

Dual Rotational Modes, Compact-Object and Distant-Object, in Quantum Many-body Systems

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Collaboration with

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Outline

1. Historical and quantal views of “rotational energy”
2. Shapes of heavy deformed nuclei
3. Dual modes of rotation, and clustering

1. & 2. TO *et al.*, EPJ-A, 61, 126 (2025);

A shorter introductory article: TO, EPJ Web of Conferences **342**, 01021 (2025).

3. TO, Volya and Itagaki, EPJ-A, 62, 108 (2026).

<https://doi.org/10.1140/epja/s10050-026-01856-x>

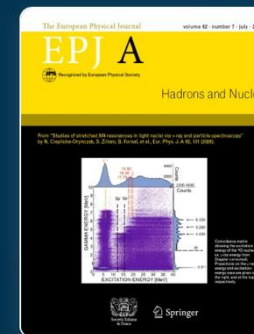
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Prevailing triaxial shapes in atomic nuclei and a quantum theory of rotation of composite objects

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EPJ Web of Conferences **342**, 01021 (2025)
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A comprehensive view of nuclear shapes, rotations and vibrations from fully quantum mechanical perspectives

Takaharu Otsuka^{1,2,3,4,*}

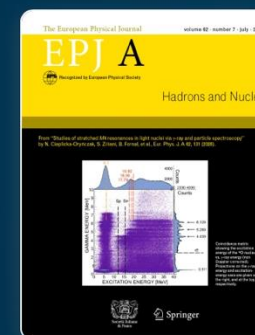
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Theoretical studies of α clustering in nuclei and beyond

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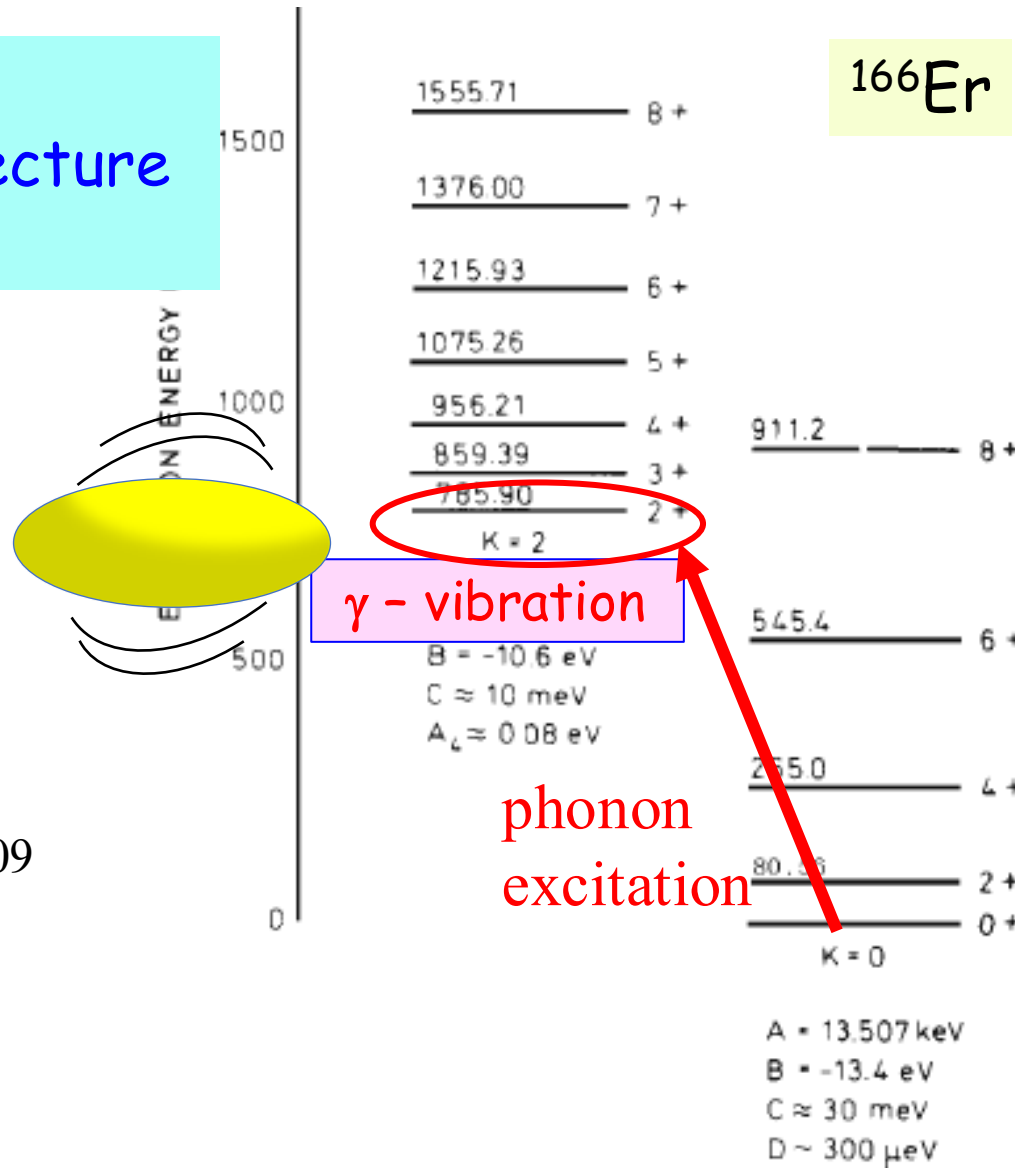


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Aage Bohr Nobel Prize Lecture (1975)

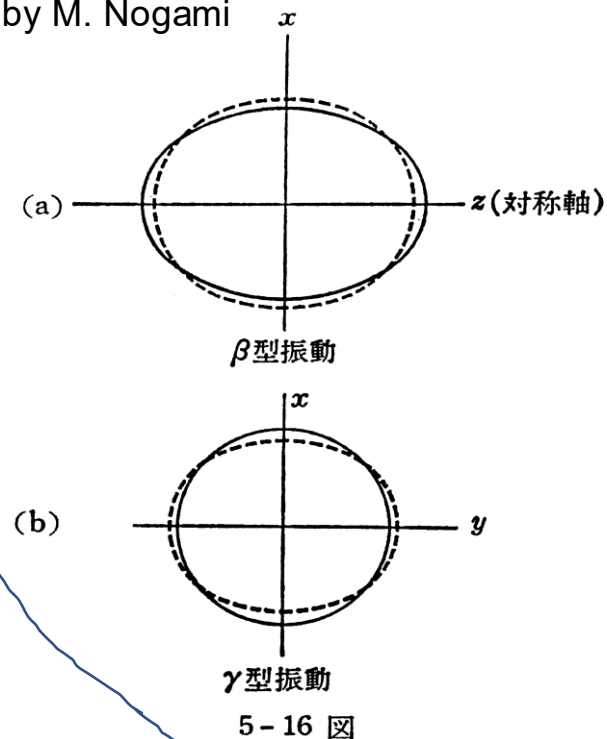


Aage N. Bohr, 1922-2009
Nobel Foundation archive



A case of the textbook example:

原子核 by M. Nogami



**Axially symmetric
prolate ellipsoid
(equilibrium)**

Fig. 9. Rotational bands in ^{166}Er . The figure is from (35) and is based on the experimental data by Reich and Cline (75). The bands are labelled by the component K of the total angular momentum with respect to the symmetry axis. The $K = 2$ band appears to represent the excitation of a mode of quadrupole vibrations involving deviations from axial symmetry in the nuclear shape.

also emphasized in
A. Bohr and B. R. Mottelson,
Nuclear Structure II
(1975, Benjamin, New York)

Origin of the $J(J+1)$ rule of rotational excitation energy

Ring & Schuck,
The Nuclear Many-Body Problem

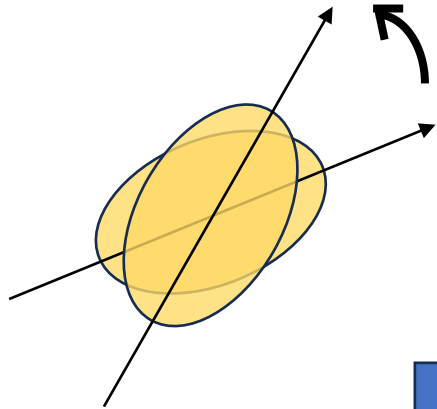
conventional description

classical mechanics

time t , angle $\Omega(t)$

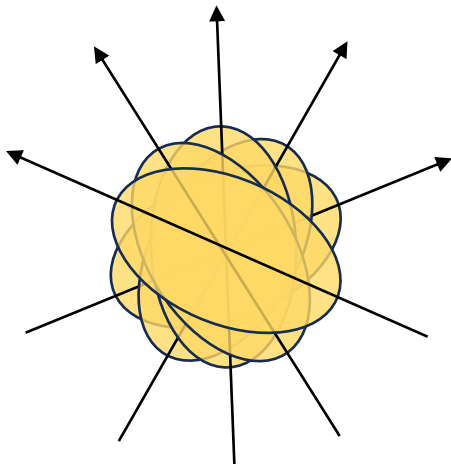
rotation of rigid body

time t_0 , angle Ω_0



quantization of free rotation of this rigid body

→ eigenstate with angular momentum $\hbar J$



- superposition of states at varying angles
- for axially symmetric shape, $J(J+1)$ rule is suggested
- just kinetic energy of free rotation

Bohr Hamiltonian

$$\hat{H}_{\text{coll}} = \frac{-\hbar^2}{2B_2} \left[\beta^{-4} \frac{\partial}{\partial \beta} \left(\beta^4 \frac{\partial}{\partial \beta} \right) + \frac{1}{\beta^2 \sin 3\gamma} \frac{\partial}{\partial \gamma} \left(\sin 3\gamma \frac{\partial}{\partial \gamma} \right) \right] + \boxed{\hat{T}_{\text{rot}}} + V(\beta, \gamma),$$

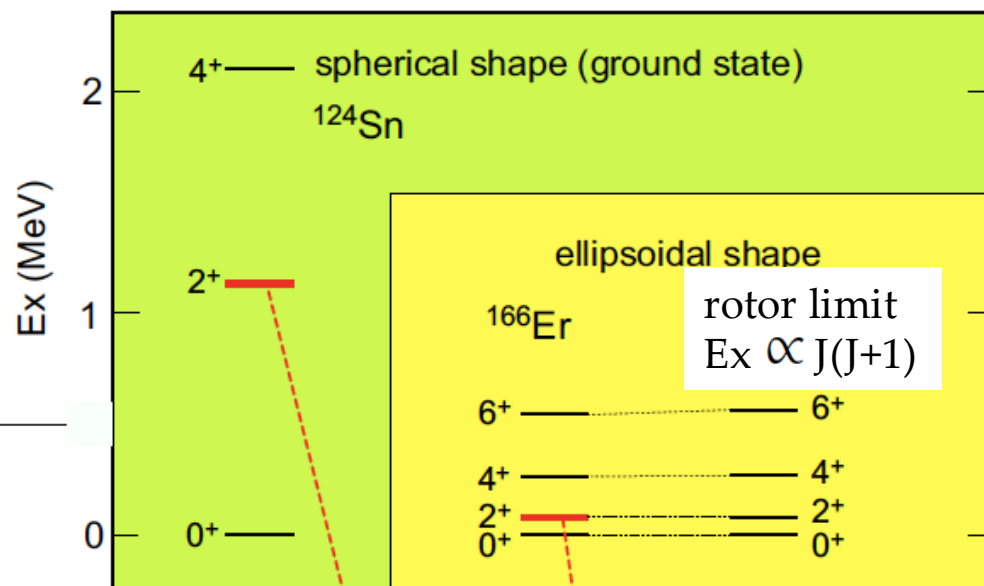
the rotational energy is found to be

$$\hat{T}_{\text{rot}} = \frac{\hat{I}_1^2}{2\mathcal{I}_1} + \frac{\hat{I}_2^2}{2\mathcal{I}_2} + \frac{\hat{I}_3^2}{2\mathcal{I}_3}.$$

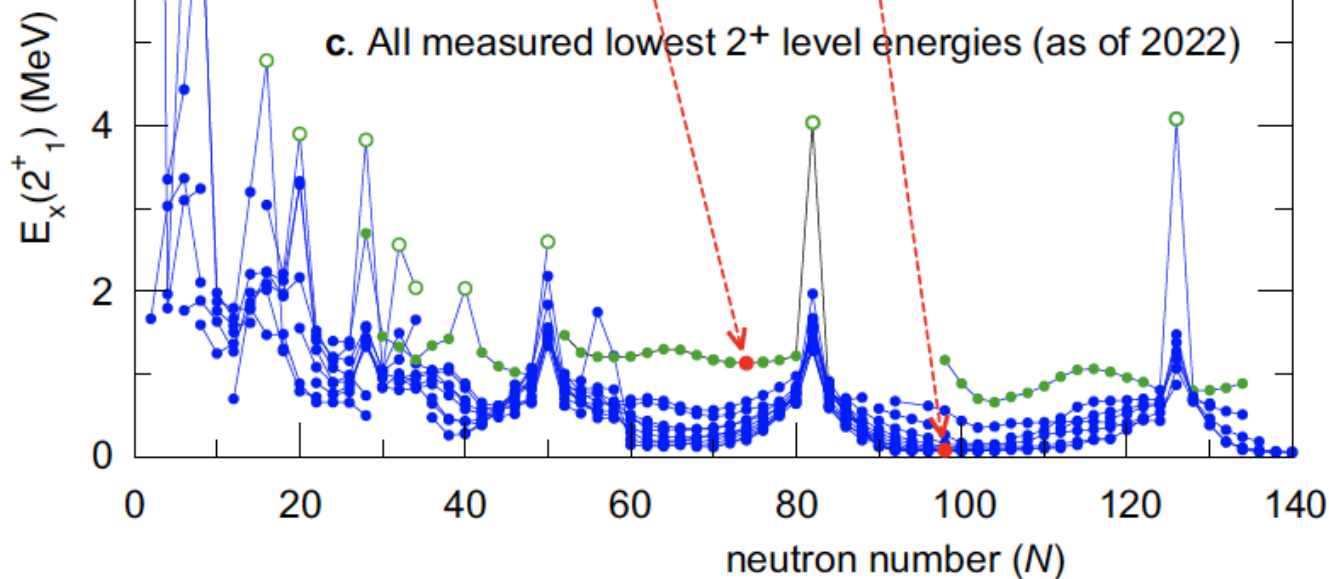
Thus, for axially symmetric shapes ($\mathcal{I}_3=0$), the rotational kinetic energy is given by

$$T_{\text{rot}} \propto J(J+1)$$

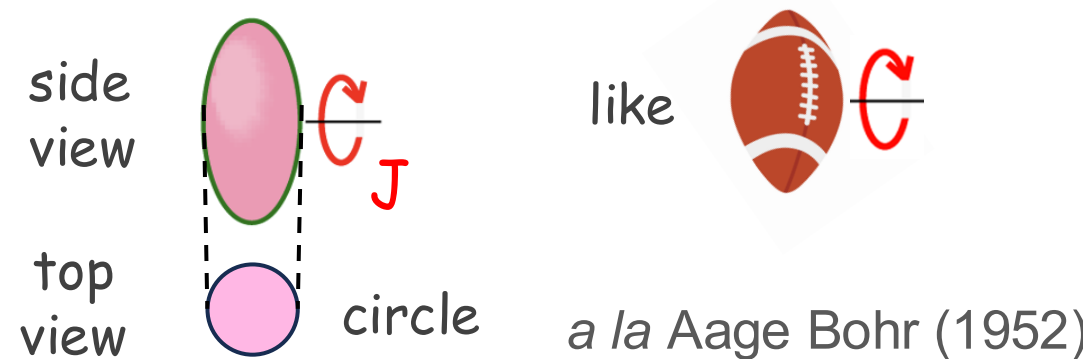
b. Level energies of atomic nuclei with spherical and ellipsoidal shapes (examples)



c. All measured lowest 2^+ level energies (as of 2022)



Conventional picture of nuclear shape and rotation



Textbooks kept teaching us for 70 years:
For strongly deformed nuclei,

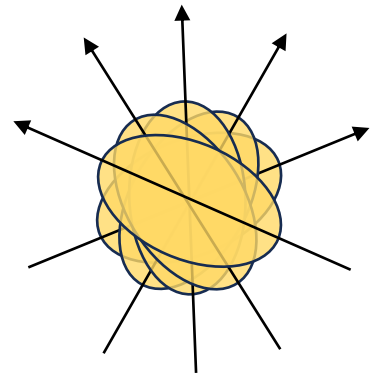
1. axially symmetric ellipsoid emerges, and rotates, *like a rugby ball*

2. $J(J+1)$ rule of excitation energy is due to **rotational kinetic energy**

3. γ band is due to γ vibration

4. if axial symmetry is broken, no good K quantum numbers remain

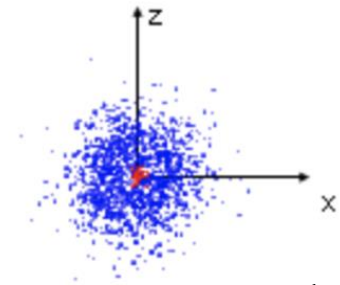
However, rotational states can be formulated in a quantum mechanical way without having such a rigid-body's free rotation picture.



Wave functions of members of a rotational band are produced by superposing a common intrinsic state oriented to various directions, so that the superposed state has a good angular momentum (J, M), by using Wigner's D function.



the same underlying ideas



Electron-cloud picture
for atoms

– An electron in an s-orbital



Cranking of an object pointing
to a fixed orientation



This concept can be materialized, by following the well-defined recipe of the angular momentum projection of a given intrinsic state.

General expression of the projection on to J and M from an intrinsic state ϕ .

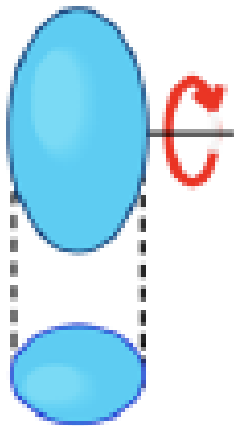
$$\Psi[\phi, J, M, K] = (2J + 1)/(8\pi^2)$$

$$\int_0^{2\pi} d\alpha \int_0^\pi d\beta \sin\beta \int_0^{2\pi} d\gamma$$

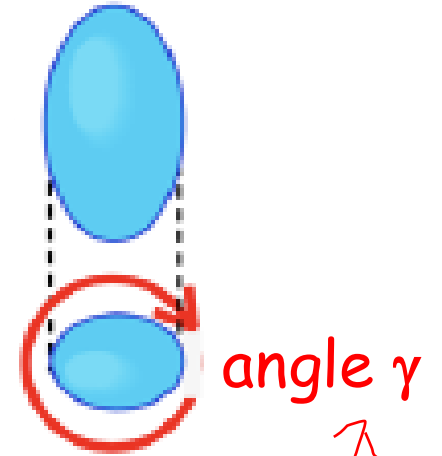
$$\{D_{M,K}^J(\alpha, \beta, \gamma)\}^* e^{i\alpha \hat{J}_z} e^{i\beta \hat{J}_y} e^{i\gamma \hat{J}_z} |\phi\rangle$$

Wigner D function

intrinsic state



angle β



angle γ

α, β, γ are Euler angles for 3-dimensional rotation.
(Do not confuse them with deformation parameters.)

We start with a simple case, $K=0$, with intrinsic state ϕ_0 .
No integration with respect to γ is needed.
We then can set $M=0$ (no integration with respect to α).

Because of the identity,

$$D_{M,K}^J(\alpha, \beta, \gamma) = e^{iM\alpha} d_{M,K}^J(\beta) e^{iK\gamma}$$

The original equation is simplified to

$$\Psi[\phi, J, M, K] = (2J + 1)/(8\pi^2) \int_0^{2\pi} d\alpha \int_0^\pi d\beta \sin\beta \int_0^{2\pi} d\gamma \{D_{M,K}^J(\alpha, \beta, \gamma)\}^* e^{i\alpha \hat{J}_z} e^{i\beta \hat{J}_y} e^{i\gamma \hat{J}_z} |\phi\rangle.$$

$$\text{if } K=M=0 \quad \propto \int_0^\pi d\beta \sin\beta d_{0,0}^J(\beta) \boxed{e^{i\beta \hat{J}_y} |\phi_0\rangle}$$

↑
Wigner's d function = Legendre polynomial

Quantum many-body derivation of rotational excitation energy

ϕ_0 : intrinsic state with $K=0$ for simplicity, e.g. by shell model

The member of angular momentum J of a rotational band

is given by the projected state $\propto \int_0^\pi d\beta \sin\beta d_{0,0}^J(\beta) e^{i\beta \hat{J}_y} |\phi_0\rangle$

→ the energy is given by

$$= \frac{2J+1}{2|\mathcal{N}_J|^2} \langle \phi_0 | H \int_0^\pi d\beta \sin\beta d_{0,0}^J(\beta) e^{i\beta \hat{J}_y} |\phi_0\rangle,$$

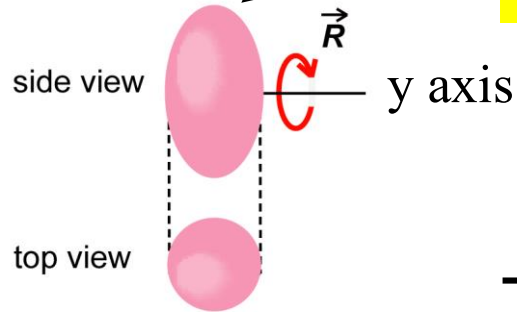
$$= \frac{2J+1}{2|\mathcal{N}_J|^2} \int_0^\pi d\beta \sin\beta d_{0,0}^J(\beta) h_y(\beta),$$

energy kernel $h_y(\beta) = \langle \phi_0 | H e^{i\beta \hat{J}_y} |\phi_0\rangle$

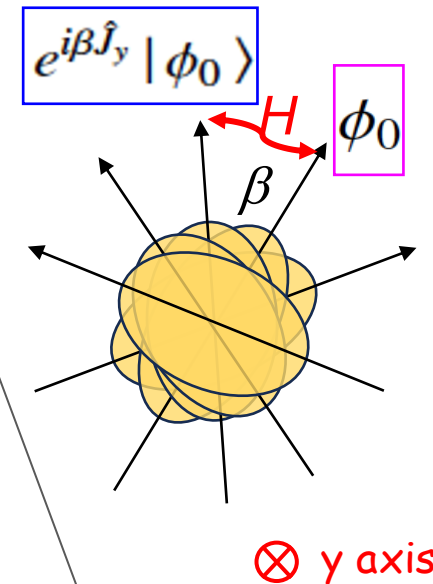
polynomial expansion: $d_{0,0}^J(\beta) = P_J(\cos\beta) \approx 1 + F_J(\cos\beta - 1) + G_J(\cos\beta - 1)^2 + \dots$

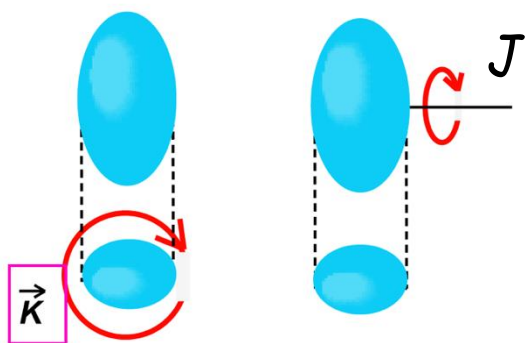
(stops at finite power)

a. nucleus (prolate)



rotation about y axis



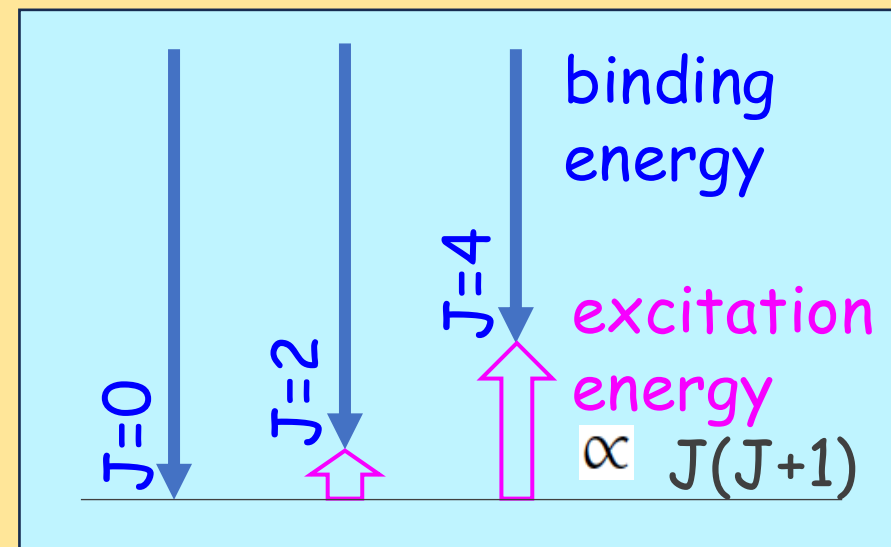


The excitation energy thus depicts the $J(J+1) - K^2$ dependence in the cases of strong deformation :

$$E_{J,K}^{(0+1)} = \frac{\tilde{e}_0}{\tilde{n}_0} + \frac{1}{2} \left\{ J(J+1) - K^2 \right\} \frac{\tilde{e}_0}{\tilde{n}_0} \left\{ \frac{\tilde{e}_1}{\tilde{e}_0} - \frac{\tilde{n}_1}{\tilde{n}_0} \right\}$$

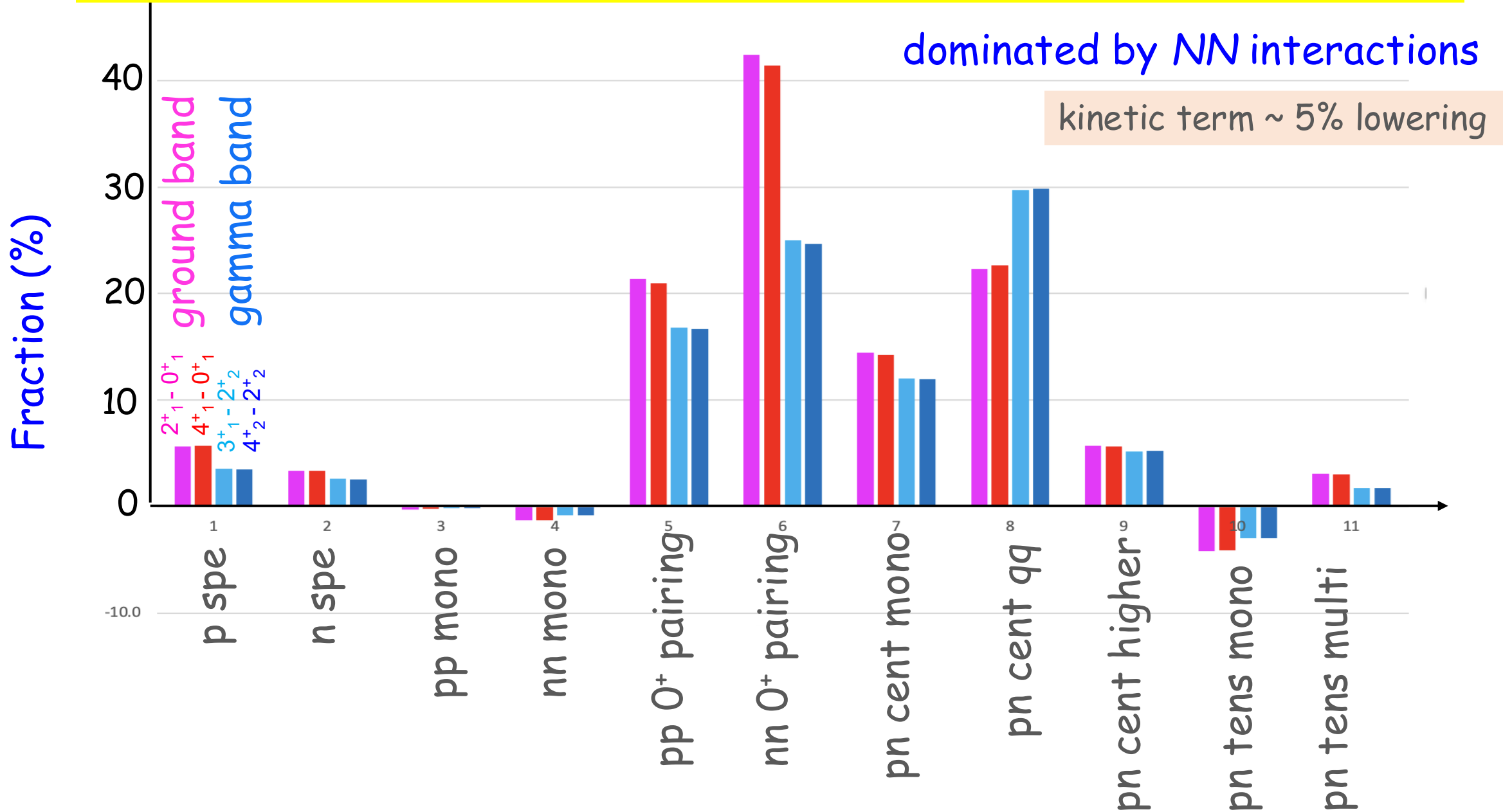
The excitation energies in the rotational band represent a loss of the binding energy as a function of J .

Almost no contribution from rotational kinetic energy (even opposite in some cases), in contrast to the conventional picture.



Note: Despite rather substantial differences from the present work, the underlying picture can be partly shared with earlier works, Peierles & Yoccoz (1957), Verhaar (1963), Kamlah (1968), Siemens & Jensen (book, 1987). The infinite Taylor expansion of Wigner d function with β^k was used in Verhaar and Siemens & Jensen, but the d function is simply polynomials like $(\cos \beta - 1)^k$, which leads to a finite expansion converging differently.

Decomposition of rotational excitation energies for two bands in ^{166}Er



Outline

1. Historical and quantal views of “rotational energy”

2. Shapes of heavy deformed nuclei

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Are atomic nuclei like
rugby ball or almond ?



1. & 2. TO *et al.*, EPJ-A, 61, 126 (2025);

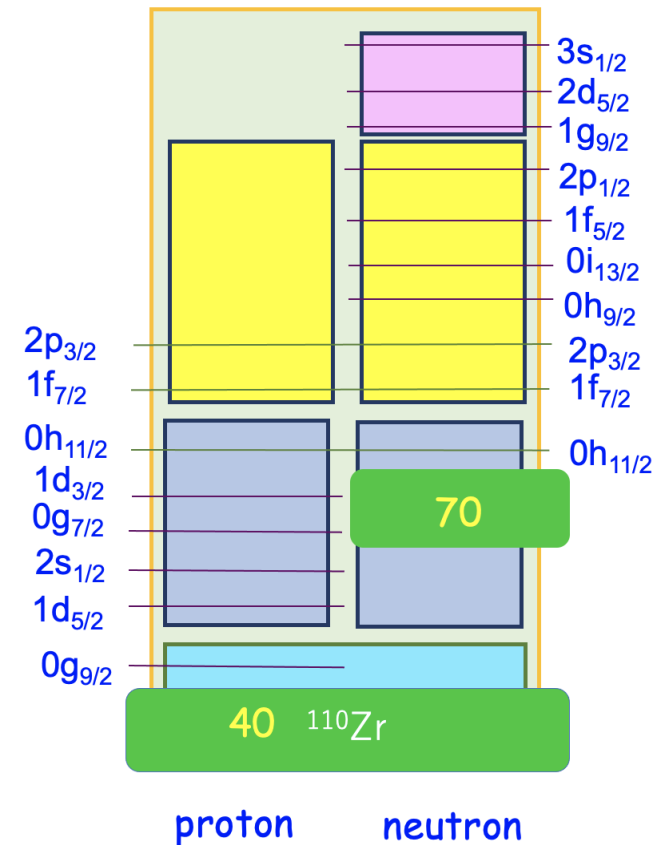
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Revisit with Monte Carlo Shell Model (CI calculation)

The model space



We performed Monte Carlo Shell Model (**MCSM**) calculations, where the largest case corresponds to the diagonalization of 3.9×10^{31} dim. matrix. The advanced version of MCSM, **Quasiparticle Vacua Shell Model (QVSM)***, was used, in order to incorporate both **pairing** and **deformation** effects on an equal footing, with ***N*-projected Bogoliubov basis vectors**. Supercomputer Fugaku of RIKEN was utilized.

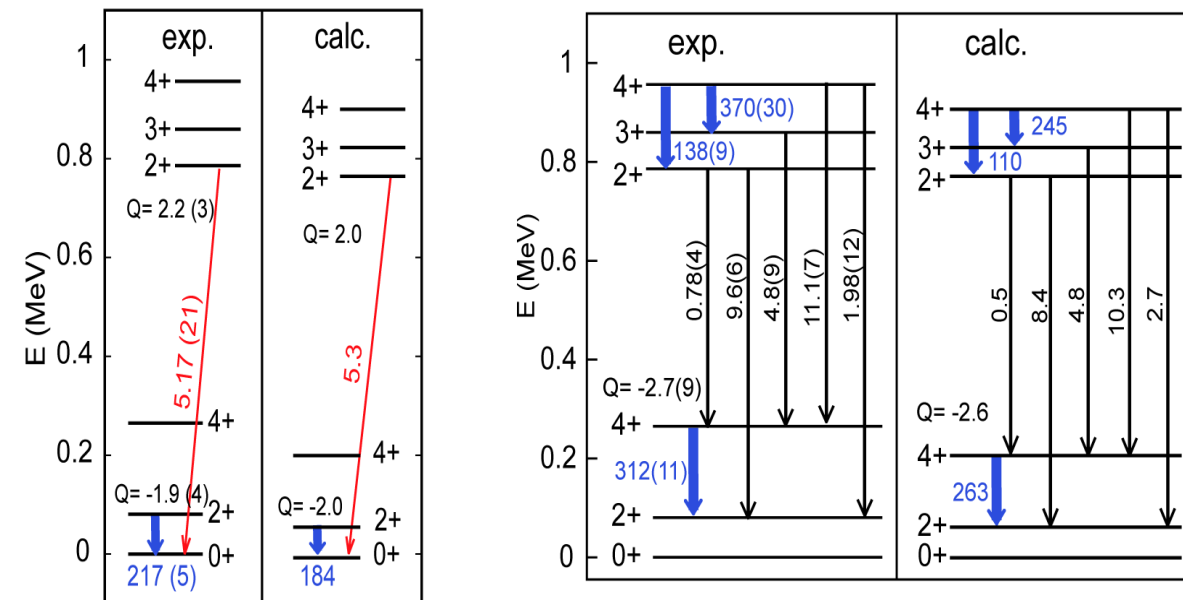
*Shimizu *et al*, PRC 103, 014312 (2021)



Effective interaction:
 $G\text{-matrix}^* + V_{\text{MU}}$
 * Brown, PRL (2000)

V_{MU} : same interaction for the description of shell evolution in exotic nuclei

c. level energies and E2 properties of ^{166}Er



Basic formulation of Monte Carlo Shell Model

N_B : number of basis vectors

eigenstate

$$|\Psi(D)\rangle = \sum_{n=1}^{N_B} c_n P^{J,\Pi} |\phi(D^{(n)})\rangle$$

amplitude

Projection op.

N_p : number of (active) particles

N_{sp} : number of single-particle states

$$|\phi(D^{(n)})\rangle = \prod_{\alpha=1}^{N_p} \left(\sum_{i=1}^{N_{sp}} a_i D_{i\alpha}^{(n)} \right) |-\rangle$$

n-th basis vector (Slater determinant)

Superposition of original single-particle state

$$E(D) = \langle \Psi(D) | H | \Psi(D) \rangle$$

Minimize $E(D)$ with respect to D utilizing Quantum MC and variational methods

Step 1 : Shift randomly matrix matrix D. (The initial guess can be taken from Hartree-Fock.)
Select the one producing the lowest $E(D)$ (rate < 0.1 %)

Step 2 : Polish D by means of the conjugate gradient (CG) method variationally.

Basic formulation of Monte Carlo Shell Model

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n-th basis vector (Slater determinant)

Superposition of original single-particle state

Bogoliubov state in the QVSM (advanced version)

$$E(D) = \langle \Psi(D) | H | \Psi(D) \rangle$$

Minimize $E(D)$ with respect to D utilizing Quantum MC and variational methods

Step 1 : Shift randomly matrix matrix D. (The initial guess can be taken from Hartree-Fock.)
Select the one producing the lowest $E(D)$ (rate < 0.1 %)

Step 2 : Polish D by means of the conjugate gradient (CG) method variationally.

Most advanced methodology in the MCSM is used

- (Ordinary) MCSM: superposed Slater determinants with angular momentum and parity projections
- **QVSM**(Quasiparticle Vacua Shell Model): superposed quasiparticle vacua with number, angular momentum, and parity projections
- **Pairing correlations** over many single-particle orbitals are already incorporated in each basis vector because of its **BCS-type** character

$$\begin{array}{ccc} \text{quasiparticle} & \nearrow & \\ \text{vacuum} & & \end{array} |\phi\rangle = \prod_p (u_p + v_p a_p^\dagger a_{\bar{p}}^\dagger) |-\rangle \begin{array}{cc} & \nwarrow \\ & \text{core (vacuum)} \end{array}$$

PHYSICAL REVIEW C **103**, 014312 (2021)

Variational approach with the superposition of the symmetry-restored quasiparticle vacua for nuclear shell-model calculations

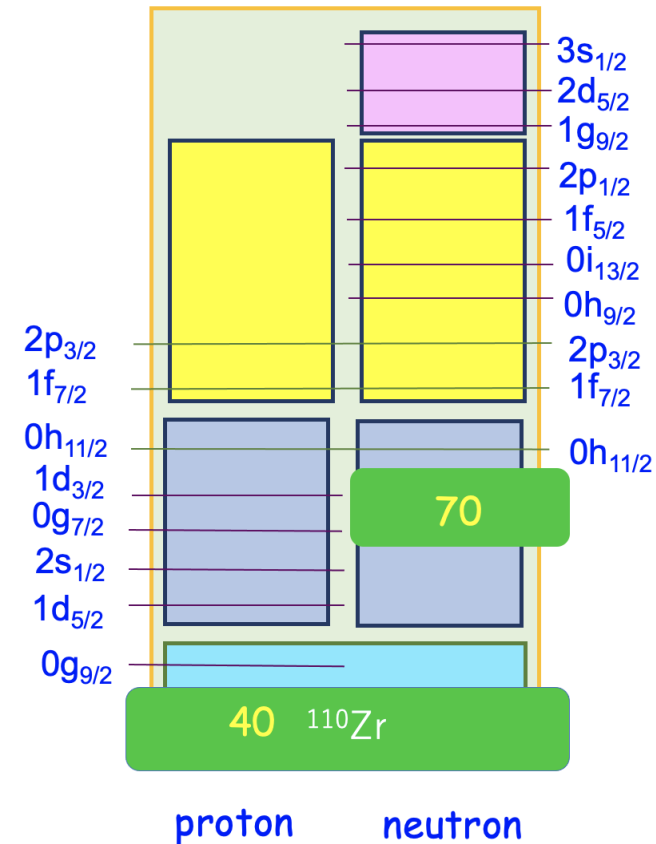
Noritaka Shimizu ^{1,*} Yusuke Tsunoda,¹ Yutaka Utsuno,^{2,1} and Takaharu Otsuka^{3,4,2}

The QVSM code was fully used, but huge computer resources were still needed.

reprise

Revisit with Monte Carlo Shell Model (CI calculation)

The model space



We performed Monte Carlo Shell Model (**MCSM**) calculations, where the largest case corresponds to the diagonalization of 3.9×10^{31} dim. matrix. The advanced version of MCSM, **Quasiparticle Vacua Shell Model (QVSM)***, was used, in order to incorporate both **pairing** and **deformation** effects on an equal footing, with ***N*-projected Bogoliubov basis vectors**. Supercomputer Fugaku of RIKEN was utilized.

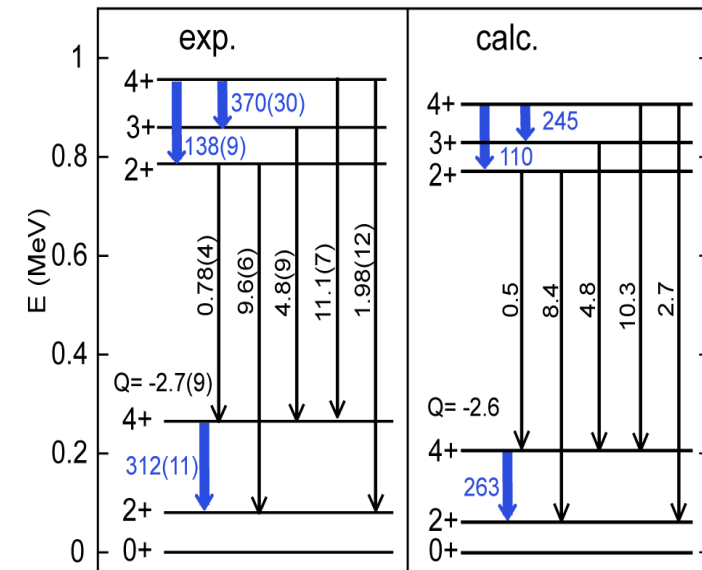
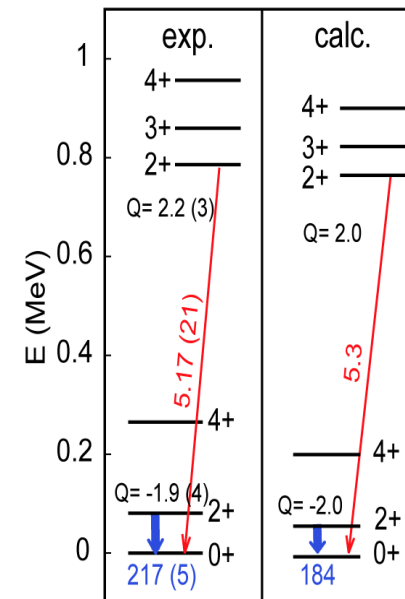
*Shimizu *et al*, PRC 103, 014312 (2021)



Effective interaction:
 $G\text{-matrix}^* + V_{MU}$
* Brown, PRL (2000)

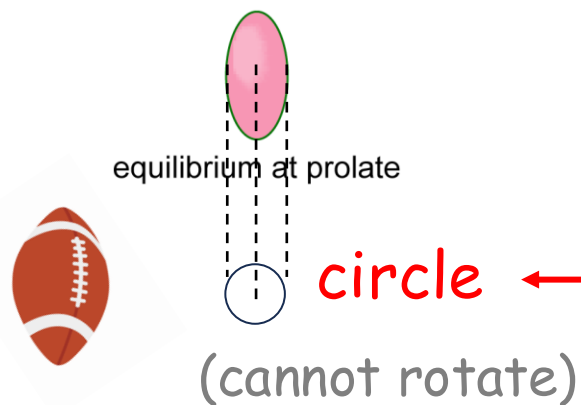
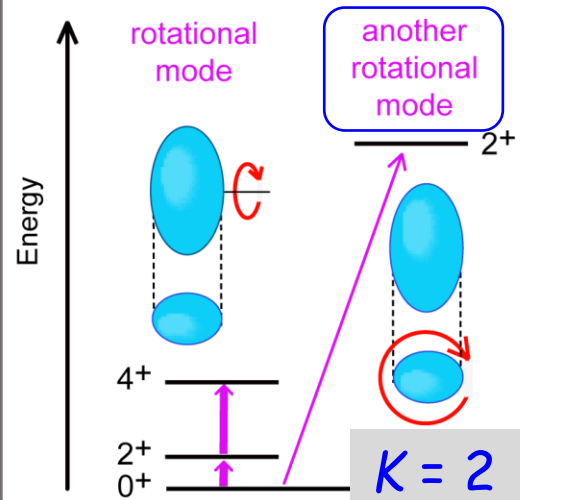
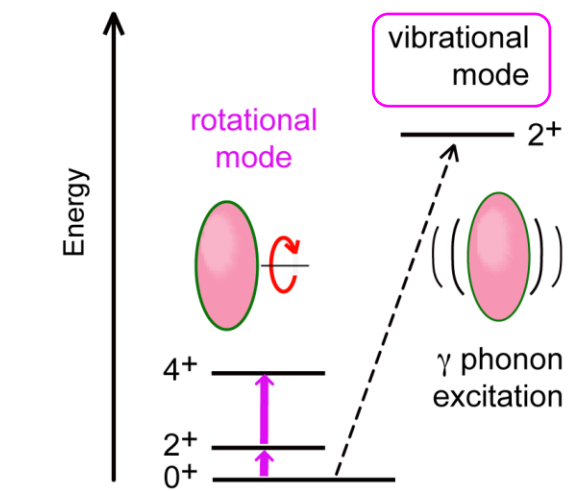
V_{MU} : same interaction for the description of shell evolution in exotic nuclei

c. level energies and E2 properties of ^{166}Er



Axially symmetric shape -a la A. Bohr-

Present view Triaxial shape



$\gamma = 0 \text{ deg.}$

circle

(cannot rotate)

$\gamma > 0 \text{ deg.}$

ellipse

side view

top view



triaxiality parameter γ (deg.)

$$\tan \gamma = \sqrt{2} \frac{Q_2}{Q_0}$$

Theoretical studies include

Davydov model for ^{166}Er (1959)

$2^+_2/2^+_1$ energy ratio $\rightarrow \gamma \sim 13 \text{ deg.}$

$B(E2) 2^+_2/2^+_1$ ratio $\rightarrow \gamma \sim 9 \text{ deg.}$

DFT approaches

Tajima et al. (1996)

dominance of prolate ($\gamma=0$) shape by Skyrme HF

Scamps, Goriely et al. (2021)

$\gamma=1.6$ (1.2) deg for ^{166}Er (^{154}Sm) by Skyrme HFB

Li et al., (2010); Yang et al. (2021)

Relativistic HB for ^{166}Er etc. $\gamma \sim 6 \text{ deg.}$,

γ smaller, mostly 0 for other nuclei of interest

Robledo et al. (2008),

PES by HFB with Gogny D1S for many

Li et al. (2009),

Rel. EDF $\rightarrow$ 5-dim coll. Hamiltonian,

Delaroche et al., (2010)

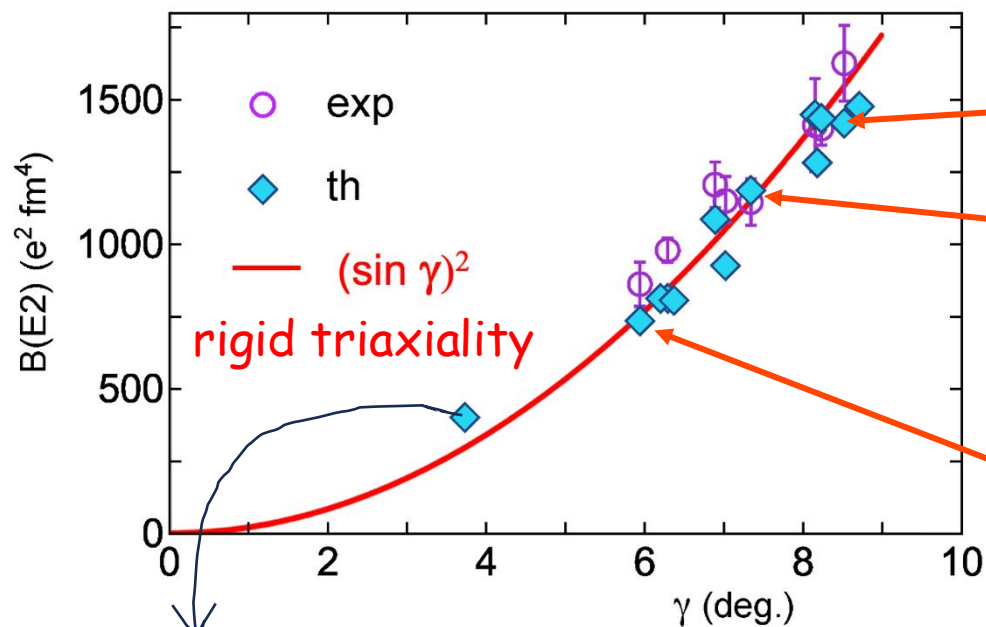
Gogny $\rightarrow$ 5-dim coll. Hamiltonian

From experimental side

Sharpey-Schafer et al.(2019)

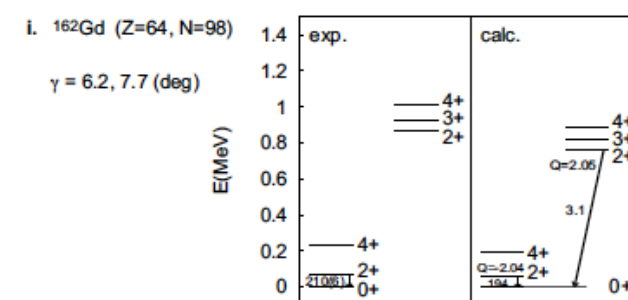
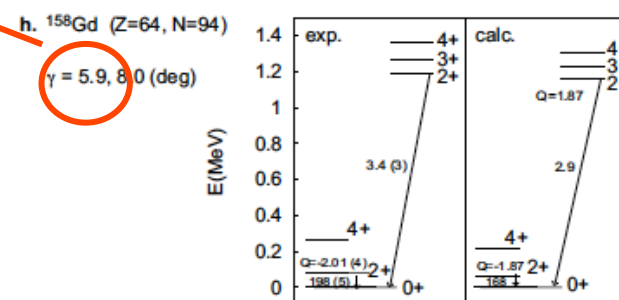
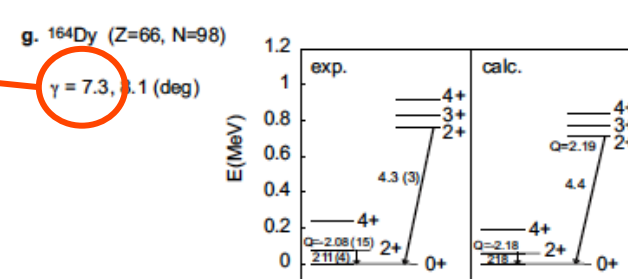
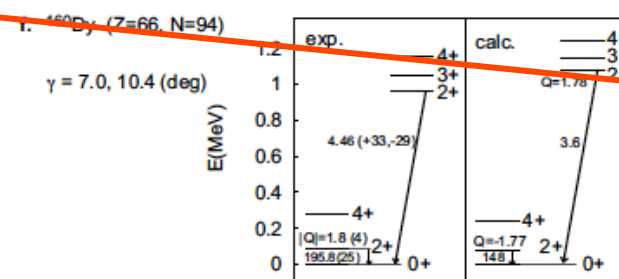
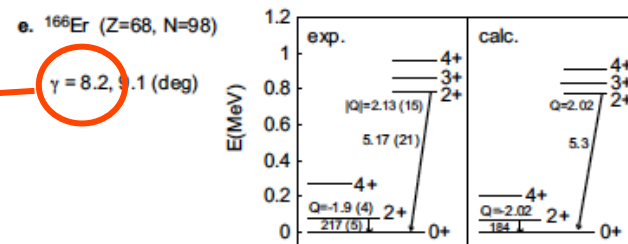
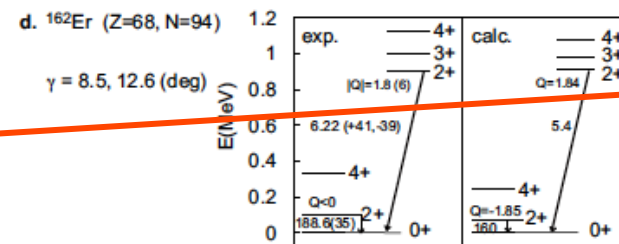
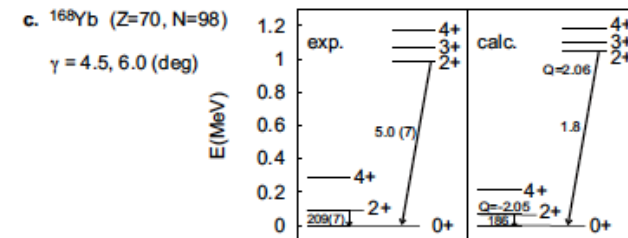
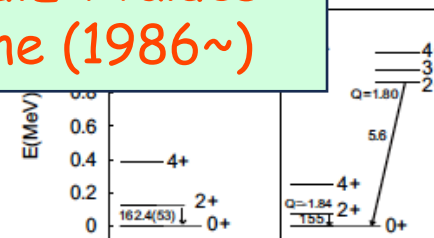
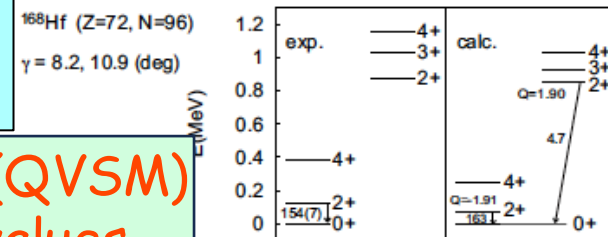
Medium triaxiality
systematically produced
by the same Hamiltonian

An experimental evidence :
clear correlation between γ
and $B(E2; 0^+_1 \rightarrow 2^+_{\text{gamma}})$



Levels, $B(E2)$'s and
Q-moments reproduced

○ : γ values by MCSM (QVSM)
~ Multiple CoulEx values
a la D. Cline (1986~)



Predicted $B(E2)$ to 2^+ at $E_x \sim 2.7$ MeV of ^{154}Sm
an example of small triaxiality

Two origins and two appearances of triaxiality in deformed heavy nuclei

1. Small triaxiality due to symmetry restoration with K

This mechanism alone generates γ up to 5 degrees.

This occurs in most (virtually all) strongly deformed nuclei.

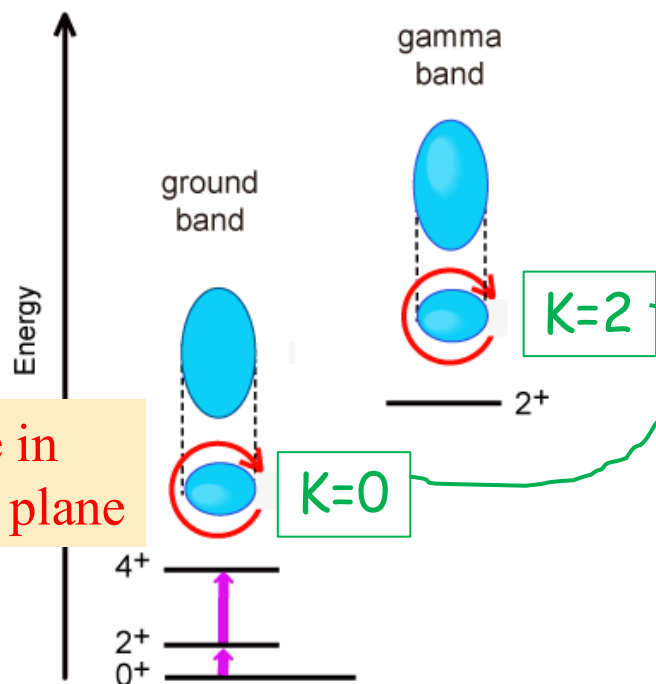
2. Medium triaxiality mainly due to monopole part of pn tensor force (through self-organization) and/or hexadecupole part of pn central force.

This mechanism enlarges γ to a range of 6 - 14 degrees (or more),
in selected heavy deformed nuclei (~half ?).

Both cases involve high-j orbitals, like $g_{9/2,7/2}$, $h_{11/2,9/2}$, $i_{13/2,11/2}$, *etc.*

This enlargement has been verified by constrained HFB calculation.

Triaxiality provides nuclei with additional binding energy !



ellipse in the xy plane

The rotational symmetry in the xy plane is broken because of this ellipse, but it is restored by projecting onto a good K value.

K conservation is discussed later.

Euler angle γ

0

$\pi/4$

$\pi/2$

$3\pi/4$

state (different representations of the 2-dim. rotational group)

(a) $K = 0$	$\Phi \propto$		+	...	+		+	...	+		+	...	+		+	...	+
(b) $K = 2$	$\Phi \propto$		+	...	+		+	...	-		+	...	-		+	...	+
(c) $K = -2$	$\Phi \propto$		+	...	-		+	...	-		+	...	+		+	...	+

Expectation value of H

finite triaxial deformation
→ more binding energy

(d) $K = 0$ (diagonal)

$$\langle K=0 | H | K=0 \rangle \propto \langle \text{ellipse} | H | \text{ellipse} \rangle + \dots + \langle \text{ellipse} | H | \text{tilted ellipse} \rangle + \dots + \langle \text{ellipse} | H | \text{vertical ellipse} \rangle + \dots + \langle \text{ellipse} | H | \text{tilted ellipse} \rangle + \dots + \langle \text{ellipse} | H | \text{vertical ellipse} \rangle$$

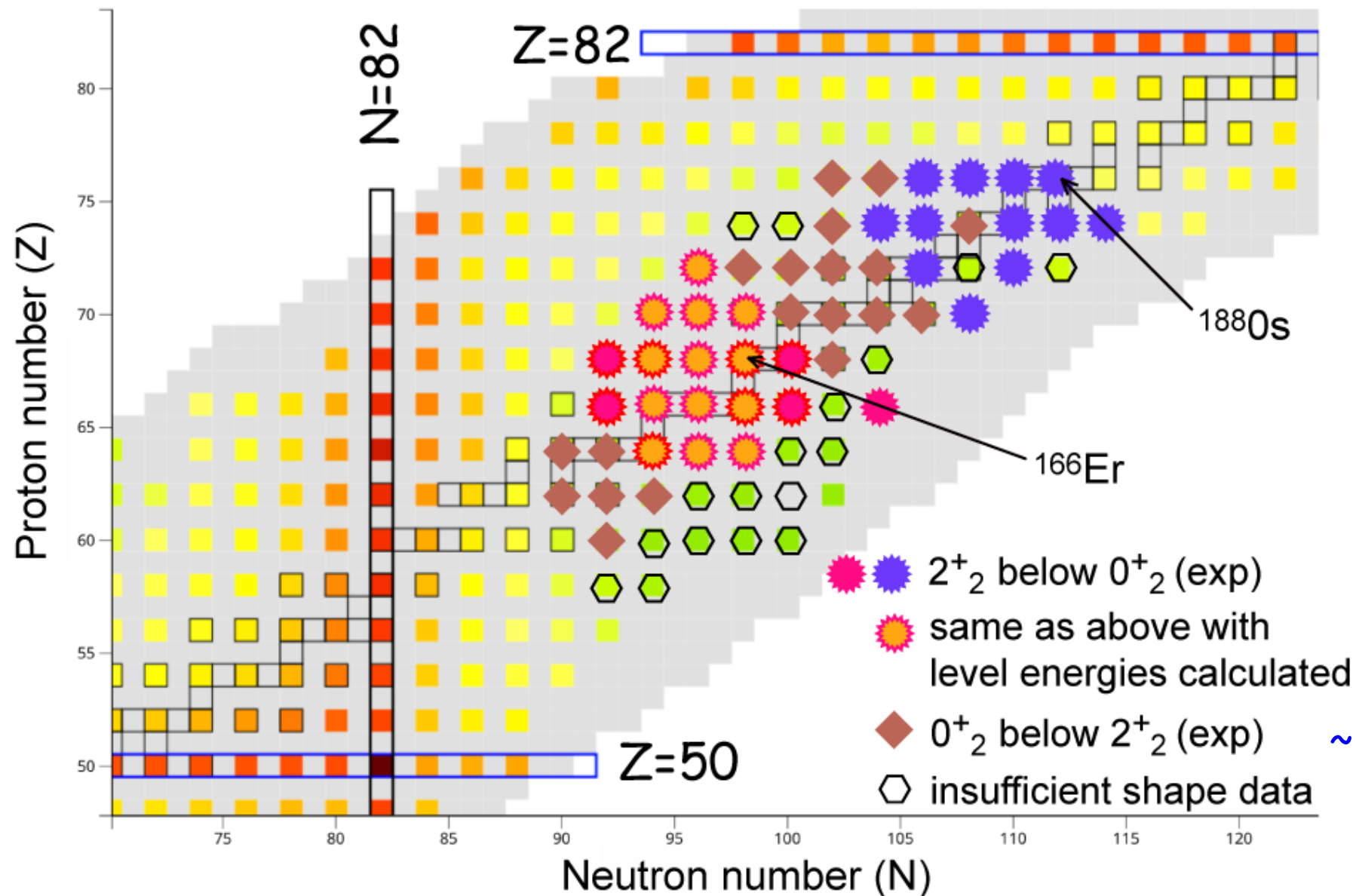
(e) $K = 2 + K = -2$ (diagonal)

$$\langle K=2 \& -2 | H | K=2 \& -2 \rangle \propto \langle \text{ellipse} | H | \text{ellipse} \rangle + \dots + 0 \langle \text{tilted ellipse} | H | \text{tilted ellipse} \rangle + \dots + \langle \text{vertical ellipse} | H | \text{vertical ellipse} \rangle + \dots + 0 \langle \text{tilted ellipse} | H | \text{tilted ellipse} \rangle$$

opposite

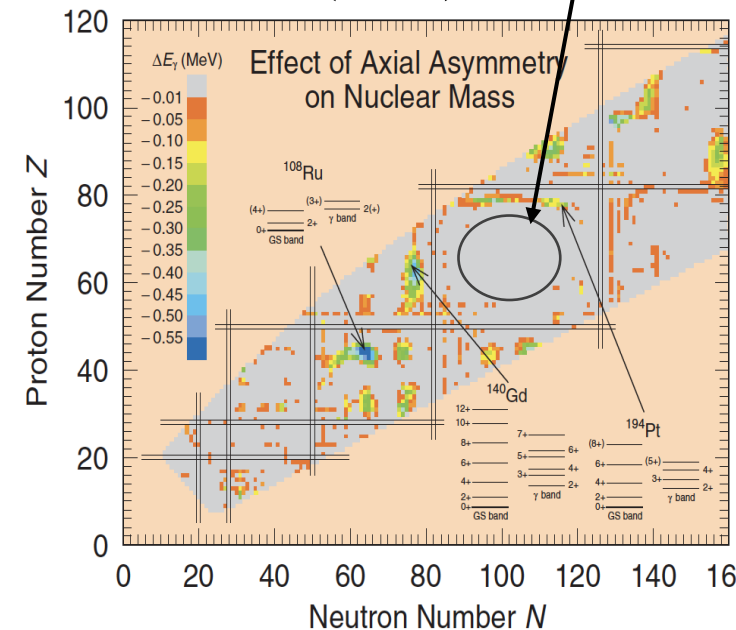
less binding energy than $K=0$

Appearance of triaxial shapes in the nuclear chart



Conventionally axially symmetric

Moller et al. (2006)

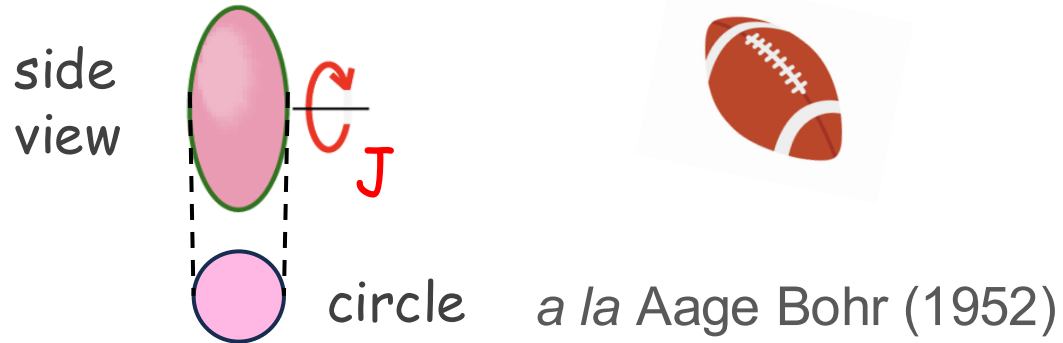


medium triaxiality

~ small triaxiality

A summary (for rotational modes)

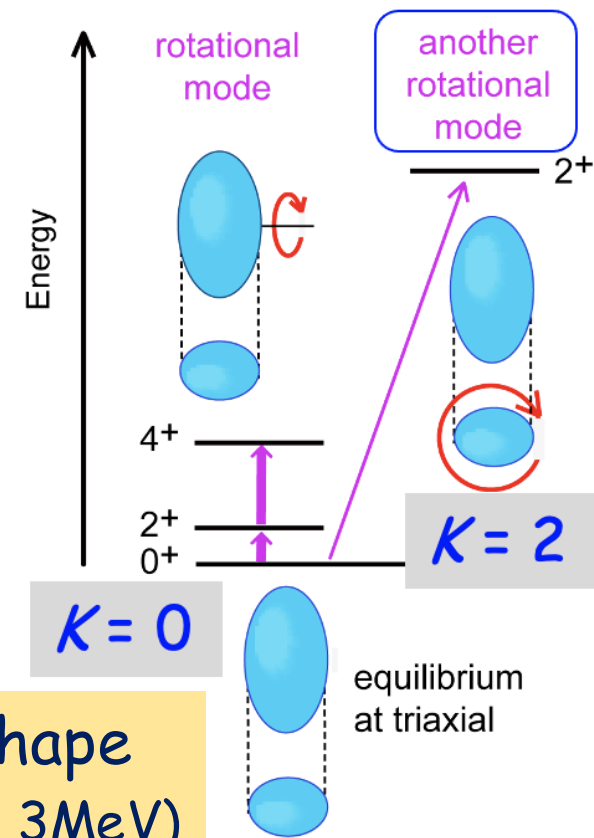
Conventional picture of strongly deformed nuclei in textbooks for 70 years



Presently ...



Novel overall view



1. axially symmetric ellipsoid emerges, and rotates, like a rugby ball

2. $J(J+1)$ rule of excitation energy is due to **rotational kinetic** energy

3. γ band is due to γ vibration

4. if axial symmetry is broken, no good K quantum numbers remain

1. Prevailing triaxial shape like an almond ($\Delta E \sim 3\text{MeV}$)

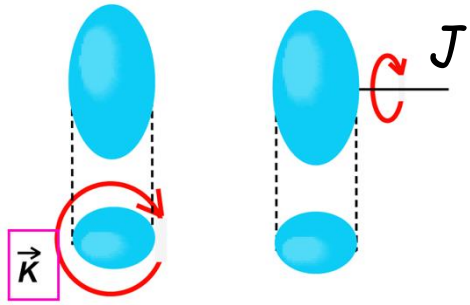
2. $J(J+1)$ rule represents the whole Hamiltonian, primarily **interactions**

3. γ band is a $K=2$ rotation

4. K quantum number is practically conserved even with triaxiality

Prevailing triaxiality $\rightarrow$ Davydov et al. (1958-9)

A digest: T. Otsuka, arXiv: 2509.08552 [nucl-th]



The excitation energy thus depicts the $J(J+1) - K^2$ dependence in the cases of strong deformation :

$$E_{J,K}^{(0+1)} = \frac{\tilde{e}_0}{\tilde{n}_0} + \frac{1}{2} \left\{ J(J+1) - K^2 \right\} \frac{\tilde{e}_0}{\tilde{n}_0} \left\{ \frac{\tilde{e}_1}{\tilde{e}_0} - \frac{\tilde{n}_1}{\tilde{n}_0} \right\}$$

a.

$$\langle \text{rotation } K' | H | \text{rotation } K \rangle \neq 0 \text{ only if } K' = K$$

$$= 0 \text{ otherwise}$$

Quantum number K is practically conserved for triaxially deformed nuclei. $\rightarrow E_x \propto J(J+1)$.

$\leftarrow K' = K$ for non-vanishing coupling

b.

$$\langle \text{rotation } K' | H | \text{rotation } K \rangle = 0 \text{ independently of } K' \text{ or } K$$

Why has this feature **not** been conceived ?

It was assumed that the intrinsic deg. of freedom (dof) and extrinsic dof can be separated (in a good approx.).

This separation does not hold due to many-body effects.

c.

$$\langle \text{rotation } K' | H | \text{rotation } K \rangle \neq 0 \text{ weaker def. more coupling}$$

Good K quantum number also holds for cluster states.

Outline

1. Historical background and “rotational energy”

2. Present view of heavy deformed nuclei

3. Dual modes of rotation, and clustering

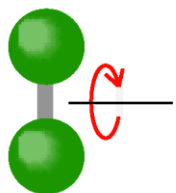
A question : Are there any cases where the excitation energy within
a collective band is due to rotational kinetic energy ?

If so, can they be explained in the same framework ?

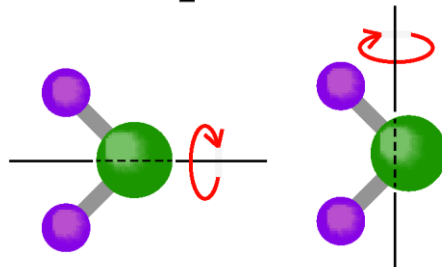
2. TO, Volya & Itagaki, EPJ-A, 61, 126 (2026)

Rotation of molecules

a. O₂ molecule



b. H₂O molecule



Rotational motion of point masses

Quantization of classical rigid body

$$E_x \propto J(J+1)$$

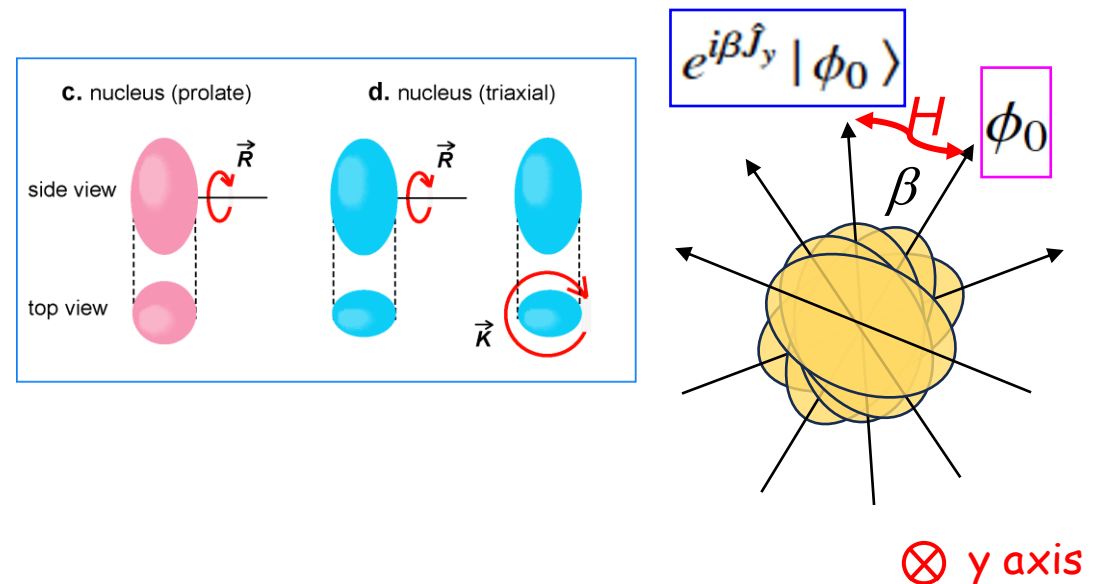
↔ $E_x \sim$ rotational kinetic energy

motivation

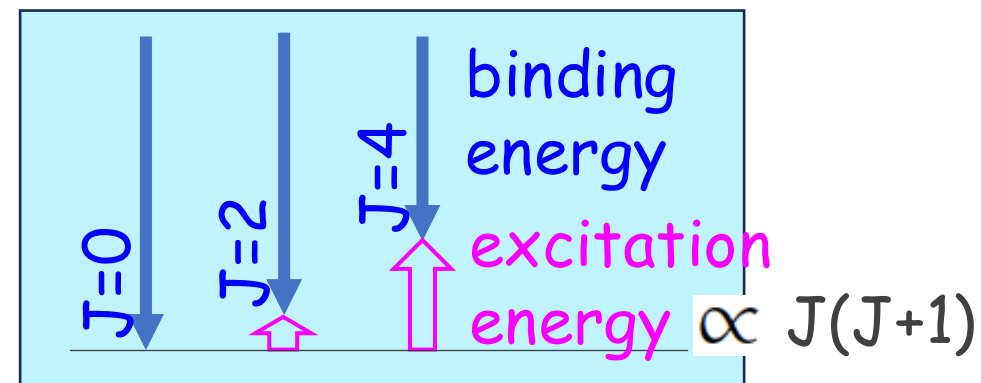


Any relation ?

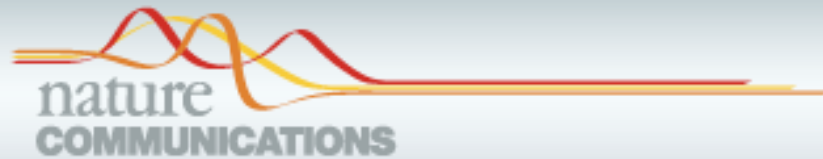
Rotational mode of nucleus discussed so far



$$E_{J,K}^{(0+1)} = \frac{\tilde{e}_0}{\tilde{n}_0} + \frac{1}{2} \left\{ J(J+1) - K^2 \right\} \frac{\tilde{e}_0}{\tilde{n}_0} \left\{ \frac{\tilde{e}_1}{\tilde{e}_0} - \frac{\tilde{n}_1}{\tilde{n}_0} \right\}$$



- No-core *ab initio* Monte Carlo Shell Model
density profile more reliable because of very minor renormalization
of wave functions, thanks to no-core *ab initio* calculation
- Be isotopes by JISP16 interaction
- C isotopes by Daejeon16 interaction



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<https://doi.org/10.1038/s41467-022-29582-0> |

ARTICLE

<https://doi.org/10.1038/s41467-022-29582-0>

OPEN



α -Clustering in atomic nuclei from first principles with statistical learning and the Hoyle state character

T. Otsuka^{1,2,3}, T. Abe^{2,4}, T. Yoshida^{4,5}, Y. Tsunoda⁴, N. Shimizu⁴, N. Itagaki⁶, Y. Utsuno^{3,4},
J. Vary⁷, P. Maris⁷ & H. Ueno²

Energy level & transition strength of ^8Be and ^{12}C

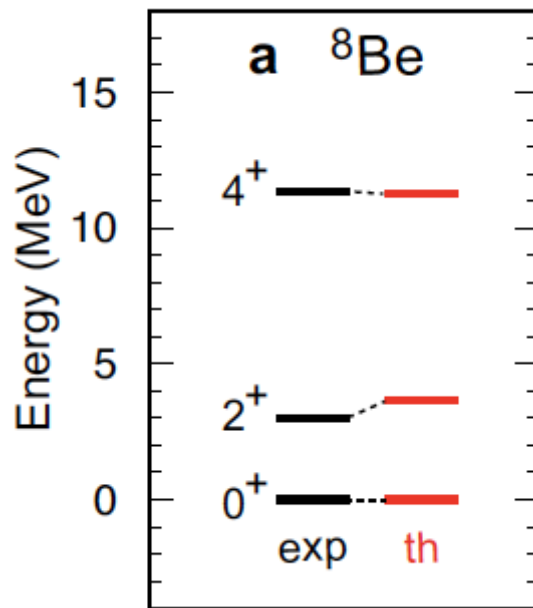
ab initio no-core MCSM + JISP 16 interaction (Shirokov et al.)

ab initio no-core MCSM + Daejeon 16 interaction (Shirokov et al.)
based on chiral EFT (Machleidt-Entem, 2011)

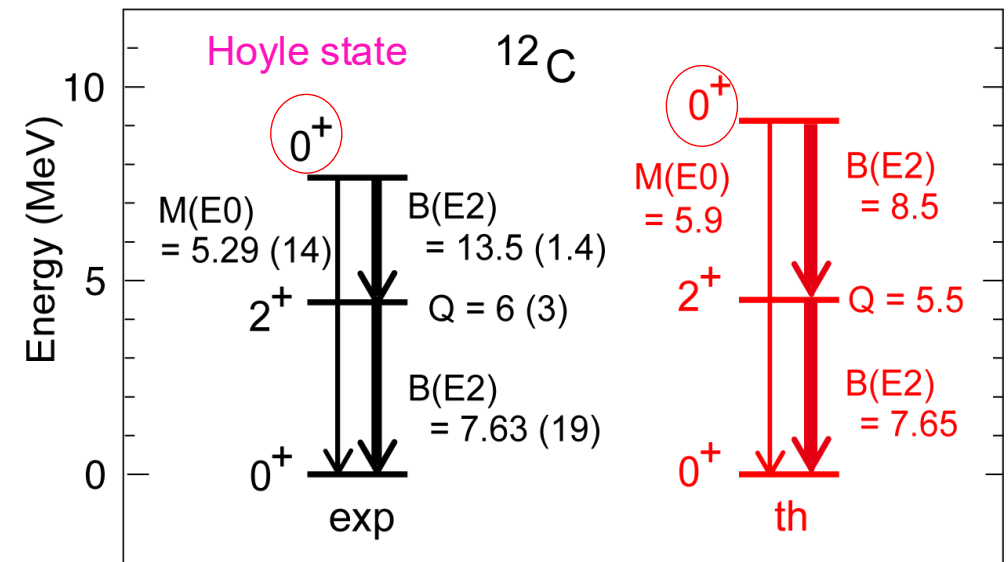
charges protons 1e
 neutrons 0e

correlation effects are explicitly treated
(no medium correction needed)

The *ab initio* calculation by Abe, Yoshida and others can reproduce some "rotational characters" very well.



Strong deformation ($\beta_2 \sim 1$, prolate) in the 0^+_{11} and 2^+_{11} states can now be described from *first principles*.

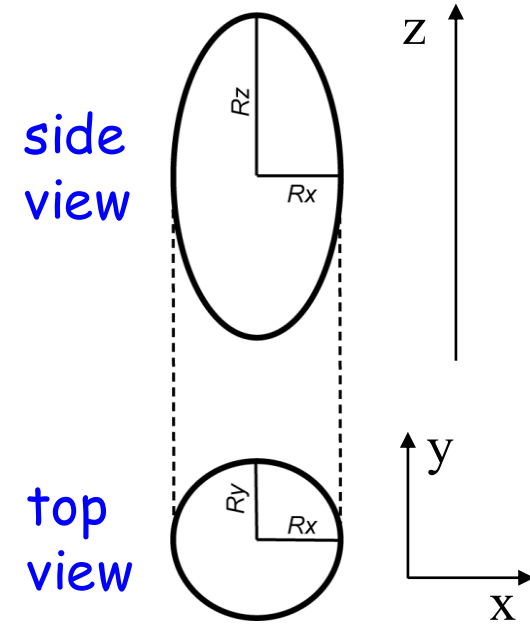
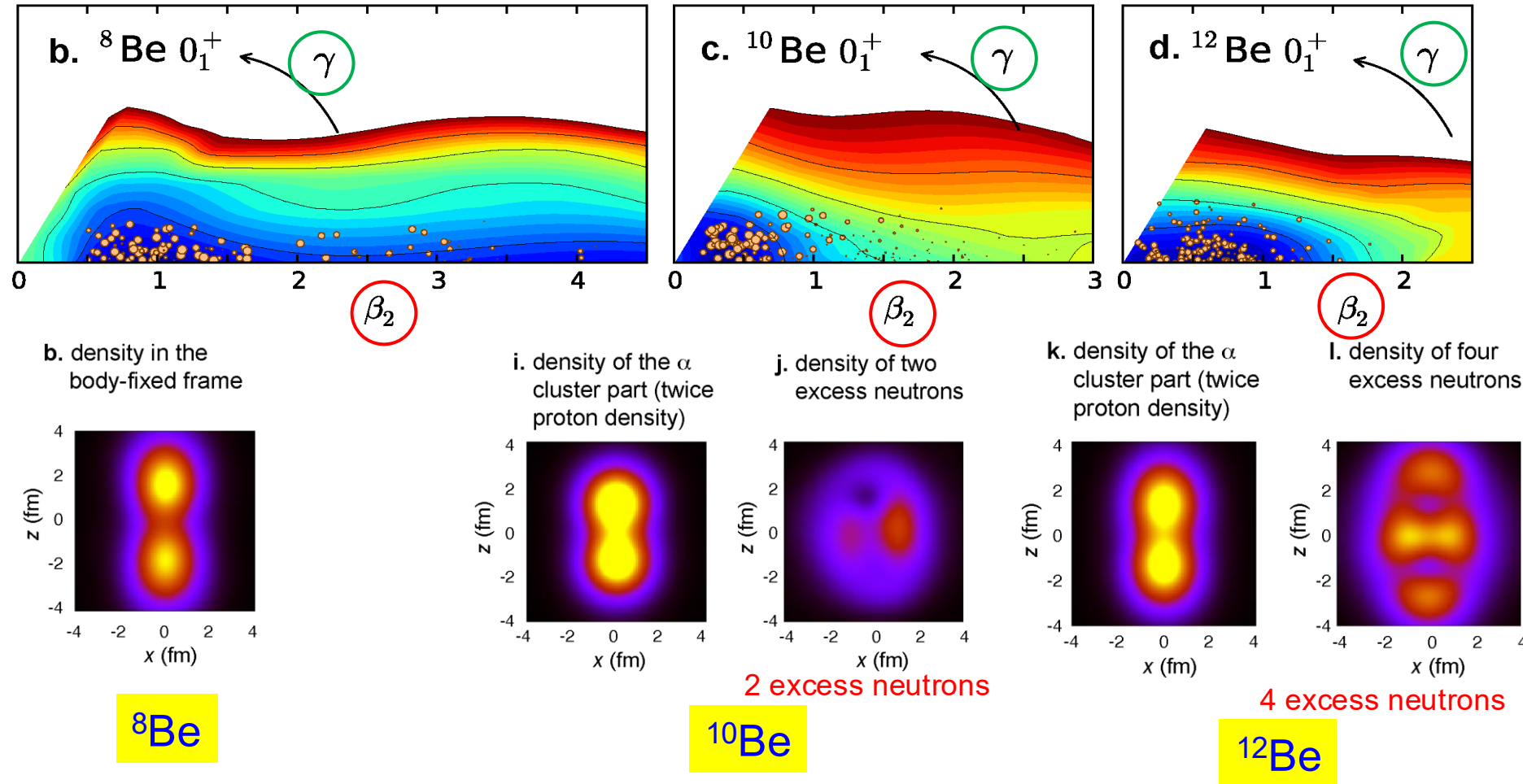


Strong deformation ($\beta_2 \sim 0.6$, oblate) in the 0^+_{11} and 2^+_{11} states can now be described from *first principles*.

T-plot analysis of 0+ states applied to Be isotopes

Quadrupole moments are used as partial coordinates

Circles represent individual basis vectors (=Slater determinant)



$$Q_0 = \langle 2z^2 - x^2 - y^2 \rangle$$

$$Q_2 = \sqrt{3/2} \langle x^2 - y^2 \rangle$$

$$\beta_2^2 \propto (Q_0^2 + 2Q_2^2)$$

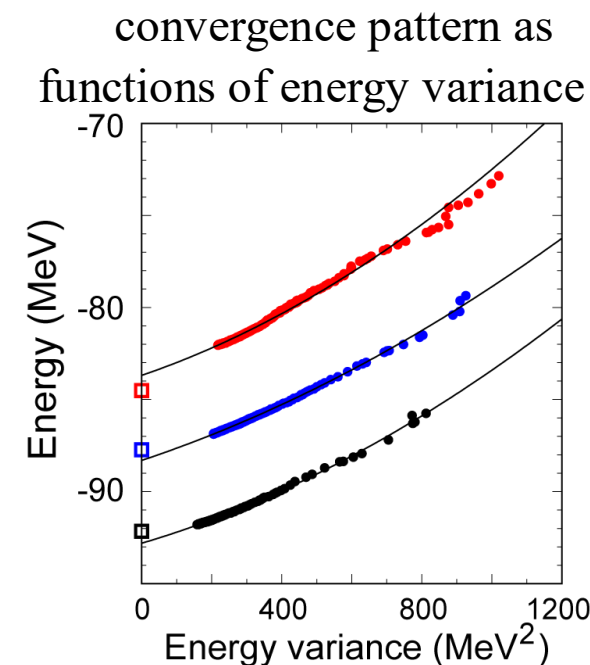
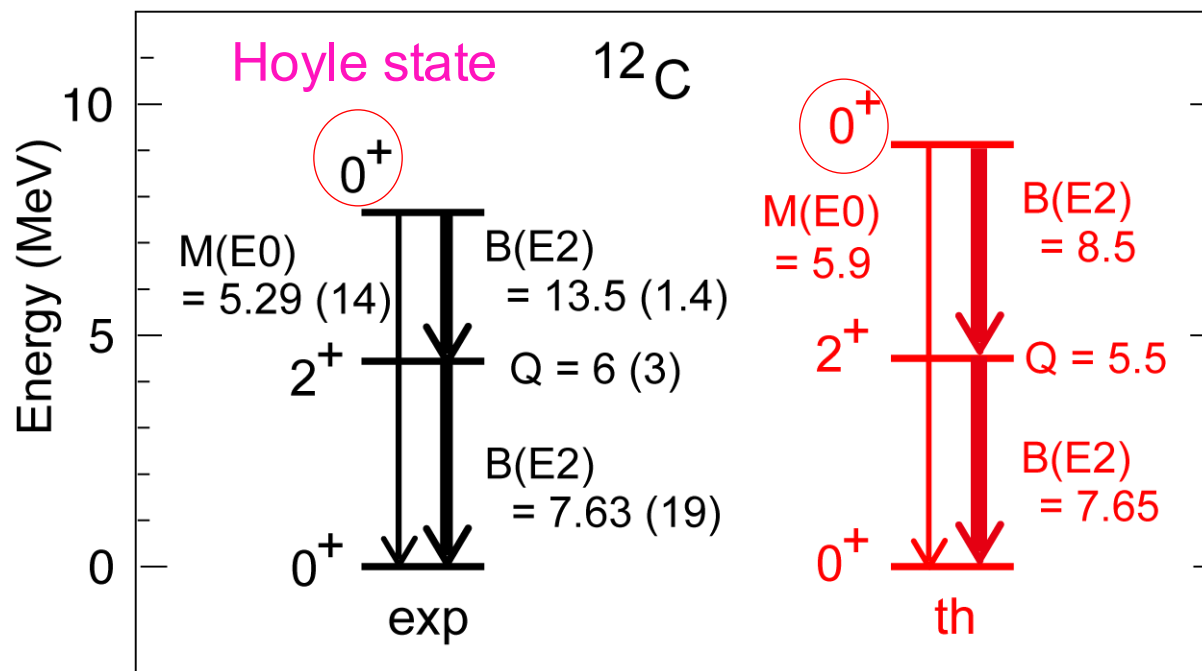
$$\tan \gamma = \sqrt{2} \frac{Q_2}{Q_0}$$

Energy level & transition strength of ^{12}C

ab initio no-core MCSM + Daejeon 16 interaction (Shirokov et al.)
based on chiral EFT (Machleidt-Entem, 2011)

charges protons 1e
 neutrons 0e

correlation effects are explicitly treated (no medium correction needed)



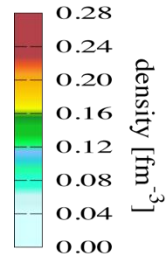
Strong deformation ($\beta_2 \sim 0.6$, oblate) in the 0^+_1 and 2^+_1 states can now be described from *first principles*.

Stringent test for the Daejeon 16 interaction and the present No-Core MCSM.

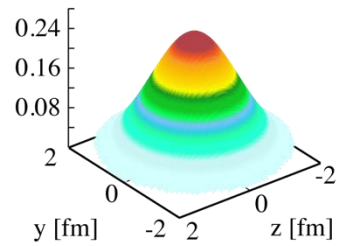
Nucleon densities in the intrinsic frame

after proper orthogonalization

a legend

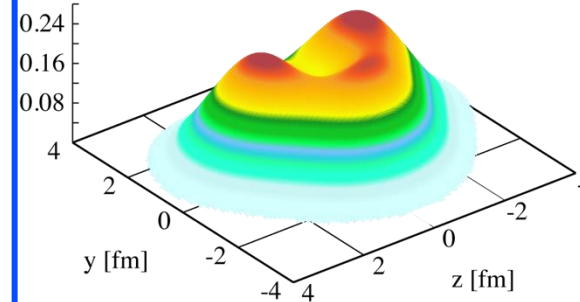


b α particle (^4He)

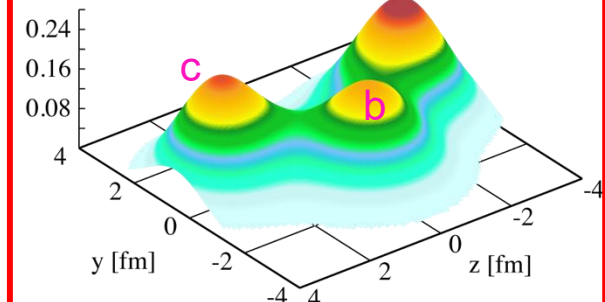


^{12}C

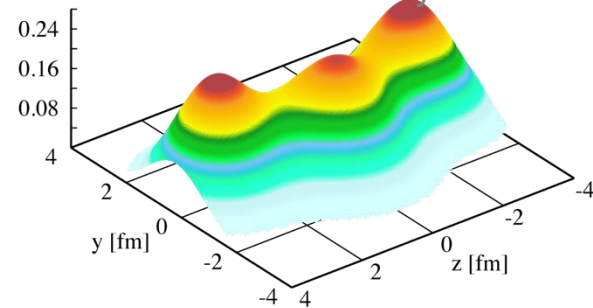
c 0_1^+ state



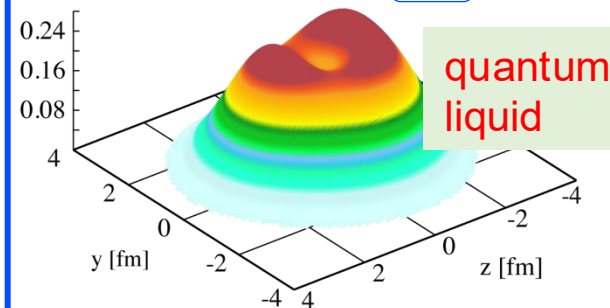
d 0_2^+ (Hoyle) state



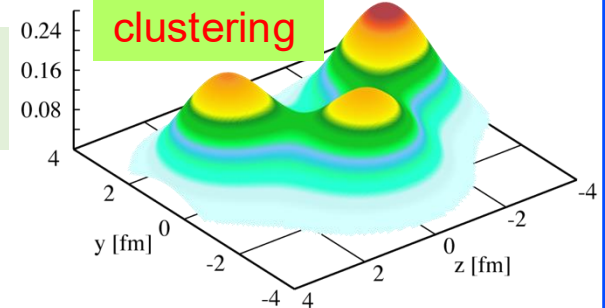
e 0_3^+ state tentatively ~ 14 MeV



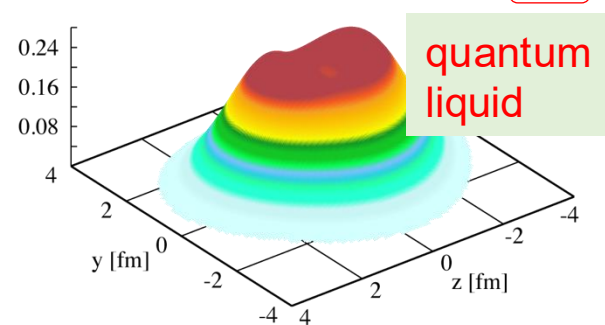
f 0_1^+ state region I 94%



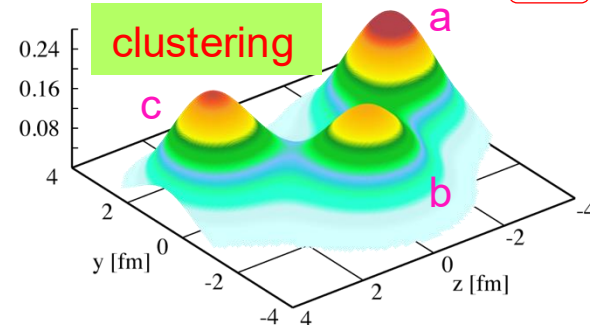
g 0_1^+ state region II 6%



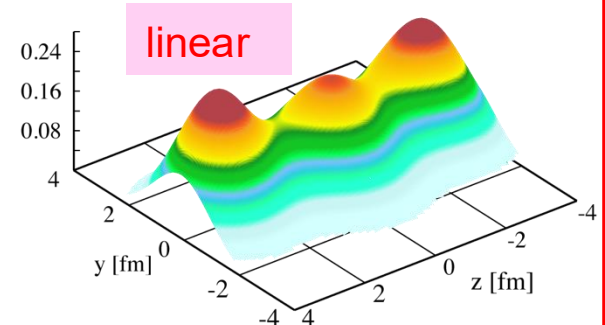
h 0_2^+ (Hoyle) state region I 33%



i 0_2^+ (Hoyle) state region II 61%



j 0_2^+ (Hoyle) state region III 6%



^{12}C : MCSM basis vectors classified by quadrupole moments (*T plot*) $\rightarrow$ decomposition

T plot circles are spread in the case of ^{12}C . A characteristic feature.

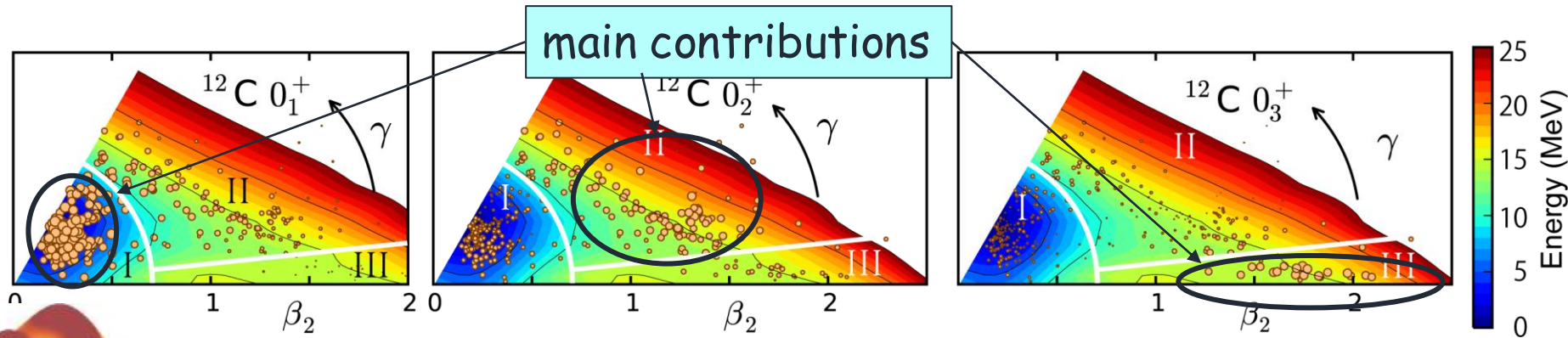
Unique structures appear at low excitation energies ... different from other nuclei

PES is divided into three

I	$\beta_2 < 0.7$, oblate basin in the PES
II	triaxial
III	very prolate

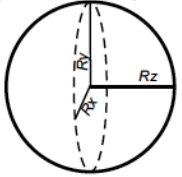
$\beta_2=0.7$, $\gamma=6^\circ$ $\rightarrow$ basis vectors decomposed into regions I, II and III

Data science
yields almost
the same
classification.

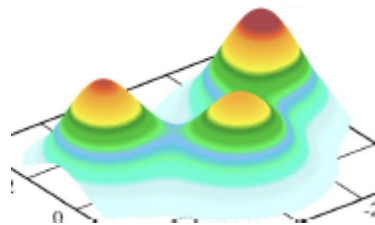


oblate
(pancake)

b. $\gamma = 60^\circ$: $R_z = R_y > R_x$



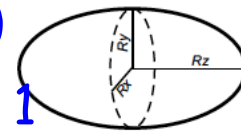
$R_z : R_y : R_x = 2 : 2 : 1$



Hoyle state

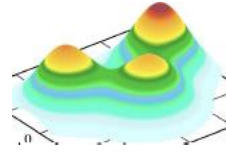
prolate (football)

$R_z : R_y : R_x = 5 : 1 : 1$



Cluster - Liquid crossover in the present no-core MCSM calc.

components of the ground state

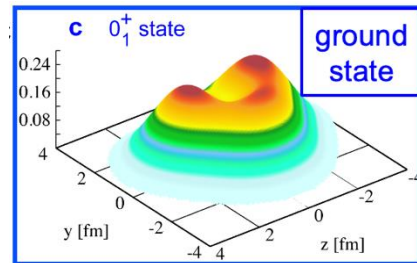
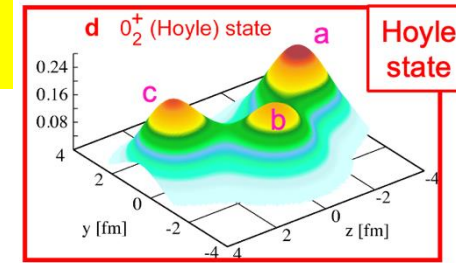


energy ↑

components of the Hoyle state

expanding

Hoyle state



Ground state

mixing

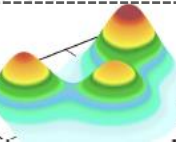
6%
94%

2.9 MeV

-80.4 MeV

Cluster
(~ bumpy density)

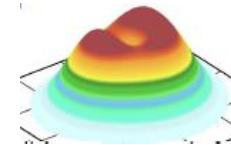
3.5 MeV



-84.2 MeV

-86.0 MeV

liquid
(~uniform density)



-91.0 MeV

compact
(closer to sphere)

1.5 MeV
-81.9 MeV
61%
33%

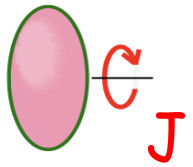
mixing (repulsive effect)
& rearrangement

Two modes of the localization emerge due to the force (no loose binding effect).

The two modes can talk, and can be mixed.

New question: Can this be a general feature for attractive short-range force ?

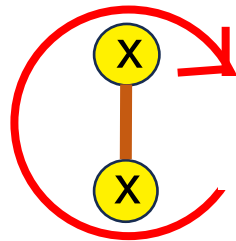
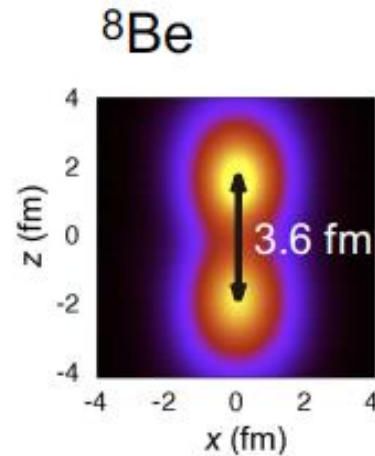
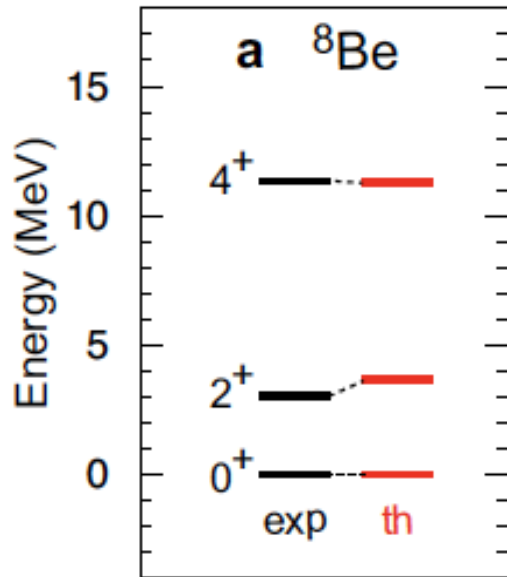
Our formulation of the rotation can be applied to the rotation of clusters.



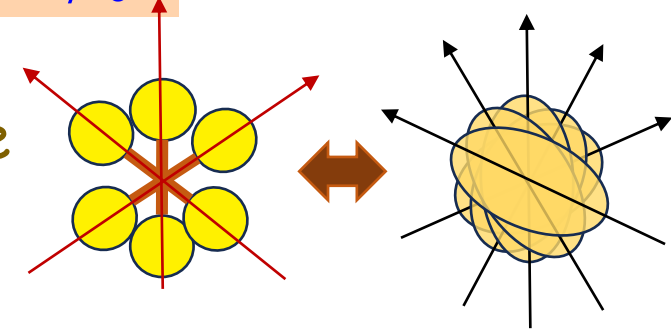
$$E_J \approx E_0 + J(J+1) \frac{1}{2} \frac{e_0}{n_0} \left\{ \frac{e_1}{e_0} - \frac{n_1}{n_0} \right\}, \text{ with } E_0 = \frac{e_0}{n_0}$$

our basic formula

di- α state below can be an intrinsic state ϕ_0



Rotation means the superposition



Different parts of Hamiltonian contribute !

$H \sim$ kinetic energy term of
 center of gravity of each cluster (x)
 + internal Hamiltonian of each cluster
 eigen energy of cluster (constant)
 + ...

ab initio no-core Monte Carlo Shell Model with JISP16 interaction

Reminder

Quantum many-body derivation of rotational excitation energy

ϕ_0 : intrinsic state with $K=0$ for simplicity, e.g. by shell model

The member of angular momentum J of a rotational band

is given by the projected state $\propto \int_0^\pi d\beta \sin\beta d_{0,0}^J(\beta) e^{i\beta \hat{J}_y} |\phi_0\rangle$

→ the energy is given by

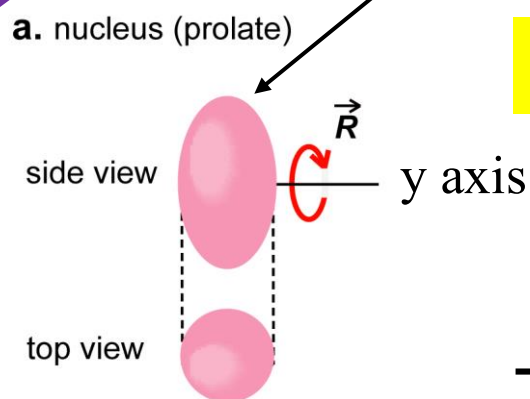
$$= \frac{2J+1}{2|\mathcal{N}_J|^2} \langle \phi_0 | H \int_0^\pi d\beta \sin\beta d_{0,0}^J(\beta) e^{i\beta \hat{J}_y} |\phi_0\rangle,$$

$$= \frac{2J+1}{2|\mathcal{N}_J|^2} \int_0^\pi d\beta \sin\beta d_{0,0}^J(\beta) h_y(\beta),$$

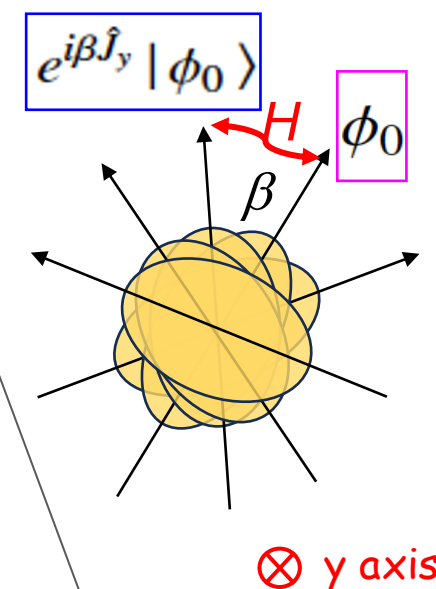
energy kernel $h_y(\beta) = \langle \phi_0 | H e^{i\beta \hat{J}_y} |\phi_0\rangle$

polynomial expansion: $d_{0,0}^J(\beta) = P_J(\cos\beta) \approx 1 + F_J(\cos\beta - 1) + G_J(\cos\beta - 1)^2 + \dots$

(stops at finite power)



rotation about y axis



Basic equation $E_J \approx E_0 + J(J+1) \frac{1}{2} \frac{e_0}{n_0} \left\{ \frac{e_1}{e_0} - \frac{n_1}{n_0} \right\}$, with $E_0 = \frac{e_0}{n_0}$.

Cluster ~ eigenstate(0^+)

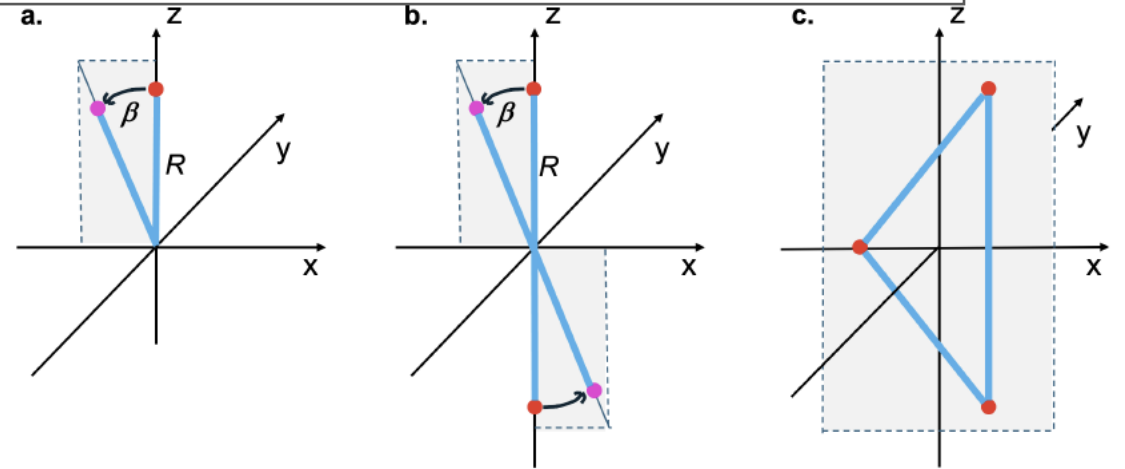
$$\begin{aligned} h_y(\beta) &= \langle \phi_0 | (H_g + H_i) e^{i\beta \hat{J}_y} | \phi_0 \rangle \\ &= \langle \phi_0 | (H_g + \epsilon) e^{i\beta \hat{J}_y} | \phi_0 \rangle \\ &= \langle \phi_0 | H_g e^{i\beta \hat{J}_y} | \phi_0 \rangle + \epsilon n_y(\beta) \end{aligned}$$

constant

$$E_J = \frac{\int_0^\pi d(\cos\beta) d_{0,0}^J(\beta) h_y(\beta)}{\int_0^\pi d(\cos\beta) d_{0,0}^J(\beta) n_y(\beta)}$$

$$H_g = -\frac{\hbar^2}{2\mathcal{I}} \frac{1}{\sin\beta} \frac{\partial}{\partial\beta} \left(\sin\beta \frac{\partial}{\partial\beta} \right) \text{ より}$$

$$\begin{aligned} h_y(\beta) &= -\frac{\hbar^2}{2\mathcal{I}} \langle \phi_0 | \frac{1}{\sin\beta} \frac{\partial}{\partial\beta} \left(\sin\beta \frac{\partial}{\partial\beta} \right) e^{i\beta \hat{J}_y} | \phi_0 \rangle, \\ &= -\frac{\hbar^2}{2\mathcal{I}} \frac{1}{\sin\beta} \frac{\partial}{\partial\beta} \left(\sin\beta \frac{\partial}{\partial\beta} \right) n_y(\beta). \end{aligned}$$



$$e_1 = \frac{\hbar^2}{2\mathcal{I}} \int d\beta (2 \cos\beta \sin\beta) n_y(\beta)$$

$$e_1 \approx + \frac{\hbar^2}{2\mathcal{I}} 2 \int d\beta (\sin\beta) n_y(\beta) = + \frac{\hbar^2}{2\mathcal{I}} 2 n_0$$

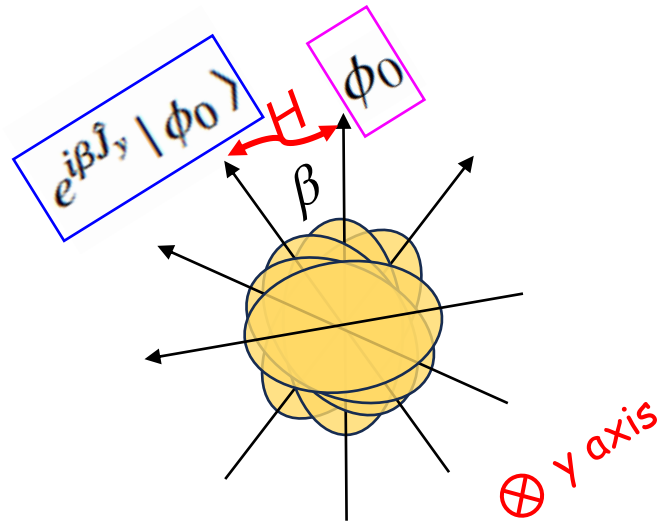
projection in quantum mechanics

$$E_J \approx E_0 + J(J+1) \frac{1}{2} \frac{e_1}{n_0} \approx \frac{\hbar^2}{2\mathcal{I}} J(J+1)$$

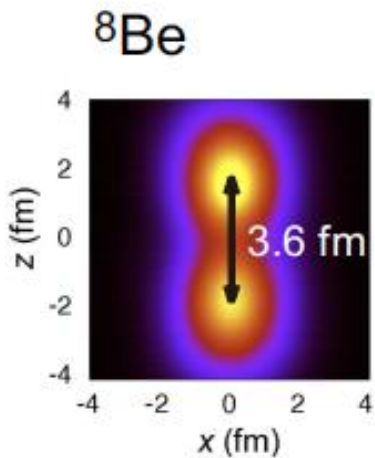
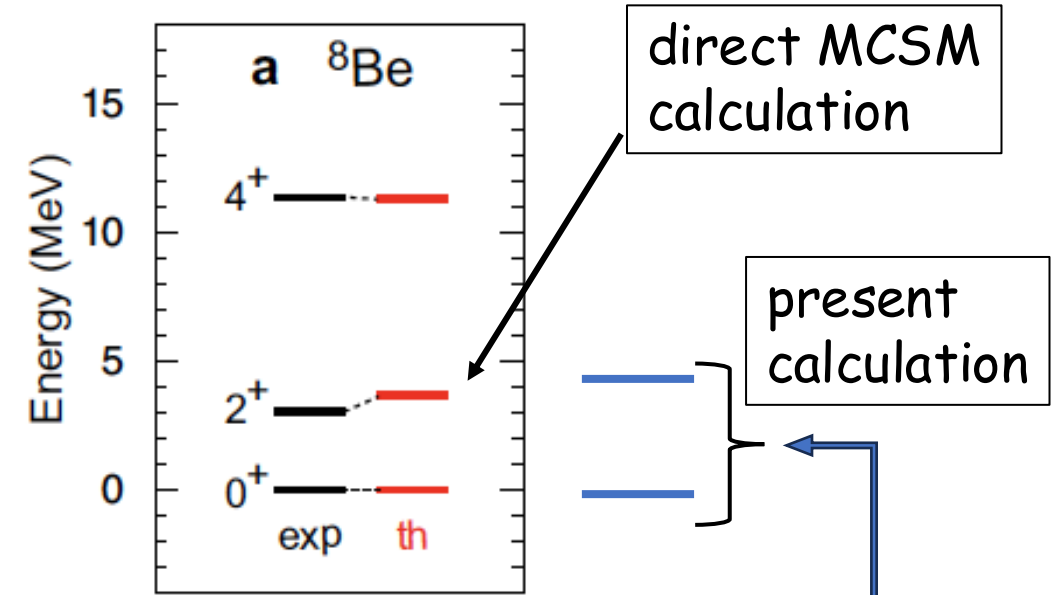
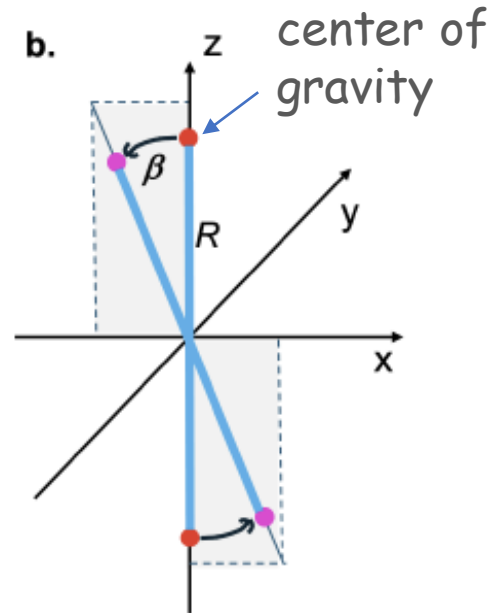
yields the same formula as free rotation

To be slightly more in detail, the same mathematical procedure is taken ...

ellipsoidal shape



clustering



Kinetic term of center of gravity of each cluster is taken, with the moment of inertia calculated from this distance given by *ab initio* no-core MCSM

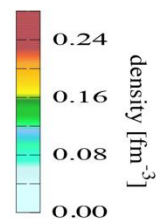
$$E_J \approx E_0 + J(J+1) \frac{1}{2} \frac{e_1}{n_0} \approx \frac{\hbar^2}{2\mathcal{I}} J(J+1),$$

$$E_0 = \frac{e_0}{n_0} = 0.$$

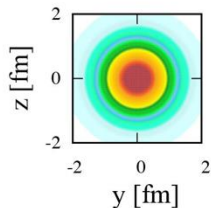
Fluctuations of center of gravity are incorporated

^{12}C case

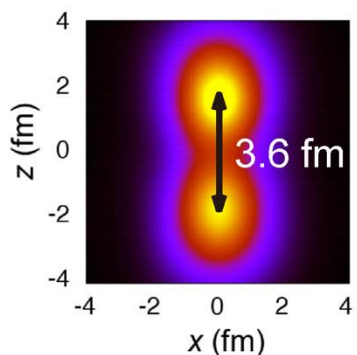
a legend



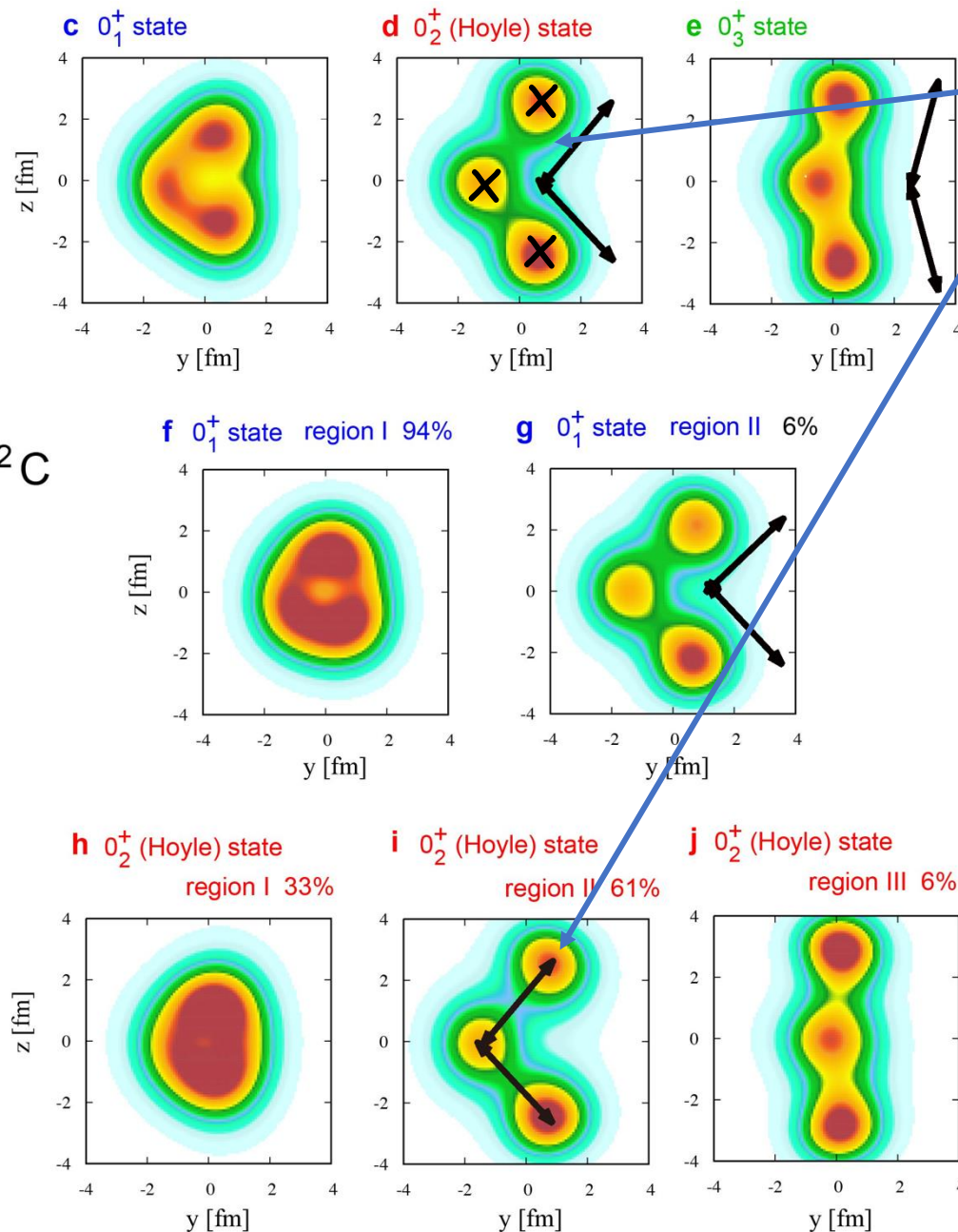
b α particle (^4He)



^8Be



^{12}C



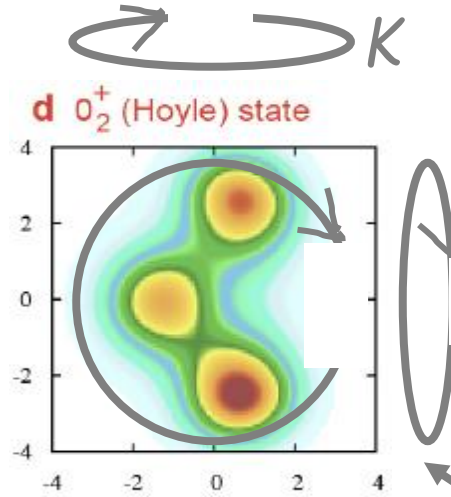
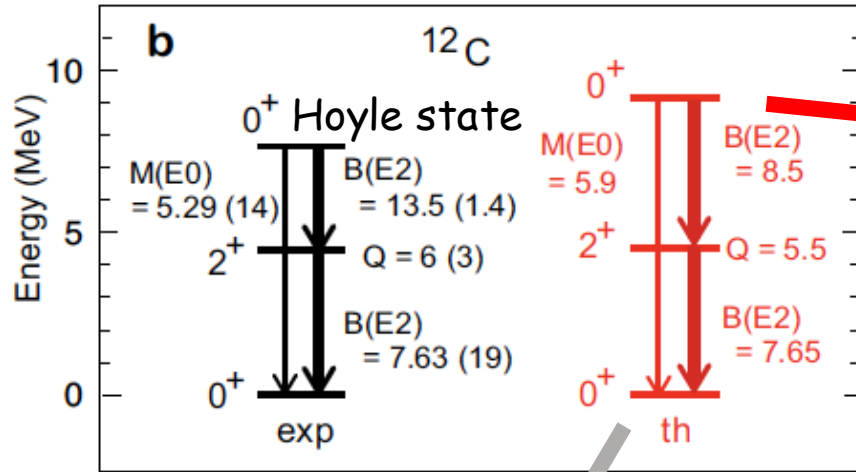
How do they "rotate" ?

We can look at center of gravity of cluster (x).

By using actual coordinates given by no-core MCSM calculations,
rotational ex. energy
 $\sim 0.25\text{-}0.30 J(J+1)$
with panel d

Here, two axes give slightly different coefficients
→ averaged with $K=0$ in many-body calculation

A similar story for ^{12}C with more impact

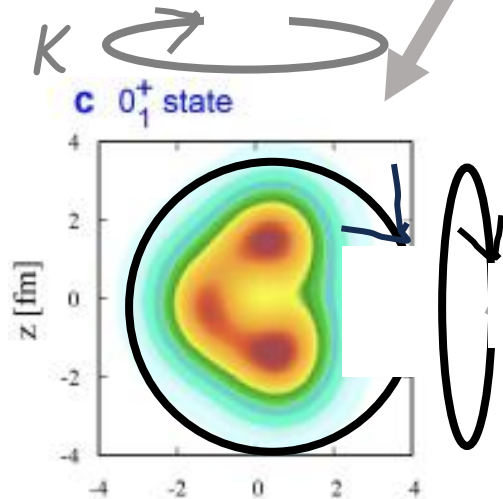


Hoyle band:
a possible rotational band
built on the Hoyle state

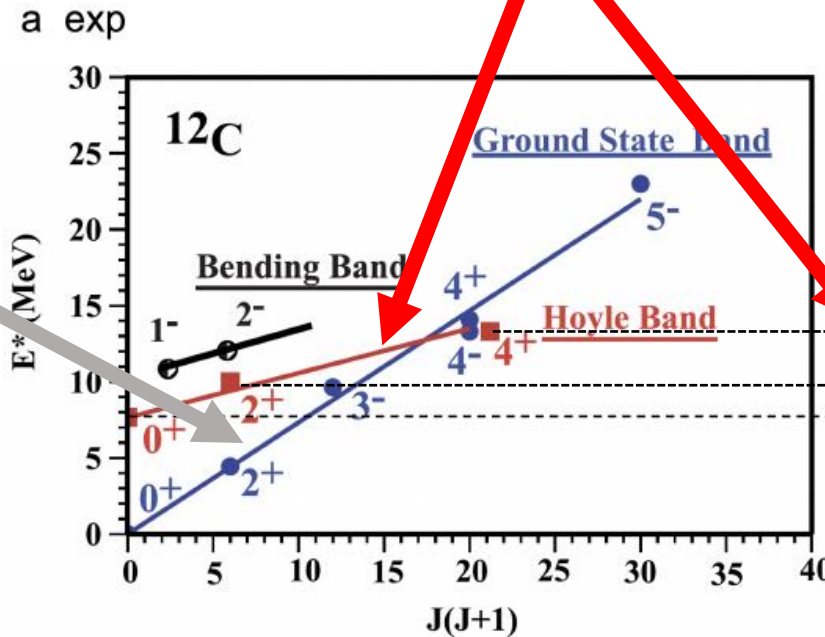
Triaxial : three axes classically

Quantum mechanically,
Hoyle band is a $K=0$ band

These two axes are "mixed"
quantum mechanically.



The averaging is included
in the MCSM calculation.



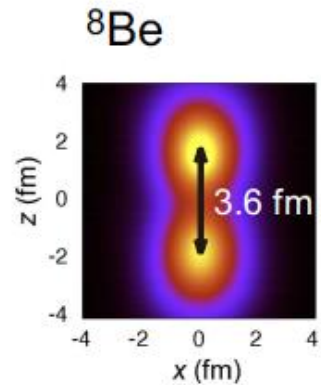
this calc.

Due to triaxiality,
rotational excitation
energies are estimated
somewhere in this range.

Distant-object Rotation clusters

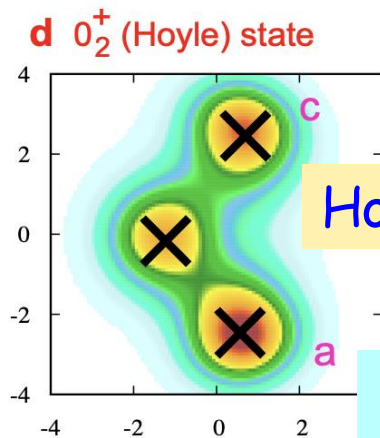
rotational motion of center of gravity of individual cluster

cluster ~ internally eigenstate



$$E_x \propto J(J+1)$$

$\Leftrightarrow E_x \sim$ rotational kinetic energy

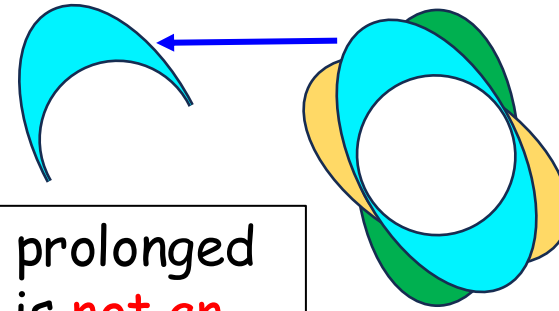


Hoyle band

Both are quantum mechanical with contributions from different parts of the Hamiltonian

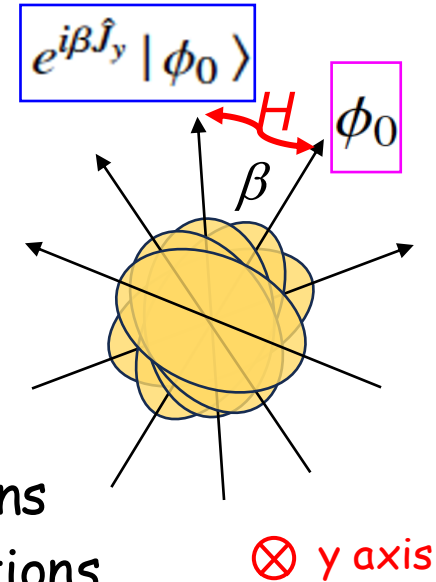
Dual modes within the same formulation

Compact-object Rotation ellipsoids

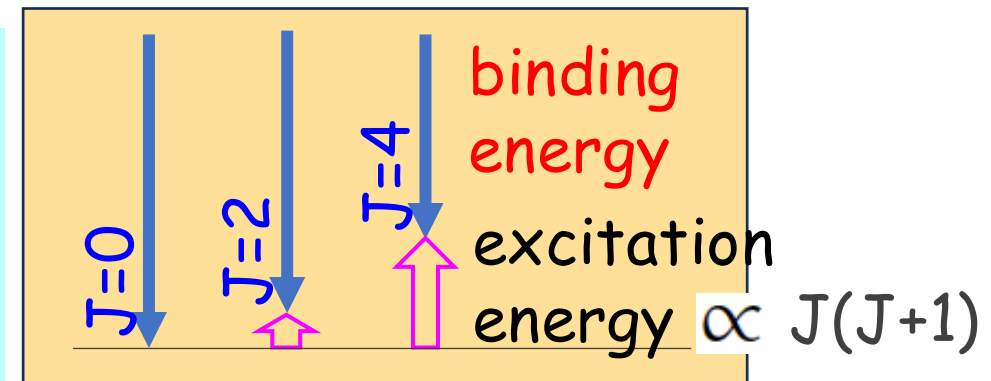


This prolonged part is not an eigenstate.

This part in different orientations are coupled primarily by interactions



$$E_{J,K}^{(0+1)} = \frac{\tilde{e}_0}{\tilde{n}_0} + \frac{1}{2} \left\{ J(J+1) - K^2 \right\} \frac{\tilde{e}_0}{\tilde{n}_0} \left\{ \frac{\tilde{e}_1}{\tilde{e}_0} - \frac{\tilde{n}_1}{\tilde{n}_0} \right\}$$



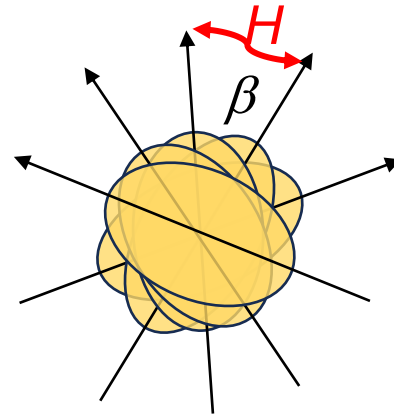
Summary

- **Duality of rotational modes** from a unified quantum mechanical description
- For heavy nuclei, **compact-object rotation** occurs

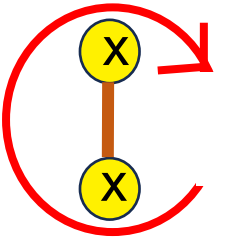
1. Prevailing triaxial shape
like an almond ($\Delta E \sim 3\text{MeV}$)
2. $J(J+1)$ rule represents the whole
Hamiltonian, primarily **interactions**



This mode emerges, if the
size of the system and the
range of the interactions
are comparable.



- If clustering states emerge, **distant-object rotation** may occur.
 $E_x = \text{kinetic energy}$. Possible extension to atomic molecules
where features similar to nuclei, e.g. triaxiality (H_2O), appear.
- **K quantum number is practically conserved even for triaxial clustering**
- ^{12}C can be an exceptional case hosting both modes within one nucleus, giving
another **fundamental significance** to Hoyle state besides nucleosynthesis

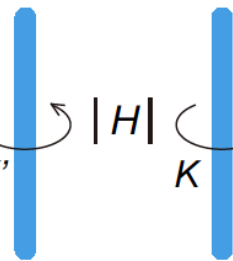


END

K quantum number is (practically) conserved, with substantial triaxiality

Robust mechanism for good K with triaxiality

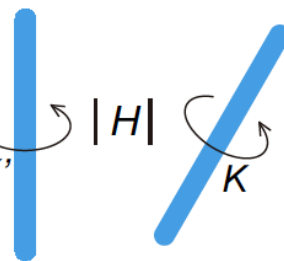
a.



$$\langle \text{rotating bar } K' | H | \text{rotating bar } K \rangle \neq 0 \text{ only if } K' = K$$

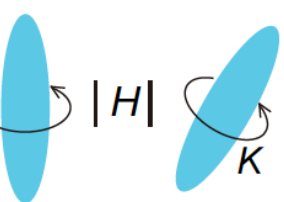
$$= 0 \text{ otherwise}$$

b.



$$\langle \text{rotating bar } K' | H | \text{tilted bar } K \rangle = 0 \text{ independently of } K' \text{ or } K$$

c.



$$\langle \text{tilted bar } K' | H | \text{tilted bar } K \rangle \neq 0 \text{ weaker def. more coupling}$$

This remains valid for clustering states !

TABLE II. Examples of overlap probabilities of $K=0^+$, 2^+ and $K=4^+$ components with selected low-lying eigenstates.

nucleus	eigenstate	$\langle \gamma \rangle^\circ$	$K=0^+$	$K=2^+$	$K=4^+$
^{166}Er	0_1^+	8.2	1.000		
	2_1^+	8.2	0.999	0.000	
	2_2^+	9.1	0.000	1.000	
	3_1^+	9.1	0.000	0.999	
	4_1^+	8.2	0.998	0.001	0.000
	4_3^+	9.5	0.000	0.000	1.000
^{158}Gd	0_1^+	5.9	1.000		
	2_1^+	6.0	0.997	0.000	
	2_2^+	8.0	0.000	1.000	
	3_1^+	8.0	0.000	0.999	
	4_1^+	6.0	0.989	0.000	0.000
	0_2^+	7.3	1.000		
^{164}Dy	2_1^+	7.3	0.997	0.000	
	2_2^+	8.1	0.000	1.000	
	3_1^+	8.1	0.000	0.999	
	4_1^+	7.4	0.990	0.001	0.000
	4_3^+	8.2	0.000	0.000	1.000
	0_1^+	8.7	1.000		
^{164}Yb	2_1^+	8.7	0.999	0.000	
	2_2^+	14.2	0.000	1.000	
	3_1^+	14.2	0.000	1.000	
	4_1^+	8.7	0.995	0.003	0.000
	4_3^+	15.1	0.005	0.000	0.994
	0_1^+	3.7	1.000		
^{154}Sm	2_1^+	3.7	0.984	0.000	
	0_2^+	12.6	1.000		
	2_2^+	12.6	0.991	0.006	
	2_3^+	13.8	0.003	0.993	
	3_1^+	13.8	0.004	0.995	
	2_4^+	5.9	0.000	0.999	
	0_1^+				
	2_1^+				
	0_2^+				

Rather strong K mixing may have been expected in traditional picture for triaxial shapes.

Its rationale is not clear to me.

K is now shown to be a good quantum number.