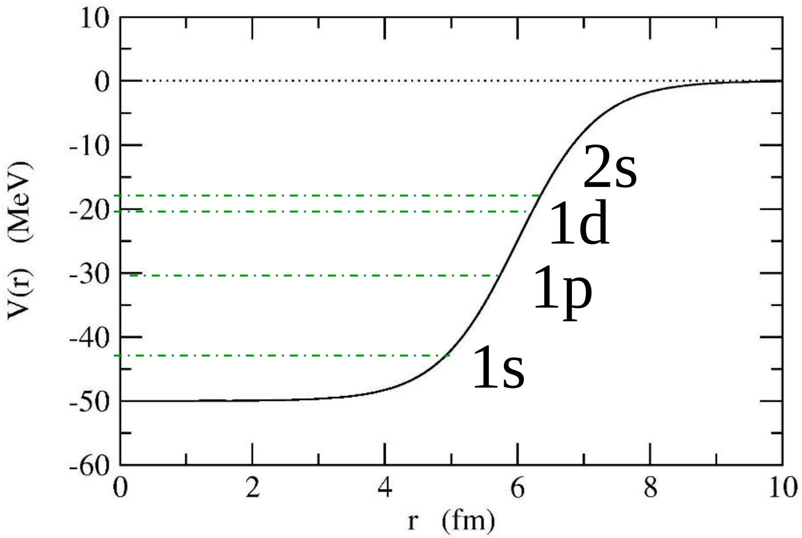
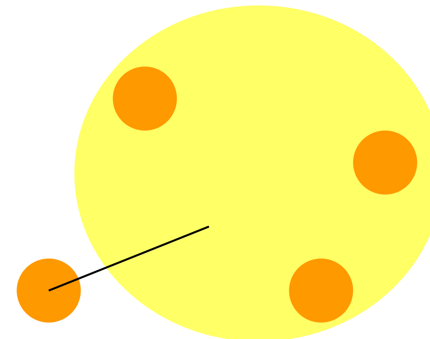
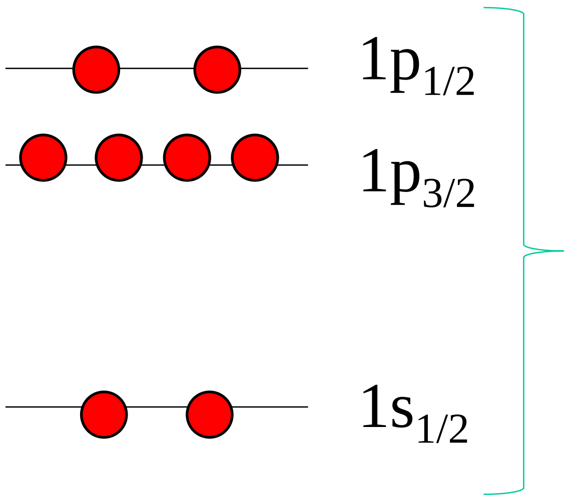
Mean-field (Hartree-Fock) Theory



平均場





shell model

naively speaking,

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

independent motion

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

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

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

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

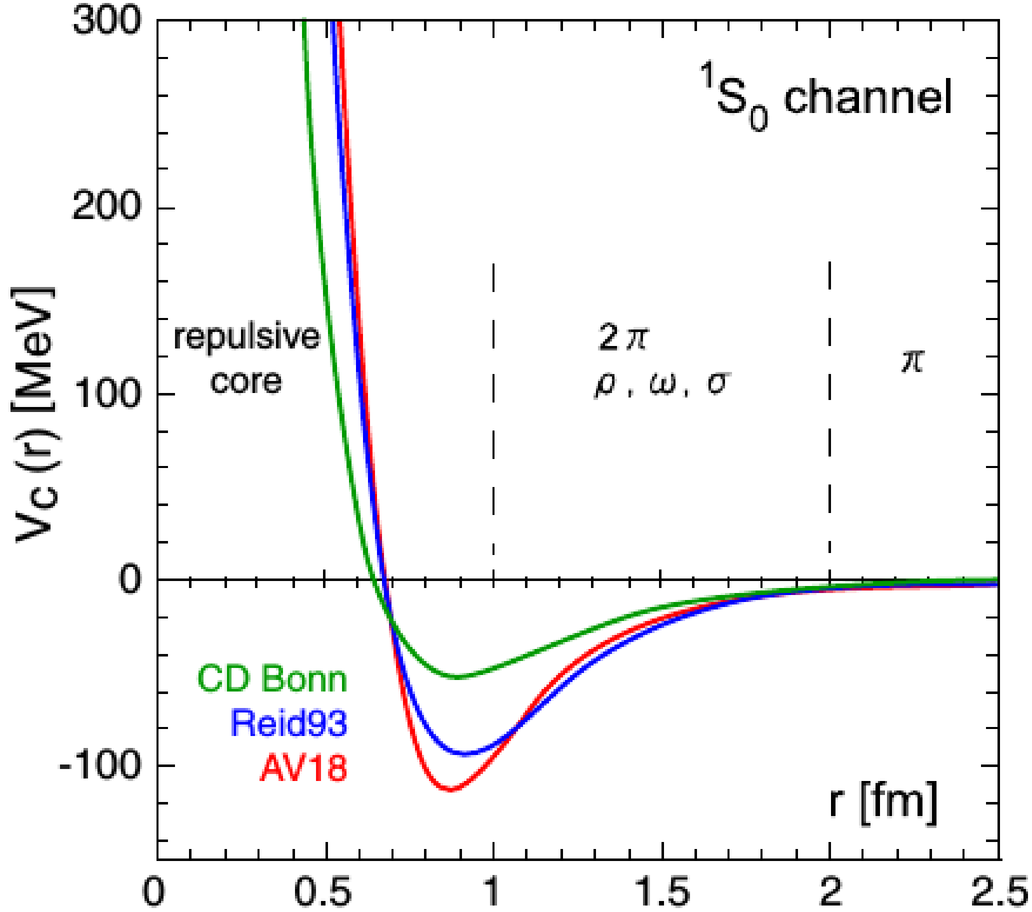
$$\to \left[-\frac{\hbar^2}{2m}\nabla^2 + \int v(\boldsymbol{r}-\boldsymbol{r}')\left(\sum_j |\psi_j(\boldsymbol{r}')|^2\right) d\boldsymbol{r}' - \epsilon_i\right]\psi_i(\boldsymbol{r})$$

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

exchange term

Hartree-Fock theory

Bare nucleon-nucleon interaction



N. Ishii, S. Aoki, and T. Hatsuda,
PRL99, 022001 (2007)

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

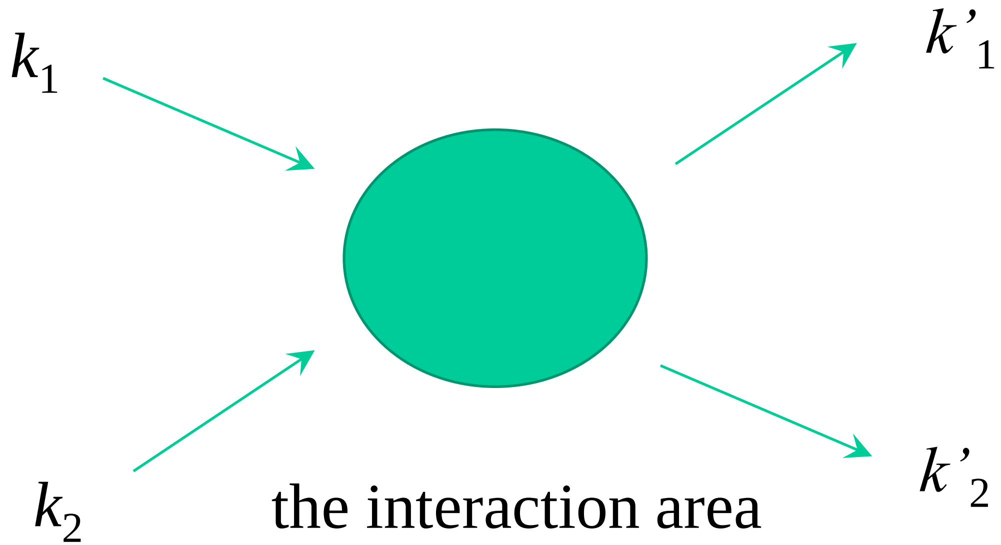
cf. magic numbers

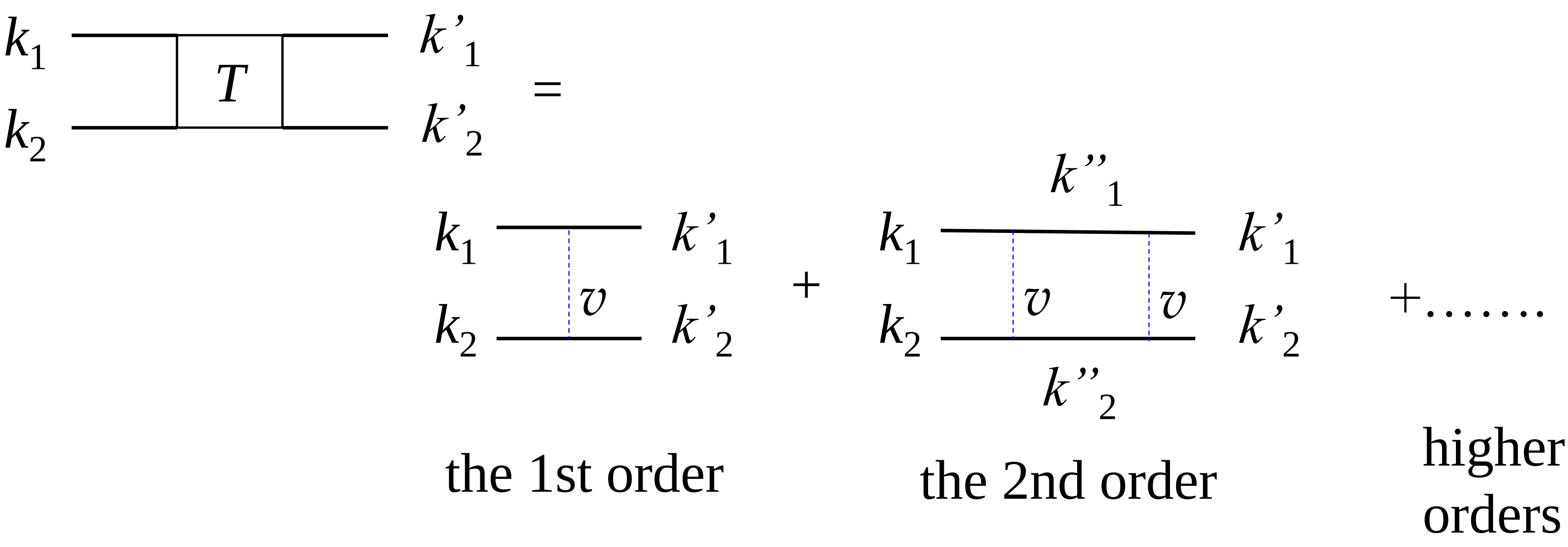
Solution: a nucleon-nucleon interaction *in medium* (effective interaction) rather than a bare interaction

↑

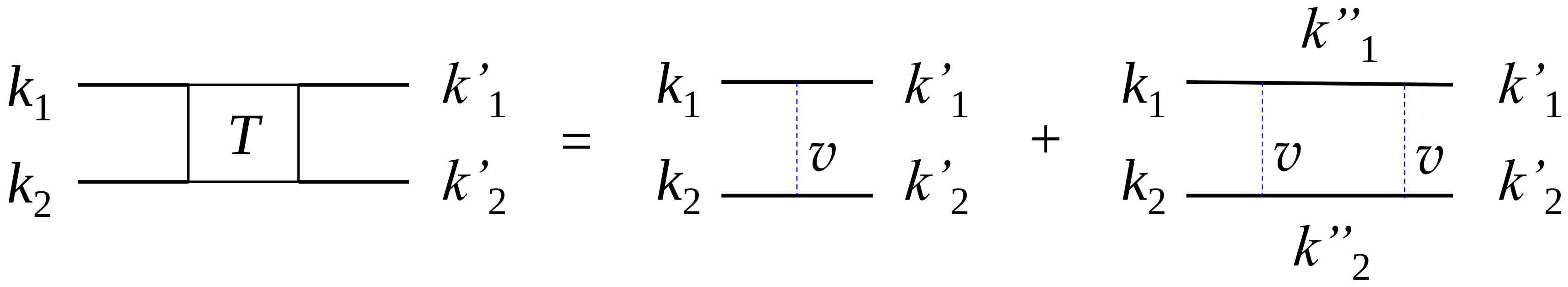
Bruckner's G-matrix

- Firstly, two-body (multiple) scattering *in vacuum*





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



$+\ldots\ldots$

Lippmann-Schwinger equation

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

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

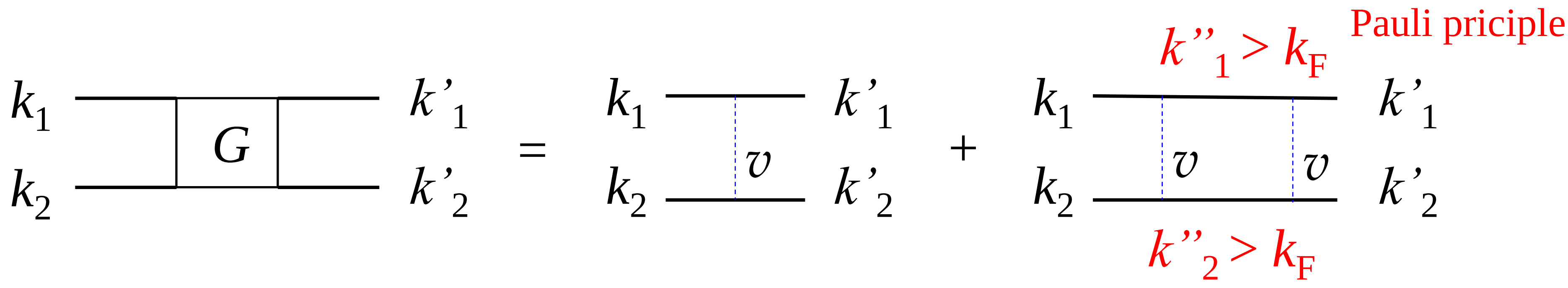
$$\Rightarrow \left(-\frac{\hbar^2}{2m}\nabla^2 - E\right)\psi = -V\psi$$

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

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

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
$k > k_F$ $\longrightarrow$ 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.

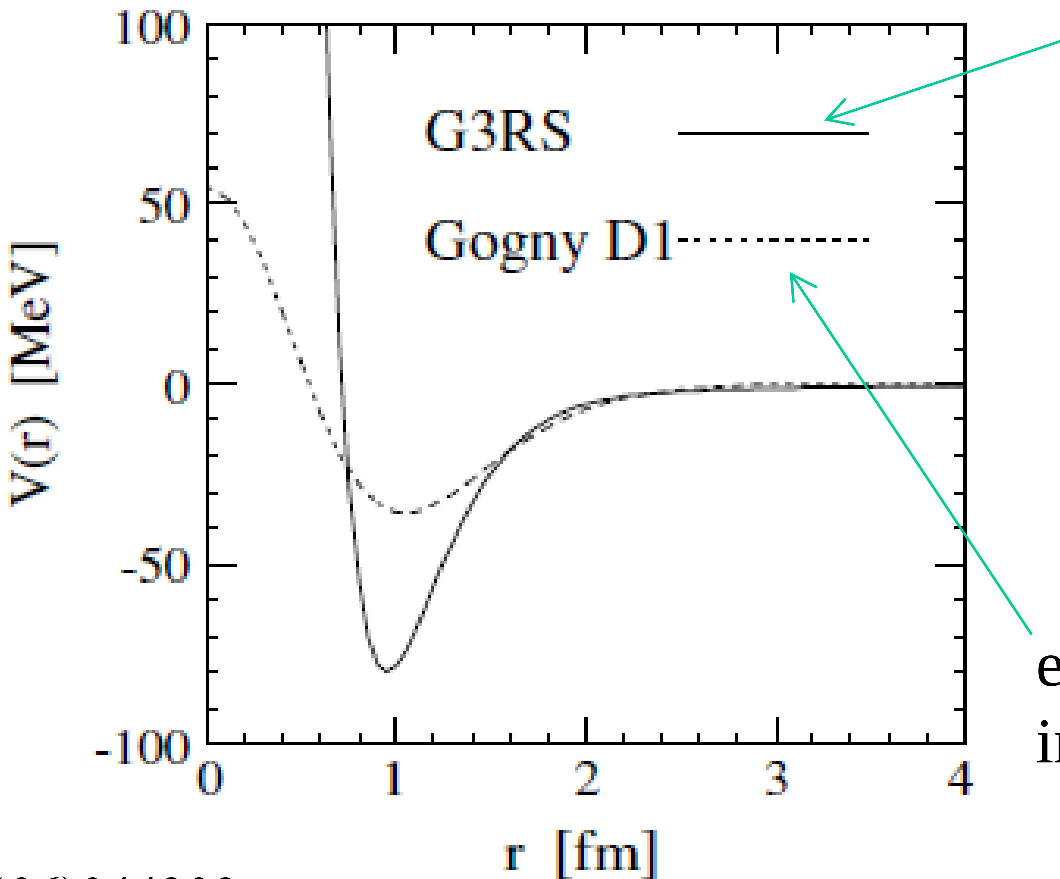


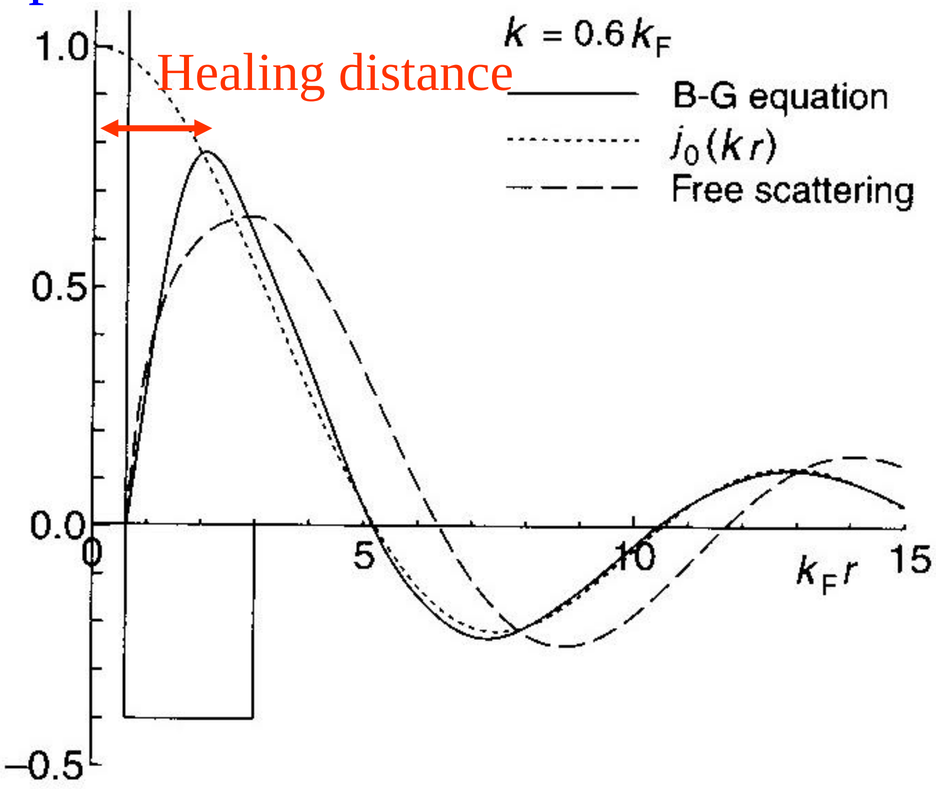
figure from
M. Matsuo,
Phys. Rev. C73('06)044309

◆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

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

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

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 ⟶ local

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

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:

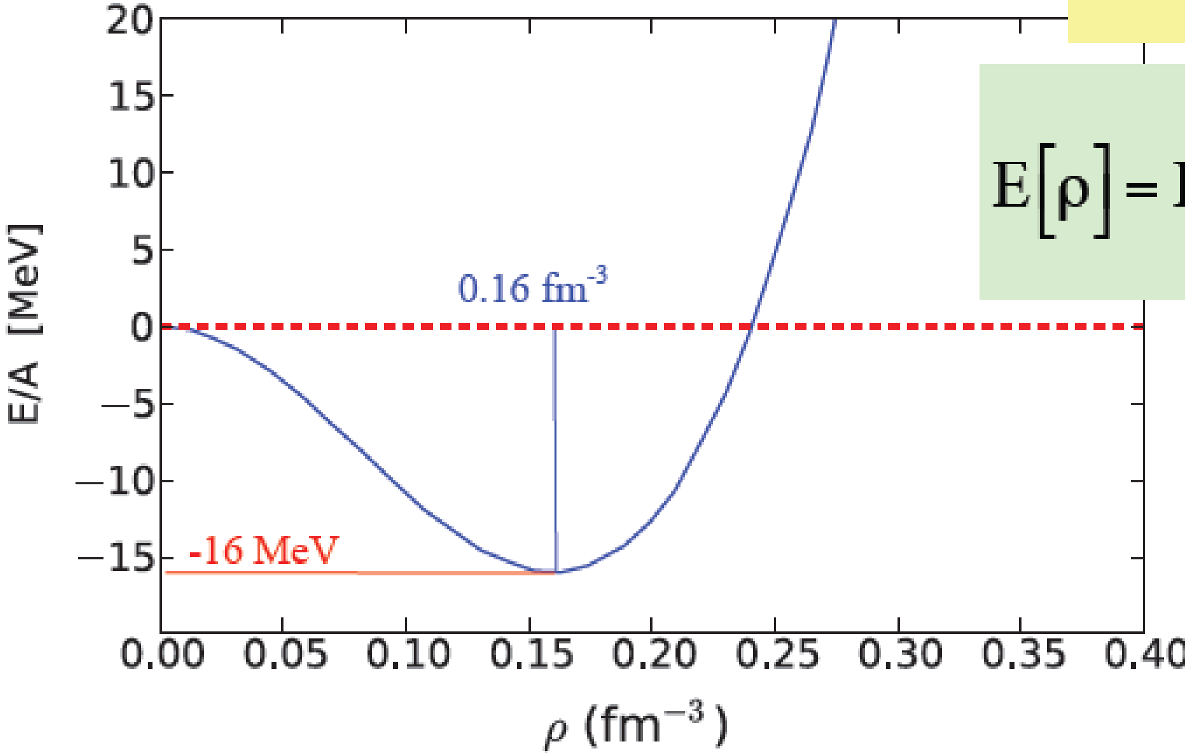
B.E. and r_{rms}: ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{90}Zr, ^{208}Pb,…..

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

Parameter sets:

SIII, SkM*, SGII, SLy4,…….

EOS of infinite nuclear matter



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

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

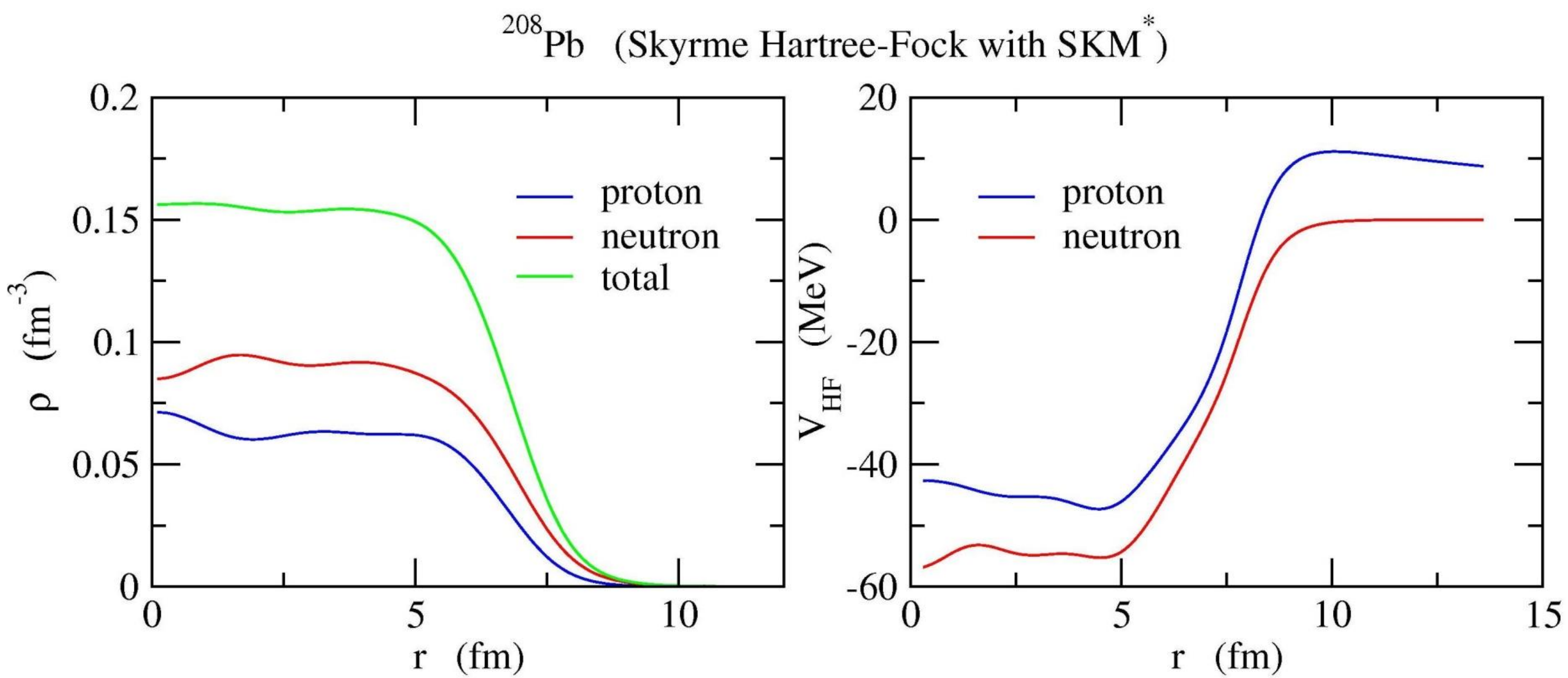
slide: Carlos Bertulani

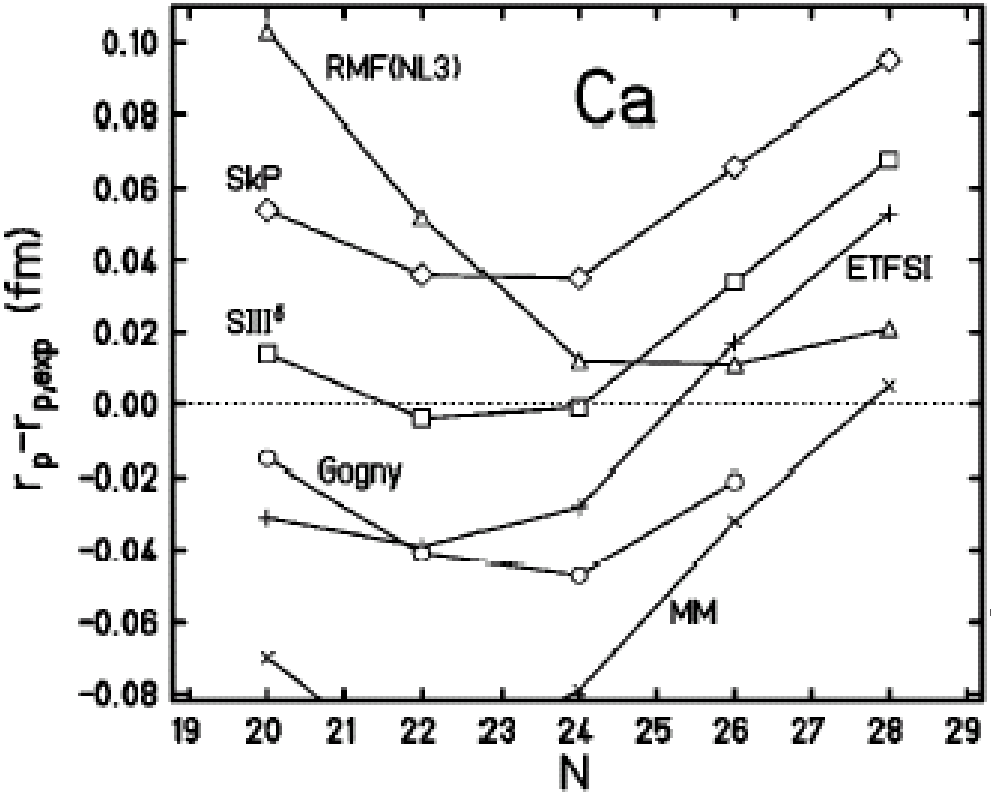
$$-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2\psi_i(\boldsymbol{r}) + \int v(\boldsymbol{r},\boldsymbol{r}')\rho_{\mathsf{HF}}(\boldsymbol{r}')d\boldsymbol{r}'\psi_i(\boldsymbol{r}) - \int \rho_{\mathsf{HF}}(\boldsymbol{r},\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\psi_i(\boldsymbol{r}')\,d\boldsymbol{r}'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

Iteration

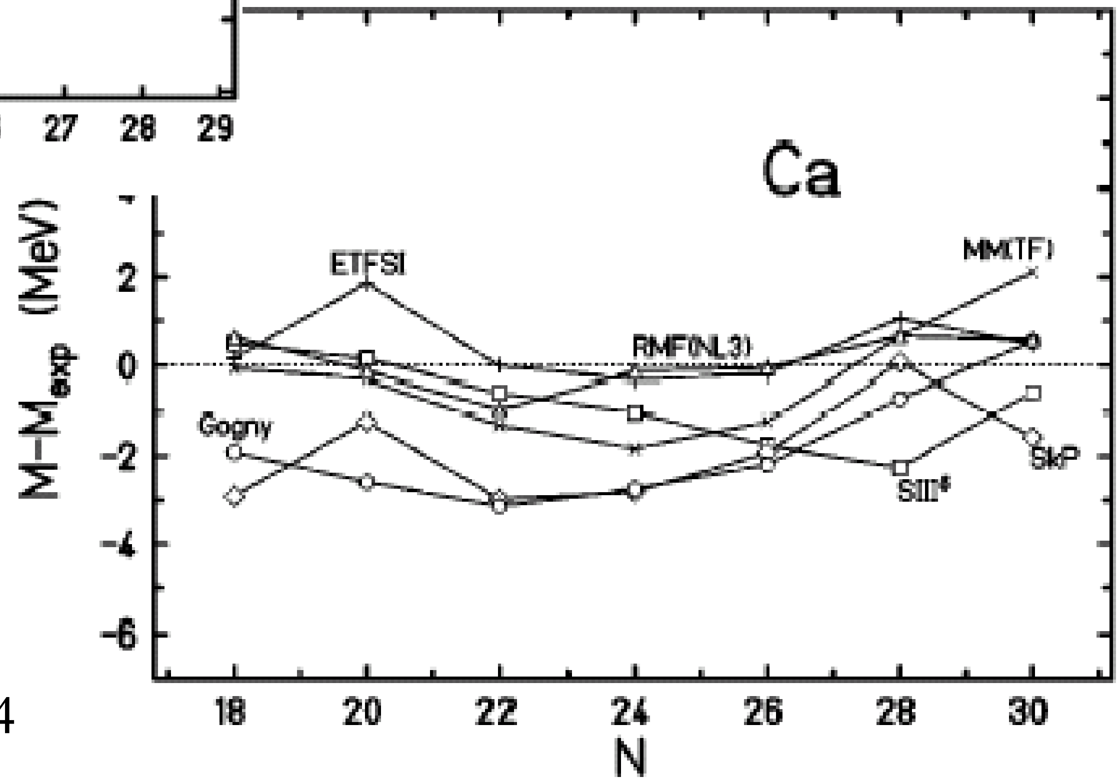
V_{HF}: depends on ψ_i $\longleftarrow$ non-linear problem

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



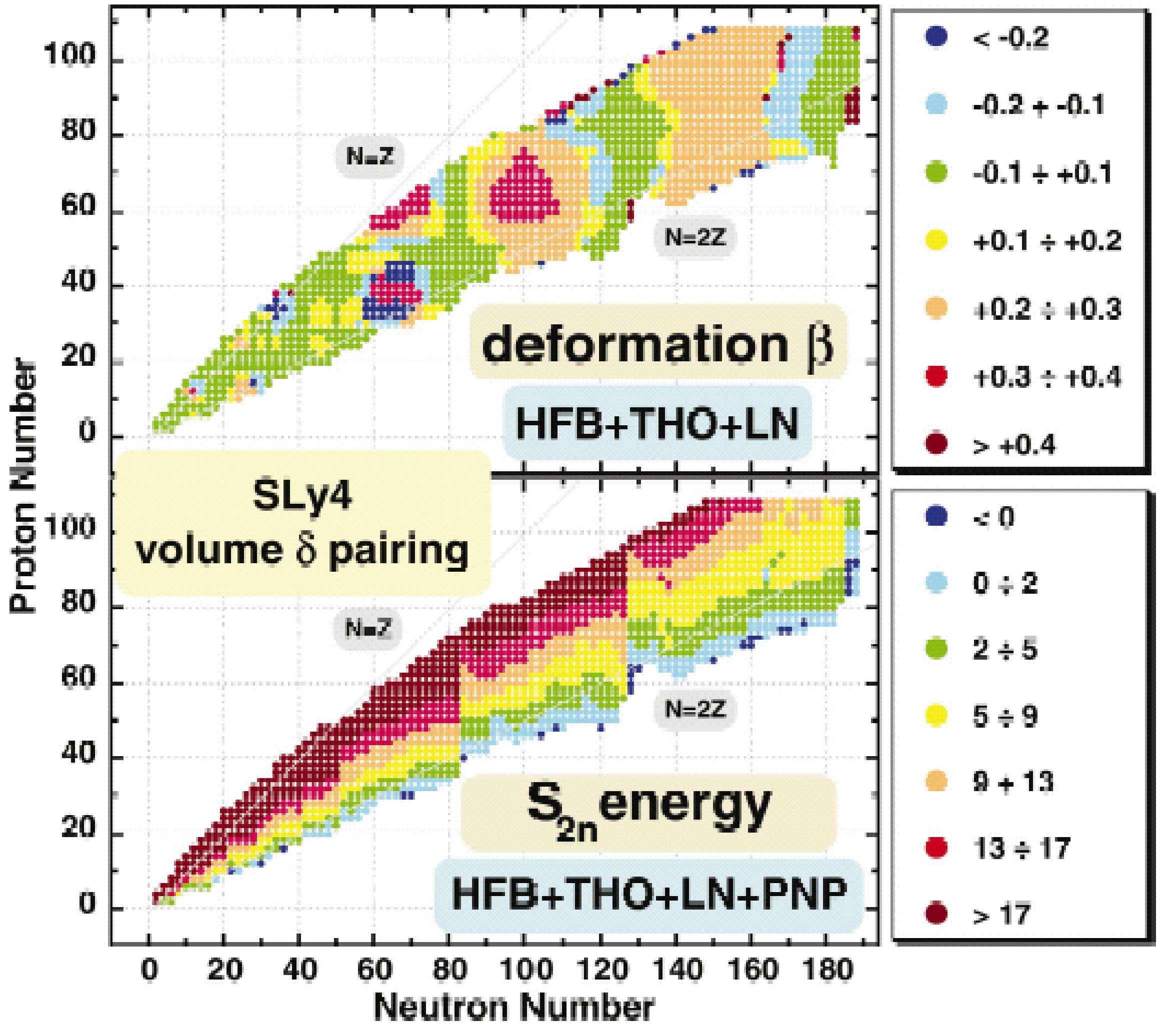


Examples of HF calculations for masses and radii



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

deformation and two-neutron separation energy



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

Mean-field approximation and deformation

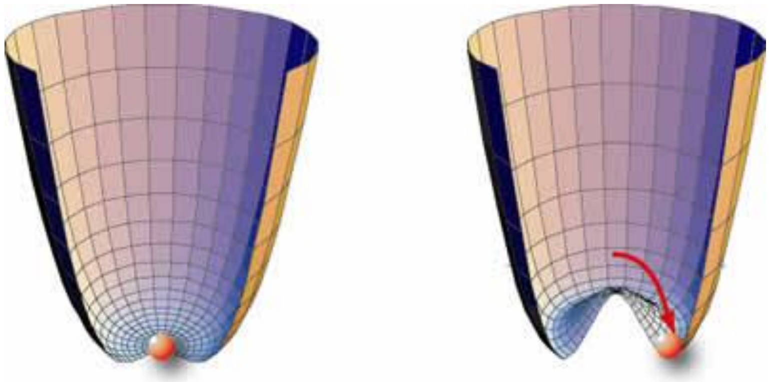
平均場近似＝2体場→1体場に近似

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

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

$\Psi_{\rm MF}$: ハミルトニアン H が持っている対称性を持たなくてもいい

"対称性の自発的破れ"



Ψ_{MF} ：ハミルトニアン H が持っている対称性を持たなくてもいい

典型的な例

- 並進対称性: 原子核の平均場近似(DFT)では常に破れる

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

$\Psi_{\rm MF}$ ：ハミルトニアン H が持っている対称性を持たなくてもいい

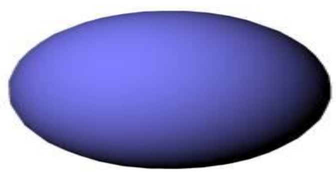
典型的な例

➢ 並進対称性: 原子核の平均場近似（DFT）では常に破れる

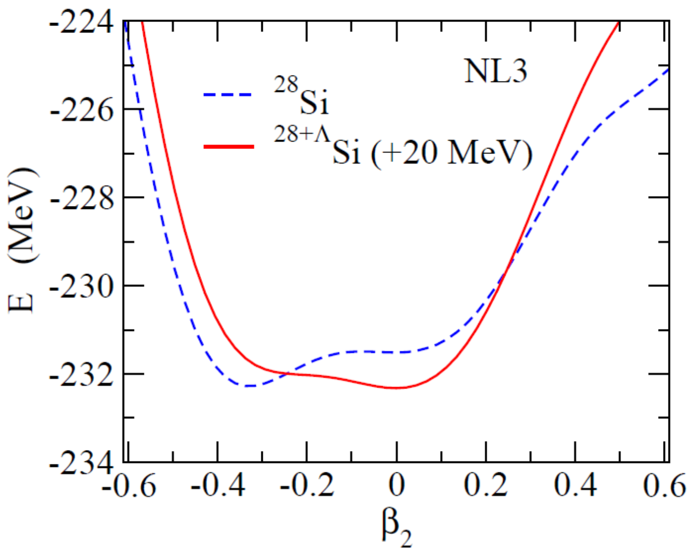
$$H = -\sum_{i=1}^{A}\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i - \boldsymbol{r}_j) \rightarrow \sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\nabla_i^2 + V_{\rm MF}(\boldsymbol{r}_i)\right)$$

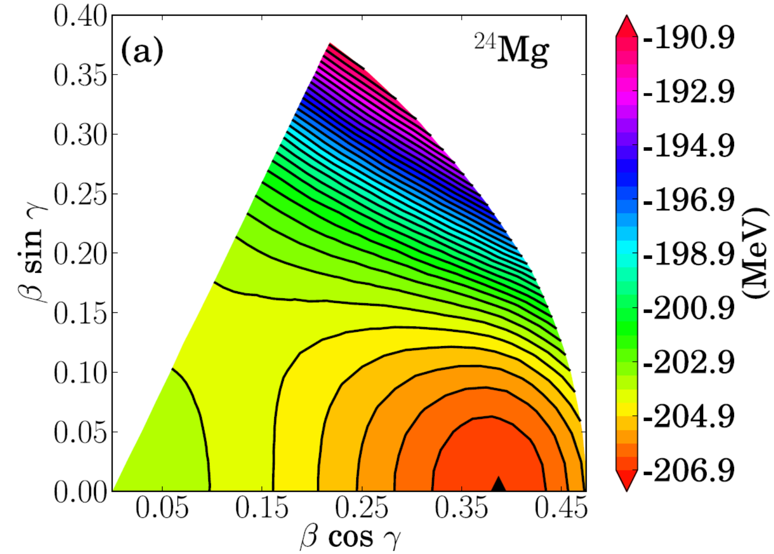
➢ 回転対称性

変形した基底状態



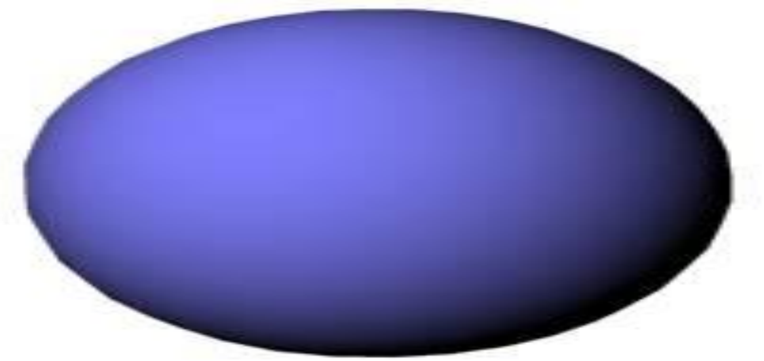
$\rightarrow V(r,\theta)$





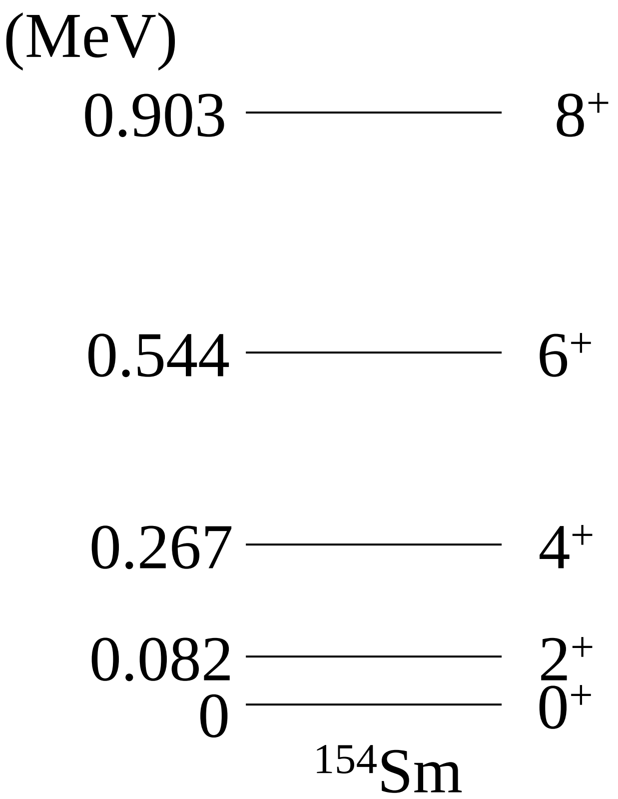
Nuclear Deformation

実験的な証拠

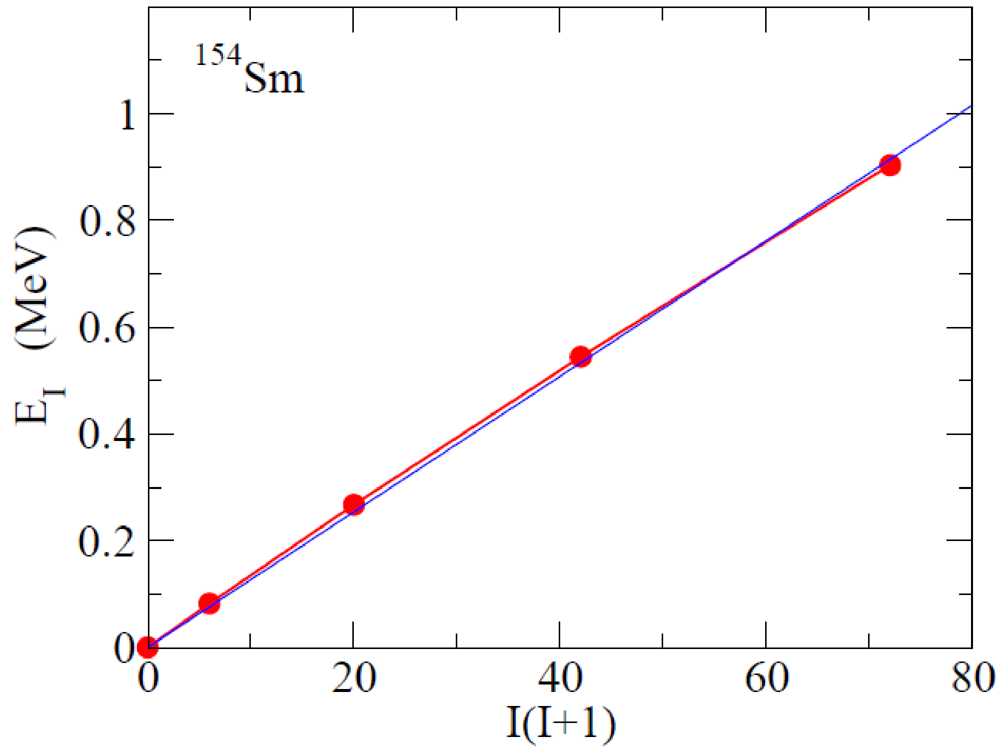


Nuclear Deformation

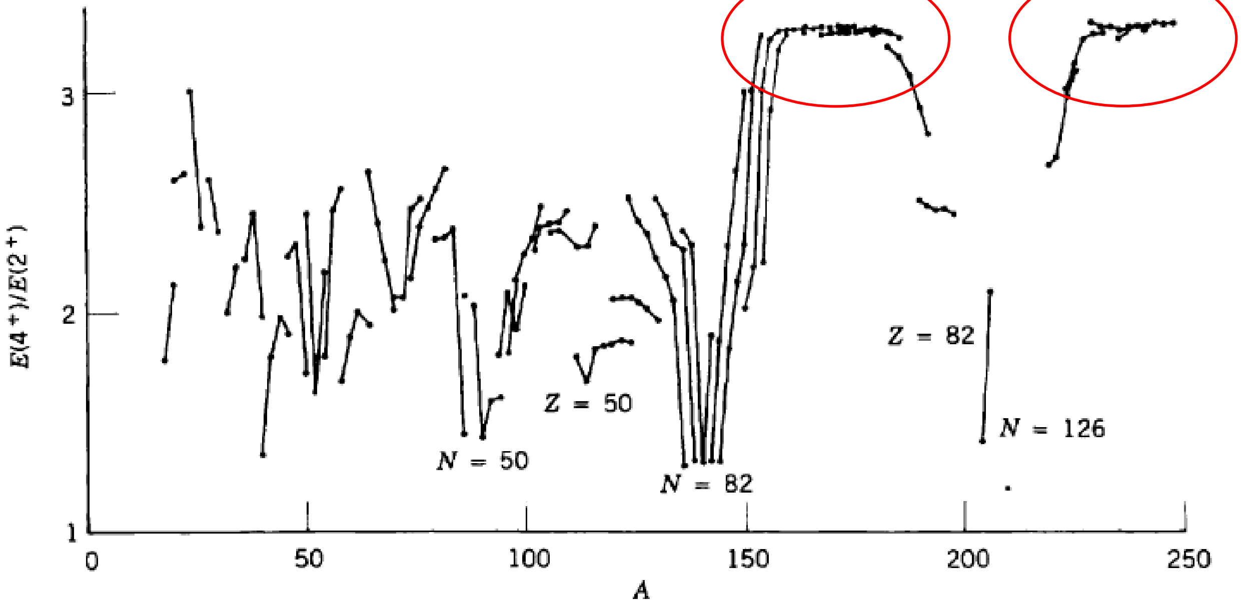
Excitation spectra of ^{154}Sm



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



E(4⁺)/E(2⁺)

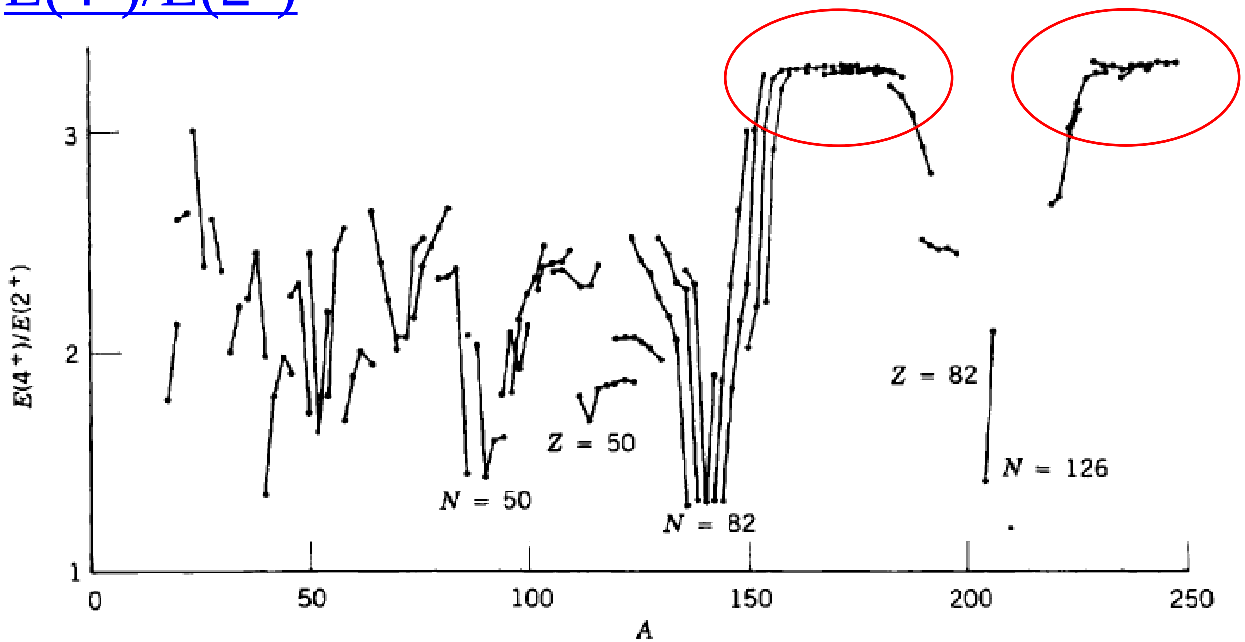


deformed nuclei:
$E(4^+)/E(2^+) \sim 3.3$

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

K.S. Krane, "Introductory Nuclear Physics"

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

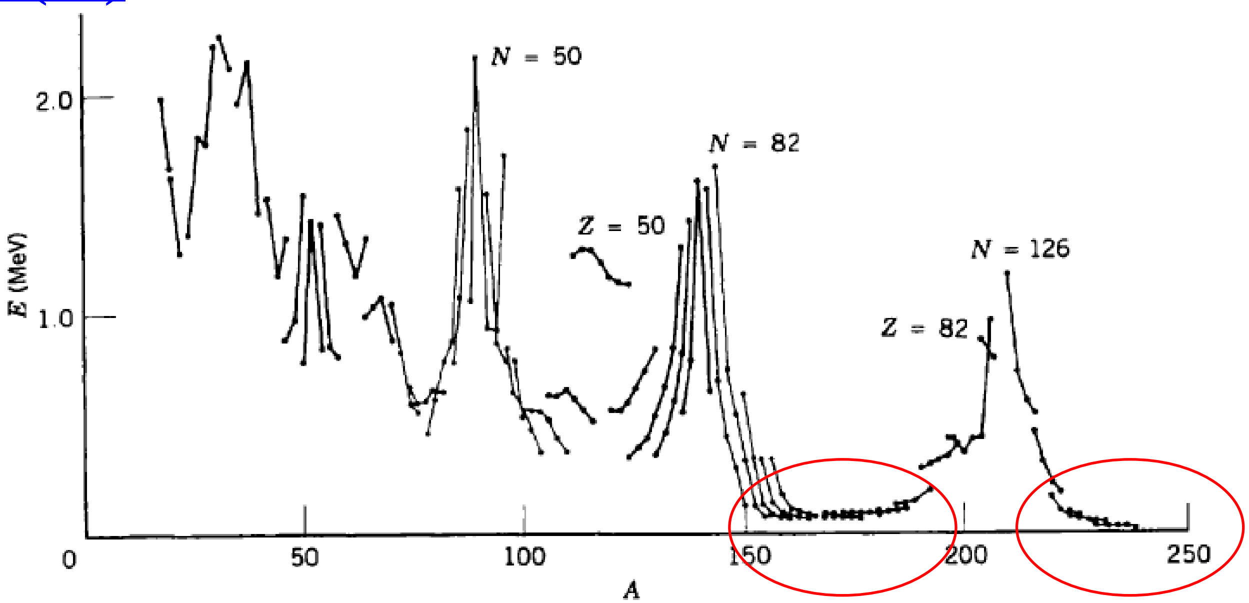


deformed nuclei:
E(4^+)/E(2^+) ~ 3.3

spherical nuclei:
E(4^+)/E(2^+) ~ 2

E(2^+)

K.S. Krane. “Introductory Nuclear Physics”

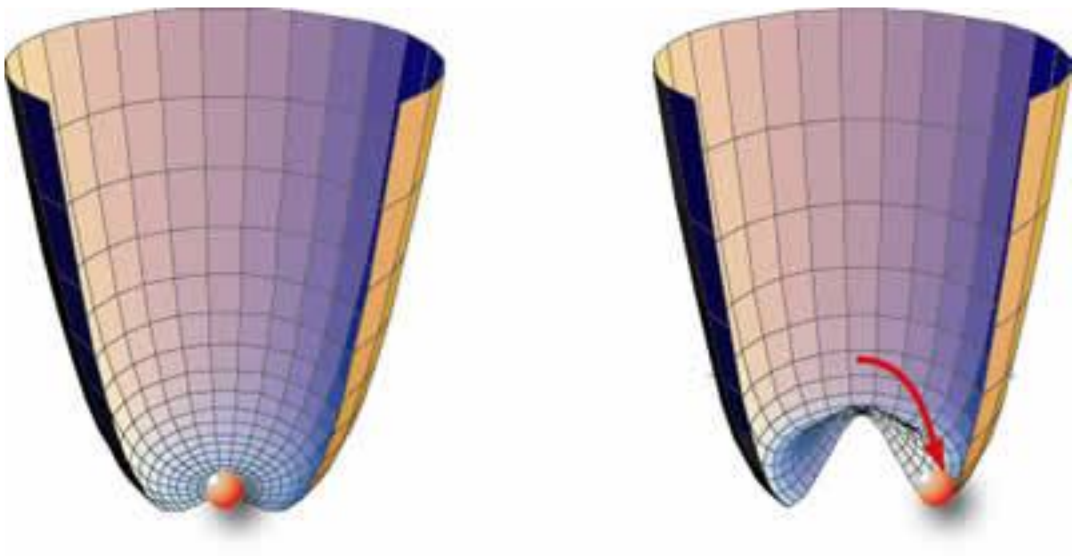


a small energy
→ spontaneously
symm. breaking

deformed nuclei

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

Quiz: spontaneous symmetry breaking

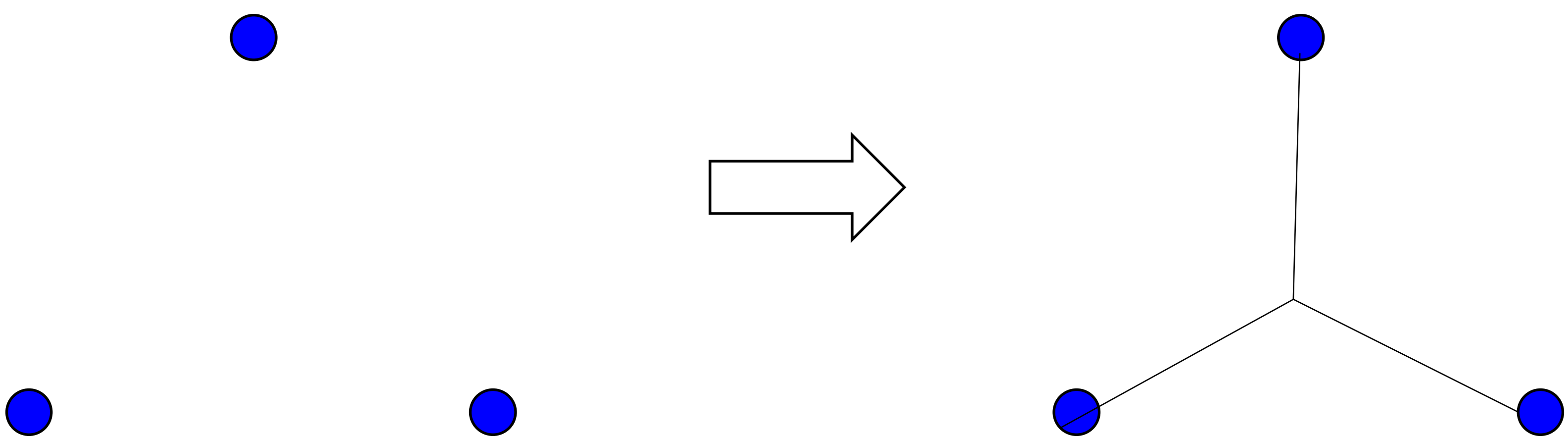
There are a few dots.

- Connect the dots.
- The number of lines is not limited.
- Two lines can cross.
- Connect the dots so that one can go from one dot to all the other dots.

How do you connect the lines if you want to make the total length of lines the shortest?

e.g.) Equilateral triangle

Connect symmetrically



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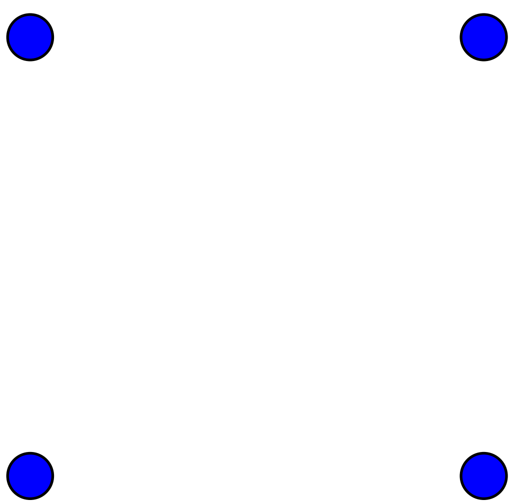
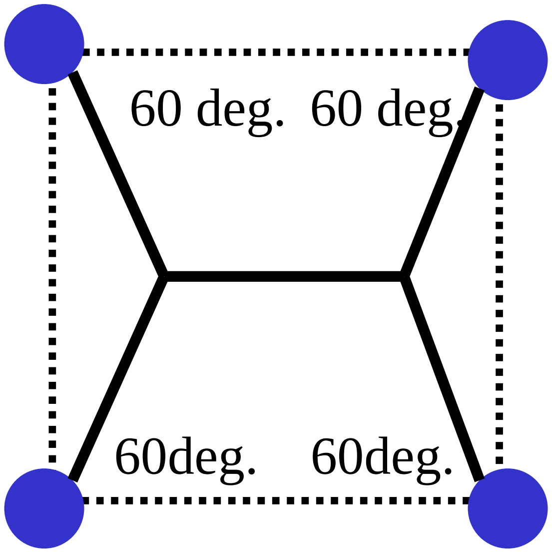
- Connect the dots so that one can go from one dot to all the other dots.

How do you connect the lines if you want to make the total length of lines the shortest?

(question) how about the case for a square?



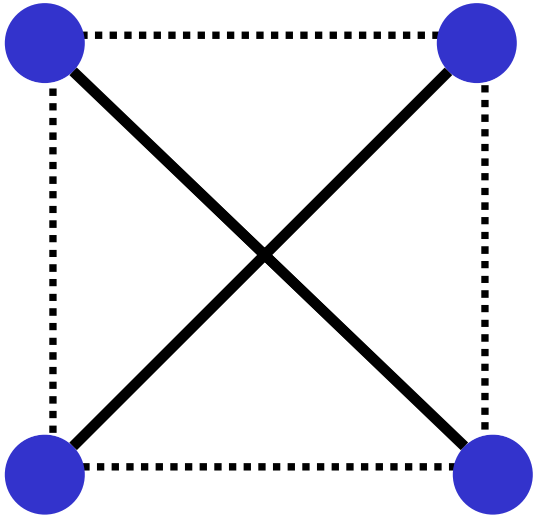
(the answer)



Length

$$4 \times \frac{1}{\sqrt{3}} + \left(1 - 2 \times \frac{1}{2\sqrt{3}}\right)$$
$$= 1 + \sqrt{3}$$
$$= 2.732\cdots$$

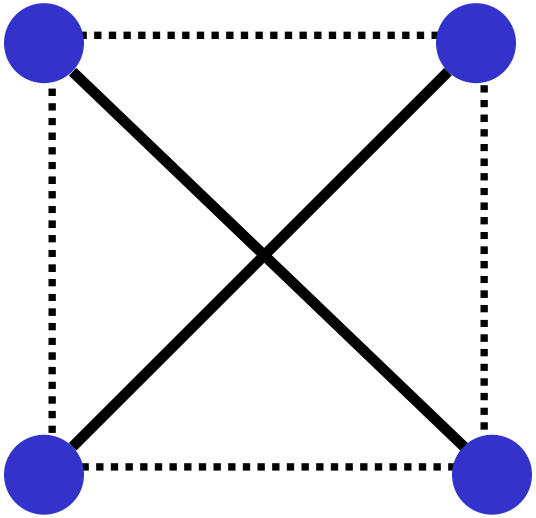
cf.



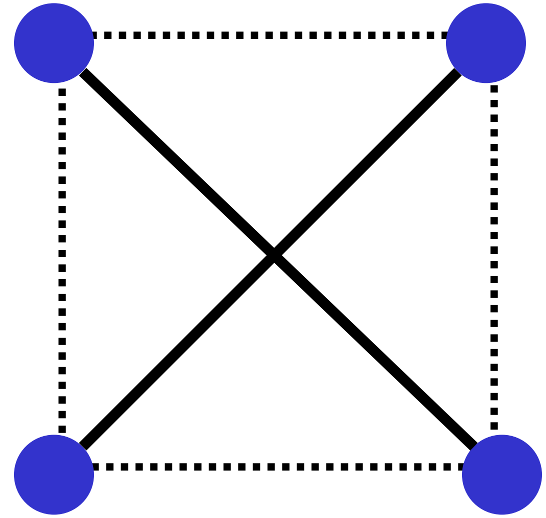
Length

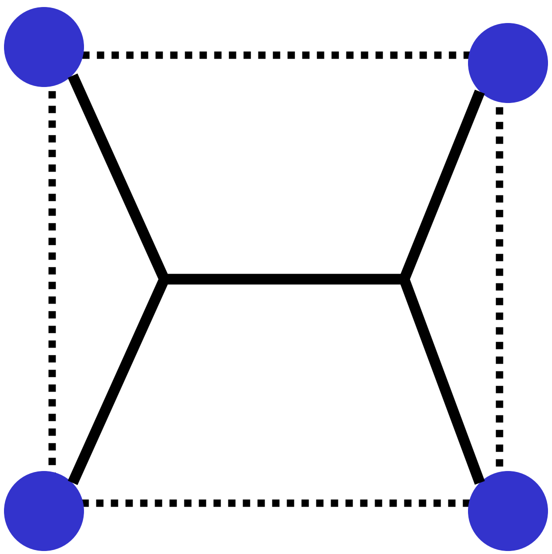
$$2 \times \sqrt{2} = 2.828\cdots$$

Ref. Takeshi Koike,
"Genshikaku Kenkyu" Vol. 52 No. 2, p. 14

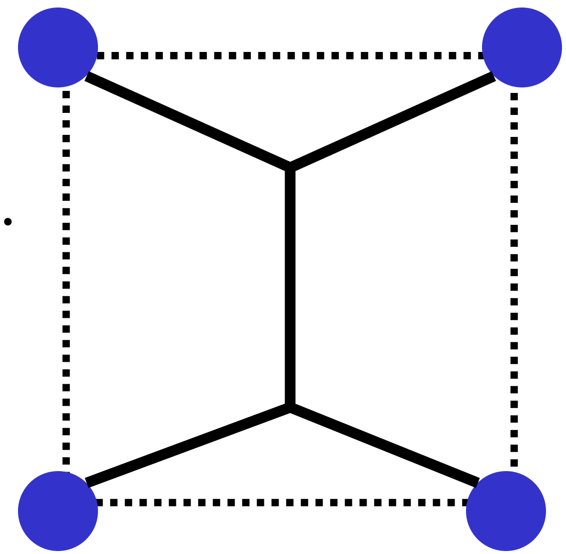


invariant with
rotation by 90 deg.





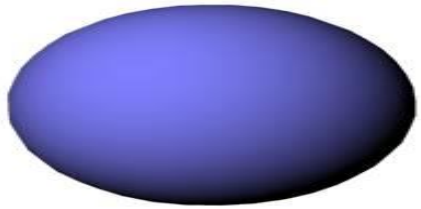
rotation by 90 deg.



a good example of spontaneous symm. breaking

Courtesy: Takeshi Koike

One-particle motion in a deformed potential



$\rightarrow V(r,\theta)$

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V(r,\theta) - E\right]\psi(\boldsymbol{r}) = 0$$

(note) $V(r,\theta)$ → 回転対称性を持っていない

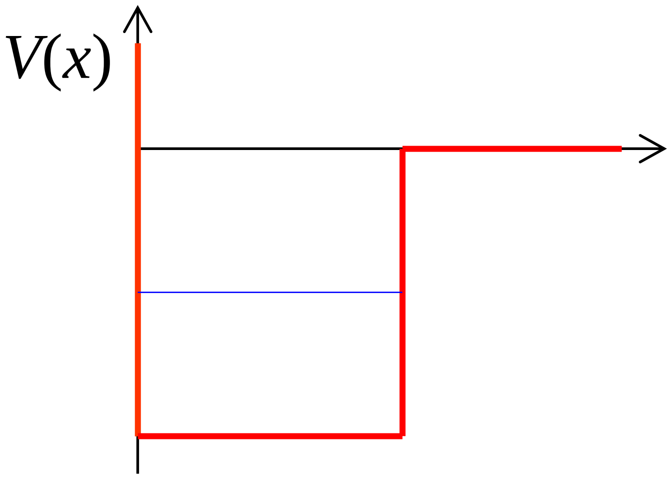
→ 角運動量がいい量子数ではない

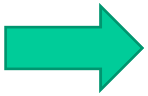
$$\psi_{nlm}(\boldsymbol{r}) = R_{nl}(r)Y_{lm}(\hat{\boldsymbol{r}}) \rightarrow \psi_{nK}(\boldsymbol{r}) = \sum_l R_{nl}(r)Y_{lK}(\hat{\boldsymbol{r}})$$

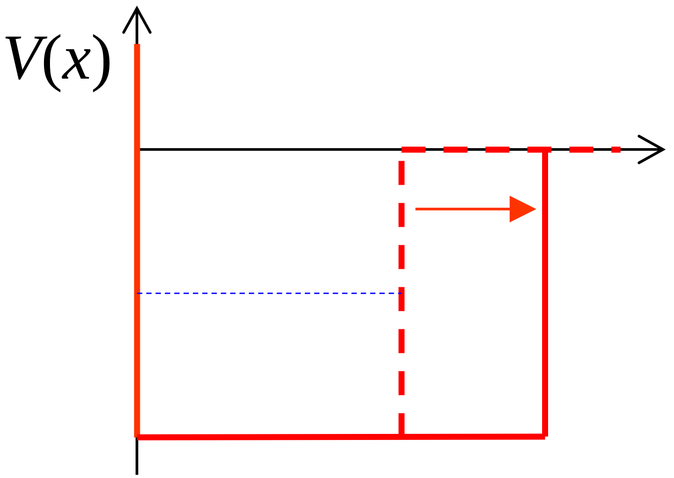
* 軸対称変形であれば l_z は保存

$$E_{nl} \rightarrow E_{nK}$$

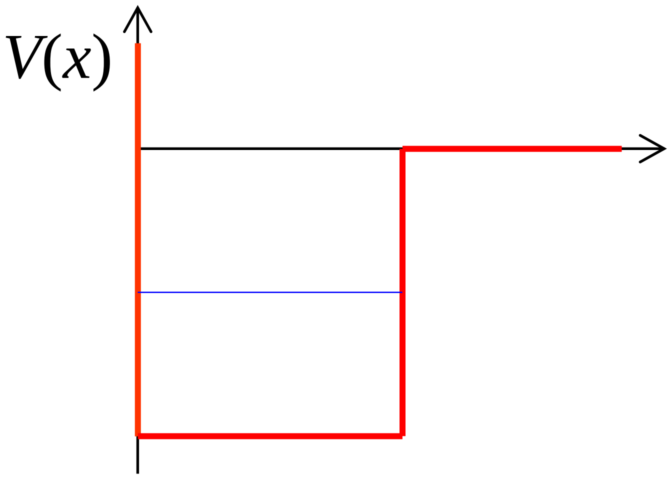
（準備）1次元井戸型ポテンシャル

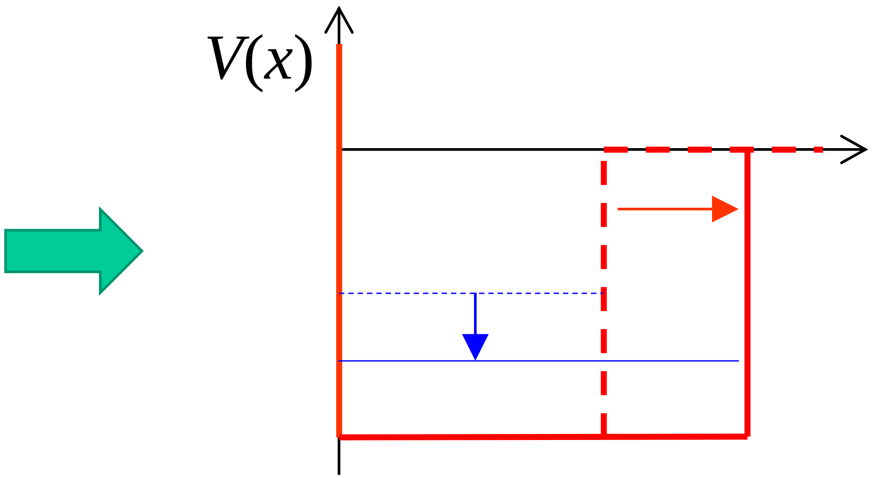




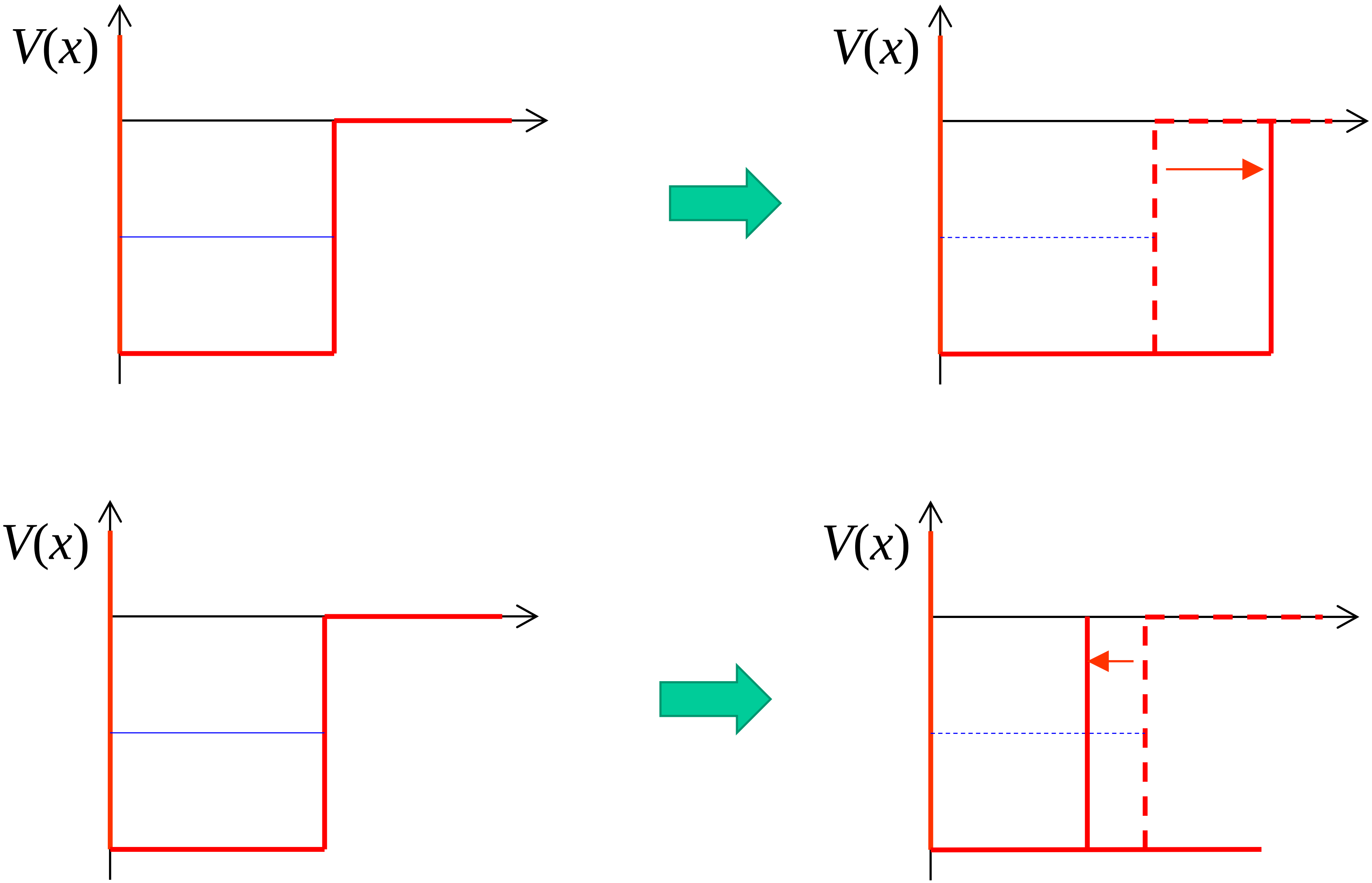


（準備）1次元井戸型ポテンシャル

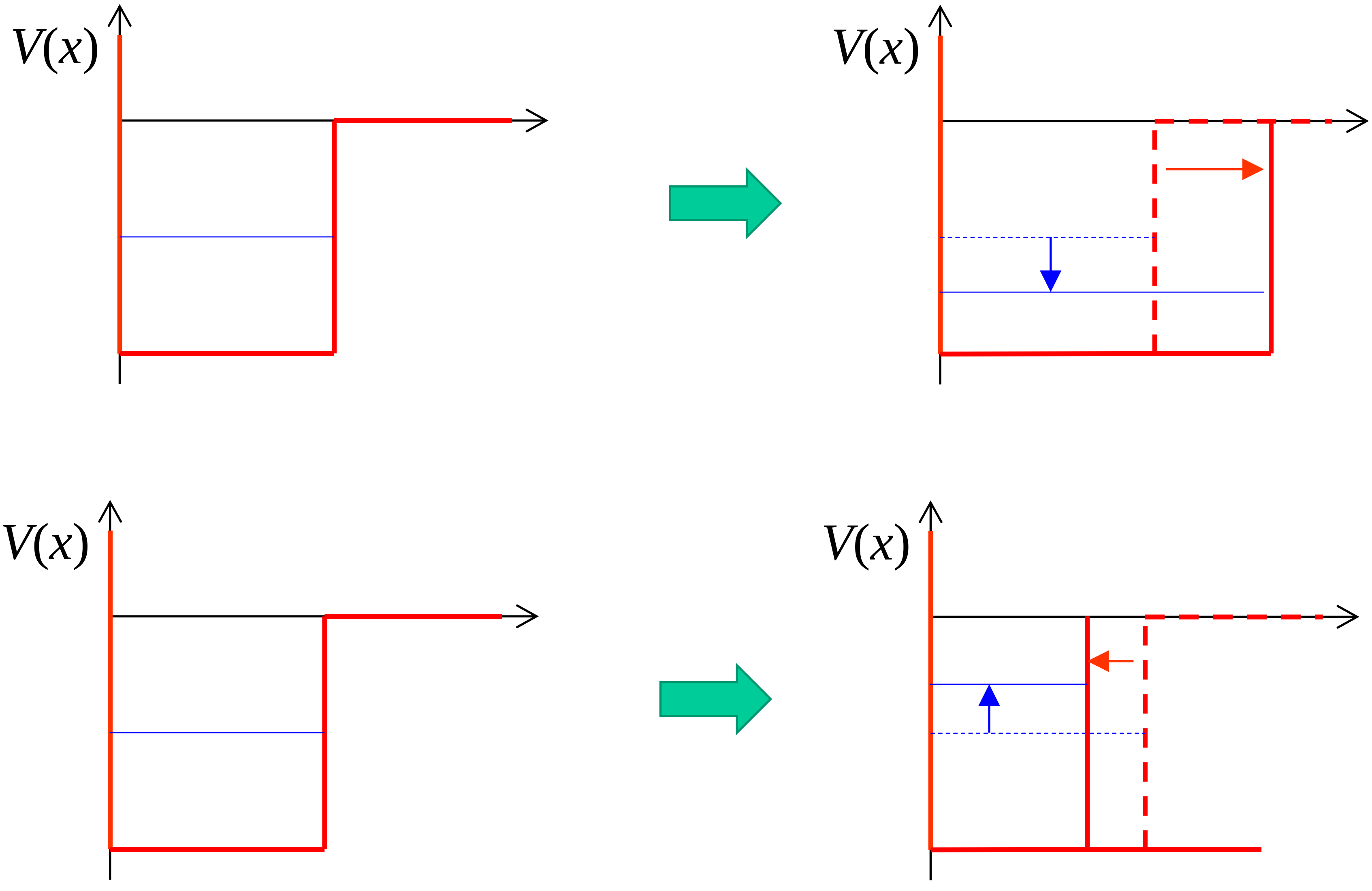




（準備）1次元井戸型ポテンシャル

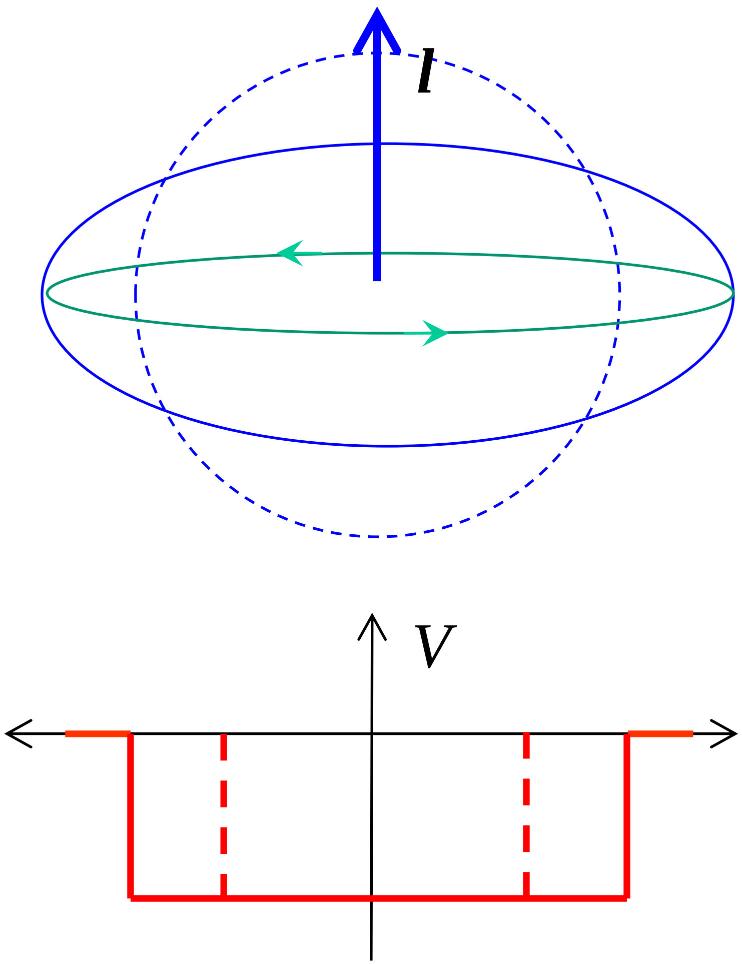


（準備）1次元井戸型ポテンシャル



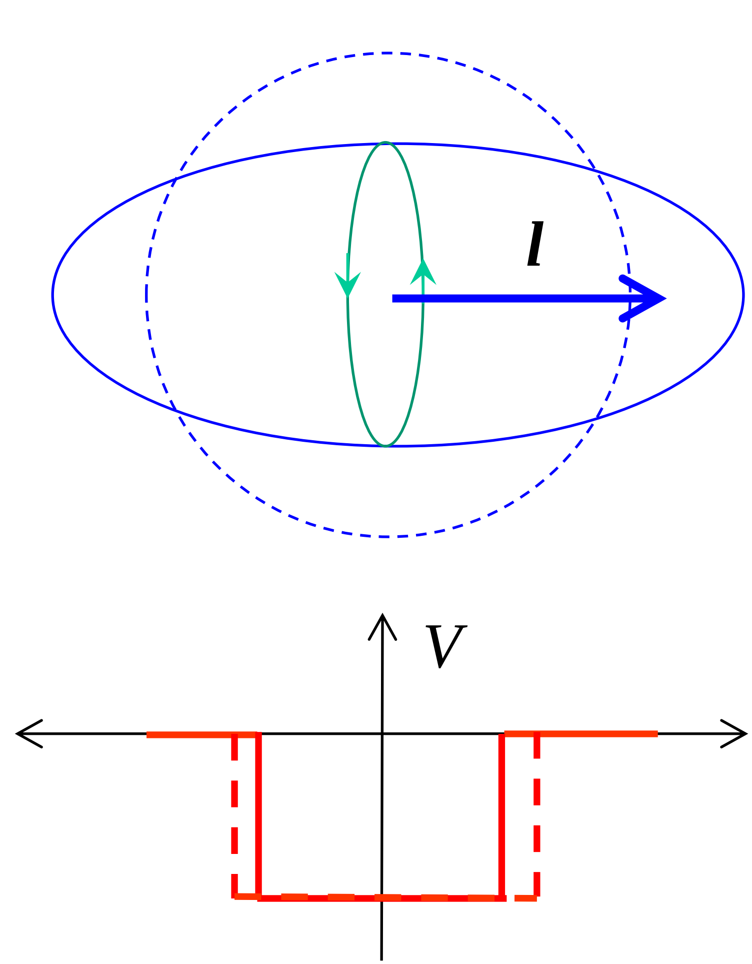
One-particle motion in a deformed potential

長軸に沿った運動



$E \rightarrow$ 小

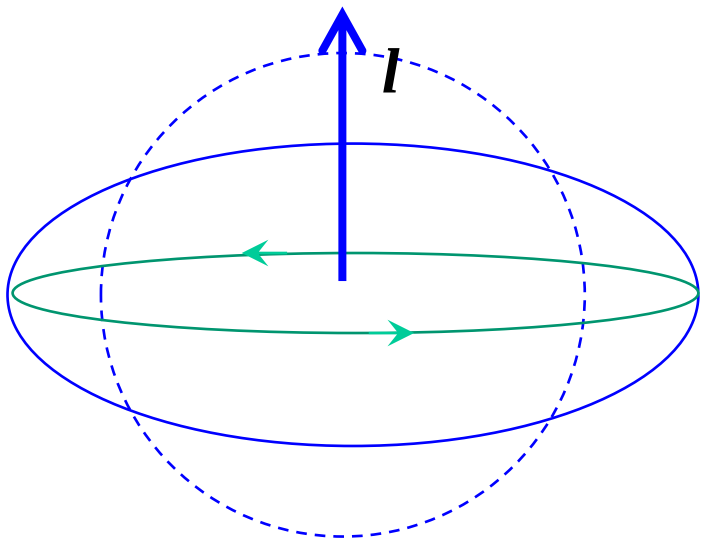
短軸に沿った運動



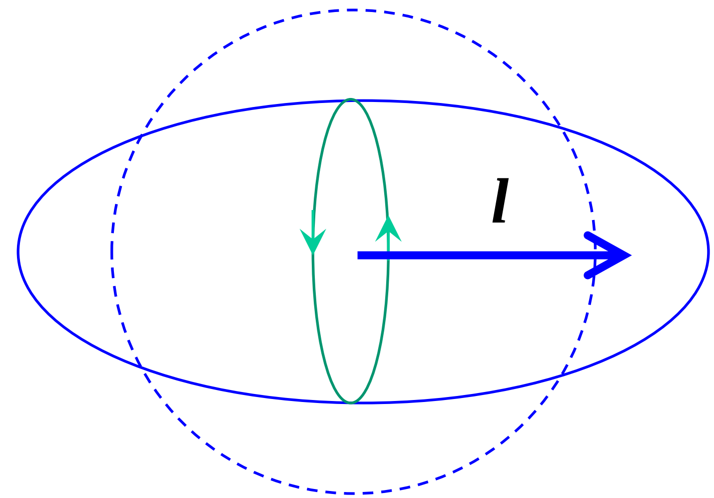
$E \rightarrow$ 大

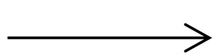
One-particle motion in a deformed potential

長軸に沿った運動

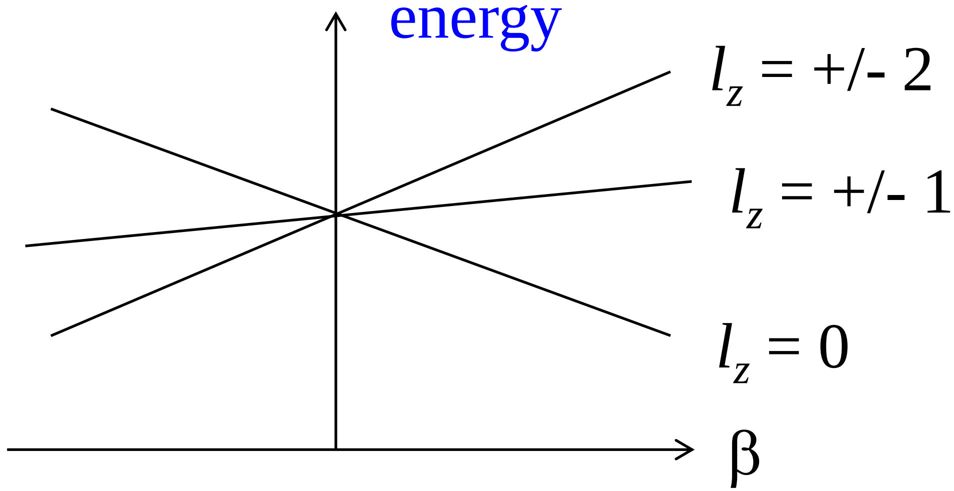


短軸に沿った運動





軌道が
スプリット



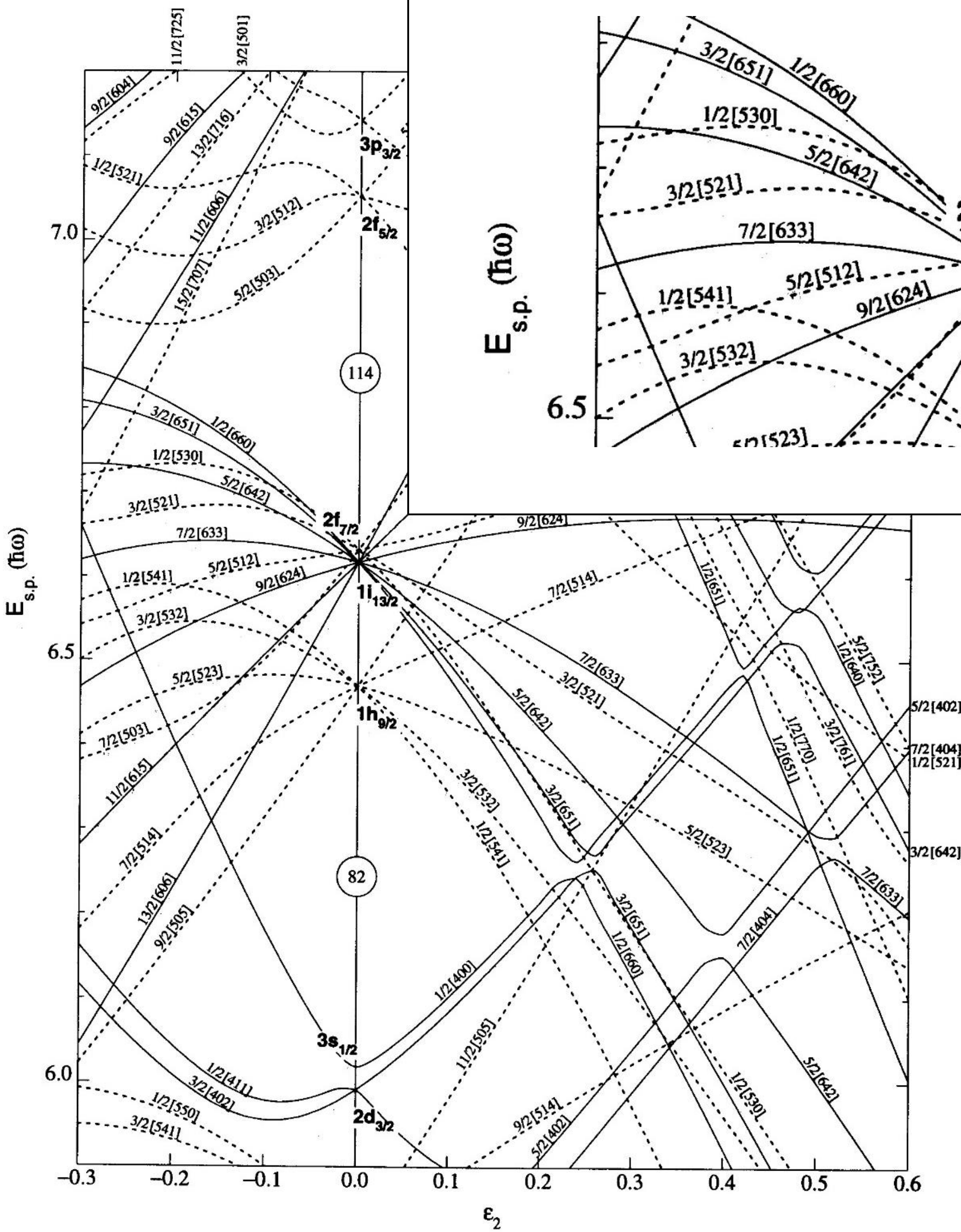
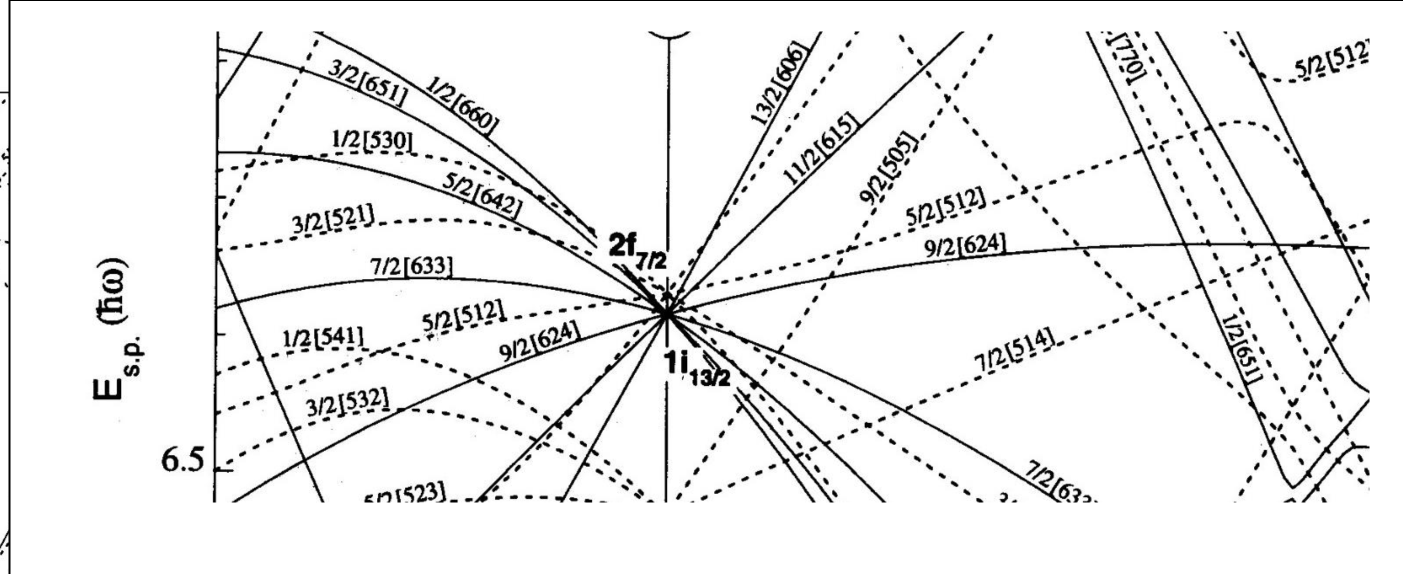


Figure 13. Nilsson diagram for protons, $Z \geq 82$ ($\varepsilon_4 = \varepsilon_2^2/6$).



Nilsson diagram

$h = T + V(r,\theta)$
の固有値