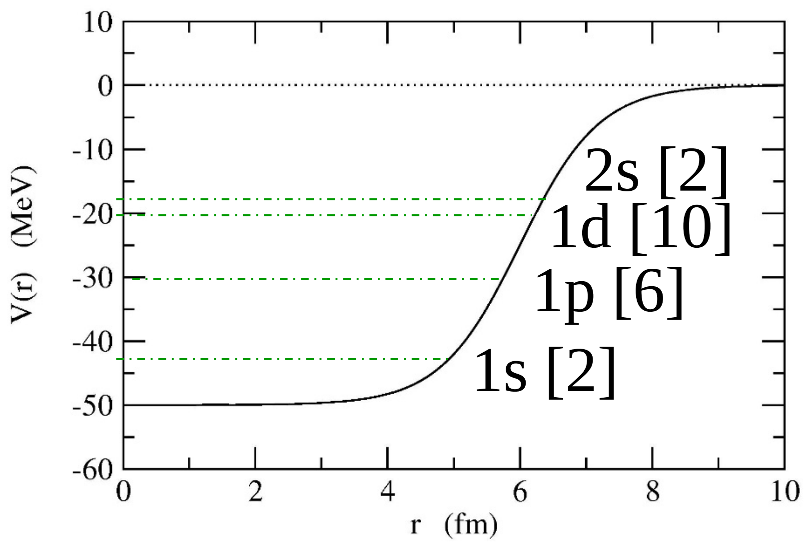
Mean-field approximation and deformation

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

f[14] → $f_{5/2}[6]$, $f_{7/2}[8]$

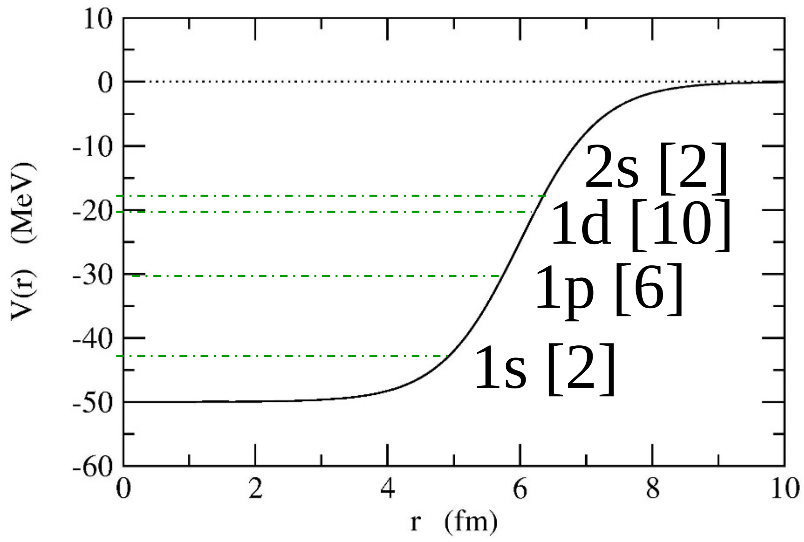
20+8 = 28

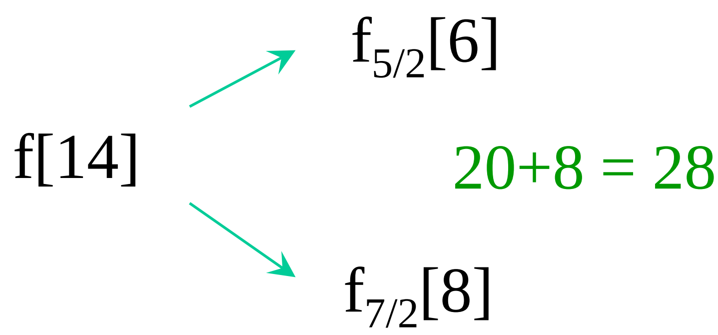
Hartree-Fock近似:核子間相互作用から平均場ポテンシャル

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

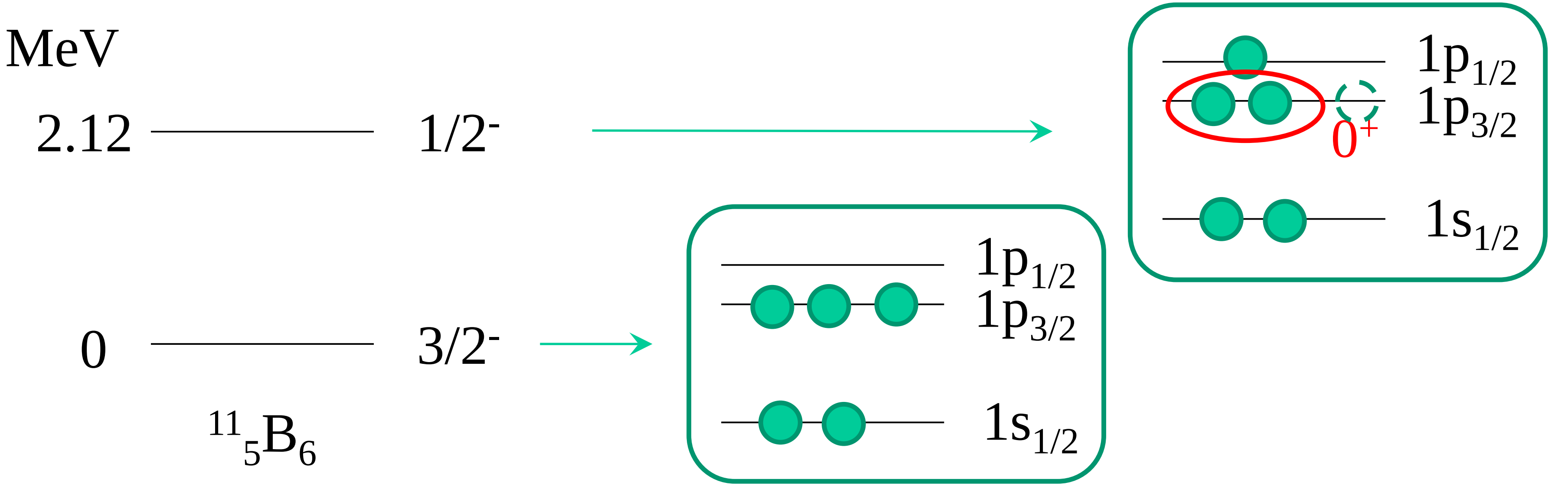
$$-\int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j \psi_j^*(\boldsymbol{r}')\psi_i(\boldsymbol{r}')\right)d\boldsymbol{r}'\psi_j(\boldsymbol{r})$$

Mean-field approximation and deformation

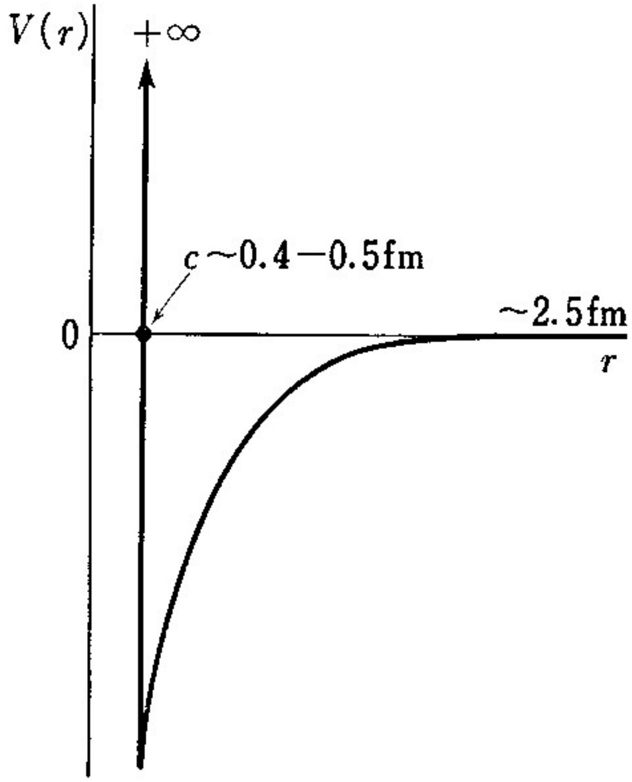




example:



Bare nucleon-nucleon interaction

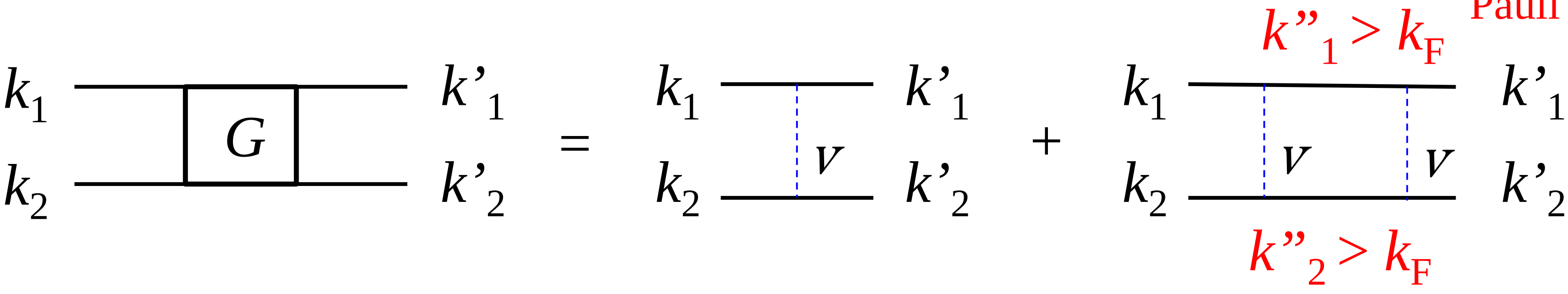


Existence of short range repulsive core

核内における核子間相互作用（媒質効果）

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

Pauli priciple



+.......

Bethe-Goldstone equation

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

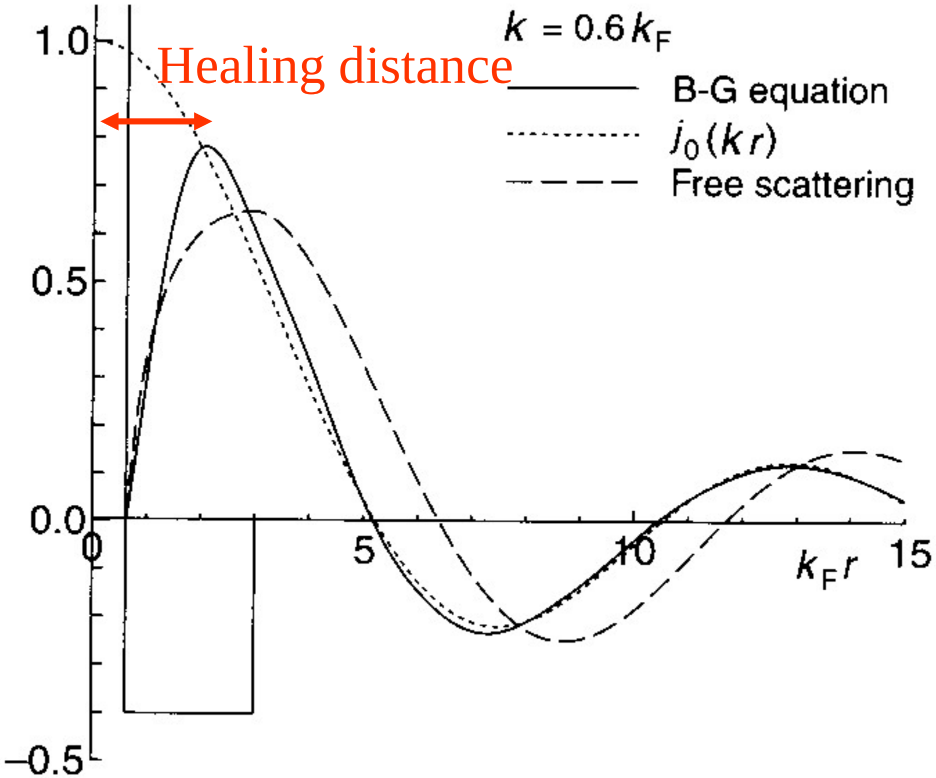
*scattering: suppressed
because intermediate states have to have
$k > k_F$ ⟶ independent particle picture

◆Hard core

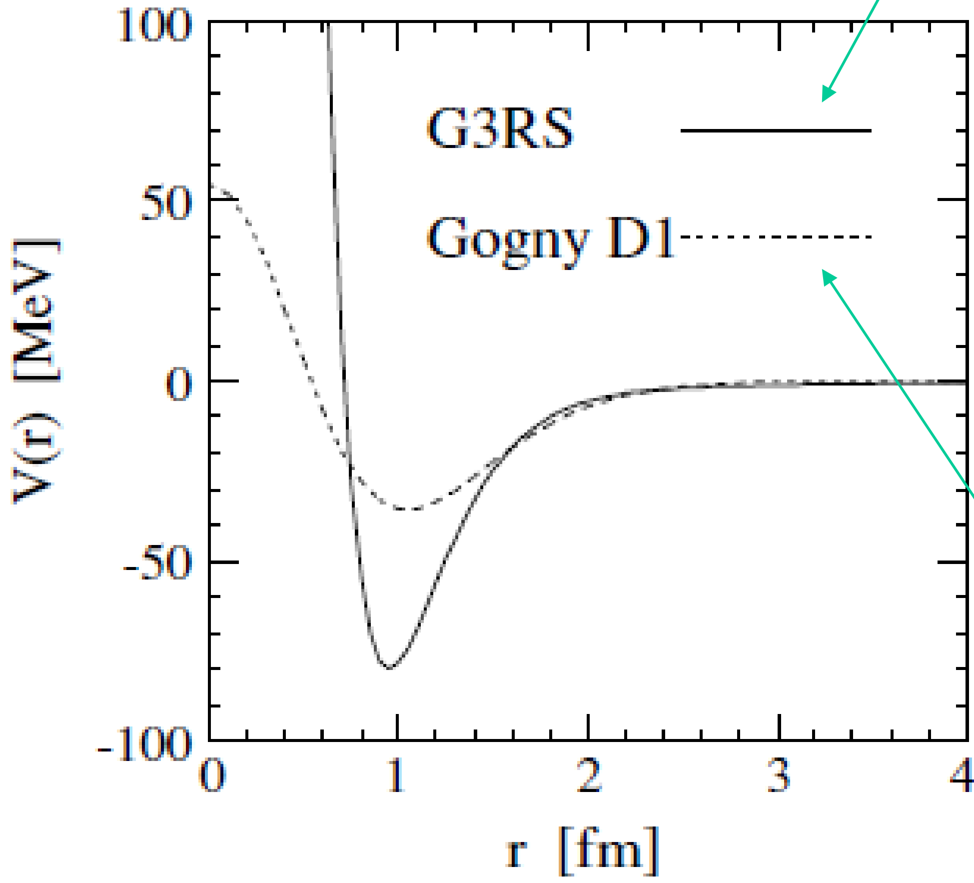
$$G = v + v\frac{Q_F}{E - H_0}G \quad \Longleftrightarrow \quad G = \frac{v}{1 - v\,\frac{Q_F}{E-H_0}}$$

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 $x_i=0$, $t_1=t_2=0$:

$$v(\boldsymbol{r},\boldsymbol{r}') = t_0\delta(\boldsymbol{r}-\boldsymbol{r}') + \frac{1}{6}t_3\delta(\boldsymbol{r}-\boldsymbol{r}')\rho^\alpha(\boldsymbol{r})$$

short-range attraction   repulsion to avoid collapse

$$+iW_0(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot\boldsymbol{k}\times\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{k}$$

spin-orbit interaction

Skyrme interaction density dependent zero-range interaction

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

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

(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 $\longrightarrow$ 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:

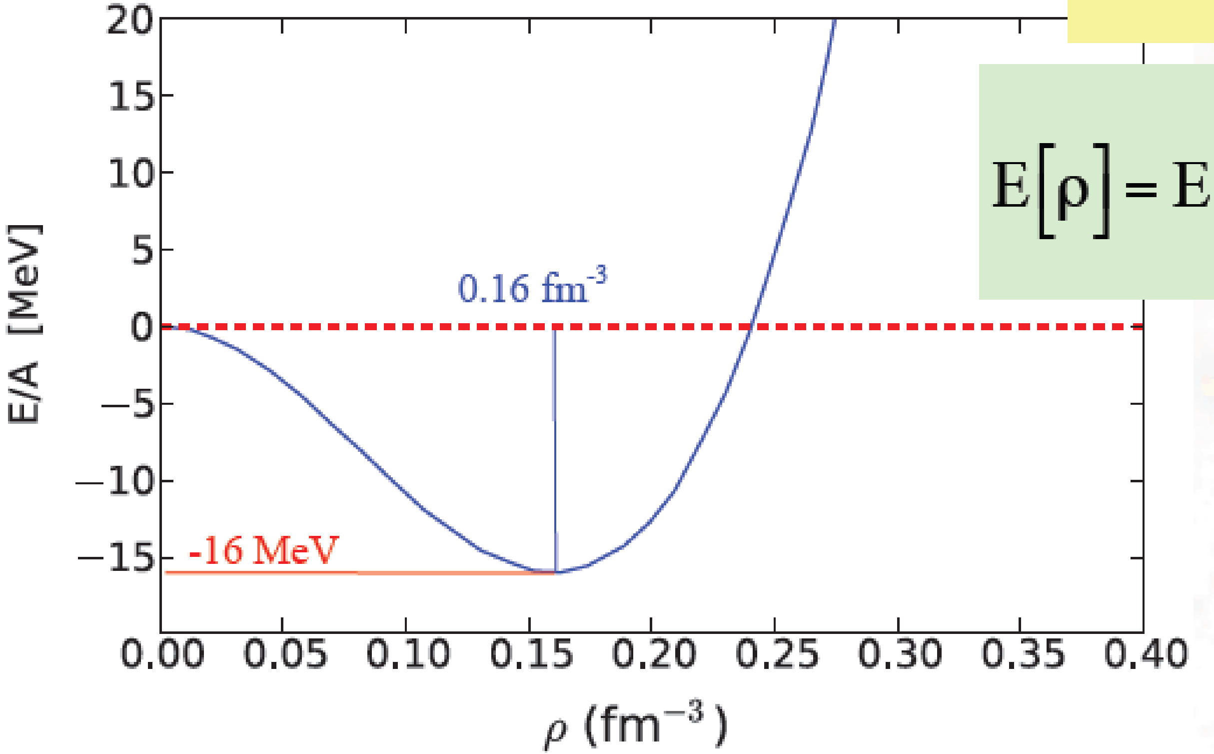
B.E. and r_{rms}: ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{208}Pb,…..

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

Parameter sets:

SIII, SkM*, SGII, SLy4,…….

EOS of infinite nuclear matter



$$K_\infty = 9\rho^2 \left.\frac{d^2\left[E(\rho)/\rho\right]}{d\rho^2}\right|_{\rho_0}$$

$$E[\rho] = E[\rho_0] + \frac{1}{18}K_\infty\left(\frac{\rho-\rho_0}{\rho_0}\right)^2$$

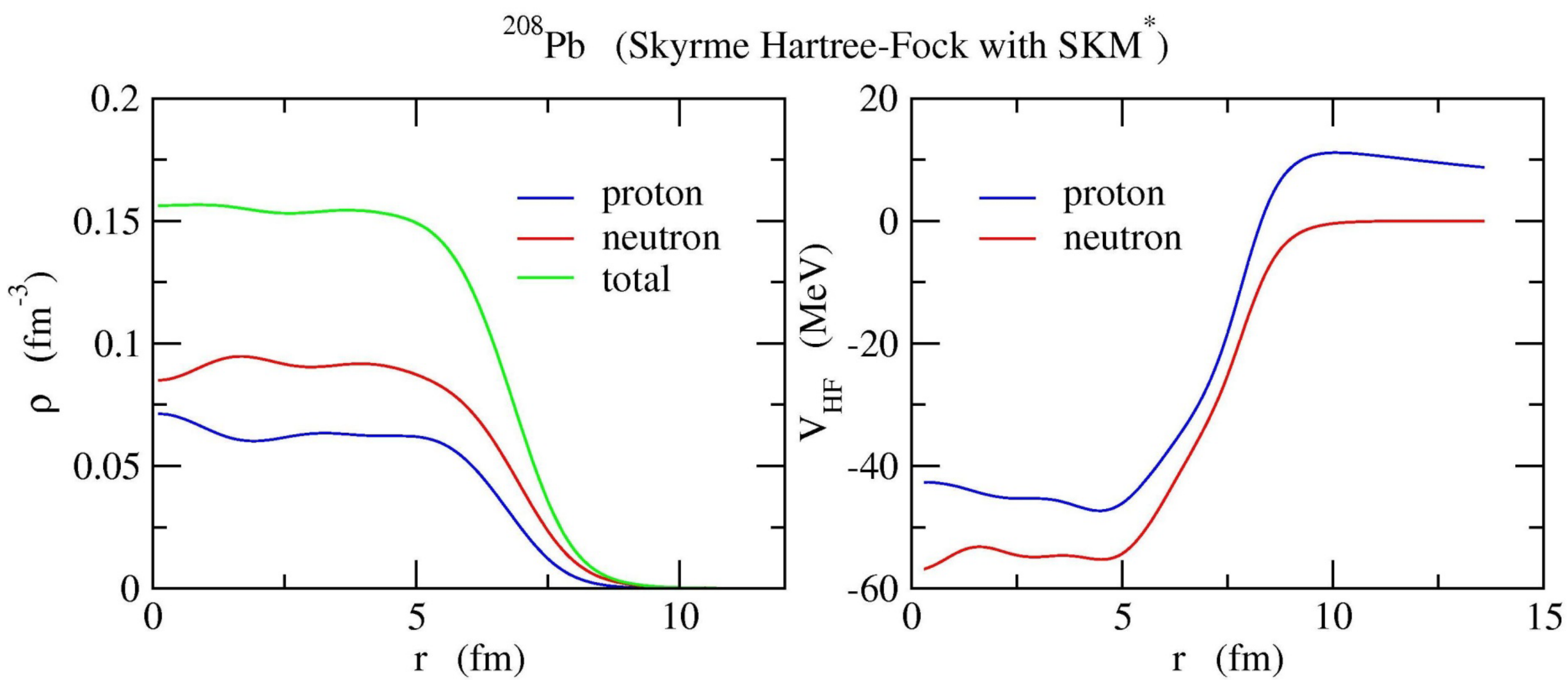
slide: Carlos Bertulani

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

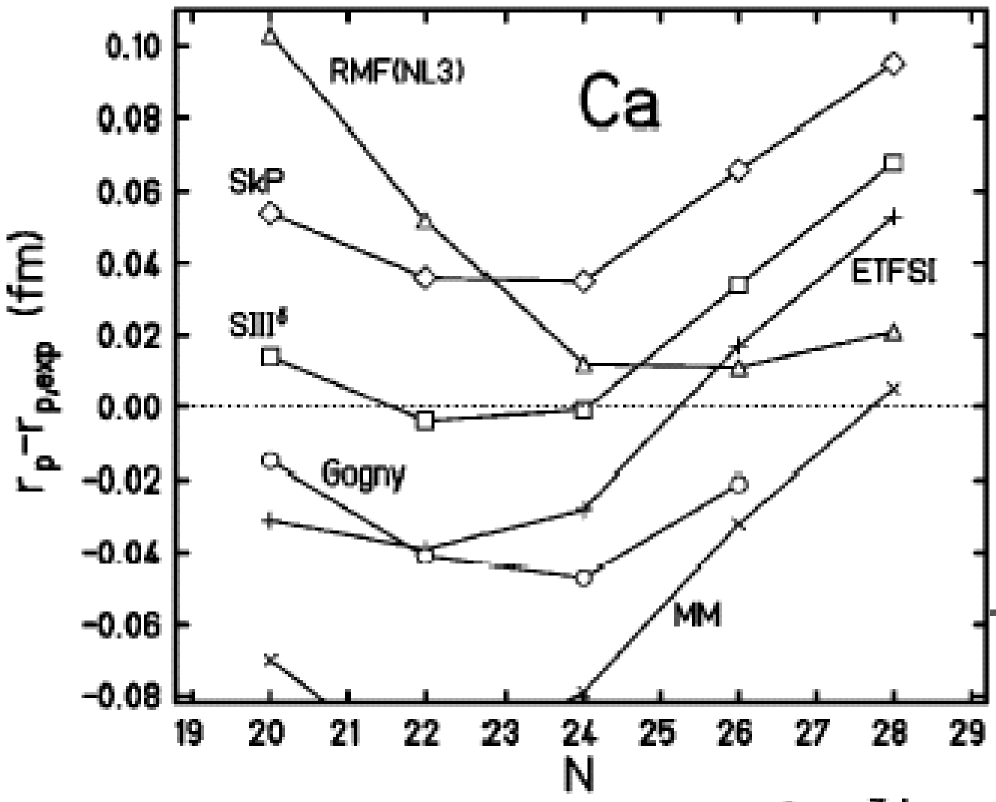
Iteration

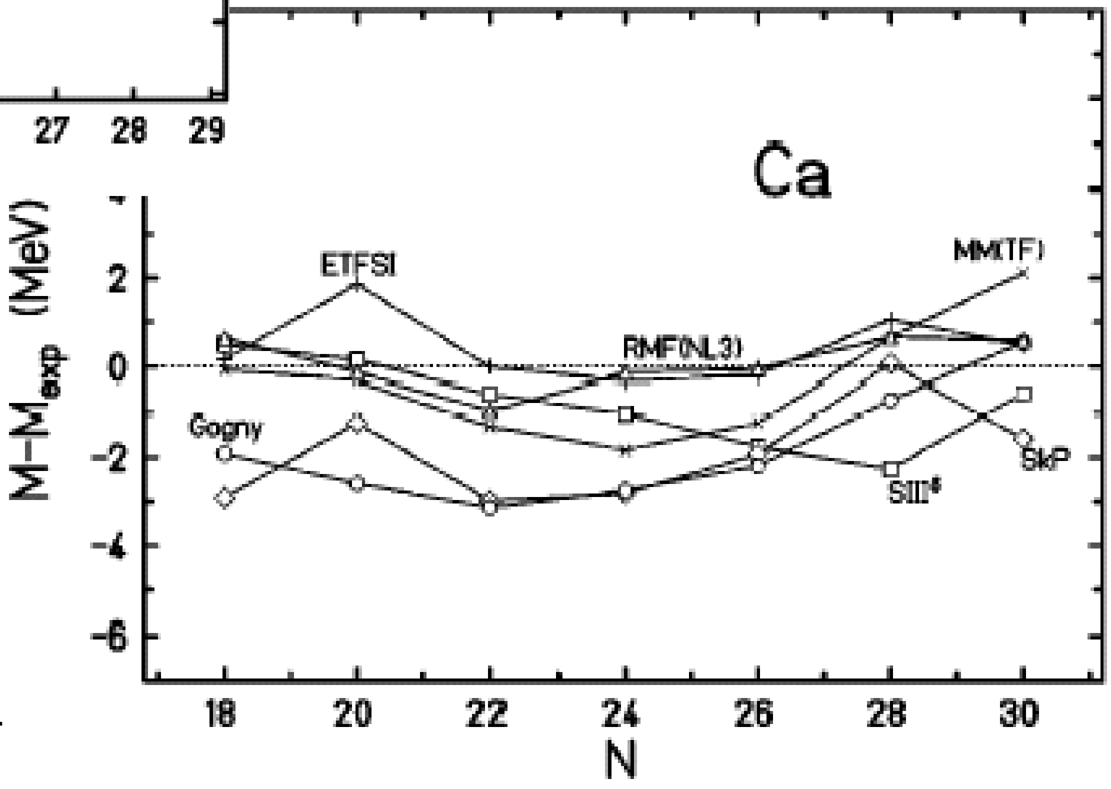
V_{HF}: depends on ψ_i $\longleftarrow$ non-linear problem

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



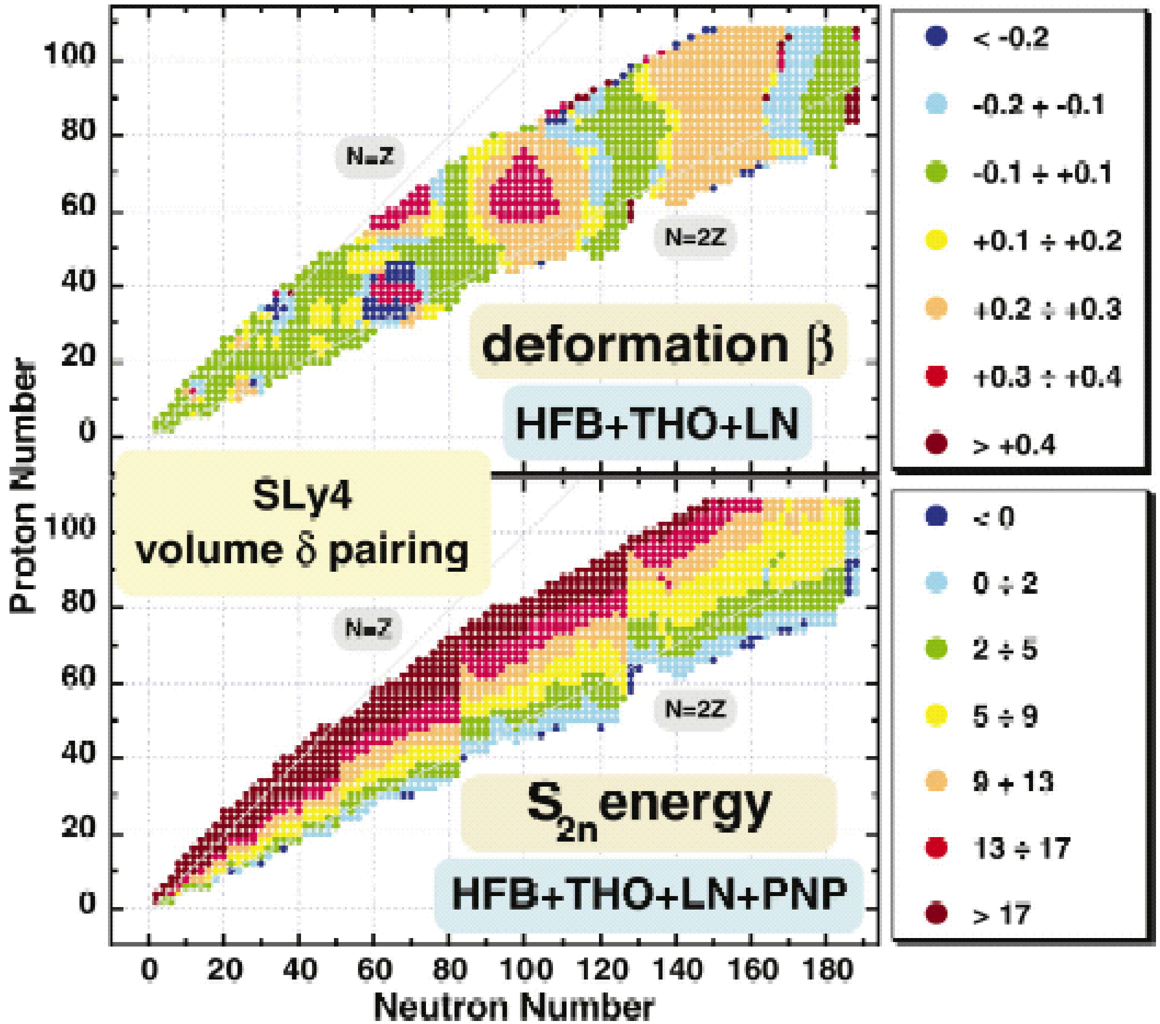
Examples of HF calculations for masses and radii





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

deformation and two-neutron separation energy



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

Density Functional Theory

With Skyrme interaction:

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

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

$H=H_0+V_{ext}$

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

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

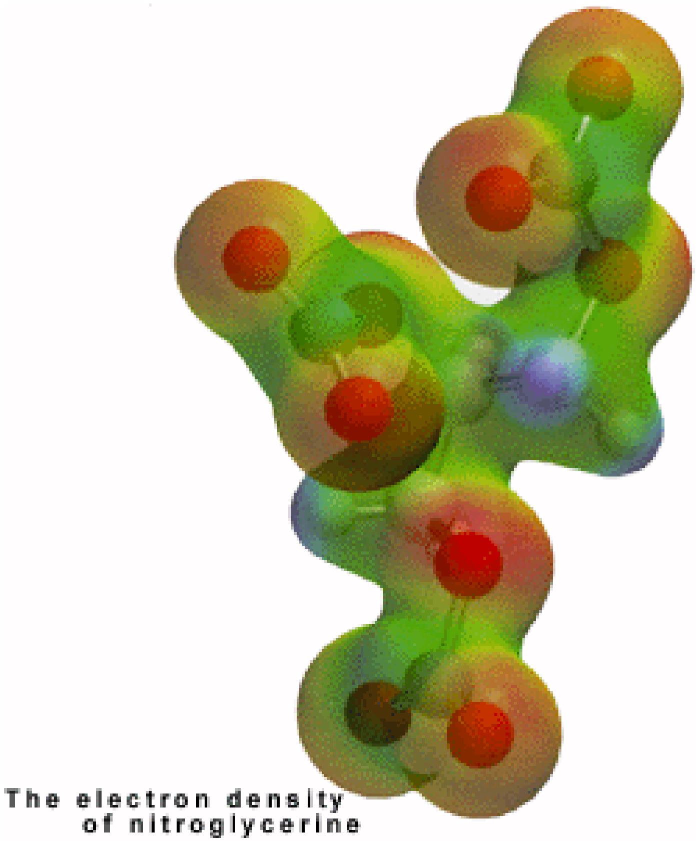
ii) Hohenberg-Kohn variational principle

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

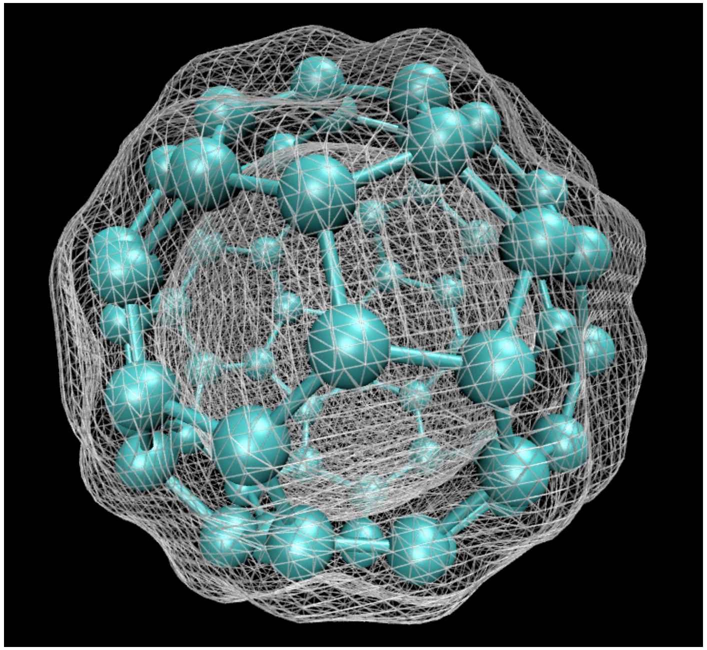
$$\Longrightarrow E[\rho] \geq E_{gs}$$

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。

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

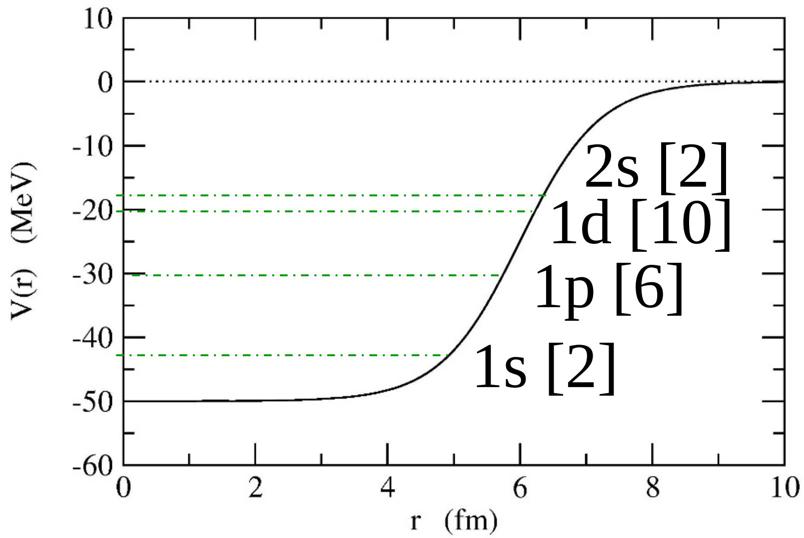


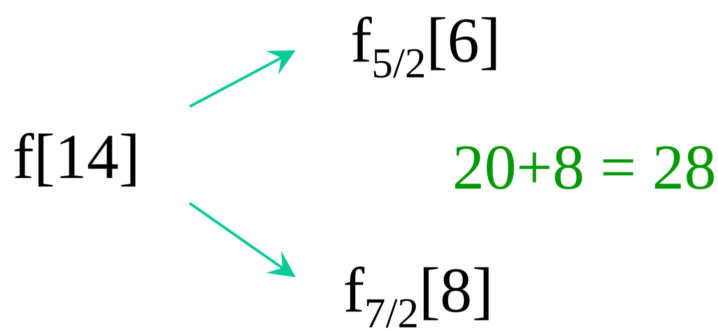
ニトログリセリンの電子密度
（Nobelprize.org より）



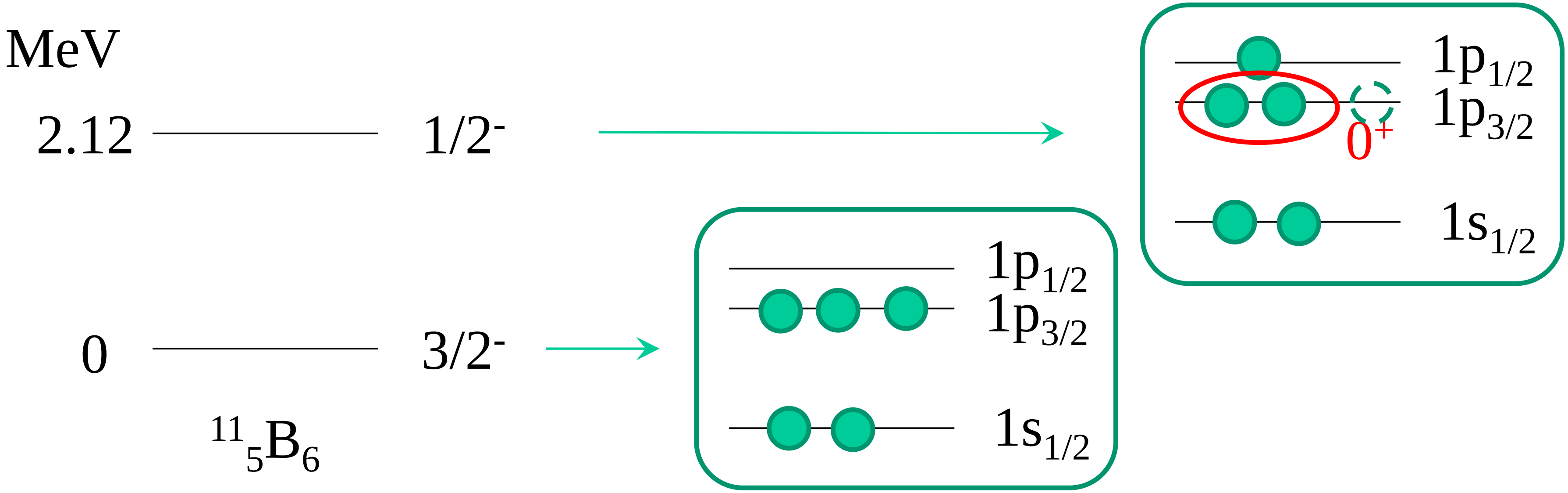
C_{60} の電子密度
（Wikipedia より）

Mean-field approximation and deformation



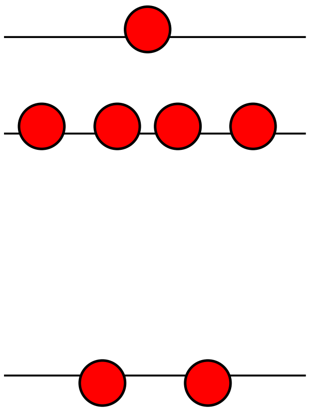


example:



同じように殻模型で$^{11}_{4}\mathrm{Be}_{7}$ のレベルを考えると。。。

殻模型（球形ポテンシャルの準位）で考えた場合：

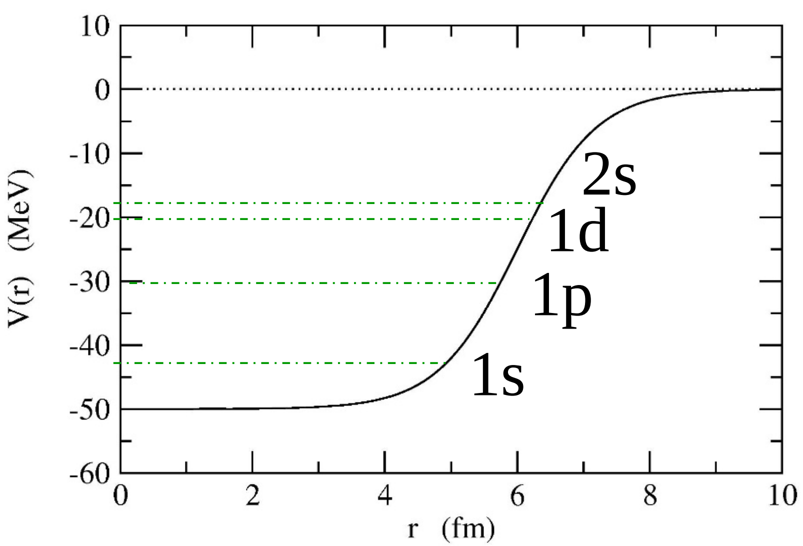


$1p_{1/2}$ [2]

$1p_{3/2}$ [4]

$1s_{1/2}$ [2]

→ ^{11}Be の基底状態は $I^{\pi} = 1/2^{-}$



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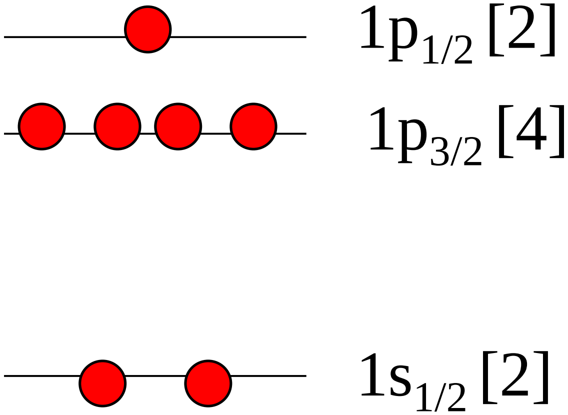
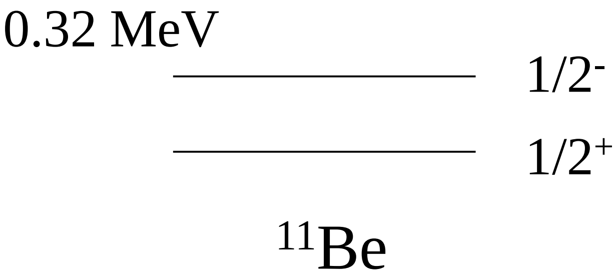


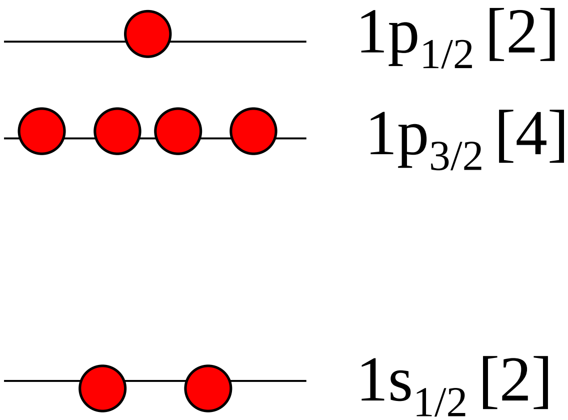
→ ^{11}Be の基底状態は $I^{\pi} = 1/2^{-}$

実際の ^{11}Be の準位を見てみると:



同じように殻模型で$^{11}_{4}Be_7$ のレベルを考えると。。。

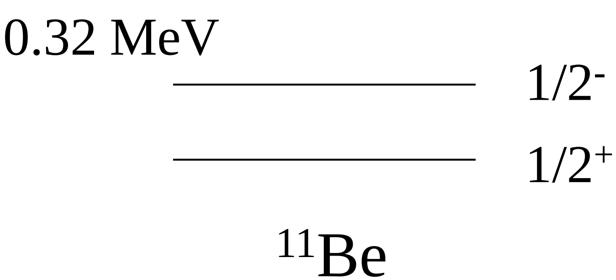
殻模型(球形ポテンシャルの準位)で考えた場合:



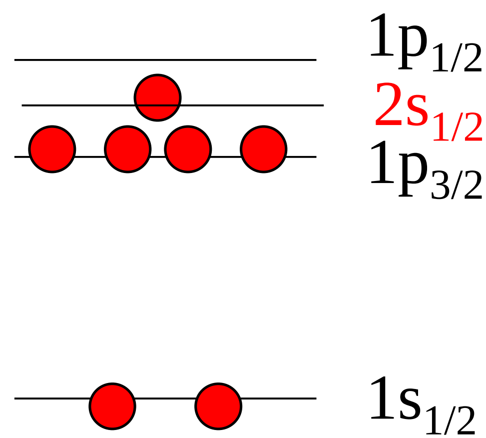
^{11}Be の基底状態は $I^{\pi} = 1/2^{-}$

かなり無理

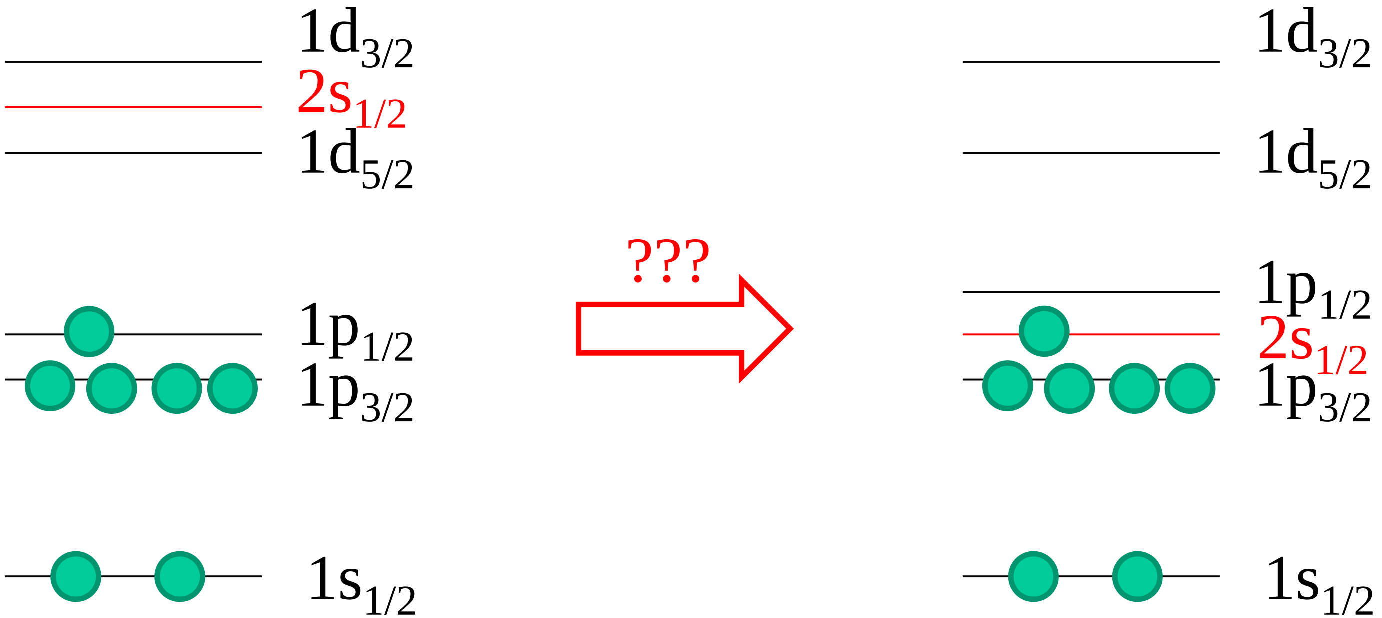
実際の ^{11}Be の準位を見てみると:



?



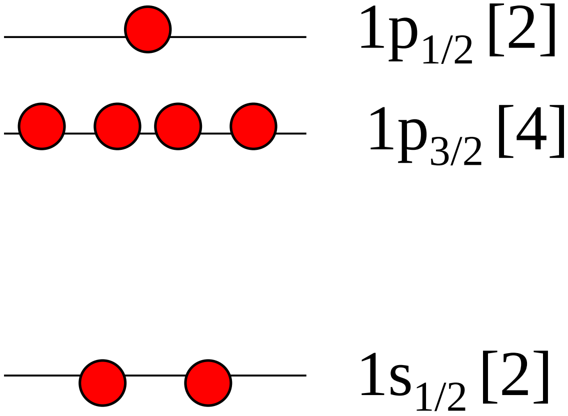
"parity inversion"



1d3/2
2s1/2
1d5/2
1p1/2
1p3/2
1s1/2
???
1d3/2
1d5/2
1p1/2
2s1/2
1p3/2
1s1/2

同じように殻模型で$^{11}_{4}\mathrm{Be}_7$ のレベルを考えると。。。

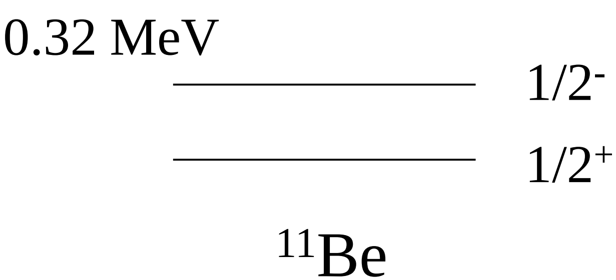
殻模型(球形ポテンシャルの準位)で考えた場合:



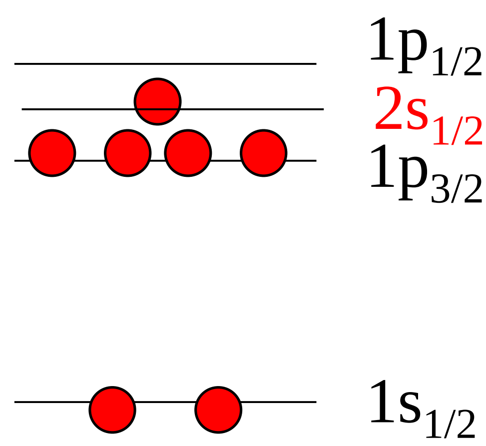
^{11}Be の基底状態は $I^{\pi} = 1/2^{-}$

かなり無理

実際の ^{11}Be の準位を見てみると:



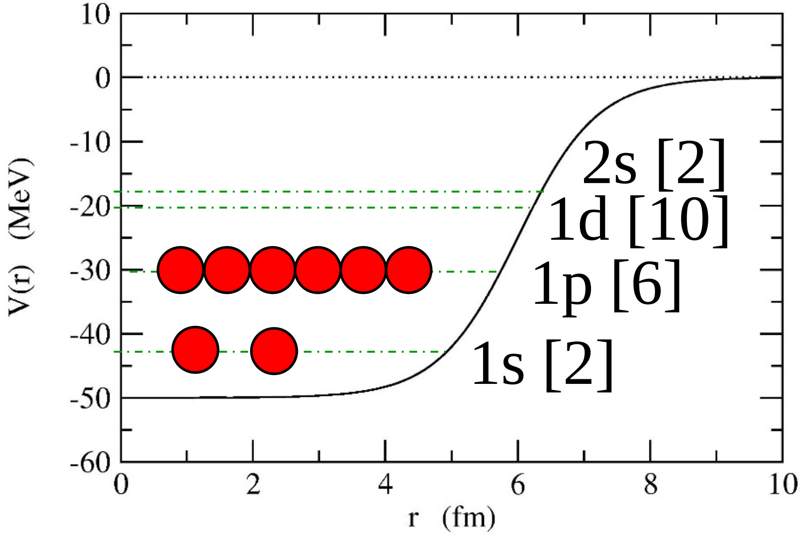
?



球形ポテンシャルに無理があるなら、変形させてみる?

Mean-field approximation and deformation

Mean-field approximation



$$H \sim \sum_i \left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{\mathrm{MF}}(\boldsymbol{r}_i) \right)$$

Slater determinant

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

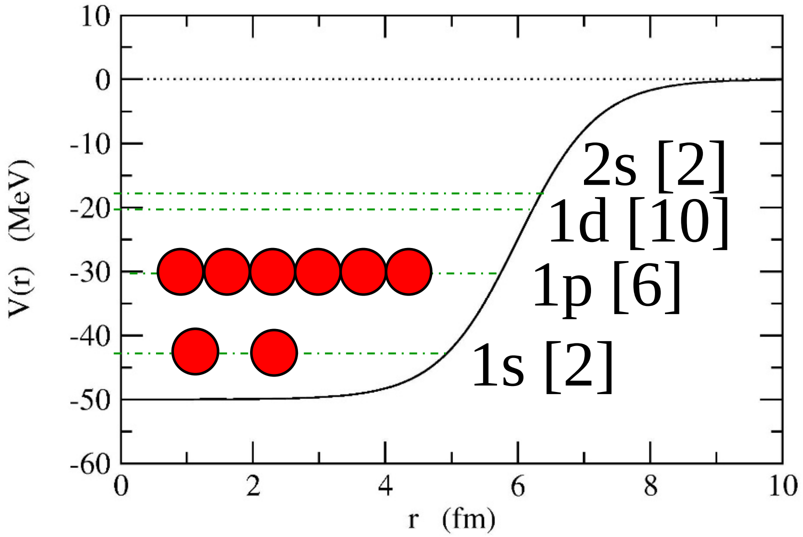
$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{MF}}(\boldsymbol{r}) \right) \psi_k(\boldsymbol{r}) = \epsilon_k \psi_k(\boldsymbol{r})$$

the original many-body *H*:

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

Mean-field approximation and deformation

Mean-field approximation



$$H \sim \sum_i \left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{\rm MF}(\boldsymbol{r}_i) \right)$$

Slater determinant

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

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\rm MF}(\boldsymbol{r}) \right)\psi_k(\boldsymbol{r}) = \epsilon_k\psi_k(\boldsymbol{r})$$

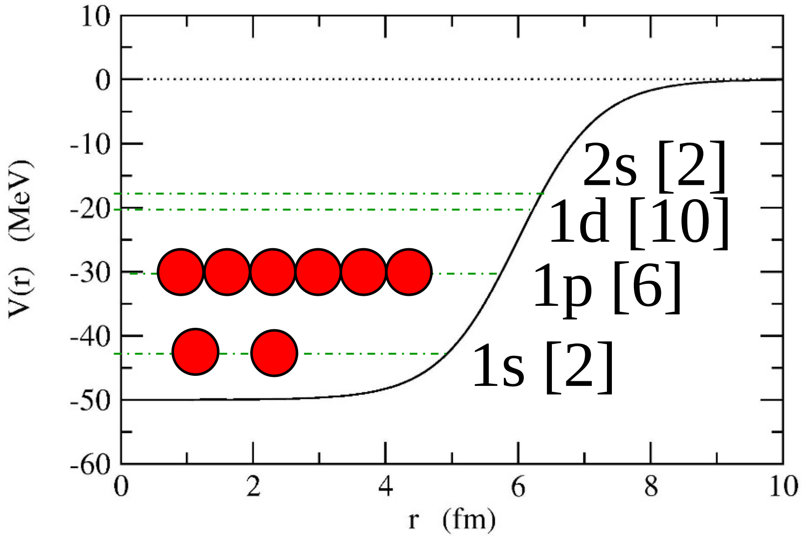
the original many-body *H*:

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

$$= \sum_{i=1}^{A} \left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_i^2 + V_{\rm MF}(\boldsymbol{r}_i) \right) + \frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i, \boldsymbol{r}_j) - \sum_i V_{\rm MF}(\boldsymbol{r}_i)$$

Mean-field approximation and deformation

Mean-field approximation



$$H \sim \sum_i \left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{\mathrm{MF}}(\boldsymbol{r}_i)\right)$$

Slater determinant

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

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\mathrm{MF}}(\boldsymbol{r})\right)\psi_k(\boldsymbol{r}) = \epsilon_k\psi_k(\boldsymbol{r})$$

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

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

"Symmetry-broken solution"
"Spontaneous Symmetry Broken"

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

Typical Examples

- Translational symmetry: always broken in nuclear systems

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

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

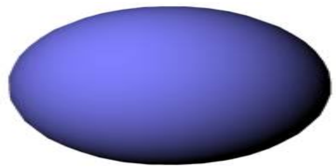
Typical Examples

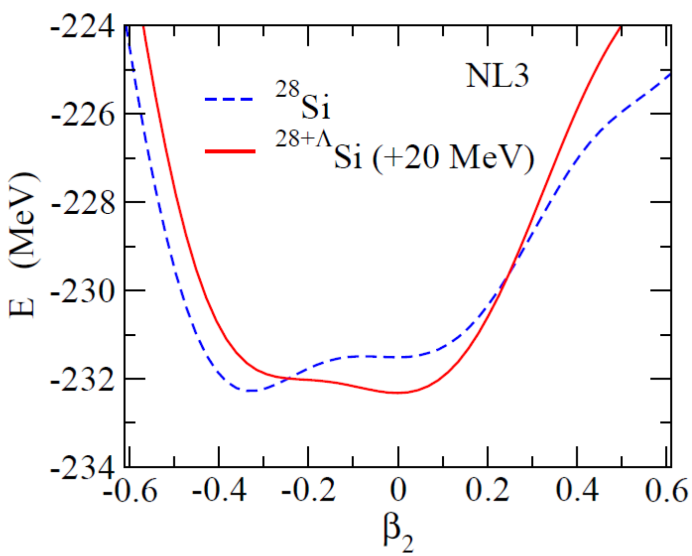
➤Translational symmetry: always broken in nuclear systems

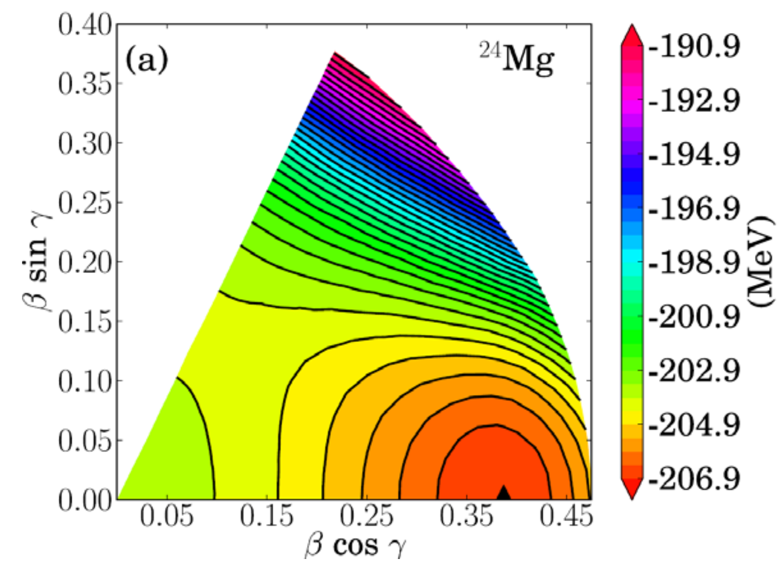
$$H = -\sum_{i=1}^{A}\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i - \boldsymbol{r}_j) \to \sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{\rm MF}(\boldsymbol{r}_i)\right)$$

➤Rotational symmetry

Deformed solution

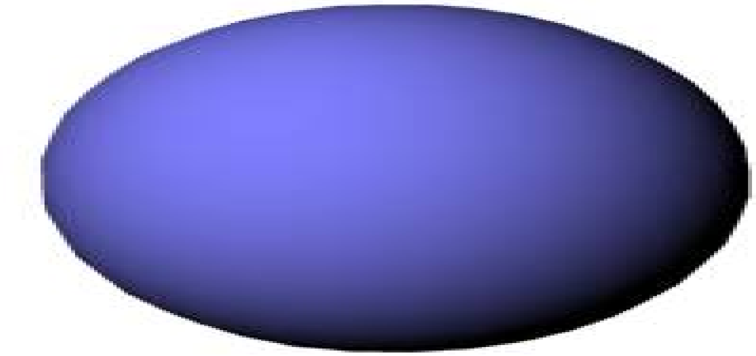






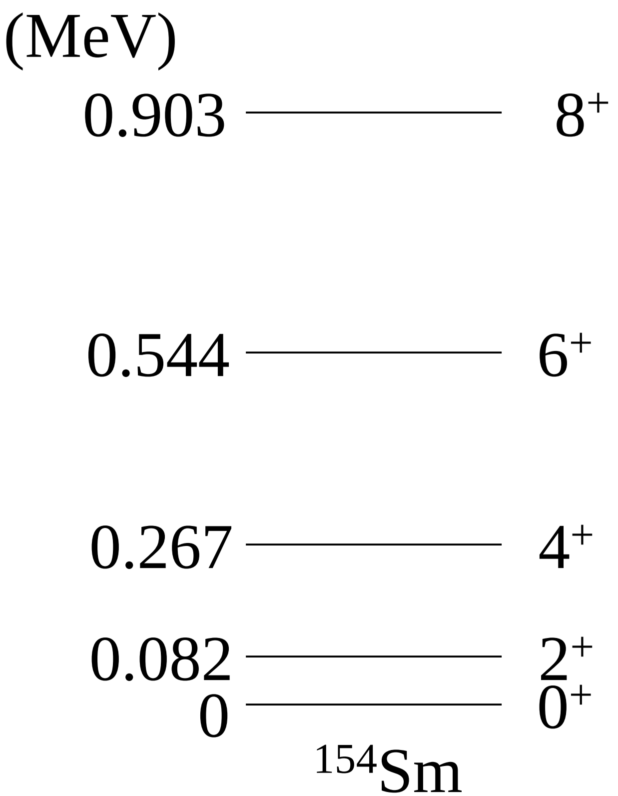
Nuclear Deformation

実験的な証拠

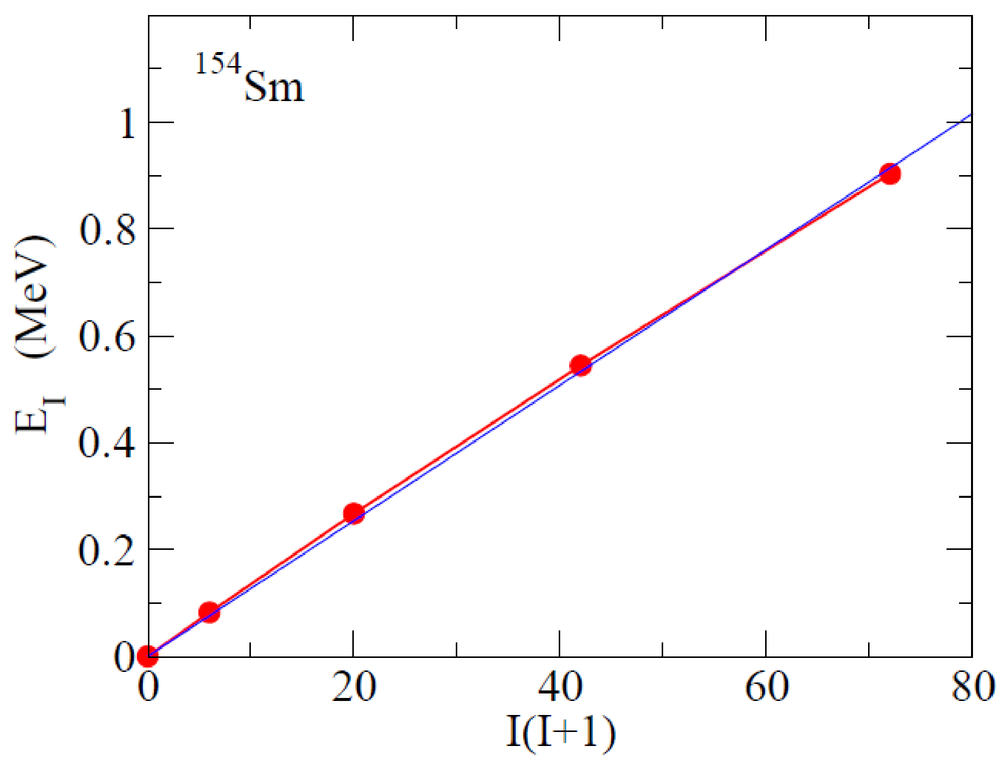


Nuclear Deformation

Excitation spectra of ^{154}Sm



$$E_I \sim \frac{I(I+1)\hbar^2}{2\mathcal{J}}$$



Nuclear Deformation

Excitation spectra of ^{154}Sm

(MeV)

0.903	8^+
0.544	6^+
0.267	4^+
0.082	2^+
0	0^+

^{154}Sm

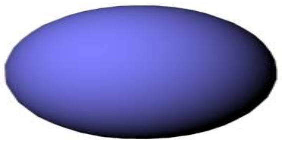
$$E_I \sim \frac{I(I+1)\hbar^2}{2\mathcal{J}}$$

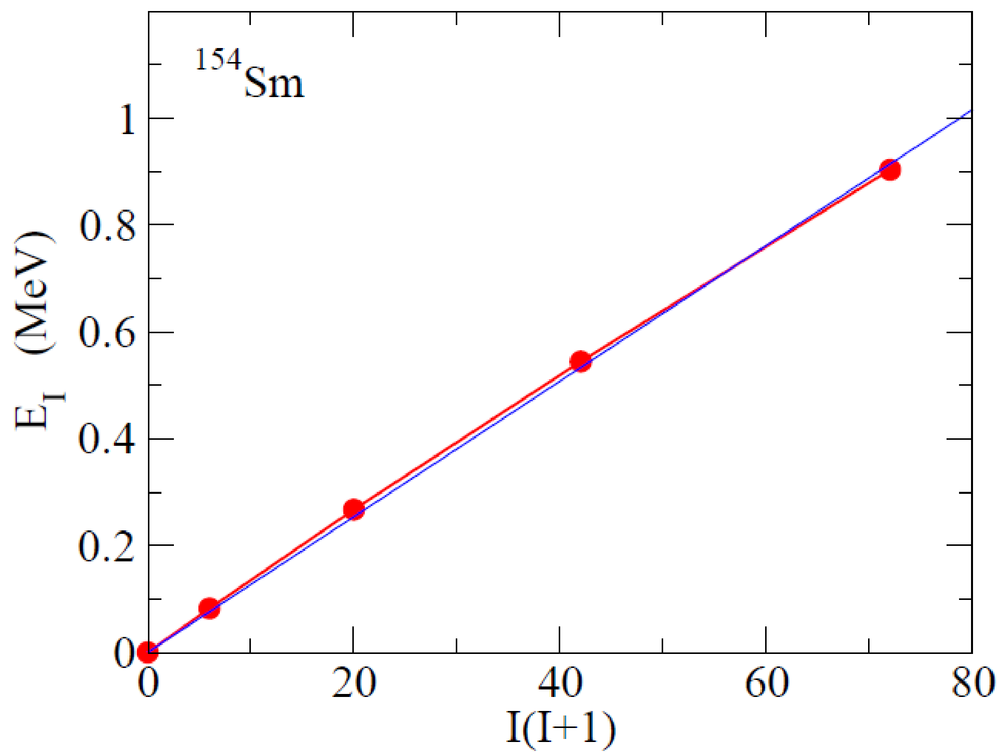
cf. Rotational energy of a rigid body (Classical mechanics)

$$E = \frac{1}{2}\mathcal{J}\omega^2 = \frac{I^2}{2\mathcal{J}}$$

$$(I = \mathcal{J}\omega, \ \omega = \dot{\theta})$$

^{154}Sm is deformed





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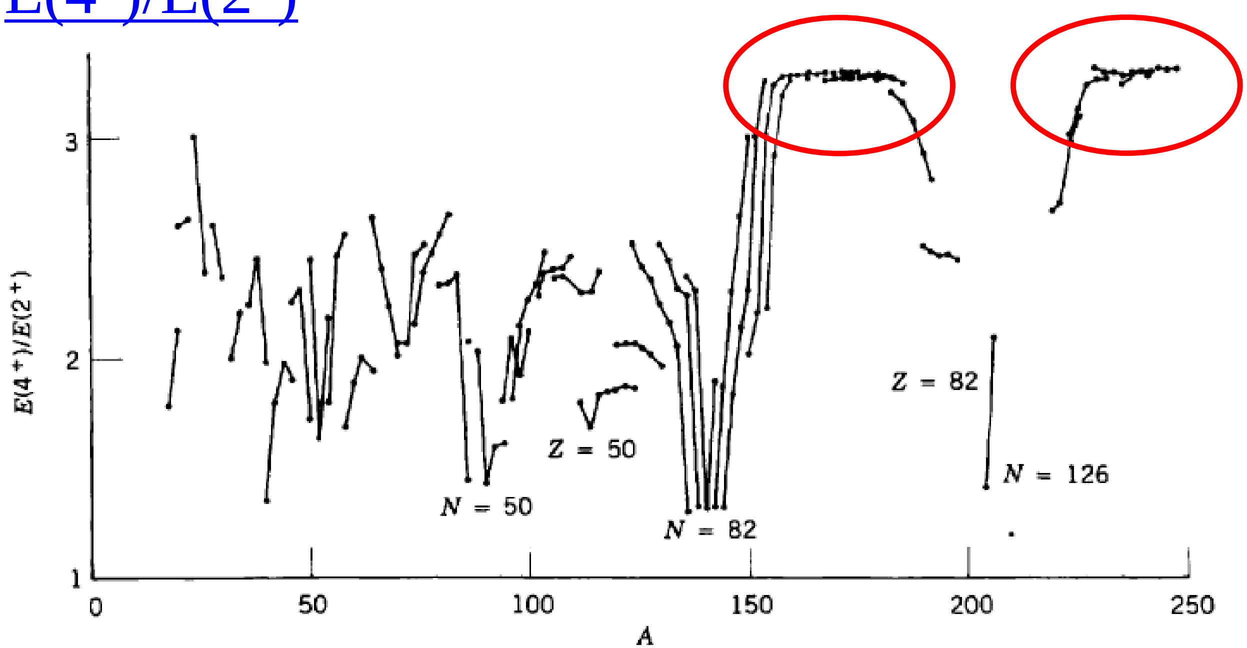
$$\Longrightarrow E_2 \propto 2 \times 3 = 6, \quad E_4 \propto 4 \times 5 = 20$$

$$\Longrightarrow E_4/E_2 = 20/6 = 3.3333\cdots$$

E(4⁺)/E(2⁺)

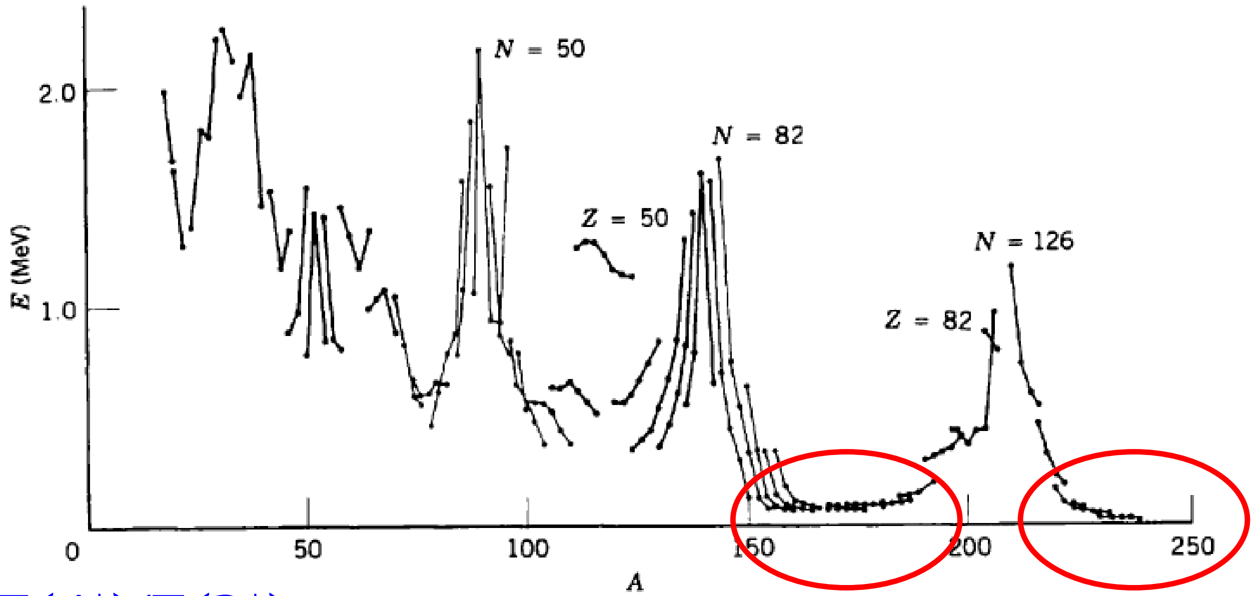


deformed nuclei:
$E(4^+)/E(2^+) \sim 3.3$

spherical nuclei:
$E(4^+)/E(2^+) \sim 2$

K.S. Krane, "Introductory Nuclear Physics"

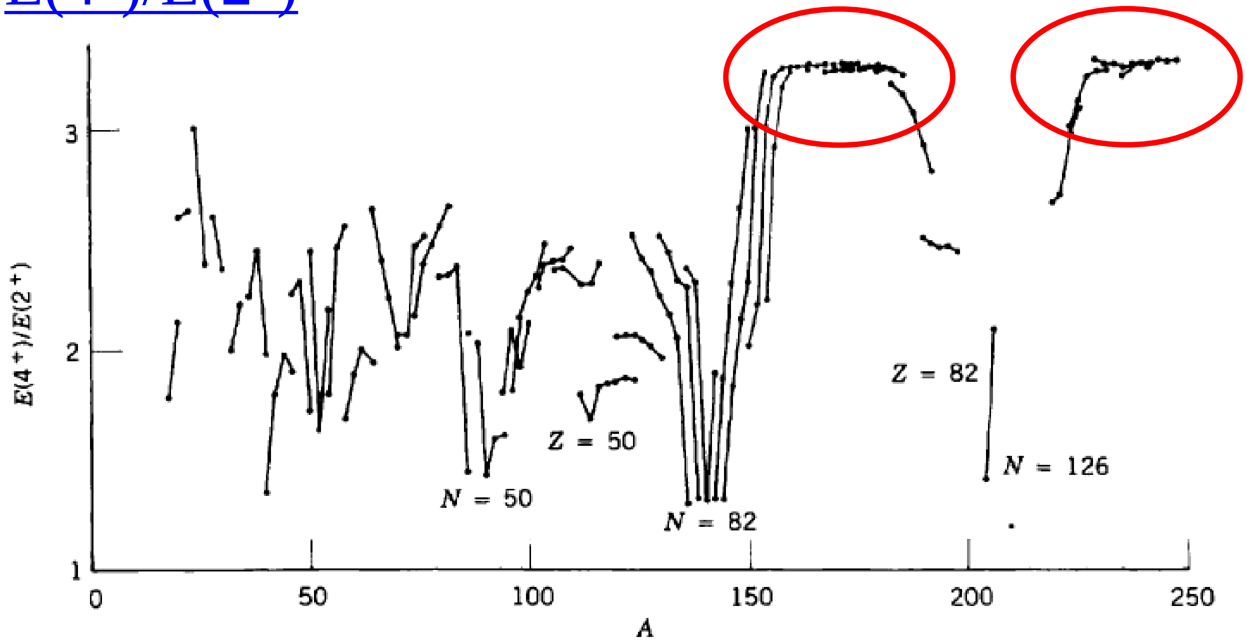
The energy of the first 2^+ state in even-even nuclei



a small energy
→ spontaneously
symm. breaking

deformed nuclei

$E(4^+)/E(2^+)$



deformed nuclei:
$E(4^+)/E(2^+) \sim 3.3$

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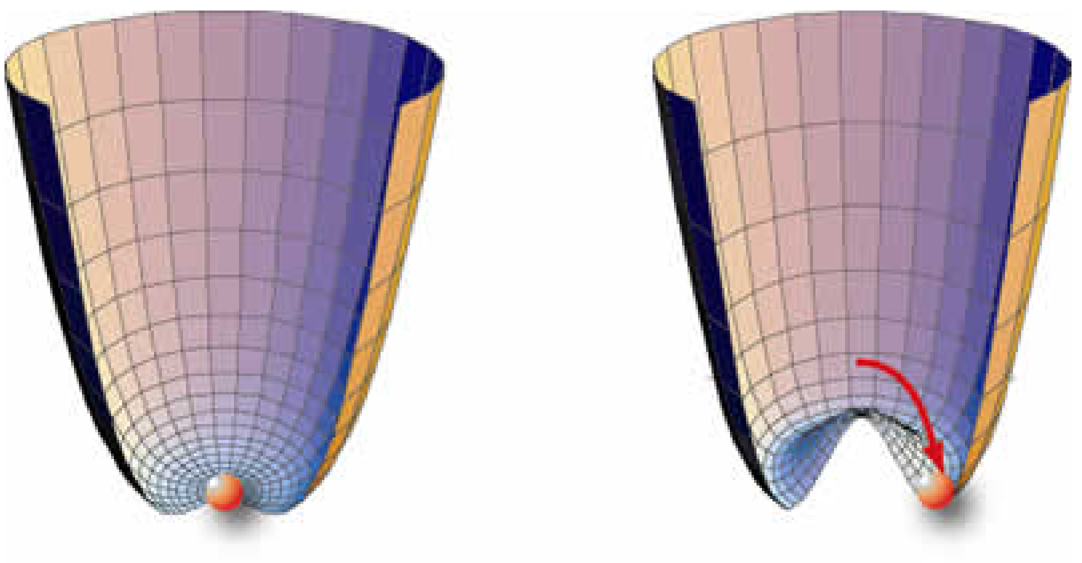
Spontaneous symmetry breaking

The vacuum state does not have (i.e, the vacuum state violates) the symmetry which the Hamiltonian has.



Nambu-Goldstone mode (zero energy mode) to restore the symmetry