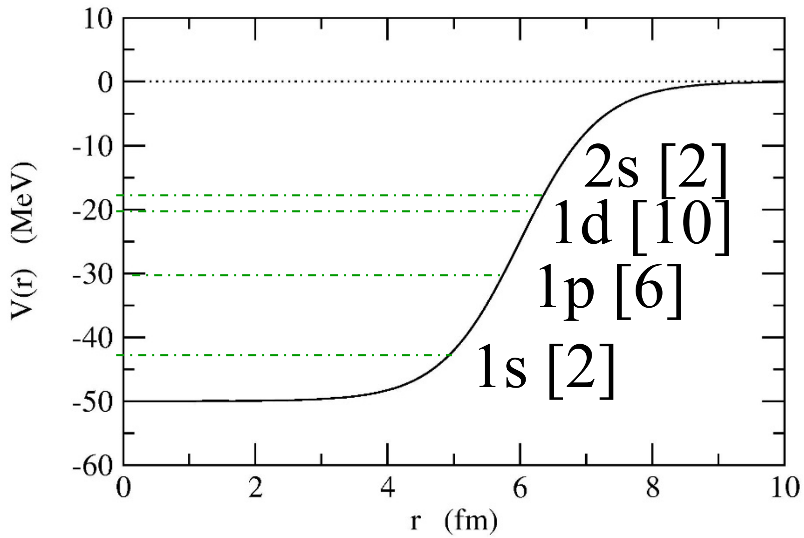
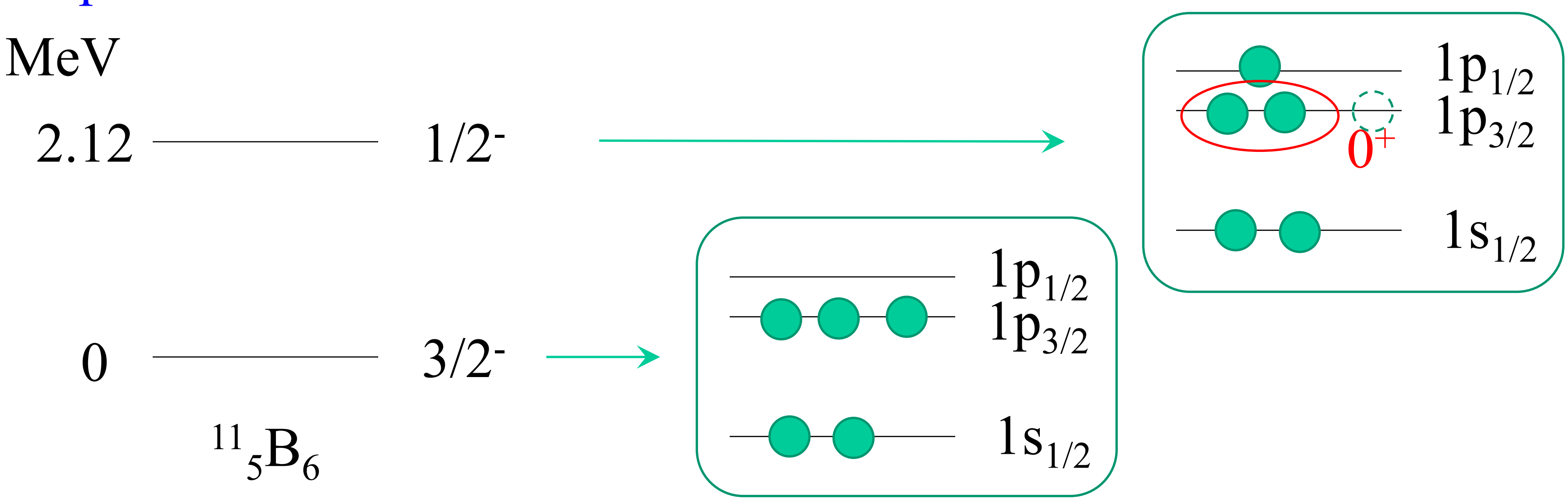
Mean-field approximation and deformation



f[14] → $f_{5/2}[6]$, $f_{7/2}[8]$

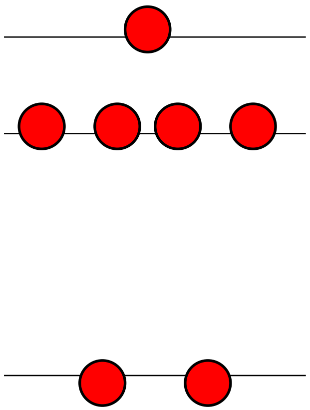
20+8 = 28

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：

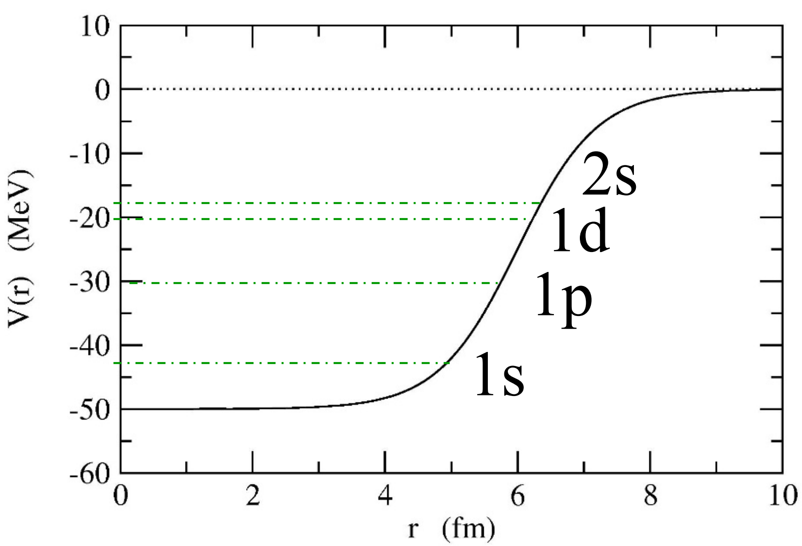


$1p_{1/2}$ [2]

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

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

^{11}Be の基底状態は $I^\pi = 1/2^-$



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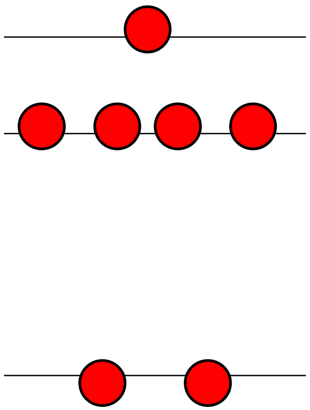

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$1s_{1/2}$ [2]

^{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:

0.32 MeV

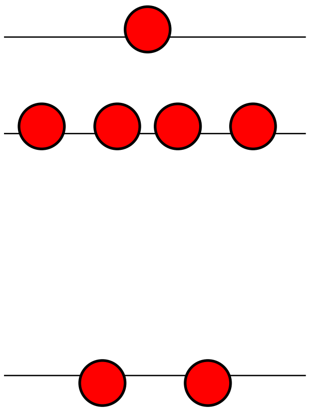
$1/2^{-}$

$1/2^{+}$

^{11}Be

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：



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かなり無理

実際の ^{11}Be の準位を見てみると:

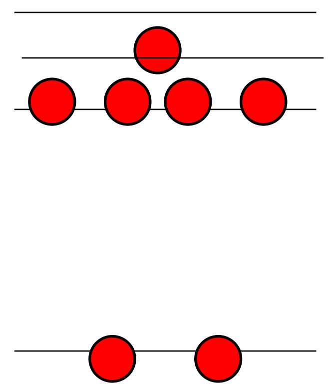
0.32 MeV

$1/2^{-}$

$1/2^{+}$

^{11}Be

?



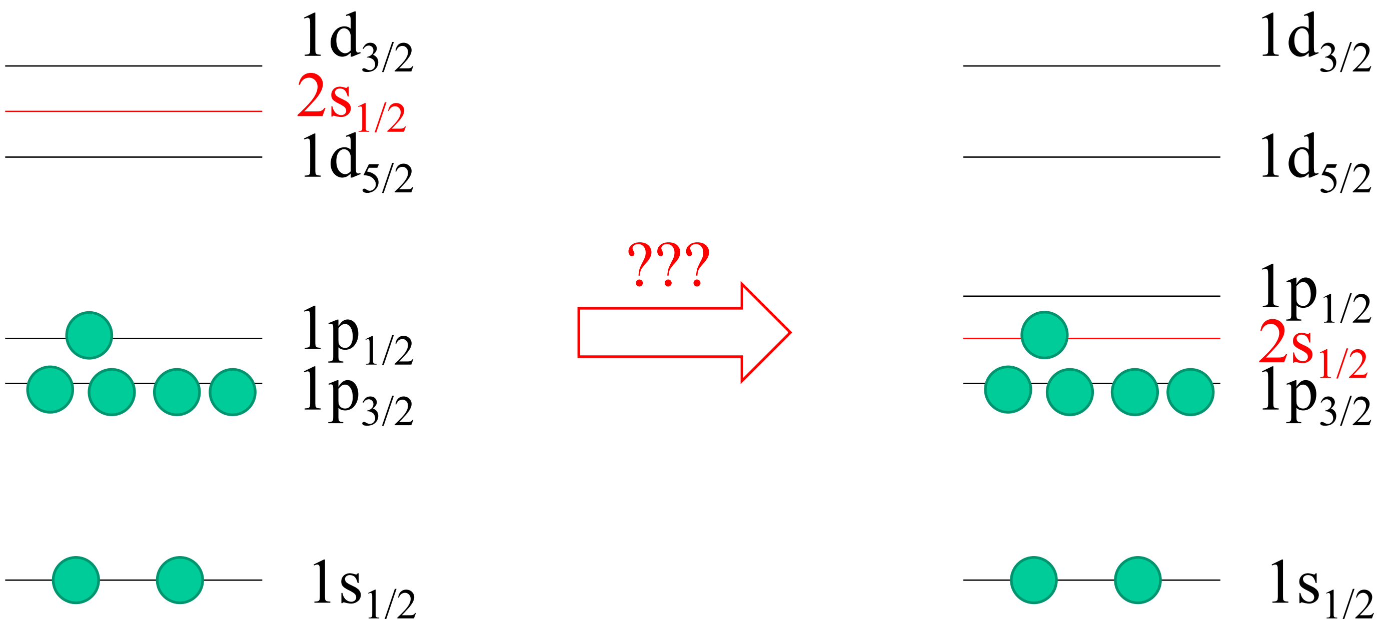
$1p_{1/2}$

$2s_{1/2}$

$1p_{3/2}$

$1s_{1/2}$

“parity inversion”



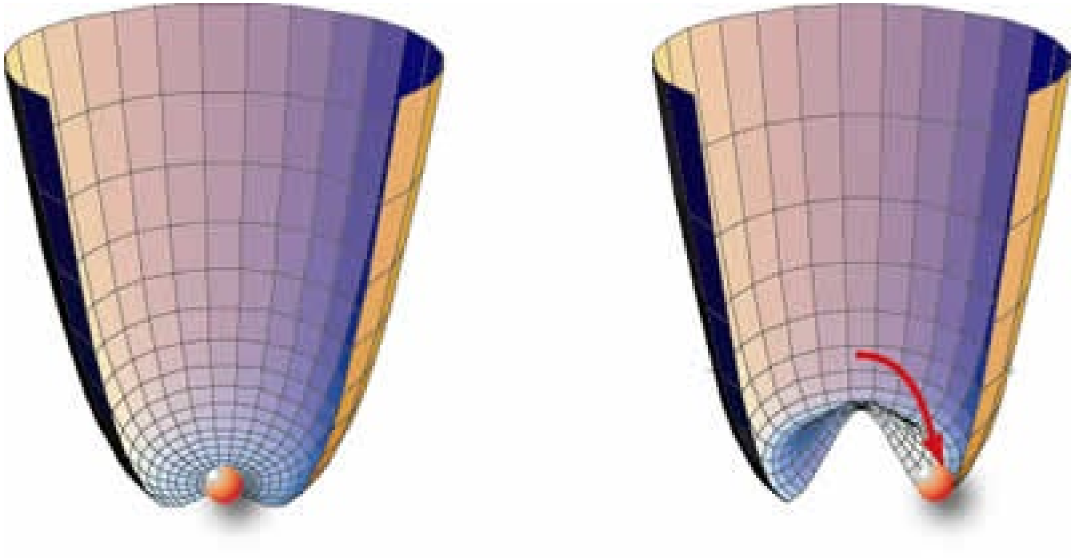
球形ポテンシャルに無理があるなら、変形させてみる?

Mean-field approximation and deformation

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

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

"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DFTでは常に破れる

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

$\Psi_{\rm MF}$ ：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

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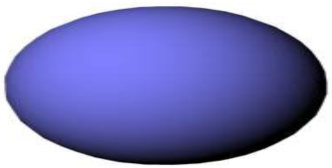
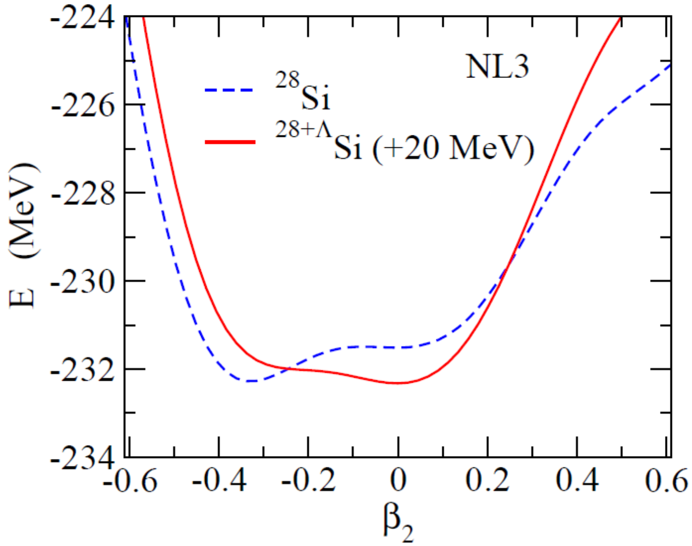
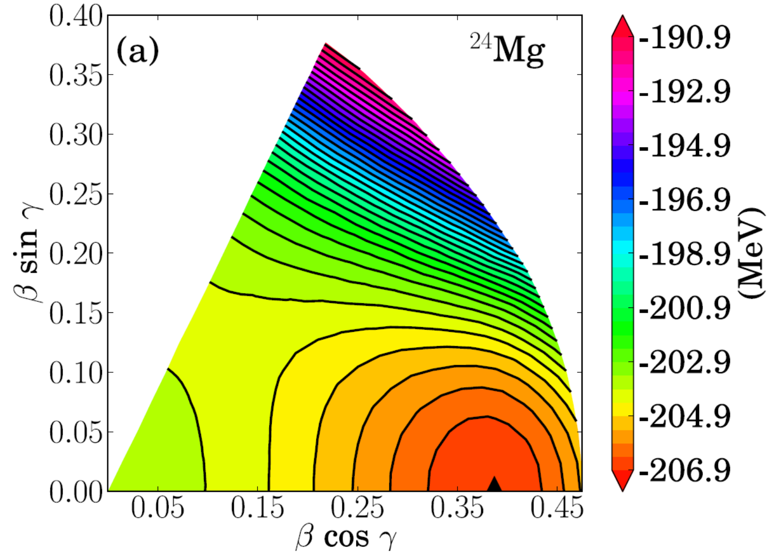
- **回転対称性**



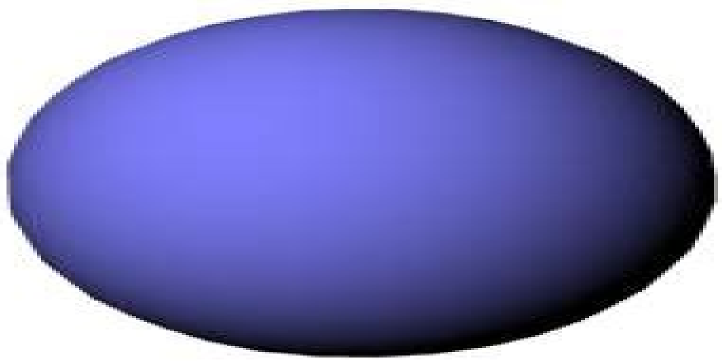
変形した基底状態





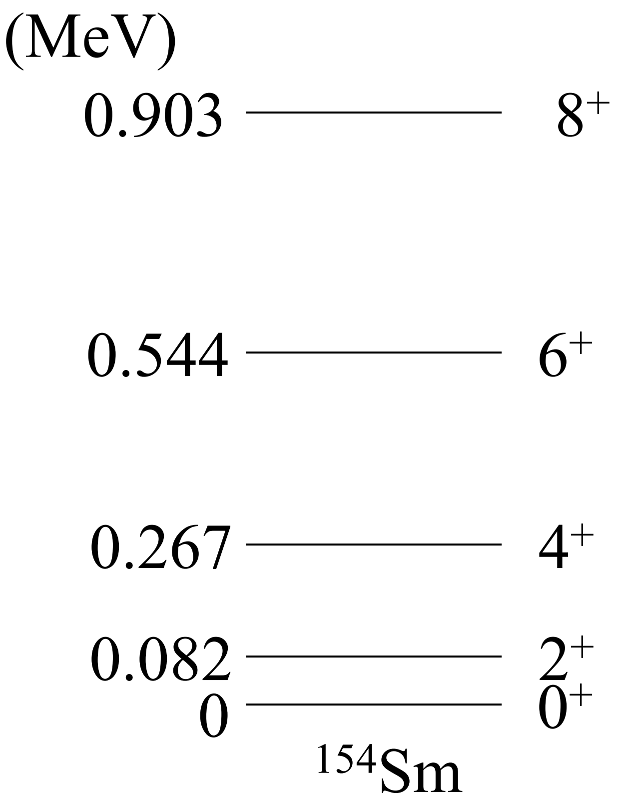
Nuclear Deformation

実験的な証拠

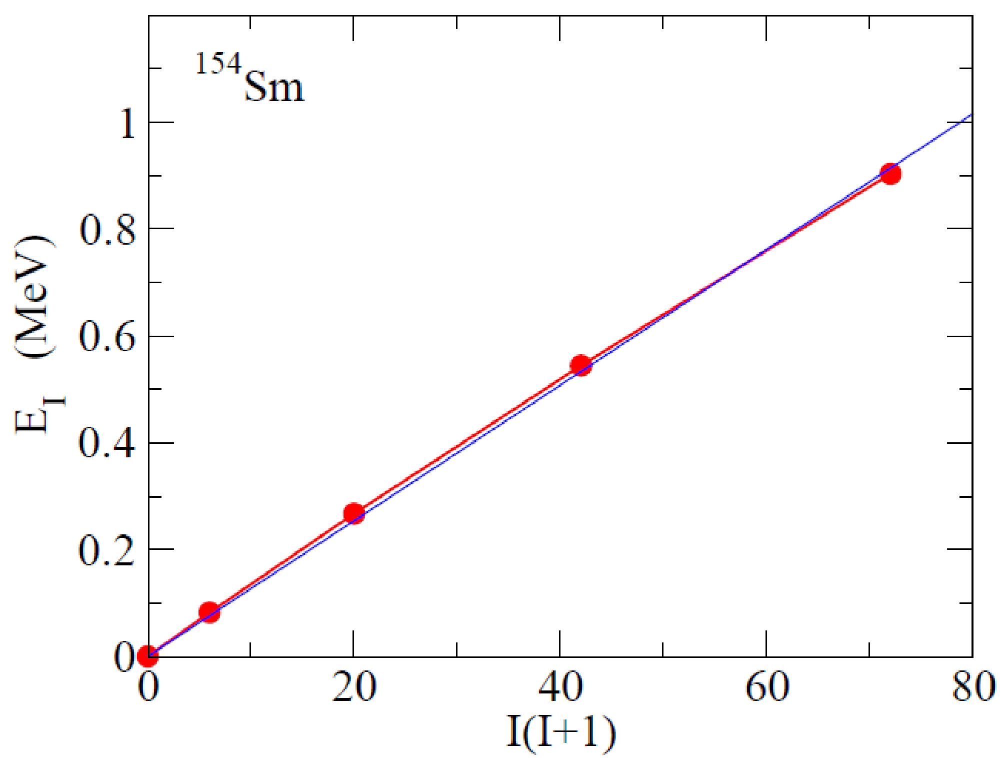


Nuclear Deformation

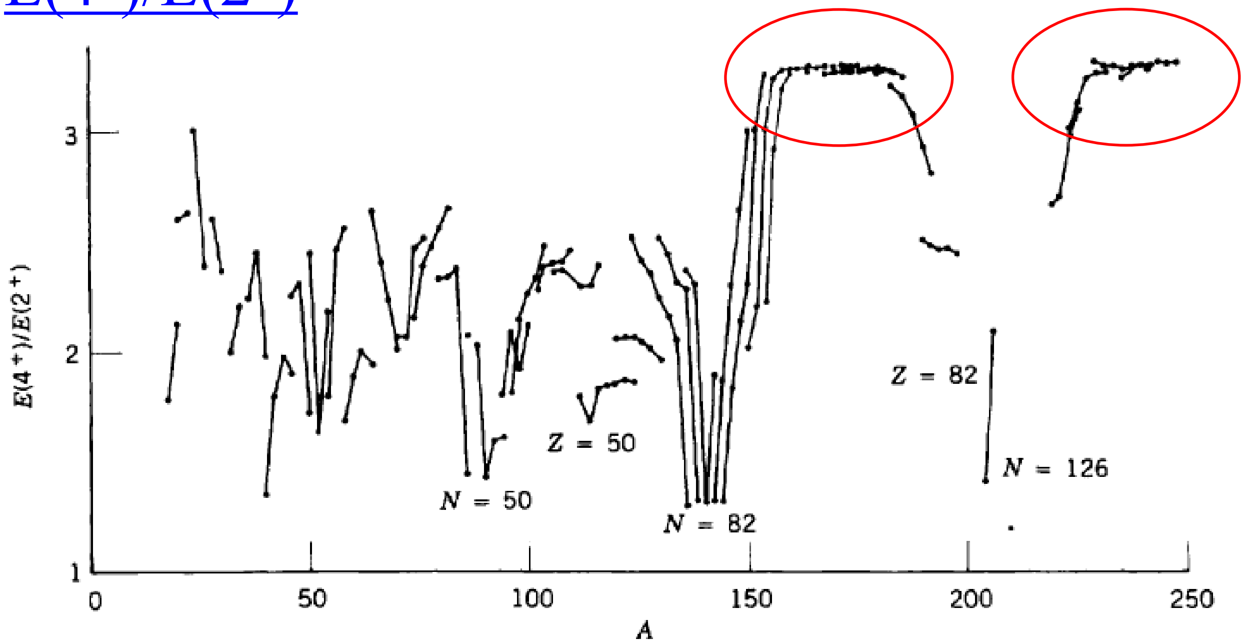
Excitation spectra of ^{154}Sm



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



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

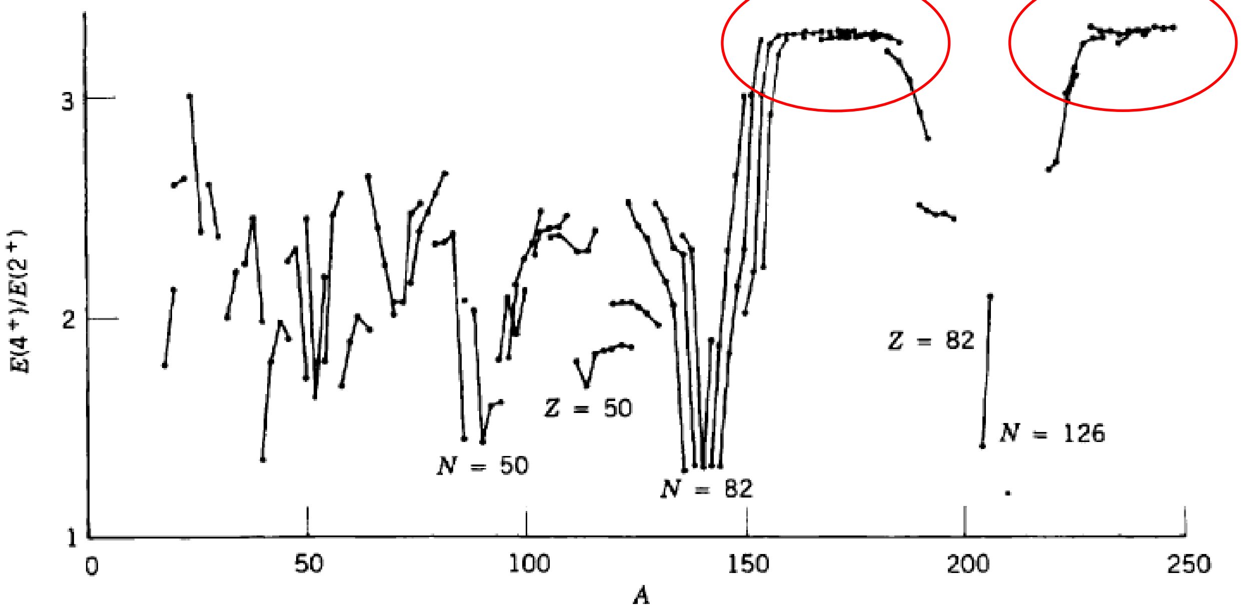


deformed nuclei:
$E(4^+)/E(2^+) \sim 3.3$

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

K.S. Krane, "Introductory Nuclear Physics"

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



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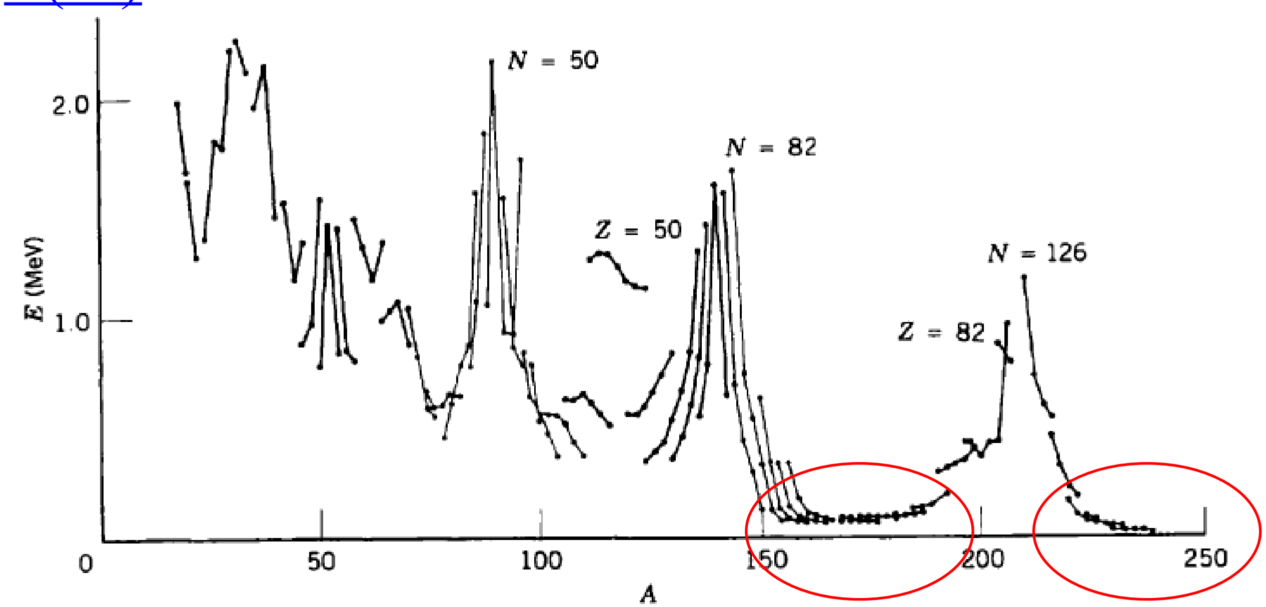
K.S. Krane. "Introductory Nuclear Physics"

$E(2^+)$

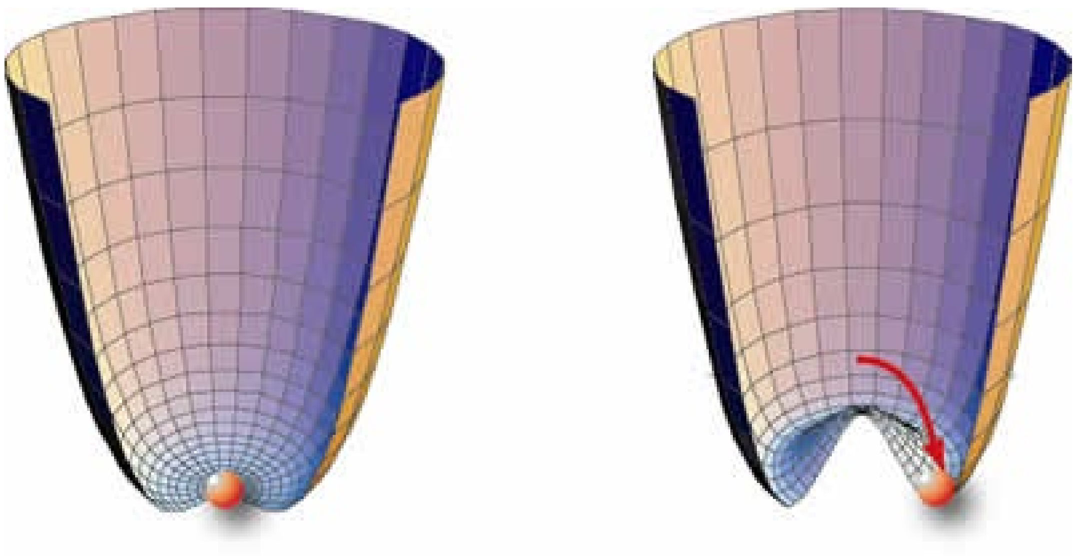


a small energy
→ spontaneously
symm. breaking

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

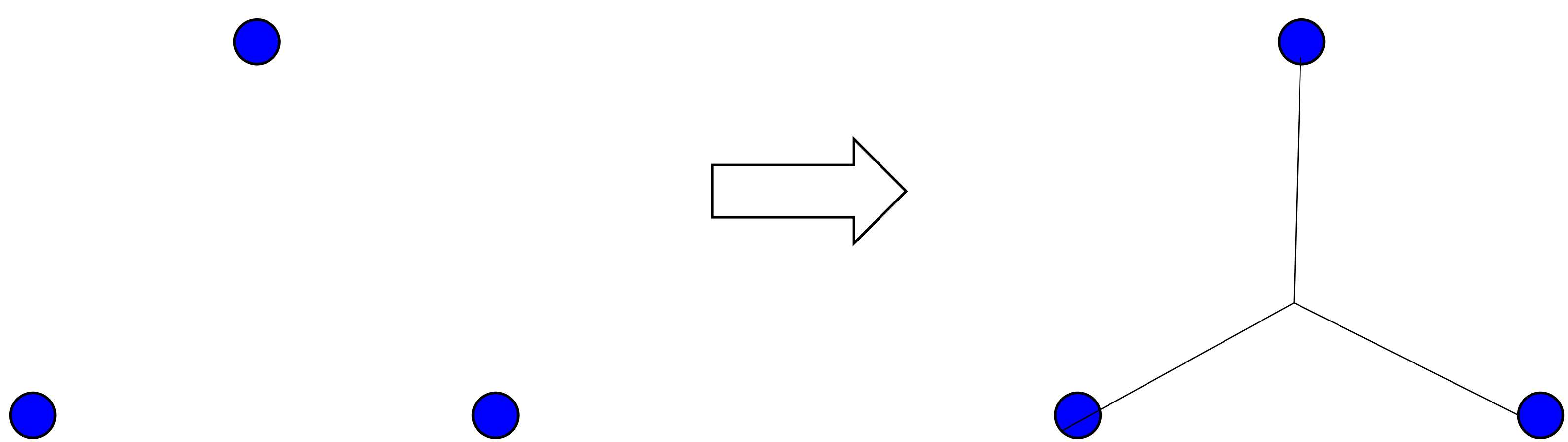
There are a few dots.

- 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



Quiz: spontaneous symmetry breaking

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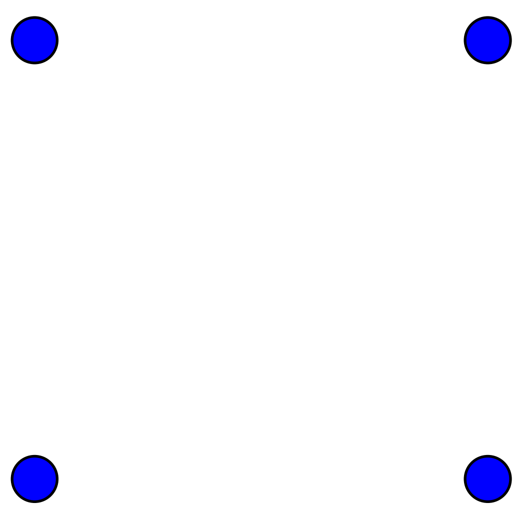
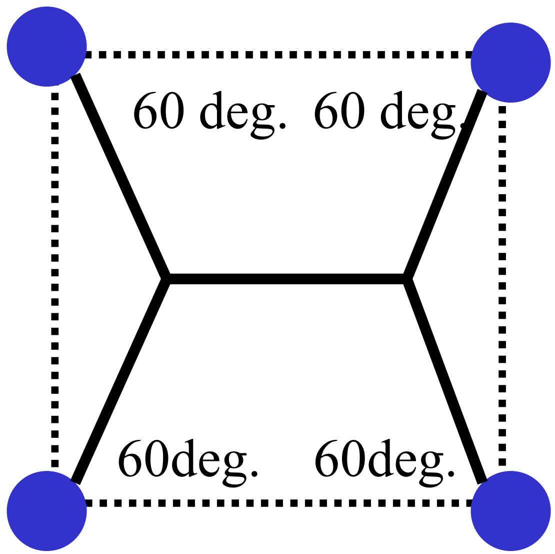
- Two lines can cross.
- Connect the dots so that one can go from one dot to all the other dots.

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

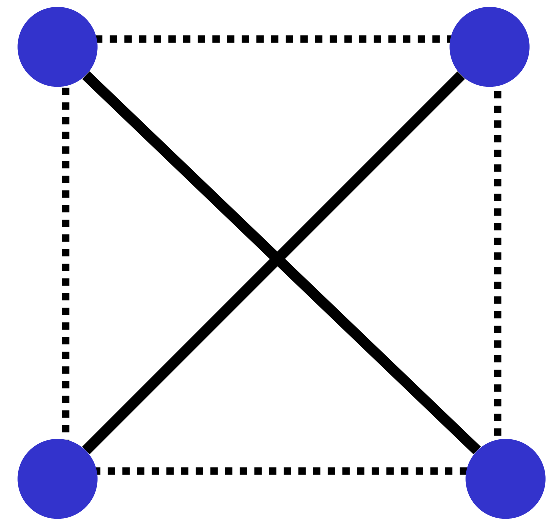
(question) how about the case for a square?



(the answer)



cf.



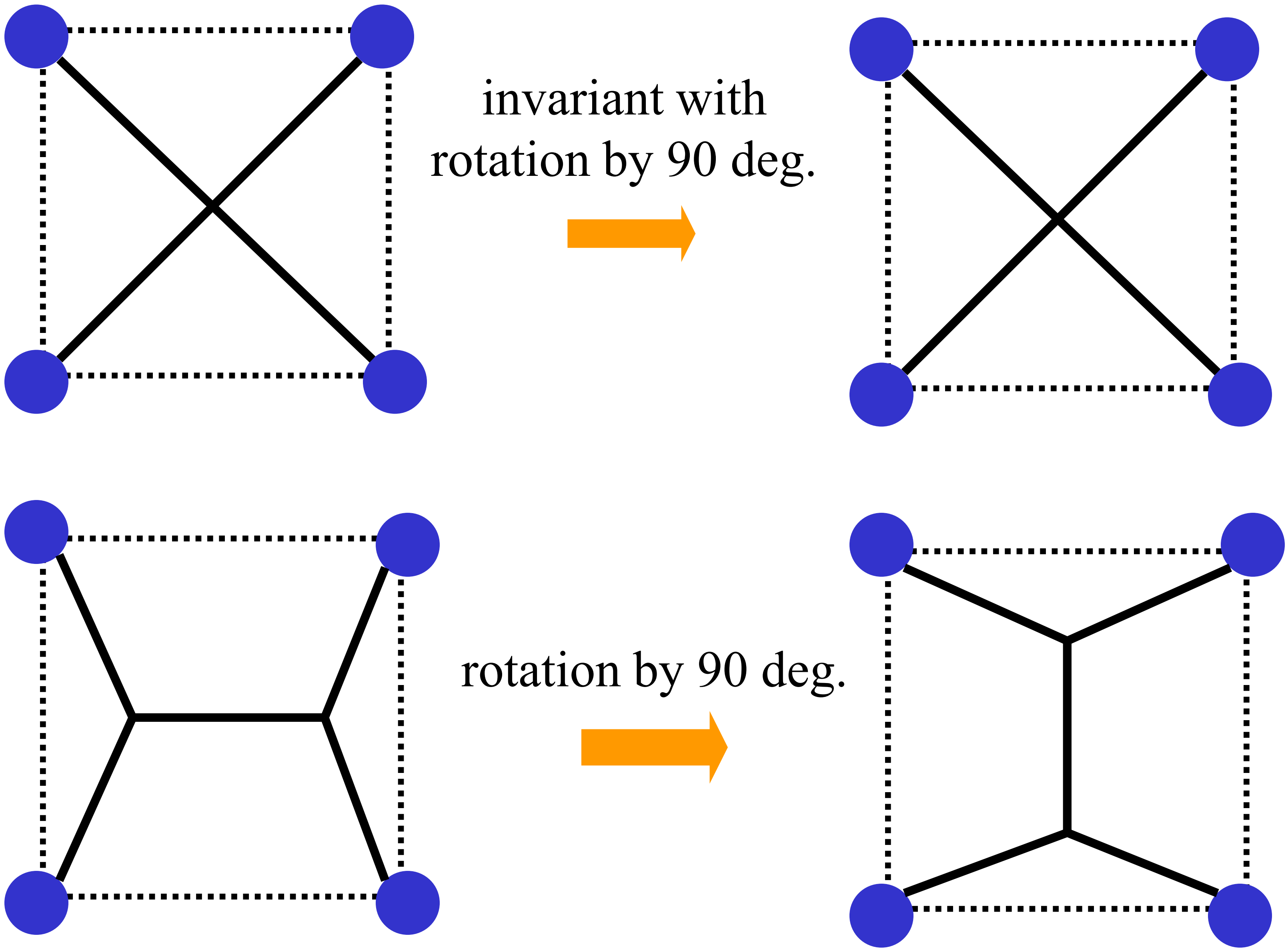
Length

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

Length

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

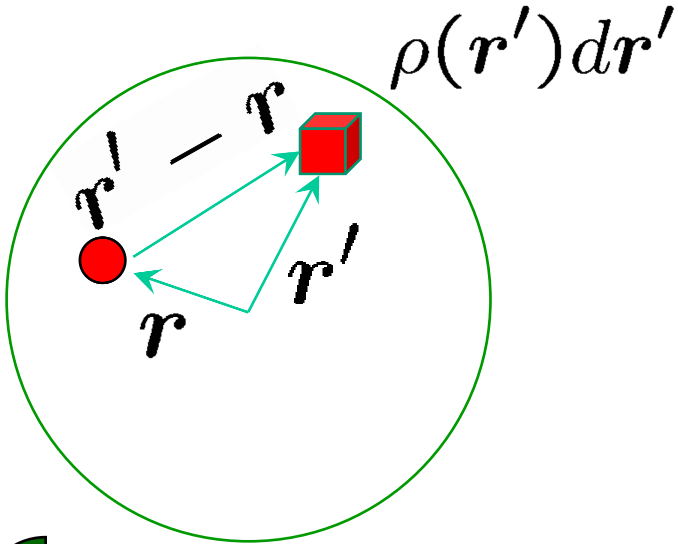
Ref. Takeshi Koike,
"Genshikaku Kenkyu" Vol. 52 No. 2, p. 14



a good example of spontaneous symm. breaking

Courtesy: Takeshi Koike

One-particle motion in a deformed potential

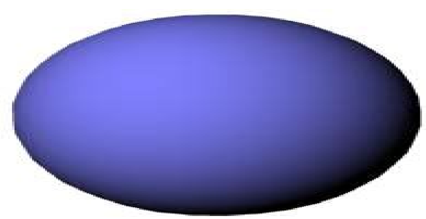


naively speaking,

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

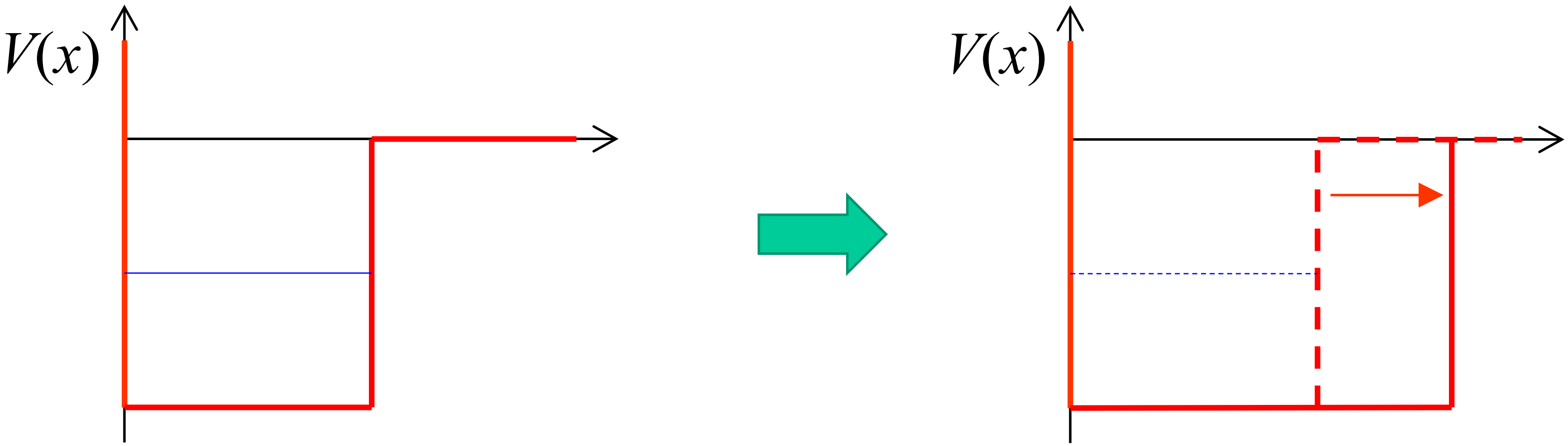
$$\boxed{V(\boldsymbol{r}) \sim \int v(\boldsymbol{r},\boldsymbol{r}')\rho(\boldsymbol{r}')d\boldsymbol{r}' \sim -g\rho(\boldsymbol{r}) \quad \text{if} \quad v(\boldsymbol{r},\boldsymbol{r}') = -g\delta(\boldsymbol{r}-\boldsymbol{r}')}$$

$\rightarrow V(r)$



$\rightarrow V(r,\theta)$

（準備）1次元井戸型ポテンシャル



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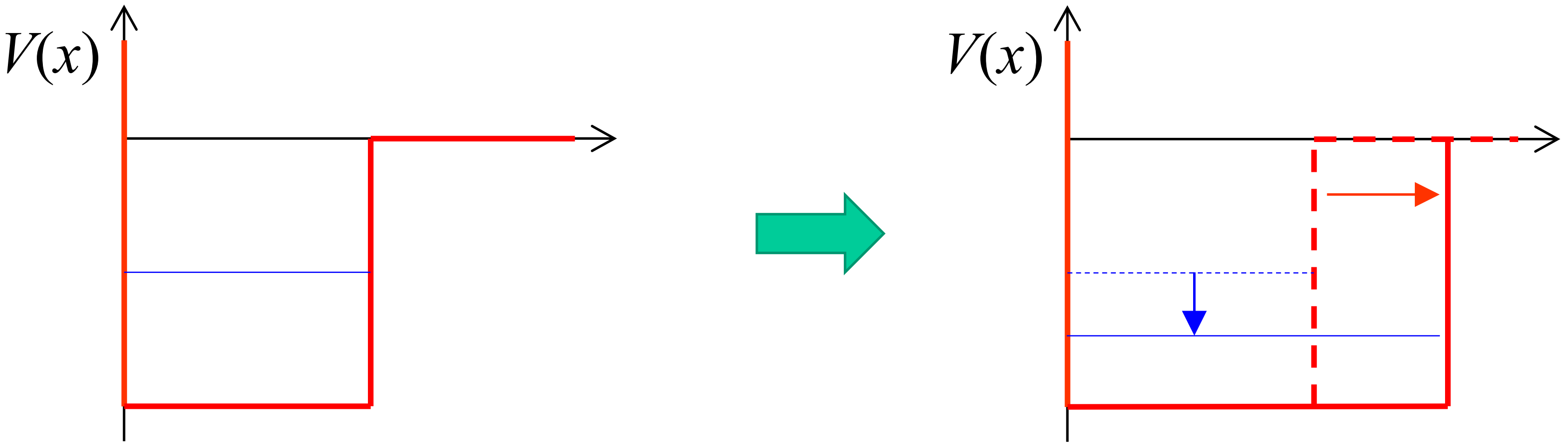
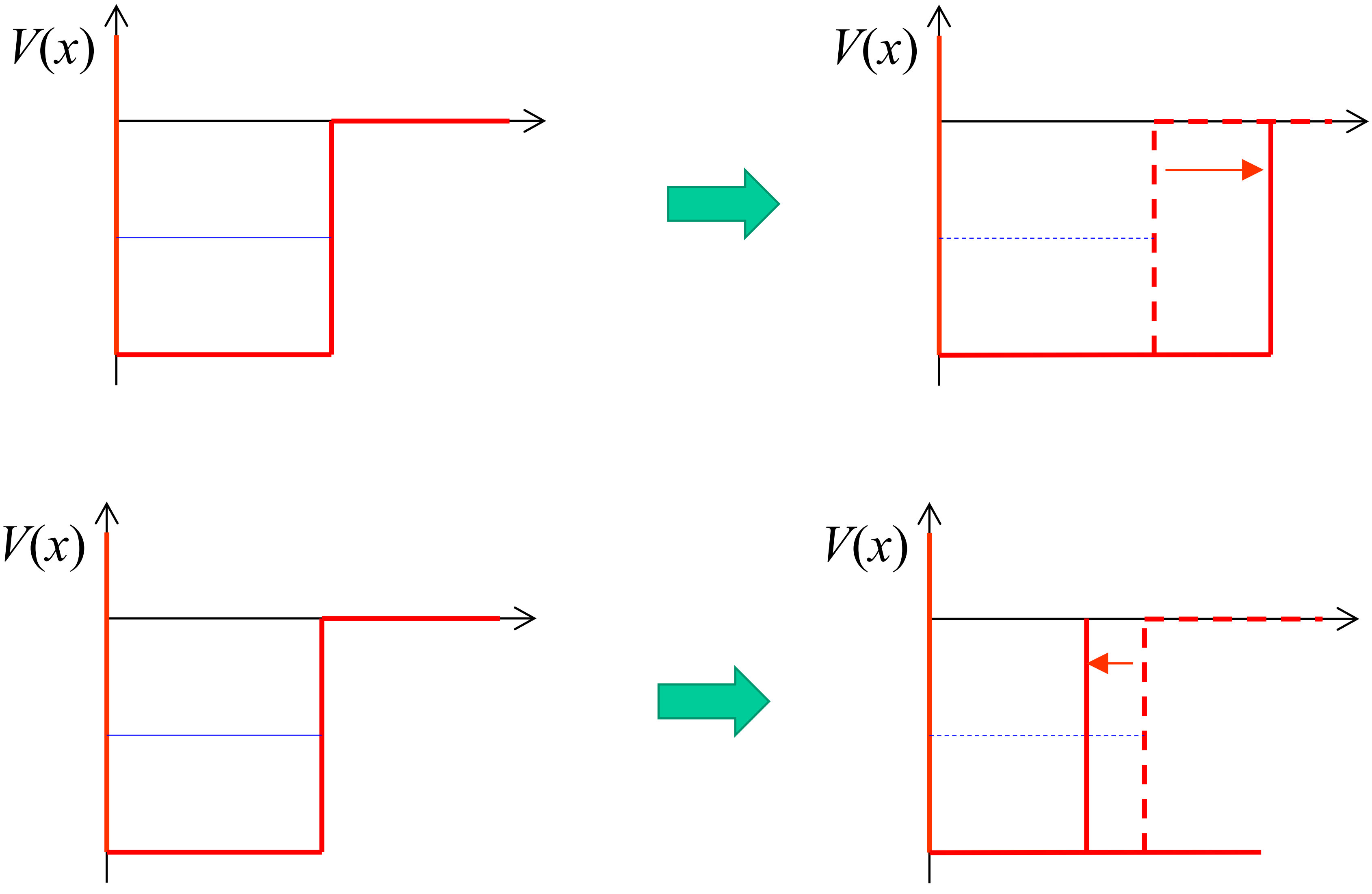
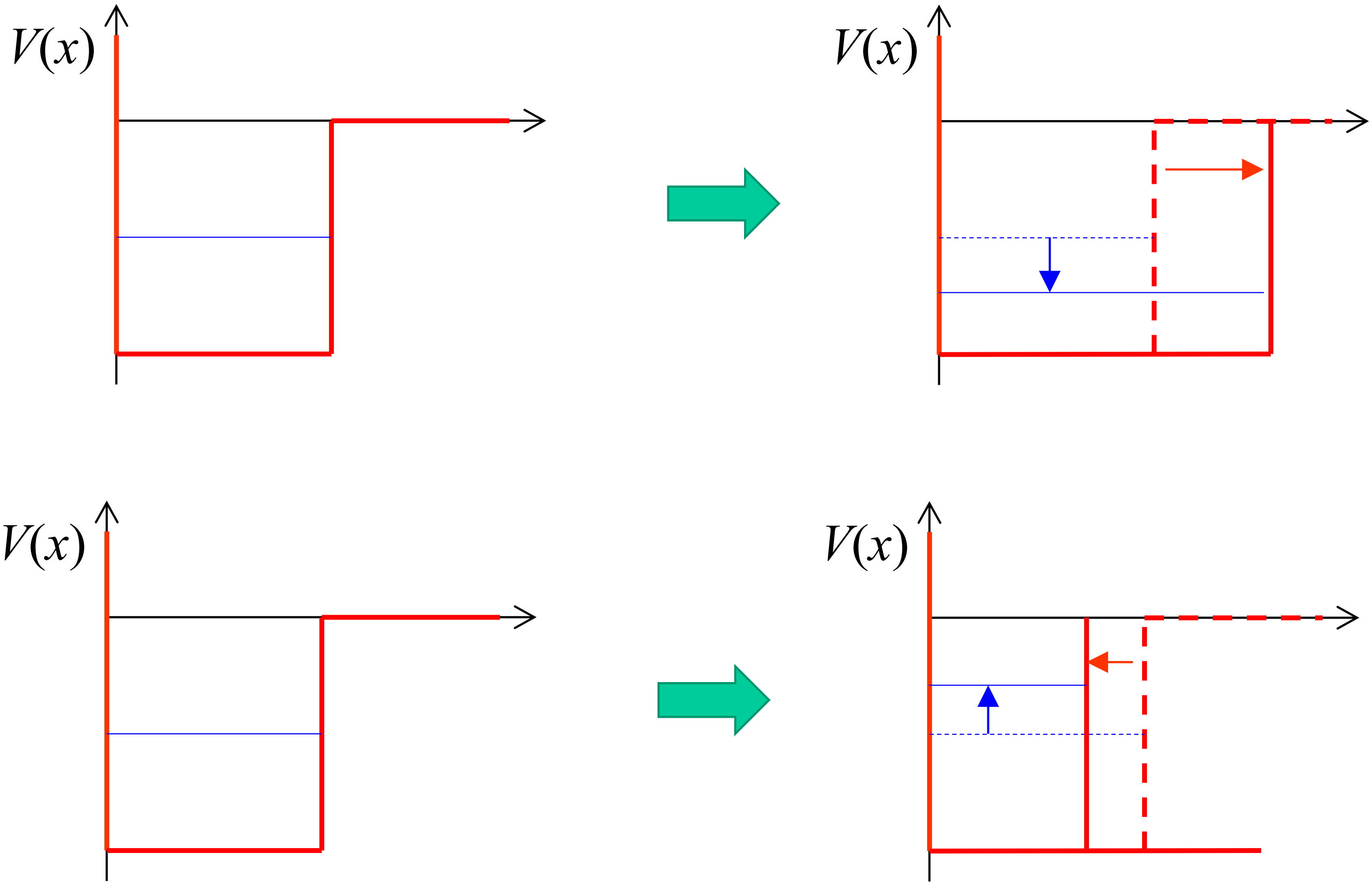


（準備）1次元井戸型ポテンシャル

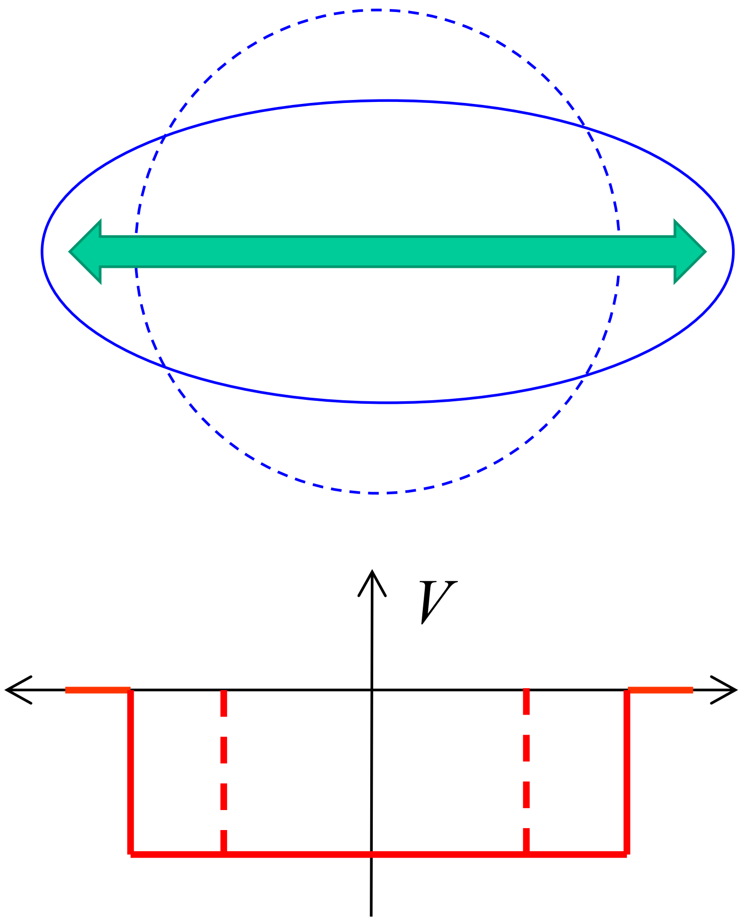


（準備）1次元井戸型ポテンシャル



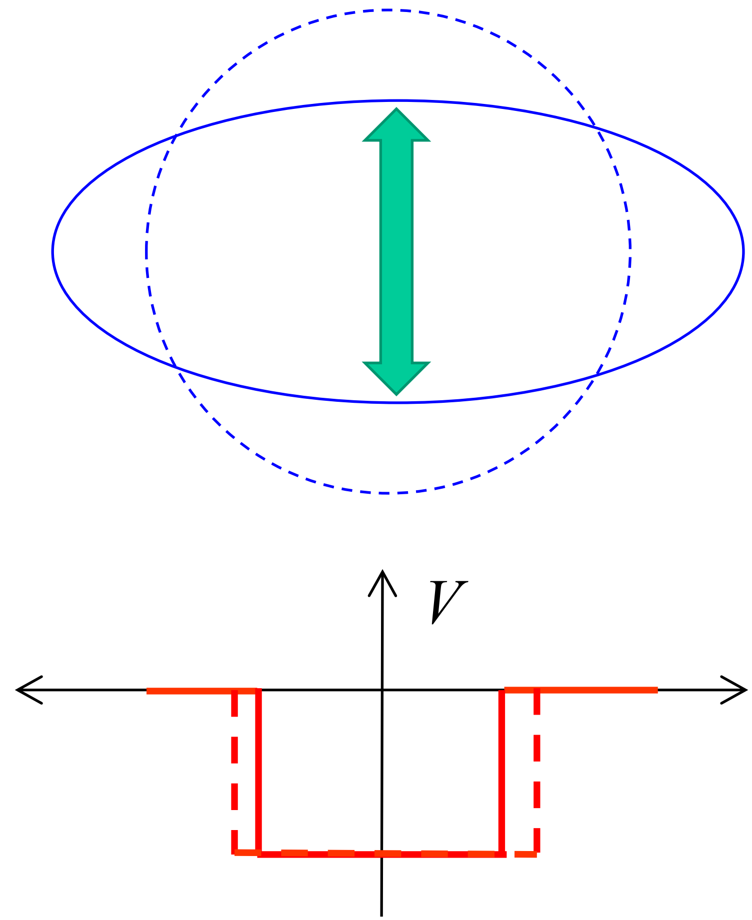
One-particle motion in a deformed potential

長軸に沿った運動



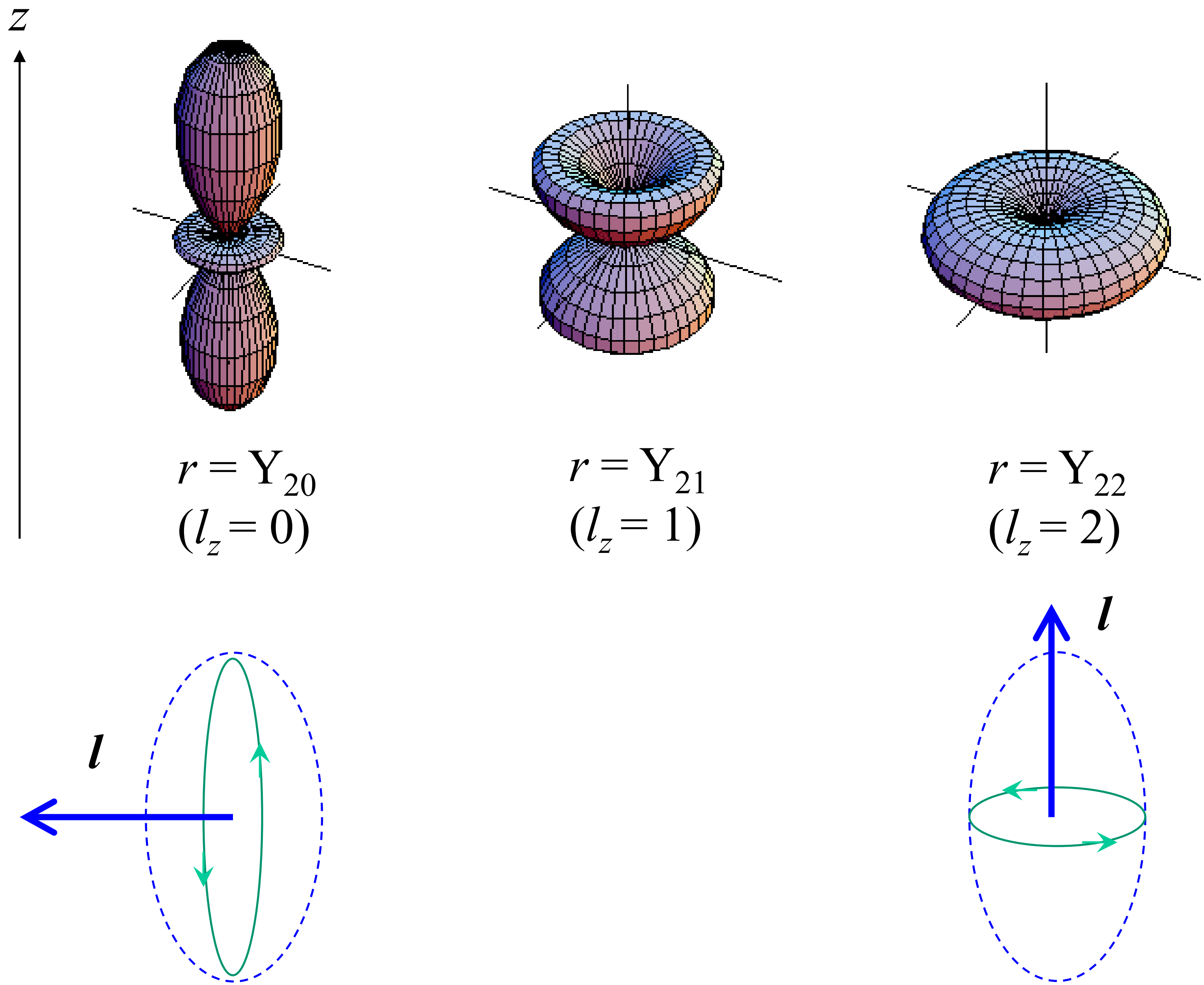
$E \rightarrow$ 小

短軸に沿った運動



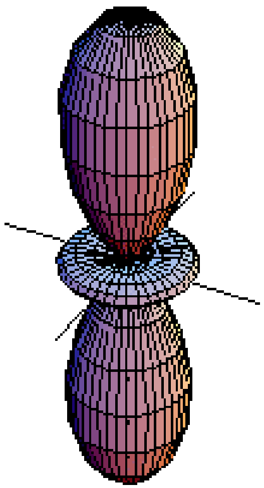
$E \rightarrow$ 大

$l = 2$

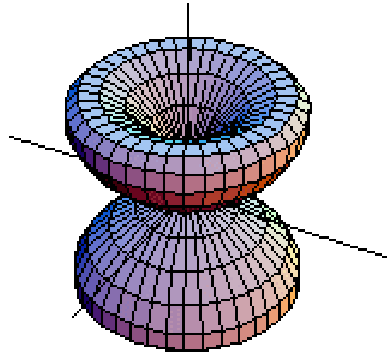


$l = 2$

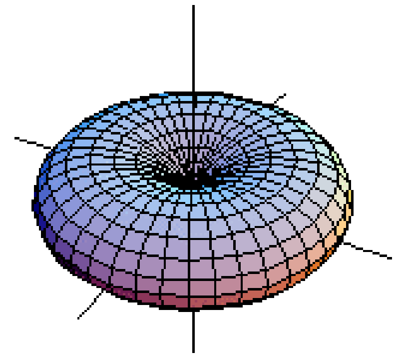
z



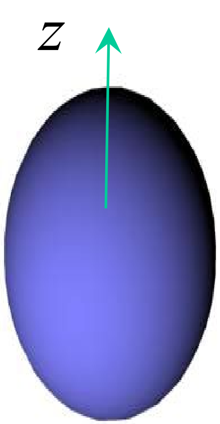
$r = Y_{20}$
$(l_z = 0)$



$r = Y_{21}$
$(l_z = 1)$



$r = Y_{22}$
$(l_z = 2)$

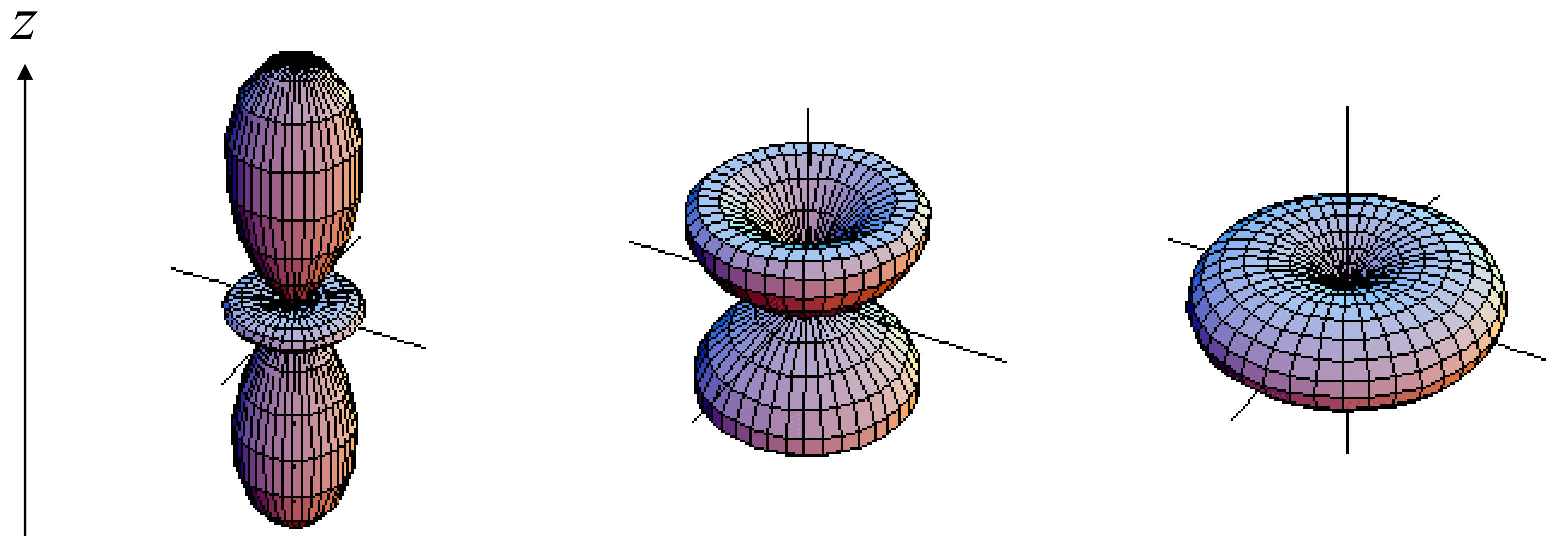


なら

$E \rightarrow$ 小

$E \rightarrow$ 大

$l = 2$

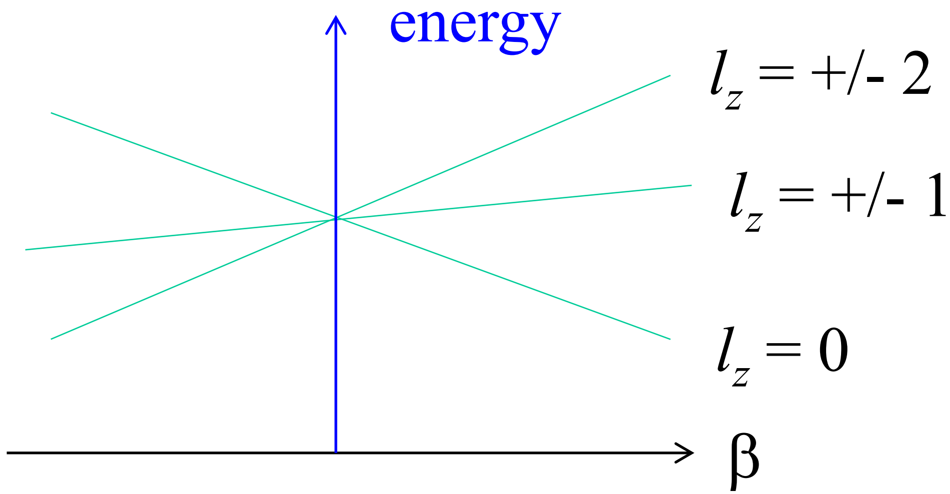


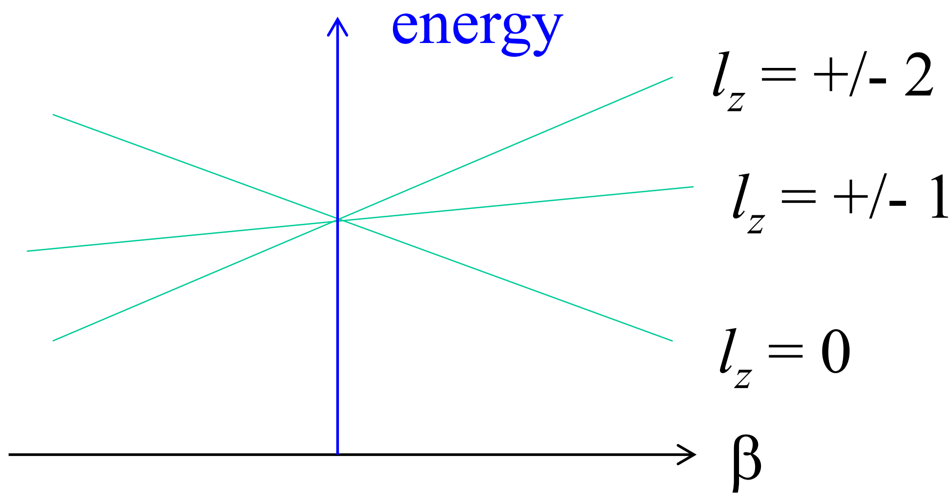
$r = Y_{20}$ $(l_z = 0)$

$r = Y_{21}$ $(l_z = 1)$

$r = Y_{22}$ $(l_z = 2)$

軌道が
スプリット





波動関数

(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

$$\phi_{nll_z}(r,\theta,\phi) \to \phi_{nl_z}(r,\theta,\phi) = \sum_l \psi_{nl}(r) Y_{ll_z}(\theta,\phi)$$

いろいろな角運動量成分が混じる

＊軸対称変形であれば l_z は保存

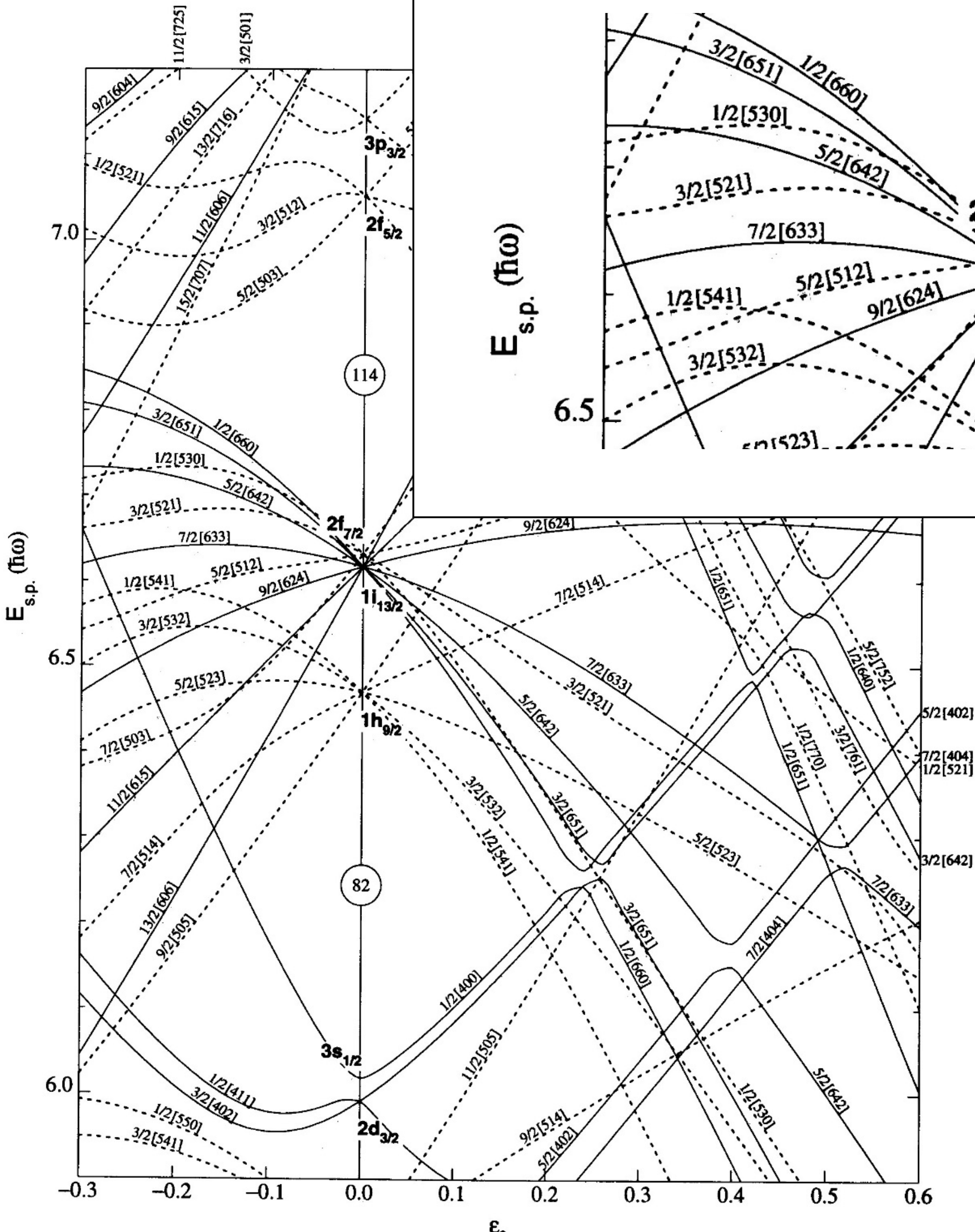
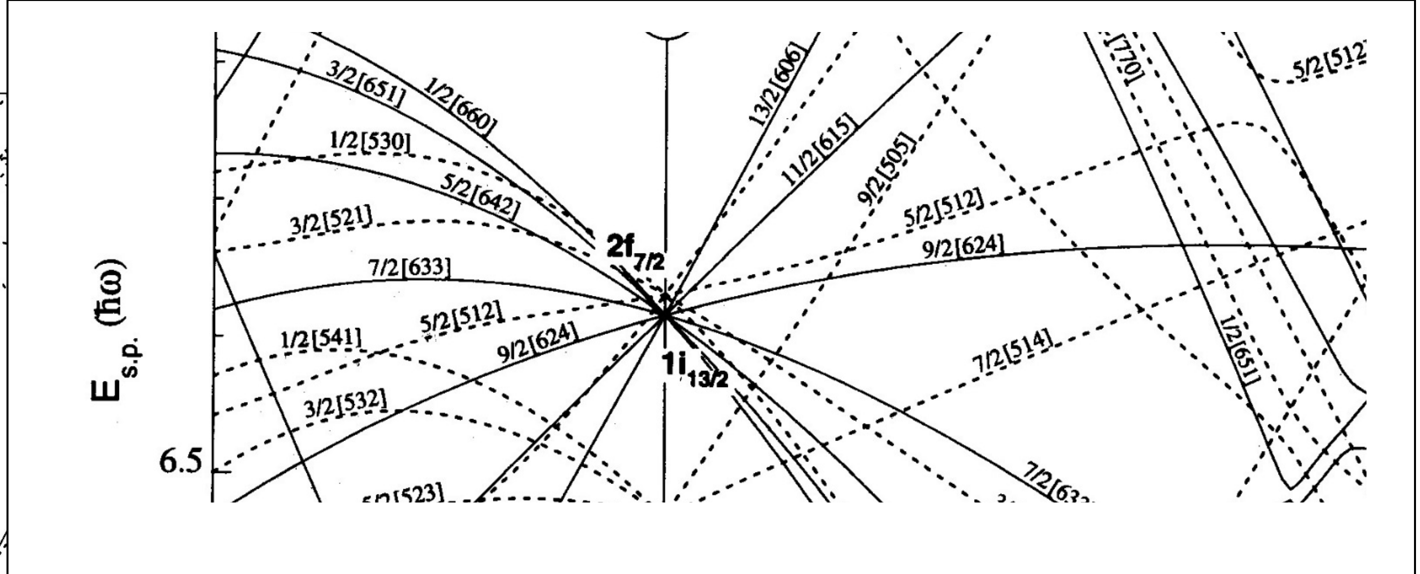


Figure 13. Nilsson diagram for protons, Z ≥ 82 ($\varepsilon_4 = \varepsilon_2^2/6$).

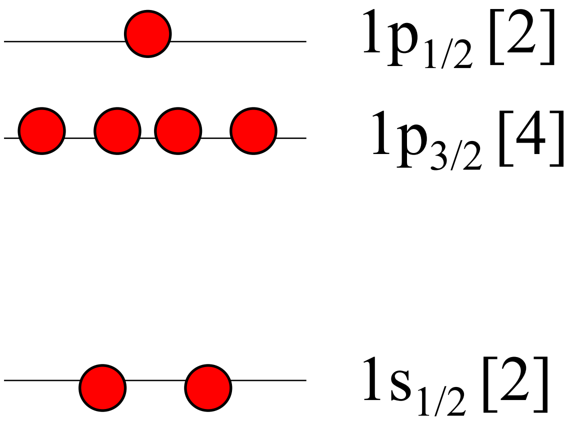


Nilsson diagram

$h = T + V(r,\theta)$
の固有値

殻模型による$^{11}_{4}Be_7$ のレベル

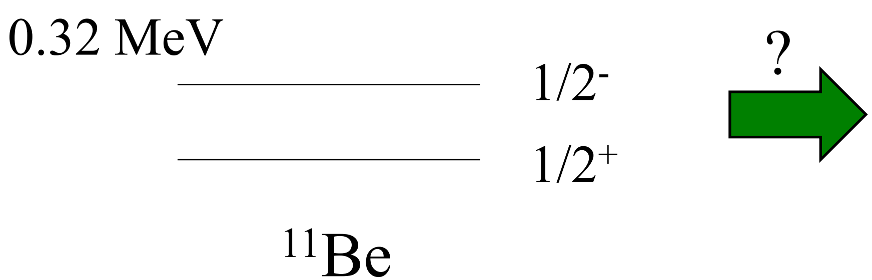
殻模型（球形ポテンシャルの準位）で考えた場合：

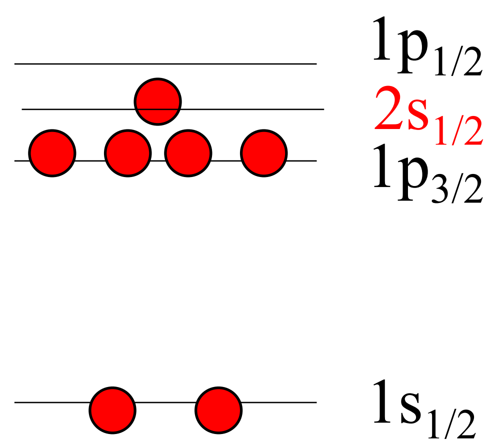


^{11}Be の基底状態は $I^{\pi} = 1/2^{-}$

かなり無理

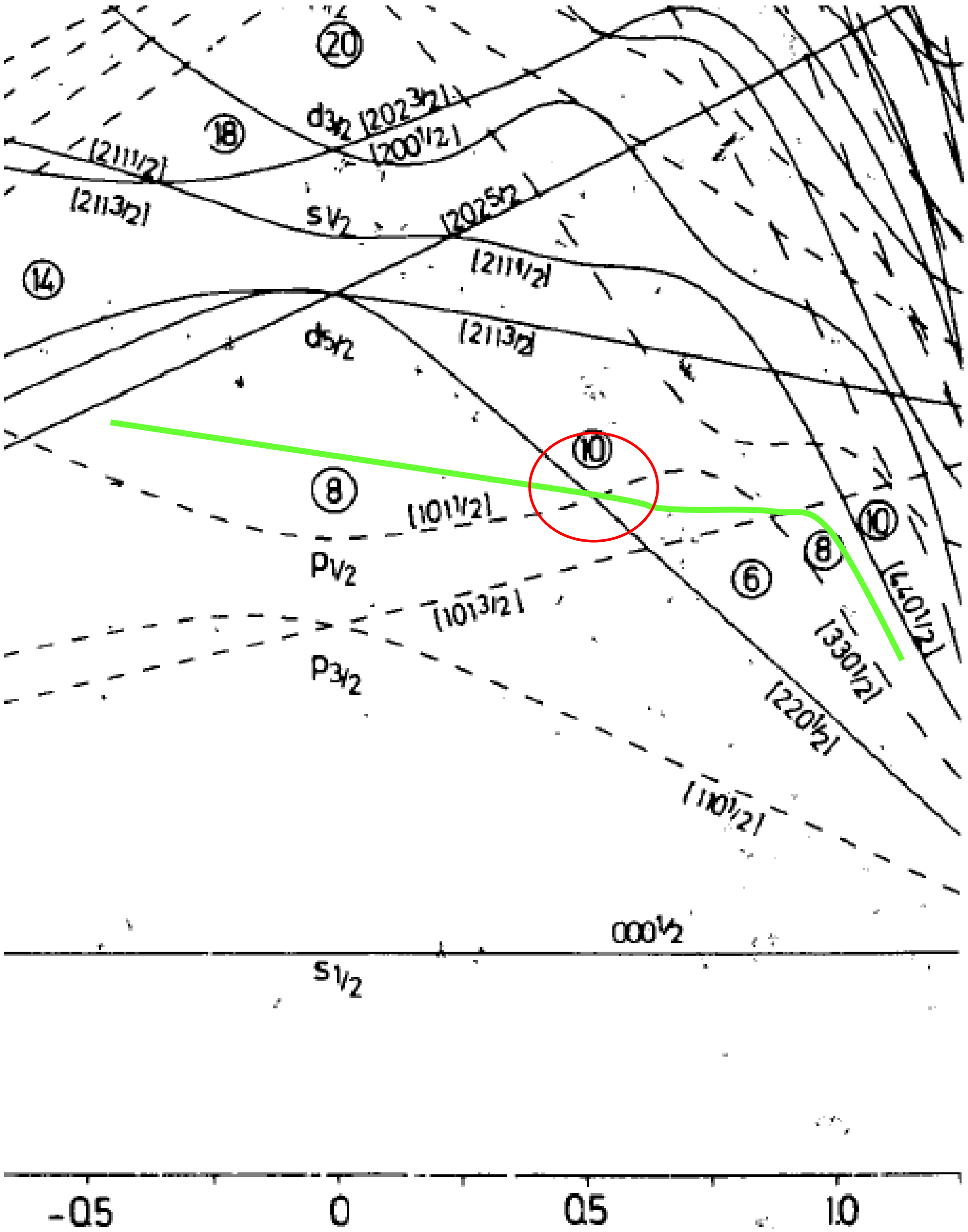
実際の ^{11}Be の準位を見てみると:



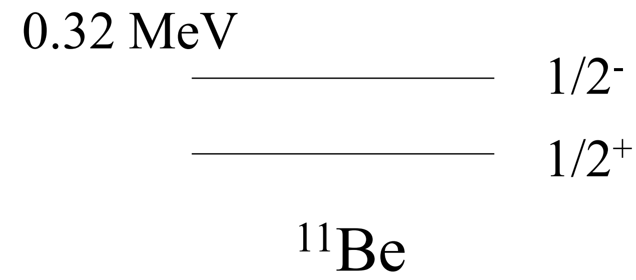


"parity inversion"

$^{11}{}_{4}Be_{7}$

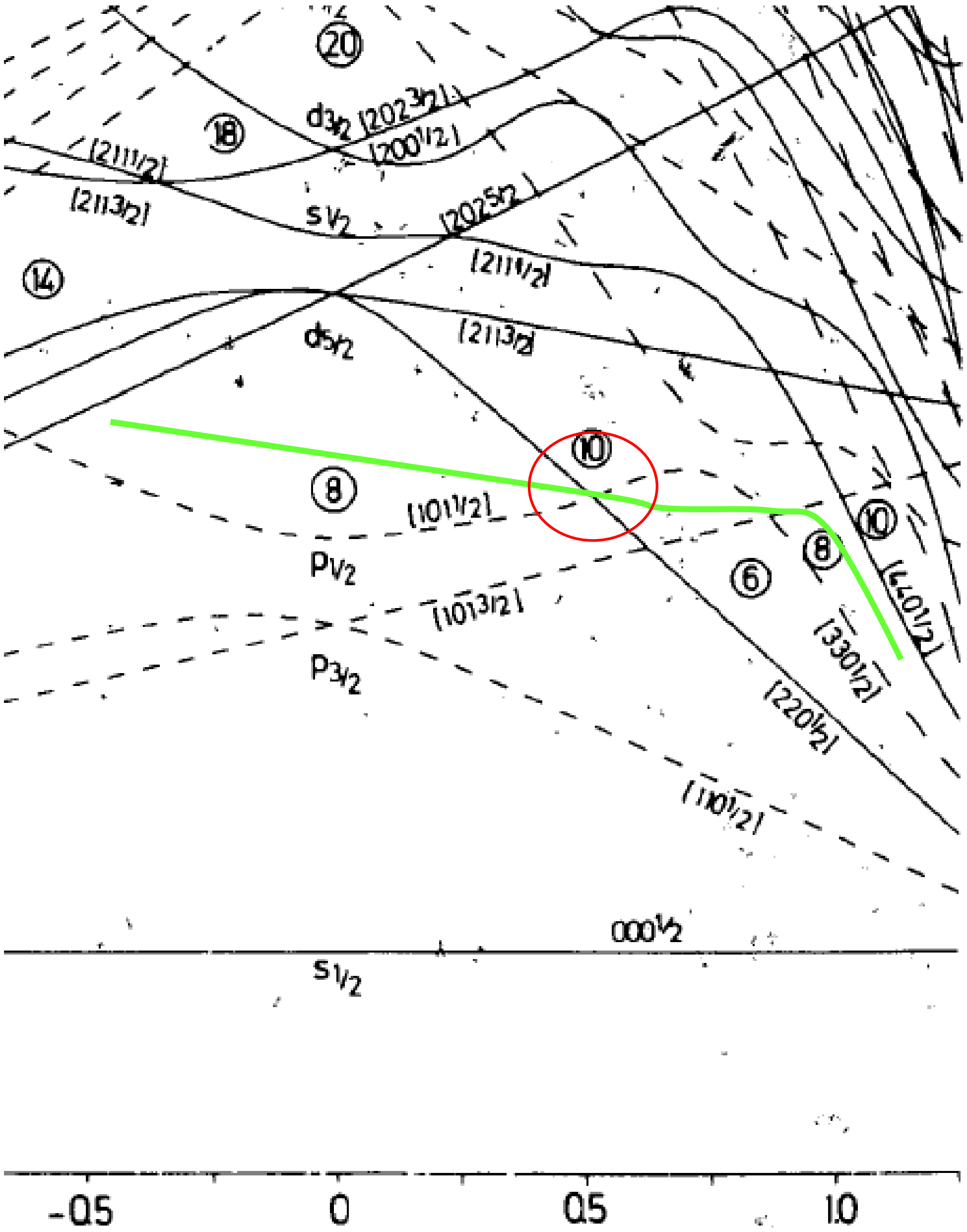


deformation parameter



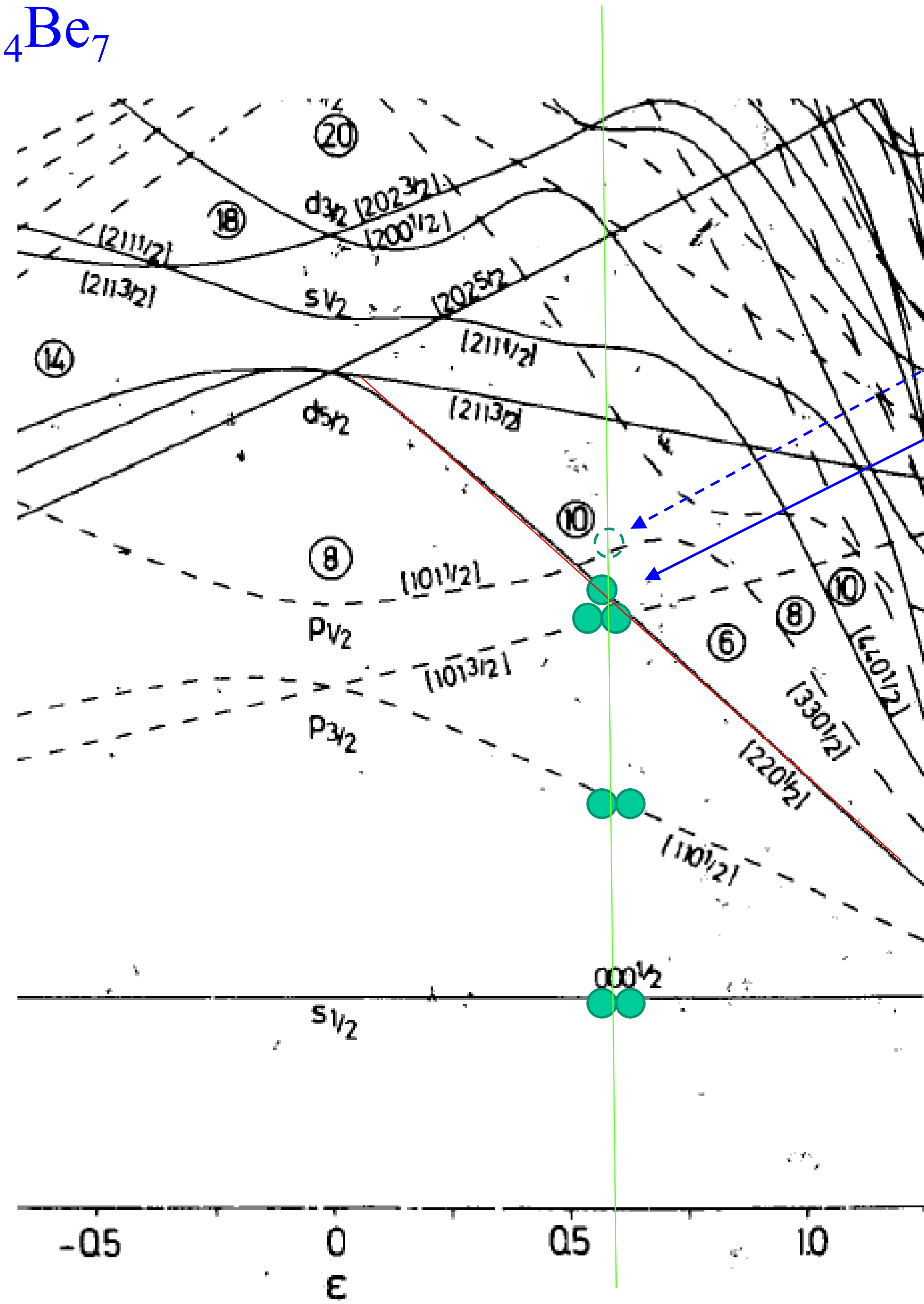
- ✓ 7番目の中性子の入る軌道を探す
（それぞれの軌道に2つずつ中性子をつめる）

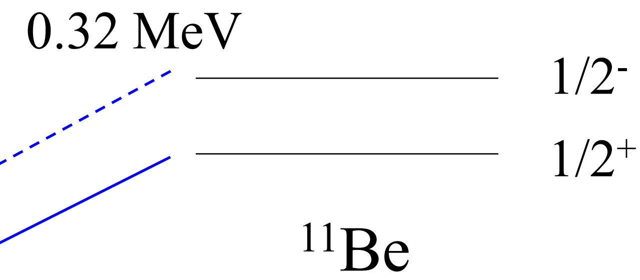
$^{11}{}_{4}Be_{7}$



deformation parameter

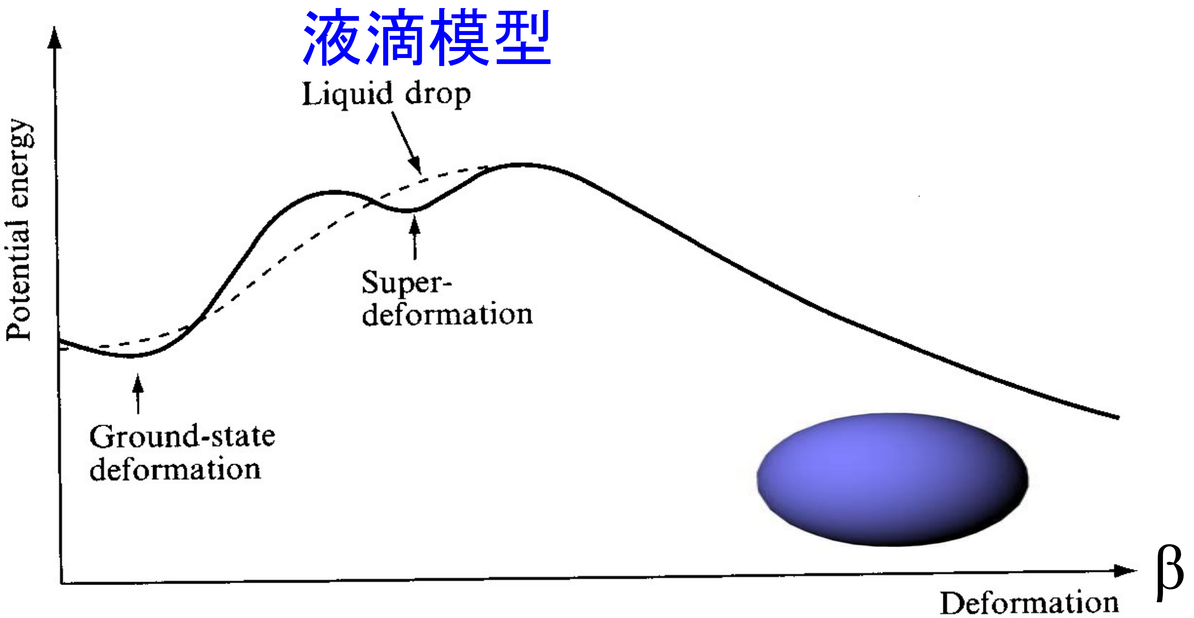
$^{11}_{4}Be_{7}$





- ✓ 7番目の中性子の入る軌道を探す
（それぞれの軌道に2つずつ中性子をつめる）

原子核の変形と殻効果



$$E(\beta) = E_{LDM}(\beta) + E_{\mathrm{shell}}(\beta)$$

液滴模型→常に球形が基底状態

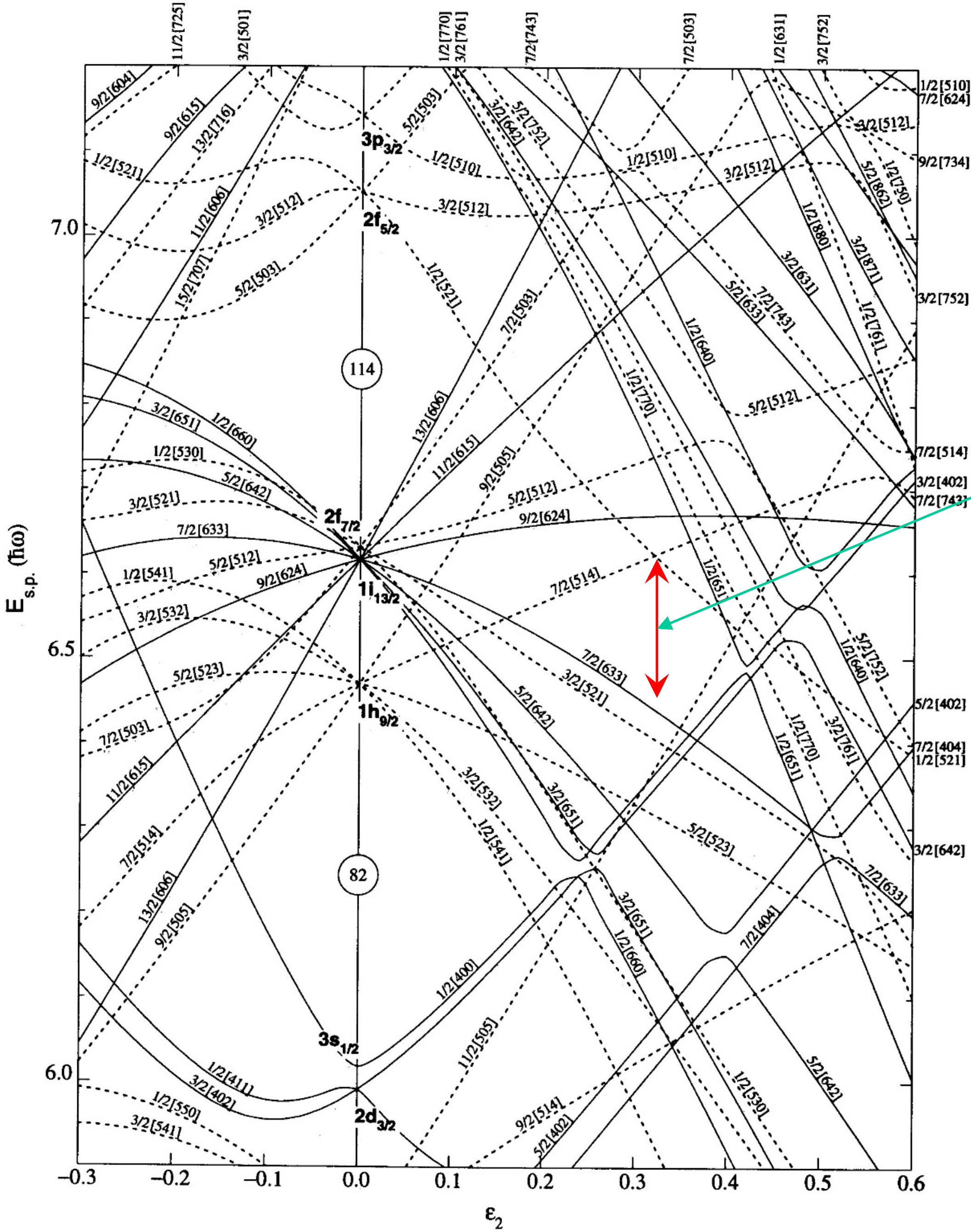
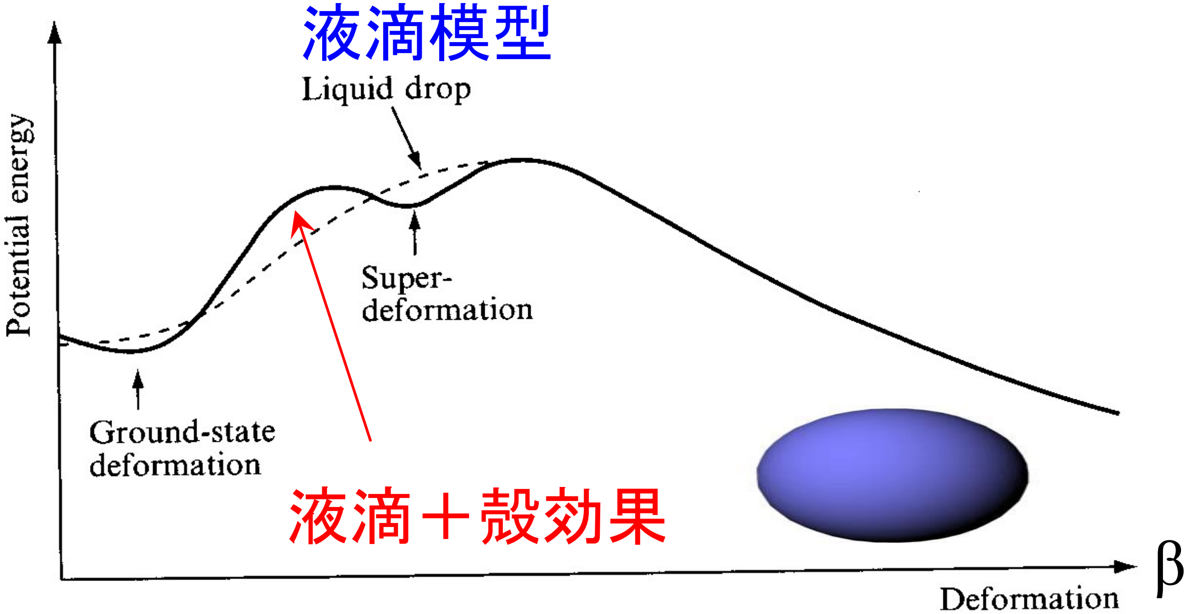
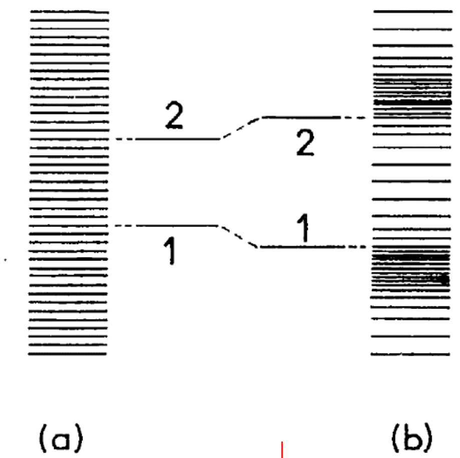


Figure 13. Nilsson diagram for protons, $Z \geq 82$ ($\varepsilon_4 = \varepsilon_2^2/6$).

変形することにより
ギャップが開く

Nilsson diagram





準位にギャップが開くと原子核が安定になる

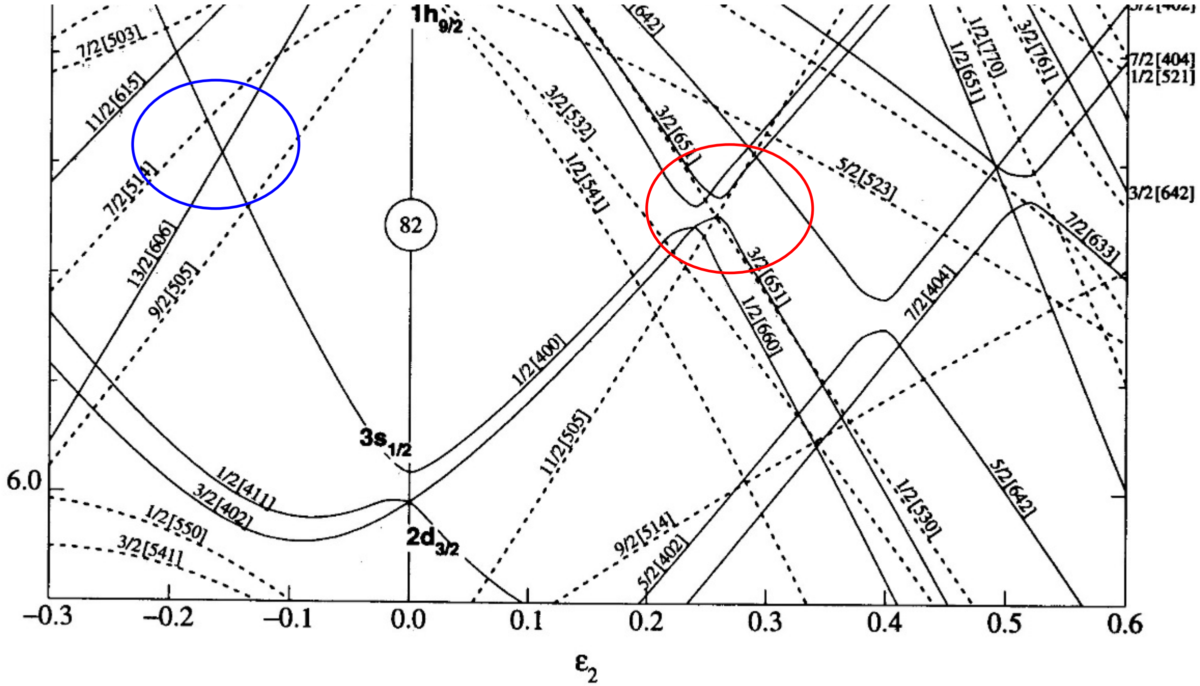
$$E(\beta) = E_{LDM}(\beta) + E_{\text{shell}}(\beta)$$

原子核が変形

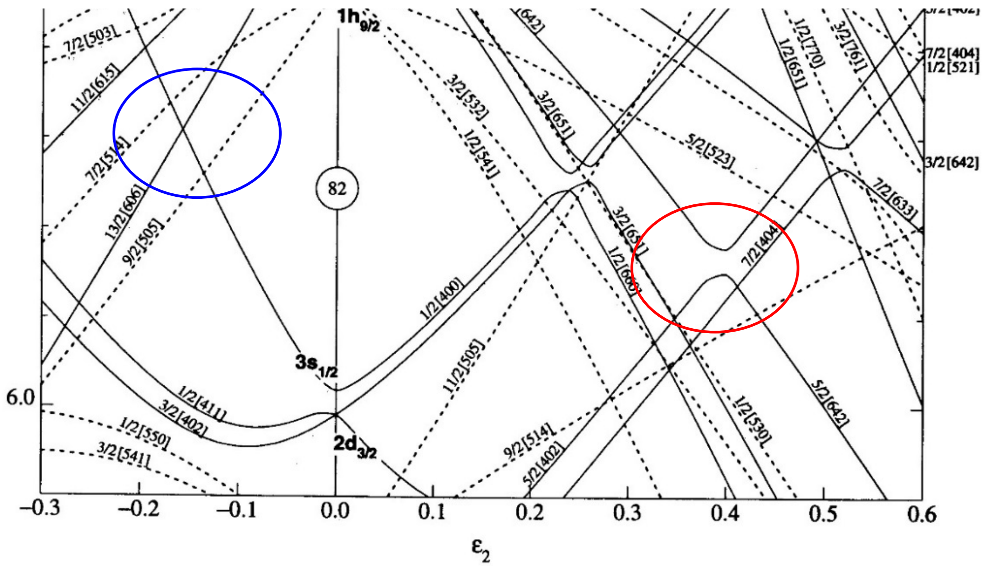
→ 核子が感じるポテンシャルも変形

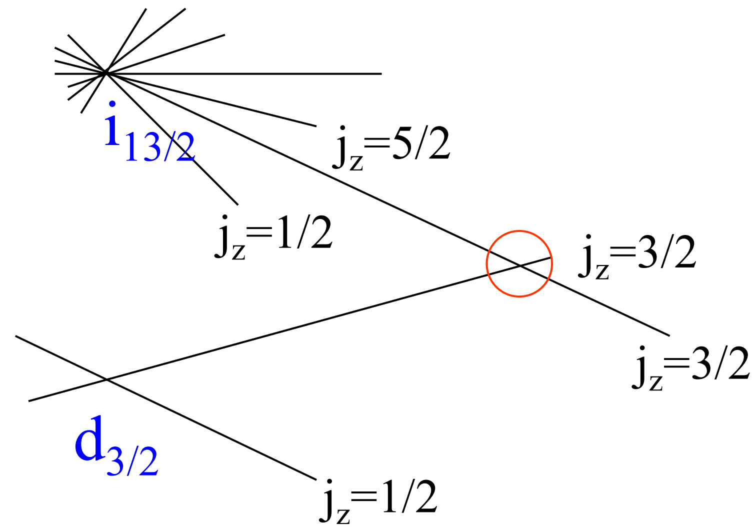
→ 変形度によって異なる量子力学的補正（殻効果）

➢ ニルソン図で準位が反発しているように見えるのは何でですか?



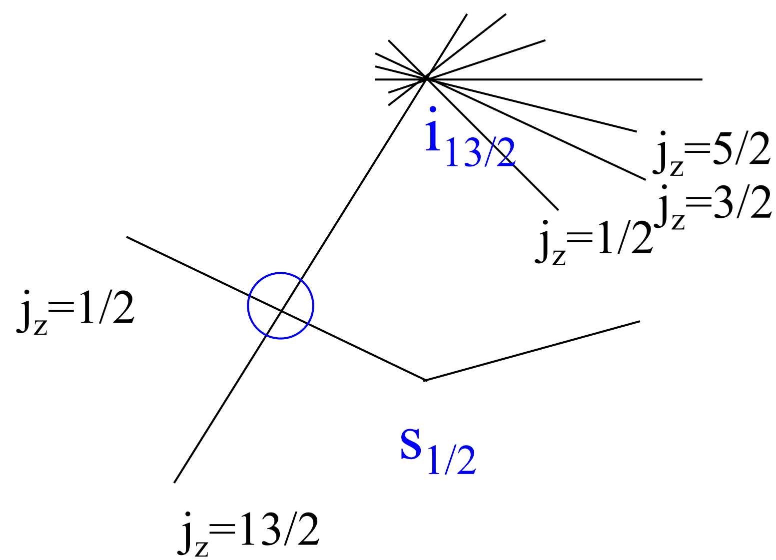
➢ ニルソン図で準位が反発しているように見えるのは何でですか?





同じ量子数を持つ準位は交わらない

（量子数が違うと交わってもよい）



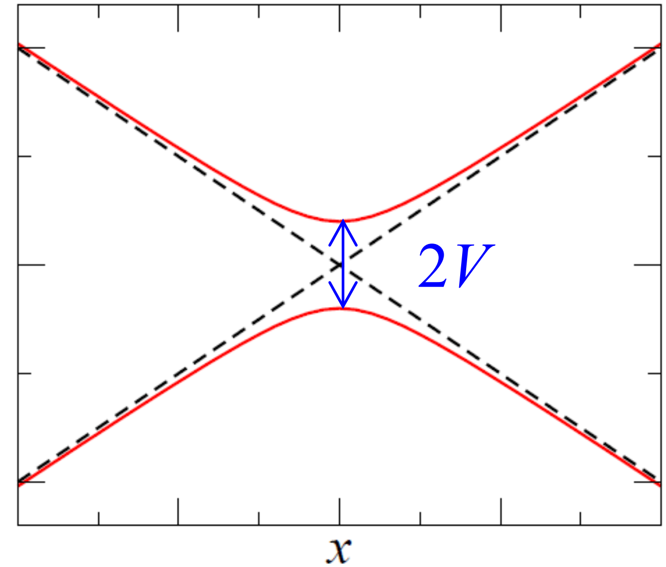
「ノイマン-ウィグナーの定理」

準位交差の問題：同じ量子数を持つ2つの状態は交差しない

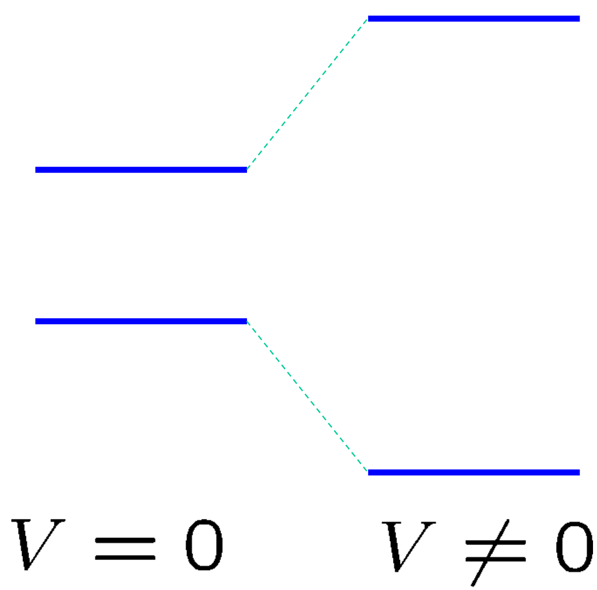
「ノイマン-ウィグナーの定理」

$$\begin{pmatrix} -\epsilon x & V \\ V & \epsilon x \end{pmatrix}$$

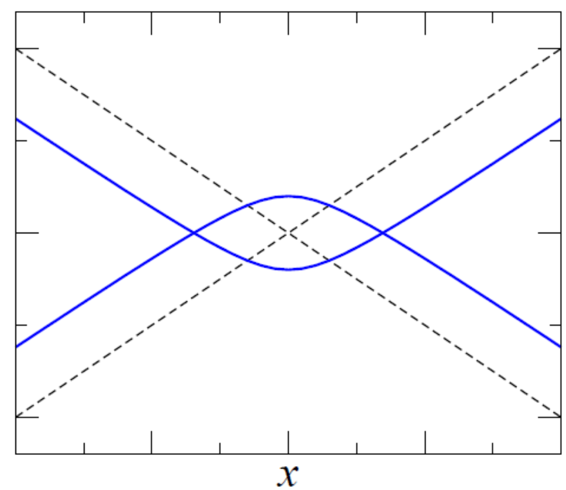
対角化 $\rightarrow \lambda_{\pm}(x) = \pm\sqrt{\epsilon^2 x^2 + V^2}$



「疑似交差」、「準位反発」

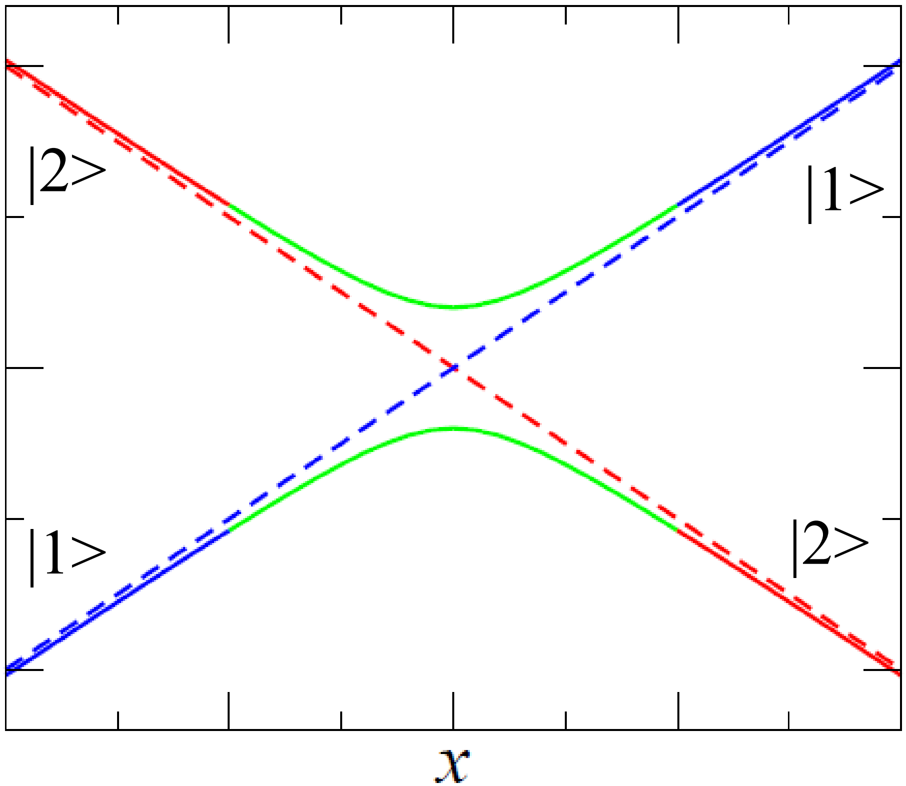


V の符号によらず必ず反発



このようになることはない

x がゆっくりと変化すると断熱的に状態が |1> から |2> へ変化
（断熱遷移）



Landau-Zener の式:

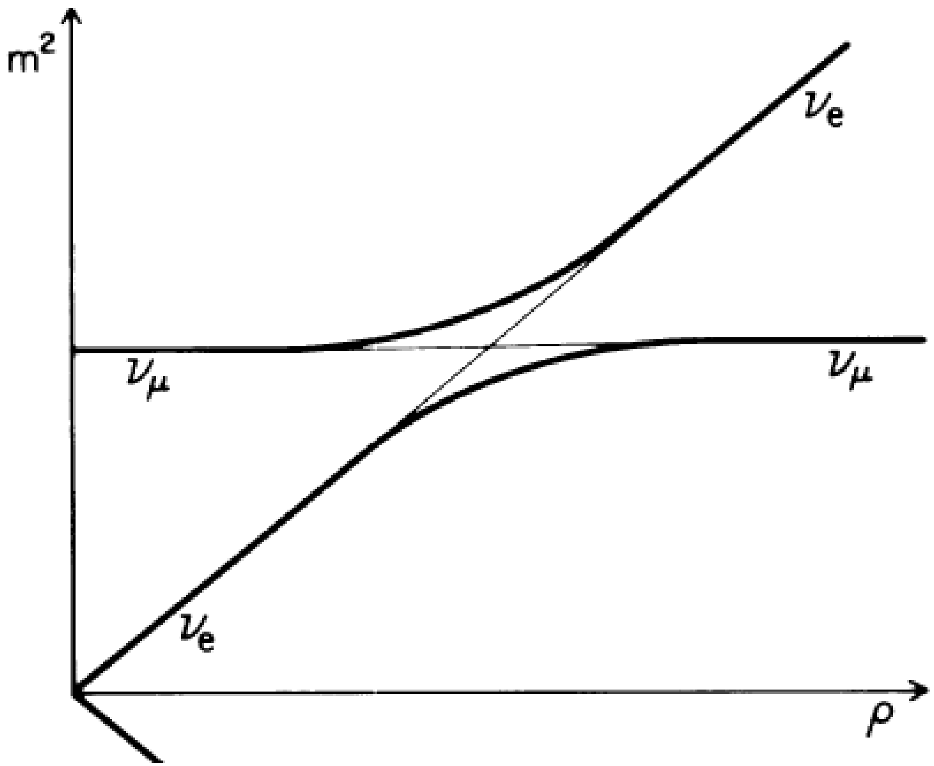
$$P(|1\rangle \to |1\rangle) = \exp\left(-\frac{2\pi V^2}{\hbar|\dot{x}| \cdot 2\epsilon}\right)$$

cf. ニュートリノ振動と準位交差問題

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\Psi_e\\ \Psi_\mu\end{pmatrix}=\left[\begin{pmatrix}E+A(r) & 0\\ 0 & E\end{pmatrix}+a\begin{pmatrix}-\cos 2\theta & \sin 2\theta\\ \sin 2\theta & \cos 2\theta\end{pmatrix}\right]\begin{pmatrix}\Psi_e\\ \Psi_\mu\end{pmatrix}$$

$$E=\frac{1}{2}(m_1^2+m_2^2),\qquad a=\frac{1}{2}(m_2^2-m_1^2)$$

電子ニュートリノと
物質中の電子との相互作用



物質中で共鳴的に
ニュートリノ振動が起こる
= MSW 効果

Ref.
H.A. Bethe, PRL56(‘86)1305,
W.C. Haxton, PRL57(‘86)1271

レポート問題3

(i) 3次元非等方調和振動子

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega_z^2 z^2 + \frac{1}{2}m\omega_\perp^2(x^2+y^2)$$

$$\begin{aligned} \omega_\perp &= \omega_0(1+\frac{\epsilon}{3}) \\ \omega_z &= \omega_0(1-\frac{2}{3}\epsilon) \end{aligned}$$

を考える。ε を 0 から 1 まで変化させるとき、ε = 0 の時の基底状態、第一励起状態、第二励起状態のエネルギーはどのように変化するか図示せよ。

(ii) 同様に ε を 0 から -1 まで変化させるとどうなるか?

＊(i) と (ii) をまとめて答えてもOK

レポート問題4

多体系の波動関数 $|\Psi\rangle$ が角運動量の固有状態 $|\Psi_{IK}\rangle$ の重ね合わせとして

$$|\Psi\rangle = \sum_I C_I |\Psi_{IK}\rangle$$

で与えられているとする。ここで、I は多体系全体の角運動量の大きさ、K はその z 成分である（K は保存しているとする）。この状態を角度 Ω だけ回転した様態を考える。

$$|\Psi_\Omega\rangle = \hat{\mathcal{R}}(\Omega)|\Psi\rangle = \sum_{I,M} C_I |\Psi_{IM}\rangle\langle\Psi_{IM}|\hat{\mathcal{R}}(\Omega)|\Psi_{IK}\rangle$$

ここで、 $\hat{\mathcal{R}}(\Omega)$ は回転の演算子である。WignerのD関数の定義

$$D^I_{MK}(\Omega) = \langle\Psi_{IM}|\hat{\mathcal{R}}(\Omega)|\Psi_{IK}\rangle$$

及び直交性 $\int d\Omega D^{I*}_{MK}(\Omega) D^{I'}_{M'K'}(\Omega) = \frac{8\pi^2}{2I+1}\delta_{I,I'}\delta_{M,M'}\delta_{K,K'}$

を用いて $|\Psi_{\text{proj}}\rangle = \int d\Omega\, D^{I*}_{MK}(\Omega)|\Psi_\Omega\rangle = \int d\Omega\, D^{I*}_{MK}(\Omega)\hat{\mathcal{R}}(\Omega)|\Psi\rangle$

が $|\Psi_{IM}\rangle$ に比例することを示せ。

Angular Momentum Projection

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

(deformed HF solution)

(note)

$$\langle\Psi_\Omega|H|\Psi_\Omega\rangle = \langle\Psi|\underbrace{\hat{\mathcal{R}}^{-1}H\hat{\mathcal{R}}}_{=\,\mathrm{H}\ \text{(for rot. symmetric Hamiltonian)}}|\Psi\rangle = \langle\Psi|H|\Psi\rangle$$

a better wf: a superposition of rotated wave functions

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

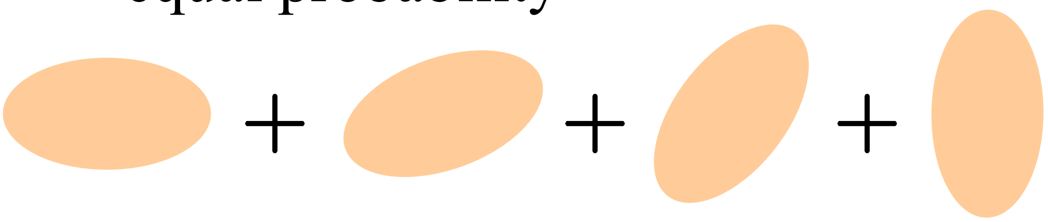
$f(\Omega) \longleftarrow$ variational principle $\langle\delta\Psi_{\rm proj}|H-E|\Psi_{\rm proj}\rangle = 0$

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

(note) For 0^+ state

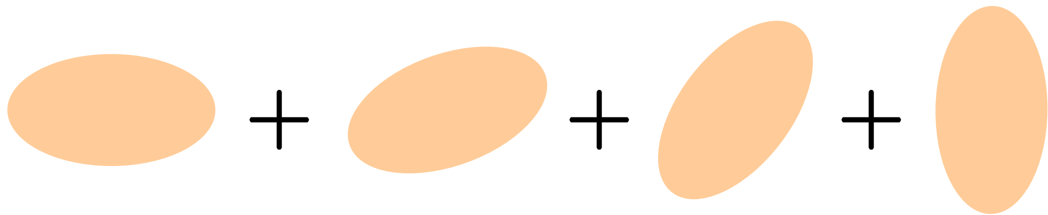
0^+: no preference of direction (spherical)

→ Mixing of all orientations with an equal probability



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

(note) For 0^+ state



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

other states:

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

(for K=0)

"angular momentum projection"

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

$f(\Omega) \longleftarrow$ variational principle

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

(Hill-Wheeler equation)
cf. Generator Coordinate Method

Solution: Wigner's D-function $\boxed{f(\Omega) = D^{I*}_{MK}(\Omega)}$

(note)

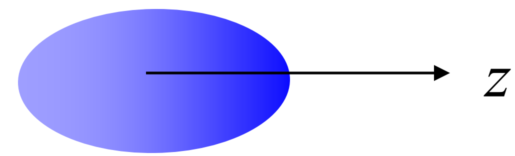
$$\hat{\mathcal{R}}(\Omega)|\phi_{IK}\rangle = \sum_M |\phi_{IM}\rangle \underbrace{\langle\phi_{IM}|\hat{\mathcal{R}}(\Omega)|\phi_{IK}\rangle}_{D^I_{MK}(\Omega)}$$

$$D^I_{M0}(\phi,\theta,\chi) = \sqrt{\frac{4\pi}{2I+1}}Y^*_{IM}(\theta,\phi)$$

$$\int d\Omega D^{I*}_{MK}(\Omega)D^{I'}_{M'K'}(\Omega) = \frac{8\pi^2}{2I+1}\delta_{I,I'}\delta_{M,M'}\delta_{K,K'}$$

Projection Operator

Consider a HF state with the axial symmetry



$$|\Psi\rangle = \sum_I C_I |\Psi_{IK}\rangle$$

$\rightarrow$ rotated state:

$$|\Psi_\Omega\rangle = \hat{\mathcal{R}}(\Omega)|\Psi\rangle = \sum_{I,M} C_I\, D^I_{MK}(\Omega)|\Psi_{IM}\rangle$$

$$\boxed{\begin{aligned} |\Psi_{\mathrm{proj}}\rangle &= \int d\Omega\, D^{I*}_{MK}(\Omega)|\Psi_\Omega\rangle \\ &= \frac{8\pi^2}{2I+1} C_I\,|\Psi_{IM}\rangle \end{aligned}}$$

or

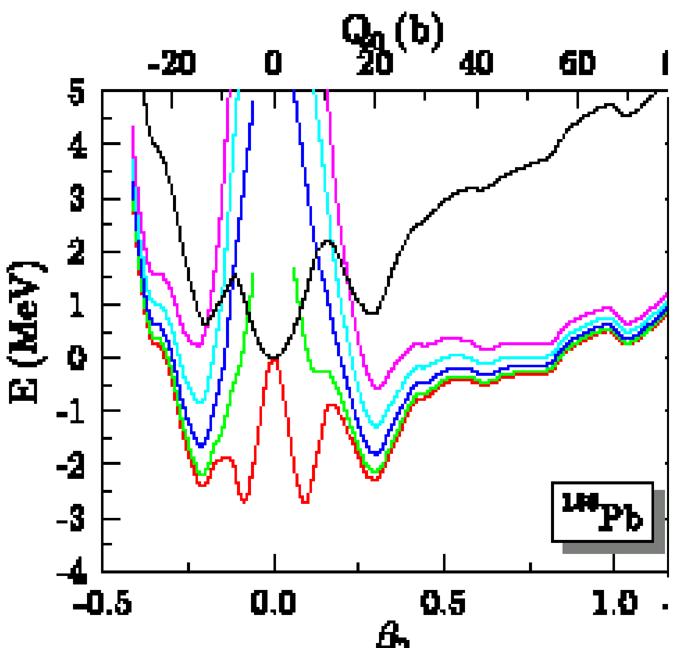
$$\hat{P}^I_{MK} = \frac{2I+1}{8\pi^2}\int D^{I*}_{MK}(\Omega)\hat{\mathcal{R}}(\Omega)\, d\Omega = |IM\rangle\langle IK|$$

Projected wave function:

$$|\Psi_{IM}\rangle = \hat{P}^{I}_{MK}|\Psi\rangle = \frac{2I+1}{8\pi^2}\int d\Omega\, D^{I*}_{MK}(\Omega)\hat{\mathcal{R}}(\Omega)\,|\Psi\rangle$$

Projected energy surface:

$$\boxed{E_I = \frac{\langle\Psi_{IM}|H|\Psi_{IM}\rangle}{\langle\Psi_{IM}|\Psi_{IM}\rangle} = \frac{\langle\Psi|\hat{P}^{I}_{KM}H\hat{P}^{I}_{MK}|\Psi\rangle}{\langle\Psi|\hat{P}^{I}_{KM}\,\hat{P}^{I}_{MK}|\Psi\rangle}}$$



Constrained HF

0^+

2^+

4^+

Calculation and Figure: M. Bender

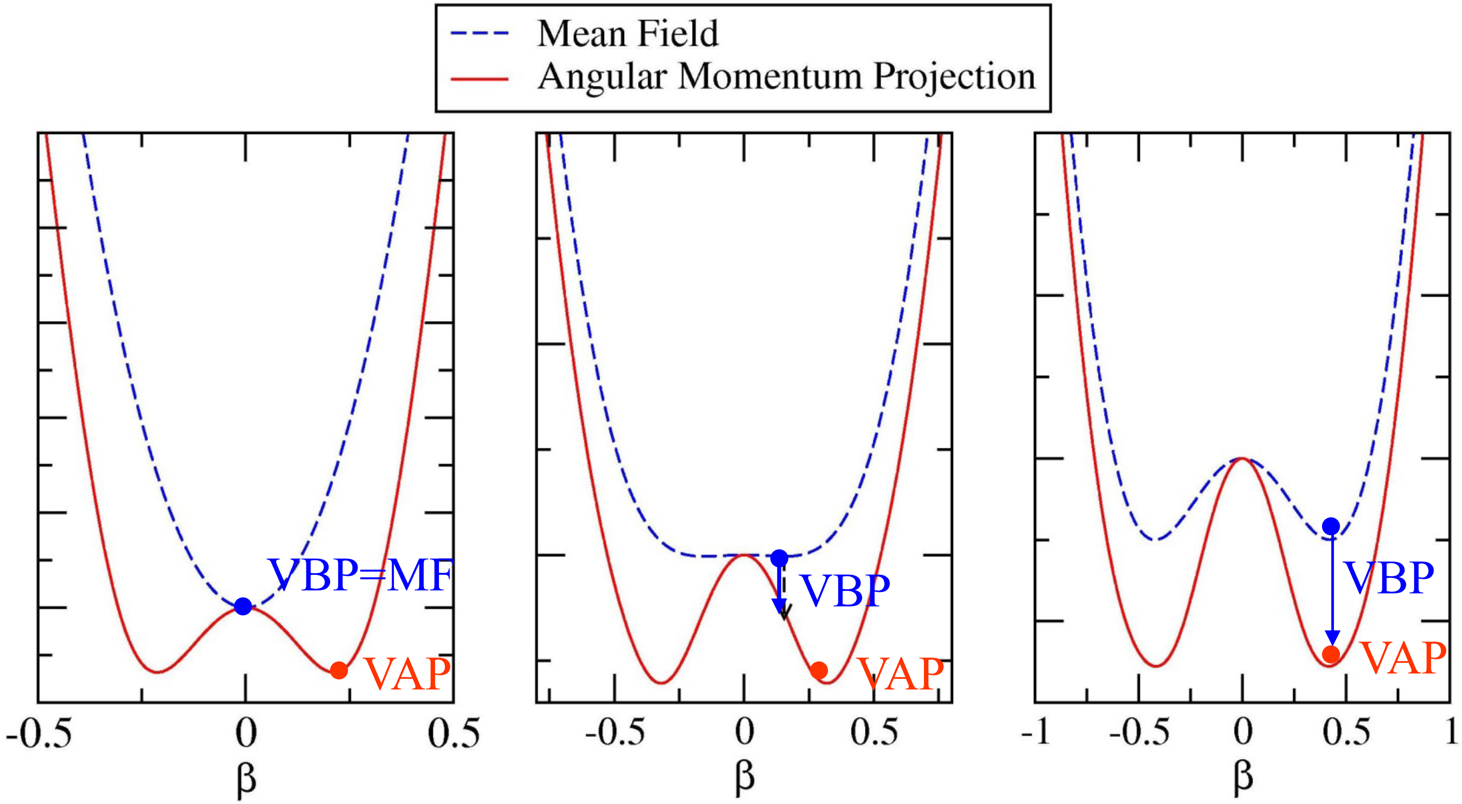
VAP v.s. VBP

- **Variation *Before* Projection (VBP)**

$$\text{minimize } \langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle \longrightarrow |\Psi_{IM}\rangle = \hat{P}^I_{MK}|\Psi\rangle$$

- **Variation *After* Projection (VAP)**

$$|\Psi_{IM}\rangle = \hat{P}^I_{MK}|\Psi\rangle \longrightarrow \text{minimize } \langle\Psi_{IM}|H|\Psi_{IM}\rangle/\langle\Psi_{IM}|\Psi_{IM}\rangle$$



VBP:
simple, but does not work for small deformation. Also, a discontinuity problem

VAP:
robust, but very expensive