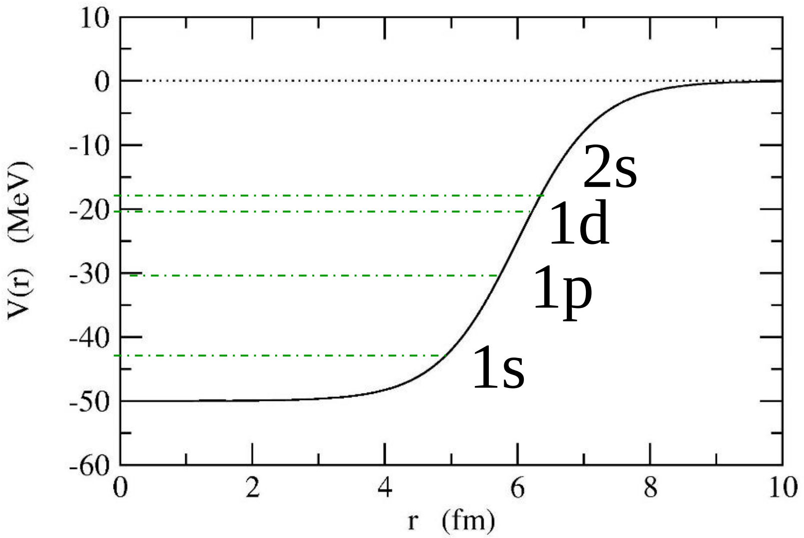
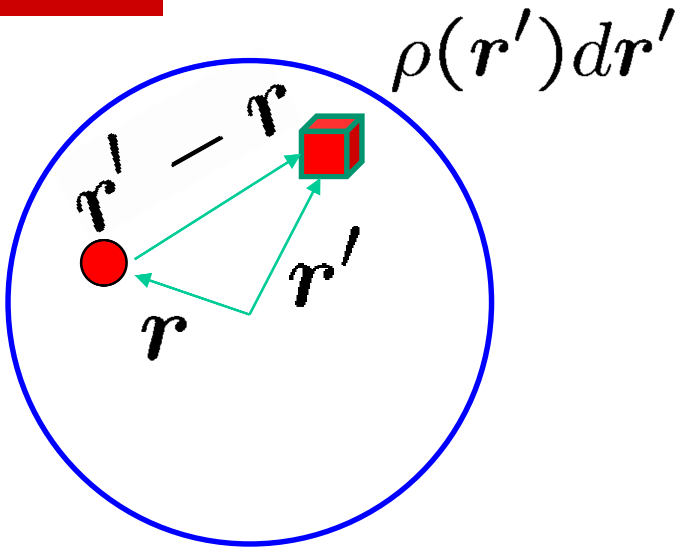
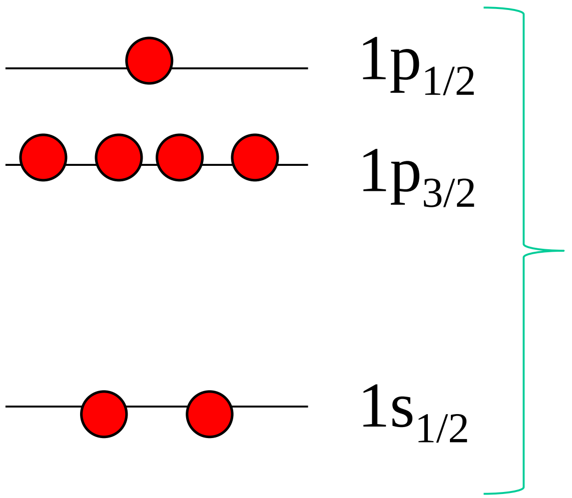
# Mean-field (Hartree-Fock) Theory




naively speaking,

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




shell model

independent motion

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

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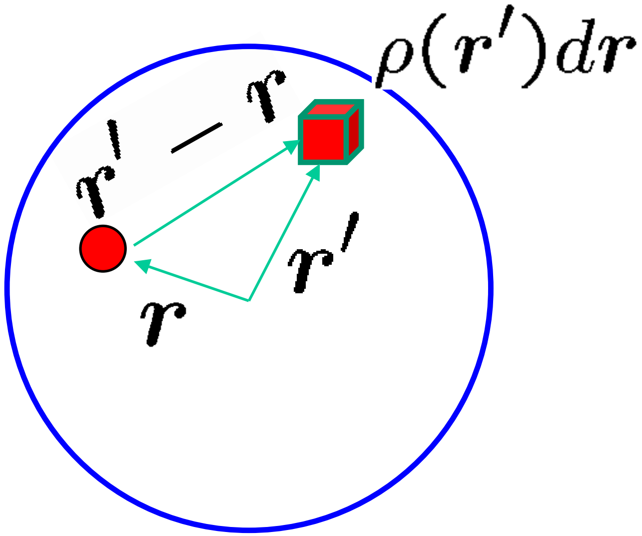



naively speaking,

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

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

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

the potential depends on the solutions

# Mean-field (Hartree-Fock) Theory

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

the potential depends on the solutions

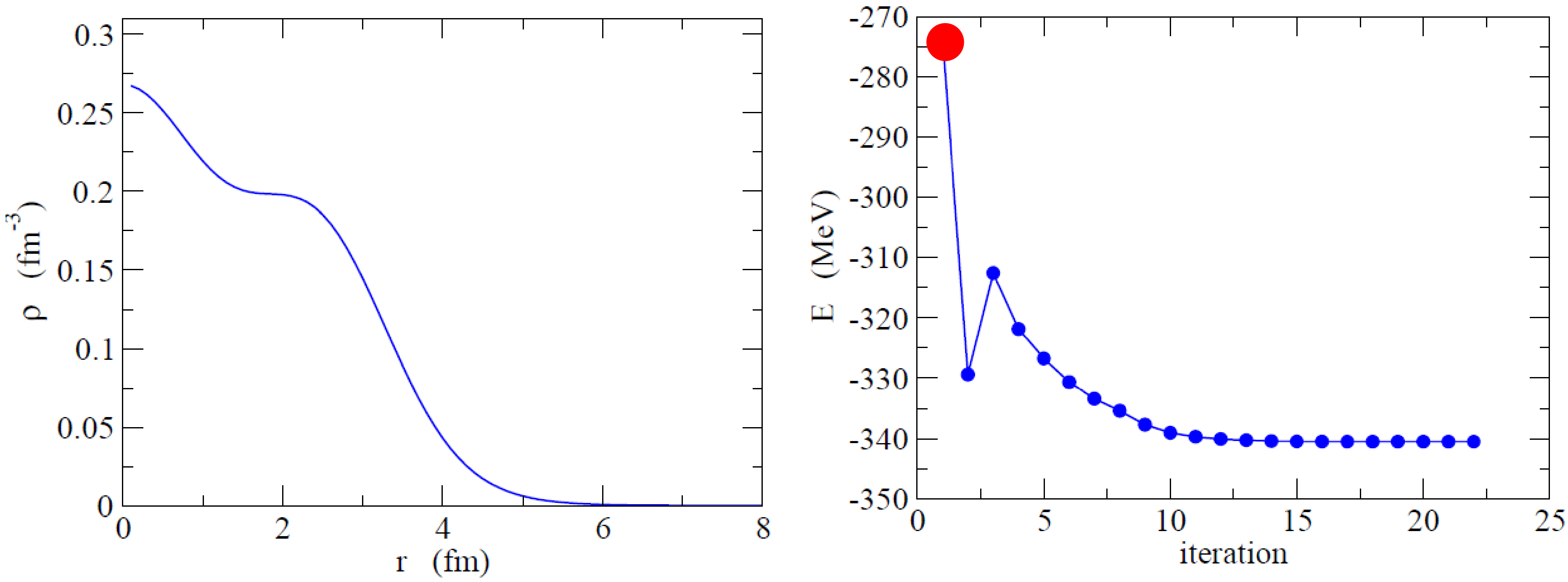
→ self-consistent solutions

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

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

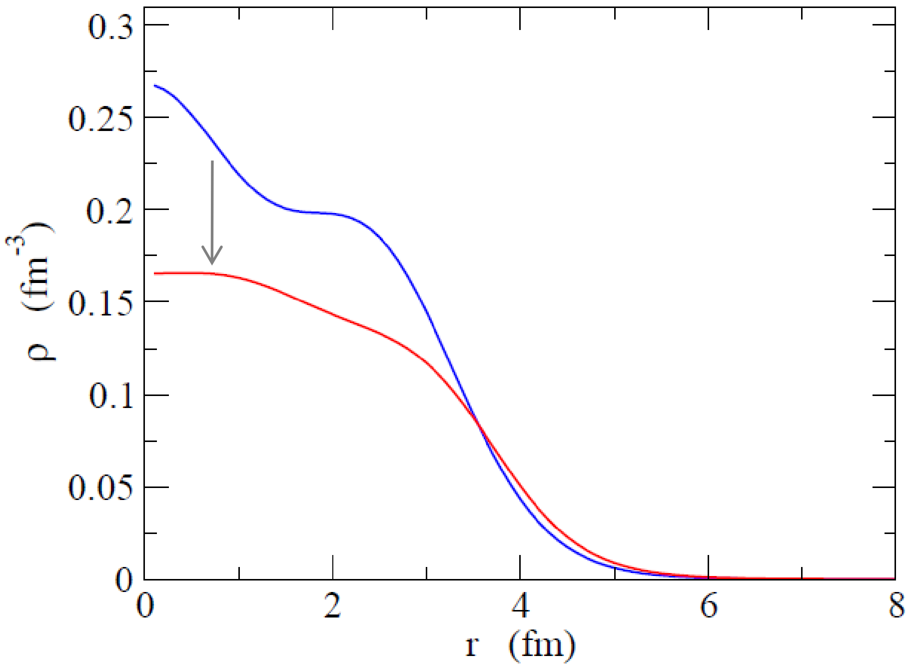
"self-consistent mean-field theory"

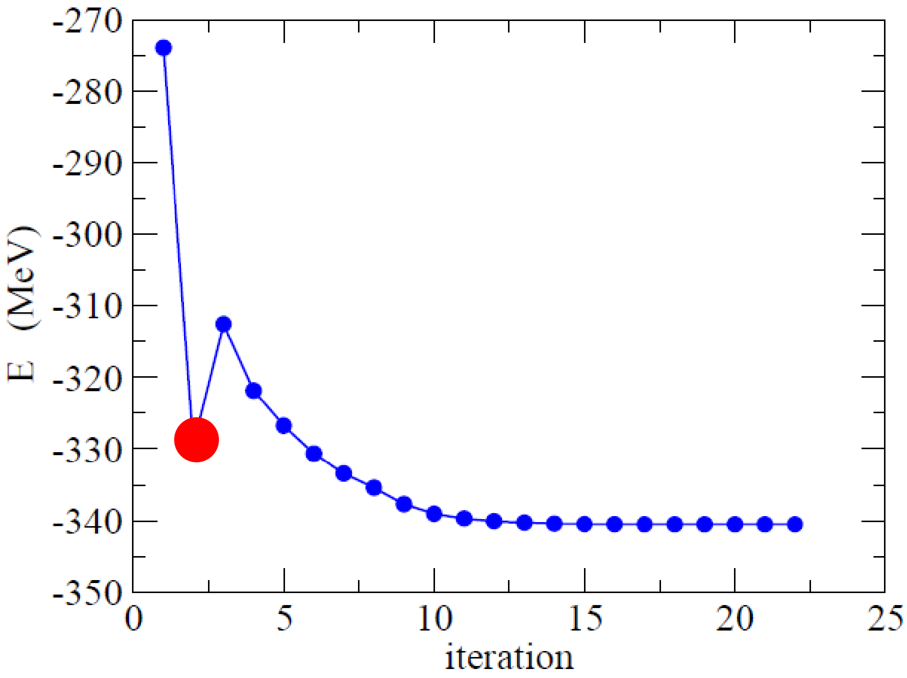
# Skyrme-Hartree-Fock calculations for $^{40}$Ca




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

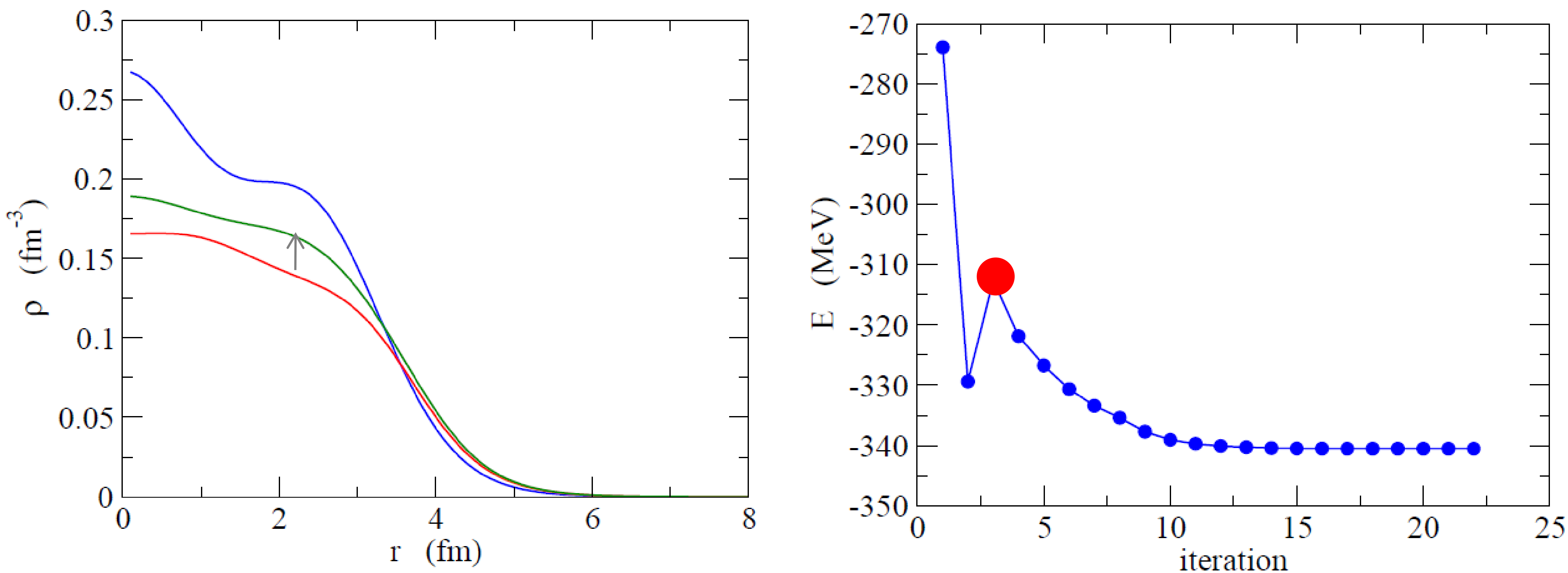
# Skyrme-Hartree-Fock calculations for $^{40}$Ca



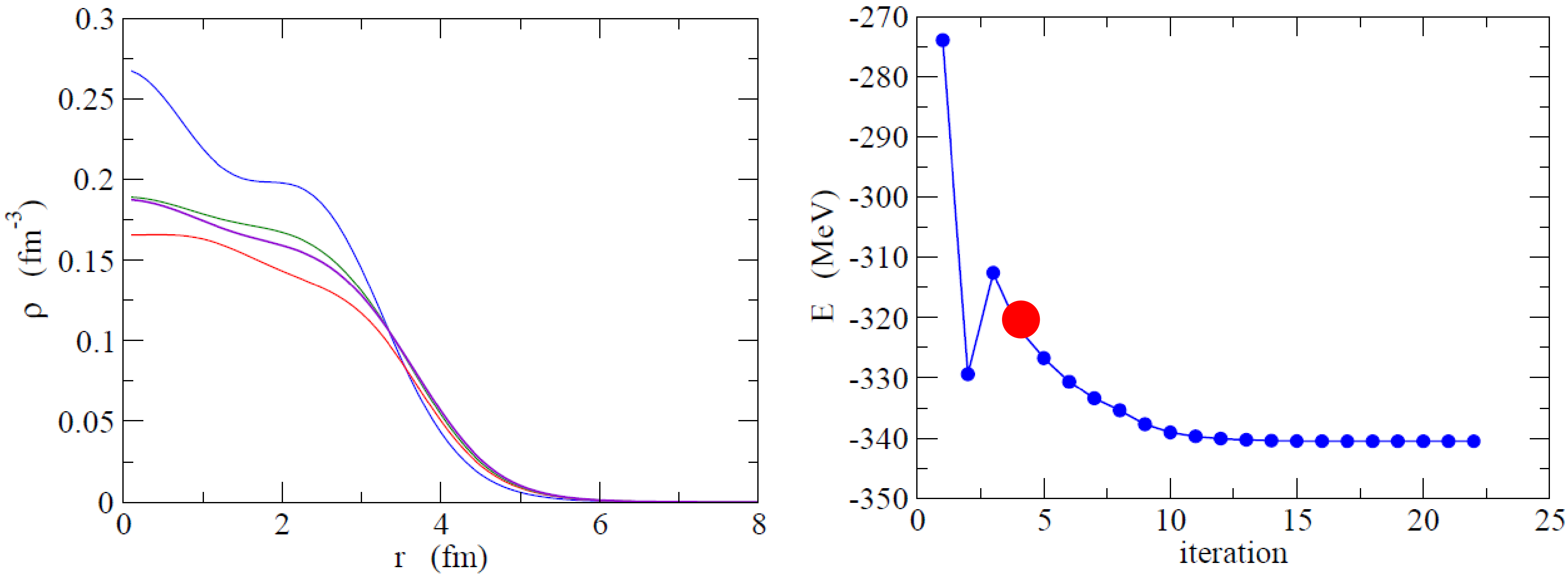

optimize the density by taking into account the nucleon-nucleon interaction

# 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

# Variational Principle (Rayleigh-Ritz method)

optimization ⟷ variational principle

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

$H$ : many-body Hamiltonian

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

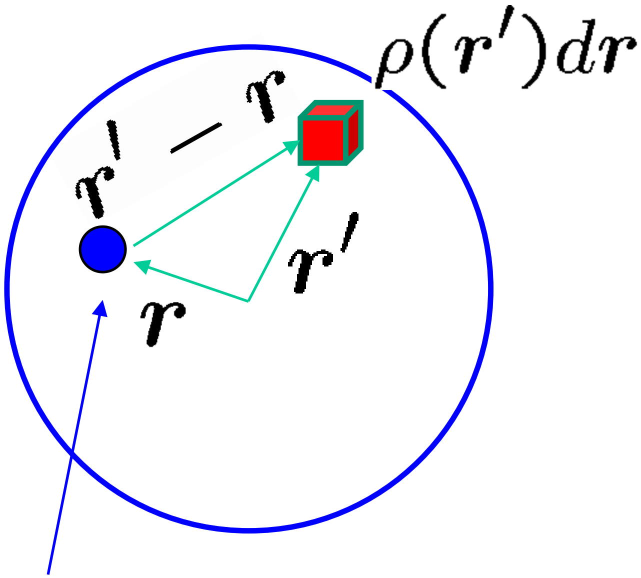
← many-body wave function for independent particles

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

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

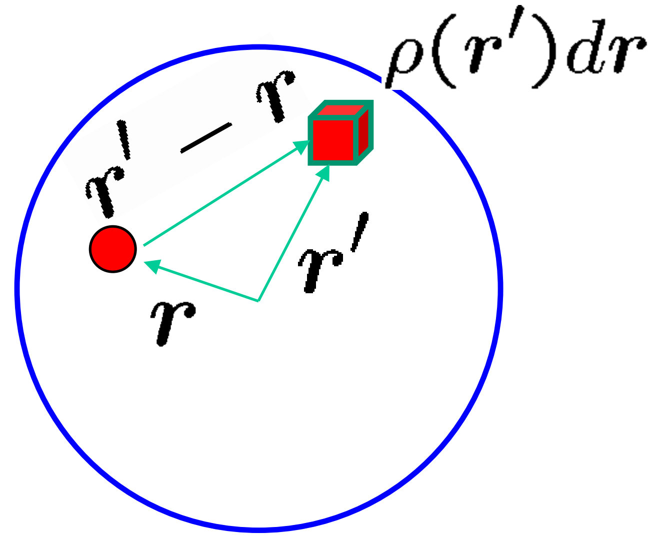
# Mean-field (Hartree-Fock) Theory

<u>electro-static potential</u>




test charge

<u>nucleus</u>




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

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

anti-symmetrization

nucleon: fermion

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

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

Slater determinat

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

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

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

exchange term

Hartree-Fock theory

anti-symmetrization

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

non-local potential

# Hartree-Fock Method and Symmetries

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

2body →1 body approximation

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

Slater determinant

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

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

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

"Symmetry-broken solution"

"Spontaneous Symmetry Broken"

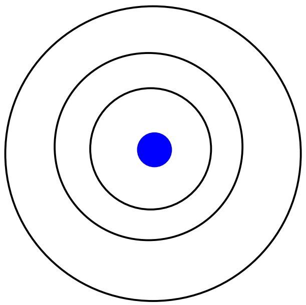
$\Psi_{\rm HF}$ : does not necessarily possess the symmetries that $H$ has.

Typical Examples

- Translational symmetry: always broken in nuclear systems

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

(cf.) atoms

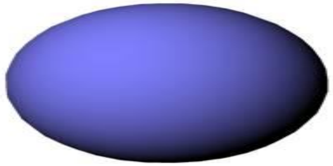


nucleus in the center

⟶ 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

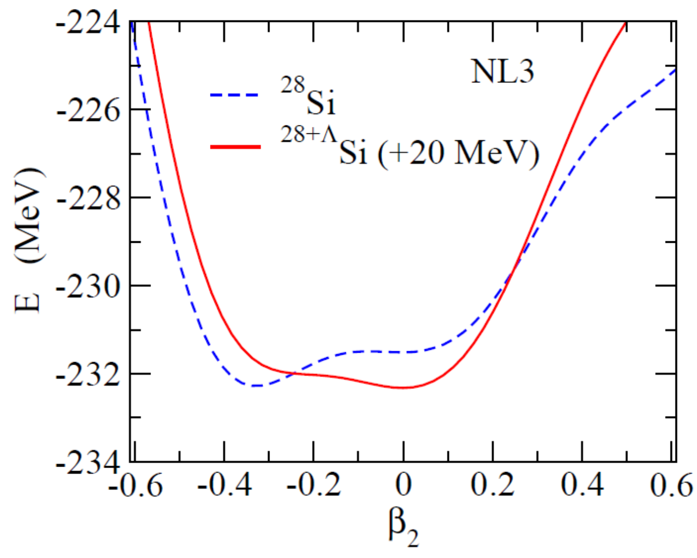
# Constrained Hartree-Fock method

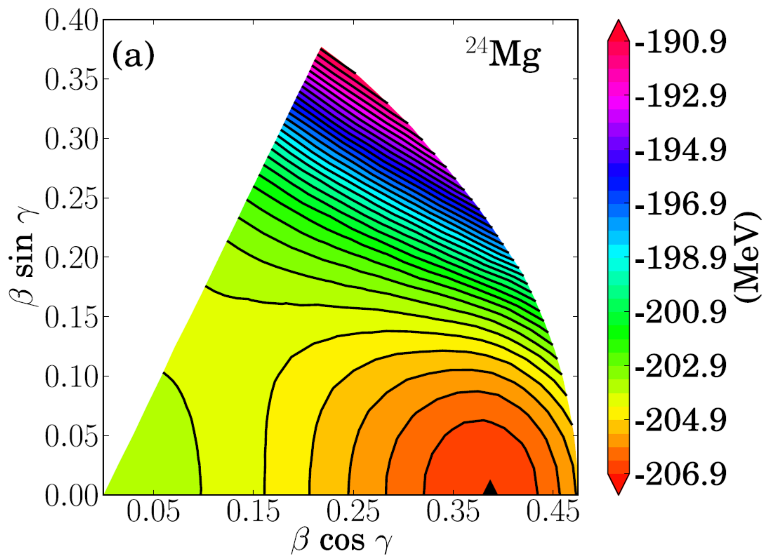
minimize $H' = H - \lambda \hat{Q}_{20}$ with a Slater determinant w.f.

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

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

⟶ $E(\beta)$ : potential energy curve



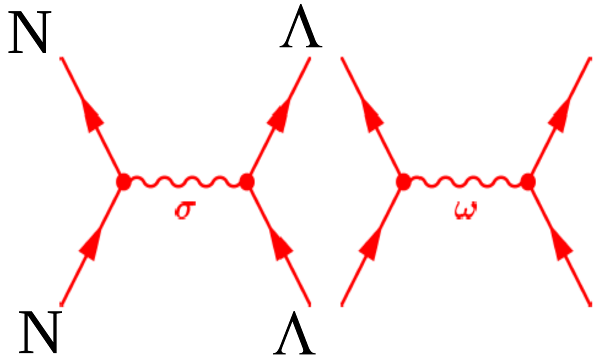

$E(\beta,\gamma)$ : potential energy surface

# RMF calculations for deformed hypernuclei

Hypernuclei: nucleus + Lambda particle

Effect of a Λ particle on nuclear shapes?

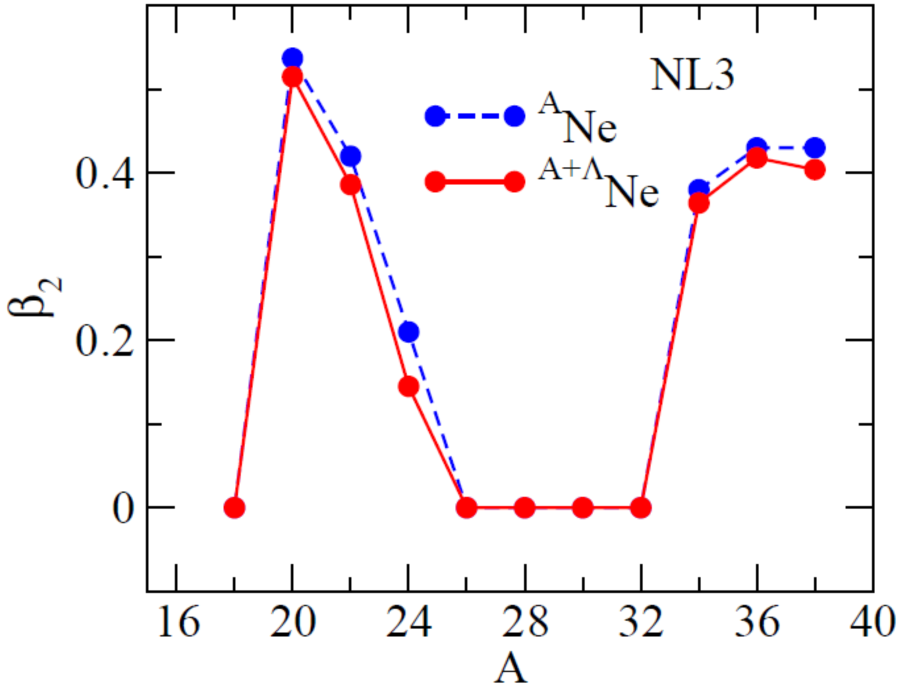
Relativistic Mean-field model



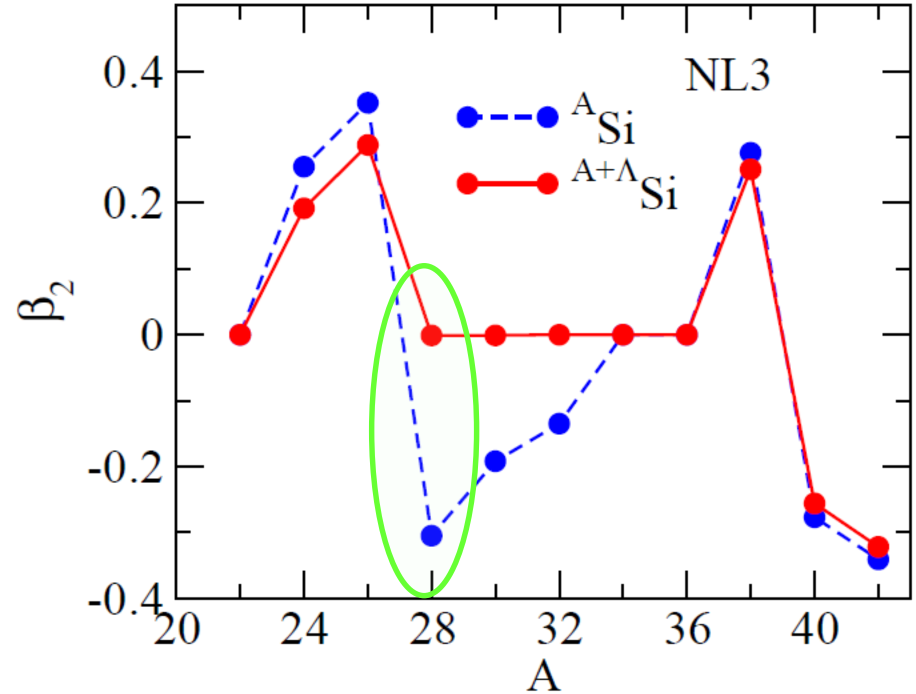

nucleon-nucleon interaction
via meson exchange

Λσ and Λω couplings

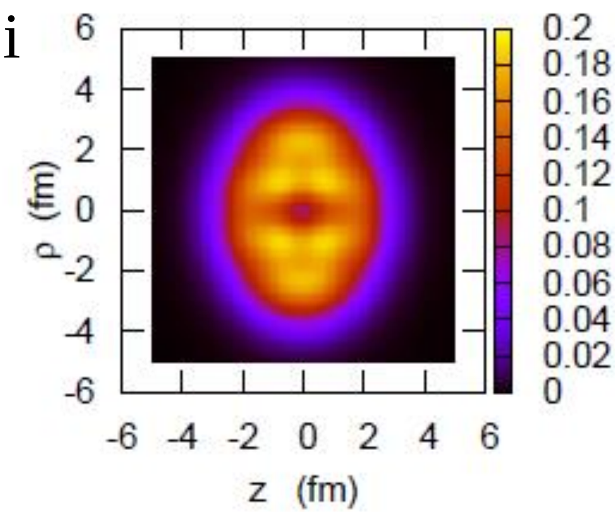
Ne isotopes




Si isotopes

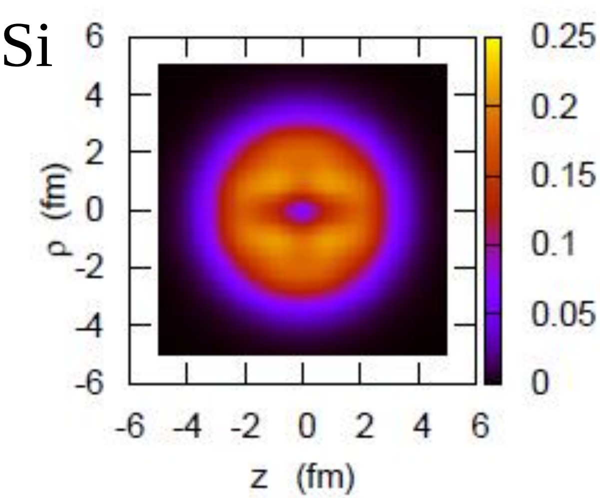



$^{28}$Si



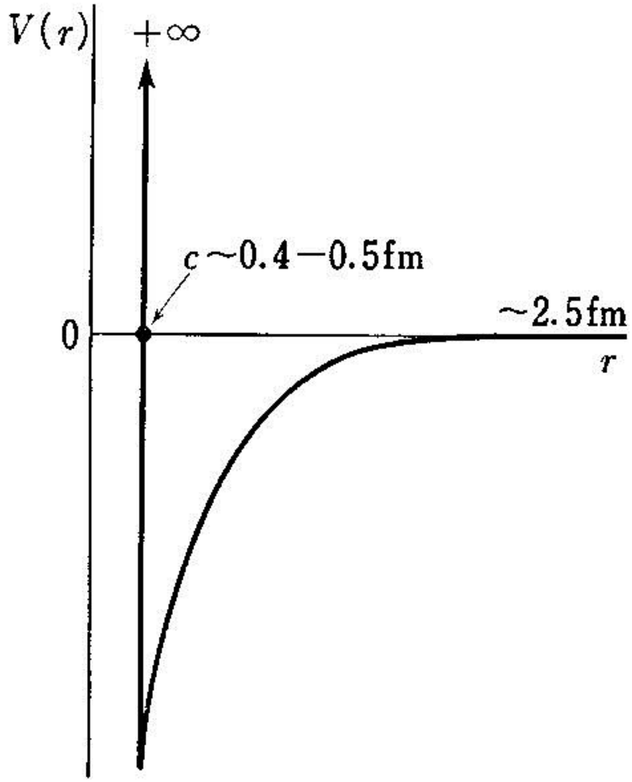

$\xrightarrow{\Lambda}$

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




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

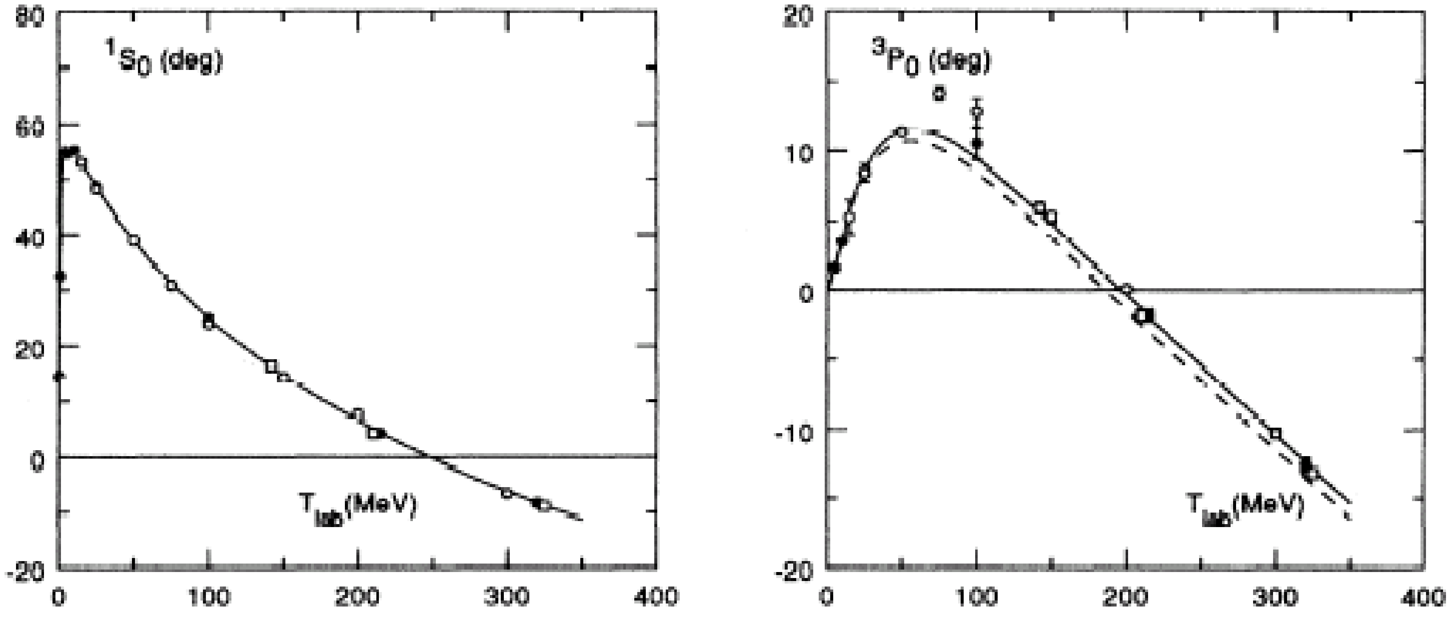
# Bare nucleon-nucleon interaction




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:

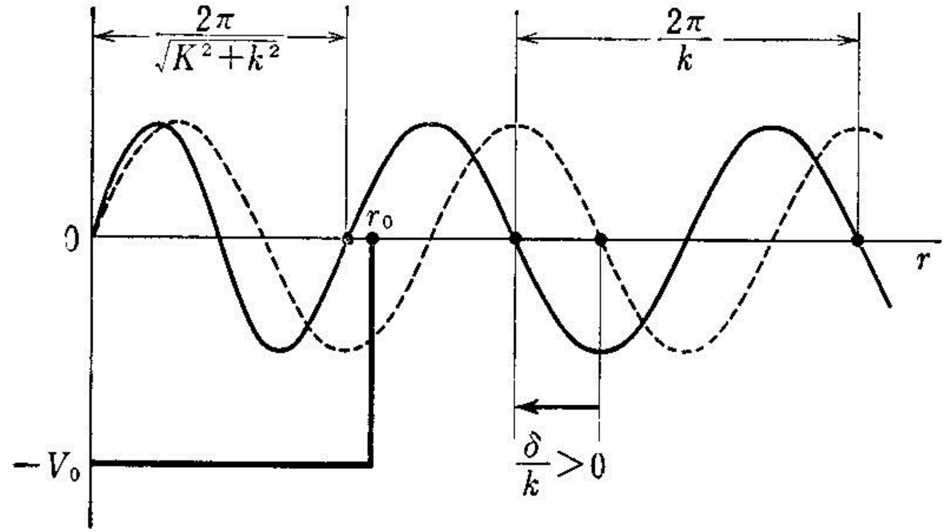
Radial wave function

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

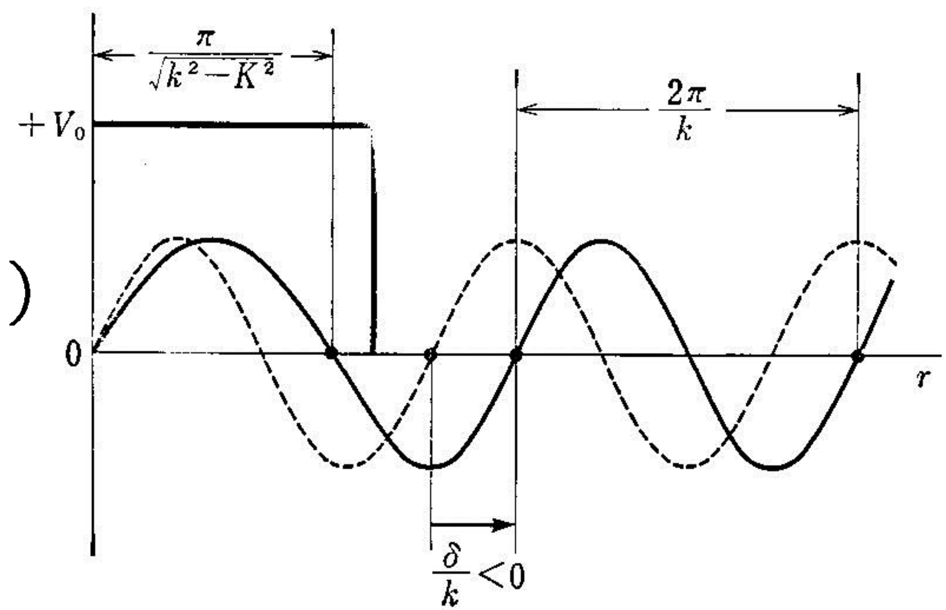
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E\right] u_l(r) = 0$$

Asymptotic form:

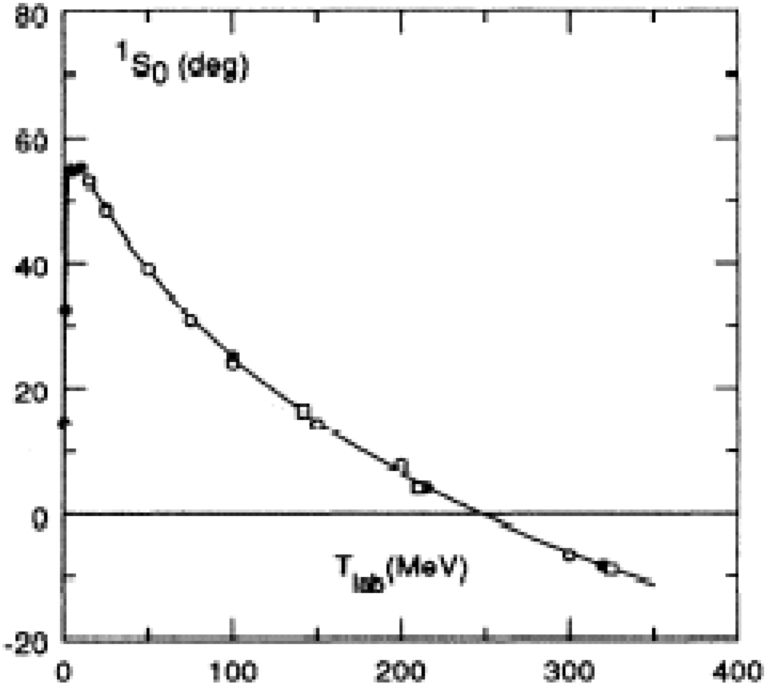
$$u_l(r) \;\rightarrow\; \sin(kr - l\pi/2 + \delta_l) \quad (r \rightarrow \infty)$$

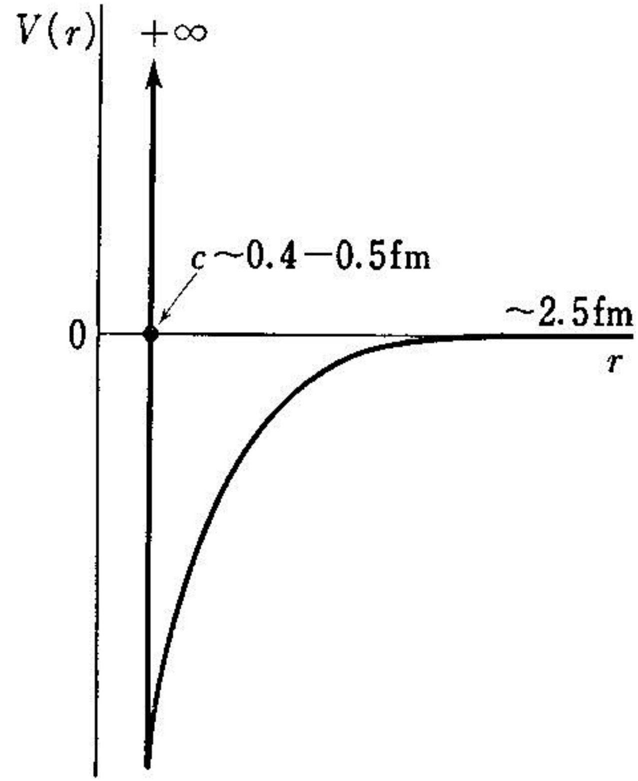



（a） 引 力




（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

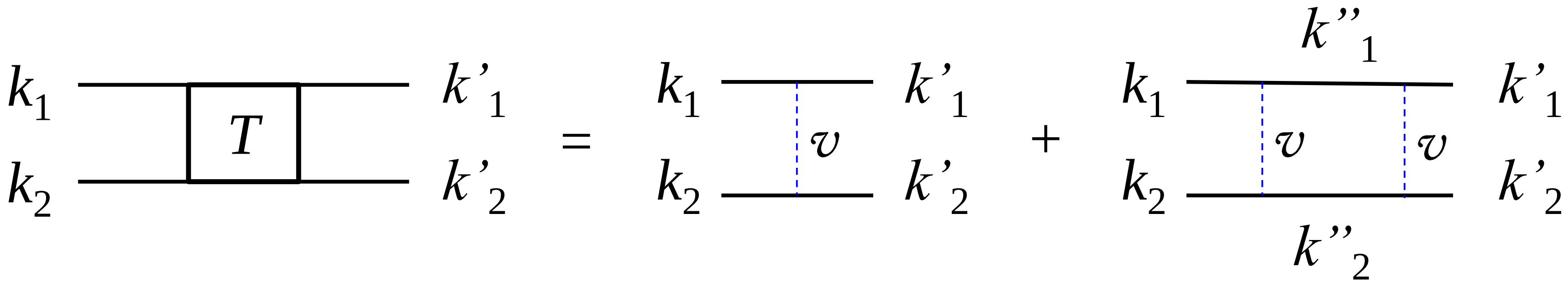
…..but the HF picture seems to work in nuclear systems

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

⇑

Bruckner's G-matrix

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

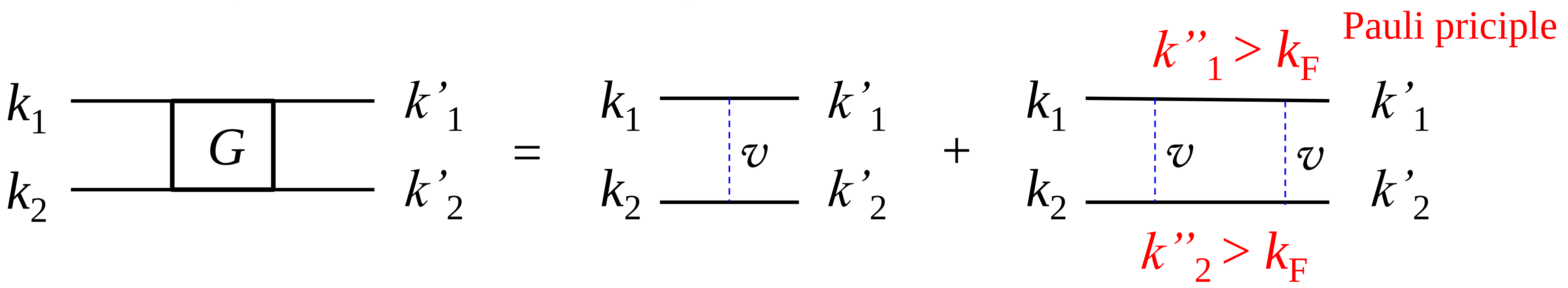



+.......

Lippmann-Schwinger equation

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

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




+.......

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

Bethe-Goldstone equation

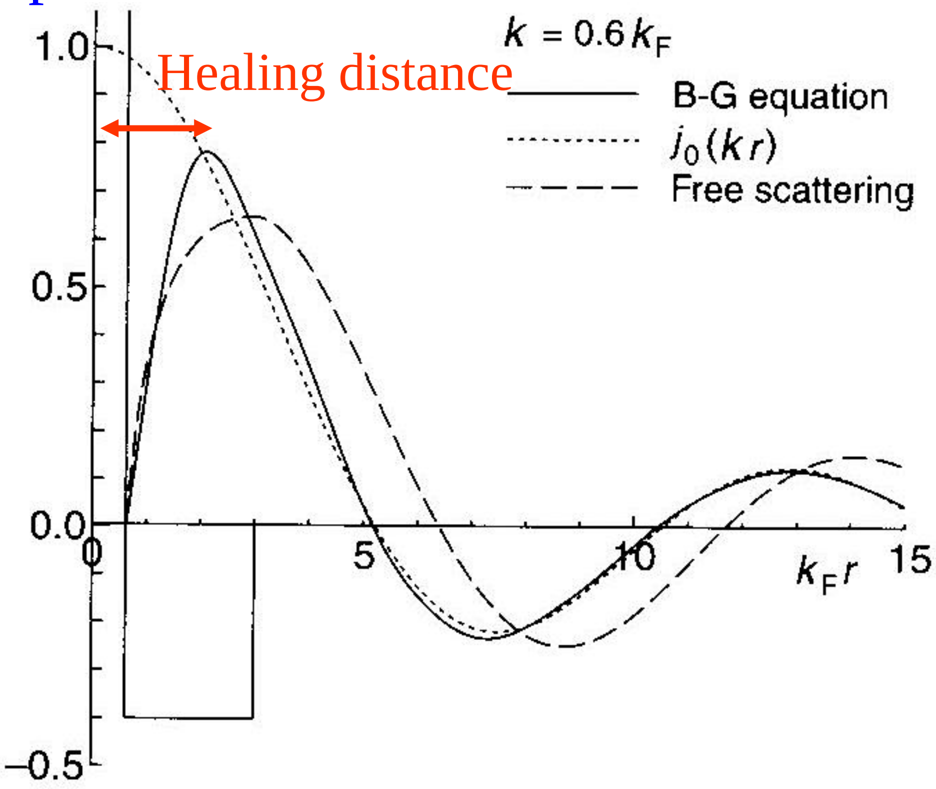
$$G = v + v\frac{Q_F}{E - H_0}G$$

◆Hard core

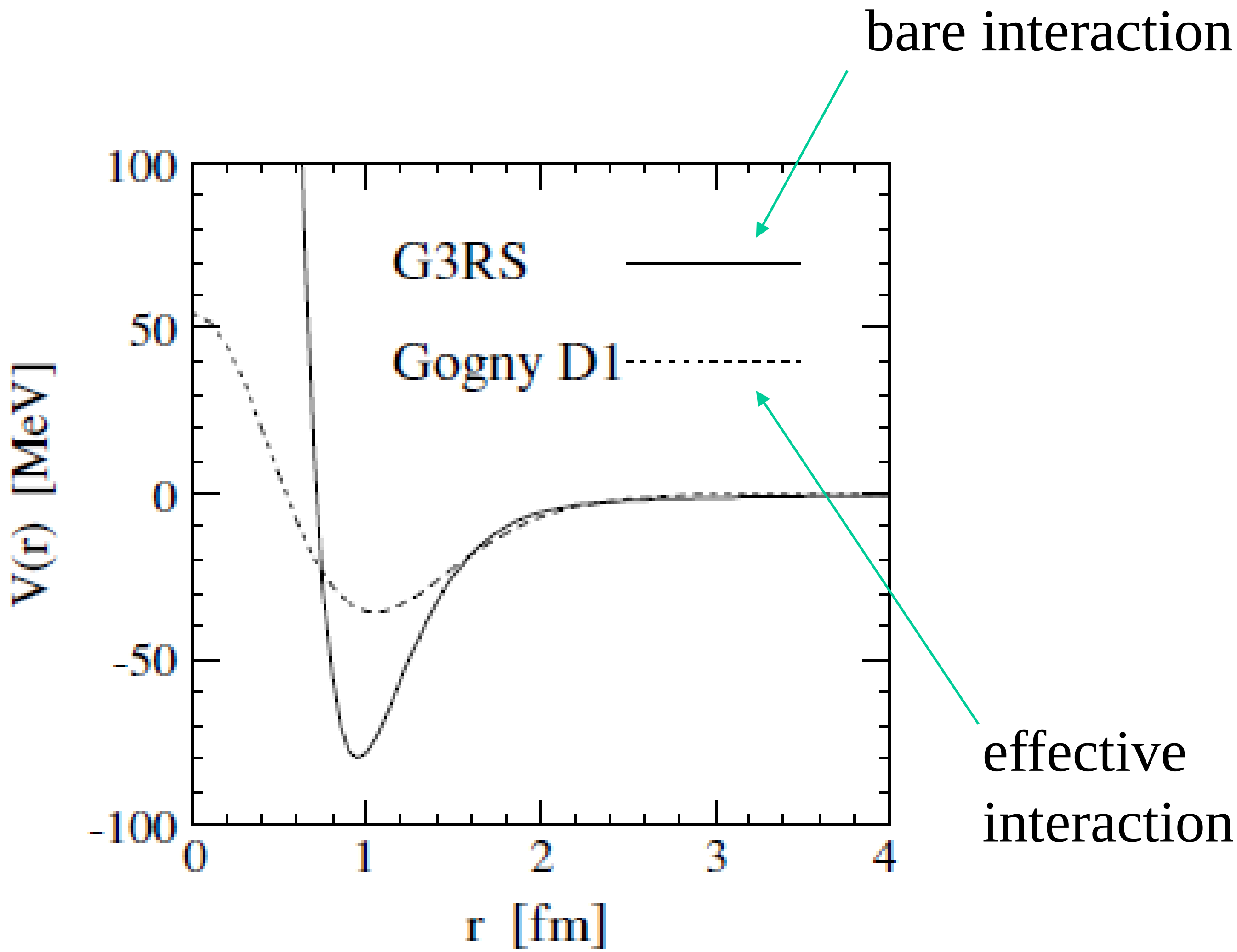
$$G = v + v\frac{Q_F}{E - H_0}G \quad \Longleftrightarrow \quad G = \frac{v}{1 - vQ_F/(E - H_0)}$$

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    density dependent zero-range interaction

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

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

the exchange potential → local

(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*, $\rho_{eq}$ ,….

Parameter sets:

SIII, SkM*, SGII, SLy4,…….

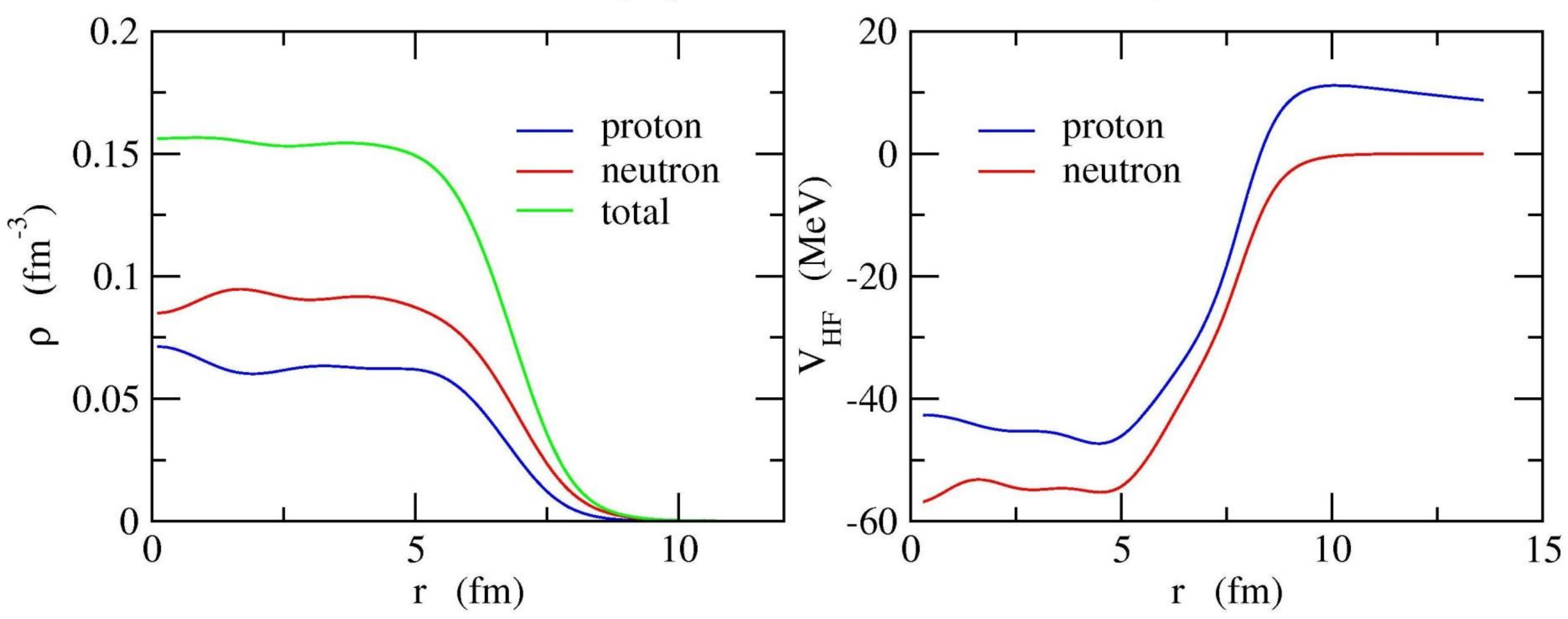
$$-\frac{\hbar^2}{2m}\nabla^2\psi_i(\boldsymbol{r}) + \int v(\boldsymbol{r},\boldsymbol{r}')\rho_{\mathsf{HF}}(\boldsymbol{r}')d\boldsymbol{r}'\psi_i(\boldsymbol{r}) - \int \rho_{\mathsf{HF}}(\boldsymbol{r},\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\psi_i(\boldsymbol{r}')\,d\boldsymbol{r}' = \epsilon_i\,\psi_i(\boldsymbol{r})$$

## Iteration

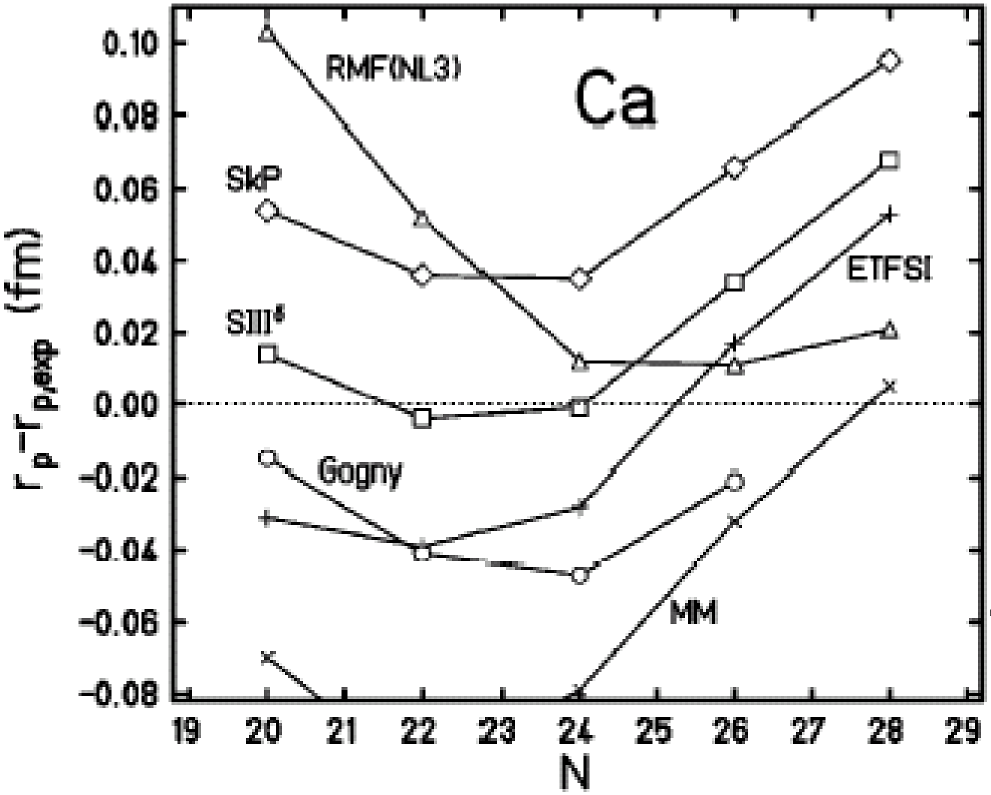
$V_{HF}$: depends on $\psi_i$ $\longleftarrow$ non-linear problem

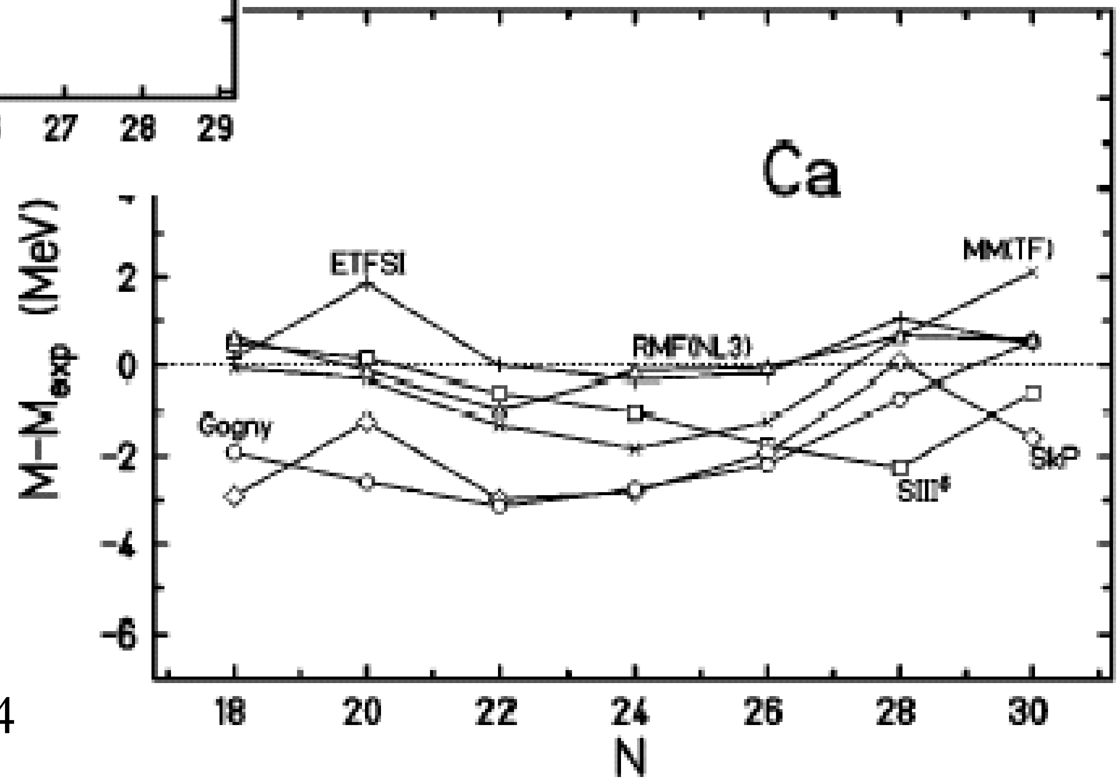
Iteration: $\{\psi_i\} \rightarrow \rho_{\mathsf{HF}} \rightarrow V_{\mathsf{HF}} \rightarrow \{\psi_i\} \rightarrow \cdots$

$^{208}$Pb (Skyrme Hartree-Fock with SKM$^*$)



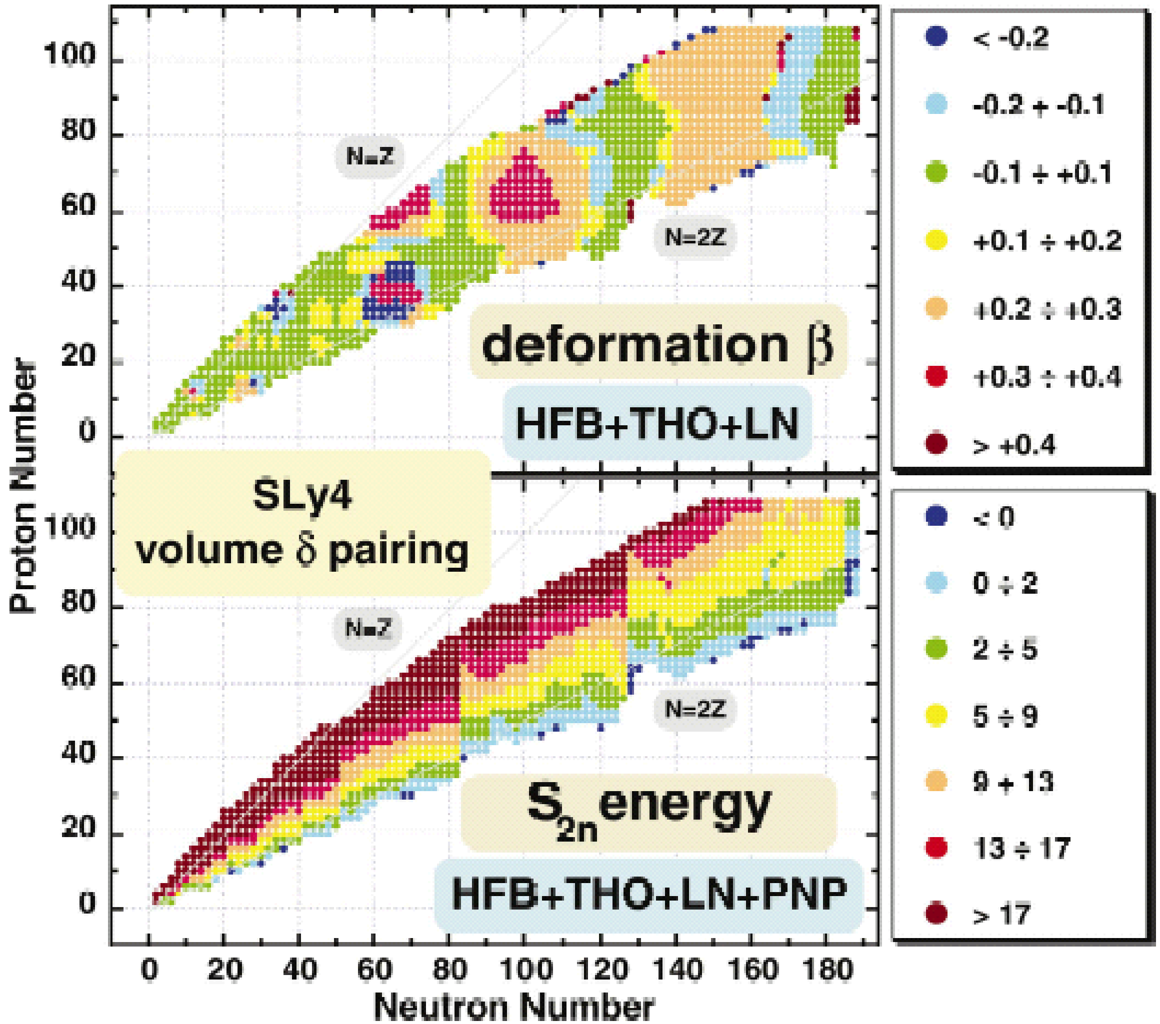
# Examples of HF calculations for masses and radii




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

# deformation and two-neutron separation energy




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