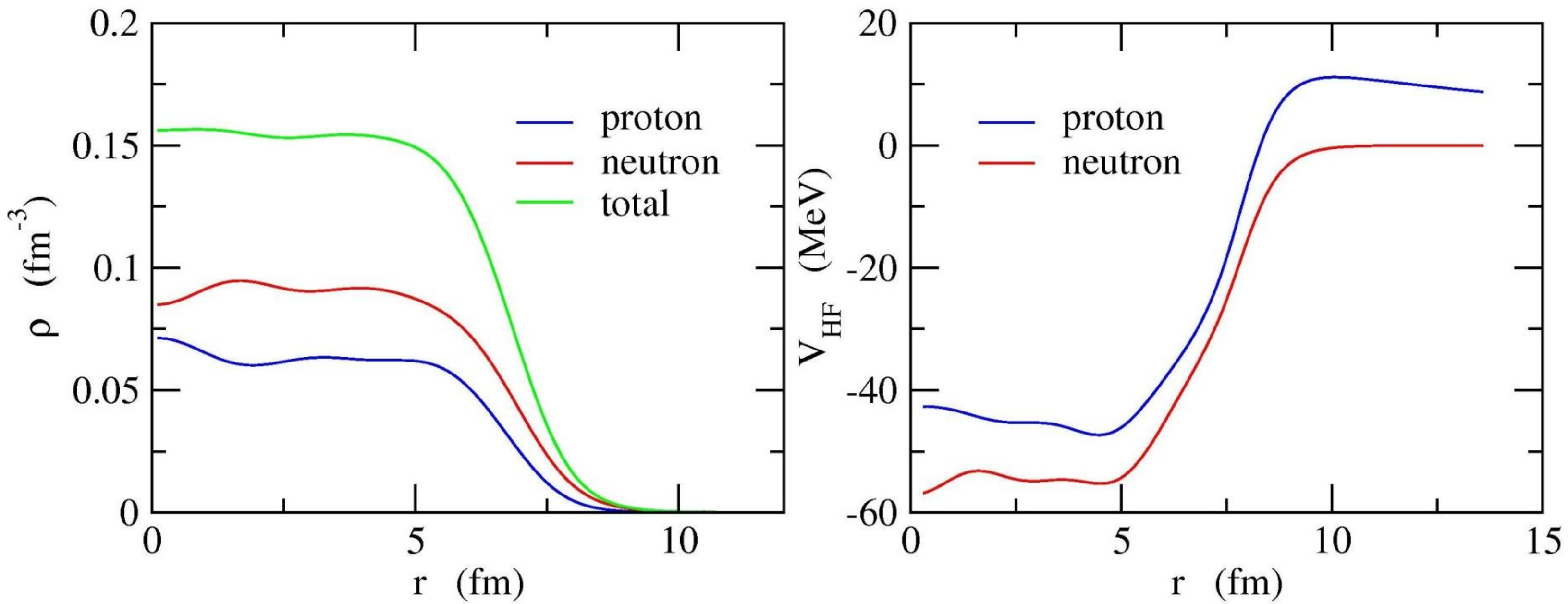
$$-\frac{\hbar^2}{2m}\nabla^2\psi_i(\boldsymbol{r}) + \int v(\boldsymbol{r},\boldsymbol{r}')\rho_{\rm HF}(\boldsymbol{r}')d\boldsymbol{r}'\psi_i(\boldsymbol{r}) - \int \rho_{\rm HF}(\boldsymbol{r},\boldsymbol{r}')v(\boldsymbol{r},\boldsymbol{r}')\psi_i(\boldsymbol{r}')\,d\boldsymbol{r}' = \epsilon_i\,\psi_i(\boldsymbol{r})$$

Iteration

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

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

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



Hartree-Fock Method and Symmetries

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

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

Slater determinant

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

⇐ 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"

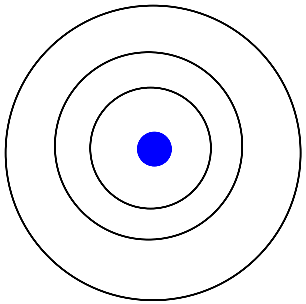
Ψ_{HF} : does not necessarily possess the symmetries that H has.

Typical Example

➢ Translational symmetry: always broken in nuclear systems

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

(cf.) atoms



nucleus in the center

→ translational symmetry: broken from the begining

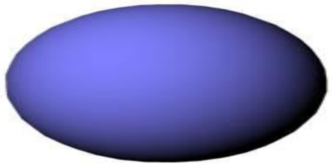
Symmetry Breaking

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 → later in this lecture

➢ Rotational symmetry

Deformed solution



$$
\begin{aligned}
H &= -\sum_{i=1}^{A}\frac{\hbar^2}{2m}\boldsymbol{\nabla}_i^2 + \frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i,\boldsymbol{r}_j) \\
&= \underbrace{\sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\boldsymbol{\nabla}_i^2 + V_{\mathsf{HF}}(i)\right)}_{h_{\mathsf{HF}}} + \underbrace{\frac{1}{2}\sum_{i,j}^{A} v(\boldsymbol{r}_i,\boldsymbol{r}_j) - \sum_i V_{\mathsf{HF}}(i)}_{V_{\mathsf{res}}}
\end{aligned}
$$

$$
\begin{aligned}
V_{\mathsf{res}} &= \frac{1}{2}\sum_{i,j} v_{\mathsf{res}}(\boldsymbol{r}_i,\boldsymbol{r}_j) \\
&= \frac{1}{2}\sum_{i,j}\sum_{\lambda,\mu} v_\lambda(r_i,r_j)Y_{\lambda\mu}(\hat{\boldsymbol{r}}_i)Y^*_{\lambda\mu}(\hat{\boldsymbol{r}}_j) \\
&\sim \frac{1}{2}\sum_{i,j}\left(\chi_1\, r_iY_1(\hat{\boldsymbol{r}}_i)\cdot r_jY_1(\hat{\boldsymbol{r}}_j) + \chi_2\, r_i^2Y_2(\hat{\boldsymbol{r}}_i)\cdot r_j^2Y_2(\hat{\boldsymbol{r}}_j) + \cdots\right)
\end{aligned}
$$

(note) $\langle\Psi_{\mathsf{HF}}|rY_{1\mu}|\Psi_{\mathsf{HF}}\rangle = \langle\Psi_{\mathsf{HF}}|r^2Y_{2\mu}|\Psi_{\mathsf{HF}}\rangle = 0$

for spherical HF state

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

$$V_{\mathrm{res}} \sim \frac{1}{2} \sum_{i,j} \left(\chi_1 \, r_i Y_1(\hat{\boldsymbol{r}}_i) \cdot r_j Y_1(\hat{\boldsymbol{r}}_j) + \chi_2 \, r_i^2 Y_2(\hat{\boldsymbol{r}}_i) \cdot r_j^2 Y_2(\hat{\boldsymbol{r}}_j) + \cdots \right)$$

(note) $\langle \Psi_{\mathrm{HF}} | r Y_{1\mu} | \Psi_{\mathrm{HF}} \rangle = \langle \Psi_{\mathrm{HF}} | r^2 Y_{2\mu} | \Psi_{\mathrm{HF}} \rangle = 0$

for spherical HF state

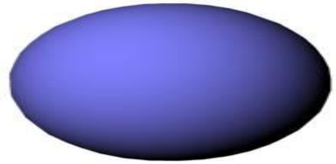
As χ_2 becomes large, it is better to include a part of v_{res} in h_{HF}.

$\longrightarrow$ **deform Ψ_{HF}**

$\longrightarrow$ $\langle \Psi_{\mathrm{HF}} | r^2 Y_{2\mu} | \Psi_{\mathrm{HF}} \rangle \neq 0$

$\longrightarrow$ $V_{\mathrm{HF}}(i) \to V_{\mathrm{HF}}(i) + \chi_2 \langle Y_{20} \rangle r^2 Y_{20}(\hat{\boldsymbol{r}}_i)$

➢ Rotational symmetry



Deformed solution

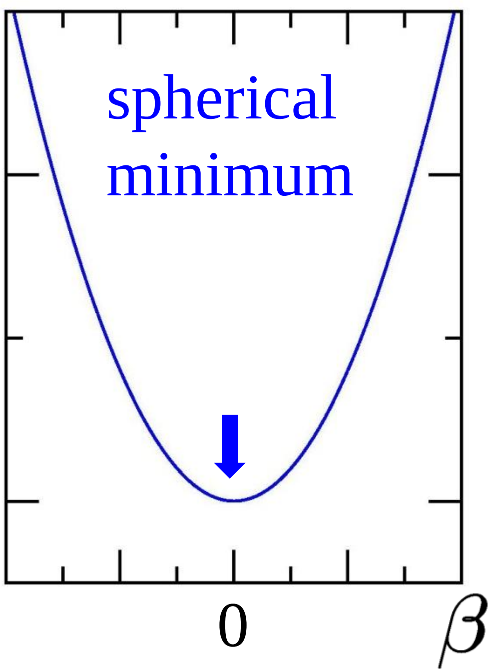
Constrained Hartree-Fock method

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

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

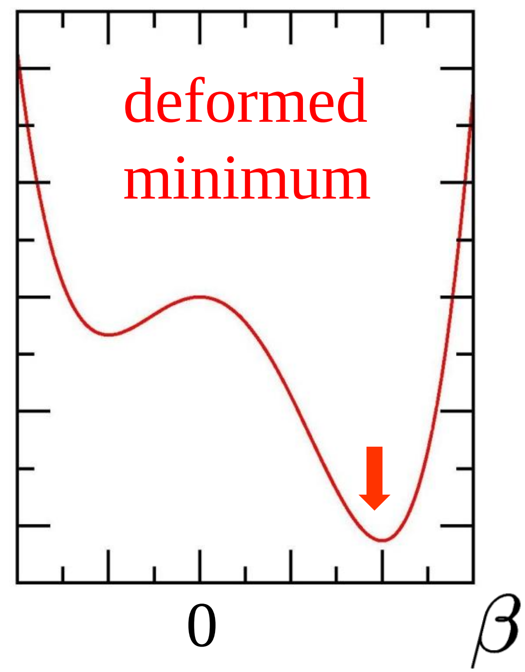
λ : Lagrange multiplier, to be determined so that $\langle \hat{Q}_{20} \rangle = Q \propto R^2\beta$

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



"phase transition"

v a/o N → large



2008年のノーベル物理学賞

"for the discovery of the mechanism of spontaneous broken symmetry in subatomic physics"

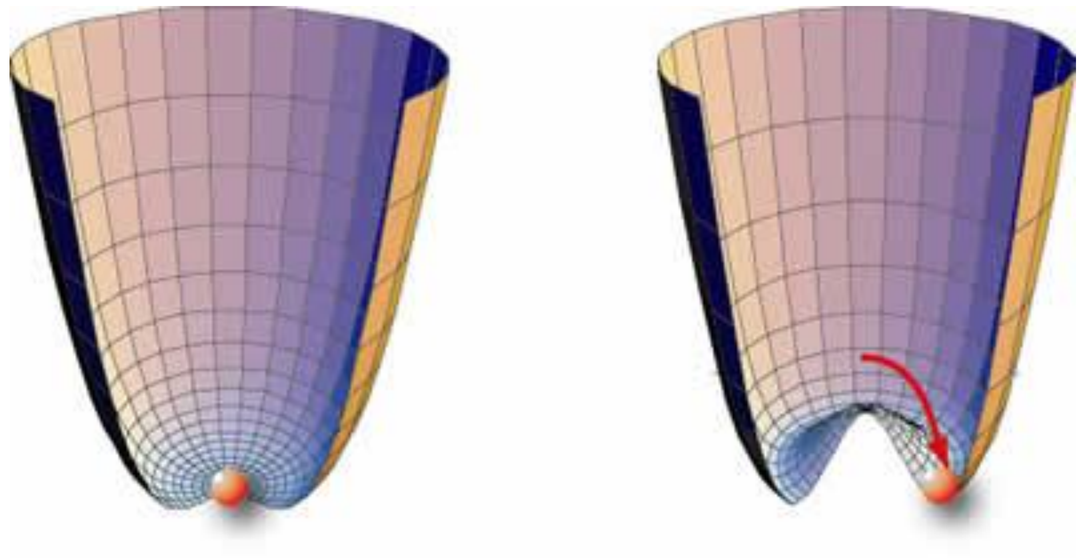
南部陽一郎

"for the discovery of the origin of the broken symmetry which predicts the existence of at least three families of quarks in nature"

小林誠、益川敏英

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)

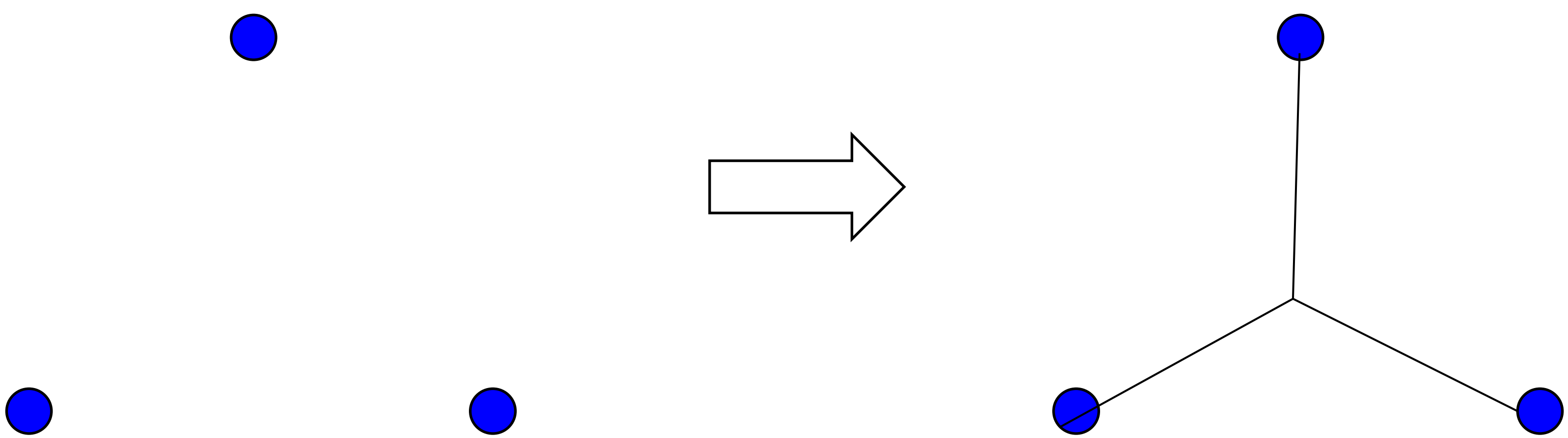
頂点が何個かある

- 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



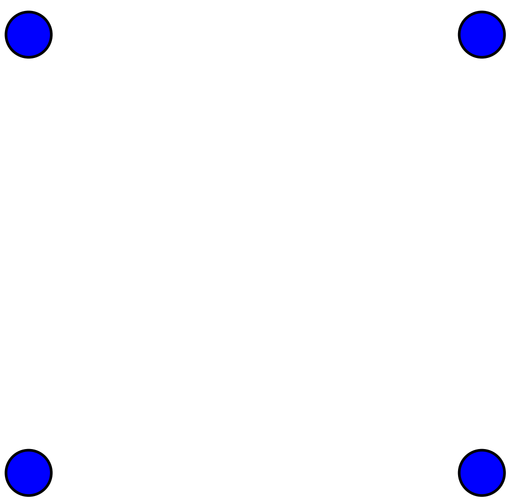
休憩(頭の体操)

頂点が何個かある

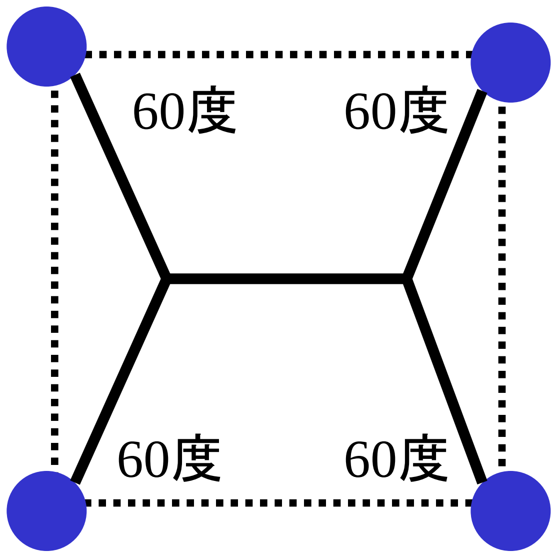
- 頂点を適当な線でつなぐ
- 何本引いてもよい
- 線は交わってもよい
- 一つの点から線を通って全ての点にいけるようにする

線の長さの合計が最短になるひき方は?

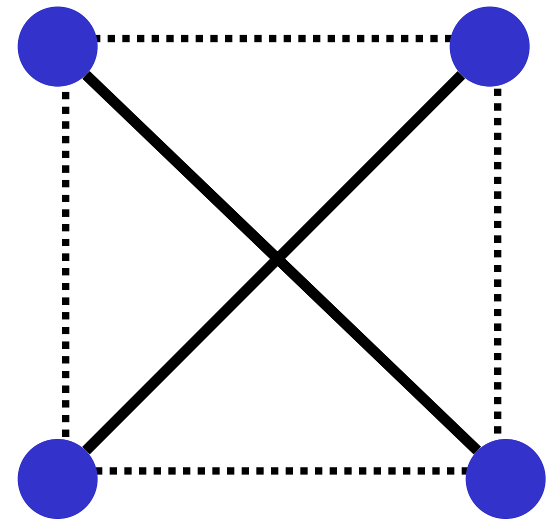
(問題)正方形の場合は?



（答え）



cf.



長さ

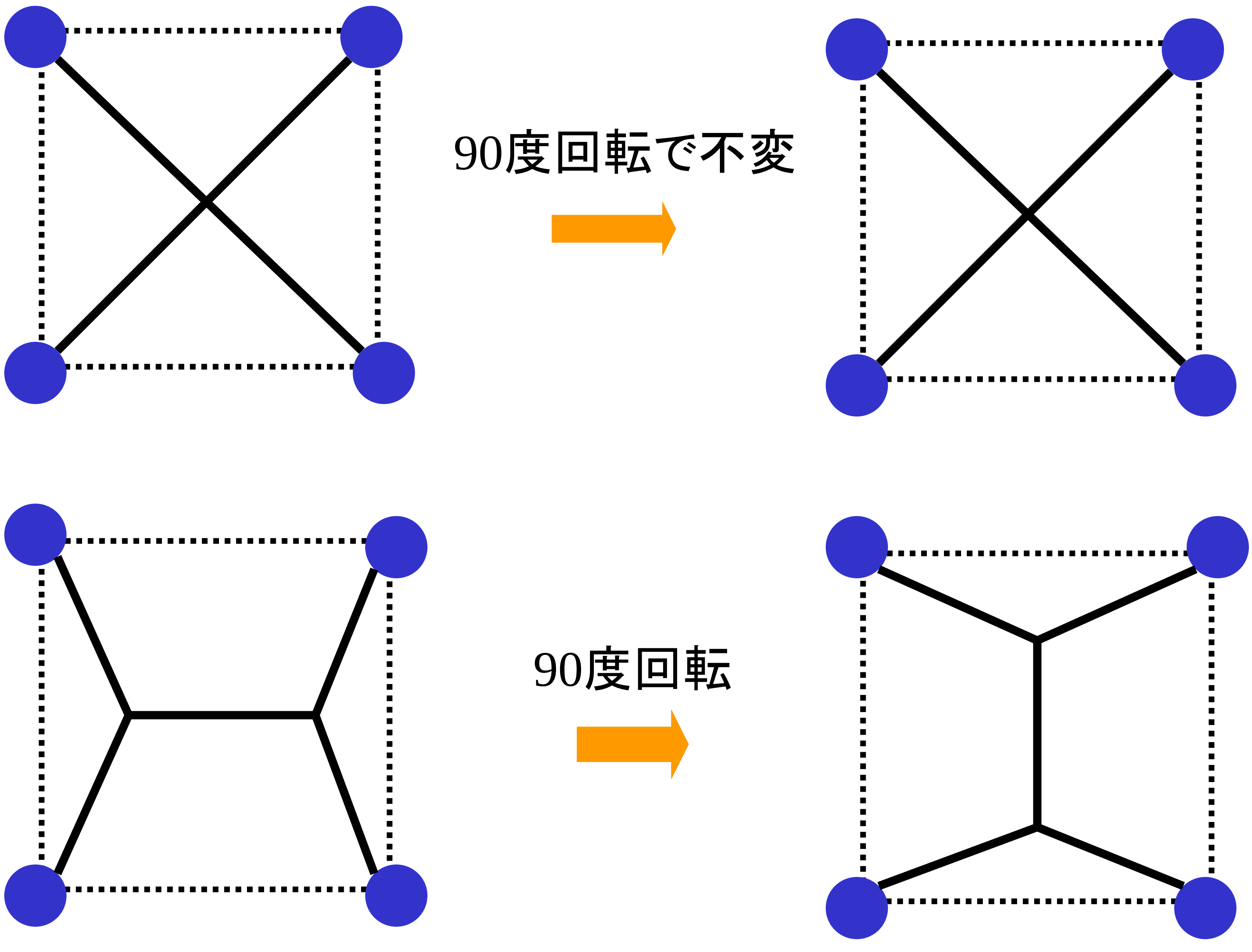
$$4 \times \frac{1}{\sqrt{3}} + \left(1 - 2 \times \frac{1}{2\sqrt{3}}\right)$$
$$= 1 + \sqrt{3}$$
$$= 2.732 \cdots$$

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

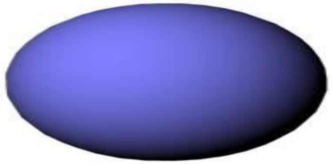


対称性の自発的破れの好例

スライド：小池武志氏（東北大学）

➢Rotational symmetry

Deformed solution

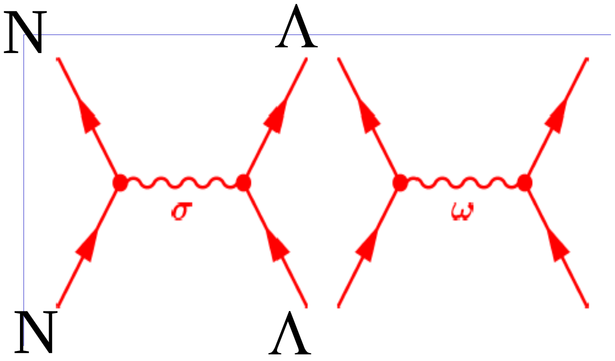


RMF calculations for deformed hypernuclei

Hypernuclei: nucleus + Lambda particle

Effect of a Λ particle on nuclear shapes?

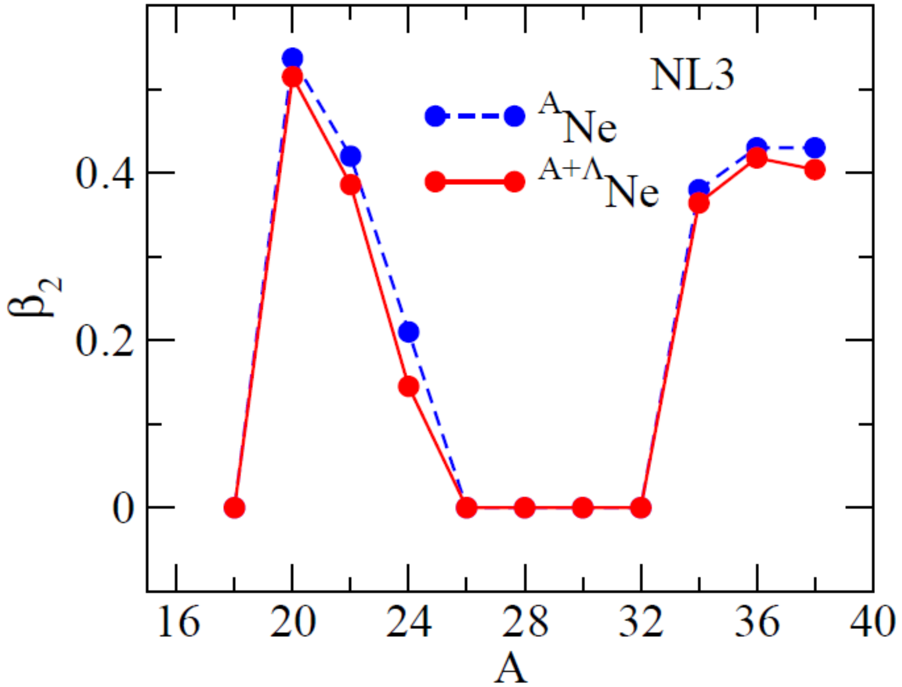
Relativistic Mean-field model



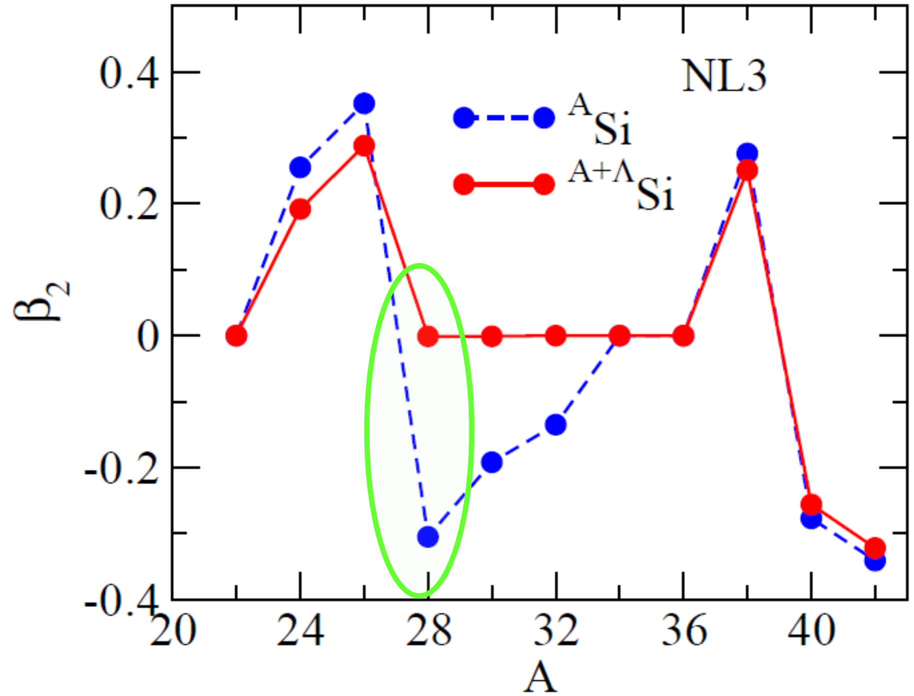
nucleon-nucleon interaction
via meson exchange

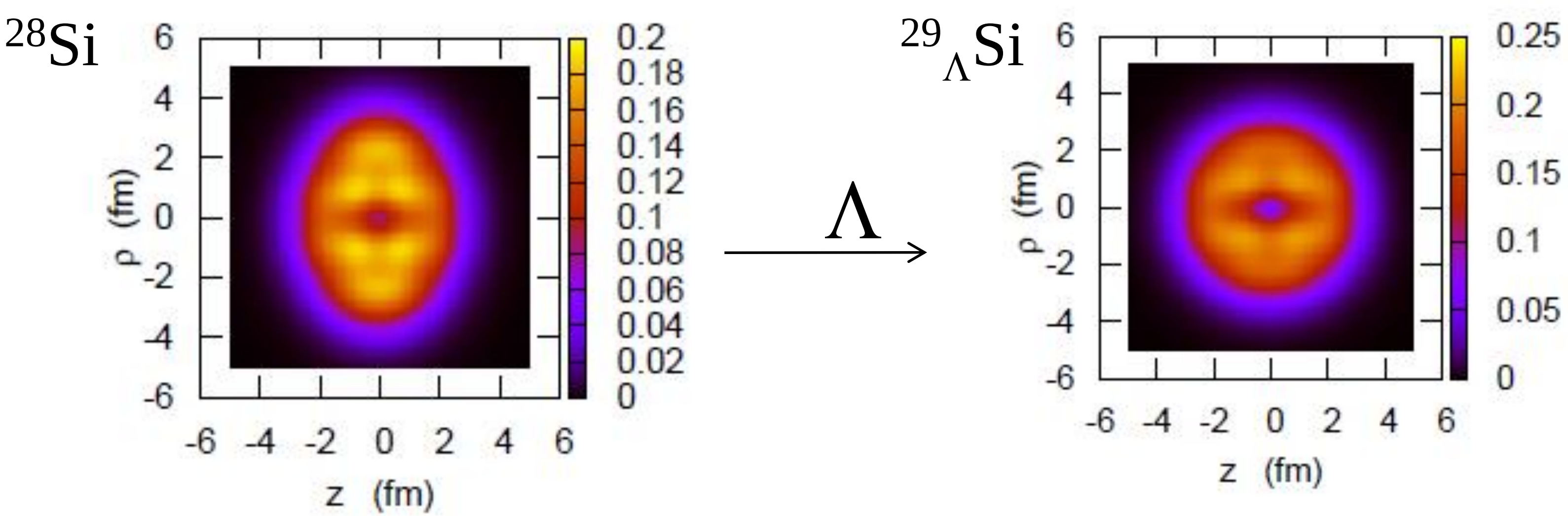
Λσ and Λω couplings

Ne isotopes



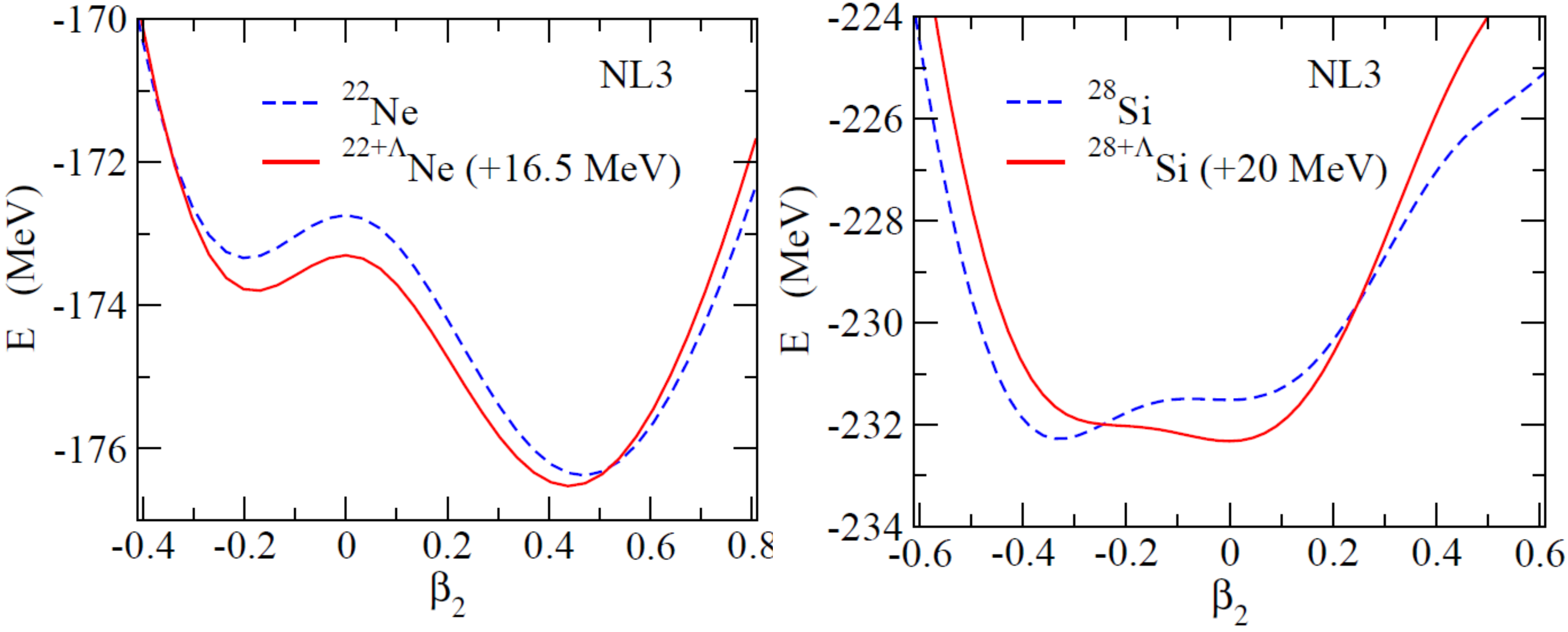
Si isotopes





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

Potential energy surface



Myaing Thi Win and K.H., 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

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

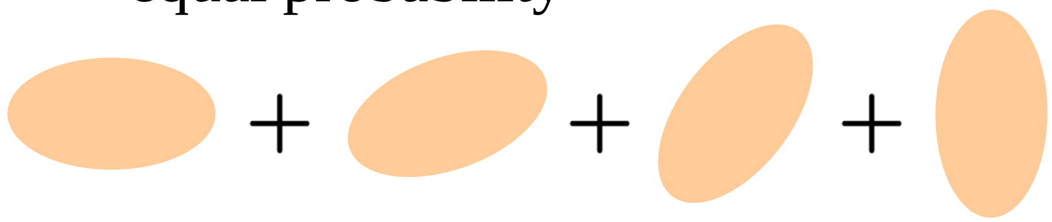
$f(\Omega) \longleftarrow$ variational principle $\langle\delta\Psi_{\rm proj}|H-E|\Psi_{\rm proj}\rangle = 0$

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

(note) For 0^+ state

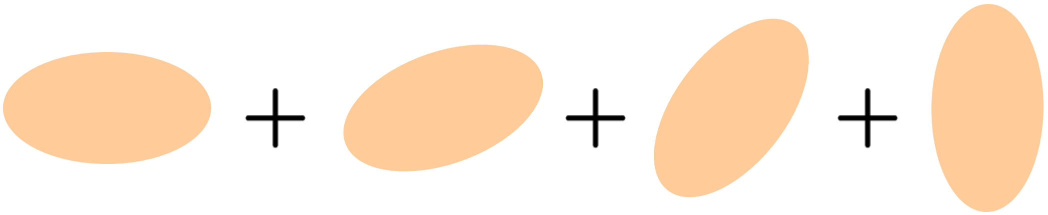
0^+: no preference of direction (spherical)

→ 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)

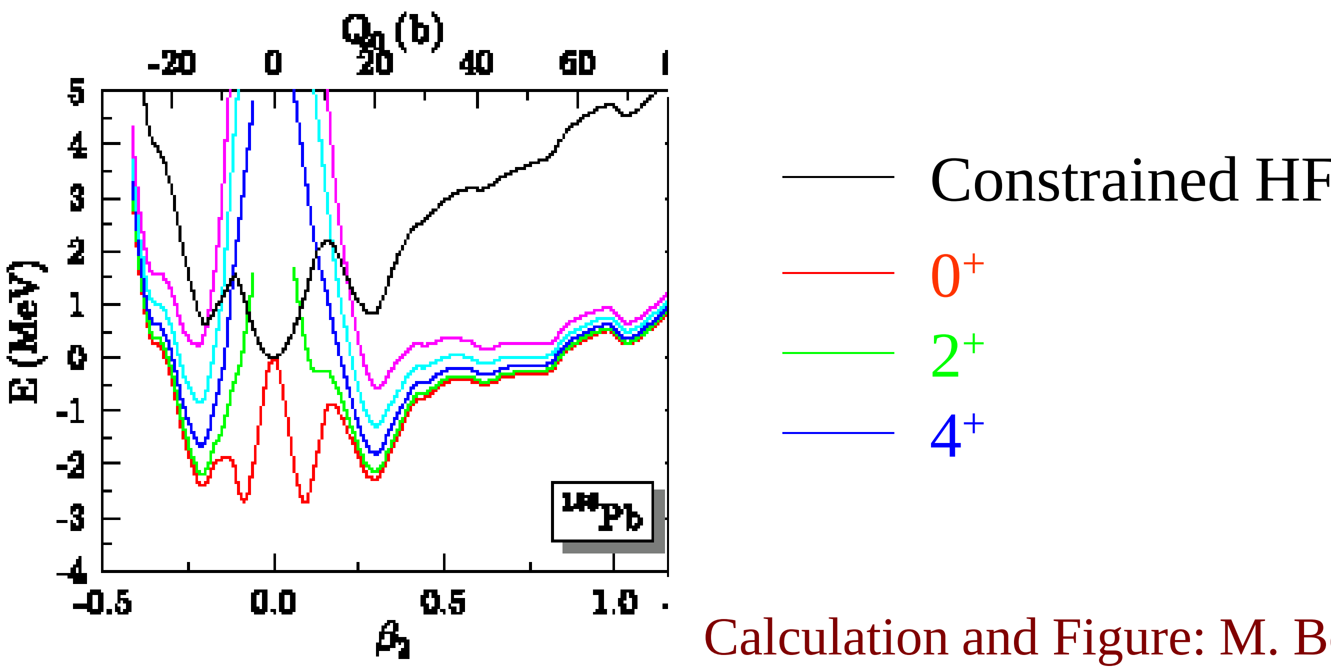
"angular momentum projection"

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:

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



Calculation and Figure: M. Bender

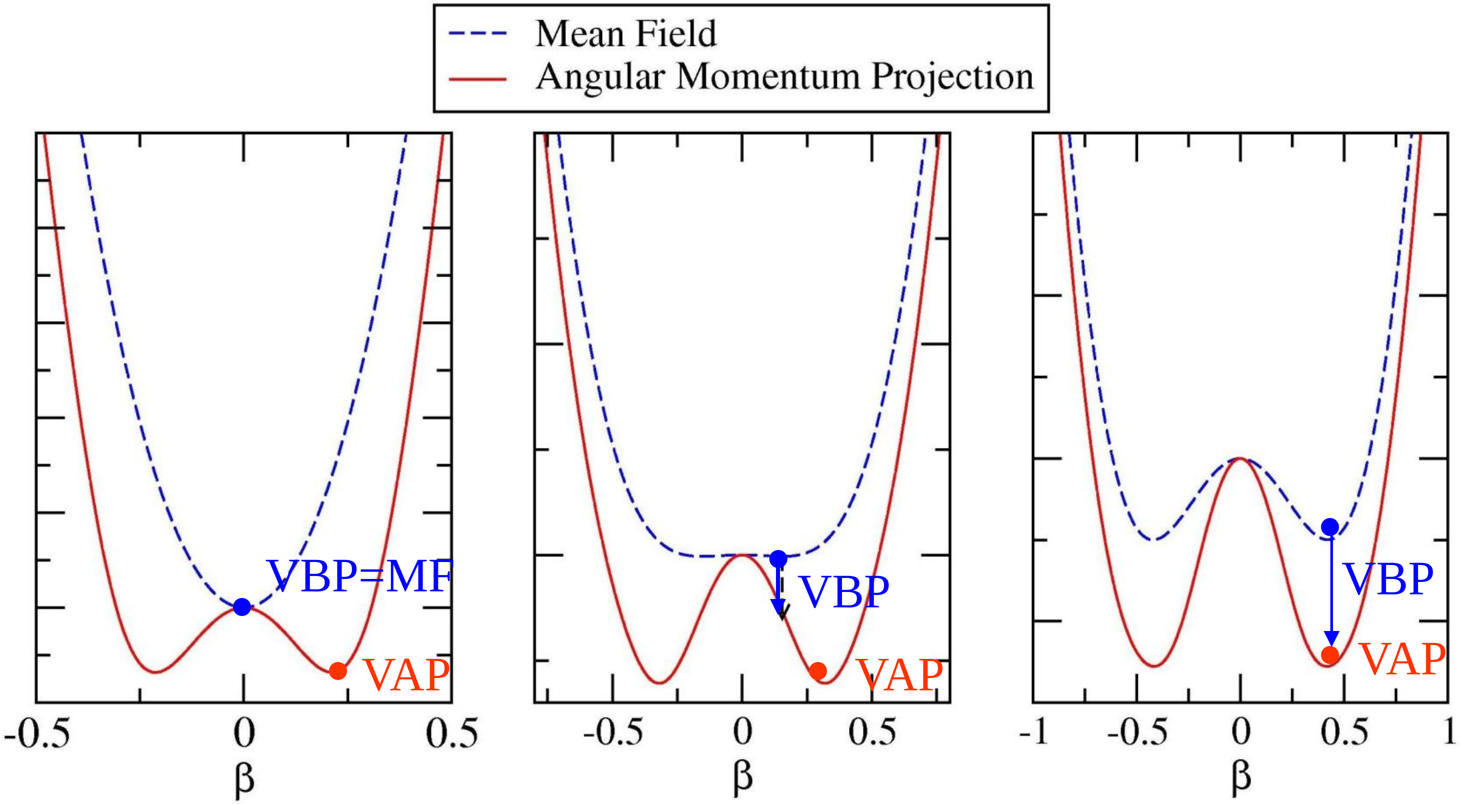
VAP v.s. VBP

- Variation *Before* Projection (VBP)

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

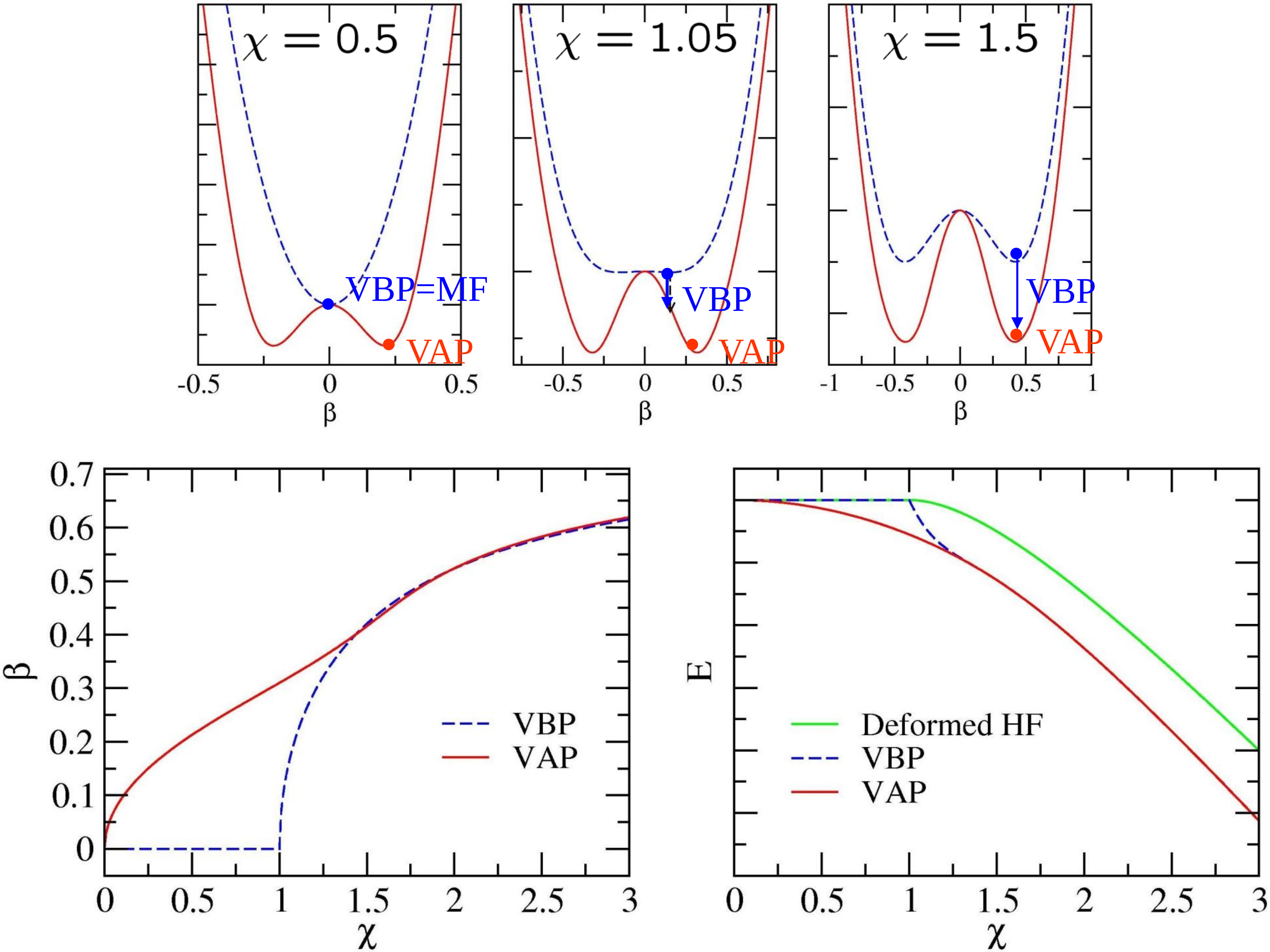
- Variation *After* Projection (VAP)

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



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

VAP:
robust, but very expensive



χ : the strength of two-body interaction (for a three-level Lipkin model)

Ref. K. Hagino, P.-G. Reinhard, G.F. Bertsch, PRC65('02)064320

Approximate Projection for large deformation

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:

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

Axial Symmetry, even-even nucleus

$$E_{0+} = \frac{\int_0^\pi \sin\theta\,\langle\Psi|H\hat{\mathcal{R}}(\theta)|\Psi\rangle\,d\theta}{\int_0^\pi \sin\theta\,\langle\Psi|\hat{\mathcal{R}}(\theta)|\Psi\rangle\,d\theta} \equiv \frac{\int_0^\pi \sin\theta\, H(\theta)\,d\theta}{\int_0^\pi \sin\theta\, N(\theta)\,d\theta}$$

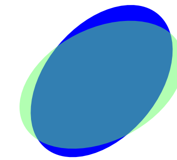
For large deformation:

$$N(\theta) \sim e^{-\alpha\theta^2}$$

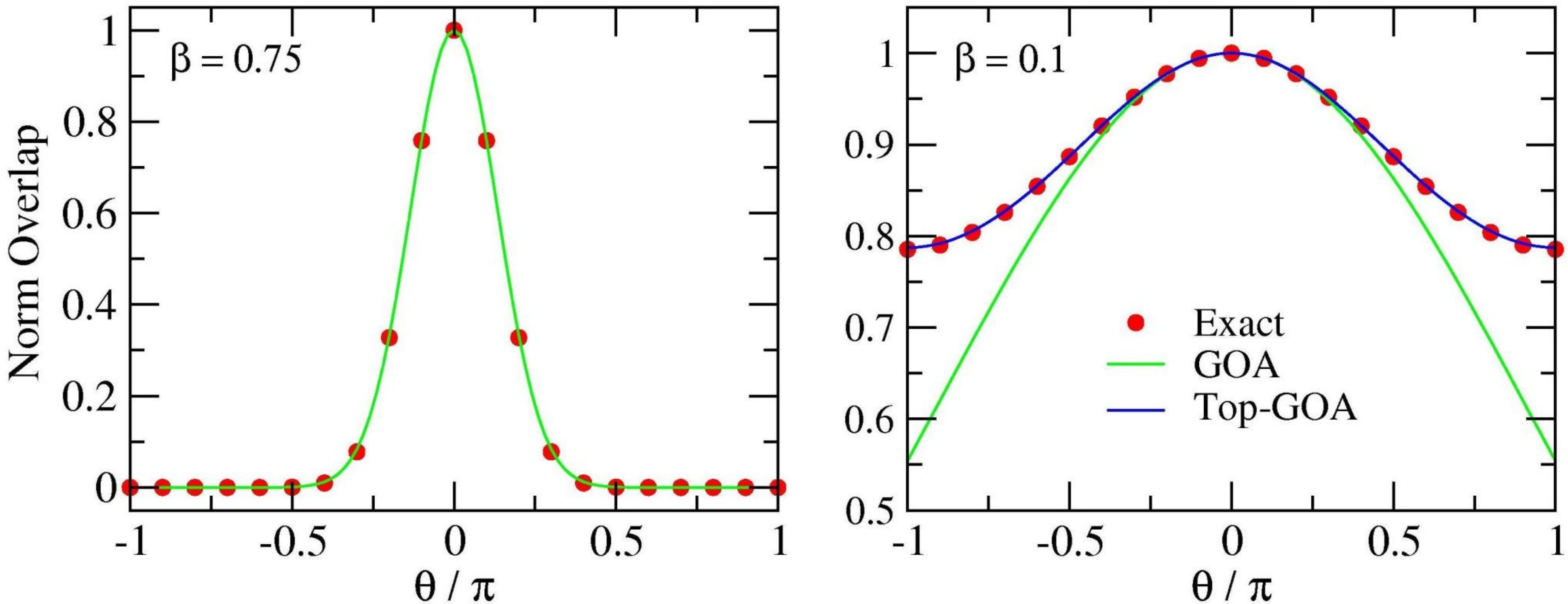
$$H(\theta) \sim N(\theta)\cdot(H_0 + H_2\,\theta^2)$$

Gaussian Overlap Approximation (GOA)

Large deformation



Small deformation



Three-level Lipkin model

K. Hagino, P.-G. Reinhard, G.F. Bertsch, PRC65('02)064320

Topological extension of GOA (top-GOA)

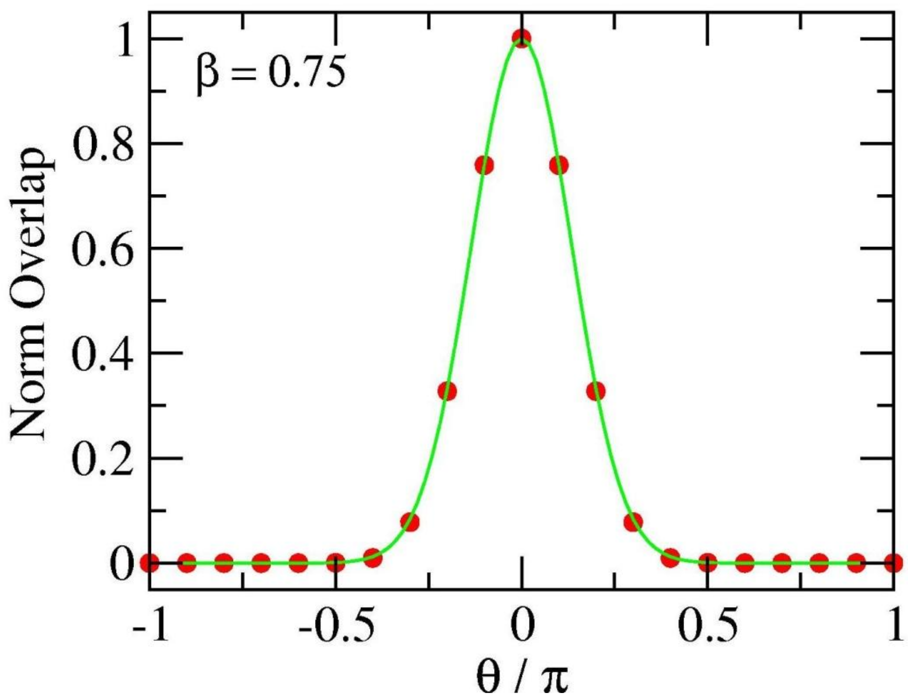
K. Hagino, P.-G. Reinhard, G.F. Bertsch, PRC65('02)064320

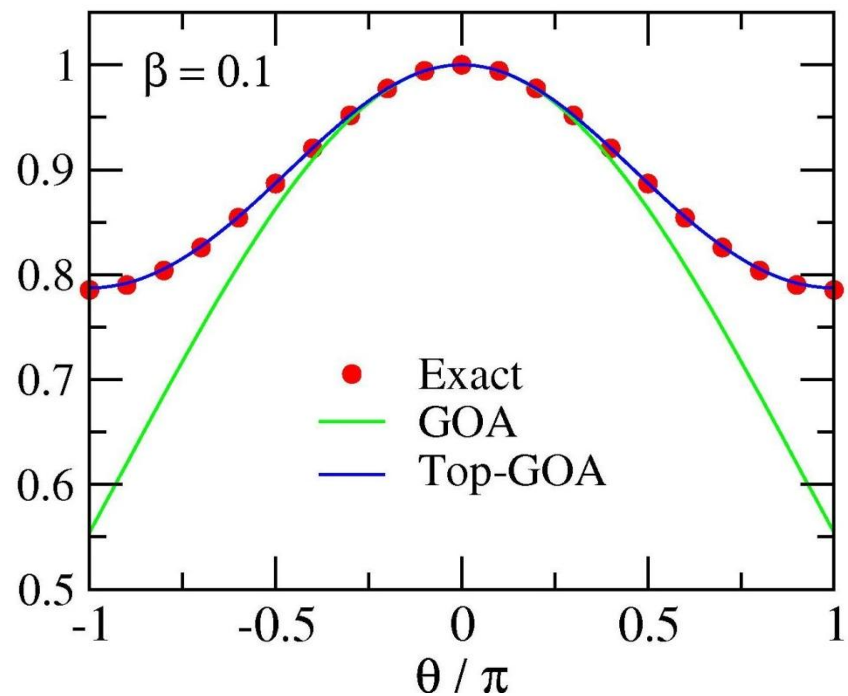
$N(\theta), \quad H(\theta)$: periodicity of 2π

$$N(\theta) \sim \exp(-4\alpha \sin^2(\theta/2))$$
$$H(\theta) \sim N(\theta) \cdot (H_0 + 4H_2 \sin^2(\theta/2))$$

(Top-GOA)

(note) $\cos\theta = 1 - 2\sin^2(\theta/2) \sim \exp(-2\sin^2(\theta/2))$





→ VAP calculations: feasible