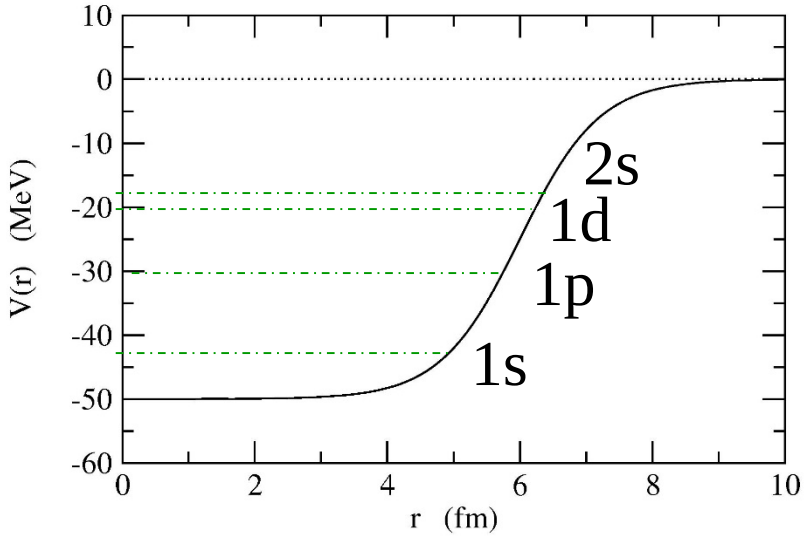
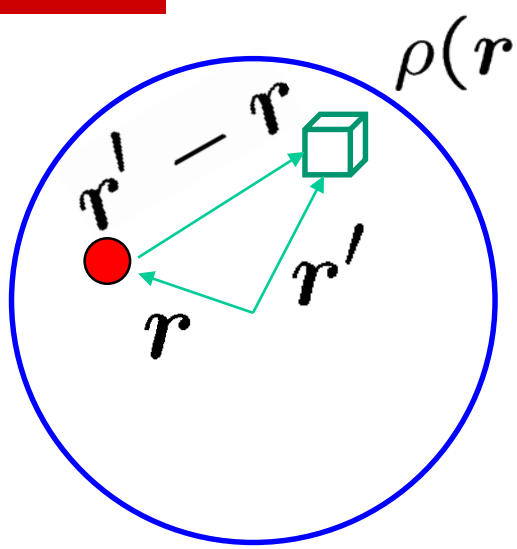
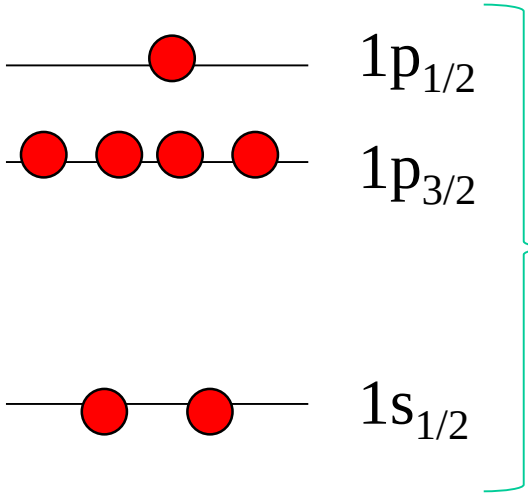
Mean-field (Hartree-Fock) Theory







shell model

naively speaking,

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

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

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

the potential depends on the solutions

→ self-consistent solutions

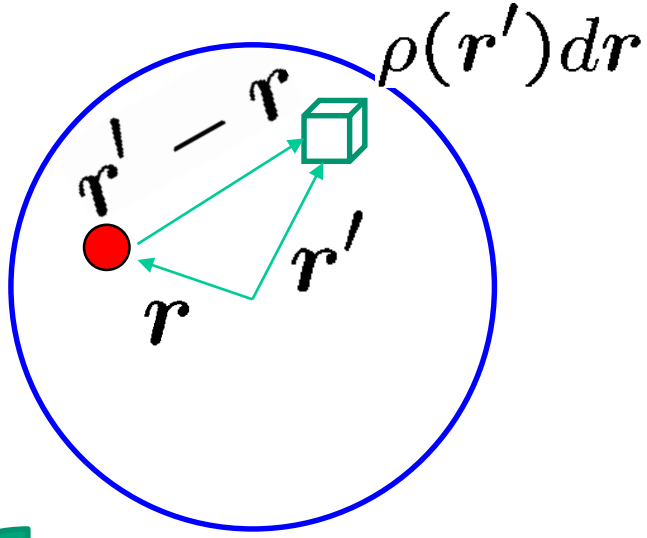
Iteration: $\{\psi_i\} \to \rho \to V \to \{\psi_i\} \to \cdots$

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

"self-consistent mean-field theory"

* 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
* 変形した方がエネルギーが下がるのであれば変形させる

反対称化



$$V(r) \sim \int v(r,r')\rho(r')dr'$$

同種粒子間の相互作用
→反対称化が必要

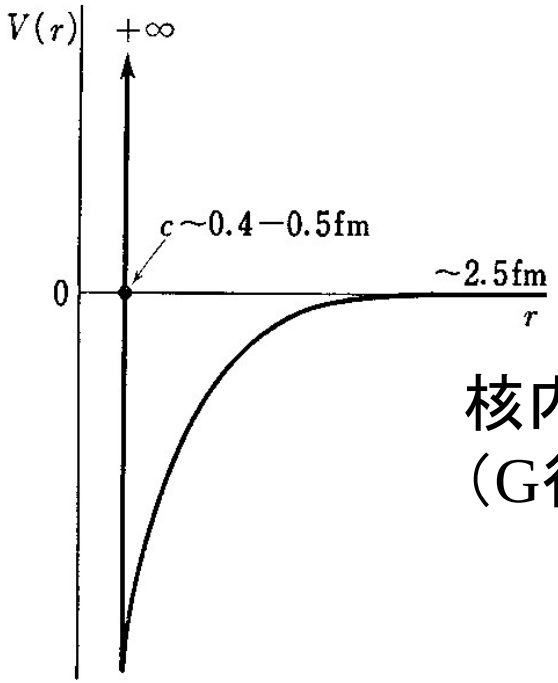
$$0 = \left[-\frac{\hbar^2}{2m}\nabla^2 + \int v(r,r')\left(\sum_j |\psi_j(r')|^2\right)dr' - \epsilon_i\right]\psi_i(r)$$

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

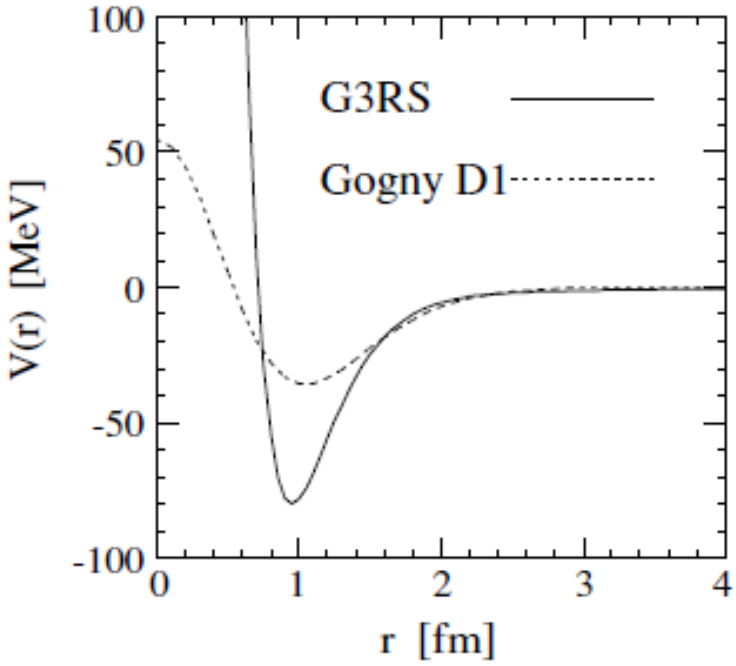
$$-\int v(r,r')\left(\sum_j \psi_j^*(r')\psi_i(r')\right)dr'\psi_j(r)$$

exchange term

有効相互作用



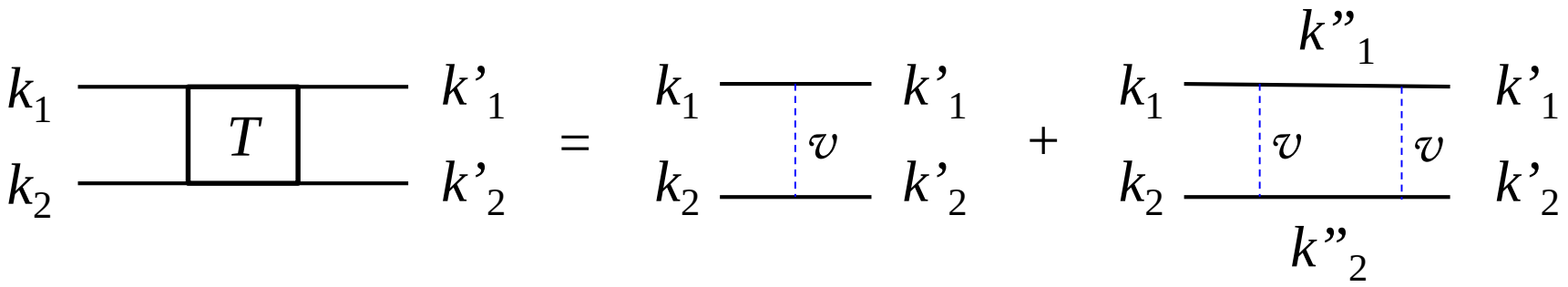
核内での多重散乱
（G行列）



Existence of short range
repulsive core

核媒質中での相互作用
（有効相互作用）

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



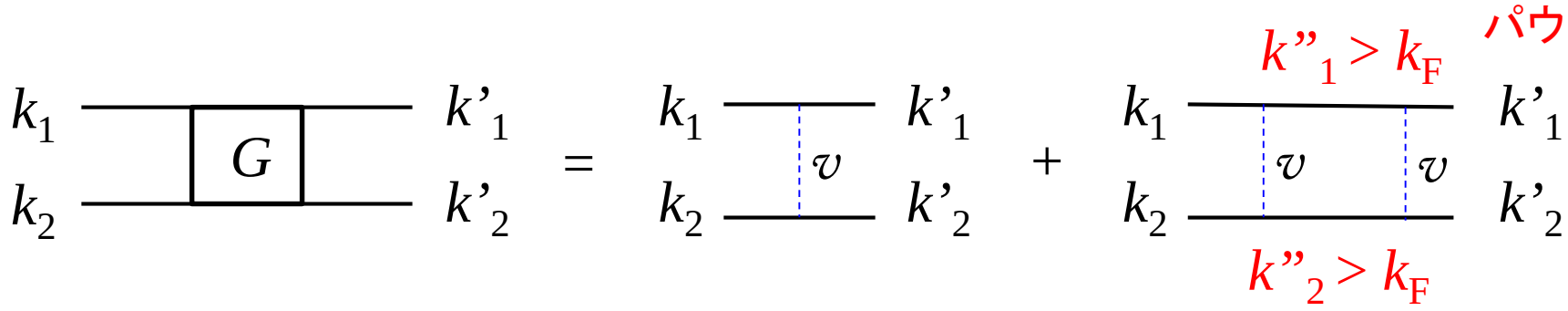
+…….

Lippmann-Schwinger equation

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

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

パウリ原理



+…….

*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

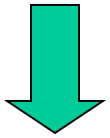
Bethe-Goldstone equation

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

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 ⟺ 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

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

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} ,….

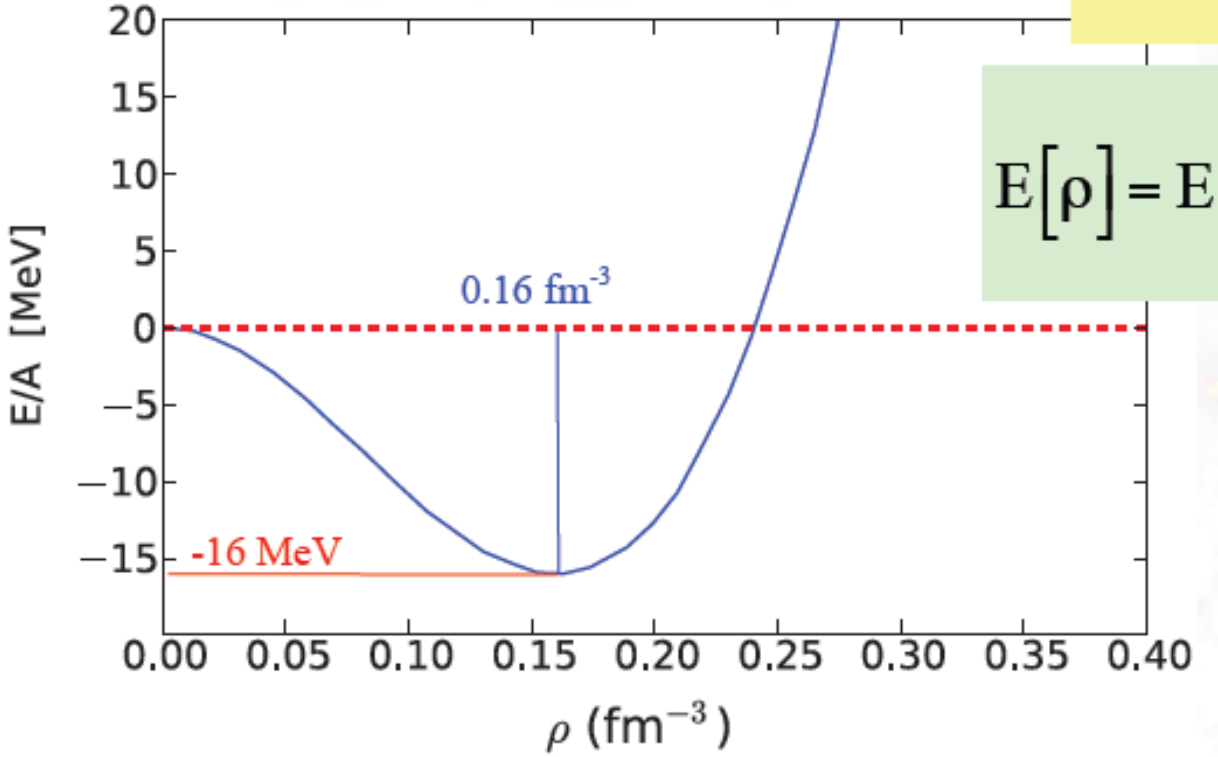
Parameter sets:

SIII, SkM*, SGII, SLy4,…….

EOS of infinite nuclear matter

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

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



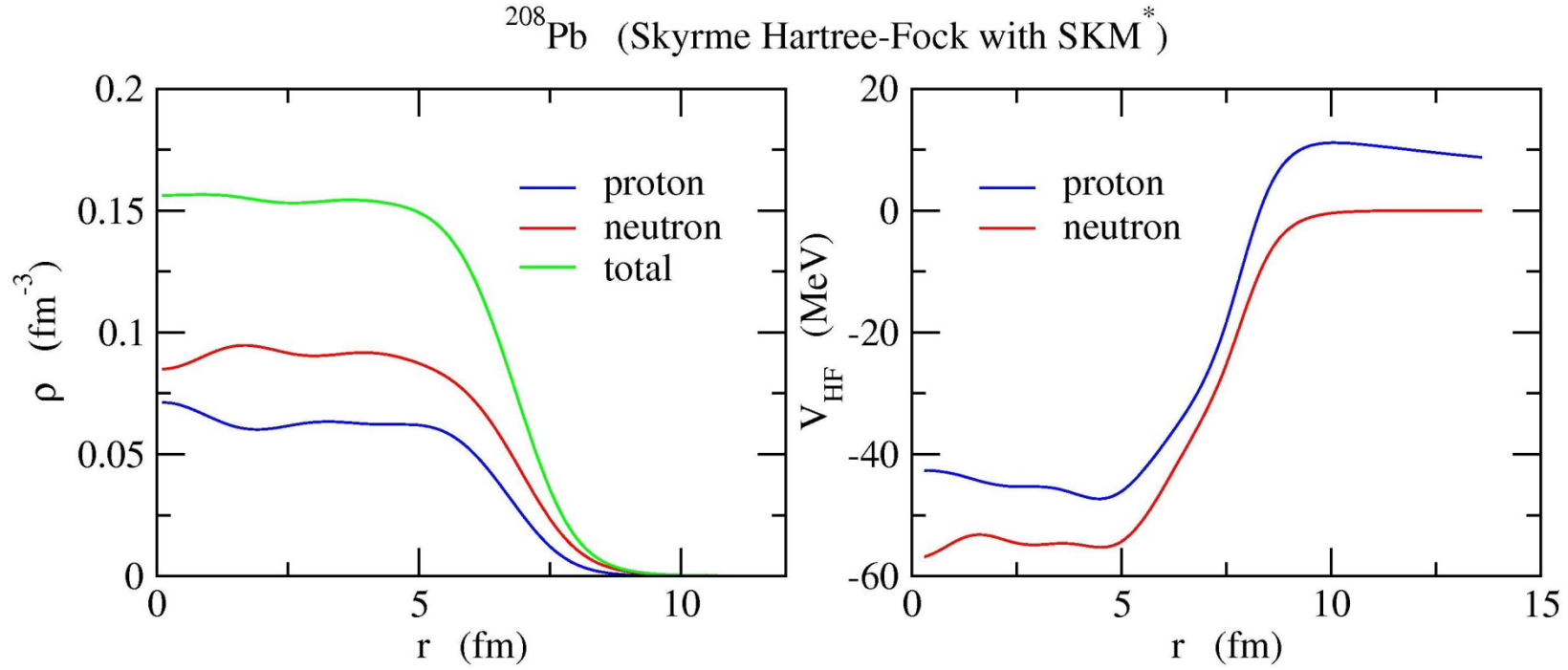
slide: Carlos Bertulani

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

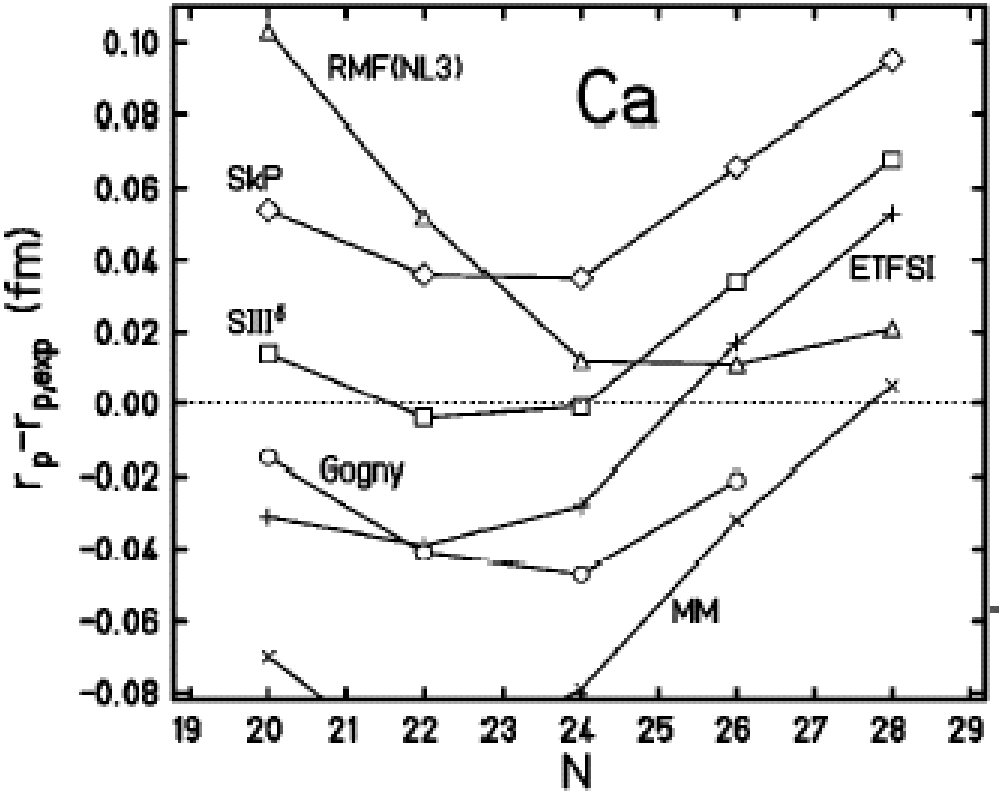
Iteration

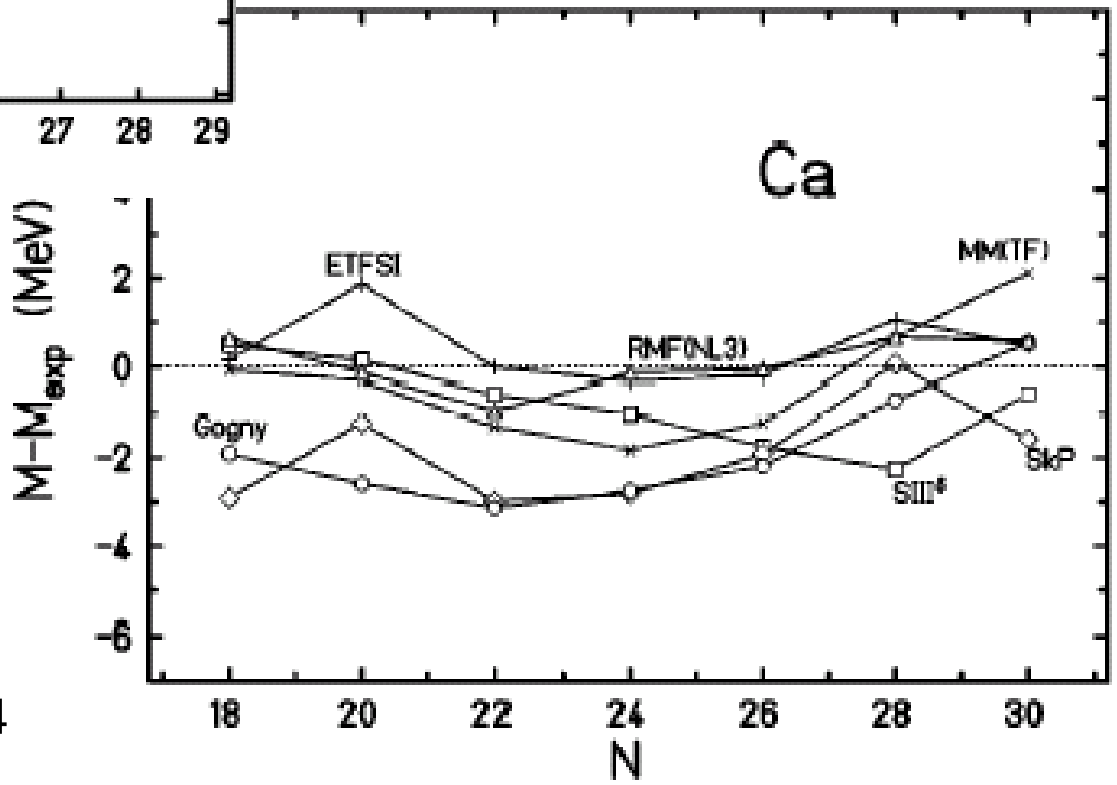
V_{HF}: depends on ψ_i ⟵ non-linear problem

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



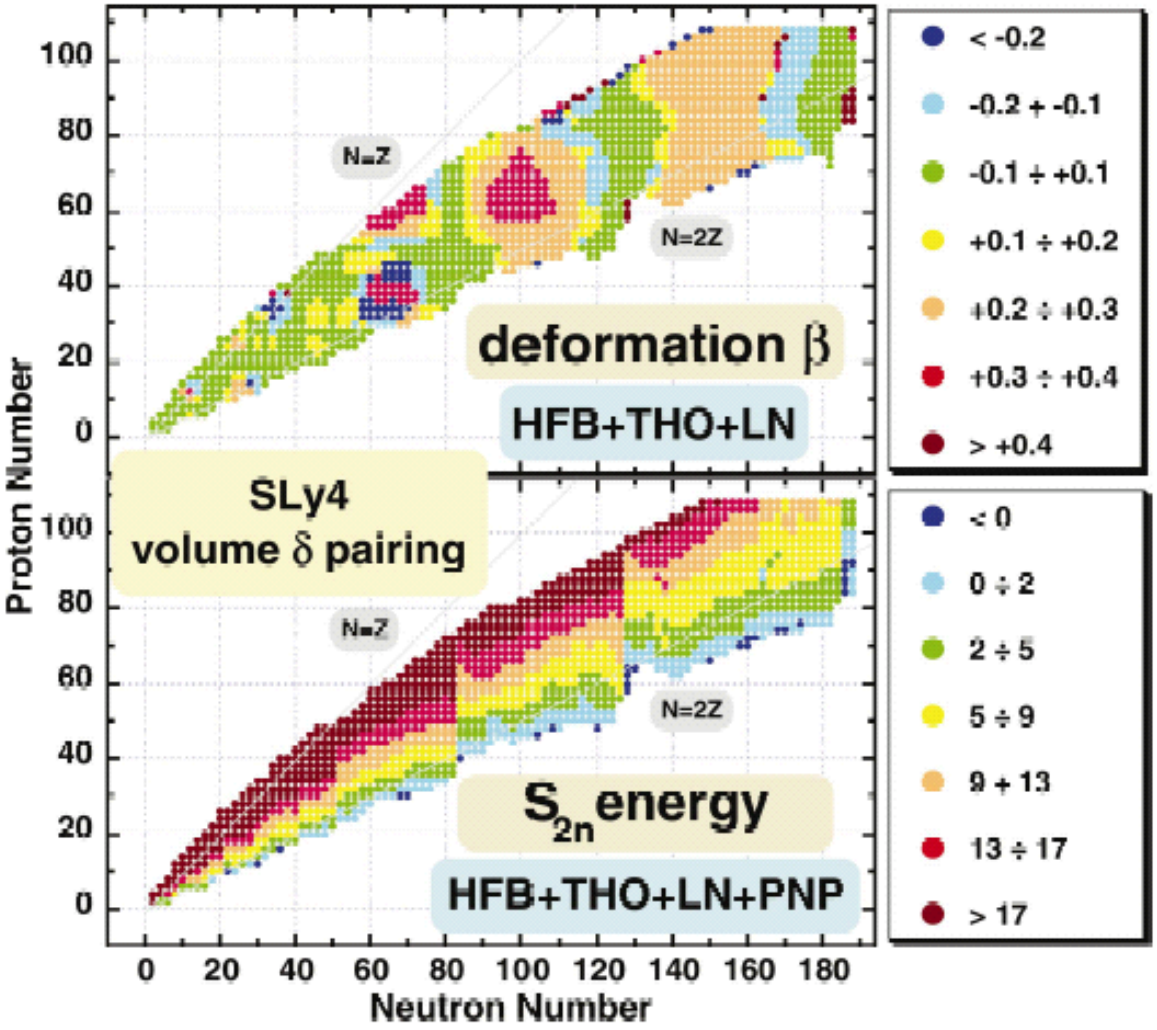
Examples of HF calculations for masses and radii





Z. Patyk et al.,
PRC59(’99)704

deformation and two-neutron separation energy



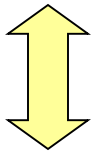
M.V. Stoitsov et al., PRC68(’03)054312

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

$H=H_0+V_{ext}$

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

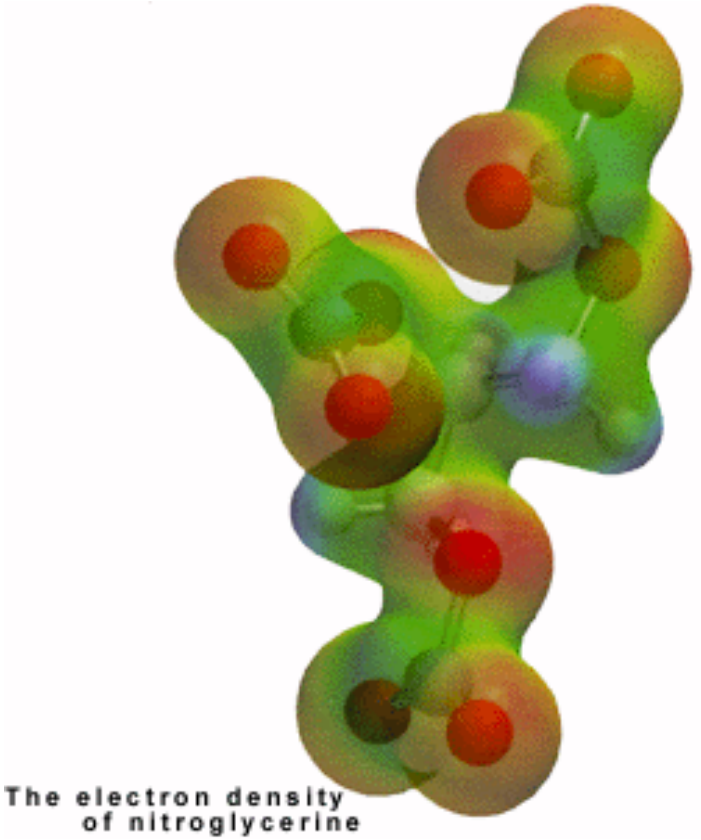
Density: the basic variable
（密度が分かれば原理的に全て分かる）

ii) Hohenberg-Kohn variational principle

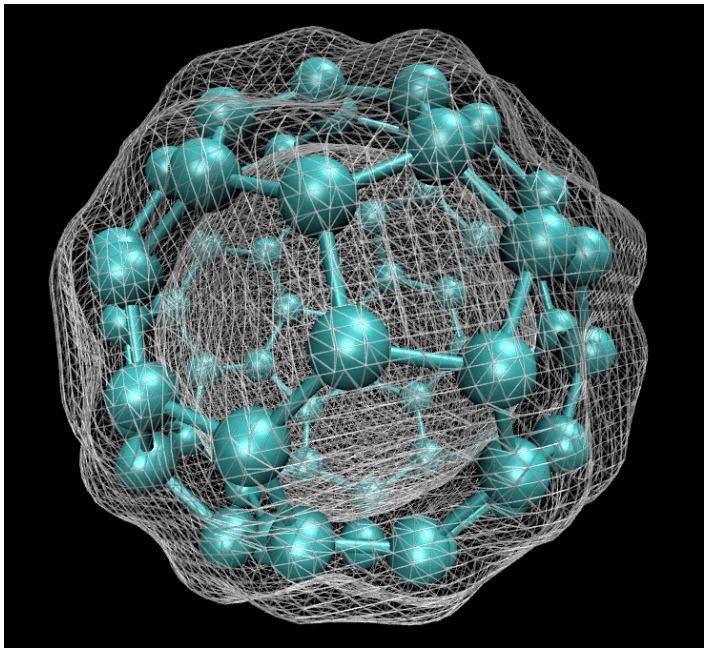
The existence of a functioal $E[\rho]$, which gives the exact g.s. energy for a given g.s. density

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

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。



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）

（参考）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)

$$
\begin{aligned}
E_1 &= \langle \Psi_1 | H_1 | \Psi_1 \rangle \\
&= \int V_1(\boldsymbol{r}) \rho(\boldsymbol{r}) d\boldsymbol{r} + \langle \Psi_1 | T + U | \Psi_1 \rangle \\
E_2 &= \langle \Psi_2 | H_2 | \Psi_2 \rangle \\
&= \int V_2(\boldsymbol{r}) \rho(\boldsymbol{r}) d\boldsymbol{r} + \langle \Psi_2 | T + U | \Psi_2 \rangle
\end{aligned}
$$

(note)

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

$$
\xrightarrow{?} E_1 + E_2 < E_1 + E_2
$$

（参考）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

Hartree-Fock 近似と対称性の自発的破れ

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

the potential depends on the solutions

→ 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.

* 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
* 変形した方がエネルギーが下がるのであれば変形させる

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

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

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_{HF}, but not of H

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

"Symmetry-broken solution"

"Spontaneous Symmetry Broken"

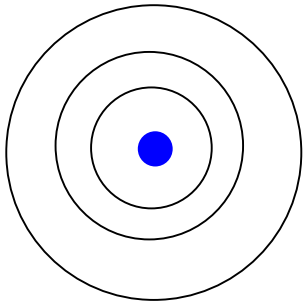
Ψ_{HF} : does not necessarily possess the symmetries that H has.

Typical Example

- Translational symmetry: always broken in nuclear systems

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

(cf.) atoms



nucleus in the center

⟶ translational symmetry: broken from the begining

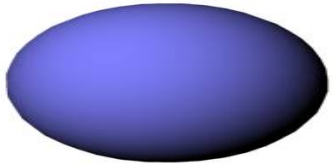
Symmetry Breaking

Advantage: a large part of many-body correlation can be taken into account without losing the independent particle picture

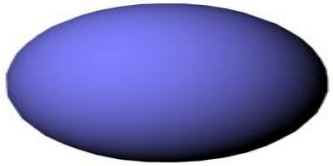
Disadvantage: a need to restore the symmetry (in principle) to compute experimental observables ⟶ projection method

- Rotational symmetry

Deformed solution



➢ Rotational symmetry



Deformed solution

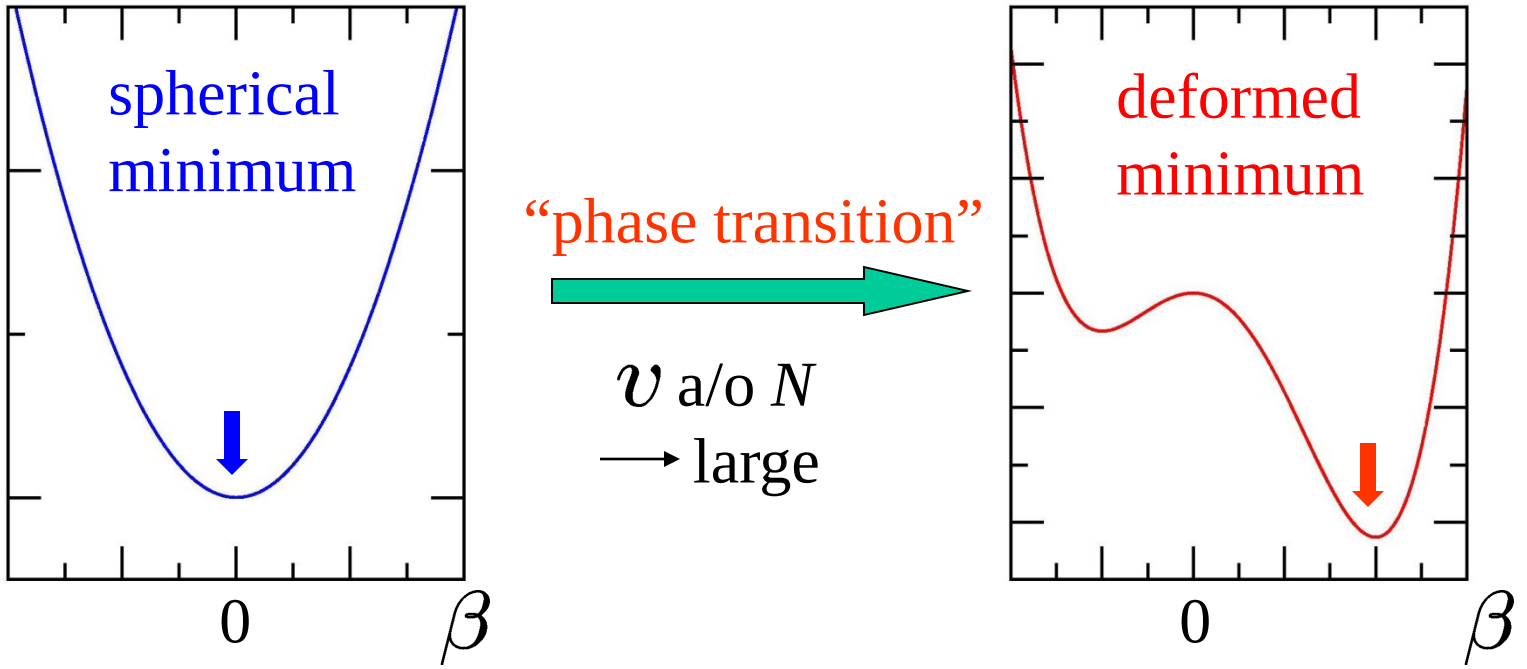
Constrained Hartree-Fock method

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

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

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

$\langle \Psi_{\mathrm{CHF}} | H | \Psi_{\mathrm{CHF}} \rangle$



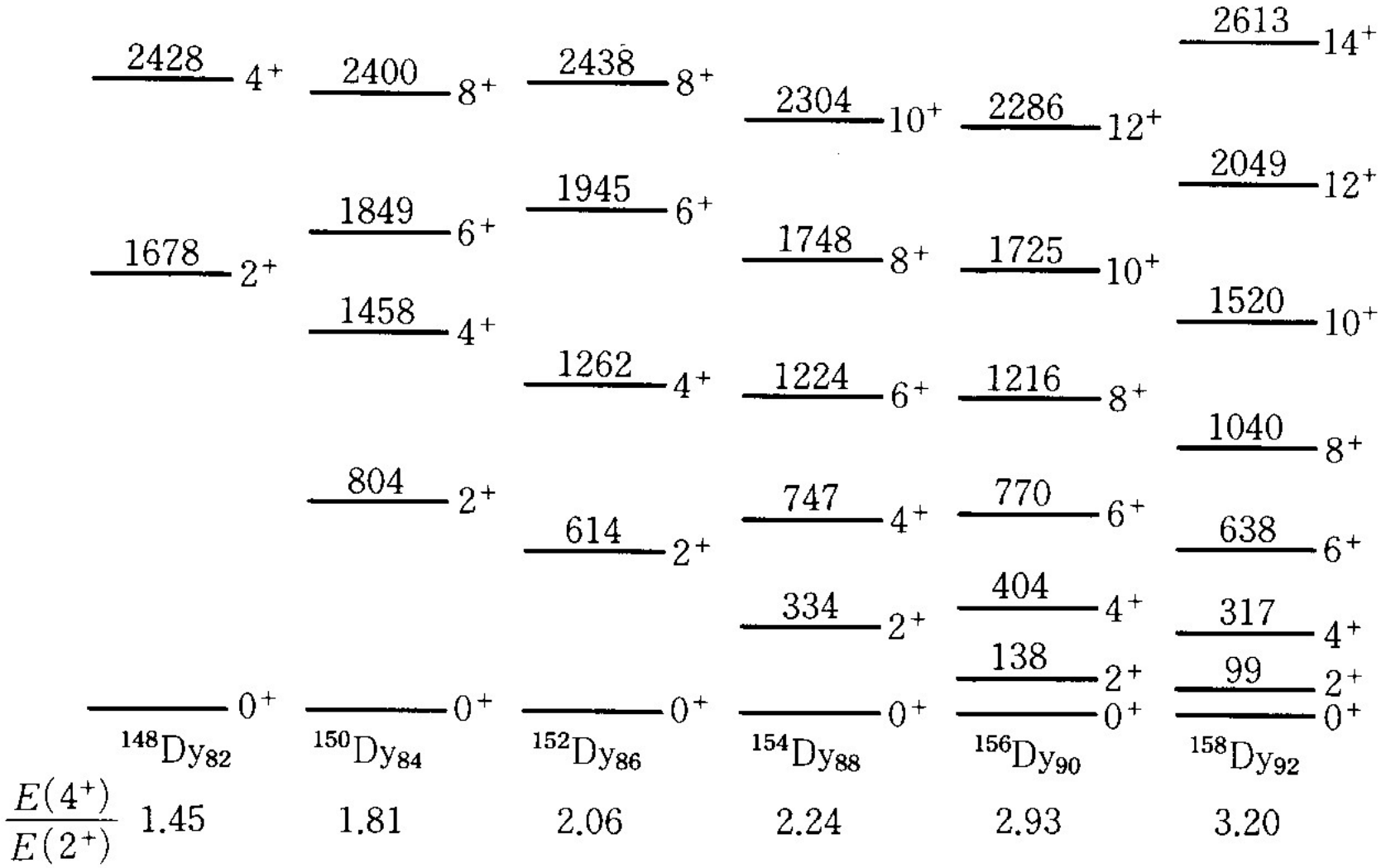
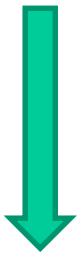


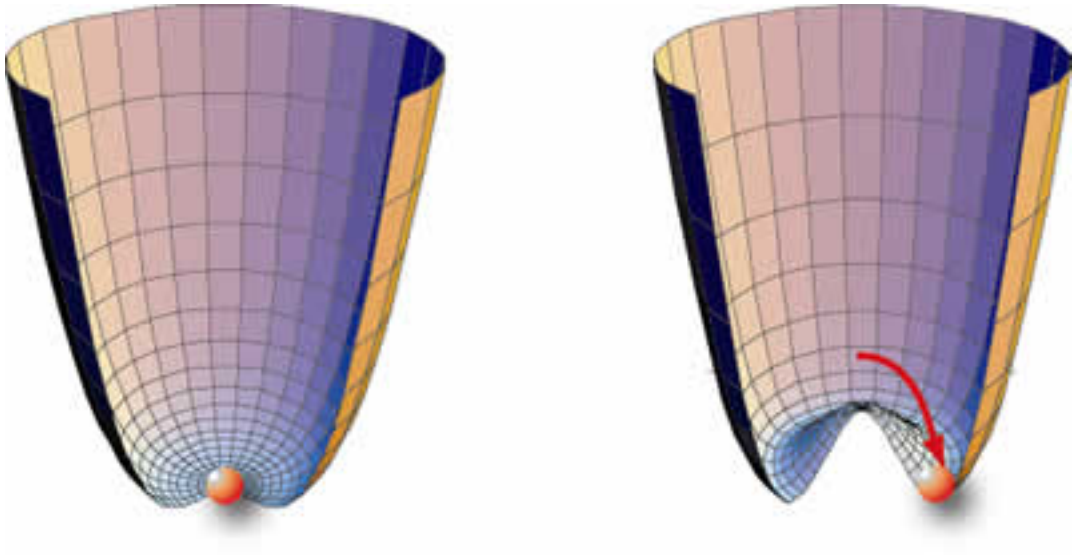
図 3-4 Dy アイソトープの低励起スペクトル．励起エネルギーの単位は keV.

市村、坂田、松柳
「原子核の理論」より

対称性の自発的破れ

ハミルトニアンが持つ対称性を、真空が持たない（破る）。





（対称性を回復するように
南部・ゴールドストン・モード（ゼロ・モード）
が発生）

休憩（頭の体操）

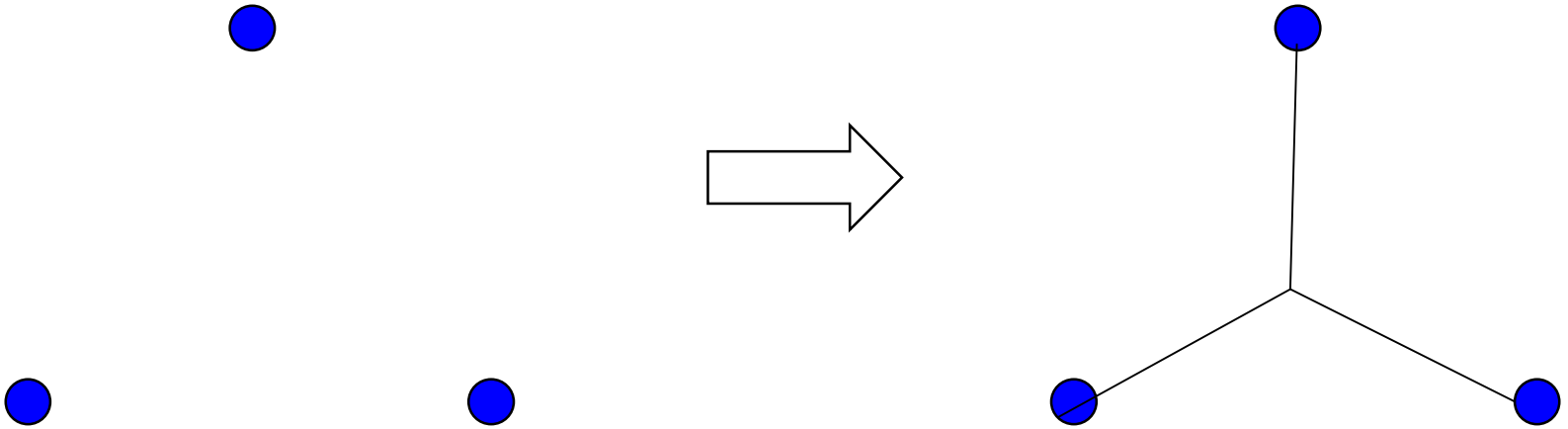
頂点が何個かある

- 頂点を適当な線でつなぐ
- 何本引いてもよい
- 線は交わってもよい
- 一つの点から線を通って全ての点にいけるようにする

線の長さの合計が最短になる線のひき方は?

例）正三角形の場合

対称となるように引く



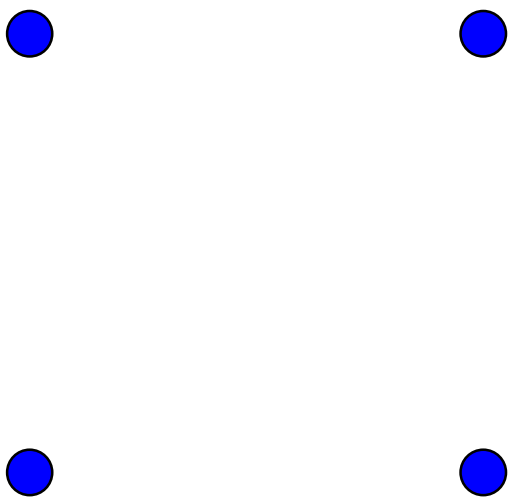
休憩（頭の体操）

頂点が何個かある

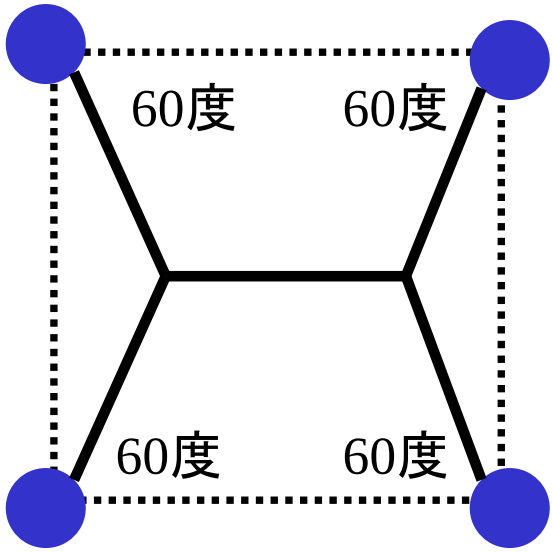
- 頂点を適当な線でつなぐ
- 何本引いてもよい
- 線は交わってもよい
- 一つの点から線を通って全ての点にいけるようにする

線の長さの合計が最短になるひき方は?

（問題）正方形の場合は?



（答え）



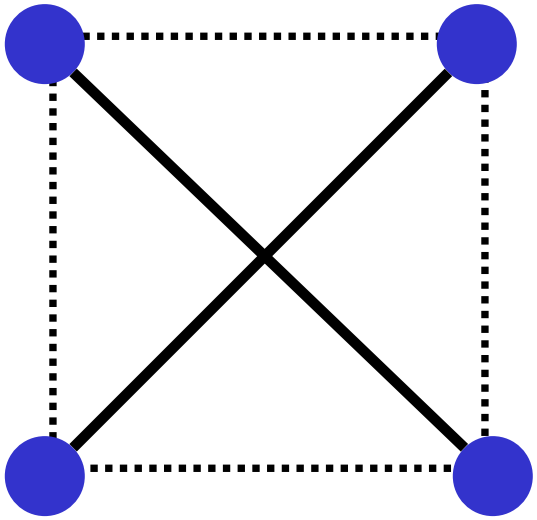
長さ

$$4 \times \frac{1}{\sqrt{3}} + \left(1 - 2 \times \frac{1}{2\sqrt{3}}\right)$$

$$= 1 + \sqrt{3}$$

$$= 2.732\cdots$$

cf.

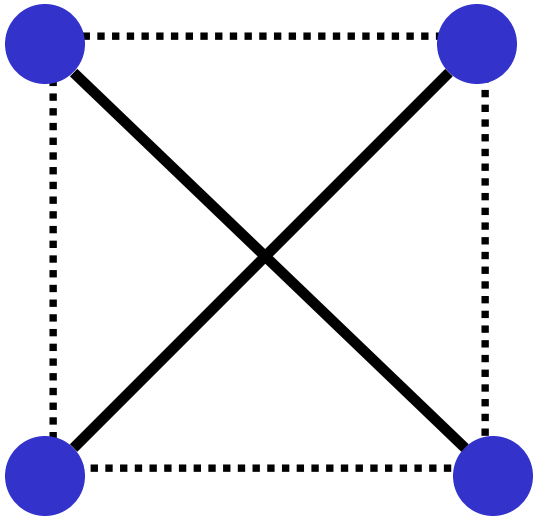


長さ

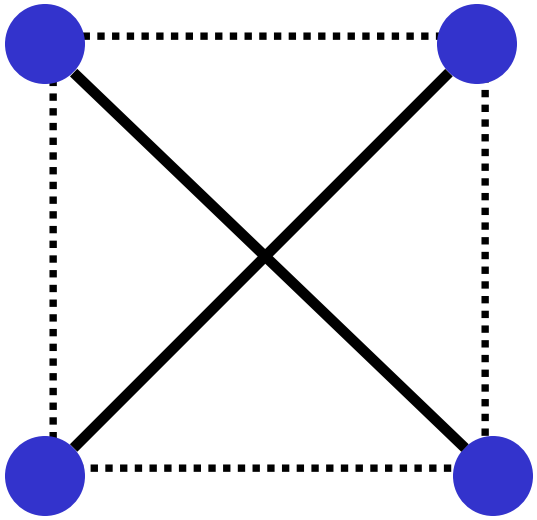
$$2 \times \sqrt{2} = 2.828\cdots$$

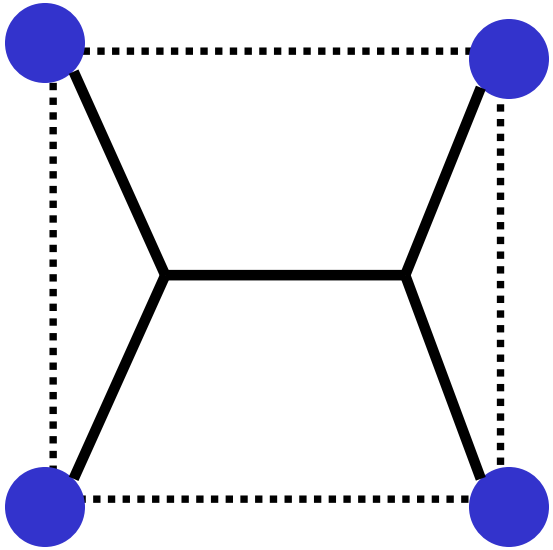
参考：

小池武志「原子核研究」Vol. 52 No. 2, p. 14

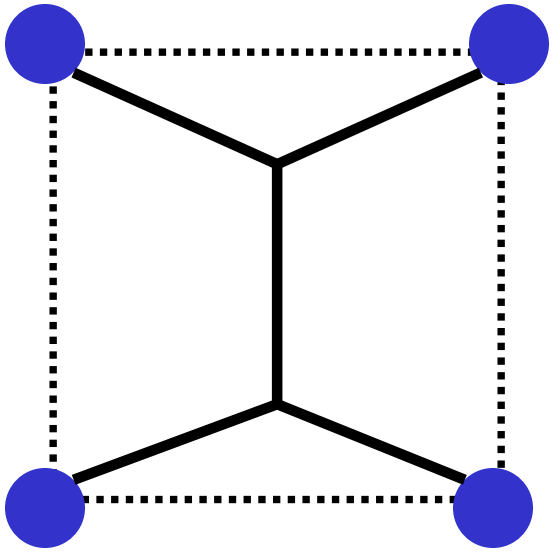


90度回転で不変





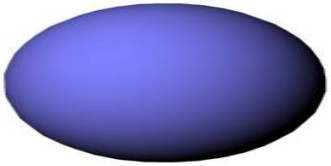
90度回転



対称性の自発的破れの好例

スライド：小池武志氏（東北大学）

➢Rotational symmetry



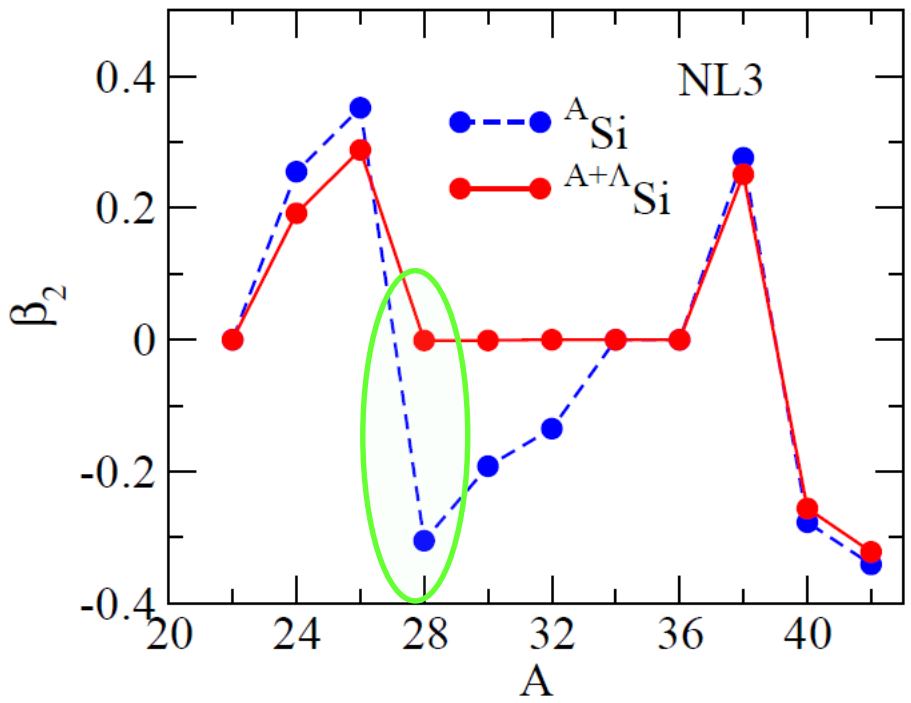
Deformed solution

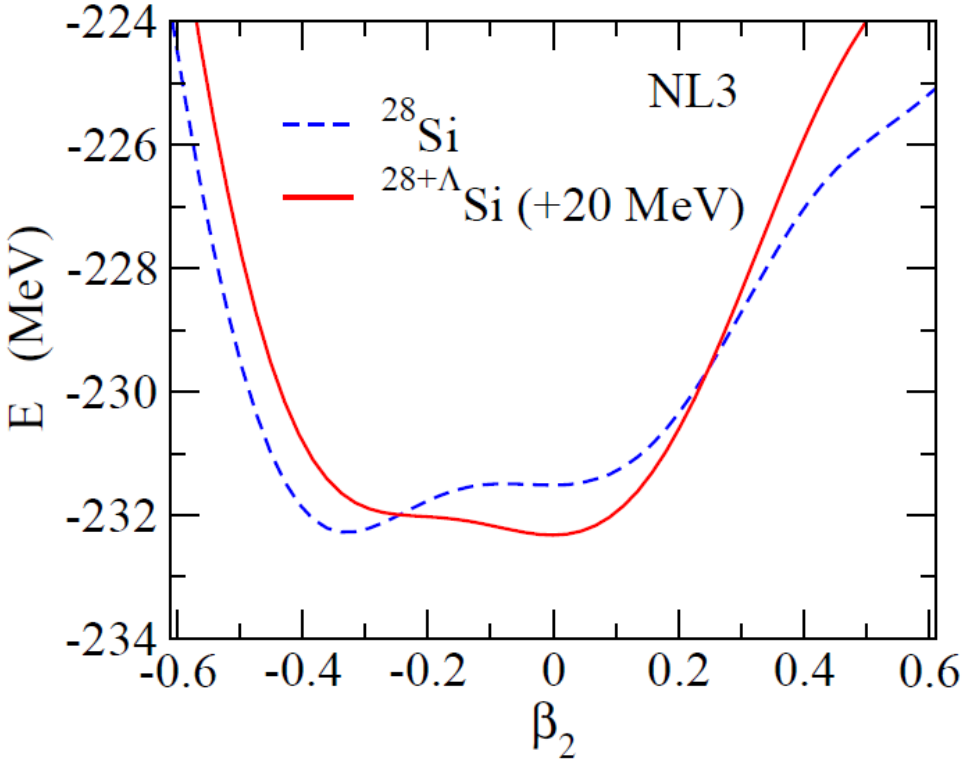
Hypernuclei: nucleus + Lambda particle

Effect of a Λ particle on nuclear shapes?

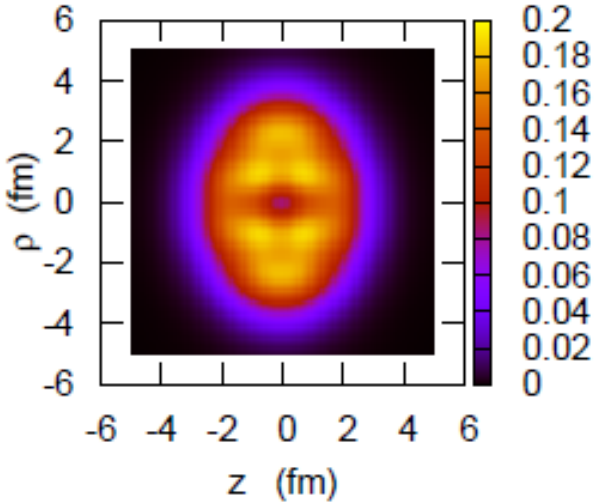
Λ粒子を原子核の形につけるとどうなるのか?
→ハートリー・フォック法では最適な形が自動的にでてくる
（Λ粒子による原子核の形の変化が自動的にでる）

Si isotopes



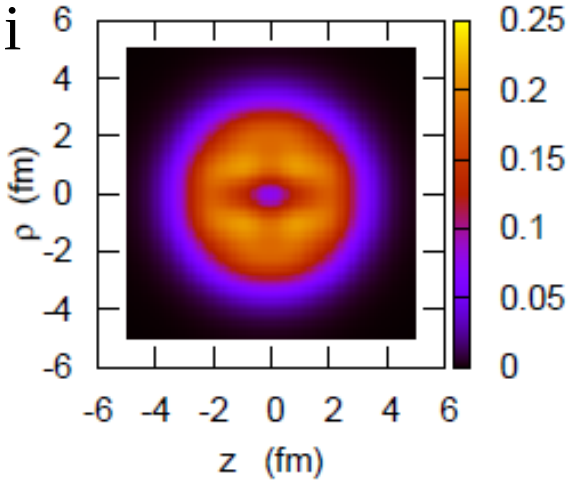


^{28}Si



Λ

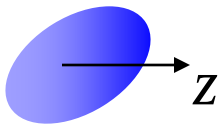
$^{29}_{\Lambda}$Si

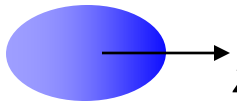


Myaing Thi Win and K.Hagino, PRC78(‘08)054311

Angular Momentum Projection

Rotated wave function: $|\Psi_\Omega\rangle = \hat{\mathcal{R}}(\Omega)|\Psi\rangle$





(deformed HF solution)

(note)

$$\langle\Psi_\Omega|H|\Psi_\Omega\rangle = \langle\Psi|\underbrace{\hat{\mathcal{R}}^{-1}H\hat{\mathcal{R}}}|\Psi\rangle = \langle\Psi|H|\Psi\rangle$$

= H (for rot. symmetric Hamiltonian)

a better wf: a superposition of rotated wave functions

$$|\Psi_{\text{proj}}\rangle = \int d\Omega\, f(\Omega)|\Psi_\Omega\rangle$$

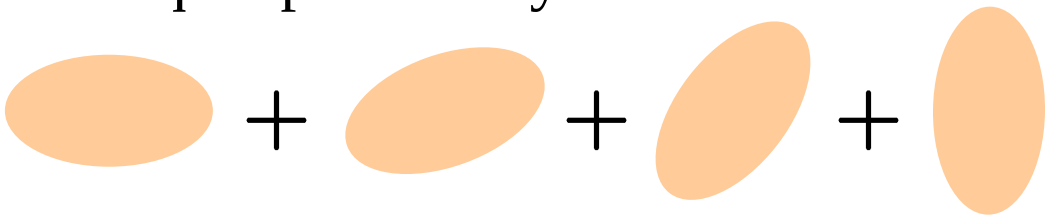
$f(\Omega)$ ⟵ variational principle $\langle\delta\Psi_{\text{proj}}|H - E|\Psi_{\text{proj}}\rangle = 0$

$$\int [\langle\Psi_\Omega|H|\Psi_{\Omega'}\rangle - E\,\langle\Psi_\Omega|\Psi_{\Omega'}\rangle]\, f(\Omega')d\Omega' = 0$$

(note) For 0^+ state

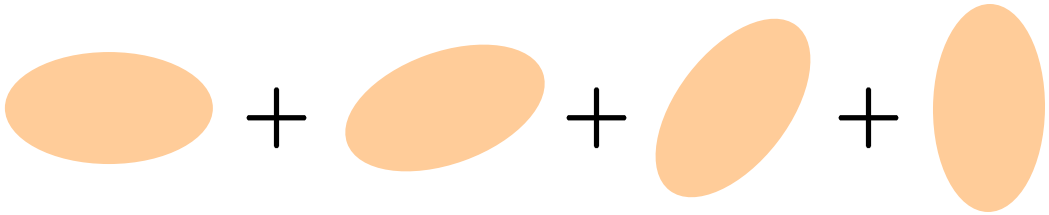
0^+: no preference of direction (spherical)

➡ Mixing of all orientations with an equal probability



$$|\Psi_{0+}\rangle = \int d\Omega \, |\Psi_{\Omega}\rangle$$

(note) For 0^+ state



$$|\Psi_{0+}\rangle = \int d\Omega\, |\Psi_\Omega\rangle$$

other states:

$$|\Psi_{IM}\rangle = \int d\Omega\, Y_{IM}(\Omega)|\Psi_\Omega\rangle$$

(for K=0)

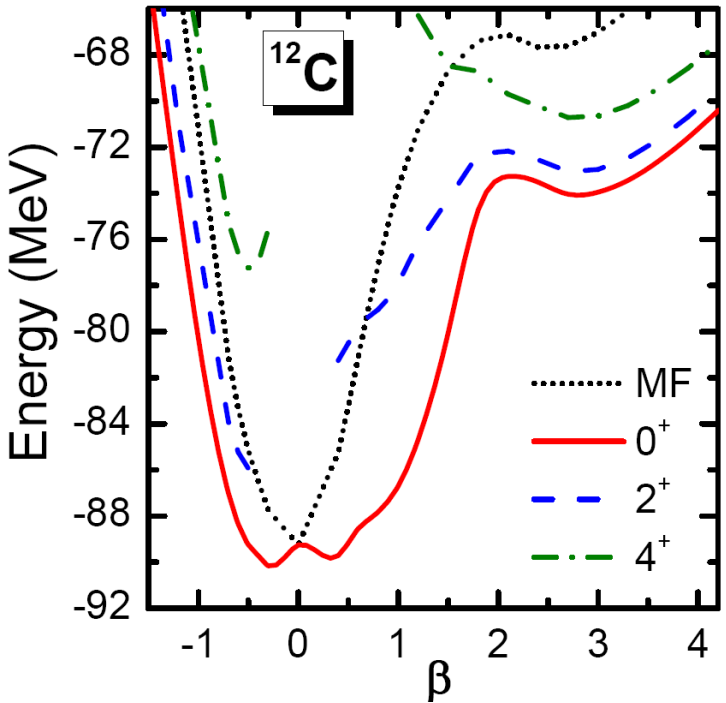
“angular momentum projection”

Projected wave function:

$$|\Psi_{IM}\rangle = \hat{P}_{IM}|\Psi\rangle = \int d\Omega\, Y_{IM}(\Omega)\hat{\mathcal{R}}(\Omega)\,|\Psi\rangle$$

Projected energy surface:

$$E_I = \frac{\langle\Psi_{IM}|H|\Psi_{IM}\rangle}{\langle\Psi_{IM}|\Psi_{IM}\rangle} = \frac{\langle\Psi|\hat{P}_{IM}H\hat{P}_{IM}|\Psi\rangle}{\langle\Psi|\hat{P}_{IM}\,\hat{P}_{IM}|\Psi\rangle}$$



Constrained HF

0^+

2^+

4^+

Calculation and Figure: Mei Hua (PC-F1)