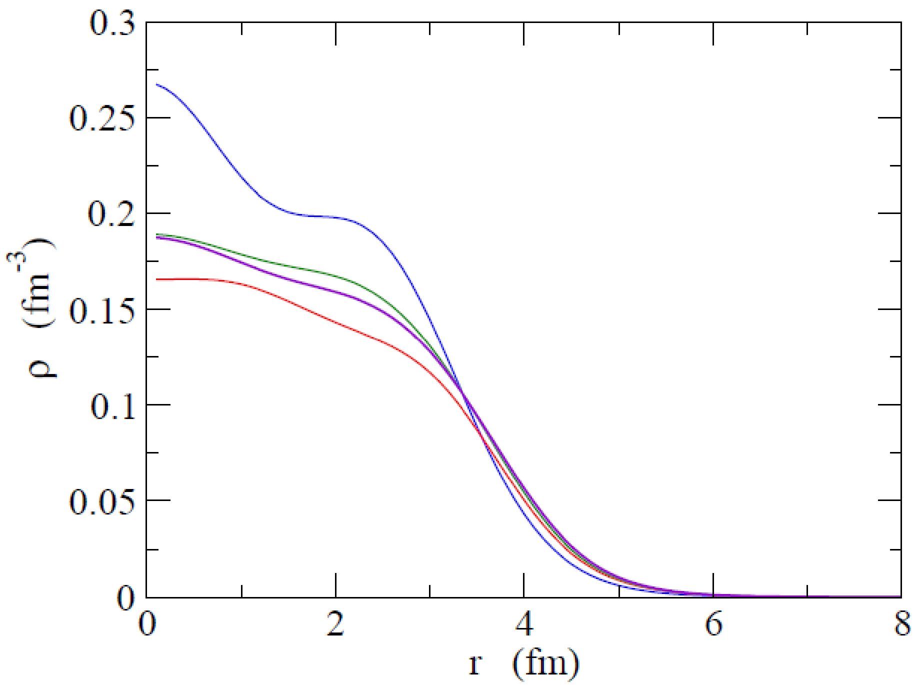
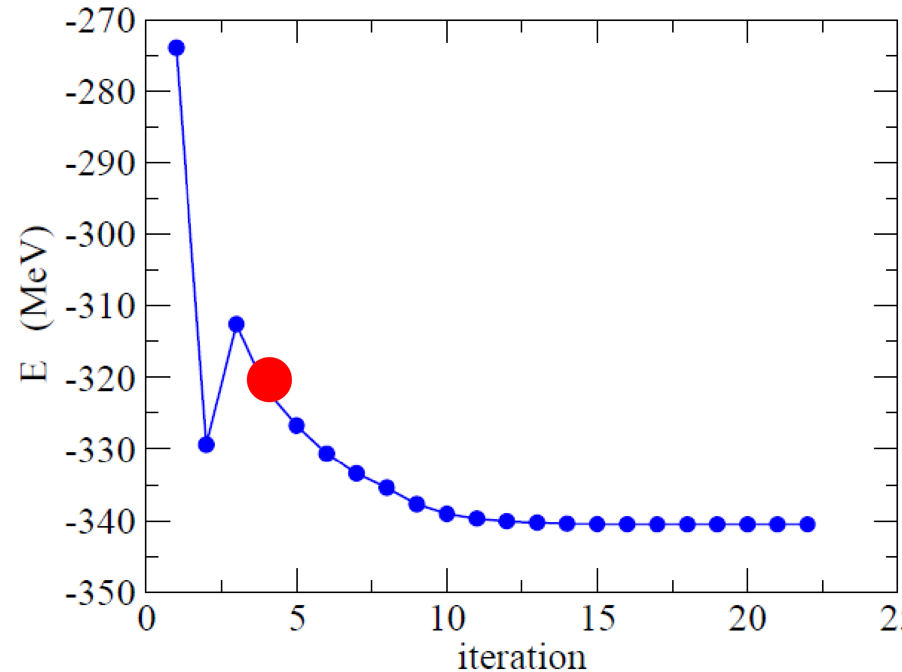




optimize the density by taking into account the nucleon-nucleon interaction

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





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

→ optimized density (and shape) can be determined automatically

Variational Principle (Rayleigh-Ritz method)

optimization $\longleftrightarrow$ variational principle

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

H : many-body Hamiltonian

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

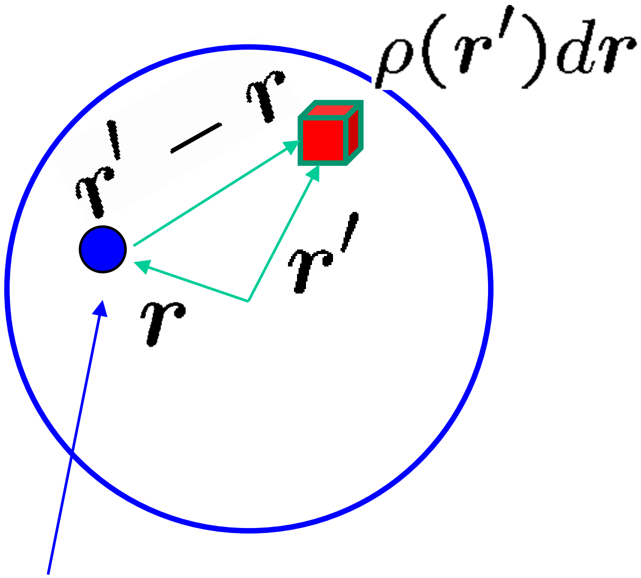
$\longleftarrow$ many-body wave function for independent particles

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

全エネルギーが最少になるようにちょっとずつ
一粒子ポテンシャルを変えていく

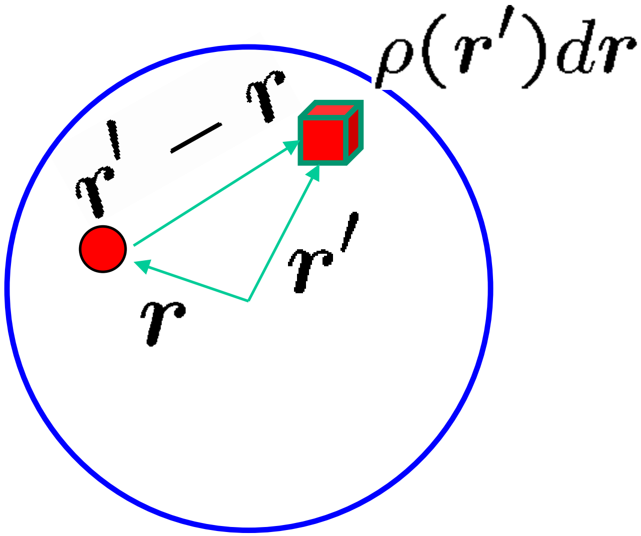
Mean-field (Hartree-Fock) Theory

電磁気の場合



テスト電子

原子核の場合



同種粒子間の相互作用
→反対称化が必要

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

anti-symmetrization

nucleon: fermion

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3 \cdots) = -\Psi(\boldsymbol{r}_2, \boldsymbol{r}_1, \boldsymbol{r}_3 \cdots)$$

$$\psi_1(\boldsymbol{r}_1)\psi_2(\boldsymbol{r}_2) \to [\psi_1(\boldsymbol{r}_1)\psi_2(\boldsymbol{r}_2) - \psi_2(\boldsymbol{r}_1)\psi_1(\boldsymbol{r}_2)]/\sqrt{2}$$

Slater determinat

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

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

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

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

Hartree-Fock Method and Symmetries

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

2体力→1体場に近似

$$= \underbrace{\sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{\rm HF}(i)\right)}_{h_{\rm HF}} + \underbrace{\frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i,\boldsymbol{r}_j) - \sum_i V_{\rm HF}(i)}_{V_{\rm res}}$$

Slater determinant

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

⇐ Eigen-state of $h_{\rm HF}$, but not of H

$\boxed{\Psi_{\rm HF} \text{ : does not necessarily possess the symmetries that } H \text{ has.}}$

"Symmetry-broken solution"

"Spontaneous Symmetry Broken"

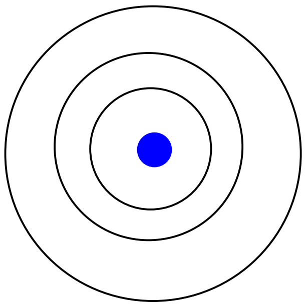
Ψ_{HF} : does not necessarily possess the symmetries that H has.

Typical Examples

➢Translational symmetry: always broken in nuclear systems

$$H = -\sum_{i=1}^{A} \frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i - \boldsymbol{r}_j) \to \sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\nabla_i^2 + \underline{\underline{V_{\mathrm{HF}}(\boldsymbol{r}_i)}}\right)$$

(cf.) atoms

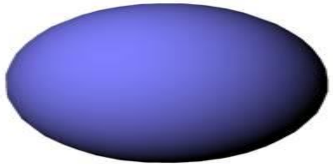


nucleus in the center

⟶ 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

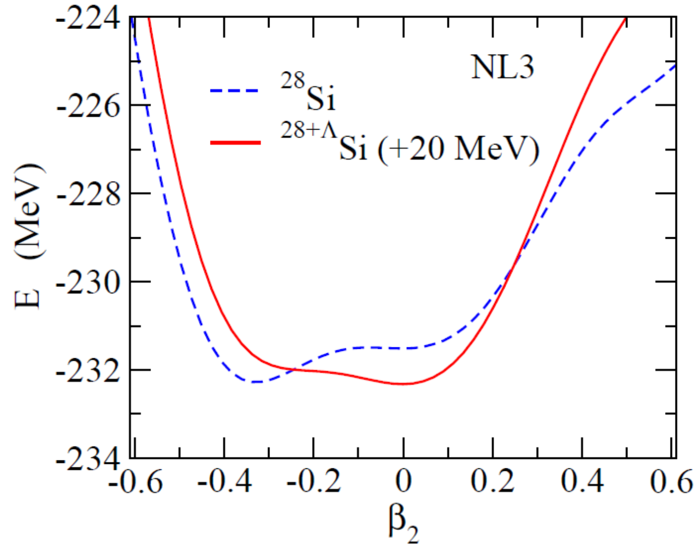
Constrained Hartree-Fock method

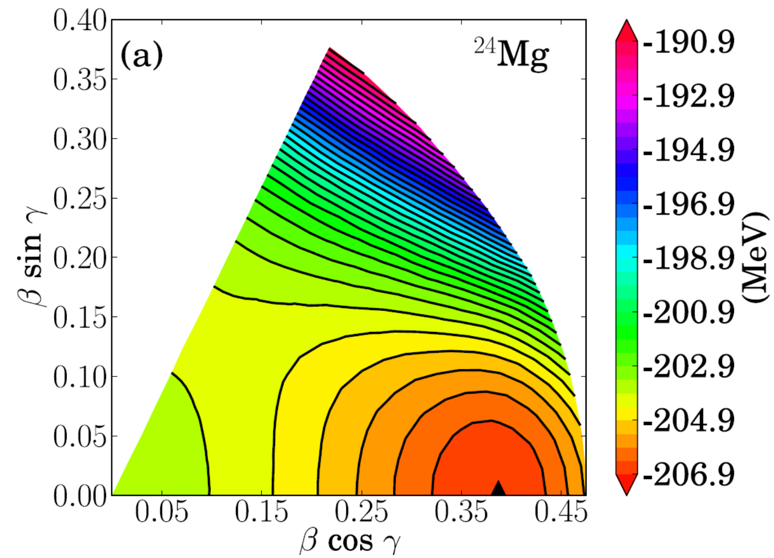
minimize $H' = H - \lambda\hat{Q}_{20}$ with a Slater determinant w.f.

$\hat{Q}_{20} = \sum_i r_i^2 Y_{20}(\hat{\boldsymbol{r}}_i)$: quadrupole operator

λ : Lagrange multiplier, to be determined so that $\langle\hat{Q}_{20}\rangle = Q \propto R^2\beta$

$\longrightarrow$ $E(\beta)$: potential energy curve





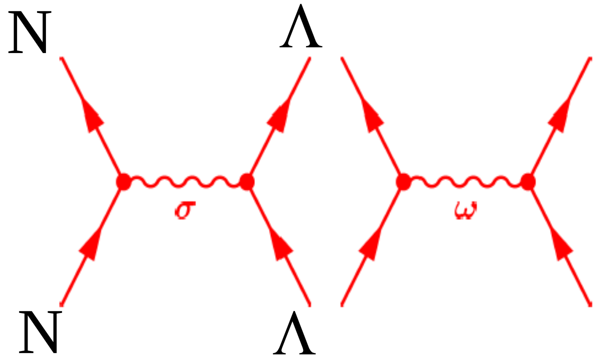
$E(\beta,\gamma)$: potential energy surface

RMF calculations for deformed hypernuclei

Hypernuclei: nucleus + Lambda particle

Effect of a Λ particle on nuclear shapes?

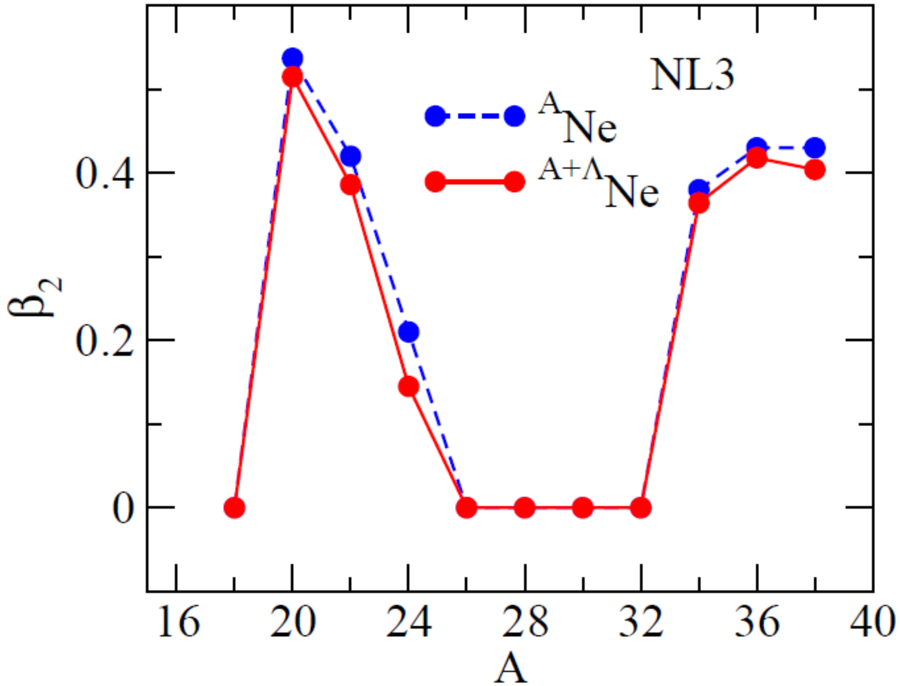
Relativistic Mean-field model



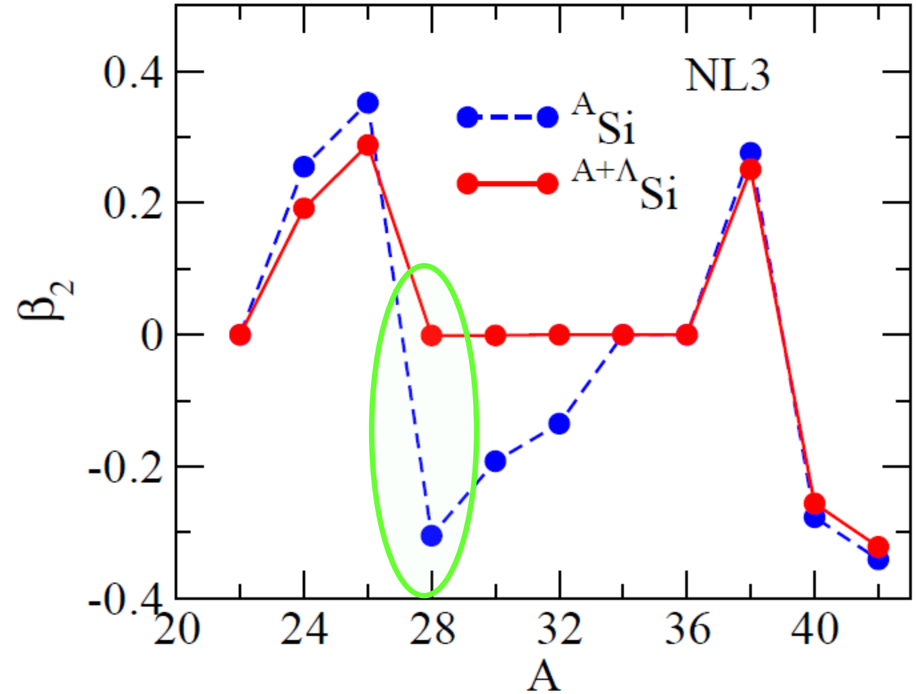
nucleon-nucleon interaction
via meson exchange

Λσ and Λω couplings

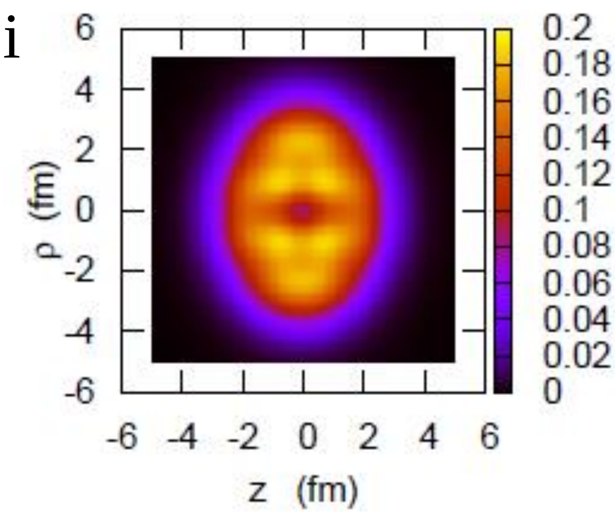
Ne isotopes



Si isotopes

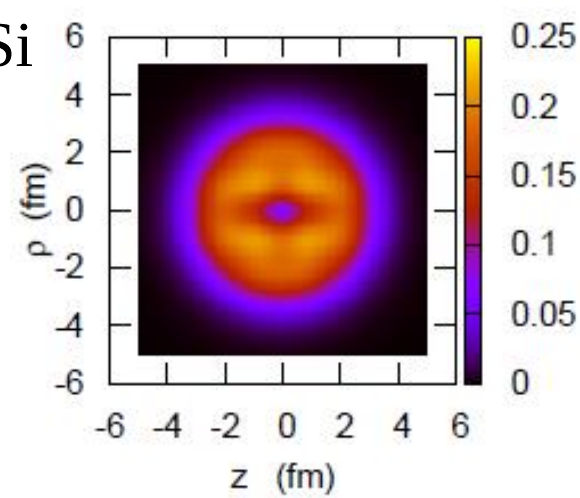


^{28}Si



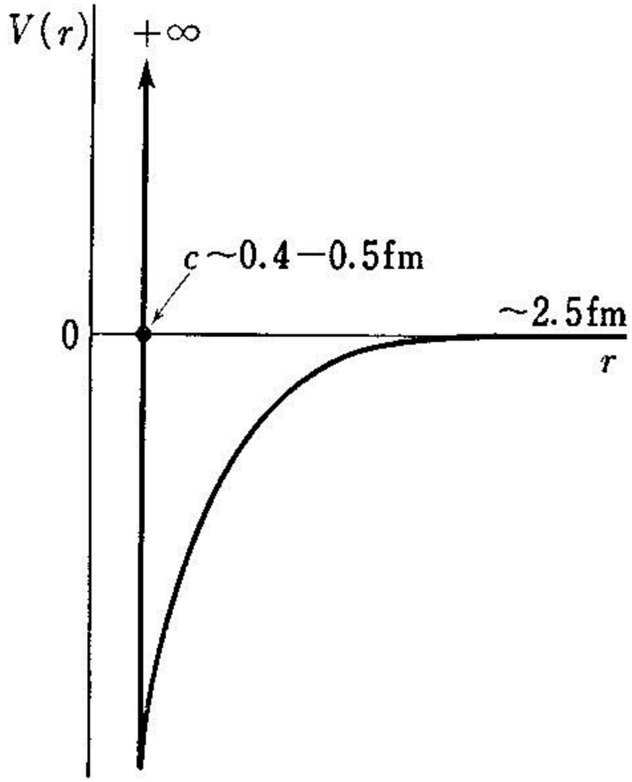
$\xrightarrow{\Lambda}$

$^{29}{}_{\Lambda}$Si



Myaing Thi Win and K.Hagino, PRC78(‘08)054311

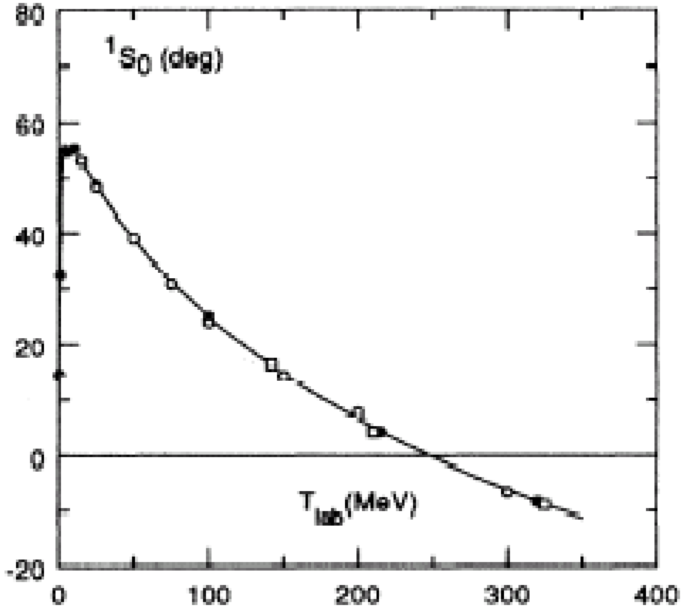
Bare nucleon-nucleon interaction

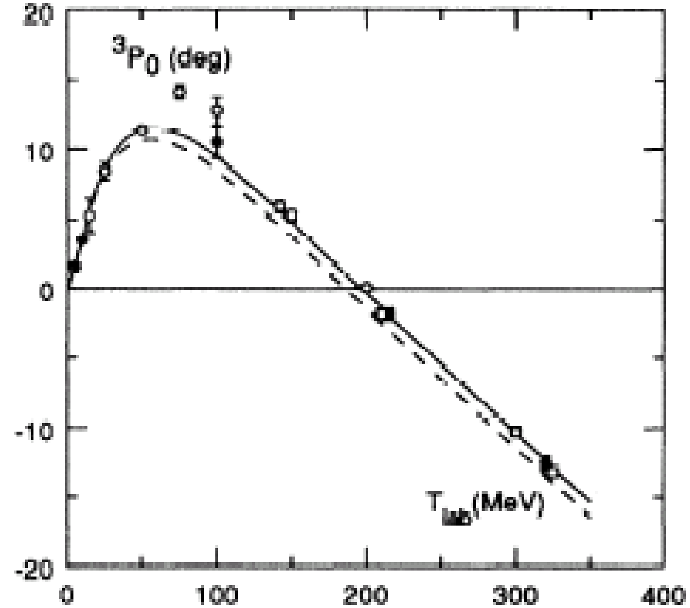


Existence of short range repulsive core

Bare nucleon-nucleon interaction

Phase shift for p-p scattering





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

Phase shift:

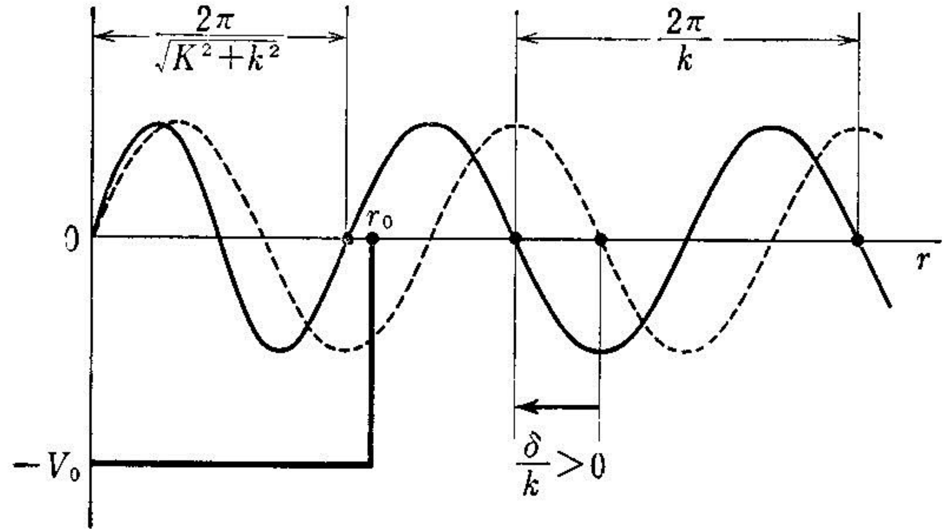
Radial wave function

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

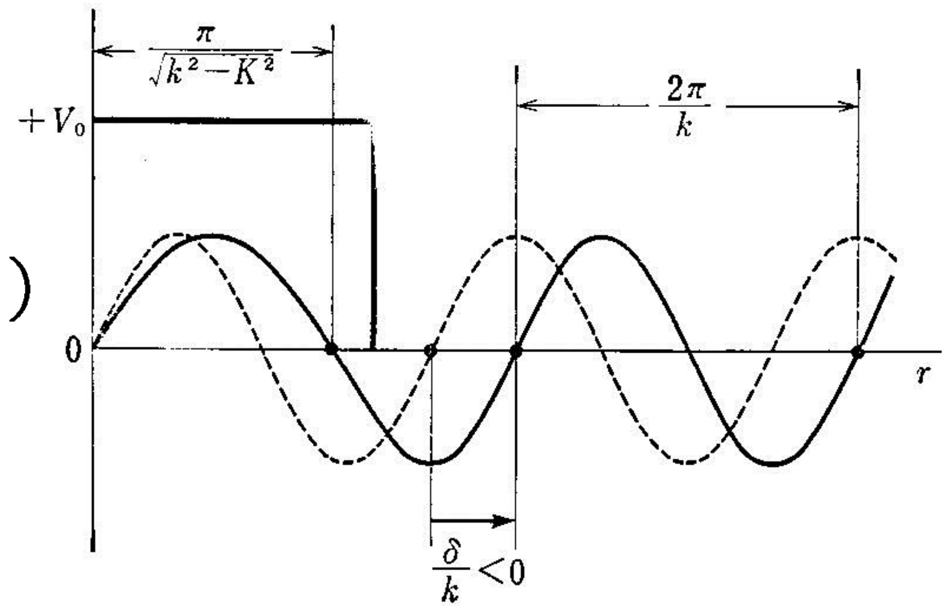
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E\right] u_l(r) = 0$$

Asymptotic form:

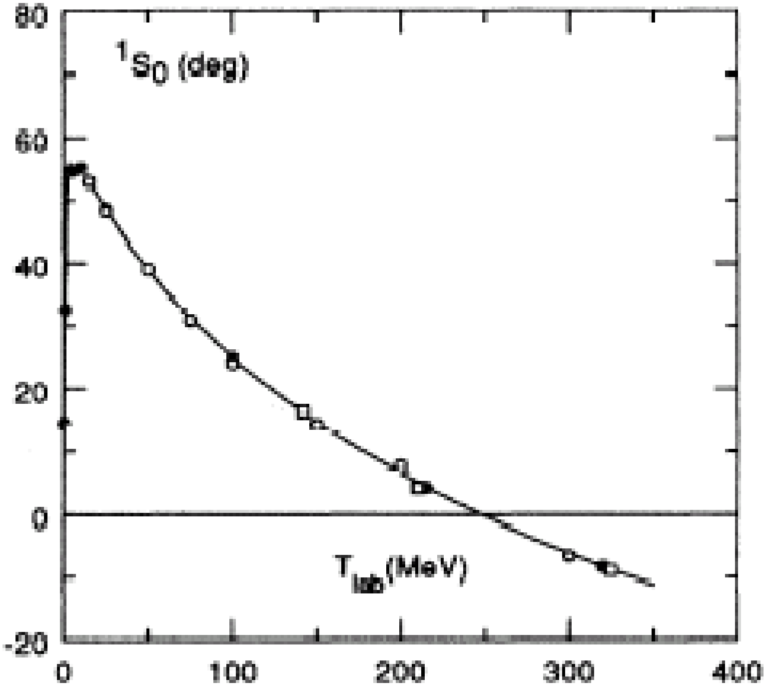
$$u_l(r) \ \to \ \sin(kr - l\pi/2 + \delta_l) \quad (r \to \infty)$$

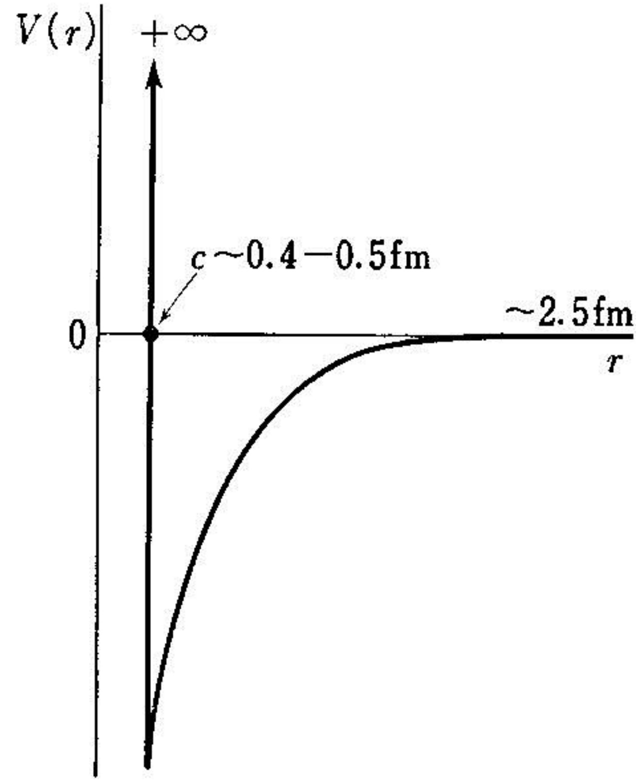


（a） 引　力



（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

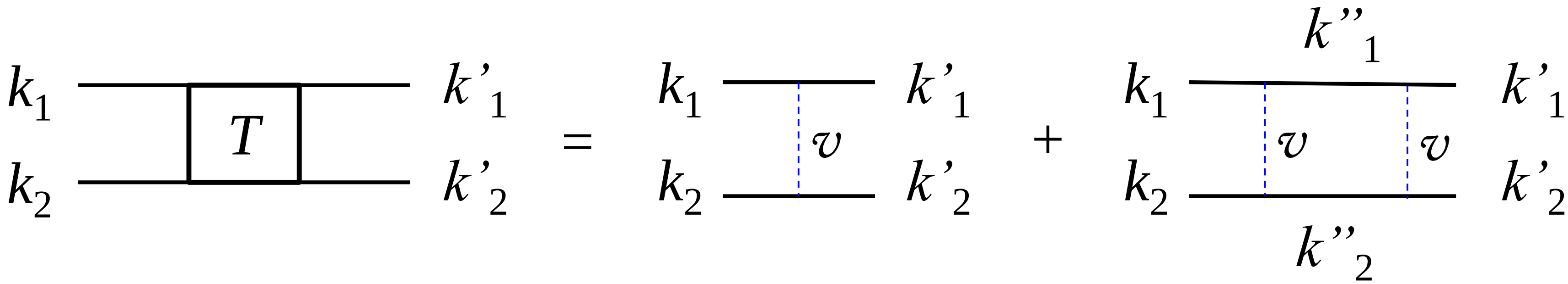
Matrix elements: diverge

…..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

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

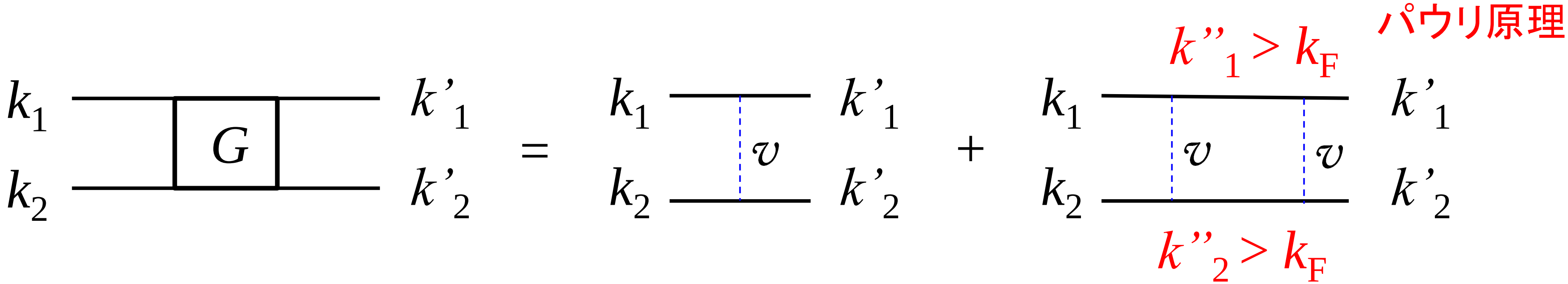


+…….

Lippmann-Schwinger equation

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

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



+…….

*中間状態で k_F 以上
に飛ばなければならないので、
散乱が抑制 → 独立粒子描像

Bethe-Goldstone equation

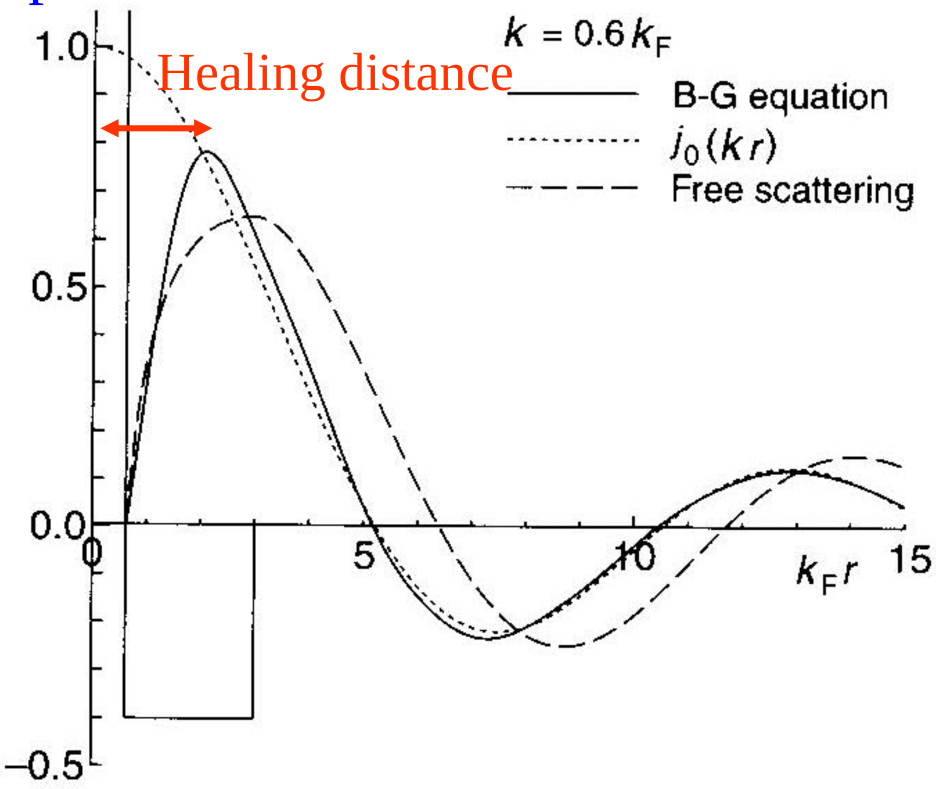
$$G = v + v\frac{Q_F}{E - H_0}G$$

◆Hard core

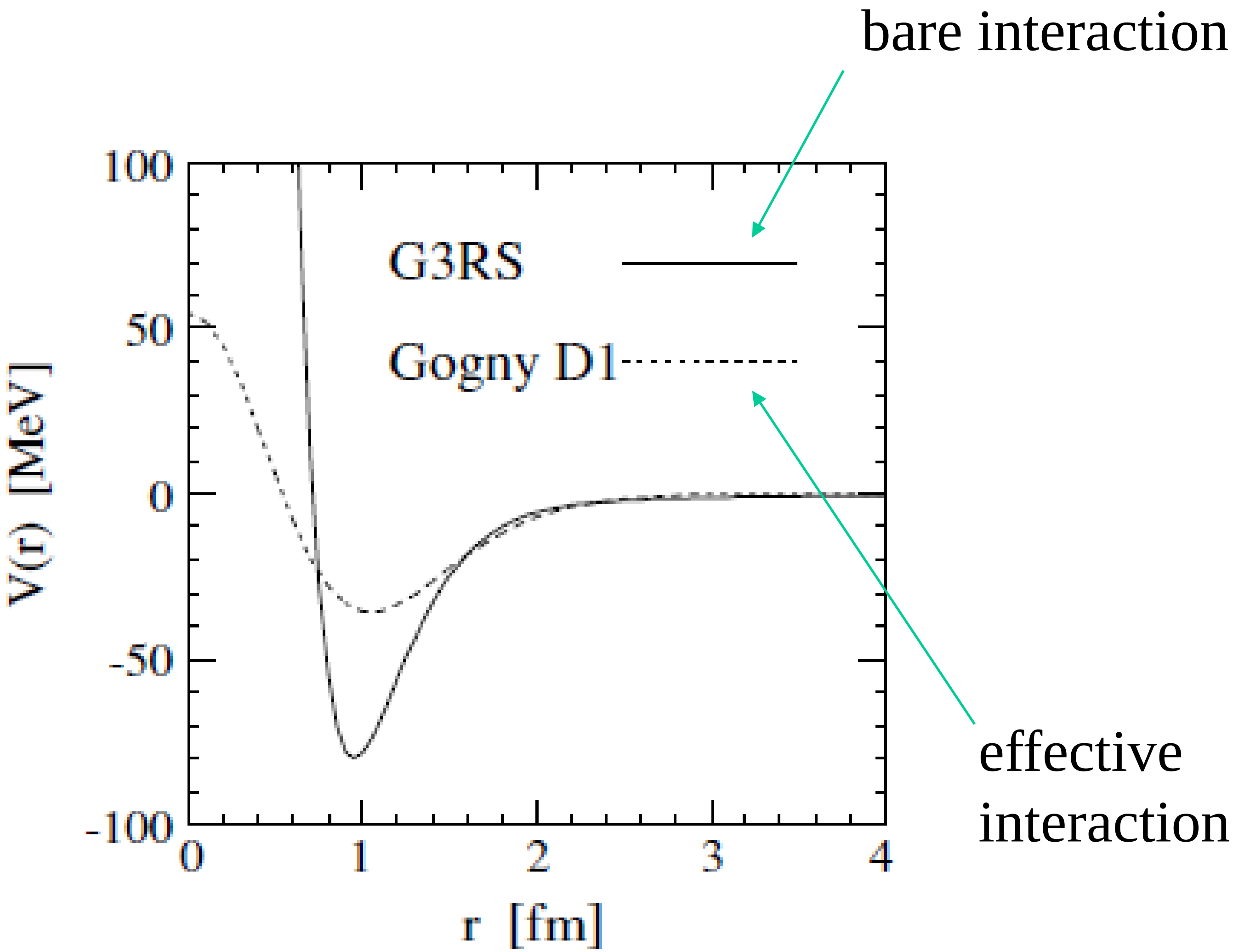
$$G = v + v\frac{Q_F}{E - H_0}G \quad \Longleftrightarrow \quad G = \frac{v}{1 - v\,Q_F/(E - H_0)}$$

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

◆Independent particle motion



→ use G instead of v in mean-field calculations



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　密度に依存するゼロ・レンジ相互作用

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

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

(note) finite range effect $\Longleftrightarrow$ 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 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:

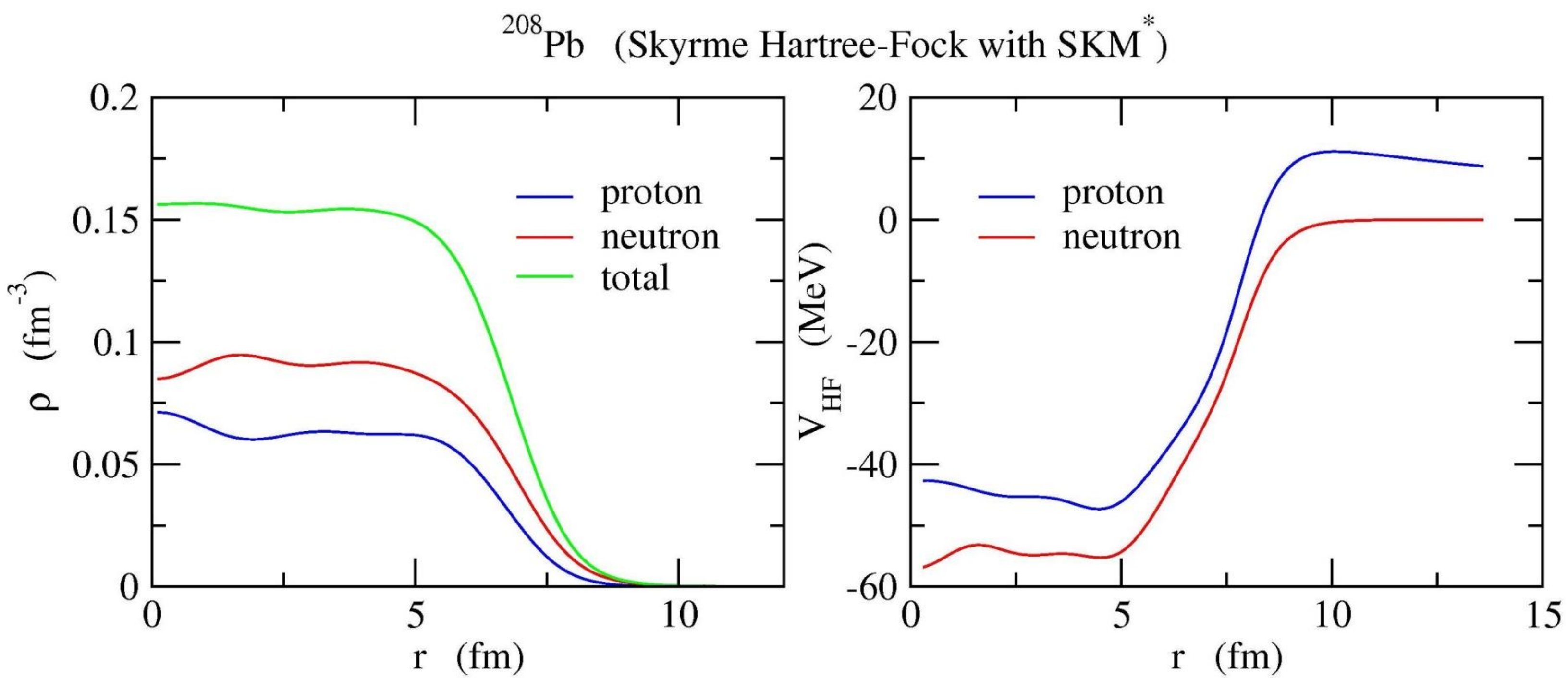
SIII, SkM*, SGII, SLy4,…….

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

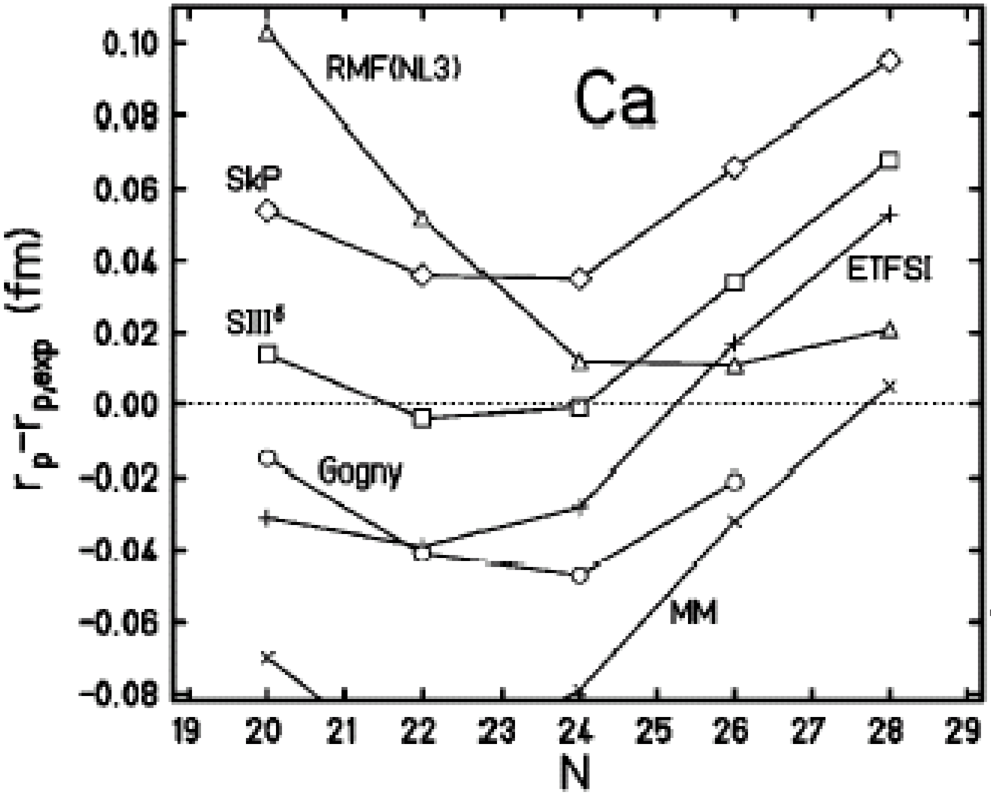
Iteration

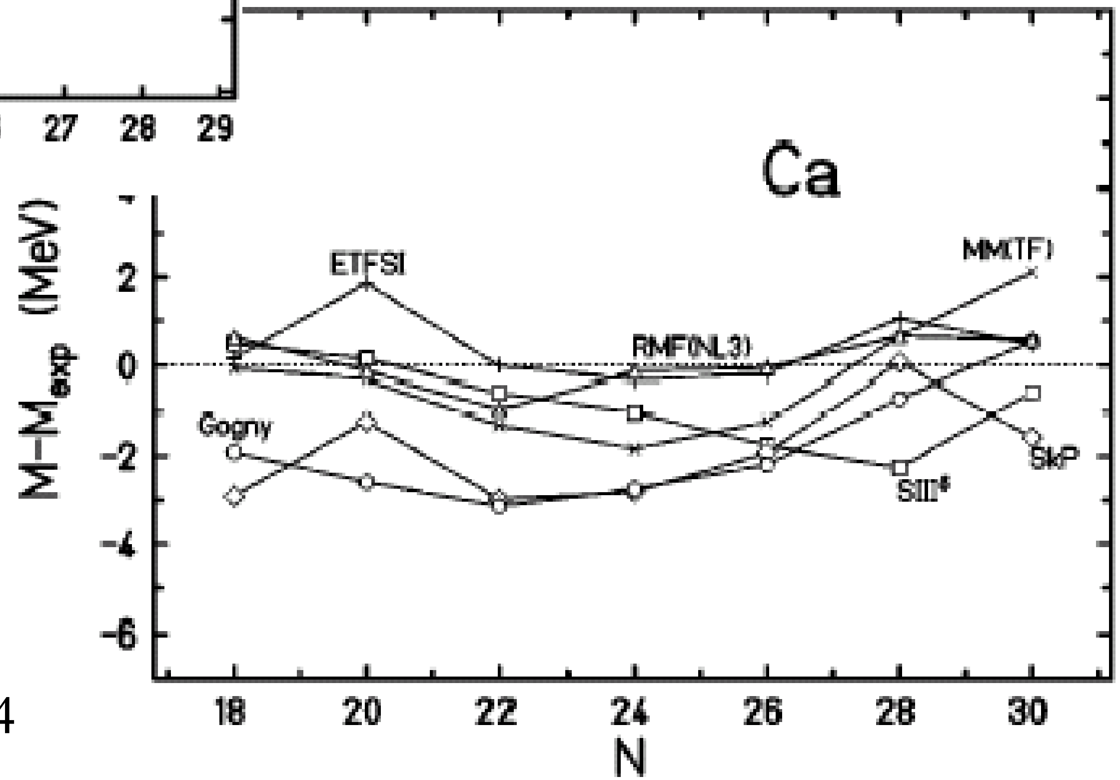
V_{HF}: depends on ψ_i $\longleftarrow$ non-linear problem

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



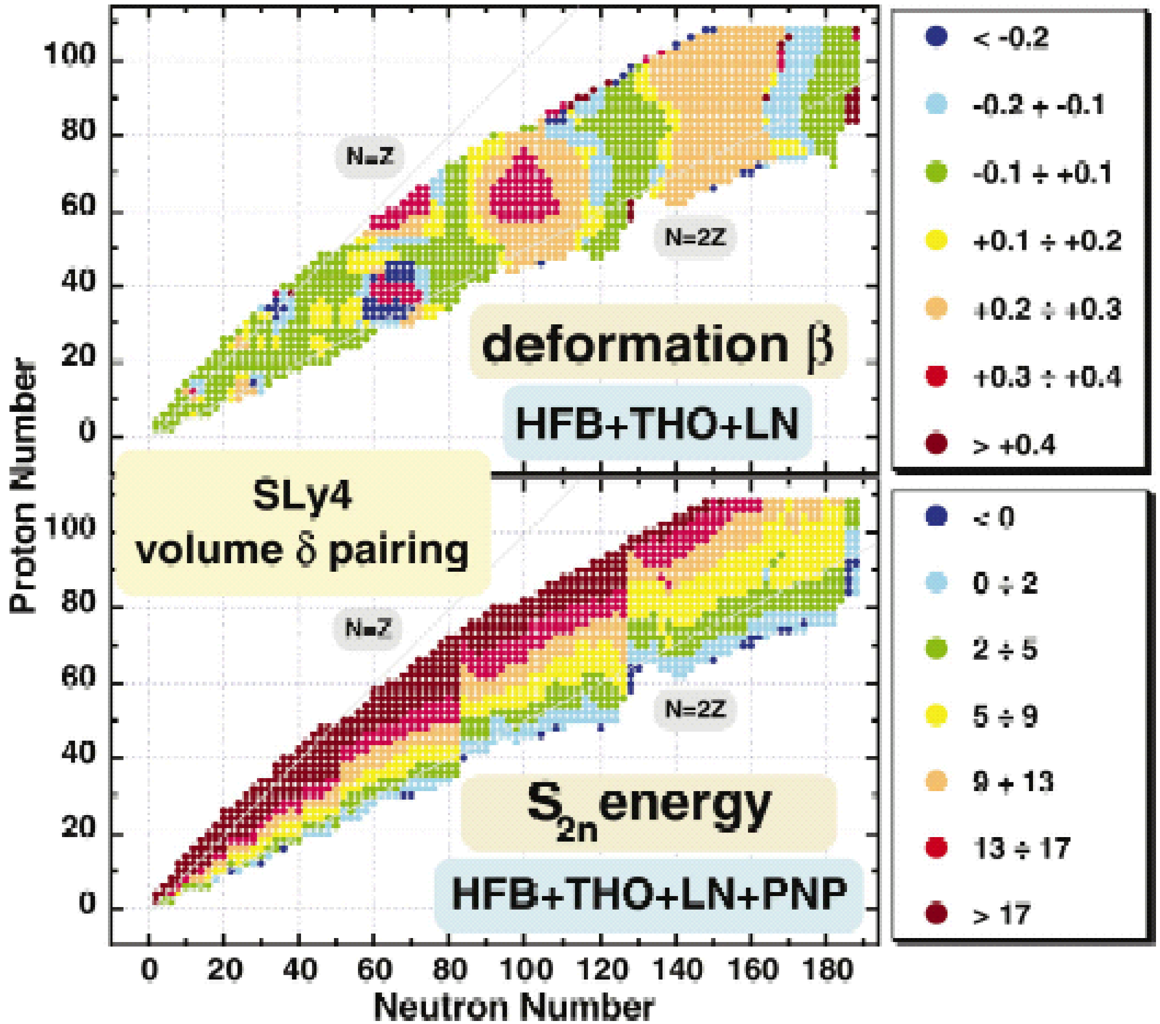
Examples of HF calculations for masses and radii





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

deformation and two-neutron separation energy



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