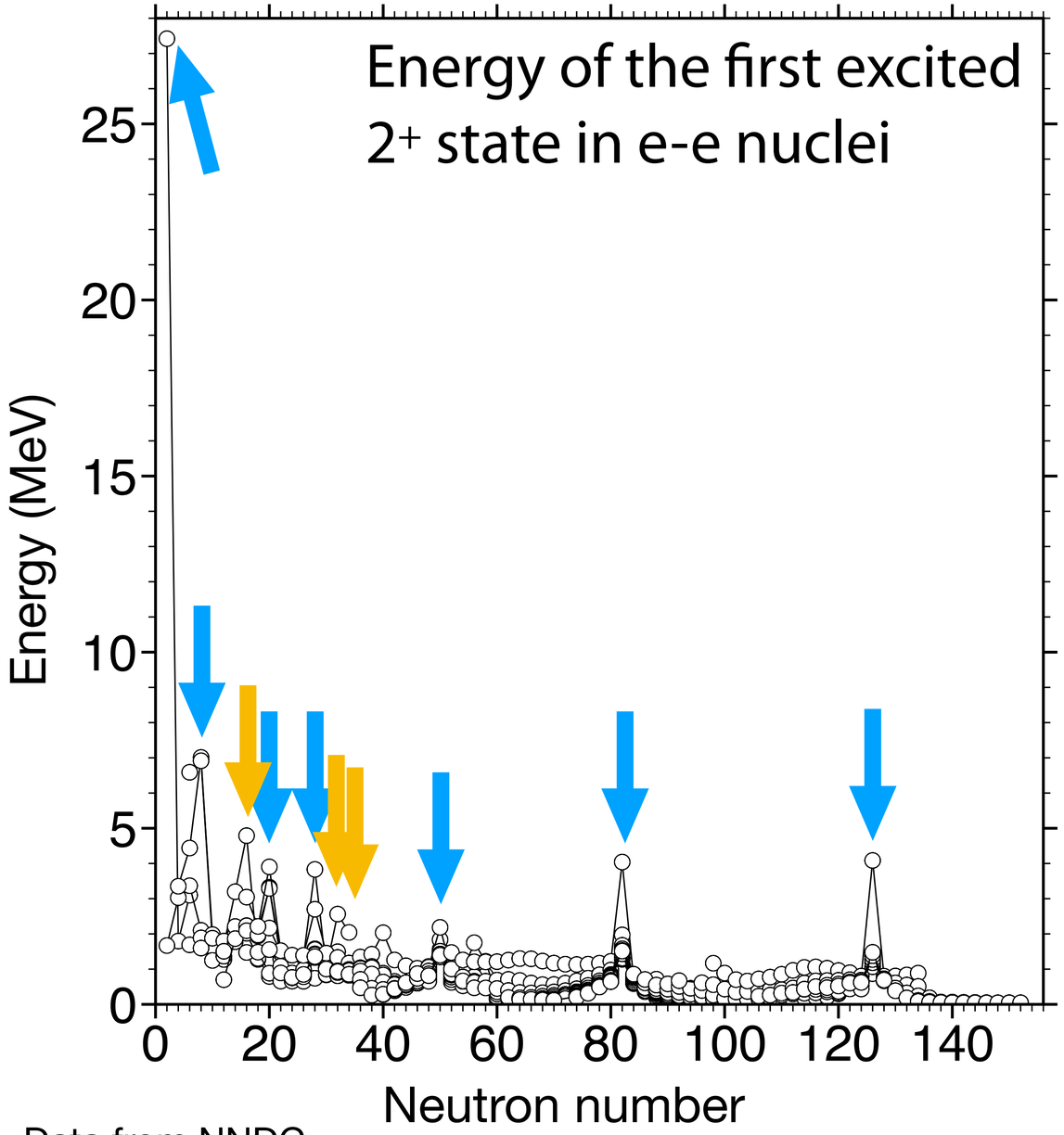
Mean-field theory for open-shell nuclei

—deformation—

Quadrupole (2^+) state energy: magic number



Data from NNDC

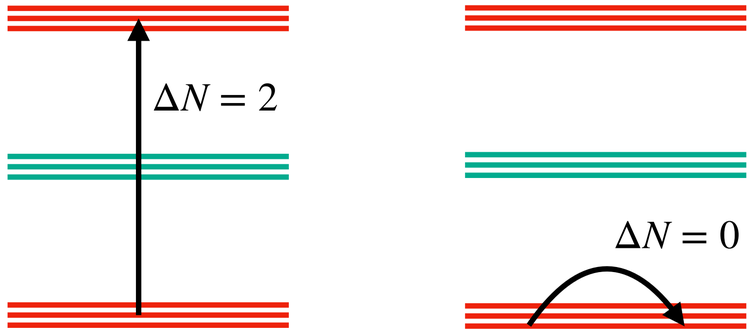
Canonical magic numbers

2, 8, 20, 28, (40), 50, 82, 126

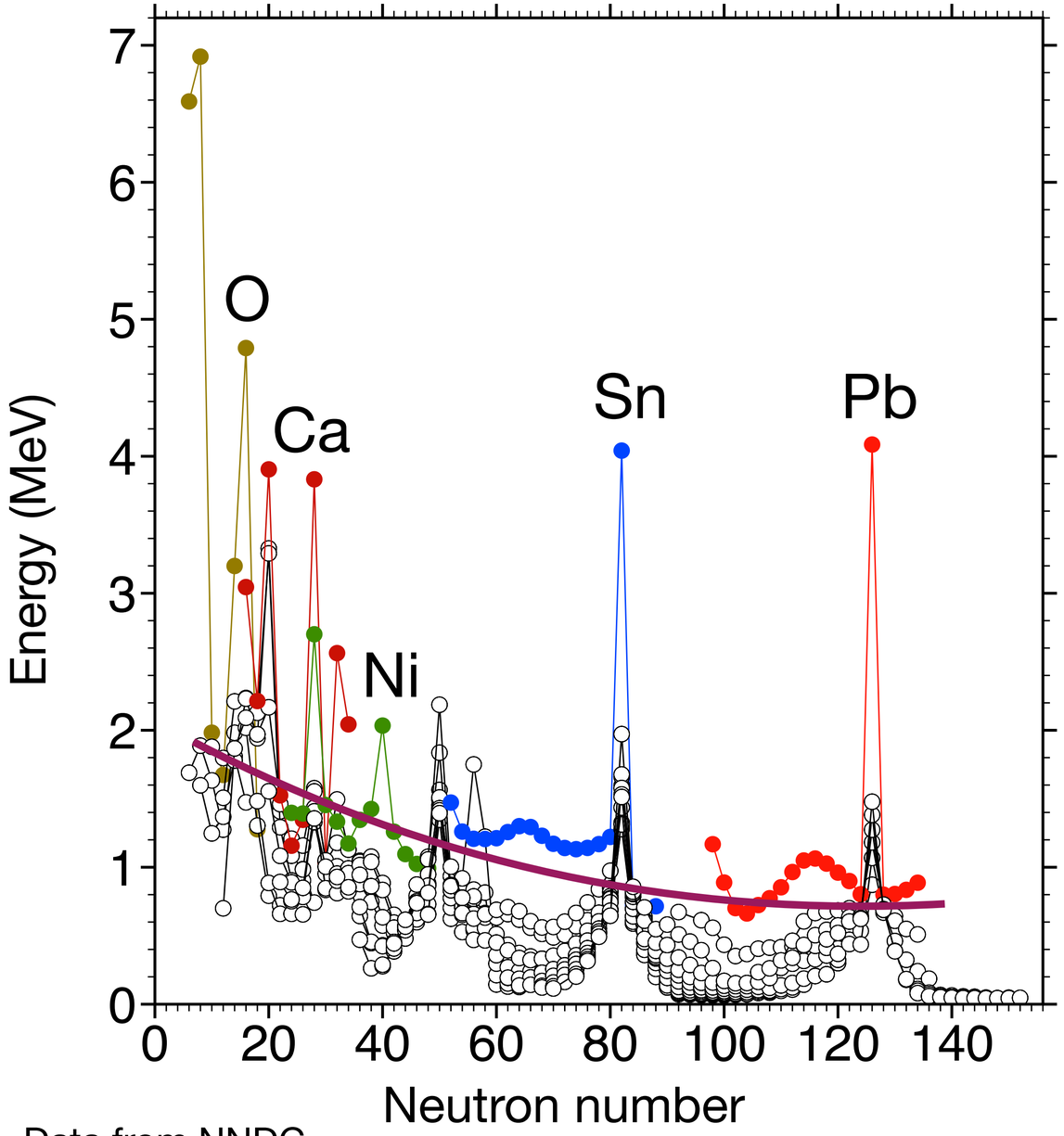
New magic numbers in neutron-rich nuclei

16, 32, 34,…

magic nuclei are hard to excite



Quadrupole (2^+) state energy: pairing



Data from NNDC

Singly-closed (Z=magic #) nuclei have

an energy gap

The ground 0^+ state is lowered by the **pairing**.

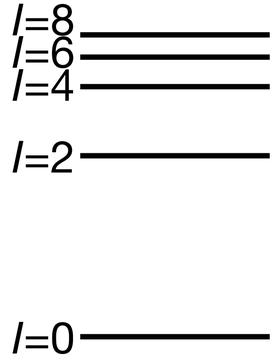
two neutrons above the magic # in a single orbital

The total spin I can be 0, 2, 4,… 2j-1.

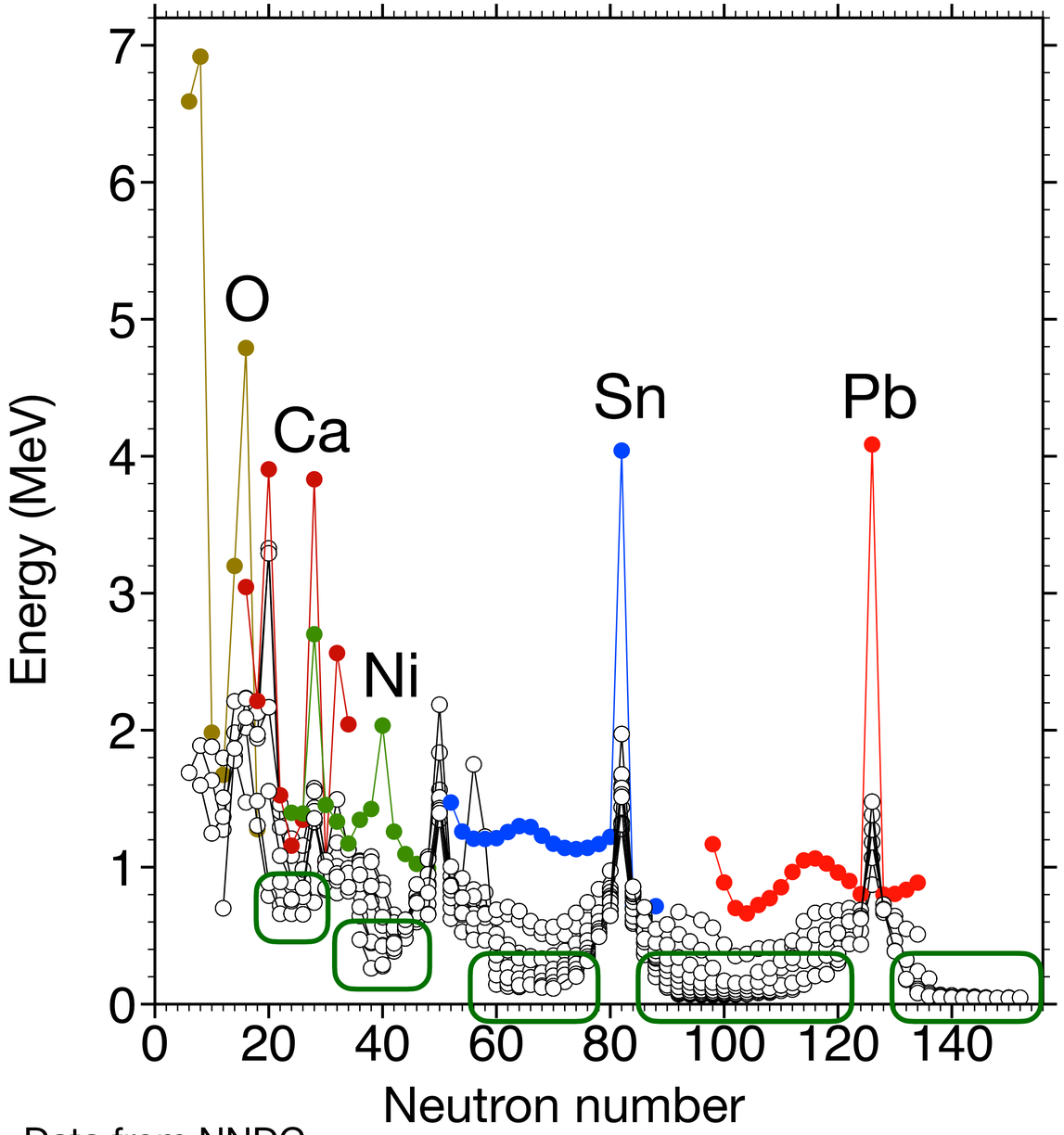
All the states are degenerated.

residual interaction

$v(1,2) = -\kappa\delta(r_1 - r_2)$



Quadrupole (2^+) state energy: zero mode



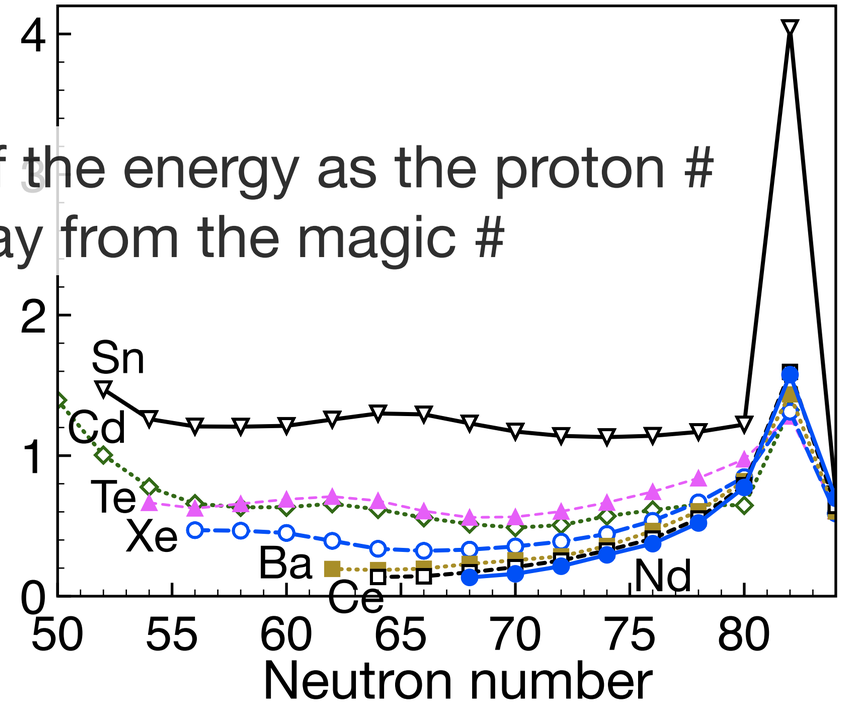
Data from NNDC

The singly-closed (Z=magic #) nuclei have

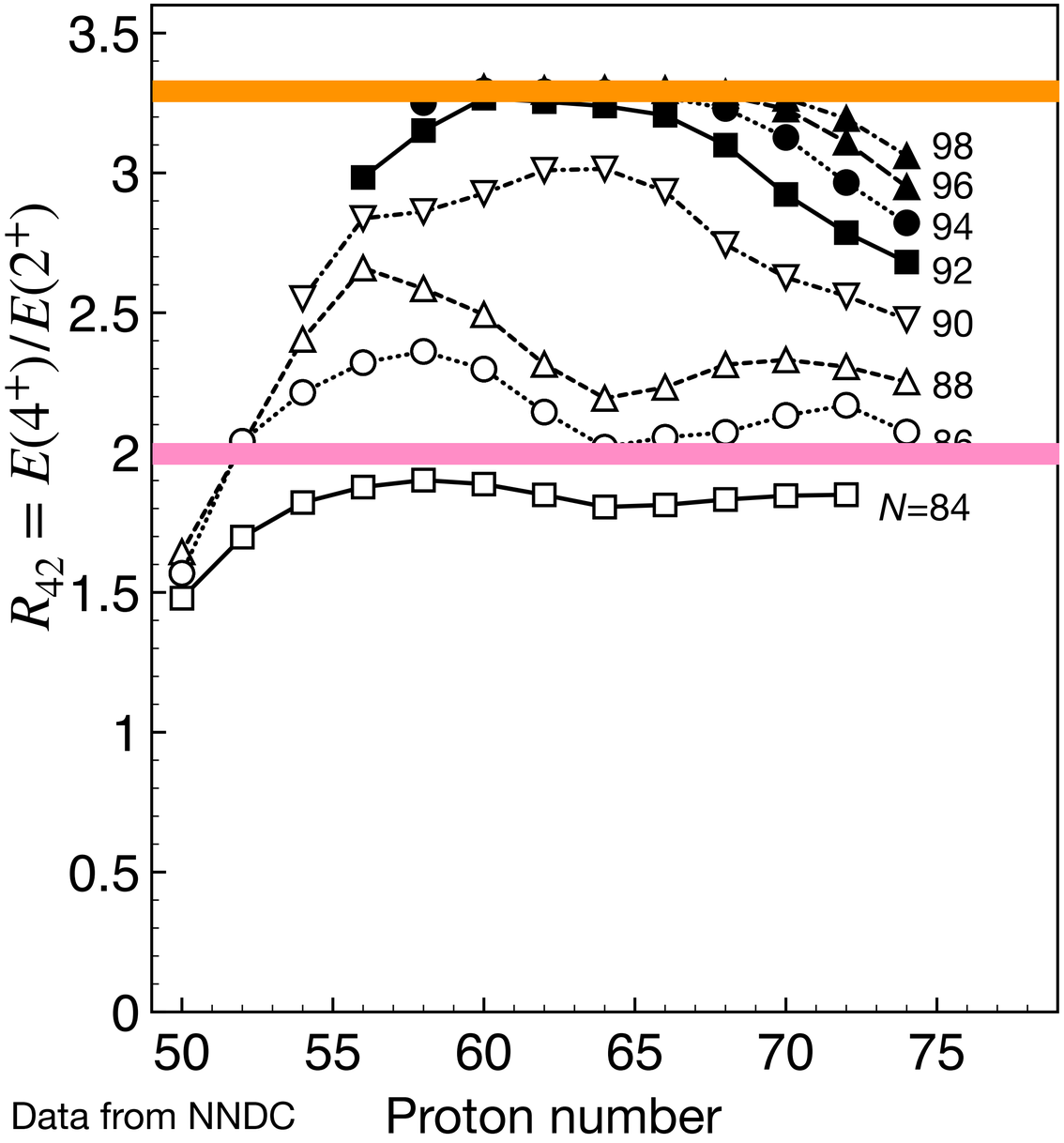
an energy gap

The ground 0^+ state is lowered by the **pairing**.

"zero-energy" mode in mid-shell nuclei



Excitation energies of 2^+ and 4^+ states



Data from NNDC

occurrence of collective excitations

Rotation ← breaking of the rotational symmetry

$$\hat{H} = \frac{\hat{I}^2}{2\mathcal{J}} \qquad E(I) = \frac{I(I+1)}{2\mathcal{J}} \qquad R_{42} = \frac{4 \times 5}{2 \times 3} = 3.33\cdots$$

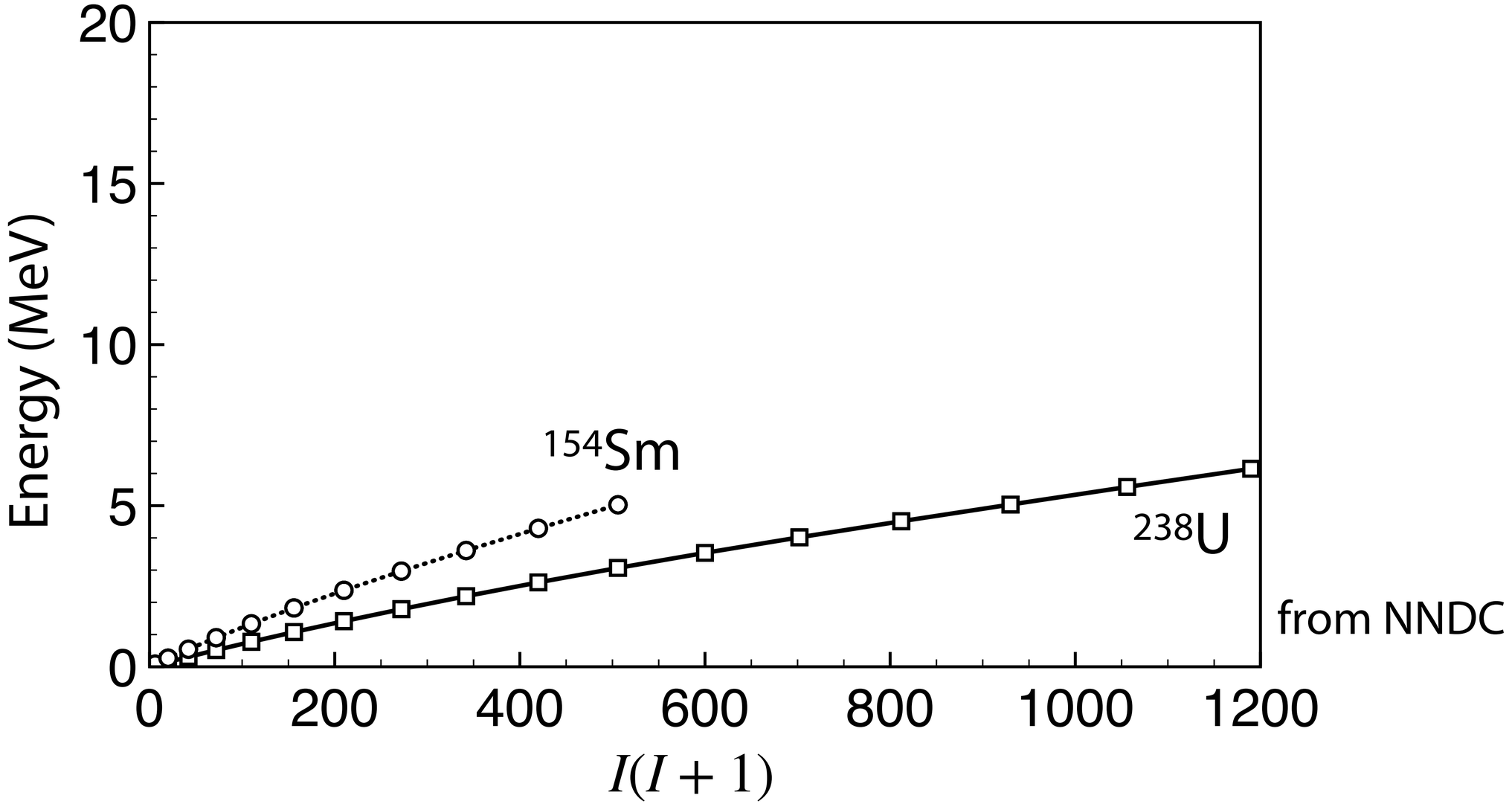
quadrupole deformation

Vibration

$$\hat{H} = \omega \hat{\Gamma}^\dagger \hat{\Gamma} \qquad E(I) = \frac{I}{2}\omega \qquad R_{42} = \frac{4}{2} = 2$$

Emergence of the rotational band

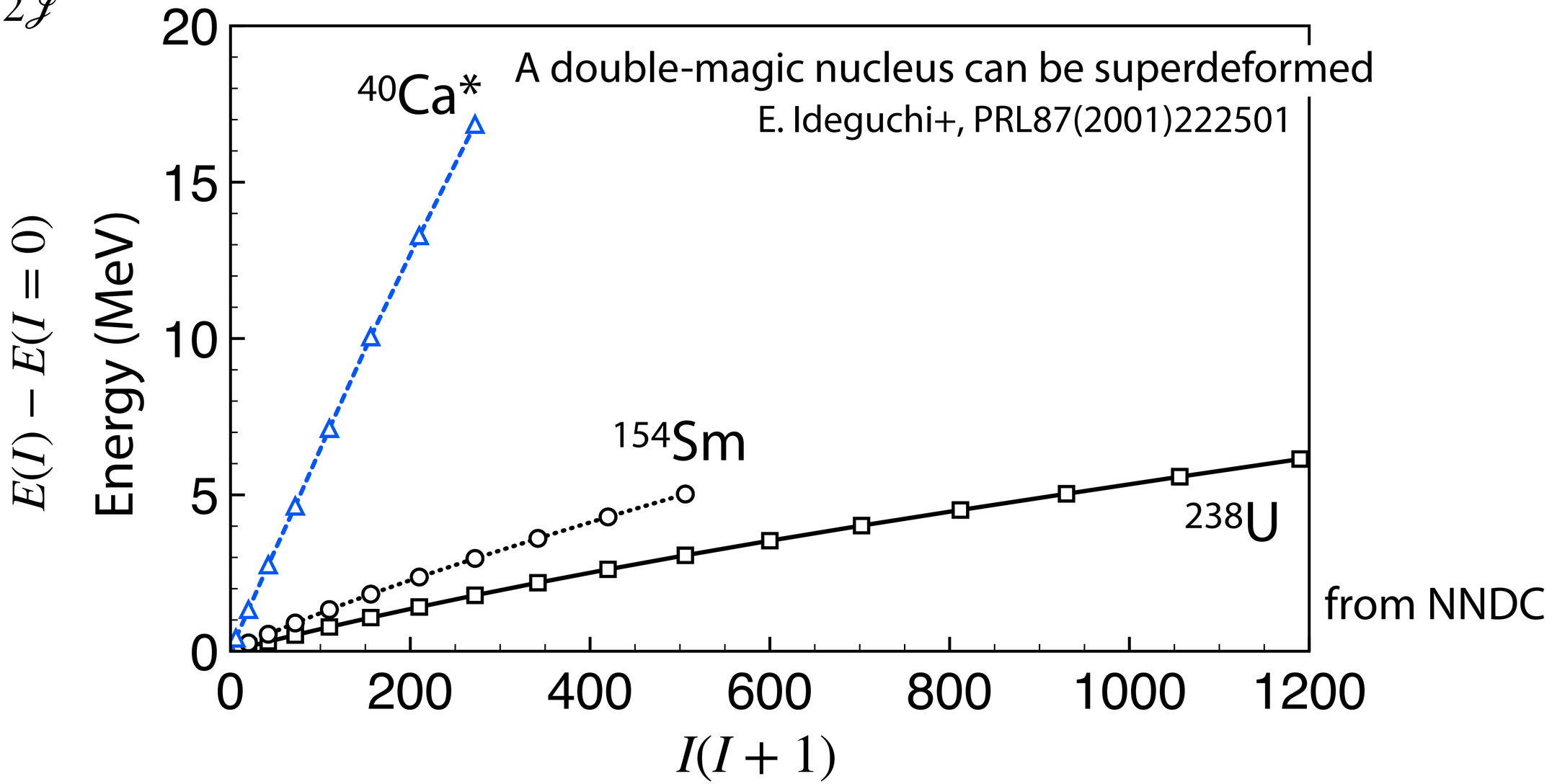
$$E = \frac{I(I+1)}{2\mathcal{J}}$$



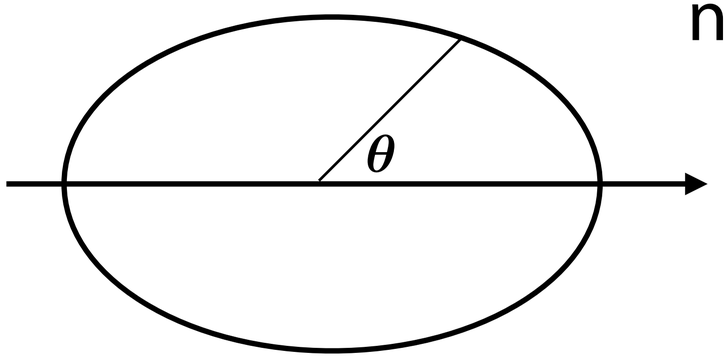
from NNDC

Emergence of the rotational band

$$E = \frac{I(I+1)}{2\mathcal{J}}$$



Some nuclei are deformed!



nuclear "surface": classical picture

$$R(\theta,\phi) = \bar{R}_0 \left(1 + \sum_{\lambda\mu} \alpha^*_{\lambda\mu} Y_{\lambda\mu}(\theta\phi) \right) \qquad \alpha_{2\mu} \neq 0$$

How to define the surface/shape of a quantal object?

$$\langle J = 0 \,|\, Y_{2\mu} \,|\, J = 0 \rangle = 0$$

one possible definition:

the nuclear shape = the shape of the mean field = that of the density

Symmetry and its breaking

$[H, \boldsymbol{J}] = 0$ The Hamiltonian is rotationally invariant: J is a good quantum number

The Hamiltonian is thus block diagonal w.r.t J.

$$H^{J=0} = H^{J=0}_{\mathrm{MF}} + H^{J=0}_{\mathrm{res}}$$

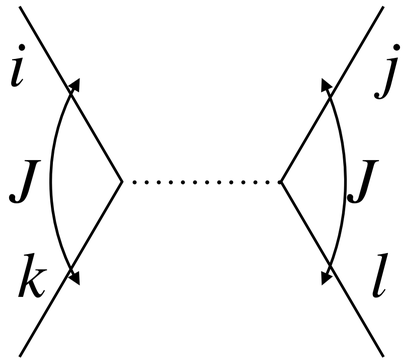
$$H^{J=0}_{\mathrm{MF}} = \sum_{\alpha} \varepsilon_{\alpha} [a^{\dagger}_{\alpha} a_{\alpha}]_0$$

s.p. orbital in the spherical MF

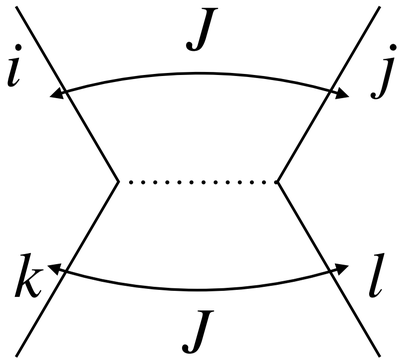
$$H^{J=0,F}_{\mathrm{res}} = \frac{1}{2} \sum_{ijkl,J} v^{F}_{ijkl}(J) : [[c^{\dagger}_i c_k]_J [c^{\dagger}_j c_l]_J]_0 :$$

$$H^{J=0,G}_{\mathrm{res}} = \sum_{ijkl,J} v^{G}_{ijkl}(J) : [[c^{\dagger}_i c^{\dagger}_j]_J [c_l c_k]_J]_0 :$$

F type



G type



angular-momentum coupling: $[A_a B_b]_{JM} = \sum_{m_a m_b} (j_a m_a j_b m_b \,|\, JM) A_{a m_a} B_{b m_b}$

Symmetry breaking

$$H_{\mathrm{MF}} = \sum_{\alpha} \varepsilon_{\alpha} \underset{J=0}{[a^{\dagger}_{\alpha} a_{\alpha}]_0} + \sum_{ij,J} \Gamma_{ij}(JM)[c^{\dagger}_{i} c_{j}]_{JM}$$

$$+ \sum_{ij,J} \left(\Delta_{ij}(JM)[c^{\dagger}_{i} c^{\dagger}_{j}]_{JM} + \Delta^{*}_{ij}(JM)[c_{b} c_{a}]_{JM} \right)$$

HF field $$\Gamma_{ij}(JM) := \sum_{kl} v^{F}_{ikjl}(J) \langle \Phi \,|\, [c^{\dagger}_{k} c_{l}]_{JM} \,|\, \Phi \rangle$$

pair field $$\Delta_{ij}(JM) := \sum_{kl} v^{G}_{ijkl}(J) \langle \Phi \,|\, [c_{l} c_{k}]_{JM} \,|\, \Phi \rangle$$

breaking of the particle number

appearance of the fields with $J > 0$ $\Longleftrightarrow$ **the rotational symmetry is broken**

Symmetry breaking of the mean fields

$|\phi\rangle$:Slater det. density matrix: $\rho_{ij} = \langle \phi | c_j^\dagger c_i | \phi \rangle$

U_s : Unitary trans.

$[H, U_s] = 0$ the symmetry the Hamiltonian has

$|\bar{\phi}\rangle = U_s |\phi\rangle, \qquad U_s |0\rangle = |0\rangle$

trans. of $c^\dagger, c$

$$U_s c_k^\dagger U_s^\dagger = \sum_l U_{s\,lk} c_l^\dagger \qquad (U_s^\dagger c_k^\dagger U_s = \sum_l U_{s\,kl}^* c_l^\dagger)$$

$$U_s c_k U_s^\dagger = \sum_l U_{s\,lk}^* c_l \qquad (U_s^\dagger c_k U_s = \sum_l U_{s\,kl} c_l)$$

Symmetry breaking of the mean fields

density matrix for the transformed SD:

$$\bar{\rho}_{ij} = \langle \bar{\phi} | c_j^\dagger c_i | \bar{\phi} \rangle = \langle \phi | \underbrace{U_s^\dagger} c_j^\dagger \underbrace{(U_s U_s^\dagger)}_{=1} c_i \underbrace{U_s} | \phi \rangle =: \langle \phi | c_{\bar{j}}^\dagger c_{\bar{i}} | \phi \rangle$$

$$c_{\bar{j}}^\dagger := \underbrace{U_s^\dagger c_j^\dagger U_s} = \sum_k U_{s\,jk}^* c_k^\dagger, \qquad c_{\bar{i}} := \underbrace{U_s^\dagger c_i U_s} = \sum_l U_{s\,il} c_l$$

$$= \sum_{kl} U_{s\,jk}^* U_{s\,il} \rho_{lk} = (U_s \rho U_s^\dagger)_{ij}$$

$$\rho \to \bar{\rho} = U_s \rho U_s^\dagger$$

Symmetry breaking of the mean fields

$$\rho \to \bar{\rho} = U_s \rho U_s^\dagger$$

the energy is unchanged

$$[H, U_s] = 0$$

$$E[\rho] = \langle \phi \,|\, H \,|\, \phi \rangle$$

$$E[\bar{\rho}] = \langle \bar{\phi} \,|\, H \,|\, \bar{\phi} \rangle = \langle \phi \,|\, U_s^\dagger H U_s \,|\, \phi \rangle = E[\rho]$$

variation of $\delta\rho, \delta\bar{\rho} := U_s \delta\rho U_s^\dagger$

$$E[\rho + \delta\rho] = E[\bar{\rho} + \delta\bar{\rho}]$$

$$\sum_{ij} \frac{\delta E}{\delta \rho_{ji}} \delta\rho_{ij} = \sum_{ij} \frac{\delta E}{\delta \rho_{ji}}\bigg|_{\rho=\bar{\rho}} \delta\bar{\rho}_{ij} \qquad h := \frac{\delta E}{\delta \rho}$$

$$\Rightarrow \quad \mathrm{tr} h[\rho]\delta\rho = \mathrm{tr} h[\bar{\rho}]\delta\bar{\rho} = \mathrm{tr} U_s^\dagger h[\bar{\rho}] U_s \delta\rho$$

$$\Rightarrow \quad h[\bar{\rho}] = U_s h[\rho] U_s^\dagger$$

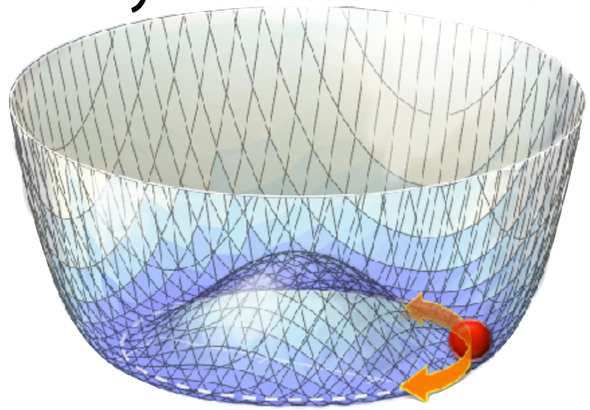
Symmetry breaking of the mean fields $h[\bar{\rho}] = U_s h[\rho] U_s^\dagger$

self-consistent symmetry

ρ is invariant under the trans. U_s: $\bar{\rho} = \rho$

$h[\bar{\rho}] = h[\rho]$ commutes with U_s

the solution of HF (mean field and density) holds the symmetry the Hamiltonian has



broken symmetry

ρ is NOT invariant under the trans. U_s : $\bar{\rho} \neq \rho$

$[h[\rho], \rho] = 0$ ➡ $[h[\bar{\rho}], \bar{\rho}] = 0$ since $[h[\bar{\rho}], \bar{\rho}] = U_s [h[\rho], \rho] U_s^\dagger = 0$

degenerate solutions

U_s is a continuous sym., infinite numbers of degenerate solutions

Symmetry breaking of the mean fields: the case of HFB

Kasuya–Yoshida, PTEP(2021)

$|\Phi\rangle \to |\bar{\Phi}\rangle = U_s|\Phi\rangle$

pair tensor: $\bar{\kappa}_{ij} = \langle\bar{\Phi}|c_j c_i|\bar{\Phi}\rangle = \langle\Phi|U_s^\dagger c_j (U_s U_s^\dagger) c_i U_s|\Phi\rangle = \sum_{kl} U_{s\,jl}\kappa_{kl}U_{s\,ik} = (U_s\kappa U_s^T)_{ij}$

then, the generalized density matrix and the HFB Hamiltonian are transformed as

$$\bar{\mathscr{R}} = \begin{pmatrix} U_s & 0 \\ 0 & U_s^* \end{pmatrix}\begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix}\begin{pmatrix} U_s^\dagger & 0 \\ 0 & U_s^T \end{pmatrix} =: \mathscr{U}_s\mathscr{R}\mathscr{U}_s^\dagger$$

$$\mathscr{H}[\bar{\mathscr{R}}] = \mathscr{U}_s\mathscr{H}\mathscr{U}_s^\dagger$$

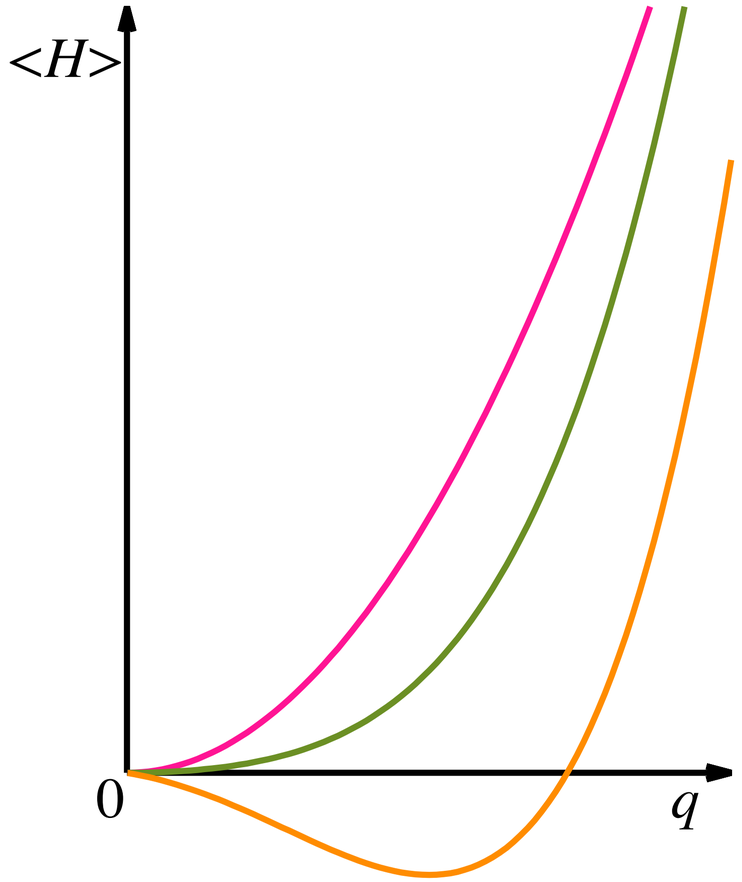
similar to the case of HF

(note) the case of the anti-unitary U_s ex. time-reversal operation

$$\mathscr{R} \to (\mathscr{U}_s\mathscr{R}\mathscr{U}_s^\dagger)^*, \qquad \mathscr{H} \to (\mathscr{U}_s\mathscr{H}\mathscr{U}_s^\dagger)^*$$

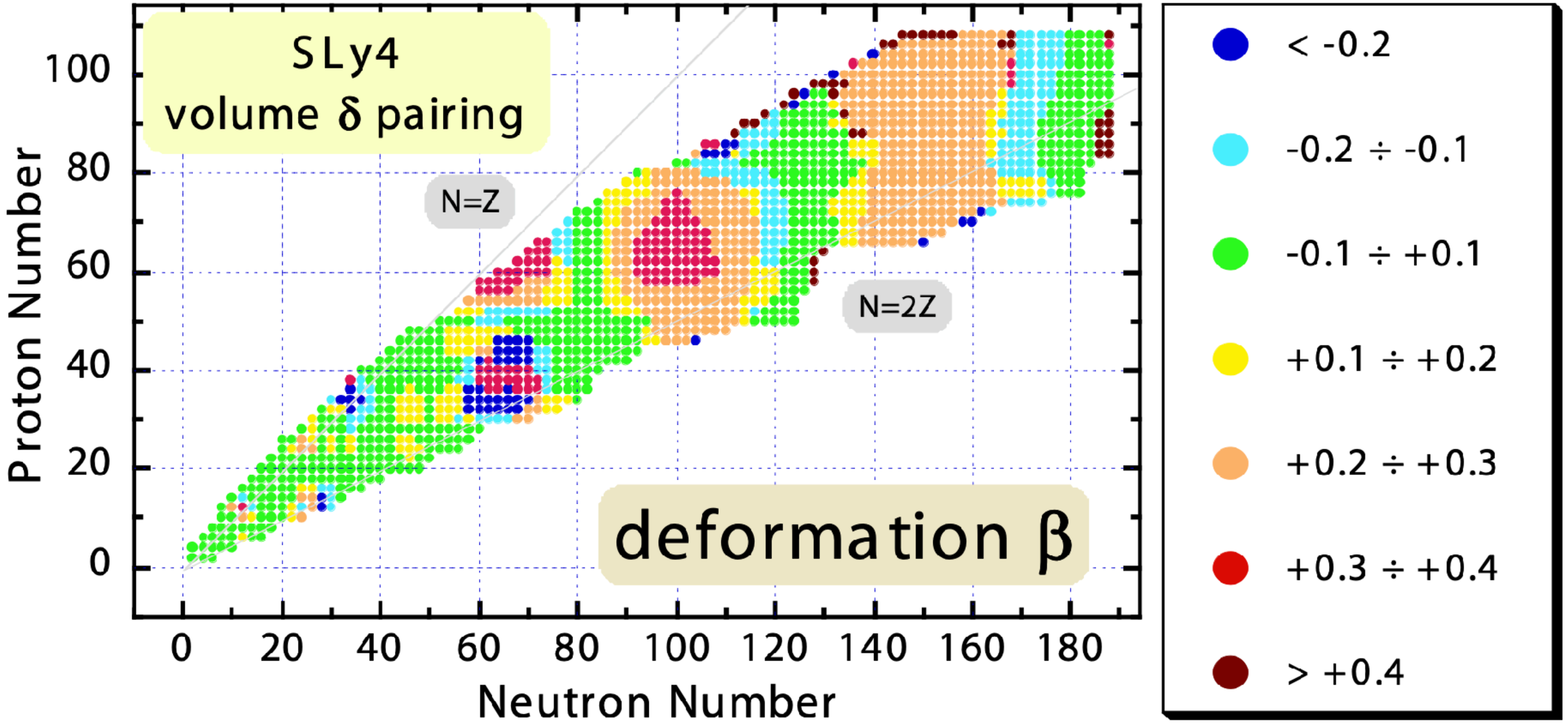
Symmetry breaking of the mean fields

pairing		**deformation**
$\langle P^\dagger \rangle \neq 0$	order para.	$\langle Q_{\lambda\mu} \rangle \neq 0$
particle-number sym.	breaking	rotational sym.
$e^{A^\dagger}\|0\rangle$	vacuum	$e^{\Gamma^\dagger}\|0\rangle$
Cooper-pair condensation		Vib.-phonon condensation
$\|\langle \Psi_0^{N+2} \| P^\dagger \| \Psi_0^N \rangle\|^2$	strong transition "rotation"	$\|\langle \Psi_i^\lambda \| Q_{\lambda\mu} \| \Psi_0 \rangle\|^2$



Predicted deformation by the HFB cal.

Stoitsov+, 2003



Phenomenological mean fields for deformed nuclei

✓anisotropic oscillator potential

$$h_{\rm HO} = \frac{1}{2m}\boldsymbol{p}^2 + \frac{m}{2}\sum_i \omega_i^2 x_i^2$$

$$= \sum_i \hbar\omega_i(\bar{p}_i^2 + \bar{x}_i^2) = \sum_i \hbar\omega_i(n_i + \frac{1}{2})$$

stretched coordinates

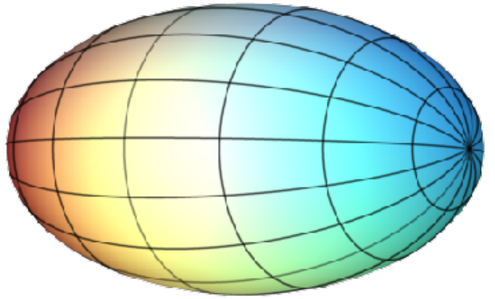
$$\bar{p}_i = \sqrt{\frac{1}{m\hbar\omega_i}}p_i, \qquad \bar{x}_i = \sqrt{\frac{m\omega_i}{\hbar}}x_i$$

$$C_i^\dagger = \frac{1}{\sqrt{2}}(\bar{x}_i - i\bar{p}_i), \qquad n_i = C_i^\dagger C_i$$

the shape of the potential: equipotential surface

$$\sum_i \omega_i^2 x_i^2 = \text{const} \quad \Longleftrightarrow \quad \frac{x^2}{R_x^2} + \frac{y^2}{R_y^2} + \frac{z^2}{R_z^2} = \text{const}$$

spheroid



under the volume conservation

$$\omega_x\omega_y\omega_z = \omega_0^3 \leftrightarrow R_xR_yR_z = R_0^3$$

$$\frac{R_i}{R_0} = \frac{\omega_0}{\omega_i}$$

$\omega_1, \omega_2, \omega_3$
or
$\omega_x, \omega_y, \omega_z$

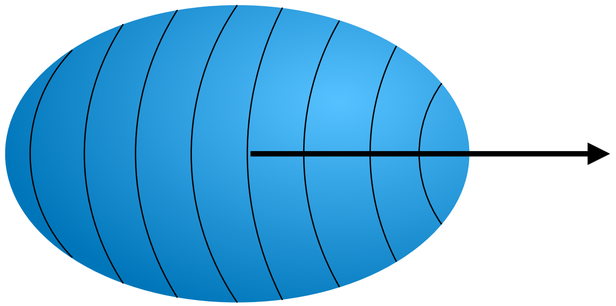
Axially-symmetric case

$$\omega_1 = \omega_2 =: \omega_\perp$$

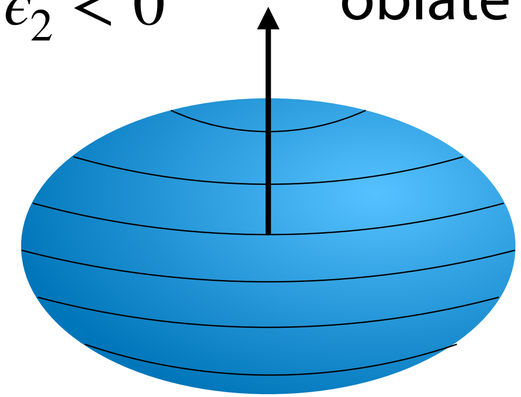
$$\omega_\perp = \omega_0(1 + \frac{1}{3}\epsilon_2)$$

$$\omega_3 = \omega_0(1 - \frac{2}{3}\epsilon_2)$$

$\epsilon_2 > 0$ prolate

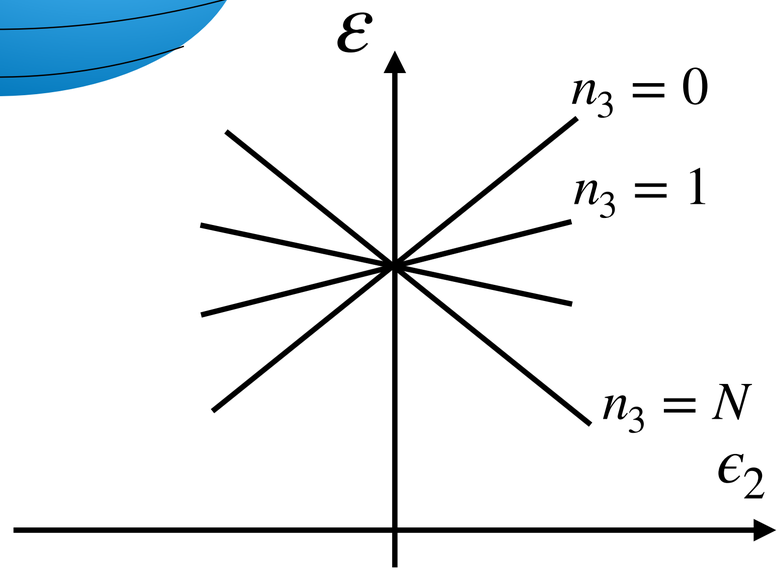


$\epsilon_2 < 0$ oblate



$$\varepsilon_{\mathrm{HO}} = \sum_i \hbar\omega_i(n_i + \frac{1}{2}) = \hbar\omega_0 \left[(N + \frac{3}{2}) + \frac{1}{3}(N - 3n_3)\epsilon_2\right]$$

$$N := n_1 + n_2 + n_3$$

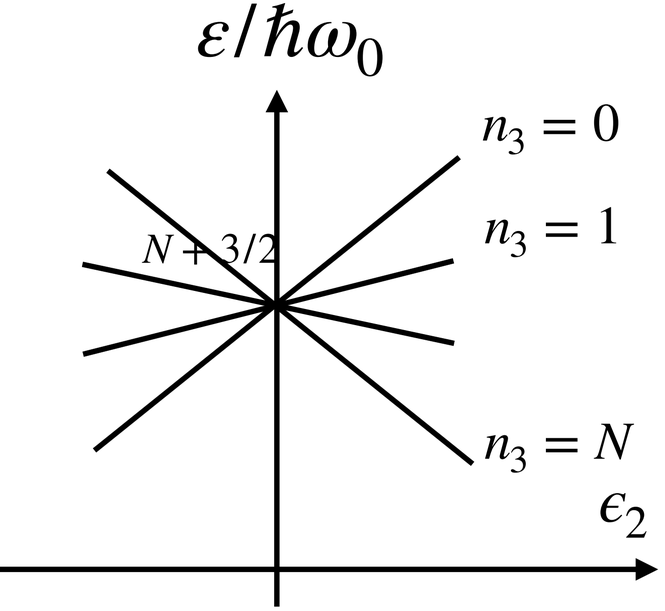


Axially-symmetric case

$$\varepsilon_{\mathrm{HO}} = \sum_i \hbar\omega_i (n_i + \frac{1}{2}) = \hbar\omega_0 \left[(N + \frac{3}{2}) + \frac{1}{3}(N - 3n_3)\epsilon_2 \right]$$

$$N := n_1 + n_2 + n_3 = 2n + \ell$$

in the spherical coordinate



degeneracy

$2(N+1)$

$2N$

2

with spin

ex.)

	$[n_1, n_2, n_3]$	$[n, \ell, \ell_z]$
$N = 0$	[0,0,0]	[0,0,0]
$N = 1$	[1,0,0]	[0,1, − 1]
	[0,1,0]	[0,1,0]
	[0,0,1]	[0,1,1]

$$2\sum_{i=0}^{N}(i+1) = (N+1)(N+2)$$

Axially-symmetric case

$$\varepsilon_{\mathrm{HO}} = \sum_i \hbar\omega_i (n_i + \frac{1}{2}) = \hbar\omega_0 \left[(N + \frac{3}{2}) + \frac{1}{3}(N - 3n_3)\epsilon_2 \right]$$

principal quantum #: $N = n_1 + n_2 + n_3 = n_+ + n_- + n_3, \quad \Lambda := l_3 = n_+ - n_-$

$[n_1, n_2, n_3] \longleftrightarrow [N, n_3, \Lambda]$

ex.)

$$\omega_1 = \omega_2 = 2\omega_3$$

$[n_1, n_2, n_3]$			$[N, n_3, \lvert\Lambda\rvert]$		
[0,0,0]			[0,0,0]		$N = 0$
[0,0,1]			[1,1,0]		$N = 1$
[1,0,0]	[0,1,0]	[0,0,2]	[1,0,1]	[2,2,0]	$N = 1$ and 2
[1,0,1]	[0,1,1]	[0,0,3]	[1,1,1]	[3,3,0]	$N = 2$ and 3

intruder = different parity

octupole correlation

spherical: $\epsilon_2 = 0$

degeneracy w.r.t N

$$(N+1)(N+2)$$

spherical magic numbers

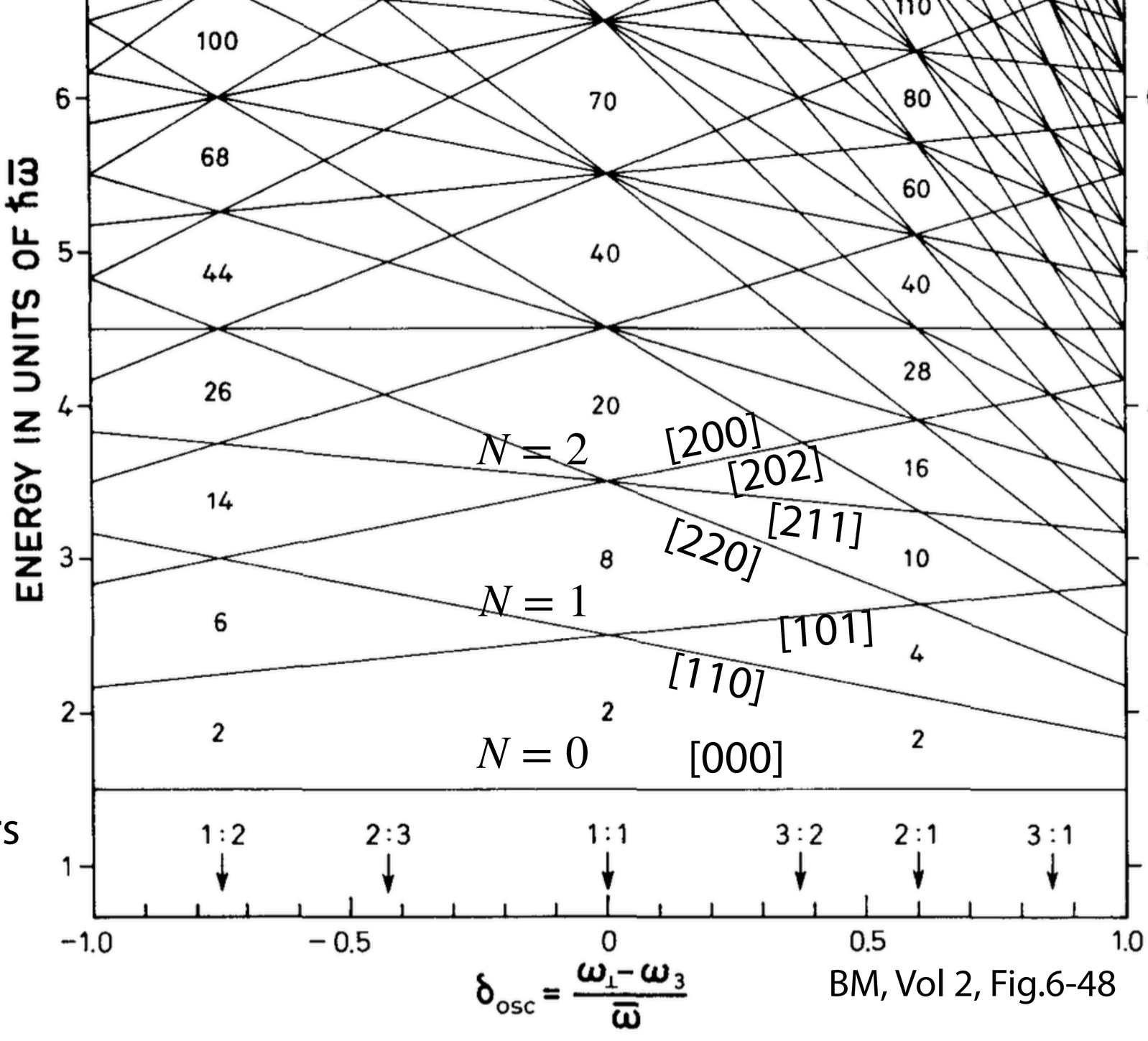
superdeformation (SD)

$$\omega_\perp / \omega_z = 2$$

$$\epsilon_2 = 0.6$$

a new type of degeneracy appears

SD magic numbers



BM, Vol 2, Fig.6-48

Nilsson model

$$h = h_{\mathrm{HO}} + h_{ls+ll}$$

$$h_{\mathrm{HO}} = \frac{1}{2m}\boldsymbol{p}^2 + \frac{m}{2}\sum_i \omega_i^2 x_i^2$$

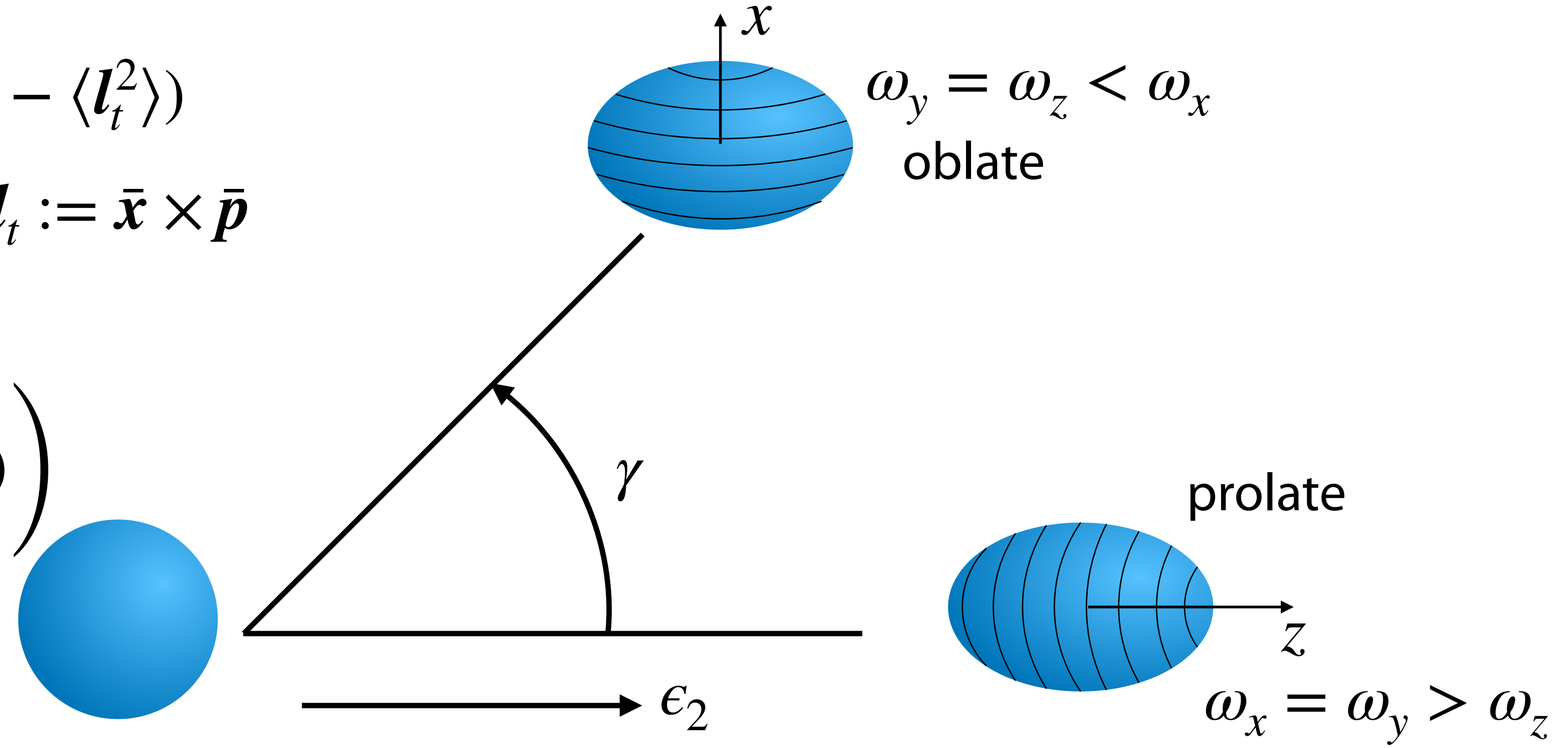
$$= \sum_i \hbar\omega_i(\bar{p}_i^2 + \bar{x}_i^2) = \sum_i \hbar\omega_i(n_i + \frac{1}{2})$$

$$h_{ls+ll} = v_{ls}\boldsymbol{l}_t \cdot \boldsymbol{s} + v_{ll}(\boldsymbol{l}_t^2 - \langle \boldsymbol{l}_t^2 \rangle)$$

$$\boldsymbol{l}_t := \bar{\boldsymbol{x}} \times \bar{\boldsymbol{p}}$$

not necessarily axial symmetric

$$\omega_i = \bar{\omega}_0 \left(1 - \frac{2}{3}\epsilon_2 \cos(\gamma + \frac{2\pi}{3}i)\right)$$



Asymptotic quantum numbers

$h_{\mathrm{Nil}} = h_{\mathrm{HO}} + h_{ls+ll}$

h_{ls+ll} is not diagonal in the HO basis

treated as perturbations at large deformations

good quantum # in an axially and reflection sym. potential: $\Omega(=j_z=m), \pi$ (parity)

asymptotic quantum #: $|Nn_3\Lambda\Omega^\pi\rangle$

principal quantum # : $N = n_1 + n_2 + n_3 = n_+ + n_- + n_3$

$\Lambda := l_3 = n_+ - n_-, \quad \Omega = \Lambda + \Sigma$

$$|\Omega^\pi, k\rangle = \sum_{Nlj} C(Nljk)\,|Nlj\Omega^\pi\rangle = \sum_{Nn_3\Lambda} C'(Nn_3\Lambda k)\,|Nn_3\Lambda\Omega^\pi\rangle$$

spherical HO basis deformed HO basis

Examples of the Nilsson diagram

relatively simple in light nuclei

——— $\pi = +$

····· $\pi = -$

two-fold degenerated (time-reversal sym.)

$\pm\Omega$

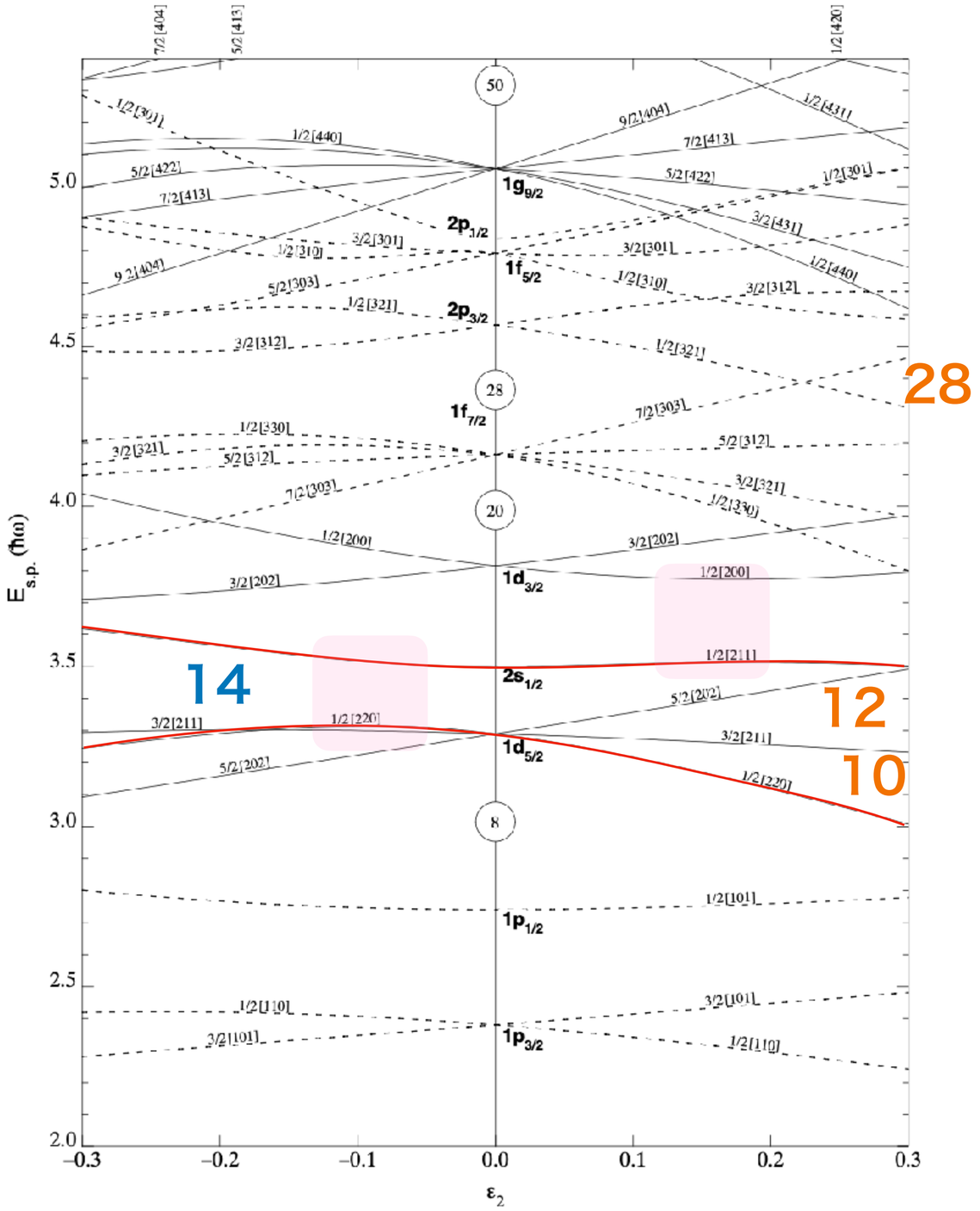
avoided crossing

for the orbitals with same Ω^{π}

deformed magic numbers

10, 12, **28** (prolate)

14 (oblate)



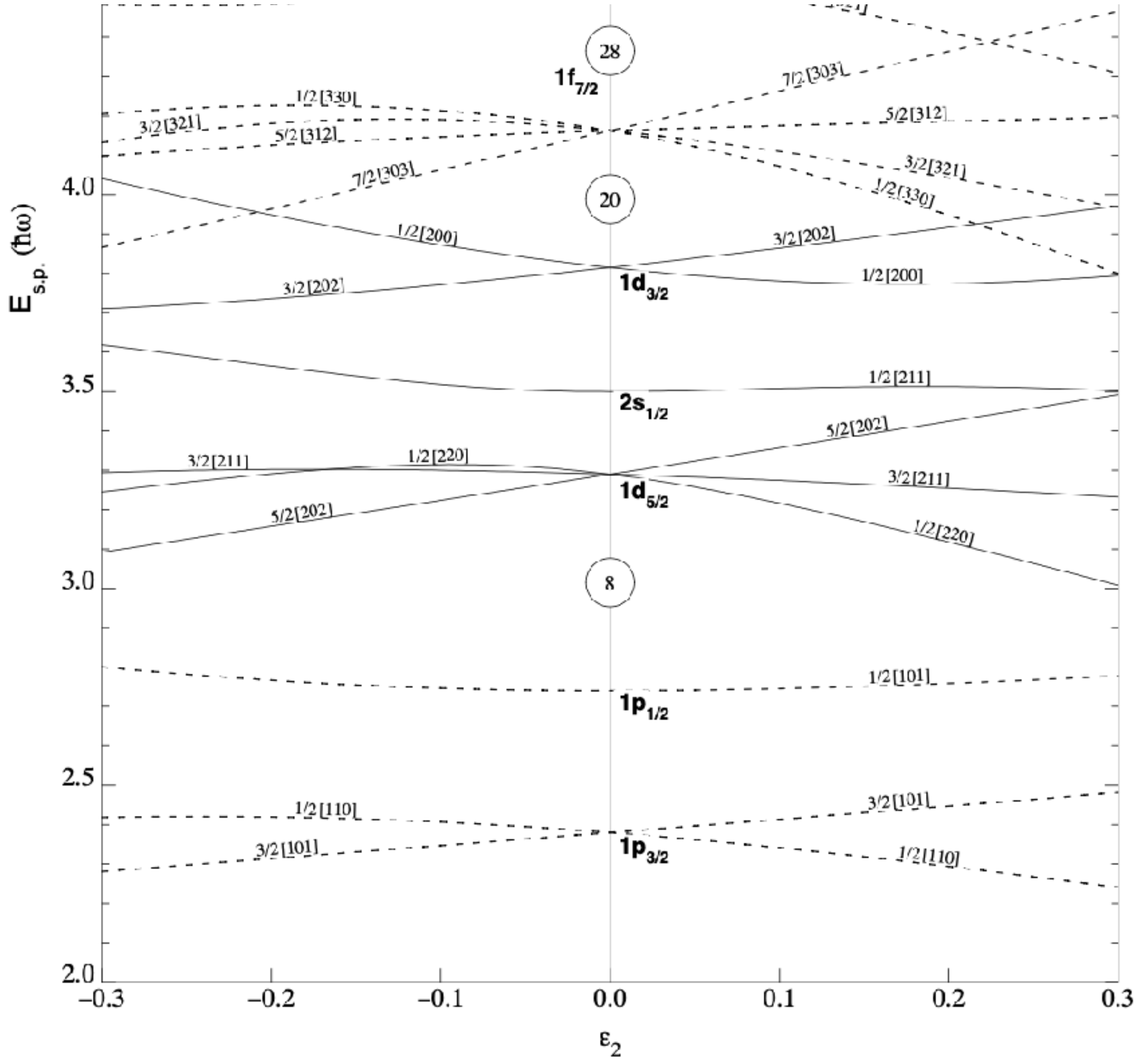
Collective motions in nuclei: rotation

An application of the Nilsson diagram

odd nuclei:

$$|\Phi_{\text{odd}}\rangle = a_i^\dagger |\Phi_{\text{HFB}}\rangle$$

nuclide	measured J^π	
$^{17}O_9$	$5/2^+$	$\nu 1d_{5/2}$
$^{15}O_7$	$1/2^-$	$\nu 1p_{1/2}$
$^{19}Ne_9$	$1/2^+$	~~$\nu 1d_{5/2}$~~ $\nu[220]1/2$

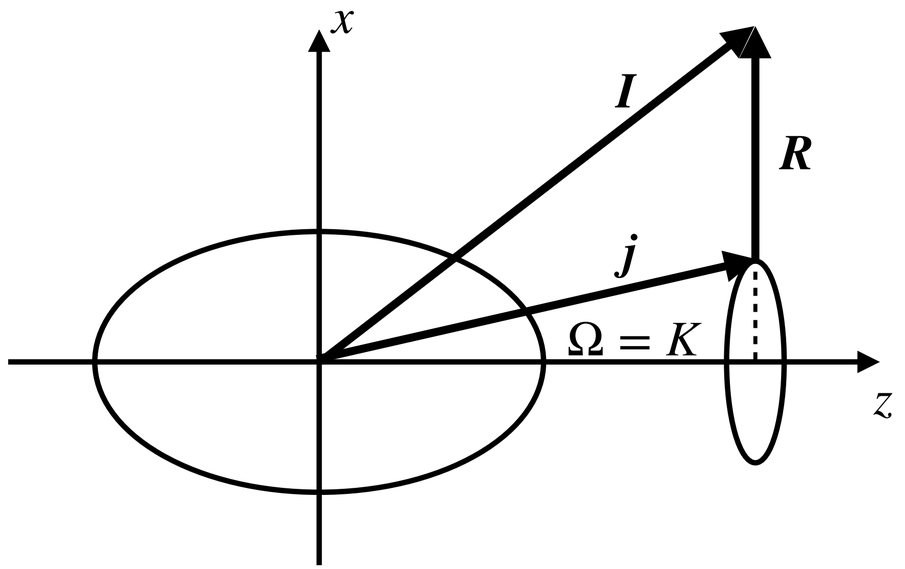


Rotational spectra

$$H_{\text{rot}} = \frac{\boldsymbol{R}^2}{2\mathcal{J}}$$

$\boldsymbol{R}$: collective spin (angular momentum) of the core

$$\Rightarrow \quad E_I = \frac{I(I+1)}{2\mathcal{J}}$$



strong coupling: deformation alignment

rotation along the perpendicular axis, 3-axis being the symmetry axis

$$H_{\text{rot}} = \frac{\boldsymbol{R}^2}{2\mathcal{J}} = \frac{1}{2\mathcal{J}}[(I_1 - j_1)^2 + (I_2 - j_2)^2]$$

$$= \frac{1}{2\mathcal{J}}[\boldsymbol{I}^2 - I_3^2 + (j_1^2 + j_2^2) - (I_+ j_- + I_- j_+)]$$

recoil Coriolis and centrifugal forces

treated in first order perturbation theory

Rotational spectra in the strong coupling

$$H = H_{\rm sp} + H_{\rm rot}$$

HF(B) single-(quasi)particle: ϕ_ν, e_ν

$$H_{\rm rot} = \frac{1}{2\mathcal{J}}[\boldsymbol{I}^2 - I_3^2 - (I_+ j_- + I_- j_+)]$$

selection rules for $j_\pm$ are $\Delta\Omega = \pm 1$

$$E_{IK} = |e_\nu - \lambda| + \frac{1}{2\mathcal{J}}[I(I+1) - K^2] \qquad K \neq \frac{1}{2}$$

for the case of $K = \frac{1}{2}$ bands

$$E_{IK} = |e_\nu - \lambda| + \frac{1}{2\mathcal{J}}[I(I+1) - K^2 + a(-1)^{I+1/2}(I+1/2)]$$

decoupling parameter

$$a = -\langle \phi_\nu | j_+ | \phi_{\bar{\nu}} \rangle$$

$\Omega = 1/2 \quad \Omega = -1/2$

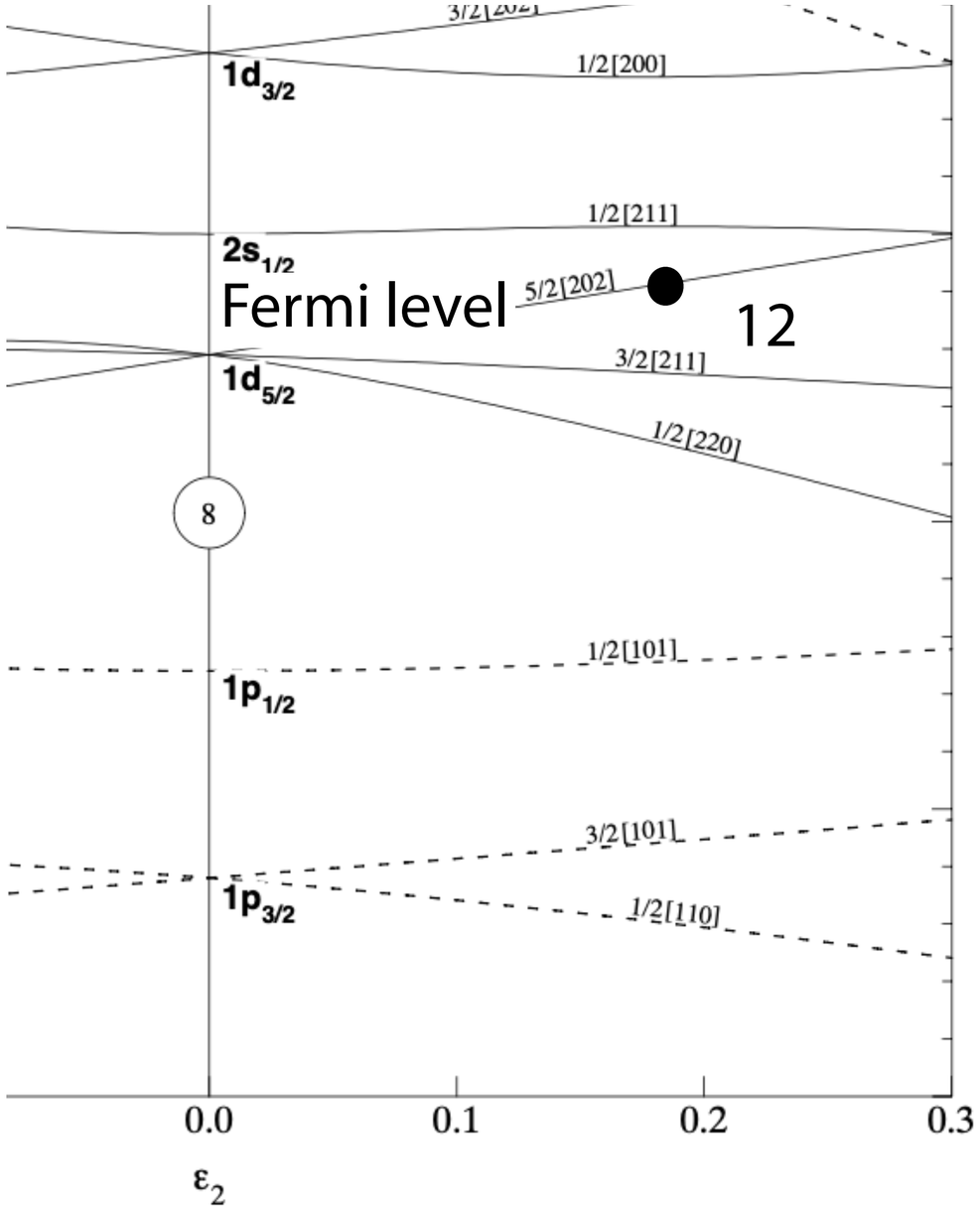
assuming

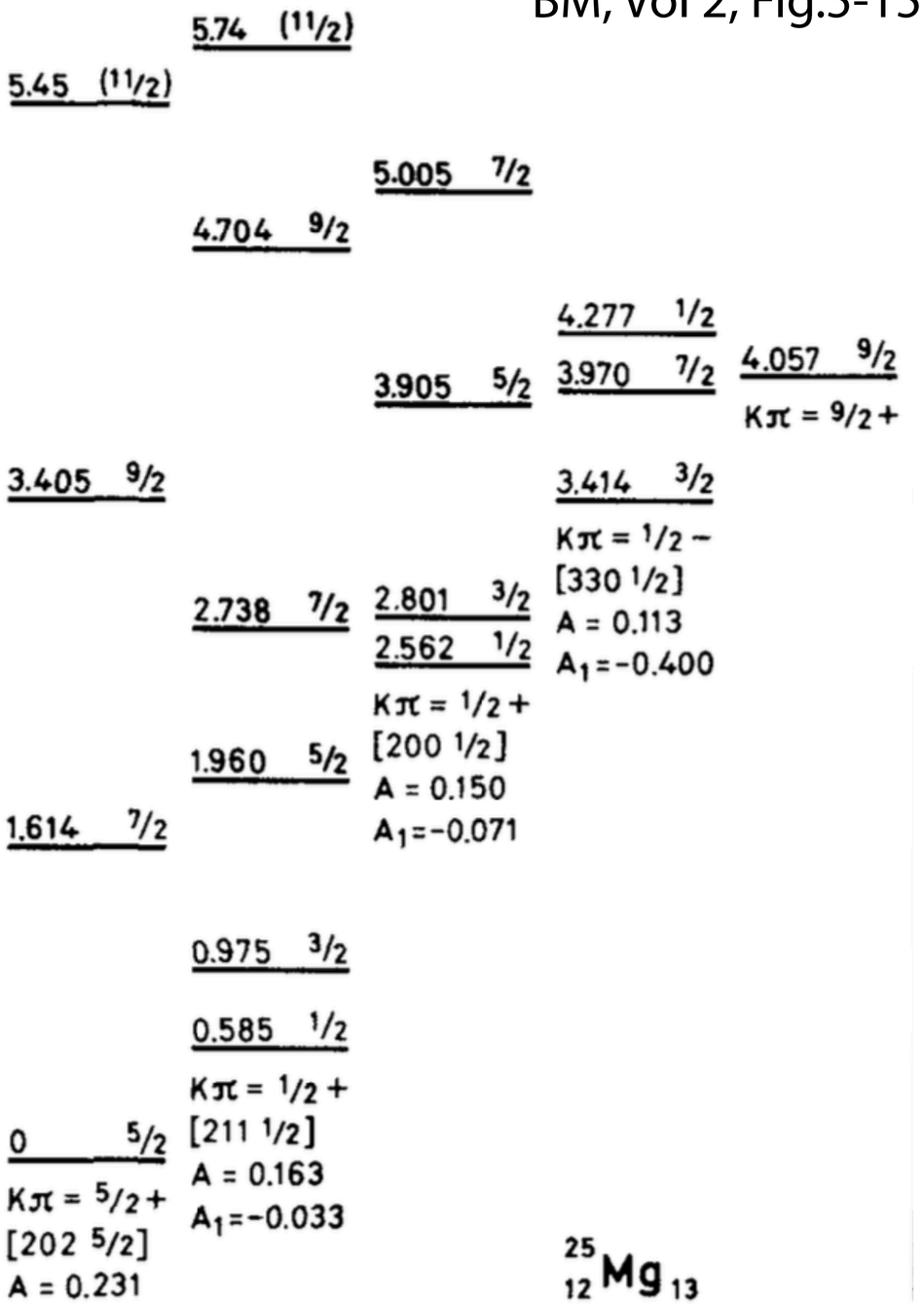
axial symmetry

reflection symmetry

$$E_{\text{rot}} = AI(I+1) + A_1(-1)^{I+1/2}(I+1/2)\delta_{K,1/2}$$

BM, Vol 2, Fig.5-15

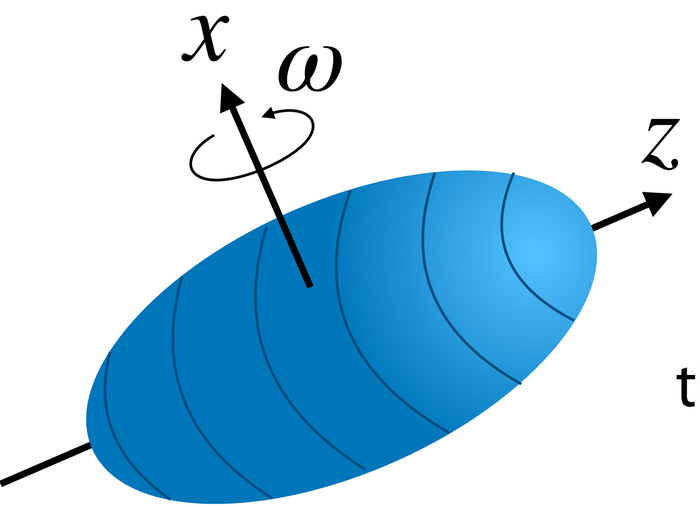




The cranking model

simultaneous description of s.p. and rotational motions

the rotation is treated **classically** within the **quantum mechanics**



$$x_1 = x$$
$$x_2 = y\cos\omega t + z\sin\omega t$$
$$x_3 = -y\sin\omega t + z\cos\omega t$$

uniform rotation along the x-axis

the time-dependent wave functions in the two systems must satisfy

$$\psi^{\omega}(x_1, x_2, x_3, t) = \psi(x, y, z, t)$$

up to the phase

$$\left(\frac{\partial\psi}{\partial t}\right)_{x,y,z} = \left(\frac{\partial\psi^{\omega}}{\partial t}\right)_{x_1,x_2,x_3} + \frac{\partial\psi^{\omega}}{\partial x_2}\frac{\partial x_2}{\partial t} + \frac{\partial\psi^{\omega}}{\partial x_3}\frac{\partial x_3}{\partial t}$$

$$\frac{\partial x_2}{\partial t} = \omega x_3, \quad \frac{\partial x_3}{\partial t} = -\omega x_2$$

$$\rightarrow \quad \frac{\partial\psi(x, y, z, t)}{\partial t} = \left(\frac{\partial}{\partial t} - i\omega\ell_1\right)\psi^{\omega}(x_1, x_2, x_3, t)$$

The cranking model

$$\frac{\partial\psi(x,y,z,t)}{\partial t} = \left(\frac{\partial}{\partial t} - i\omega\ell_1\right)\psi^{\omega}(x_1,x_2,x_3,t)$$

note:

$$\ell_1 = -i\left(x_2\frac{\partial}{\partial x_3} - x_3\frac{\partial}{\partial x_2}\right)$$

$$= -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = \ell_x$$

→ time-dependent Sch. eq.

$$i\partial_t\psi(x,y,z,t) = h\psi(x,y,z,t)$$

↓

$$i\partial_t\psi^{\omega}(x_1,x_2,x_3,t) = (h - \omega\ell_1)\psi^{\omega}(x_1,x_2,x_3,t)$$

the cranking Hamiltonian (Routhian): $\hat{H}' = \hat{H} - \omega\hat{J}_1$

↔ $\delta\langle\psi|\hat{H}|\psi\rangle = 0$ under the constraint $\langle\psi|\hat{J}_1|\psi\rangle = J_1$

ω : a Lagrange multiplier

Variational principle in a rotating frame

transformation of the frame $|\phi(\theta, I)\rangle = e^{-i\theta \hat{J}_x} |\phi_{\rm intr}(I)\rangle$

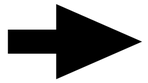
time-dependent variational principle : $\delta \langle \phi(\theta, I) | i\partial_t - \hat{H} | \phi(\theta, I)\rangle = 0$

$$\delta \langle \phi_{\rm intr}(I) | \hat{H} - i \left(\frac{1}{i} \frac{\partial \mathscr{H}}{\partial I} \hat{J}_x - \frac{\partial \mathscr{H}}{\partial \theta} \frac{\partial}{\partial I} \right) | \phi_{\rm intr}(I)\rangle = 0$$

note:

$$\frac{\partial}{\partial t} = \dot{\theta} \frac{\partial}{\partial \theta} + \dot{I} \frac{\partial}{\partial I}$$

$$i \frac{\partial}{\partial \theta} | \phi_{\rm intr}(I)\rangle = \hat{J}_x | \phi_{\rm intr}(I)\rangle$$



$$\delta \langle \phi_{\rm intr}(I) | \hat{H} - \omega_{\rm rot} \hat{J}_x | \phi_{\rm intr}(I)\rangle = 0$$

Hamilton's eq.: $\dot{\theta} = \dfrac{\partial \mathscr{H}}{\partial I} = \omega_{\rm rot}$

$$\dot{I} = - \frac{\partial \mathscr{H}}{\partial \theta} = 0$$

$$\mathscr{H}(I) := \langle \phi(\theta, I) | \hat{H} | \phi(\theta, I)\rangle = \langle \phi_{\rm intr}(I) | \hat{H} | \phi_{\rm intr}(I)\rangle$$

$$[\hat{H}, \hat{J}_x] = 0$$

Mean field in a rotating frame

$$H' = H - \omega J_x$$

$$h'|\mu\rangle = \varepsilon'_\mu |\mu\rangle \qquad \varepsilon'_\mu(\omega_{\rm rot}) \qquad \text{single-particle } \textbf{Routhian}$$

when the reflection symmetry is conserved

x-signature: $R_x = e^{-i\pi J_x}$

$$R_x|\mu\rangle = r|\mu\rangle \qquad r = \pm i$$
$$r = e^{-i\pi\alpha},\ \alpha = \pm 1/2$$

x-signature is a good quantum number

when the reflection symmetry is broken

x-simplex: πR_x

$$(x_1, x_2, x_3) \rightarrow (-x_1, x_2, x_3)$$

x-simplex is a good quantum number

* the axial symmetry can be (is usually) broken due to the Coriolis force

Signature quantum number

$$\hat{R}_x(\pi) = \exp(-i\pi\hat{J}_x)$$

$$\hat{R}_x^2(\pi)\Psi = r^2\Psi = (-1)^A\Psi$$

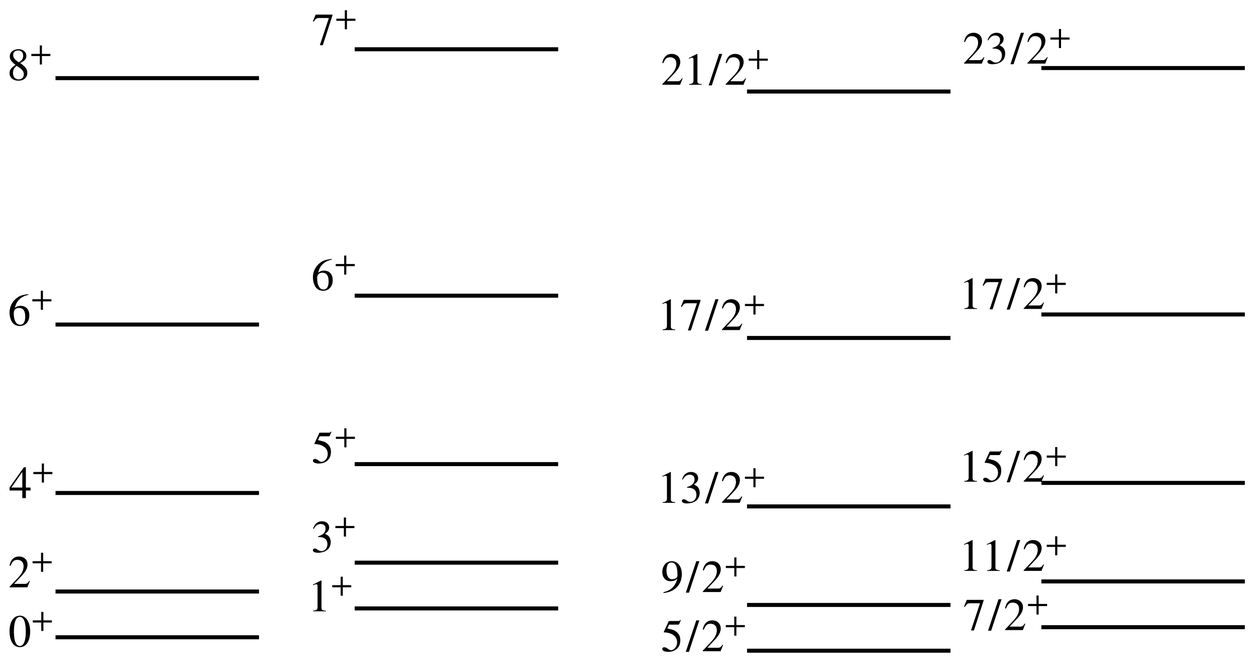
A rotation of 2π leaves the wavefunction unchanged, except for a phase factor

signature exponent quantum number:

$$r = e^{-i\pi\alpha}$$

$r = \pm 1$ (even A), $\alpha = 0,1$

$r = \pm i$ (odd A), $\alpha = \pm 1/2$



$\alpha = 0$ $\alpha = 1$ $\alpha = 1/2$ $\alpha = -1/2$

Correspondences to the experimental data

rotational frequency

$$\dot{\theta} = \frac{\partial \mathscr{H}}{\partial I} = \omega_{\mathrm{rot}} \quad \Rightarrow \quad \omega_{\mathrm{rot}}(I) \simeq \frac{dE}{dI} \approx \frac{1}{2}[E_{\mathrm{rot}}(I+1) - E_{\mathrm{rot}}(I-1)] = E_\gamma/2$$

moments of inertia

$$\mathscr{J}^{(1)} = \frac{J}{\omega_{\mathrm{rot}}} \approx \frac{2(I+1/2)}{E(I+1) - E(I-1)} = \frac{2I+1}{E_\gamma}$$

$$\mathscr{J}^{(2)} = \frac{dJ}{d\omega_{\mathrm{rot}}} \approx \frac{4}{\Delta E_\gamma}$$

note:

$$J^2 = I(I+1)$$

$$I^2 + I - J^2 = 0$$

$$I = \frac{1}{2}(-1 + \sqrt{4J^2+1})$$

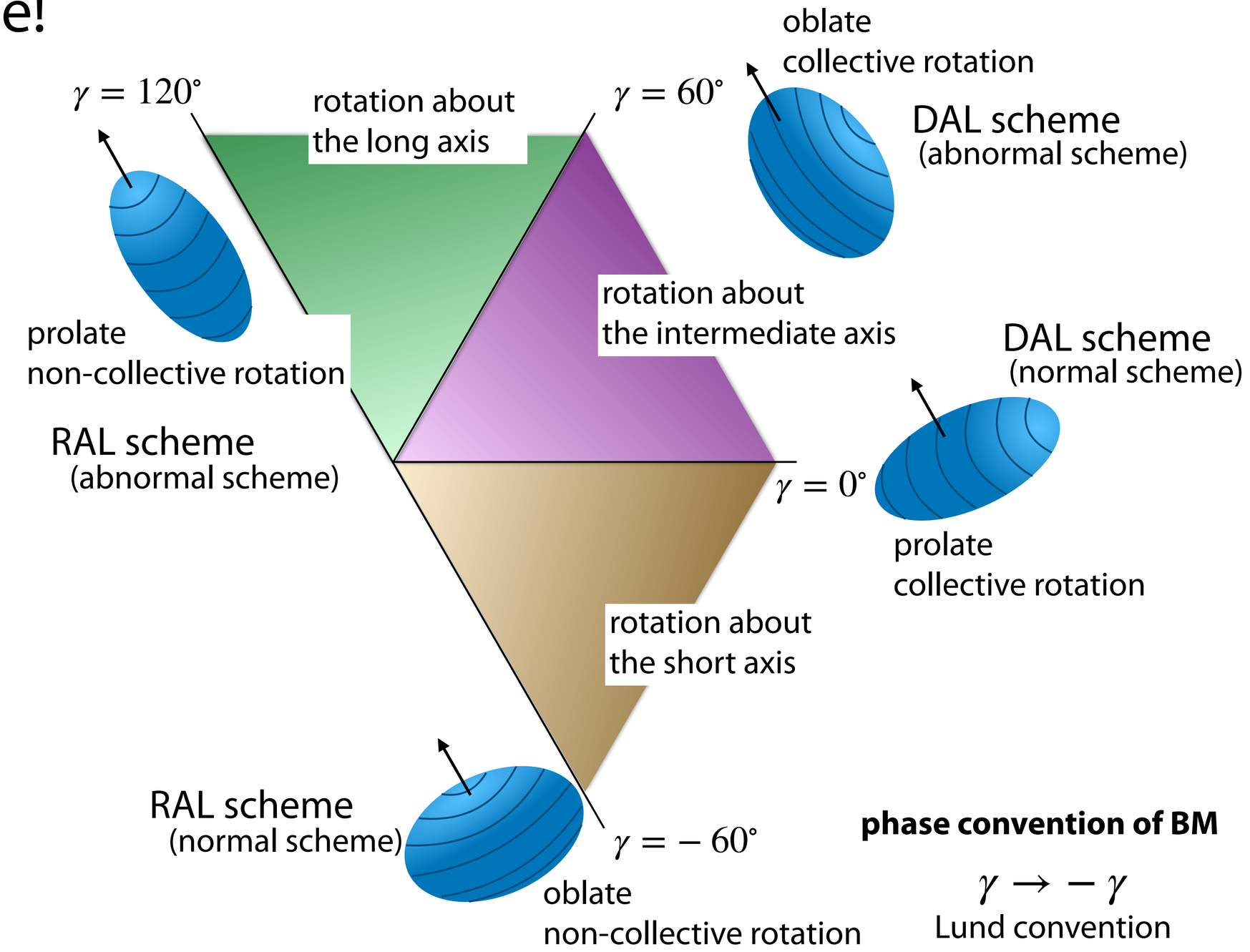
$$\simeq \frac{1}{2}(-1+2J)$$

Triaxiality plays a role!

symmetry axis
and type of deformation

rotation axis

- collective rotation
  deformation aligned
- non-collective rotation
  rotation aligned



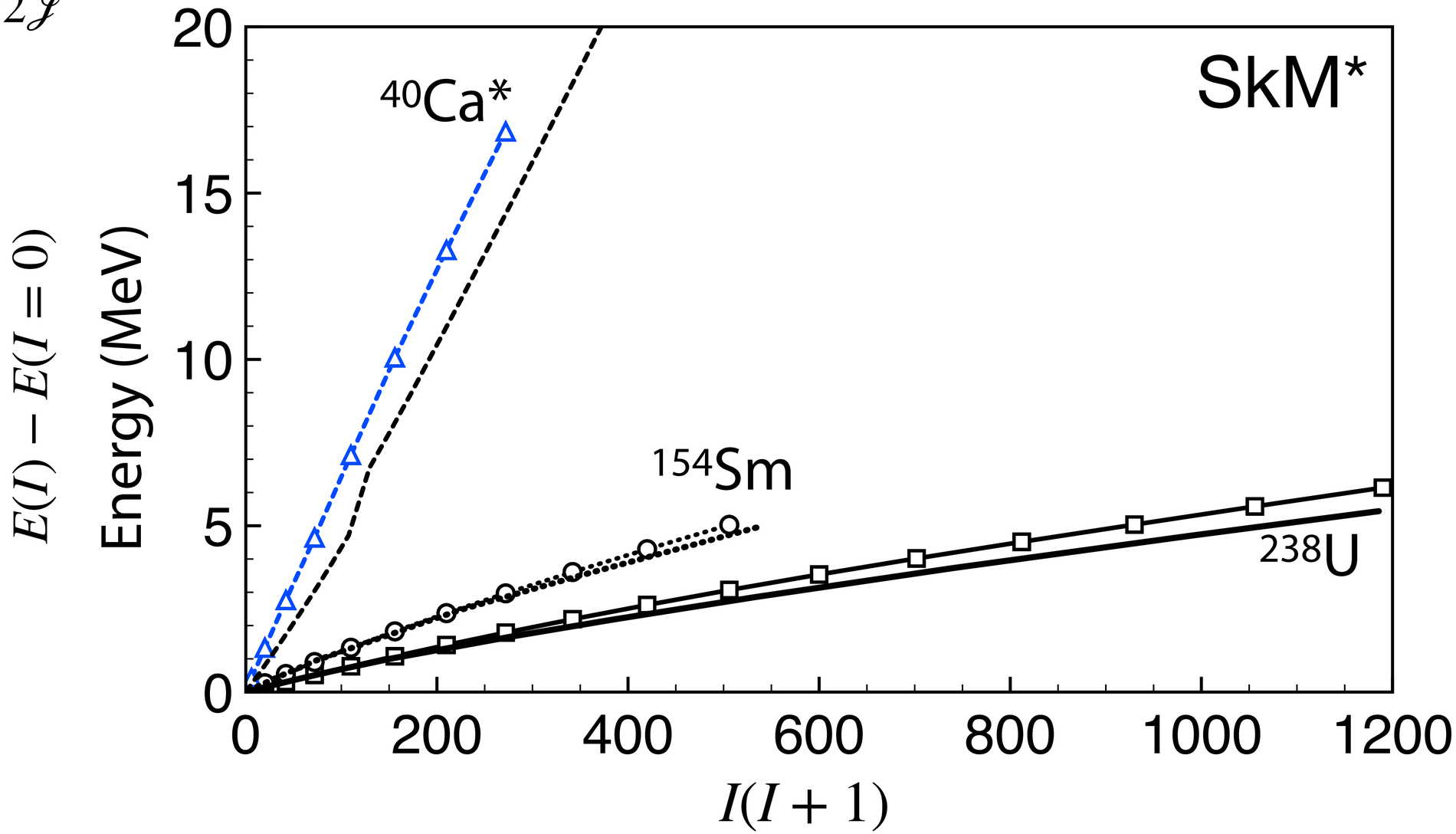
phase convention of BM

$\gamma \rightarrow -\gamma$

Lund convention

DFT for the rotational band

$$E = \frac{I(I+1)}{2\mathcal{J}}$$



Large-scale DFT calculation

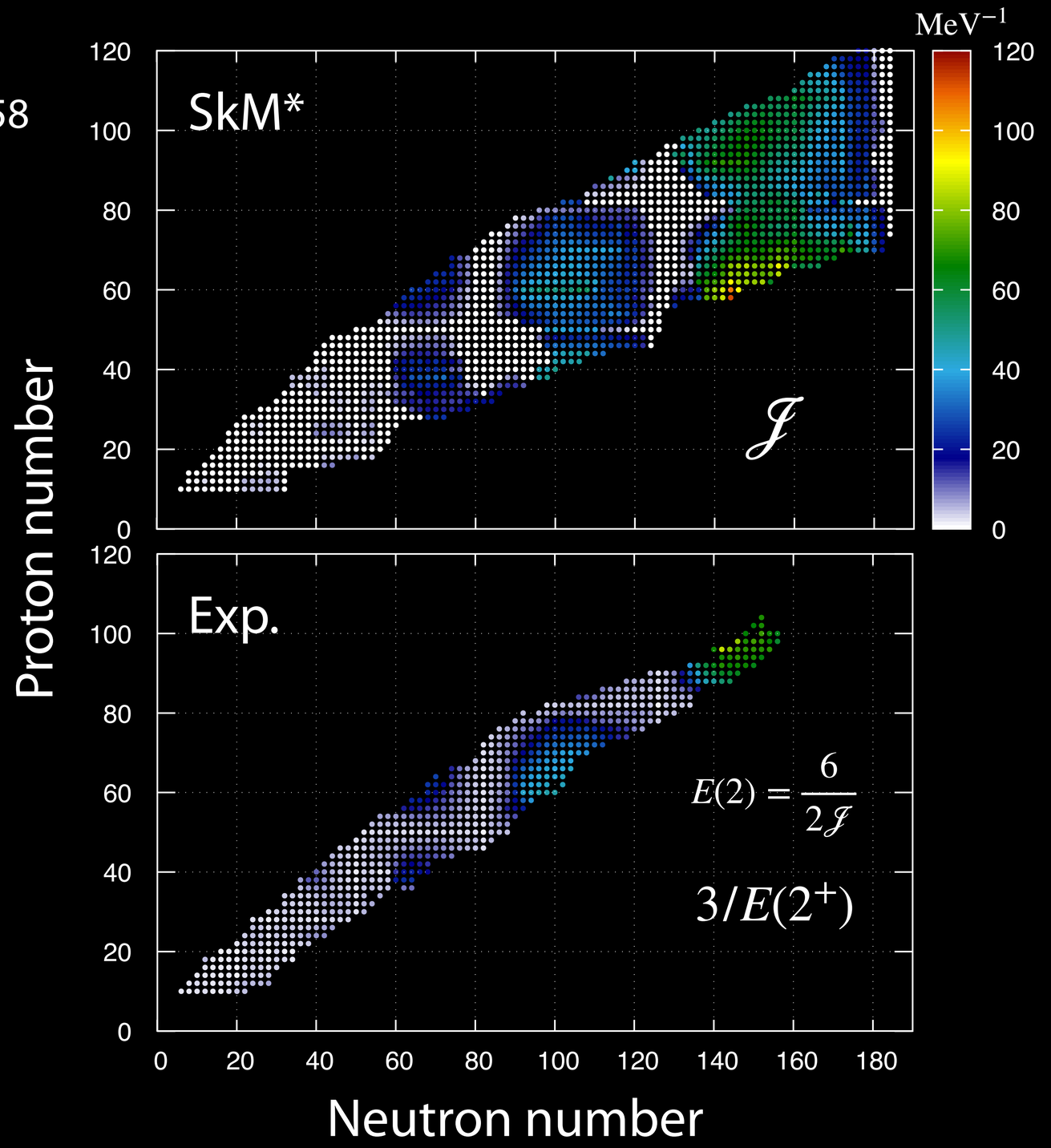
KY, PLB834(2022)137458

low $E(2^+)$ or high $1/E(2^+)$

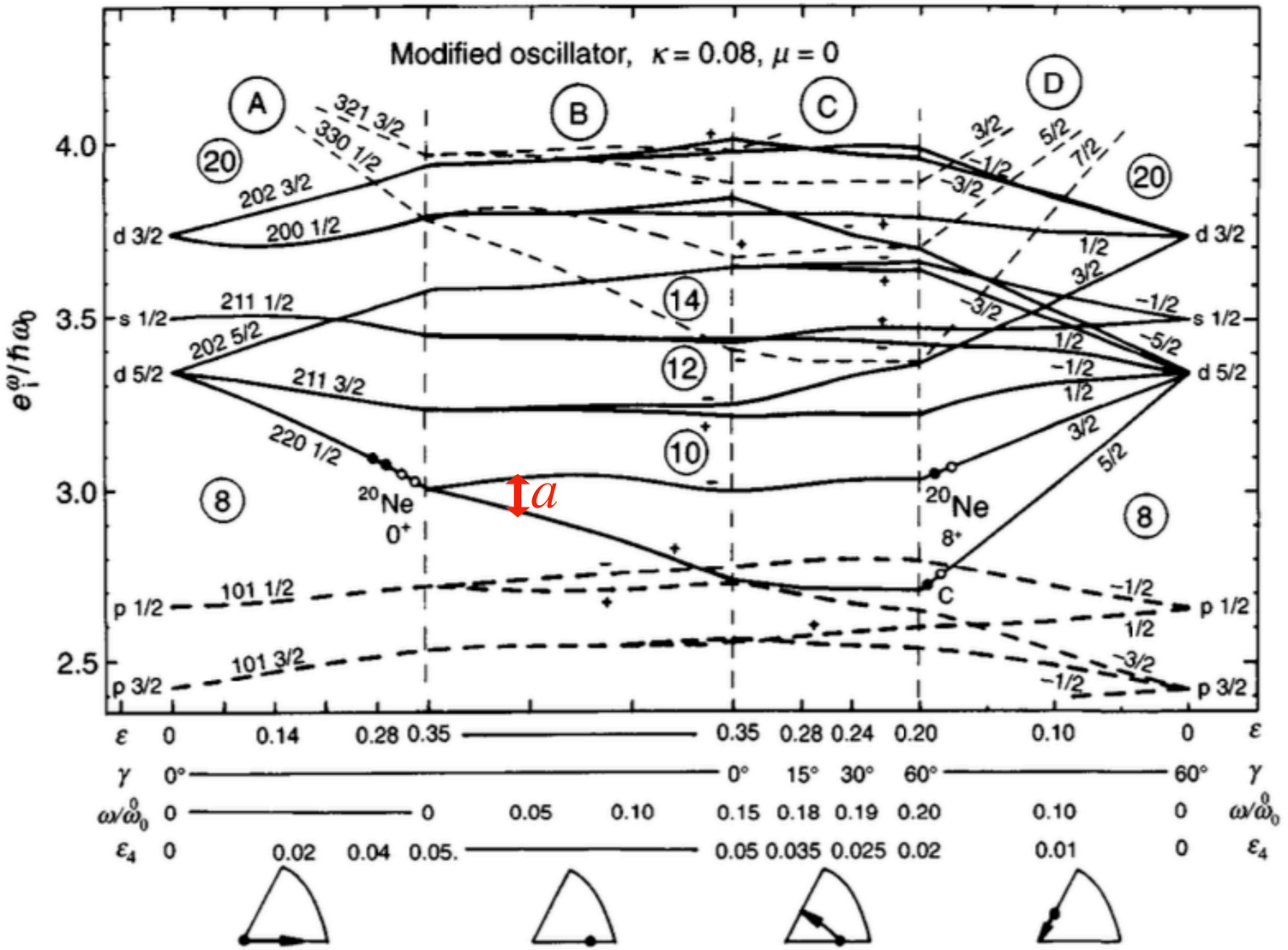
an indicator of quadrupole deformation

a patter of deformation

magic numbers

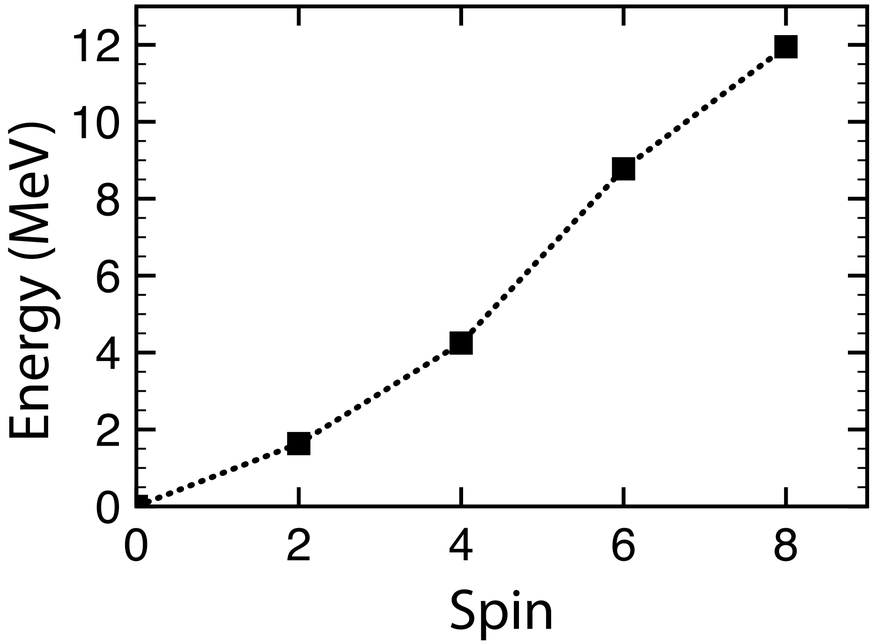


Example (1): the ground band of ^{20}Ne



Nilsson–Ragnarsson: Fig. 12.4

Exp. data for 20Ne (NNDC)



alignments:

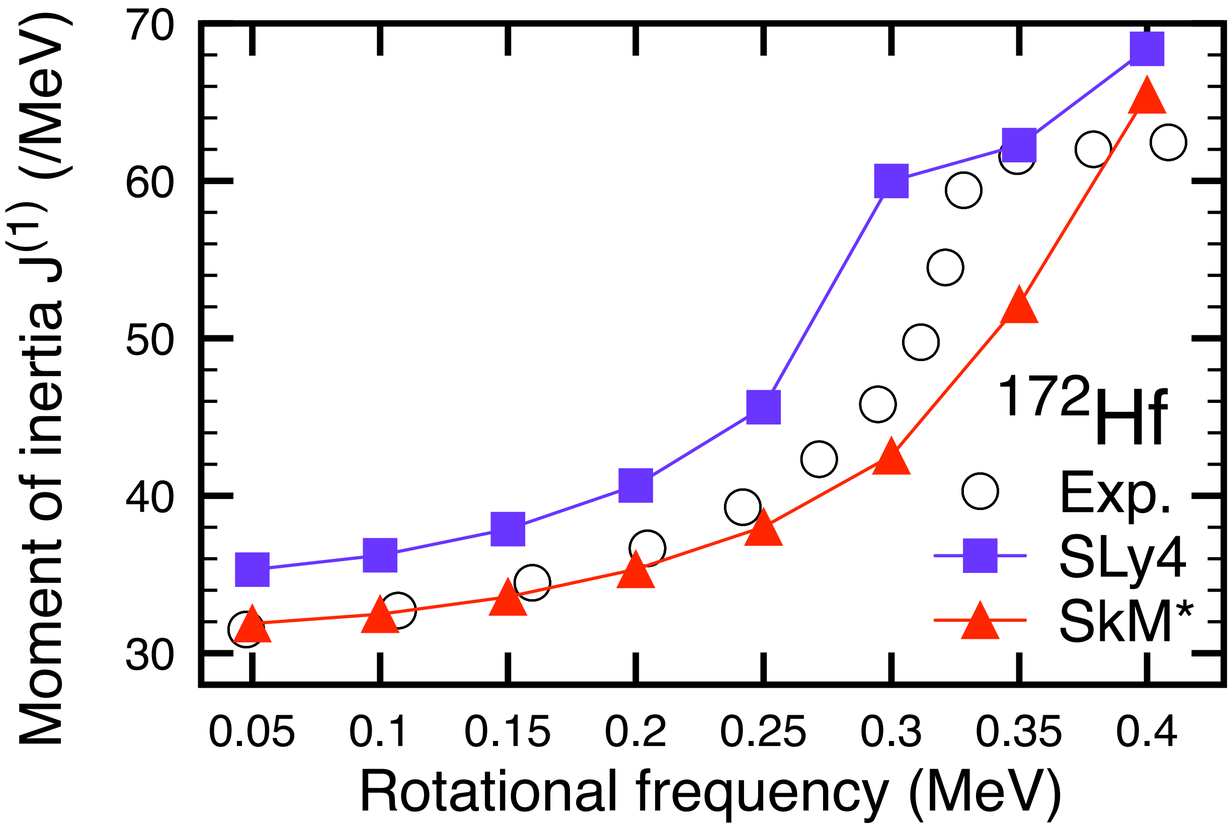
$$\langle \mu | \hat{j}_x | \mu \rangle = -\frac{d\varepsilon'_\mu}{d\omega_{\text{rot}}}$$

$$\rightarrow \pm \frac{1}{2} a$$

$$\omega_{\text{rot}} \rightarrow 0$$

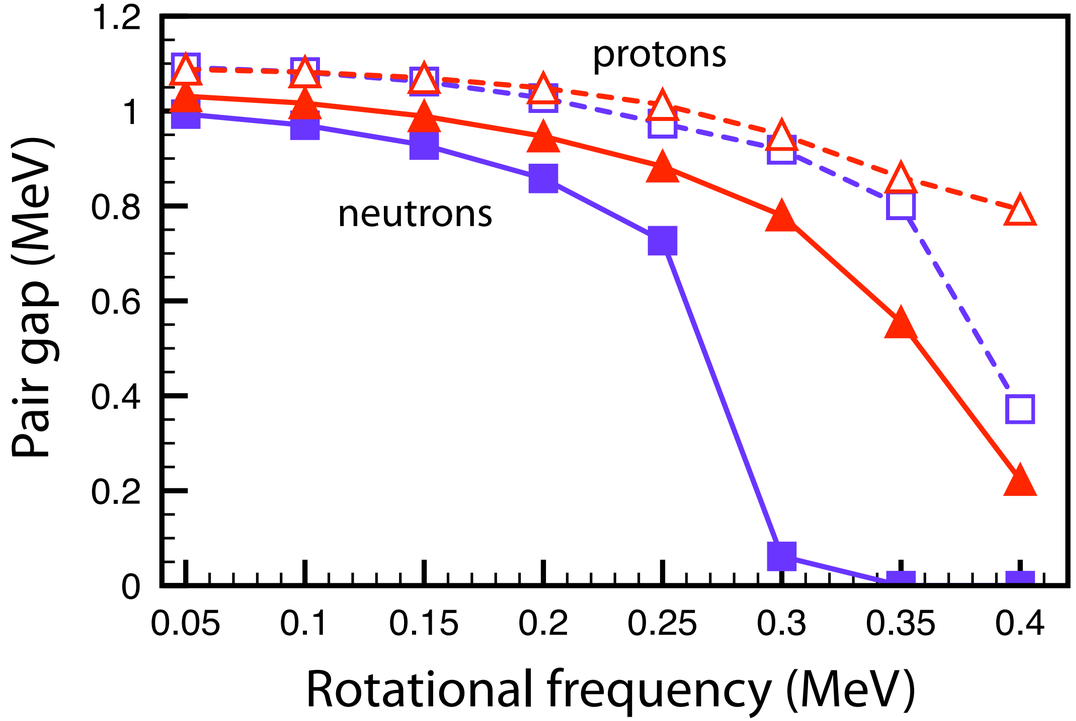
Example (2): the ground band of ^{172}Hf

KY, PRC105(2022)024313



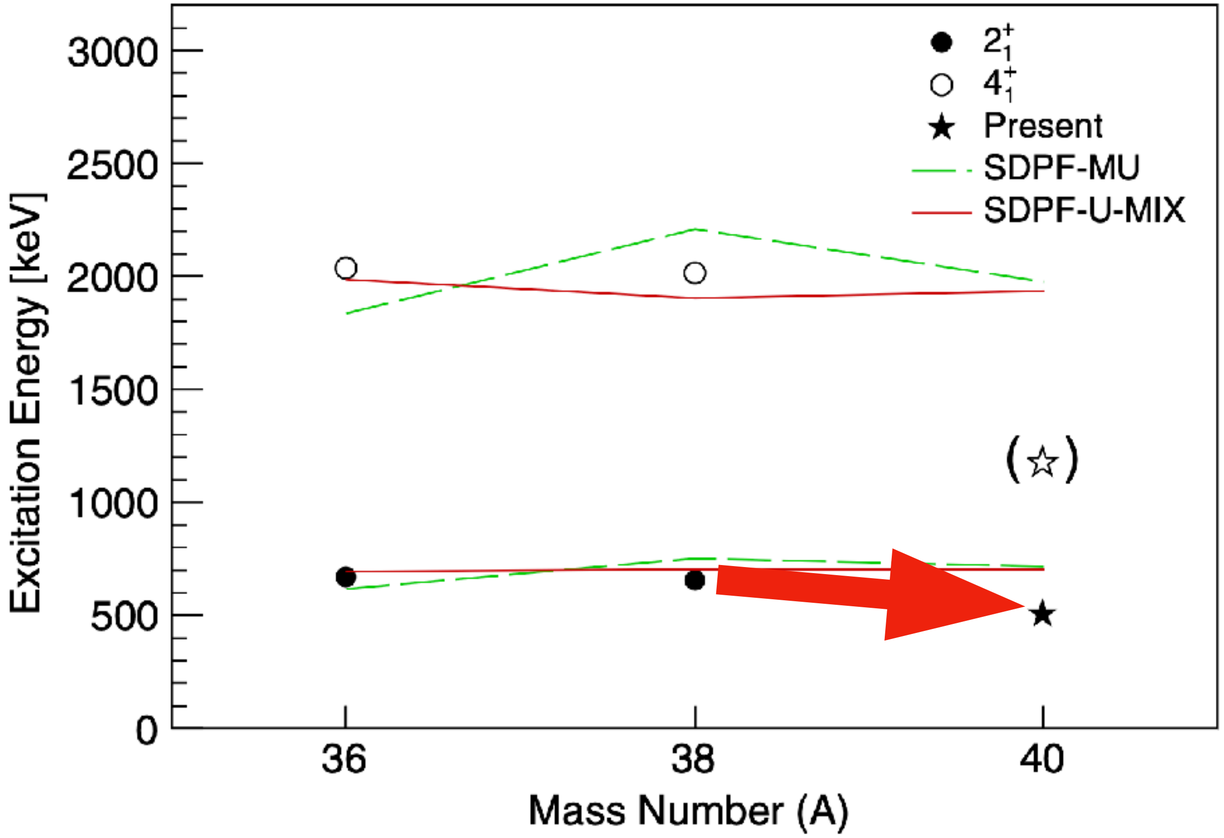
At $\omega_{\rm rot} \sim 0.3\,{\rm MeV}$

breaking of the Cooper pairs

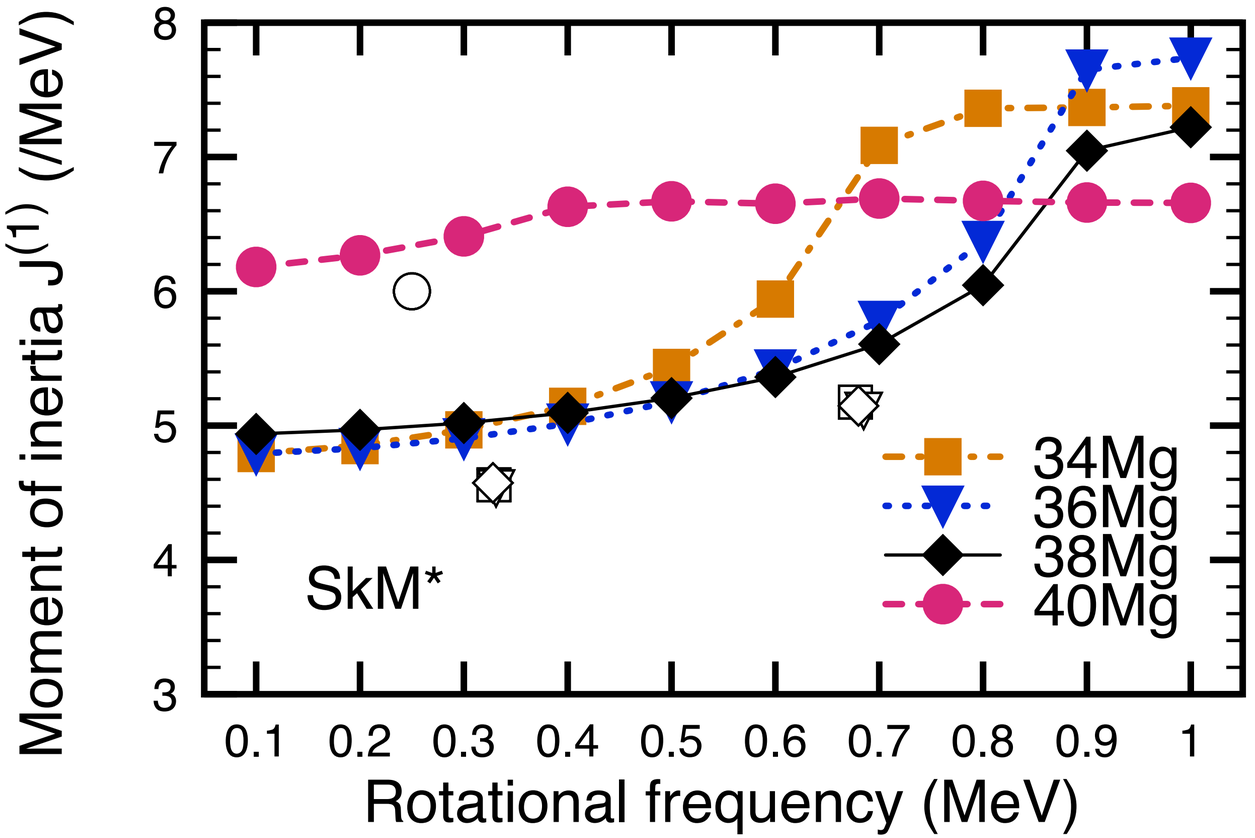


Example (3): neutron-rich Mg isotopes

Crawford+, PRL122(2019)052501



KY, PRC105(2022)024313



635(6) keV →500(14) keV

~20% decrease in energy

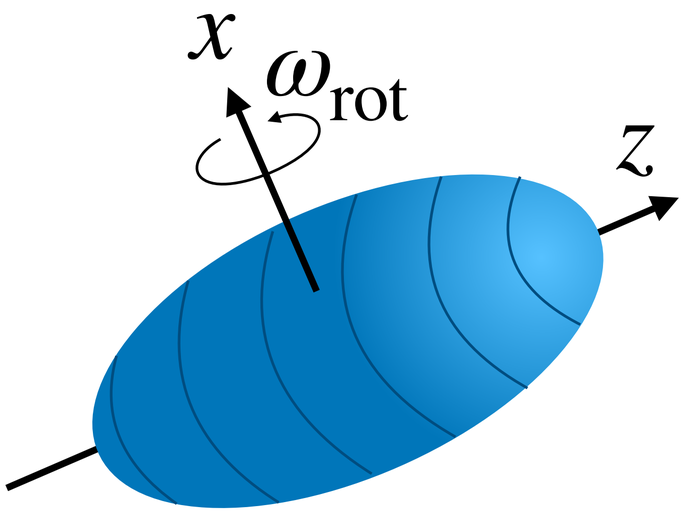
Is it a qualitatively unique feature?

weakening of the pairing

deformed shell gap at N=28

Highly deformed nuclei at high spins

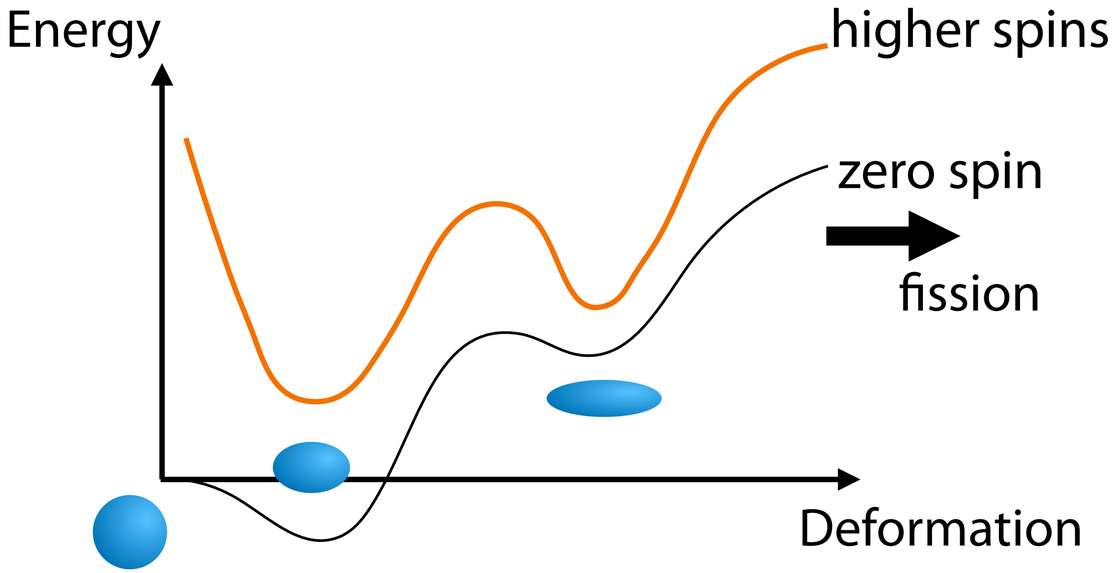
How large can a nucleus be deformed?



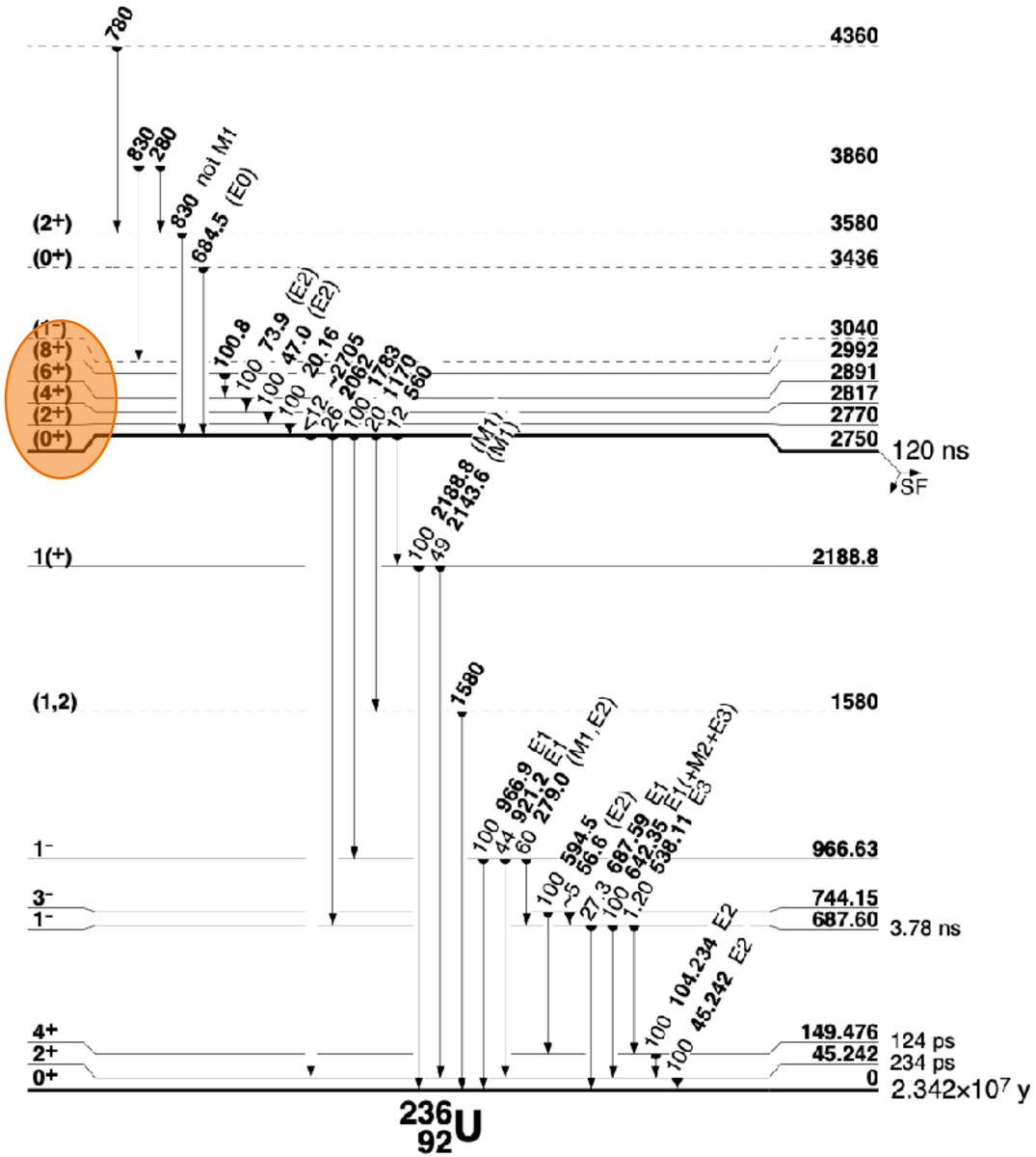
high moment of inertia for a highly-deformed nucleus

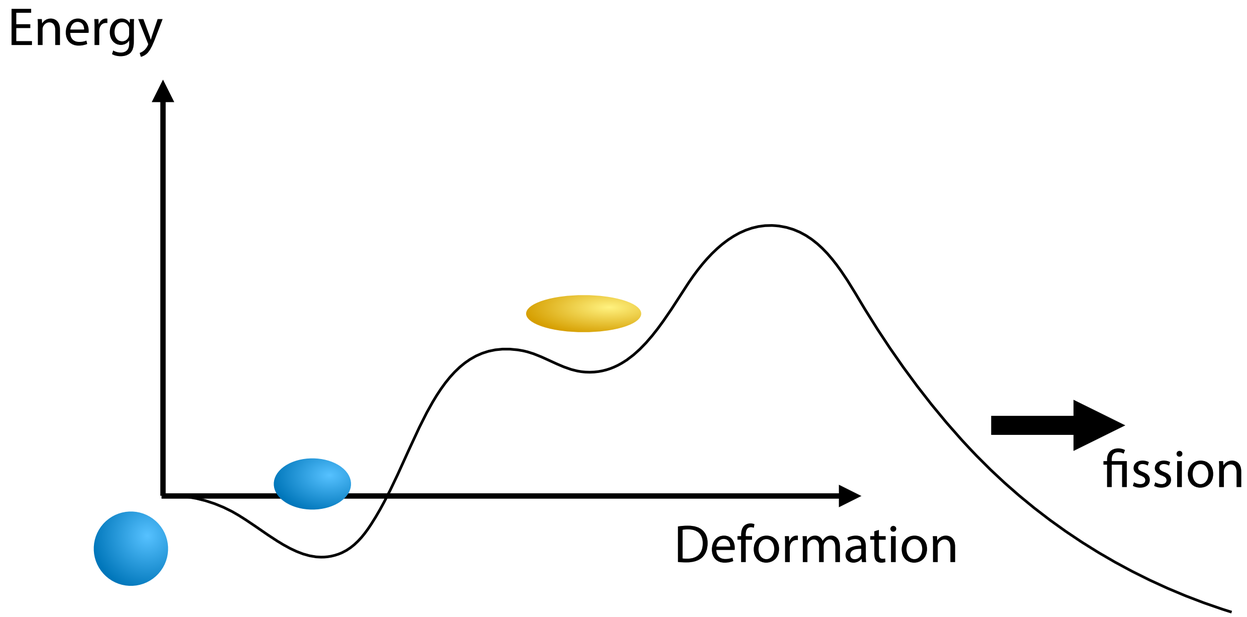
$$E = \frac{I(I+1)}{2\mathcal{J}}$$

high-deformed nuclei are energetically favored at high spins



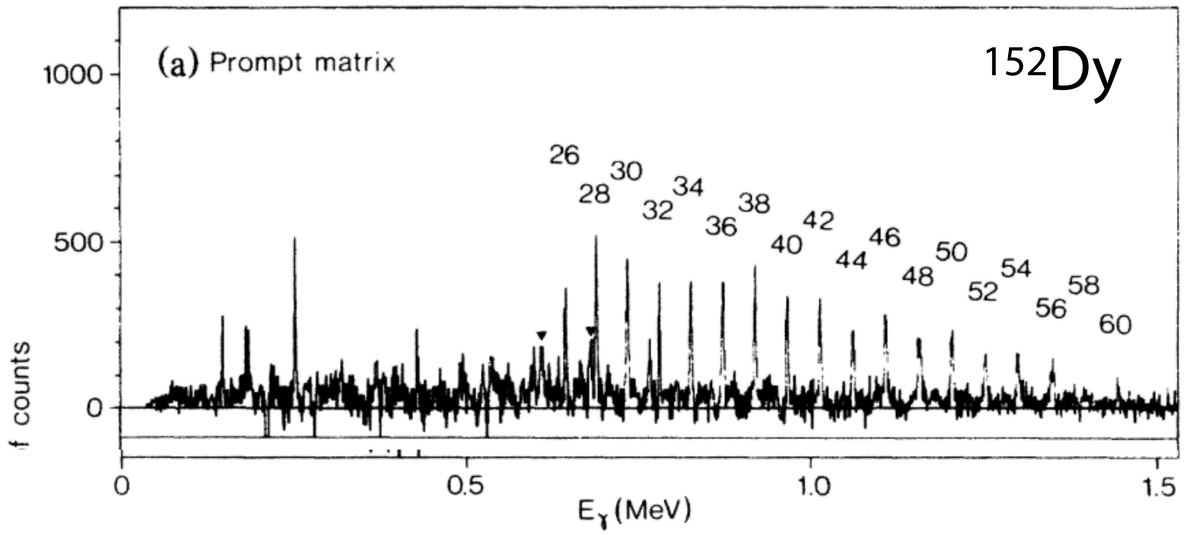
Superdeformed shape as a fission isomer





Superdeformed band

Twin+, PRL57(1986)811



low-energy heavy-ion fusion reaction

$^{108}\mathrm{Pd}(^{48}\mathrm{Ca},4n)^{152}\mathrm{Dy}$

neutron deficient

rotational frequency

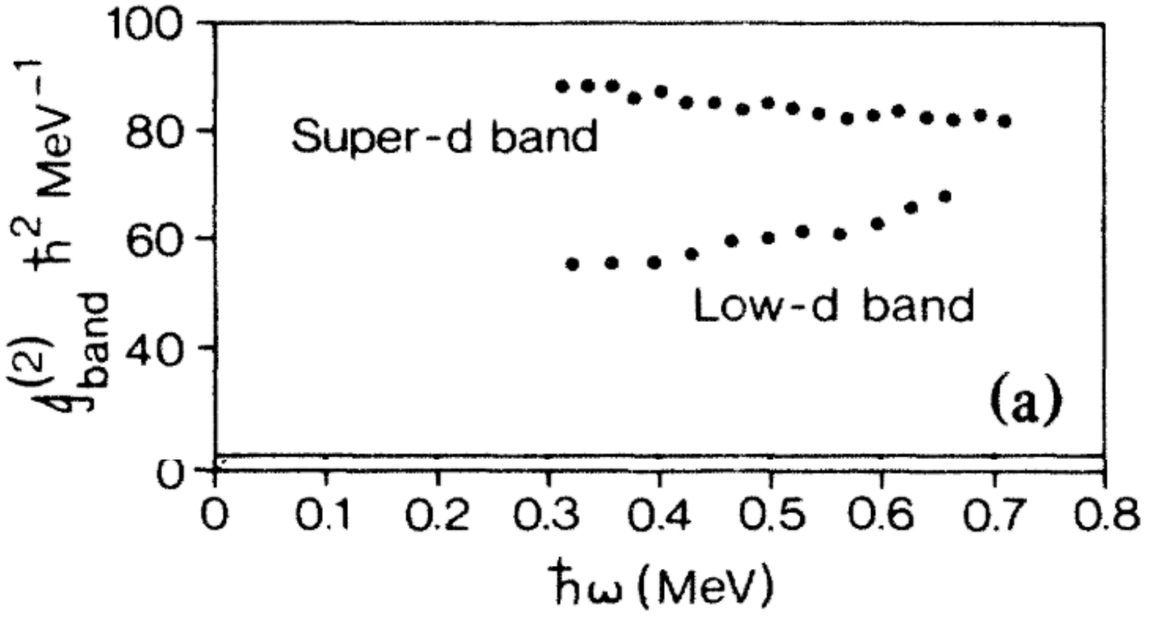
$$\omega_{\mathrm{rot}}(I) = \frac{\partial E}{\partial I}$$

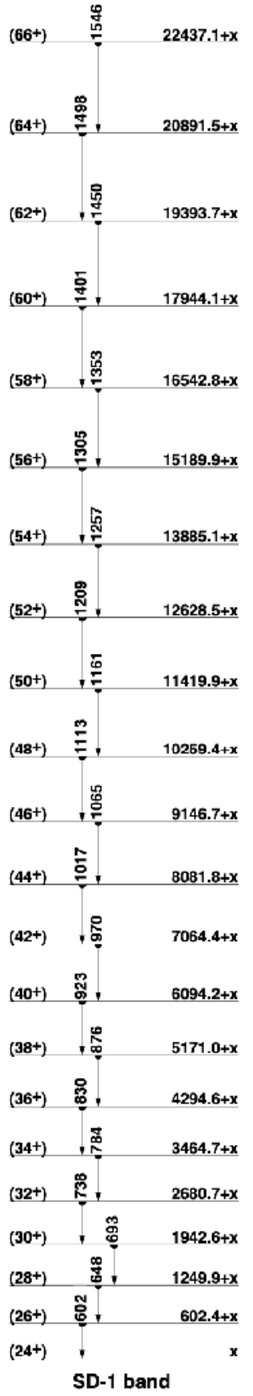
$$\approx \frac{E(I+1) - E(I-1)}{2} = \frac{E_\gamma(I)}{2}$$

moment of inertia

$$\mathcal{J}^{(2)} := \frac{dI}{d\omega_{\mathrm{rot}}} = \left(\frac{d^2E}{dI^2}\right)^{-1} = \frac{4}{\Delta E_\gamma}$$

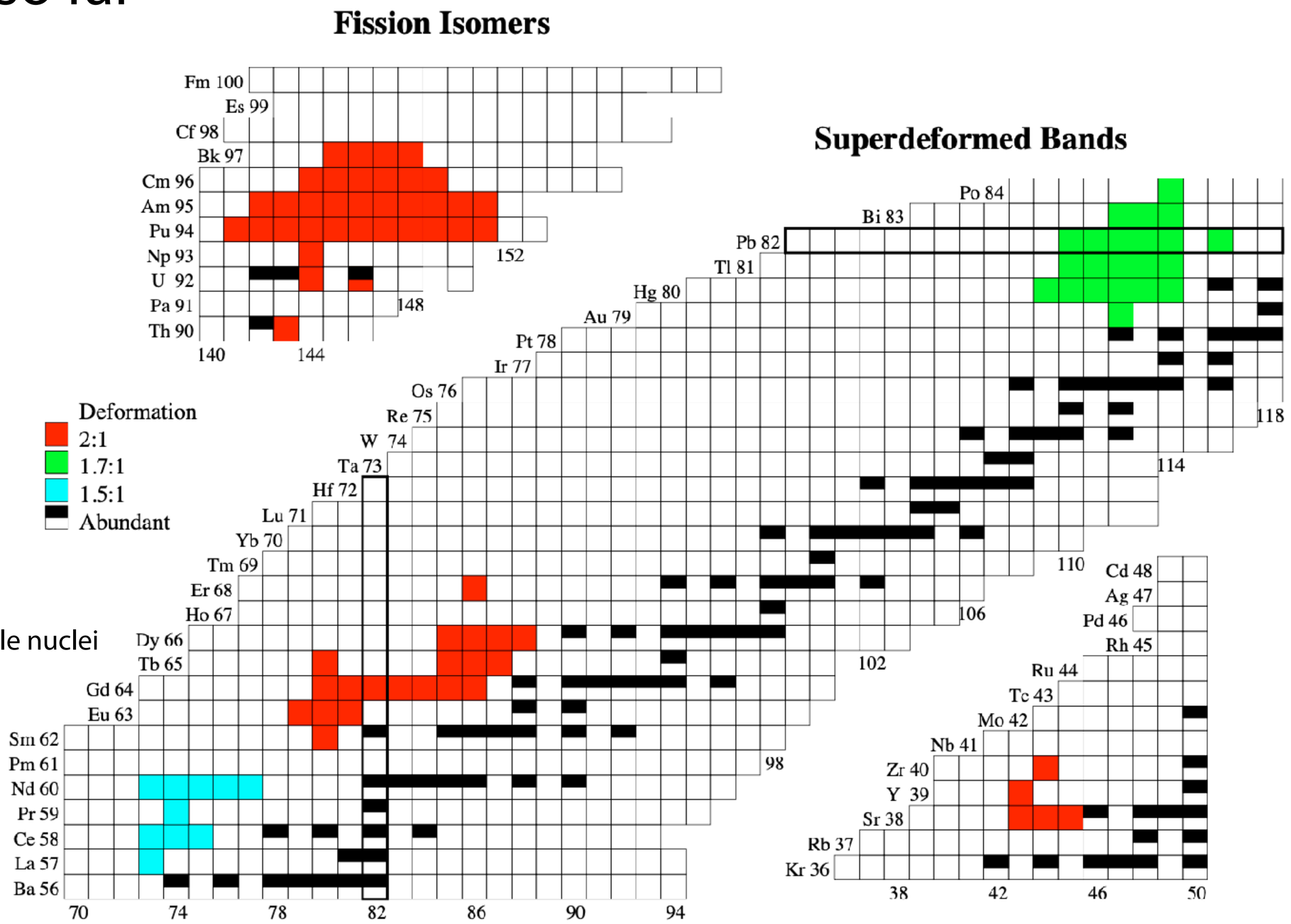
no need of the spin identification





SD discovered so far

Nucl. Data Sheets 78, 1 (1996)

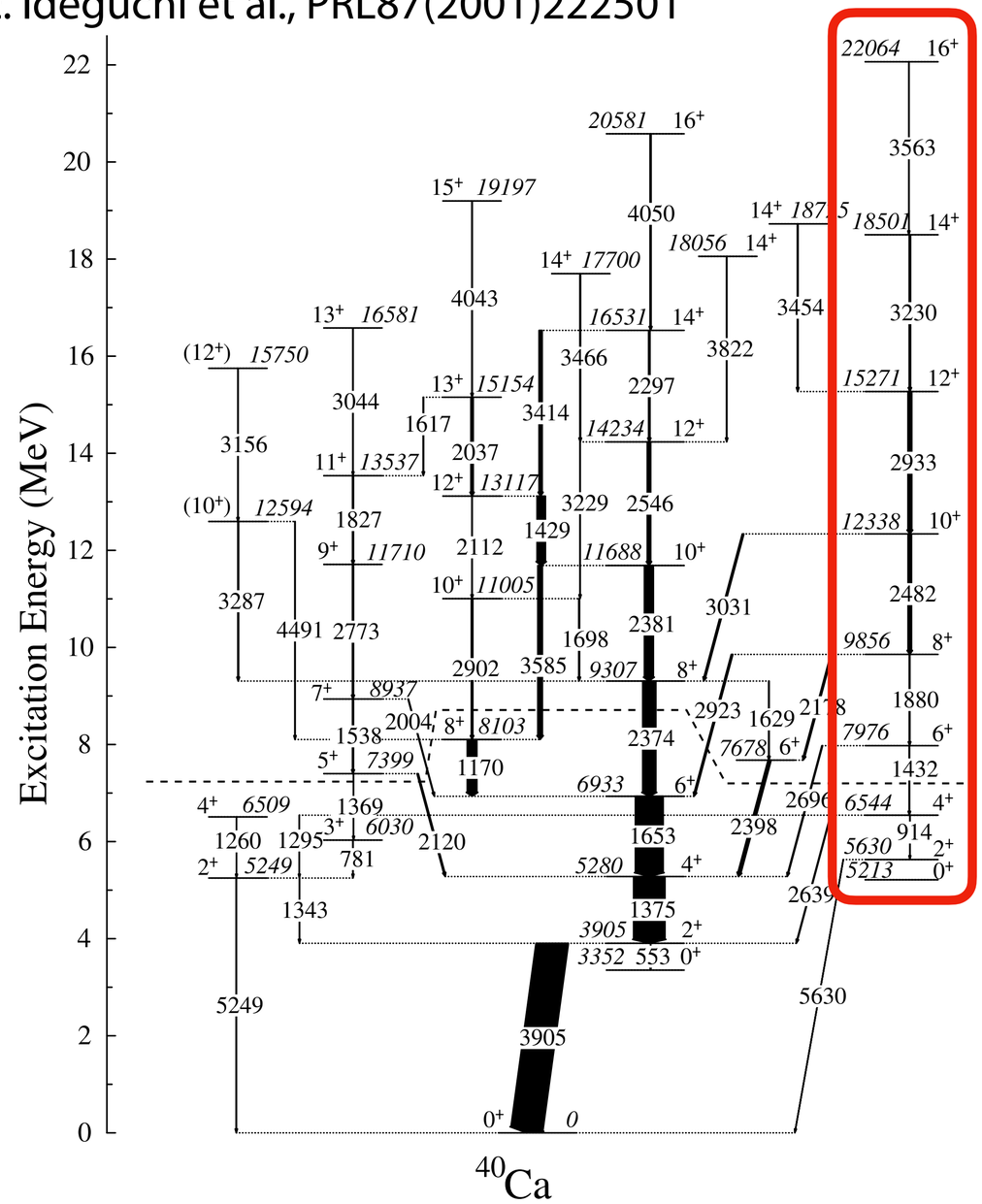


proton rich nuclei

due to the fusion of stable nuclei

SD band in a doubly-magic nucleus: ^{40}Ca

E. Ideguchi et al., PRL87(2001)222501



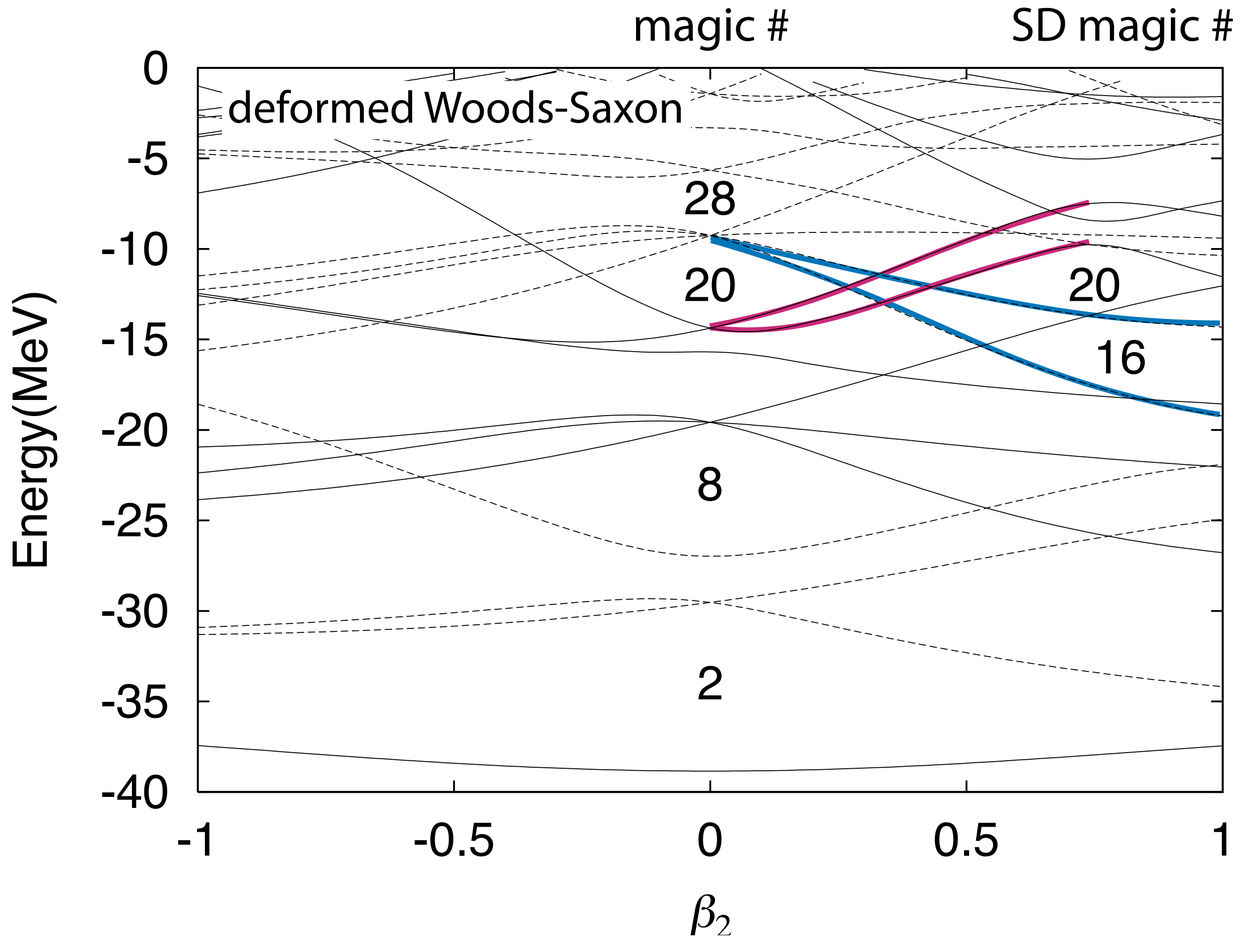
$$\hbar\omega_0 = 41 \times A^{-1/3} \simeq 12\ (\mathrm{MeV})$$

$$E(0_2^+) \sim E(\mathrm{2p2h}) \simeq 2\hbar\omega_0 \simeq 24\ (\mathrm{MeV})$$

$$E(0_{\mathrm{SD}}^+) \sim E(\mathrm{mpmh}) \simeq \mathrm{m}\hbar\omega_0$$

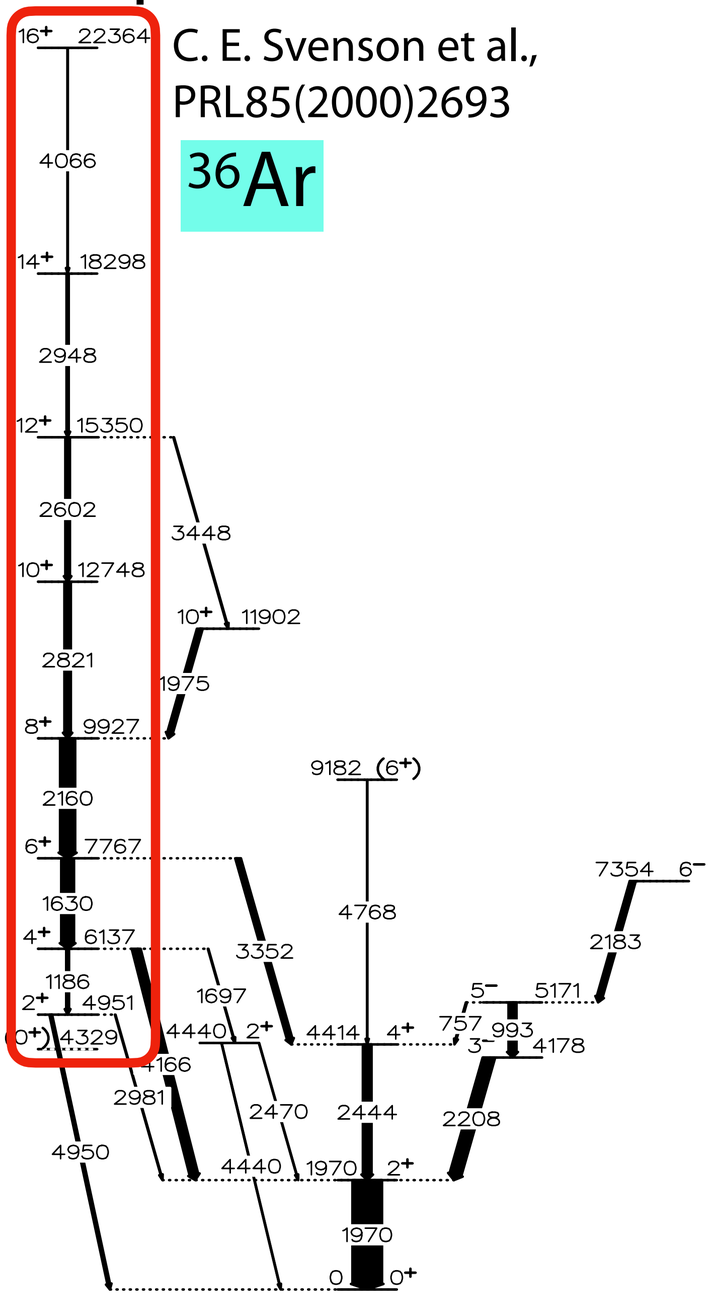
coherent shell effect of protons and neutrons

w/spin-orbit int. $E(\mathrm{8p8h}) \sim 40\ (\mathrm{MeV})$

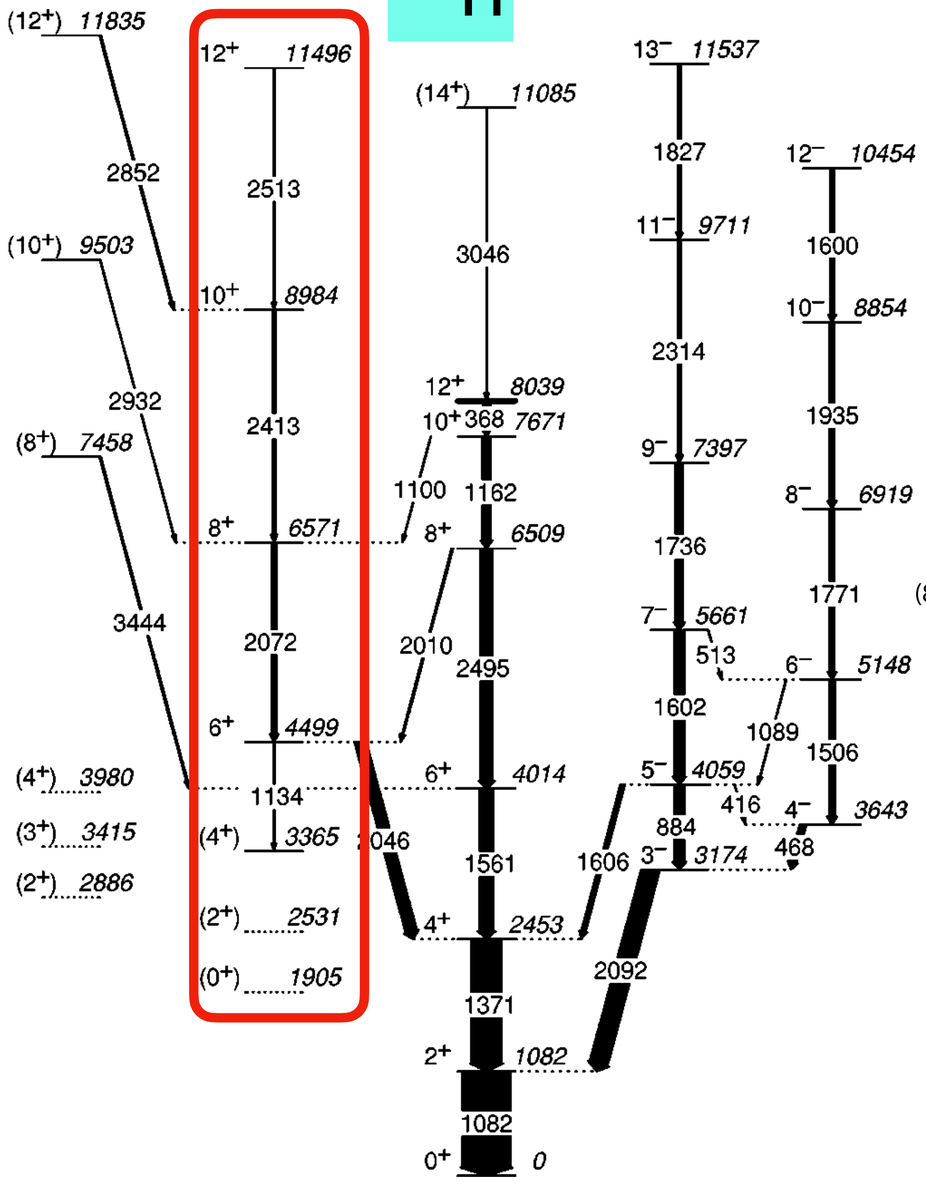


Superdeformation around ^{40}Ca: a new island of SD

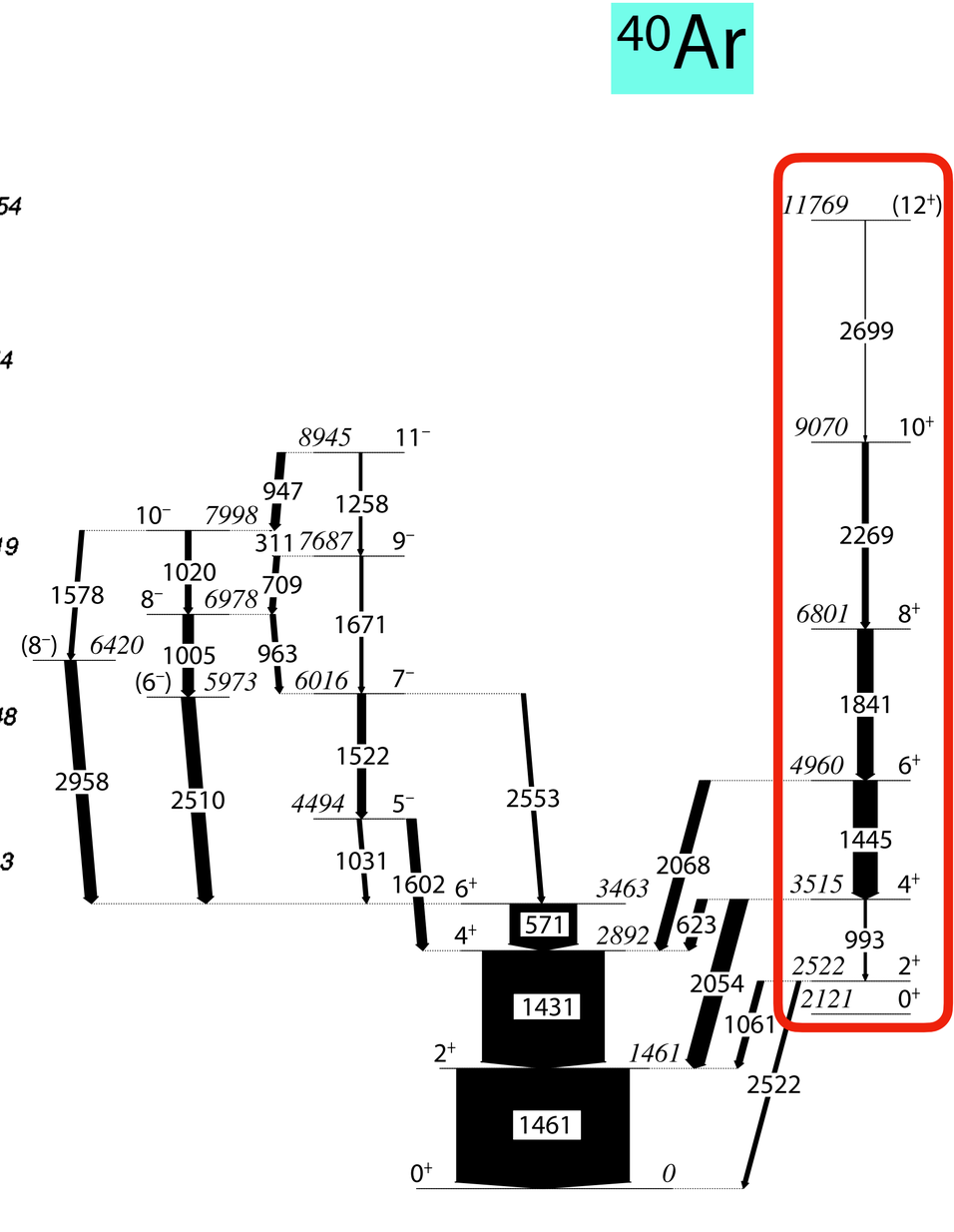
C. E. Svenson et al., PRL85(2000)2693



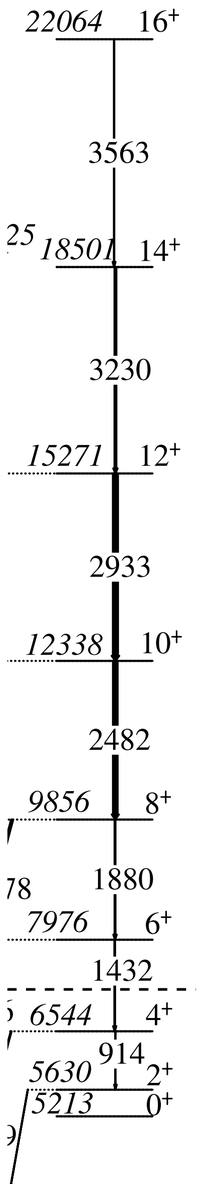
C. D. O'Leary et al., PRC61(2000)064314



E. Ideguchi et al., PLB686(2010)18



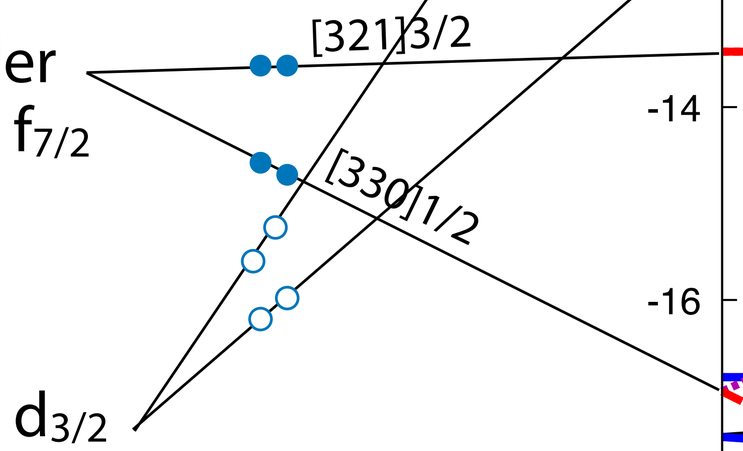
Single-particle Routhians



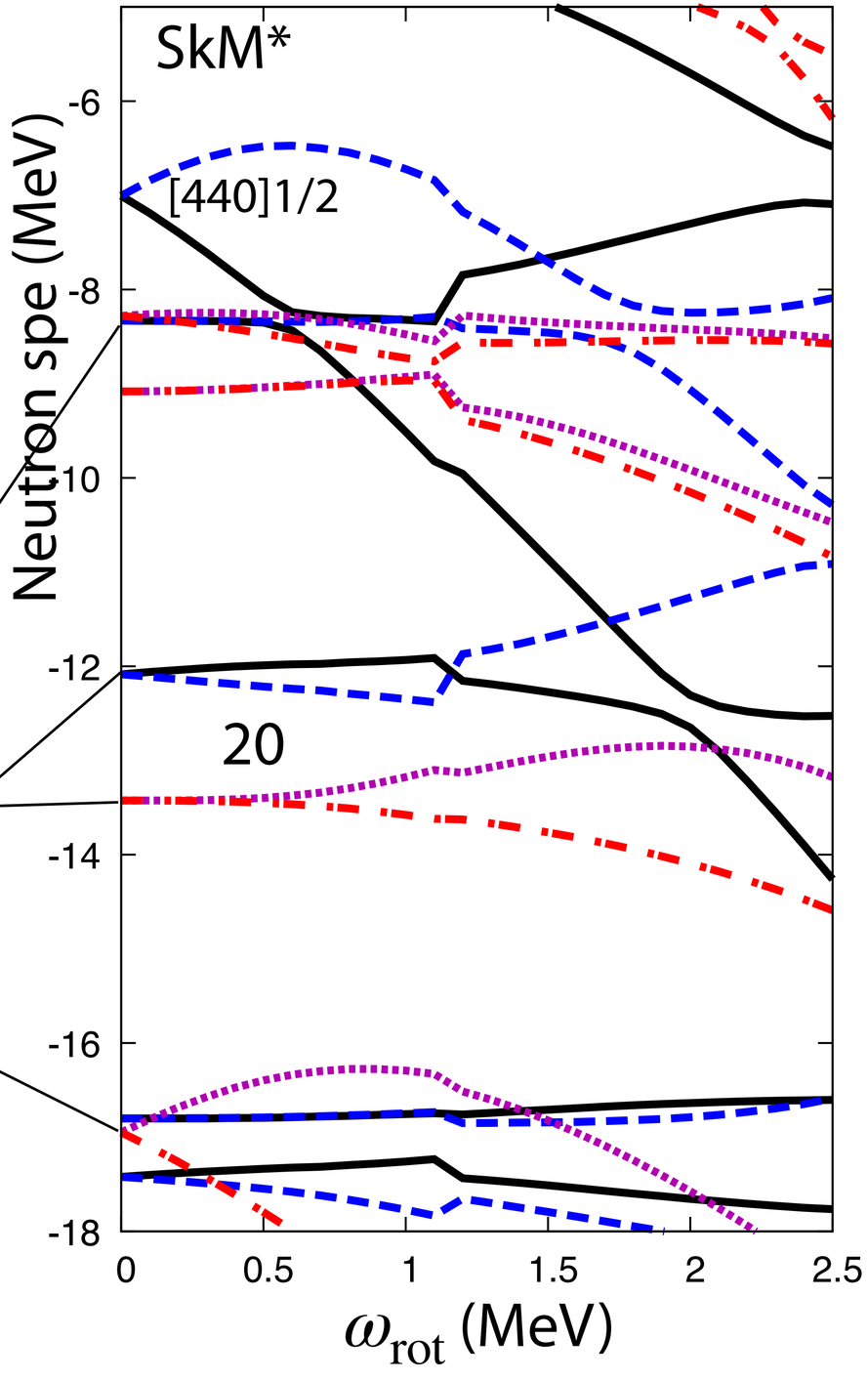
SD band up to $\omega_{\rm rot} \simeq 1.8$ MeV
is observed

SD gap at 20 remains up to
$\omega_{\rm rot} \simeq 2$ MeV

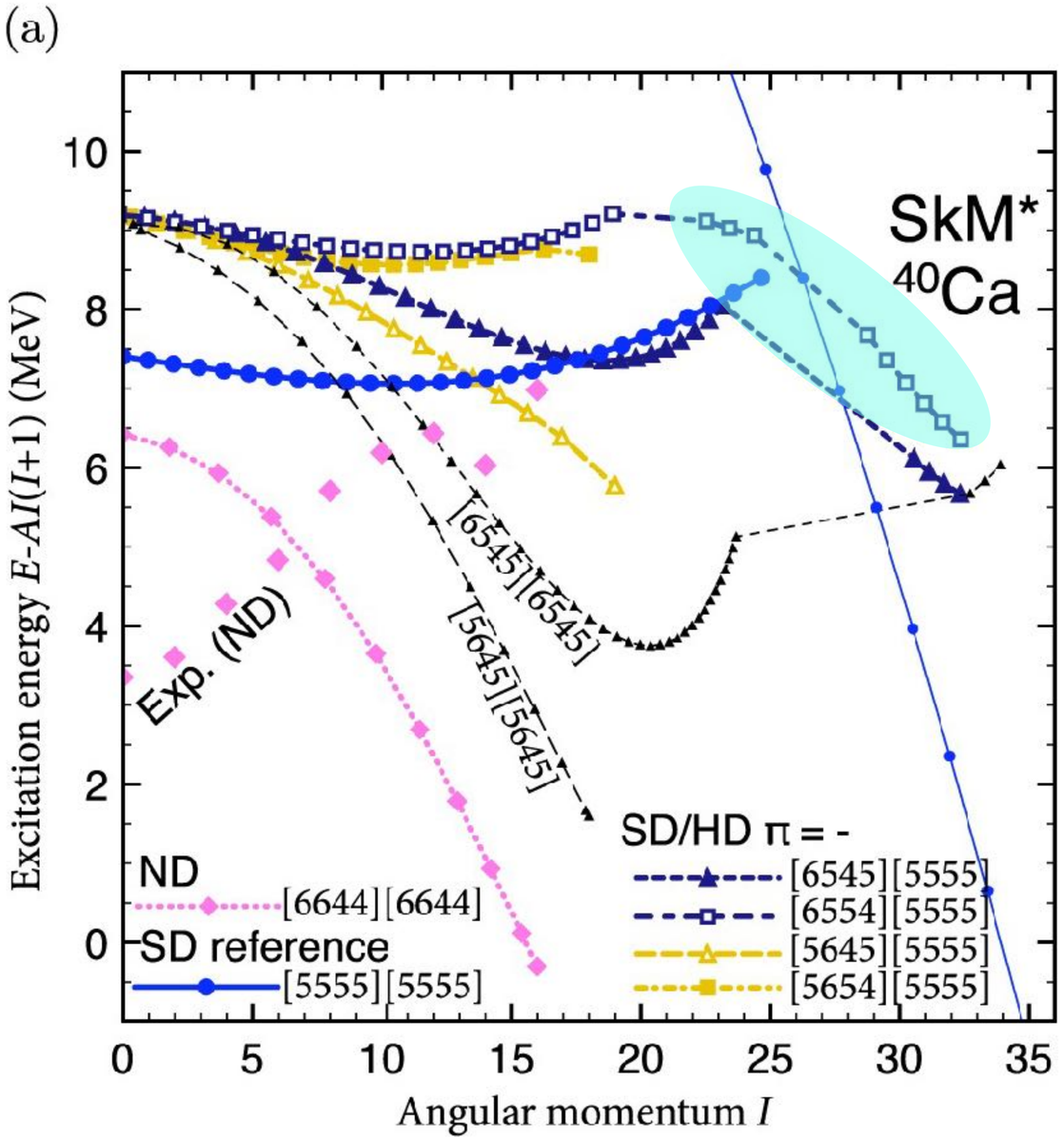
$N = 3$ intruder



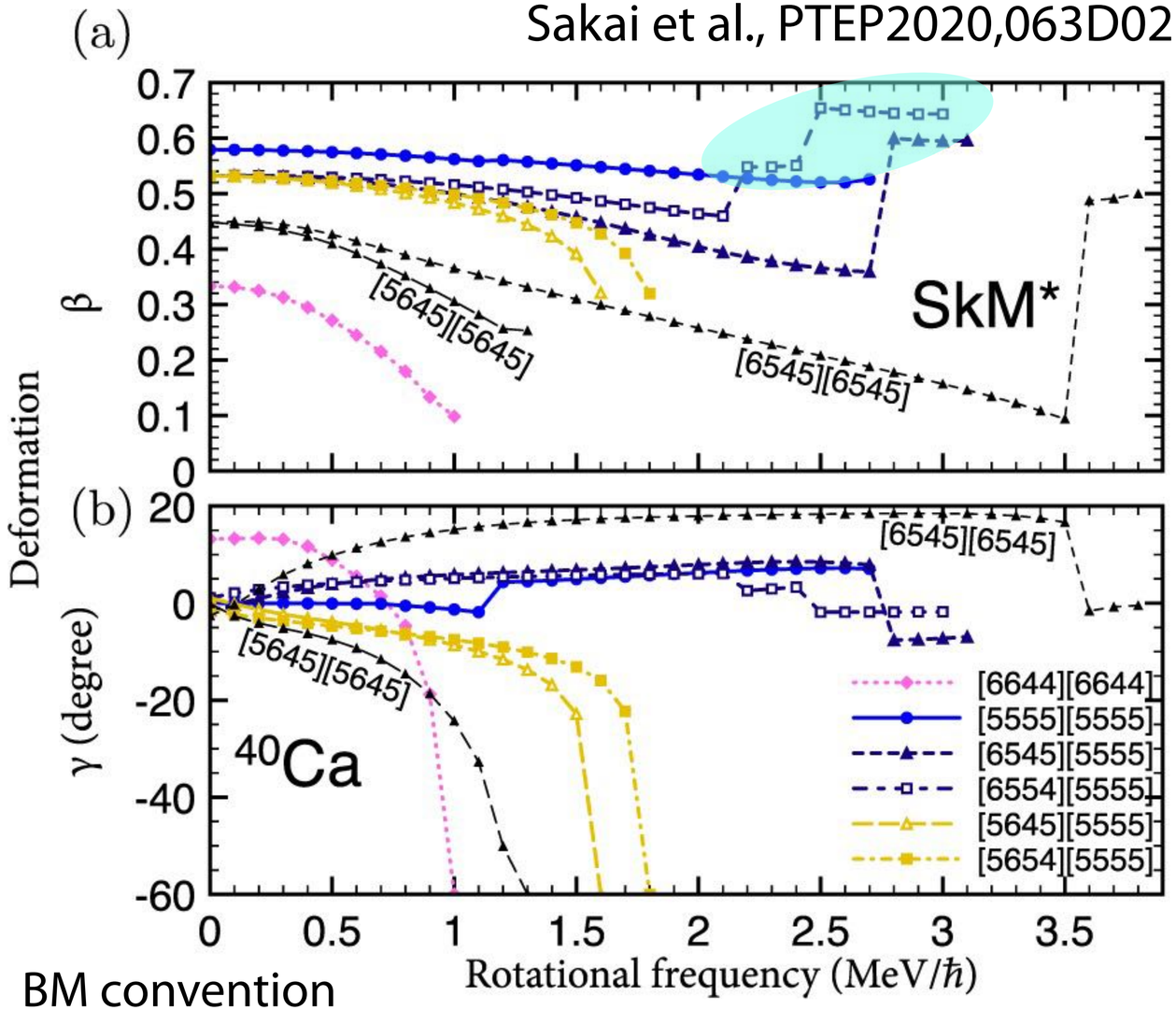
4p4h excitation



What would be expected beyond $I \simeq 20$?



Sakai et al., PTEP2020,063D02

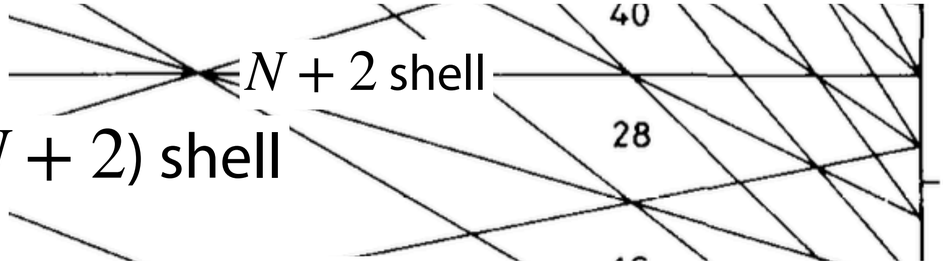


BM convention

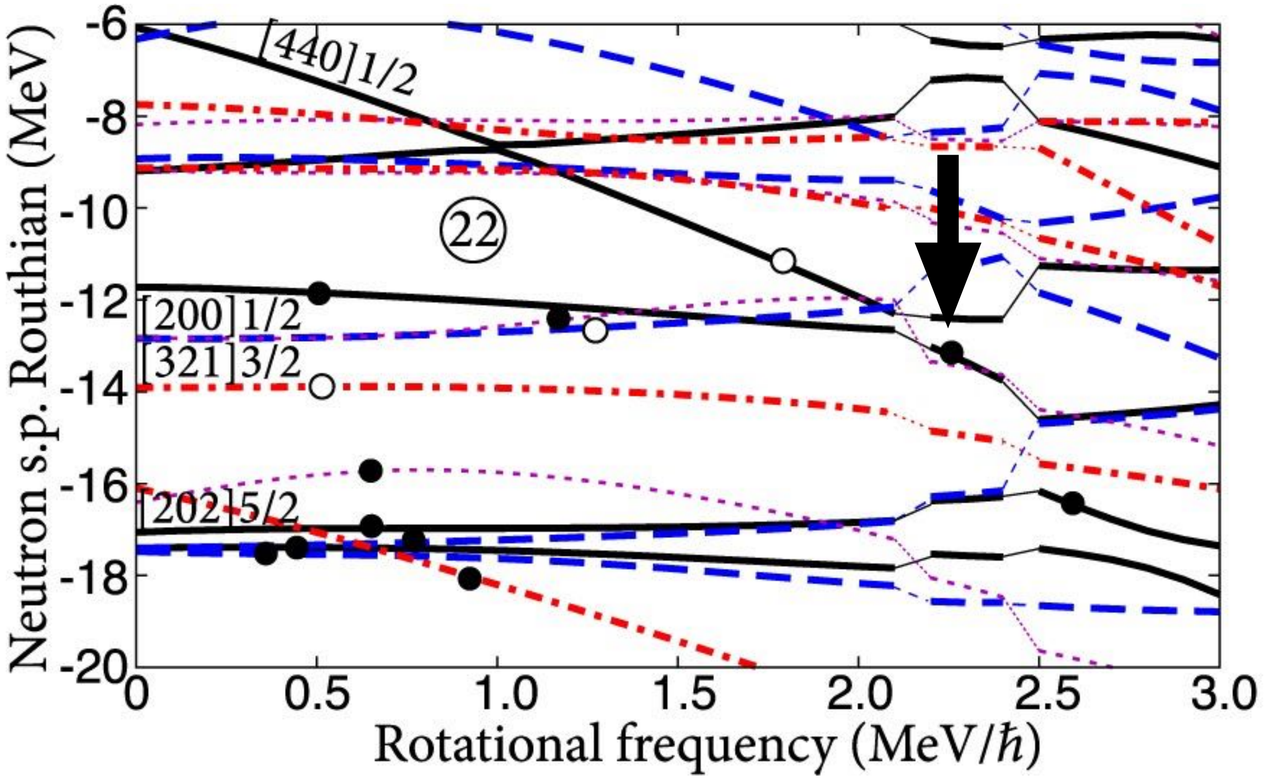
$\gamma = -60°$: band termination

Higher deformation than SD

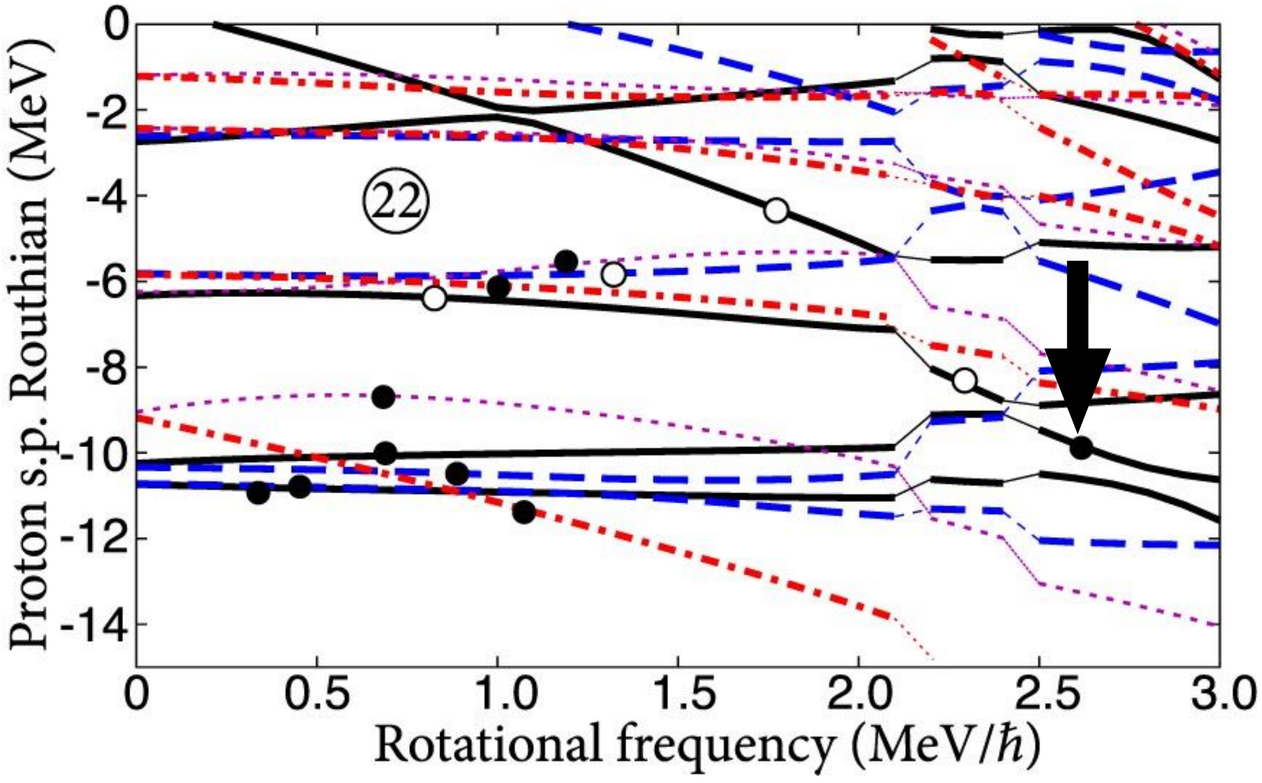
Hyperdef.: neutrons and protons in the hyper-intruder $(N+2)$ shell



a neutron occupies the g shell



a proton occupies the g shell

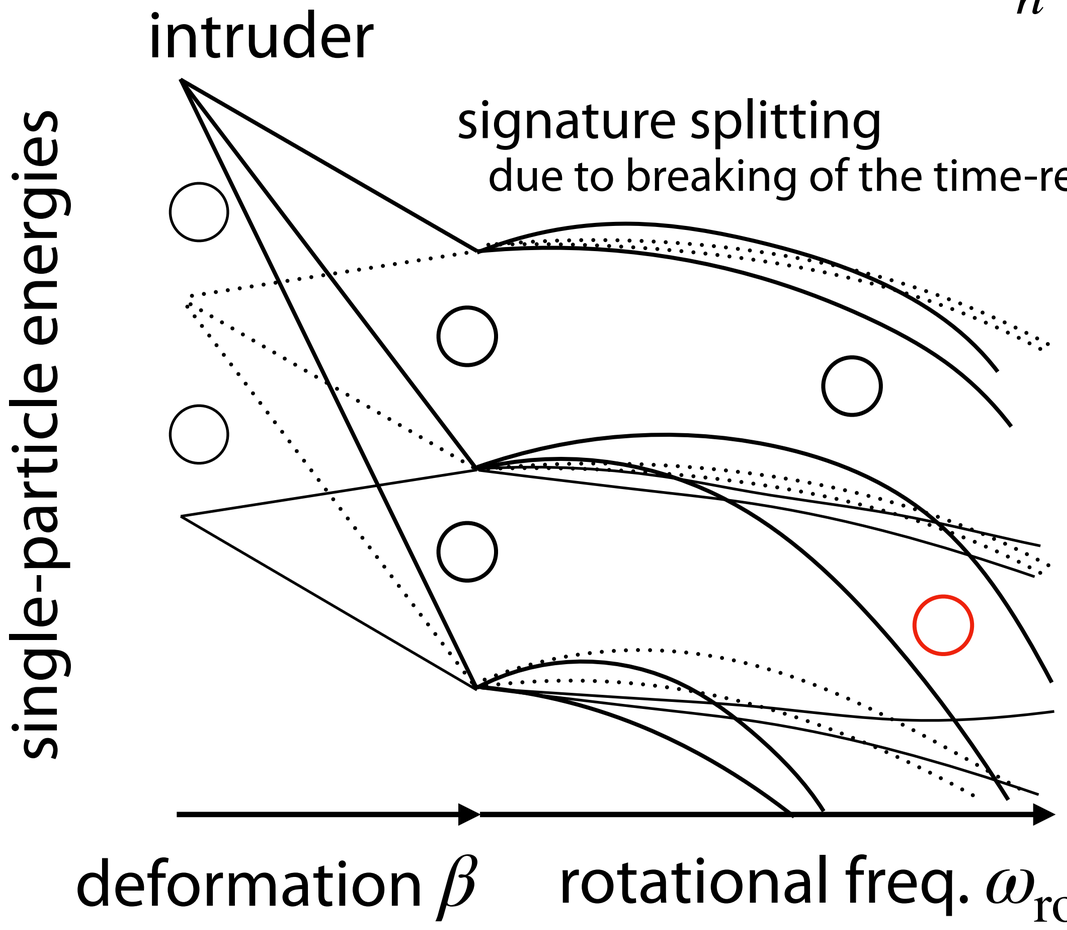


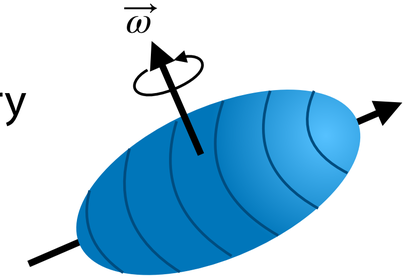
Quasi-hyperdeformation: gateway of HD

Sakai–Yoshida–Matsuo, PTEP(2020)063D02

$$h(\beta)\phi_i(\beta) = \epsilon_i(\beta)\phi_i(\beta) \qquad h'(\beta,\omega_{\rm rot})\phi_i(\beta,\omega_{\rm rot}) = \epsilon_i'(\beta,\omega_{\rm rot})\phi_i(\beta,\omega_{\rm rot})$$

$$h' = h - \omega_{\rm rot} j_x$$





shell gap: rotating-deformed magic number

involving one-more nucleon in the intruder shell

higher-deformation than SD

appearing at non-zero spins

Density-functional theory and nuclear energy-density functional method

Density Functional Theory (DFT)

developed in quantum chemistry

$$H = -\frac{\hbar^2}{2m}\int dx\psi^\dagger(x)\nabla^2\psi(x) + \int dx\psi^\dagger(x)v_{\text{ext}}(r)\psi(x) + \frac{1}{2}\int dxdx'\psi^\dagger(x)\psi^\dagger(x')w(r,r')\psi(x')\psi(x) = T + V_{\text{ext}} + W$$

Hohenberg–Kohn theorem(1964)

The exact ground-state energy of a many-body system can be obtained by variationally minimizing an energy density functional (EDF). Moreover, there exists such a functional (existence theorem).

PHYSICAL REVIEW VOLUME 136, NUMBER 3B 9 NOVEMEBR 1964

1998

W. Kohn

Inhomogeneous Electron Gas*

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(Received 18 June 1964)

This paper deals with the ground state of an interacting electron gas in an external potential $v(\mathbf{r})$. It is proved that there exists a universal functional of the density, $F[n(\mathbf{r})]$, independent of $v(\mathbf{r})$, such that the expression $E\equiv\int v(\mathbf{r})n(\mathbf{r})d\mathbf{r}+F[n(\mathbf{r})]$ has as its minimum value the correct ground-state energy associated with $v(\mathbf{r})$. The functional $F[n(\mathbf{r})]$ is then discussed for two situations: (1) $n(\mathbf{r})=n_0+\tilde{n}(\mathbf{r})$, $\tilde{n}/n_0<<1$, and (2) $n(\mathbf{r})=\varphi(\mathbf{r}/r_0)$ with φ arbitrary and $r_0\to\infty$. In both cases F can be expressed entirely in terms of the correlation energy and linear and higher order electronic polarizabilities of a uniform electron gas. This approach also sheds some light on generalized Thomas-Fermi methods and their limitations. Some new extensions of these methods are presented.

In quantum mechanics, variation of $\delta E[\Psi] = 0$

energy functional (functional of WF) $E[\Psi] = \langle \Psi | H | \Psi \rangle$

with the normalization condition

$$\langle \Psi | \int dx \psi^\dagger(x) \psi(x) | \Psi \rangle = N$$

$$E[\Psi] \geq E_0 = E[\Psi_0]$$

$$v_{\mathrm{ext}}(r) \overset{A}{\mapsto} |\Psi_0\rangle \overset{B}{\mapsto} \rho_0(r) \qquad \rho_0(r) = \langle \Psi_0 | \psi^\dagger(r) \psi(r) | \Psi_0 \rangle$$

In DFT, 1. inverse mapping： $\rho_0(r) \mapsto |\Psi_0\rangle \mapsto v_{\mathrm{ext}}(r)$

2. density variation principle

Hohenberg–Kohn theorem (1964)

under the assumptions

1.The ground state is not degenerate.

2.For any given density, there exists at least one external potential for which that density is the ground-state density: *v*-representability

The theorem was generalized to the degenerate system (W. Kohn, 1985).

A counterexample to Assumption 2 has been found.

Theorem I: mapping $v_{\mathrm{ext}}(r) \mapsto |\Psi_0\rangle \mapsto \rho_0(r)$ is one-to-one corresponding.

① : $v_{\mathrm{ext}}(r) \Longleftrightarrow |\Psi_0\rangle$

- By Assumption 2 , the mapping is surjective.
- Injectivity is proved by contradiction:

  Suppose that external potentials $v_{\mathrm{ext}}(r), v'_{\mathrm{ext}}(r)$ differing by more than a constant give rise to an identical wave function $|\Psi_0\rangle$.

$$H|\Psi_0\rangle = [T + V_{\mathrm{ext}} + W]|\Psi_0\rangle = E_0|\Psi_0\rangle$$
$$H'|\Psi_0\rangle = [T + V'_{\mathrm{ext}} + W]|\Psi_0\rangle = E'_0|\Psi_0\rangle$$

$$[V_{\mathrm{ext}} - V'_{\mathrm{ext}}]|\Psi_0\rangle = [E_0 - E'_0]|\Psi_0\rangle$$

dividing both sides by $\langle r_1\sigma_1, \cdots, r_N\sigma_N|\Psi_0\rangle = \Psi_0(r_1\sigma_1, \cdots, r_N\sigma_N)$

At all points where the wave function $\Psi_0(r_1\sigma_1, \cdots, r_N\sigma_N)$ does not vanish,

$$\sum_{i=1}^{N}[v_{\mathrm{ext}}(r_i) - v'_{\mathrm{ext}}(r_i)] = \underbrace{E_0 - E'_0}_{\text{constant}}$$

→ contradict the assumption that $v_{\mathrm{ext}}(r), v'_{\mathrm{ext}}(r)$ is different by more than a constant

② : $|\Psi_0\rangle \Longleftrightarrow \rho_0(r)$

Suppose that two wave functions, $|\Psi_0\rangle, |\Psi_0'\rangle$ differing by more than a global phase, give rise to the same density distribution $\rho_0(r)$.

variational principle:

$$E_0 = \langle\Psi_0|H|\Psi_0\rangle < \langle\Psi_0'|H|\Psi_0'\rangle$$

$$\begin{aligned} E_0 &< \langle\Psi_0'|H' + H - H'|\Psi_0'\rangle \\ &= E_0' + \langle\Psi_0'|V_{\text{ext}} - V_{\text{ext}}'|\Psi_0'\rangle \\ &= E_0' + \int dr \rho_0(r)[v_{\text{ext}}(r) - v_{\text{ext}}'(r)] \end{aligned}$$

similarly,

$$\begin{aligned} E_0' &< \langle\Psi_0|H + H' - H|\Psi_0\rangle \\ &= E_0 + \langle\Psi_0|V_{\text{ext}}' - V_{\text{ext}}|\Psi_0\rangle \\ &= E_0 + \int dr \rho_0(r)[v_{\text{ext}}'(r) - v_{\text{ext}}(r)] \end{aligned}$$

Adding both sides yields

$$E_0 + E_0' < E_0 + E_0'$$ contradiction with the assumption

Hohenberg–Kohn (Theorem I)

$$v_{\mathrm{ext}}(r) \Longleftrightarrow |\Psi_0\rangle \Longleftrightarrow \rho_0(r) = \langle \Psi_0 | \hat{\rho}(r) | \Psi_0 \rangle$$

unique except the constant (global phase)

→ $|\Psi[\rho]\rangle$ ground-state wf is a functional of density

$$|\Psi_0\rangle = |\Psi[\rho_0]\rangle$$

→ $O[\rho] \equiv \langle \Psi[\rho] | \hat{O} | \Psi[\rho] \rangle$ ground-state expectation values a functional of density

$$E[\rho] \equiv \langle \Psi[\rho] | \hat{H} | \Psi[\rho] \rangle = F[\rho] + \int dr \rho(r) v_{\mathrm{ext}}(r)$$

$$F[\rho] \equiv \langle \Psi[\rho] | \hat{T} + \hat{W} | \Psi[\rho] \rangle$$ universal energy density functional (EDF)

→ Density variational principle (Theorem II)

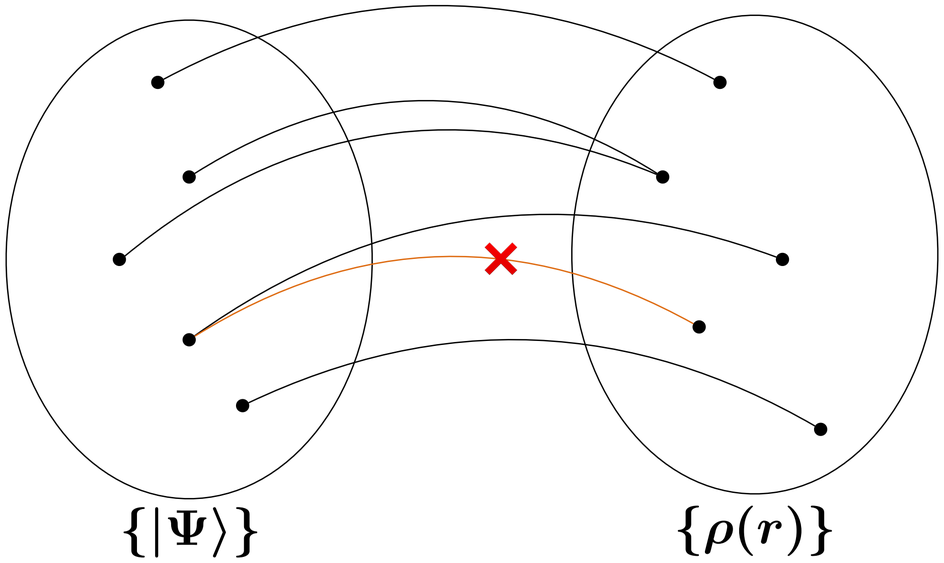
$$\rho_0(r) \neq \rho_0'(r)$$

$$E[\rho_0] < E[\rho_0'] \Longleftrightarrow E_0 = \min_{\rho(r)} E[\rho]$$

Constrained search formulation as a solution to the issue of v-rep. M. Levy, PRA26(1982)1200

For any given density, there exists at least one wave function giving that density:
N-representability

T. L. Gilbert, PRB12(1975)2111
J. E. Harriman, PRA24(1981)680



$\{|\Psi\rangle\}$ $\{\rho(r)\}$

set of many-body wave functions $\rho(r) = \langle\Psi|\psi^\dagger(r)\psi(r)|\Psi\rangle$

variational principle : $E_0 = \min_{\{|\Psi\rangle\}} [\langle\Psi|H|\Psi\rangle] = \min_{\{\rho(r)\}} \left[\min_{\{|\Psi\rangle\}_{\rho(r)}} [\langle\Psi|H|\Psi\rangle] \right]$

$$E[\rho] \equiv \min_{\{|\Psi\rangle\}_{\rho(r)}} [\langle\Psi|H|\Psi\rangle]$$ **Levy-Lieb EDF**

v- and *N*-repsentabilities

condition for the *v*-rep.

not yet proven mathematically for a general case

condition for the *N*-rep.

non-negativity

$$\rho(\vec{r}) \geq 0,$$

normalization (particle number)

$$\int d\vec{r}\rho(\vec{r}) = N,$$

continuous (finite kinetic energy)

$$\int d\vec{r} \left| \nabla \sqrt{\rho(\vec{r})} \right|^2 < \infty$$

Harriman's construction

one-dimensional without spin d.o.f for simplicity

density is non-zero in $x_1 \le x \le x_2$ $\qquad \sigma(x) = \rho(x)/N, \quad q(x) = \int_{x_1}^{x} dx' \sigma(x')$

single-particle orbitals

$$\phi_k(x) = \sqrt{\sigma(x)}\exp[2\pi i k q(x)] \qquad k = 0, \pm 1, \pm 2, \cdots$$

orbital density $\quad |\phi_k(x)|^2 = \sigma(x)$

orthonormal $\quad \int_{x_1}^{x_2} dx \phi_k(x)\phi_{k'}(x) = \delta_{kk'}$

we can construct a <u>many-body wf</u> by the Slater determinant of ϕ_k

giving any density

Practical way of DFT calculation: Kohn–Sham method

PHYSICAL REVIEW VOLUME 140, NUMBER 4A 15 NOVEMBER 1965

Self-Consistent Equations Including Exchange and Correlation Effects*

W. KOHN AND L. J. SHAM
University of California, San Diego, La Jolla, California
(Received 21 June 1965)

"Reference system" (independent particle motion in a unknown potential)

$$H = -\frac{\hbar^2}{2m}\int dx\psi^\dagger(x)\nabla^2\psi(x) + \int dx\psi^\dagger(x)v_s[\rho](r)\psi(x)$$
$$= T + V_s[\rho]$$

Kohn–Sham eq. $\left\{-\frac{\hbar^2}{2m}\nabla^2 + v_s[\rho](r)\right\}\phi_i(r) = \epsilon_i(r)$

exact ground-state density

$$\rho(r) = \langle 0|\hat{\rho}(r)|0\rangle = \sum_{i=1}^{N}|\phi_i(r)|^2$$

Kinetic energy density: $T_s[\rho] = \sum_{i=1}^{N}\langle\phi_i| - \frac{\hbar^2}{2m}|\phi_i\rangle = \sum_{i=1}^{N}\epsilon_i - \int dr v_s[\rho](r)\rho(r)$

$$v_s[\rho](r) = -\frac{\delta T_s[\rho]}{\delta\rho(r)}$$

Interacting system

density variational principle

$$\frac{\delta E[\rho]}{\delta\rho(r)} = \frac{\delta T_s[\rho]}{\delta\rho(r)} + v_{\text{ext}}(r) + \frac{\delta V_{\text{eff}}[\rho]}{\delta\rho(r)} = 0$$

$$F[\rho] = T_s[\rho] + \{F[\rho] - T_s[\rho]\}$$
$$= T_s[\rho] + V_{\text{eff}}[\rho]$$

$$v_s[\rho](r) \equiv v_{\text{ext}}(r) + \frac{\delta V_{\text{eff}}[\rho]}{\delta\rho(r)}$$

exact ground-state density of the interacting system

What is different from the mean-field approximation

$$\boldsymbol{H} = -\frac{\hbar^2}{2m}\int d\boldsymbol{x}\psi^\dagger(\boldsymbol{x})\nabla^2\psi(\boldsymbol{x}) + \int d\boldsymbol{x}\psi^\dagger(\boldsymbol{x})v_{\mathrm{ext}}(\boldsymbol{r})\psi(\boldsymbol{x})$$
$$+\frac{1}{2}\int d\boldsymbol{x}d\boldsymbol{x}'\psi^\dagger(\boldsymbol{x})\psi^\dagger(\boldsymbol{x}')w(\boldsymbol{r},\boldsymbol{r}')\psi(\boldsymbol{x}')\psi(\boldsymbol{x})$$
$$= \boldsymbol{T} + \boldsymbol{V}_{\mathrm{ext}} + \boldsymbol{W}$$

two-body interaction

neglect of the fluctuation $:\psi^\dagger\psi^\dagger\psi\psi:$

$$\int dx x_1 x_2 \Gamma(x_1, x_2) :\psi^\dagger(x_1)\psi(x_2):$$

some part of the interaction are only included in the mean field Γ

An example

$$v(x_1, x_2) = \left[t_0(1 + x_0 P_\sigma) + \frac{t_3}{6}(1 + x_3 P_\sigma)\rho^\alpha(r_1) \right] \delta(r_1 - r_2)$$

HF potential $$\Gamma_q = \frac{t_0(2+x_0)}{2}\rho - \frac{t_0(1+2x_0)}{2}\rho_q + \frac{t_3(2+x_3)}{12}\rho^{\alpha+1} - \frac{t_3(1+2x_3)}{12}\rho_q\rho^\alpha$$

neglecting spin-dependent parts

KS potential Energy density functional $F[\rho] = \langle \phi \,|\, v \,|\, \phi \rangle = \int d\vec{r}\mathscr{H}[\rho]$

$$\mathscr{H} = \frac{t_0(2+x_0)}{4}\rho^2 - \frac{t_0(1+2x_0)}{4}(\rho_\nu^2 + \rho_\pi^2) + \frac{t_3(2+x_3)}{24}\rho^{\alpha+2} - \frac{t_3(1+2x_3)}{24}\alpha\rho^\alpha(\rho_\nu^2 + \rho_\pi^2)$$

$$v_s = \frac{\delta F}{\delta \rho} = \frac{t_0(2+x_0)}{2}\rho - \frac{t_0(1+2x_0)}{2}\rho_q + \frac{t_3(2+x_3)}{24}(\alpha+2)\rho^{\alpha+1} - \frac{t_3(1+2x_3)}{24}[\alpha\rho^{\alpha-1}(\rho_\nu^2 + \rho_\pi^2) + 2\rho^\alpha\rho_q]$$

rearrangement

considered as many-body correlations beyond the HF approximation

Nuclear Energy-Density Functional (EDF)

An EDF is derived from an (effective) interaction

$$E[\rho] = \langle \Phi | \hat{V} | \Phi \rangle = \int d\vec{r} \mathscr{H}[\rho]$$

but, $E[\rho] \not\Rightarrow \hat{V}$

$|\Phi\rangle$: Slater determinant WF

In some calculation using the Skyrme-type EDF,
different types of interaction are employed in the ph and pp channels

$$E = E[\rho] + E[\rho, \kappa]$$

Skyrme-HF(B) calculation is not the Hartree–Fock one but the EDF one.

Skyrme interaction energy functional

$$\hat{v}(\vec{r}_{12}) = t_0(1 + x_0\hat{P}_\sigma)\delta(\vec{r}_{12}) + \frac{t_1}{2}(1 + x_1\hat{P}_\sigma)(\hat{\vec{k}}'^2 + \hat{\vec{k}}^2)\delta(\vec{r}_{12})$$

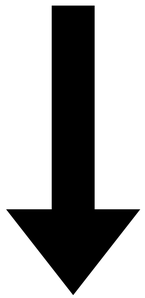
$$+t_2(1 + x_2\hat{P}_\sigma)\hat{\vec{k}}'^* \cdot \hat{\vec{k}}\delta(\vec{r}_{12}) + \frac{t_3}{6}(1 + x_3\hat{P}_\sigma)\delta(\vec{r}_{12})\rho_0^\alpha(\vec{R})$$

10 parameters

$$+iW_0(\vec{\sigma}_1 + \vec{\sigma}_2) \cdot \hat{\vec{k}}'^* \times \delta(\vec{r}_{12})\hat{\vec{k}}$$

$$E_{\text{Sky}} = \langle \Phi | \hat{V} | \Phi \rangle$$

$$= \sum_{t=0,1} \int d\vec{r}\chi_t$$



$$\vec{r}_{12} = \vec{r}_1 - \vec{r}_2, \qquad \hat{\vec{k}} = \frac{1}{2i}(\vec{\nabla}_1 - \vec{\nabla}_2), \qquad \hat{\vec{k}}' = \frac{1}{2i}(\vec{\nabla}'_1 - \vec{\nabla}'_2),$$

$$\hat{P}_\sigma = \frac{1}{2}(1 + \vec{\sigma}_1 \cdot \vec{\sigma}_2), \quad \hat{P}_\tau = \frac{1}{2}(1 + \vec{\tau}_1 \cdot \vec{\tau}_2), \quad \vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{2}$$

$$\chi_t^{\text{even}} = C_t^\rho[\rho_0]\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^\tau\rho_t\tau_t + C_t^{\nabla J}\rho_t\nabla \cdot \boldsymbol{J}_t + C_t^J\overleftrightarrow{J}_t^2$$

$$\chi_t^{\text{odd}} = C_t^s[\rho_0]\boldsymbol{s}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t \cdot \Delta\boldsymbol{s}_t + C_t^j\boldsymbol{j}_t^2 + C_t^{\nabla j}\boldsymbol{s}_t \cdot (\nabla \times \boldsymbol{j}_t) + C_t^T\boldsymbol{s}_t \cdot \boldsymbol{T}_t + C_t^{\nabla s}(\nabla \cdot \boldsymbol{s}_t)^2$$

Skyrme interaction energy functional

The coupling constants ($C_t^{\rho}, C_t^{s}, \cdots$) are expressed by the combination of the Skyrme parameters ($t_0, x_0, \cdots$).

(time-even)

$$C_0^{\tau} = \frac{1}{16}(3t_1 + 5t_2 + 4t_2x_2)$$

(time-odd)

$$C_0^{j} = -\frac{1}{16}(3t_1 + 5t_2 + 4t_2x_2) = -C_0^{\tau}$$

$$C_1^{j} = -C_1^{\tau}$$

$$C_t^{T} = -C_t^{J}, C_t^{\nabla j} = C_t^{\nabla J}$$

Galilean inv.

reduces the # of coupling constants

Skyrme interaction energy functional

$$\chi_t = C_t^{\rho}[\rho_0]\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}(\rho_t\tau_t - \boldsymbol{j}_t^2) + C_t^{\nabla J}[\rho_t\nabla\cdot\boldsymbol{J}_t + \boldsymbol{s}_t\cdot(\nabla\times\boldsymbol{j}_t)] + C_t^{J}(\boldsymbol{s}_t\cdot\boldsymbol{T}_t - \overleftrightarrow{J}_t^2)$$

$$+C_t^{s}[\rho_0]\boldsymbol{s}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t\cdot\Delta\boldsymbol{s}_t + C_t^{\nabla s}(\nabla\cdot\boldsymbol{s}_t)^2$$

16 coupling constants

(time-even)

$$C_0^{\rho} = \frac{3}{8}t_0 + \frac{3}{48}t_3\rho^{\alpha}$$

$$C_1^{\rho} = -\frac{1}{8}t_0(2x_0+1) - \frac{1}{48}t_3(2x_3+1)\rho^{\alpha}$$

(time-odd)

$$C_0^{s} = \frac{1}{8}t_0(2x_0-1) + \frac{1}{48}t_3(2x_3-1)\rho^{\alpha}$$

$$C_1^{s} = -\frac{1}{8}t_0 - \frac{1}{48}t_3\rho^{\alpha}$$

determined by the int. parameters

fixed by the static properties!

Skyrme energy-density functional

$$\mathscr{E} = \frac{\hbar^2}{2m}\tau_0 + \sum_{t=0}^{1}(\chi_t^{\text{even}} + \chi_t^{\text{odd}}) + \sum_{\tau=n,p}\tilde{\chi}_\tau + \mathscr{E}_{\text{Coul}}$$

$t = 0$: iso-scalar neutron + proton

$t = 1$: iso-vector neutron - proton

$$\chi_t^{\text{even}} = C_t^{\rho}[\rho_0]\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}\rho_t\tau_t + C_t^{J0}J_t^2 + C_t^{J1}\boldsymbol{J}_t^2 + C_t^{J2}\underline{\mathrm{J}}_t^2 + C_t^{\nabla J}\rho_t\nabla\cdot\boldsymbol{J}_t$$

$$\chi_t^{\text{odd}} = C_t^{s}[\rho_0]\boldsymbol{s}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t\cdot\Delta\boldsymbol{s}_t + C_t^{T}\boldsymbol{s}_t\cdot\boldsymbol{T}_t + C_t^{j}\boldsymbol{j}_t^2 + C_t^{\nabla j}\boldsymbol{s}_t\cdot(\nabla\times\boldsymbol{j}_t) + C_t^{\nabla s}(\nabla\cdot\boldsymbol{s}_t)^2 + C_t^{F}\boldsymbol{s}_t\cdot\boldsymbol{F}_t$$

Skyrme energy-density functional

$$\hat{\rho}(\boldsymbol{r}st,\boldsymbol{r}'s't') = \langle\Phi\,|\,\psi^{\dagger}(\boldsymbol{r}'s't')\psi(\boldsymbol{r}st)\,|\,\Phi\rangle$$

$$\rho_k(\boldsymbol{r},\boldsymbol{r}') = \sum_{stt'} \hat{\rho}(\boldsymbol{r}st,\boldsymbol{r}'st')\tau^k_{t't}$$

$$\boldsymbol{s}_k(\boldsymbol{r},\boldsymbol{r}') = \sum_{ss'tt'} \hat{\rho}(\boldsymbol{r}st,\boldsymbol{r}'s't')\boldsymbol{\sigma}_{s's}\tau^k_{t't}$$

time-even densities

density

$$\rho_t(\boldsymbol{r}) = \rho_t(\boldsymbol{r},\boldsymbol{r})$$

kinetic density

$$\tau_t(\boldsymbol{r}) = (\nabla\cdot\nabla')\rho_t(\boldsymbol{r},\boldsymbol{r}')\Big|_{\boldsymbol{r}=\boldsymbol{r}'}$$

tensor density

$$\overleftrightarrow{J}_t(\boldsymbol{r}) = \frac{1}{2i}(\nabla-\nabla')\otimes\boldsymbol{s}_t(\boldsymbol{r},\boldsymbol{r}')\Big|_{\boldsymbol{r}=\boldsymbol{r}'}$$

$$J_t = \sum_a J_{taa}$$

$$\boldsymbol{J}_t = \sum_{bc}\epsilon_{abc}J_{tbc}$$

$$\underline{\mathrm{J}}_{tab} = \frac{1}{2}J_{kab} + \frac{1}{2}J_{tba} - \frac{1}{3}J_t\delta_{ab}$$

time-odd densities

spin density

$$\boldsymbol{s}_t(\boldsymbol{r}) = \boldsymbol{s}_t(\boldsymbol{r},\boldsymbol{r})$$

spin kinetic density

$$\boldsymbol{T}_t(\boldsymbol{r}) = (\nabla\cdot\nabla')\boldsymbol{s}_t(\boldsymbol{r},\boldsymbol{r}')\Big|_{\boldsymbol{r}=\boldsymbol{r}'}$$

current density

$$\boldsymbol{j}_t(\boldsymbol{r}) = \frac{1}{2i}(\nabla-\nabla')\rho_t(\boldsymbol{r},\boldsymbol{r}')\Big|_{\boldsymbol{r}=\boldsymbol{r}'}$$

tensor kinetic density

$$\boldsymbol{F}_t(\boldsymbol{r}) = \frac{1}{2}(\nabla\otimes\nabla'+\nabla'\otimes\nabla)\boldsymbol{s}_t(\boldsymbol{r},\boldsymbol{r}')\Big|_{\boldsymbol{r}=\boldsymbol{r}'}$$

Skyrme EDF for nuclear DFT

$$\chi_t = C_t^{\rho}\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}(\rho_t\tau_t - \boldsymbol{j}_t^2) + C_t^{\nabla J}[\rho_t\nabla\cdot\boldsymbol{J}_t + \boldsymbol{s}_t\cdot(\nabla\times\boldsymbol{j}_t)] + C_t^{J}(\boldsymbol{s}_t\cdot\boldsymbol{T}_t - \overleftrightarrow{J}_t^2)$$

$$+C_t^{s}\boldsymbol{s}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t\cdot\Delta\boldsymbol{s}_t + C_t^{\nabla s}(\nabla\cdot\boldsymbol{s}_t)^2$$

16 coupling constants

independent

A pioneering work toward this direction:

Bender–Dobaczewski–Engel–Nazarewicz, PRC65(2002)054322

C_1^s as a free coupling constant

$$C_1^s = -\frac{1}{8}t_0 - \frac{1}{48}t_3\rho^{\alpha} \qquad C_1^s = \frac{1}{2N_0}(g_0' + g_1')$$

related to the Landau parameters

$$g_0' = N_0(2C_1^s + 2C_1^T\beta\rho^{2/3})$$

$$g_1' = -2N_0C_1^T\beta\rho^{2/3}$$

$$\beta = (3\pi^2/2)^{2/3}$$

$$v_{\mathrm{res}}(\mathbf{r},\mathbf{r}') = N_0^{-1}[g_0'\delta(\mathbf{r}-\mathbf{r}') + g_1'\mathbf{k}'\cdot\delta(\mathbf{r}-\mathbf{r}')\mathbf{k}](\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}')(\boldsymbol{\tau}\cdot\boldsymbol{\tau}')$$

Examples of Skyrme-type EDD

✓SkM* J. Bartel *et al*., NPA386 (1982) 79

Fission barrier height of ^{240}Pu

➡ rare-earth and actinides

✓SLy4 E. Chabanat *et al*., NPA627 (1997) 710
E. Chabanat *et al*., NPA635 (1998) 231

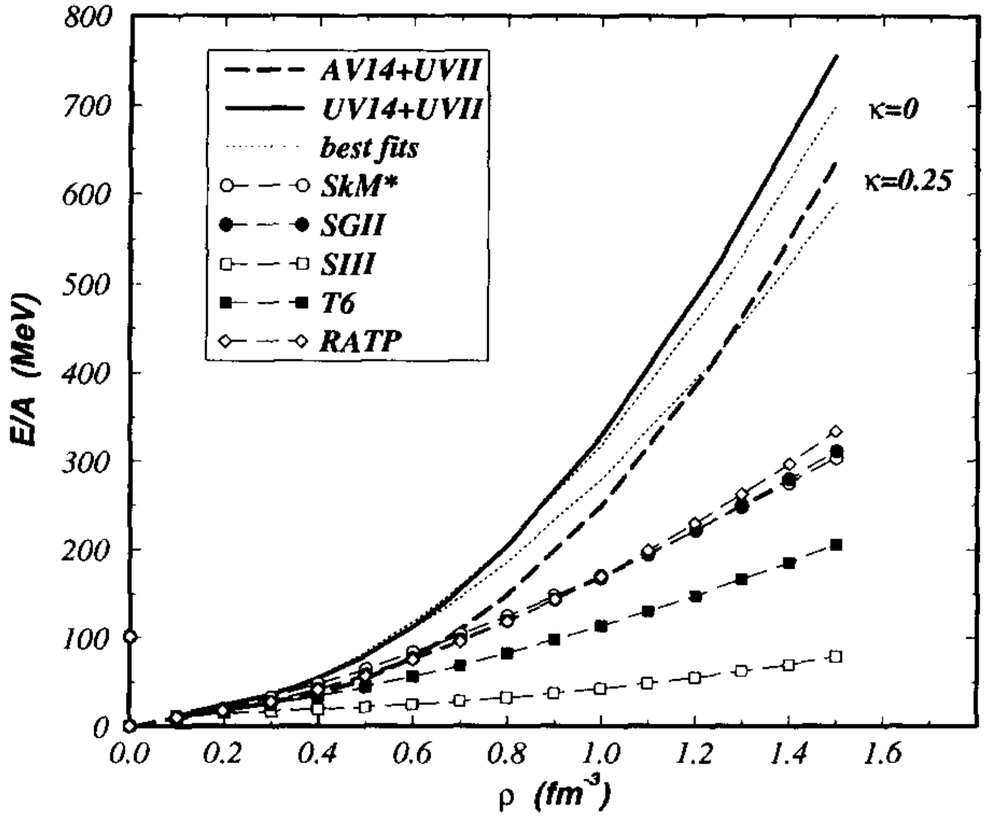
Microscopic EoS of neutron matter
R.B. Wiringa *et al*., PRC38 (1988) 1010

➡ neutron-rich nuclei

✓SGII H. Sagawa and N.V. Giai, PLB106 (1981) 379

Excitation energy of Gamow–Teller resonance in ^{208}Pb

➡ spin-isospin response



UNEDF project

→ NUCLEI(Nuclear Computational Low-Energy Initiative)

Building a Universal Nuclear Energy-Density Functional

by the researchers in nuclear theory, applied mathematics, computational science and computer science

M. Kortelainen *et al.*, PRC89 (2014) 054314

$$\chi^2(x) = \frac{1}{n_d - n_x} \sum_{i=1}^{D_T} \sum_{j=1}^{n_i} \left(\frac{s_{i,j}(x) - d_{i,j}}{w_i} \right)^2$$

$$n_d = \sum_i^{D_T} n_i$$

$$D_T = 5, \quad n_d = 130, \quad n_x = 14$$

15 parameters including ph and pp channels

130 experimental data

mass of spherical (29) and deformed (47) nuclei
charge radius (28)
odd-even staggering (13)
fission isomer (4)
spin-orbit splitting in spe (9)

RMS deviation

Observable	UNEDF0	UNEDF1	UNEDF2	No.
E	1.428	1.912	1.950	555
E ($A < 80$)	2.092	2.566	2.475	113
E ($A \geqslant 80$)	1.200	1.705	1.792	442

Ground state properties

$$\delta E[\rho, \tilde{\rho}, \tau, J] = 0$$

→ Skyrme Kohn-Sham-Bogoliubov (KSB) equation

$$\sum_{\sigma'} \begin{pmatrix} h^q(r,\sigma,\sigma') - \lambda^q & \tilde{h}^q(r,\sigma,\sigma') \\ \tilde{h}^q(r,\sigma,\sigma') & -(h^q(r,\sigma,\sigma') - \lambda^q) \end{pmatrix} \begin{pmatrix} \varphi^q_{1,\alpha}(r,\sigma') \\ \varphi^q_{2,\alpha}(r,\sigma') \end{pmatrix} = E_\alpha \begin{pmatrix} \varphi^q_{1,\alpha}(r,\sigma) \\ \varphi^q_{2,\alpha}(r,\sigma) \end{pmatrix}$$

$$h^q = -\nabla \cdot \frac{\hbar^2}{2m^*_q} \nabla + U_q + U_C \delta_{q,\pi} - iB_q \cdot (\nabla \times \sigma),$$

$$\tilde{h}_q = \frac{V_0^{(q)}}{2} F(r) \tilde{\rho}_q$$

$$\frac{\hbar^2}{2m^*_q} = \frac{\hbar^2}{2m} + b_1\rho - b'_1\rho_q$$ effective mass: finite range of the interaction (momentum dependence)

$$U_q = b_0\rho - b'_0\rho_q + b_1\tau - b'_1\tau_q + \frac{b_3}{3}(\alpha+2)\rho^{\alpha+1} - \frac{b'_3}{3}\left[\alpha\rho^{\alpha-1}\sum_q \rho_q^2 + 2\rho^\alpha\rho_q\right]$$

$$-b_4\nabla\cdot J - b'_4\nabla\cdot J_q - b_2\nabla^2\rho + b'_2\nabla^2\rho_q + \frac{\delta F}{\delta\rho}\sum_q \tilde{\rho}_q^2$$ rearrangement

$$B_q = b'_1 J_q + b_4\nabla\rho + b'_4\nabla\rho_q$$

Application to deformed nuclei

coordinate-space representation

30 points for each direction

dimension of the KSB matrix $4N = 4 \times N_x \times N_y \times N_z \sim 10^5$

the size of nucleus gradually increases as $A^{1/3}$ → the box size also does

a few tens to hundred iterations are needed to get the convergence

↓ computationally demanding

✓Expansion with the basis function

HO basis "HFODD"

two-basis method

HFB Hamiltonian in the HF basis

B. Gall *et al.*, Z. Phys. A348 (1994) 183

→ a large number of basis states are required to describe the drip-line nuclei

✓Assumption of the axial symmetry

Vanderbilt

E. Teran *et al.*, PRC67 (2003) 064314

Oak Ridge

J. C. Pei *et al.*, PRC78 (2008) 064306 (the reflection sym.)

Kyoto–Orsay

KY and N.V. Giai, PRC78 (2008) 014305

(the reflection sym.)

Niigata

H. Oba and M. Matsuo, PTP120 (2008) 143

axial symmetry $[\mathcal{H}, \hat{R}_z] = 0$

$\Leftrightarrow$

rotation along the z-axis $\hat{R}_z(\phi) = \exp(-i\phi\hat{j}_z/\hbar)$ $[\mathcal{H}, \hat{j}_z] = 0$

eigenstates

$$\mathcal{H}\begin{pmatrix}\varphi_{1,i}(\varrho,z,\phi,\sigma)\\ \varphi_{2,i}(\varrho,z,\phi,\sigma)\end{pmatrix} = E_i\begin{pmatrix}\varphi_{1,i}(\varrho,z,\phi,\sigma)\\ \varphi_{2,i}(\varrho,z,\phi,\sigma)\end{pmatrix},$$

$$\hat{j}_z\begin{pmatrix}\varphi_{1,i}(\varrho,z,\phi,\sigma)\\ \varphi_{2,i}(\varrho,z,\phi,\sigma)\end{pmatrix} = \hbar\Omega_i\begin{pmatrix}\varphi_{1,i}(\varrho,z,\phi,\sigma)\\ \varphi_{2,i}(\varrho,z,\phi,\sigma)\end{pmatrix}$$

cylindrical coordinate $r = (\varrho, z, \phi)$

parity is also a good quantum number when assuming the reflection sym.

wave functions

$$\varphi_i(\varrho,z,\phi,\sigma) = \begin{pmatrix}\varphi_i^+(\varrho,z)e^{i\Lambda_i^-\phi}\\ \varphi_i^-(\varrho,z)e^{i\Lambda_i^+\phi}\end{pmatrix} \qquad \Lambda_i^\pm = \Omega_i \pm 1/2$$

for each Ω (block diagonal)

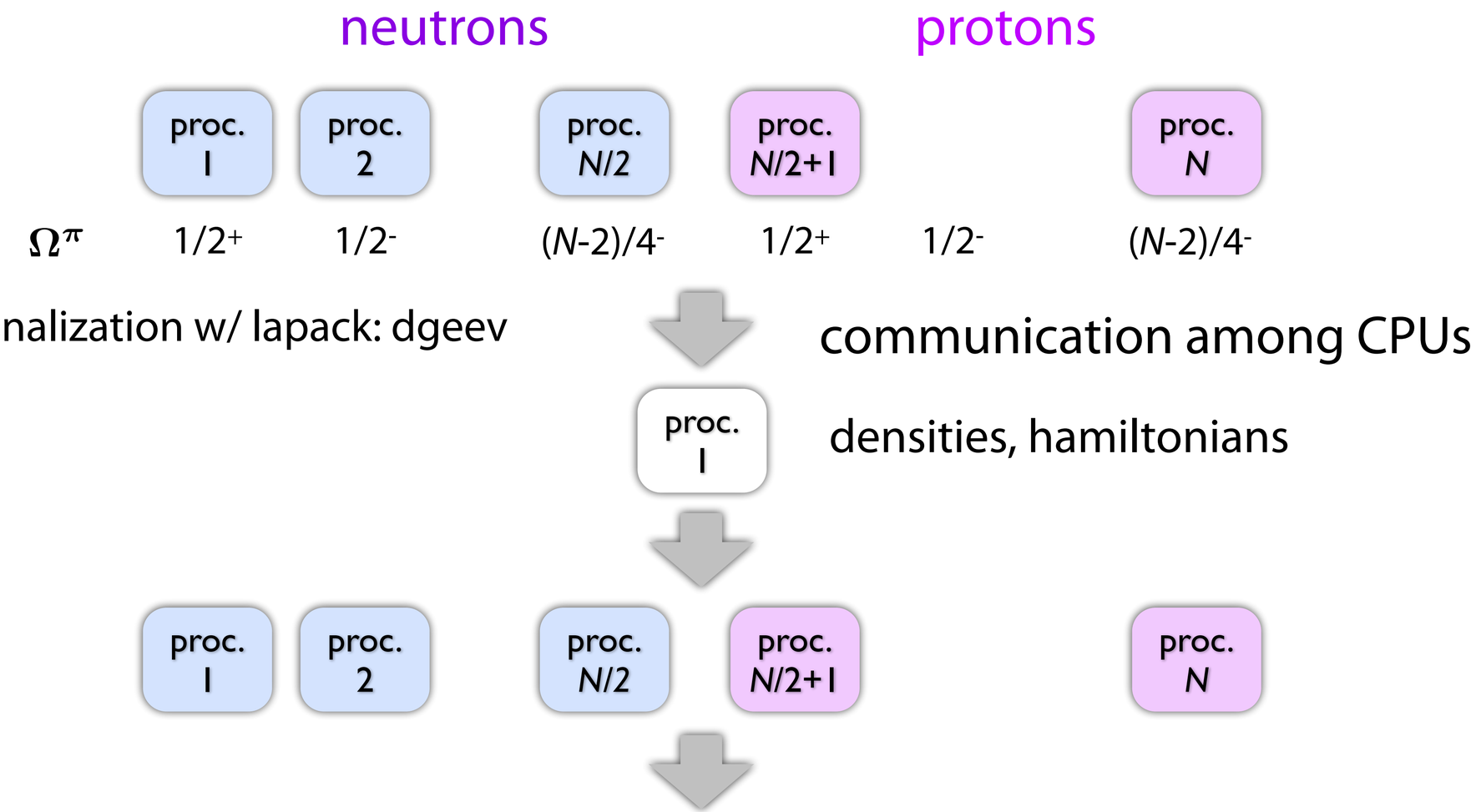
$$\begin{pmatrix} h_{\uparrow\uparrow}-\lambda & h_{\uparrow\downarrow} & \tilde{h}_{\uparrow\uparrow} & \tilde{h}_{\downarrow\uparrow}\\ h_{\downarrow\uparrow} & h_{\downarrow\downarrow}-\lambda & \tilde{h}_{\downarrow\uparrow} & \tilde{h}_{\downarrow\downarrow}\\ \tilde{h}_{\uparrow\uparrow} & \tilde{h}_{\downarrow\uparrow} & -(h_{\uparrow\uparrow}-\lambda) & -h_{\uparrow\downarrow}\\ \tilde{h}_{\downarrow\uparrow} & \tilde{h}_{\downarrow\downarrow} & -h_{\downarrow\uparrow} & -(h_{\downarrow\downarrow}-\lambda)\end{pmatrix}\begin{pmatrix}\varphi_{1,i}^+\\ \varphi_{1,i}^-\\ \varphi_{2,i}^+\\ \varphi_{2,i}^-\end{pmatrix} = E_i\begin{pmatrix}\varphi_{1,i}^+\\ \varphi_{1,i}^-\\ \varphi_{2,i}^+\\ \varphi_{2,i}^-\end{pmatrix}$$

parallelize for each Ω

dimension of the block becomes smaller $4 \times N_\rho \times N_z \sim 3000$ → easy to extend the box size for the drip-line nuclei

parallel computing

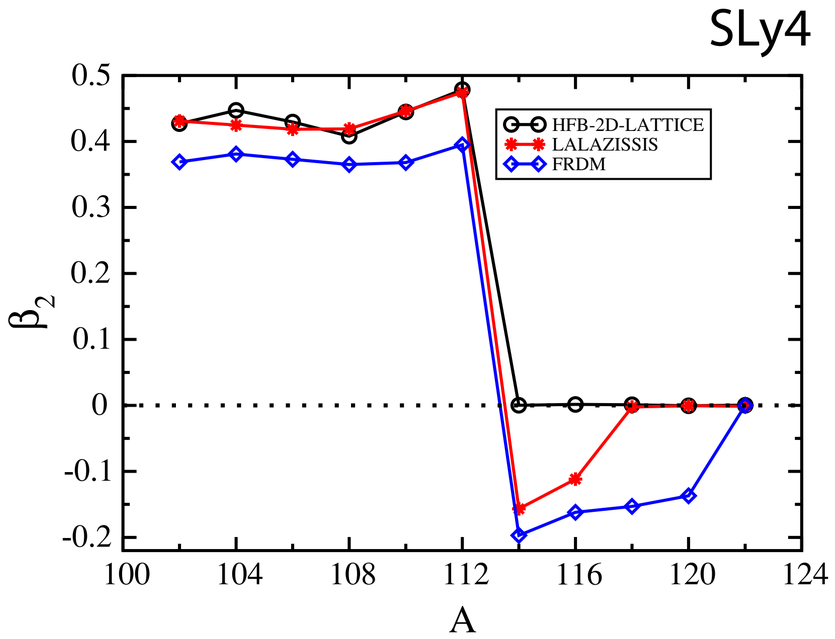
using the MPI （w/N cores: N=4n）

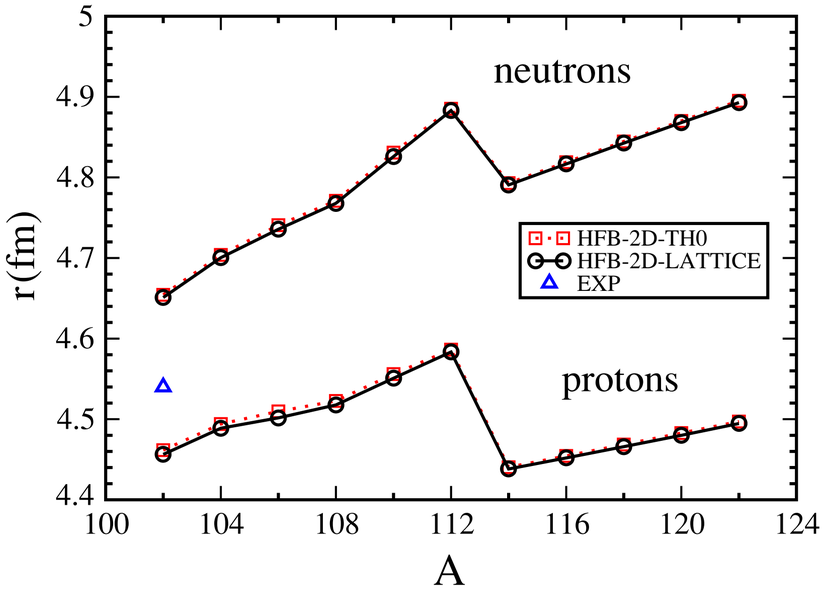


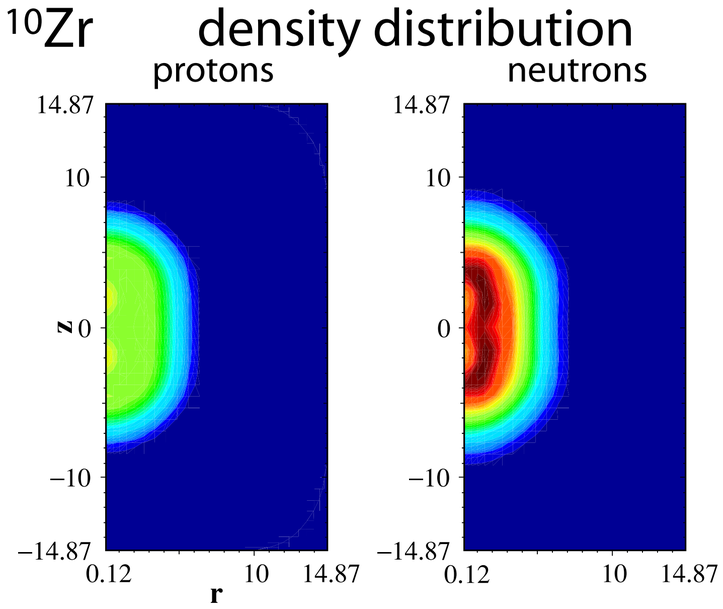
A. Baran *et al.*, PRC78(2008)014318

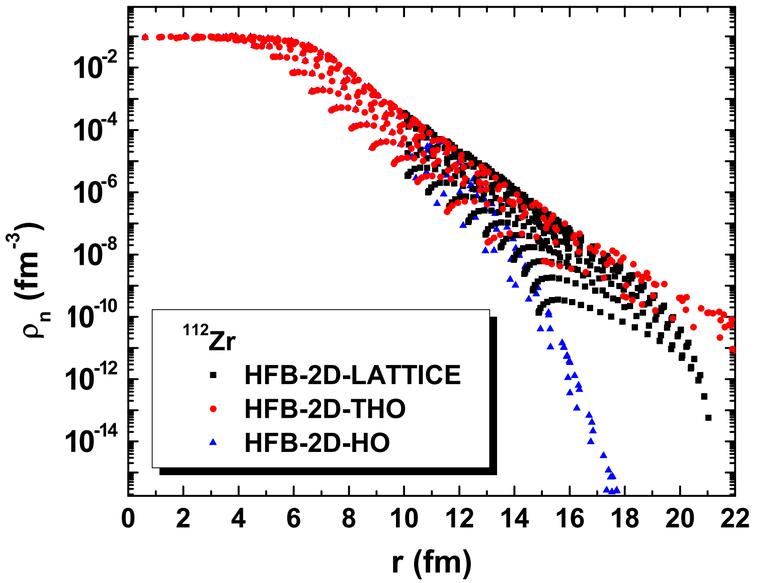
Zr isotopes: a sudden shape change

A. Blazkiewicz *et al.*, PRC71 (2005) 054321







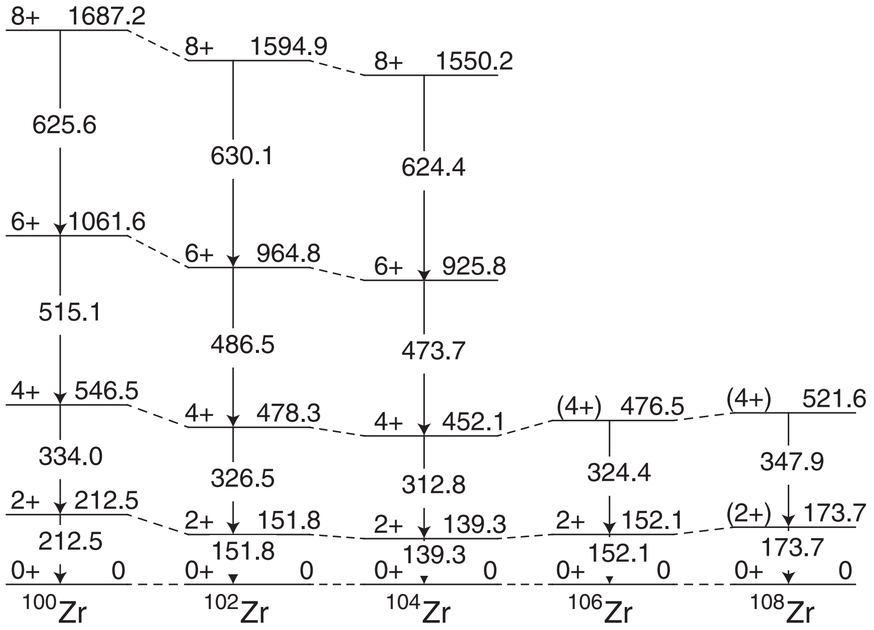


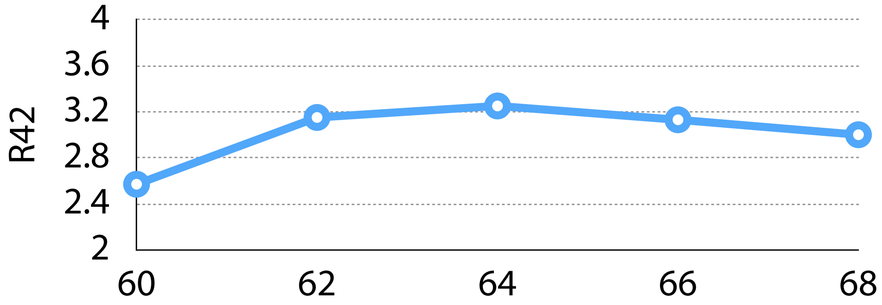
tail structure

Zr isotopes: strong deformation at *N*=64

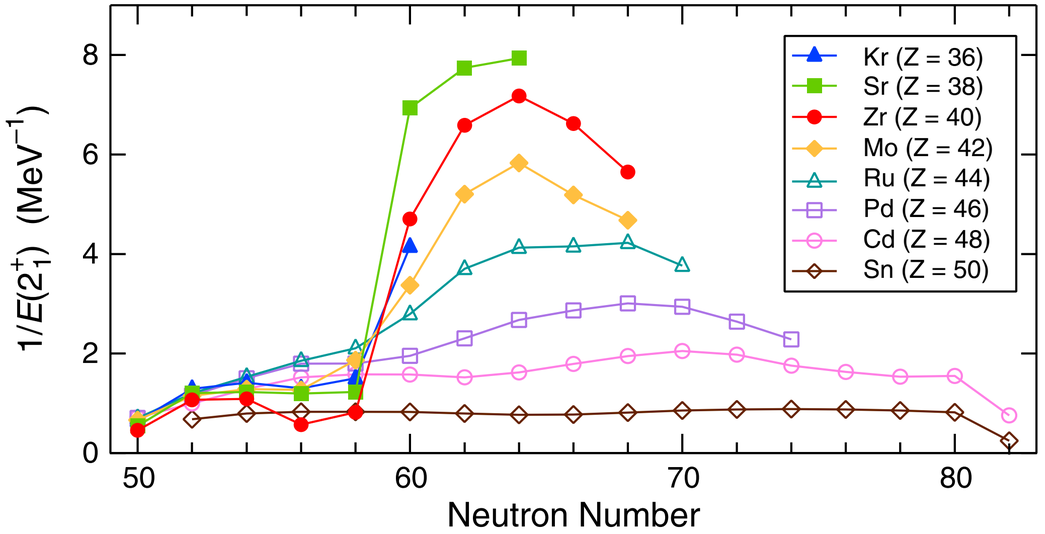
T. Sumikama *et al.*, PRL106 (2011) 202501

exp. @ RIBF

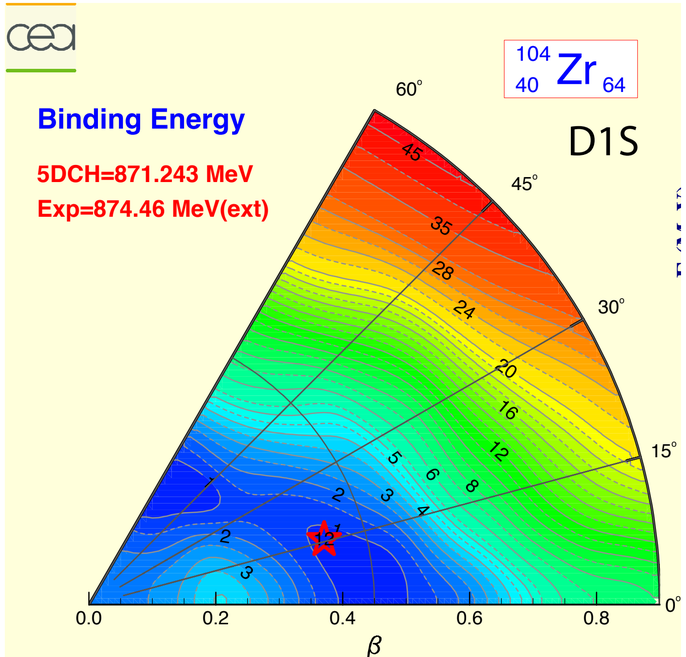




strong deformation in Zr and Sr

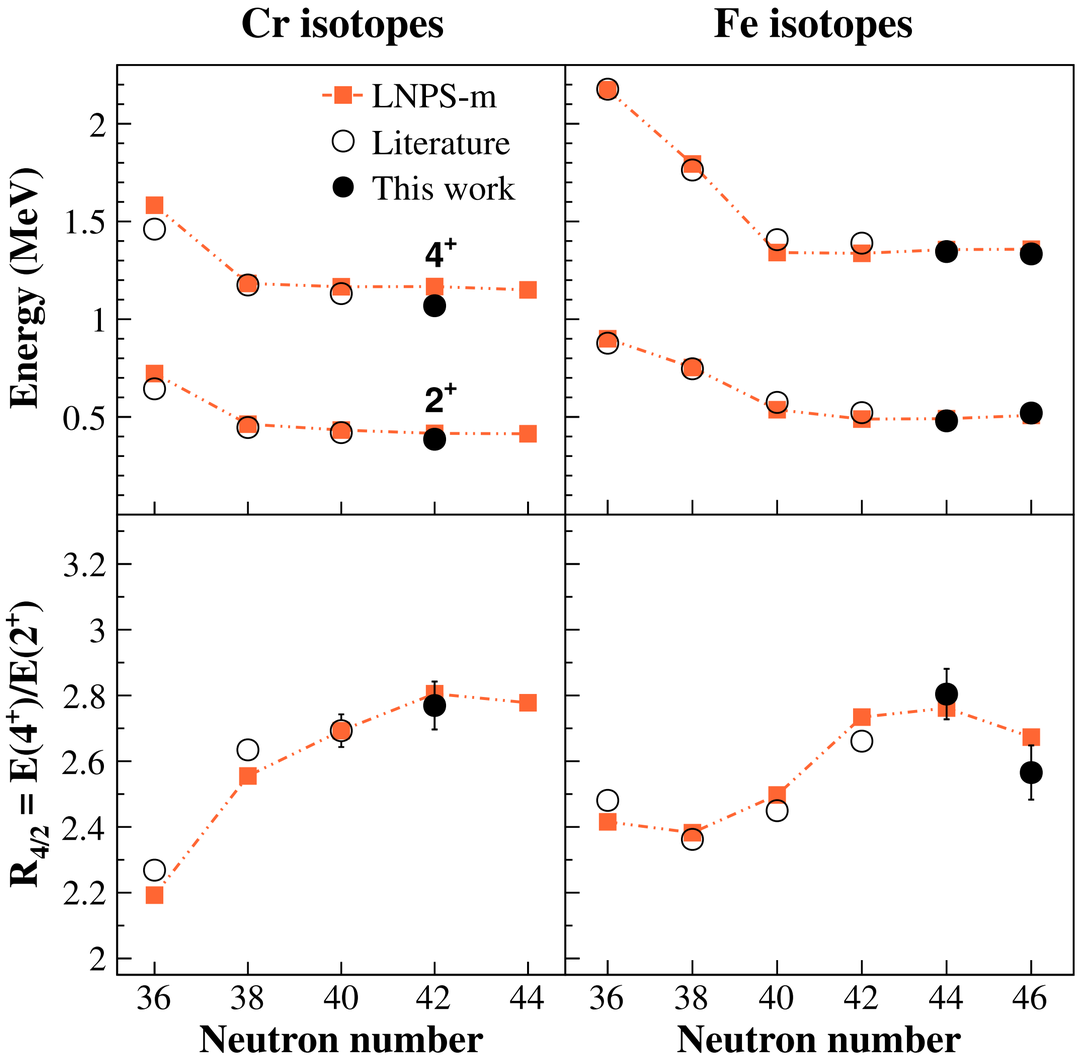


possibility of the shape coexistence

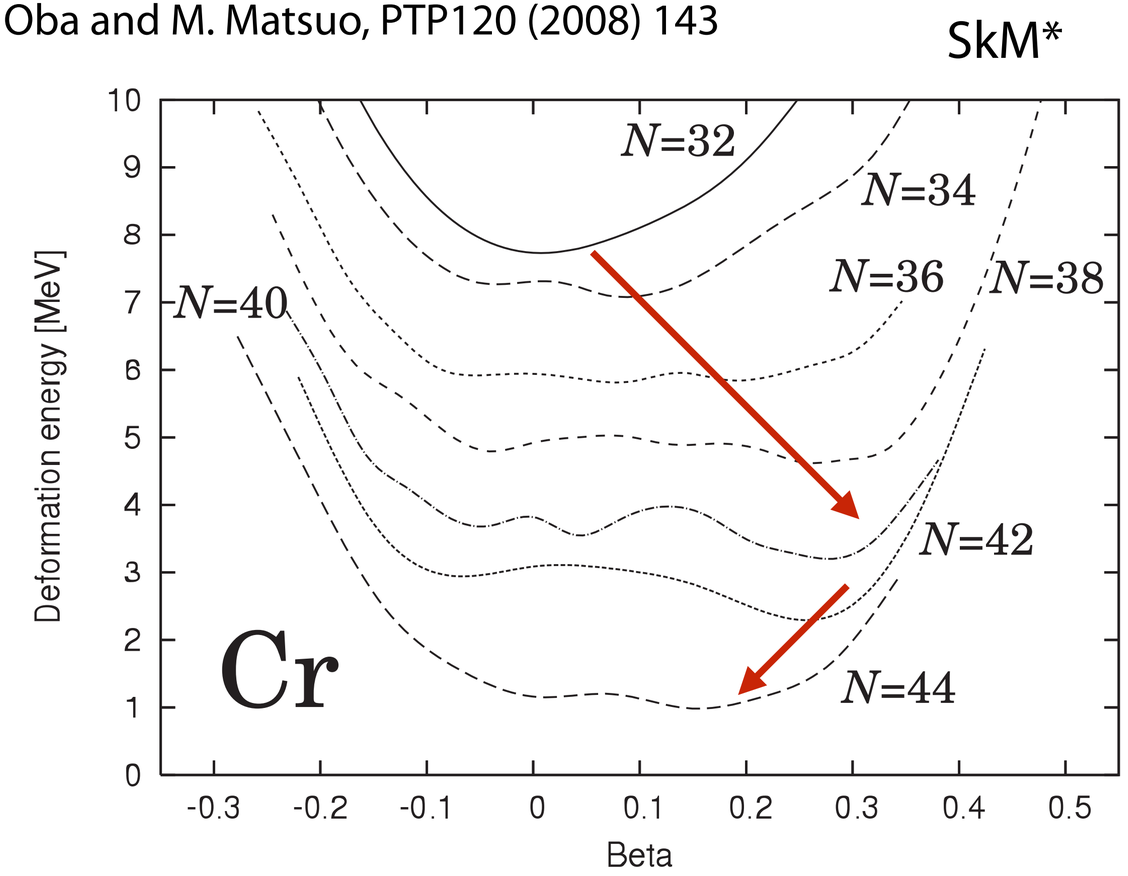


Cr–Fe isotopes: deformation at *N*=40–50

C. Santamaria *et al.*, PRL115 (2015) 192501
(p,2p)γ @ RIBF

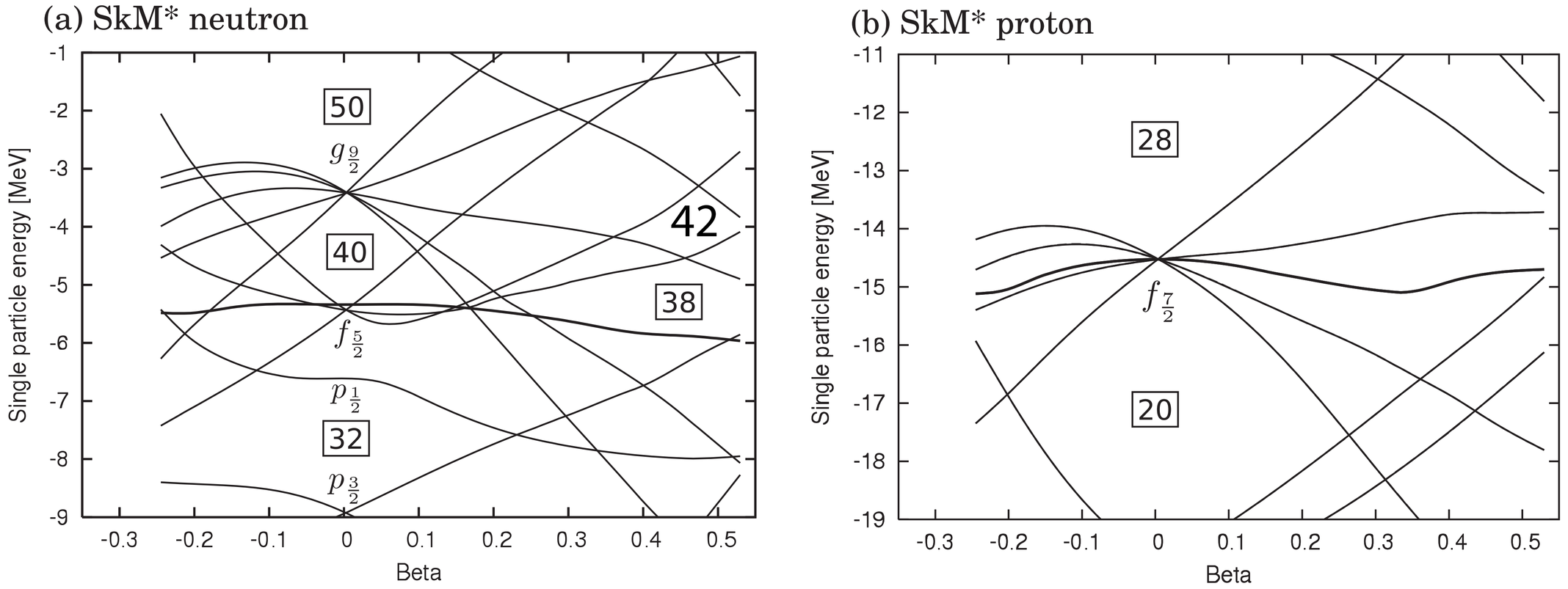


H. Oba and M. Matsuo, PTP120 (2008) 143



Nilsson diagram

H. Oba and M. Matsuo, PTP120 (2008) 143



neutrons start to occupy the $g_{9/2}$ orbital beyond N=40

high deformation at N=42

Open sources

SHF

Langanke, Maruhn, Koonin: Computational Nuclear Physics I

Chap. 2 Skyrme Hartree-Fock (P.-G. Reinhard)

HFBRAD spherical HFB in radial mesh

Bennaceur and Dobaczewski, Comp. Phys. Commun. 168, 96 (2005)

HOSPHE spherical HFB in HO basis

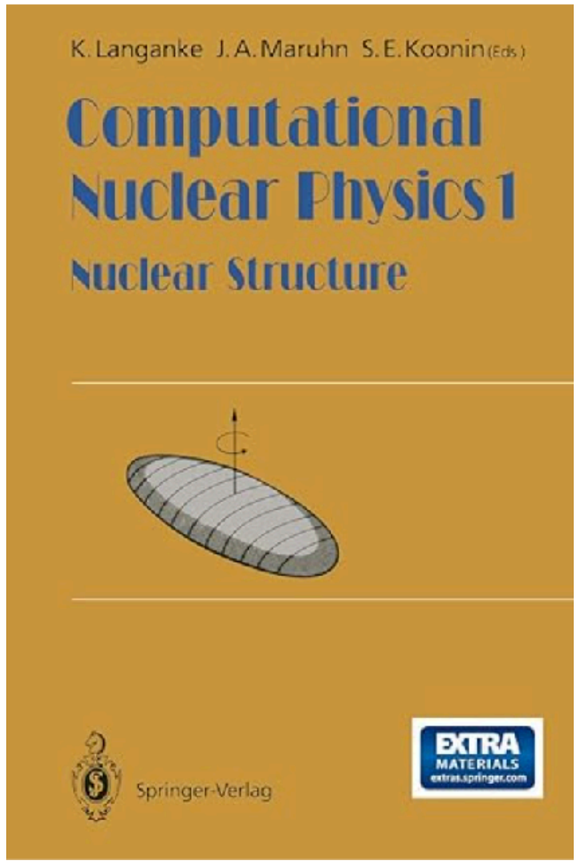
Carlsson et al., Comp. Phys. Commun. 181, 1641 (2010)

HFBTHO axial-sym. HFB in 2D HO basis

Marevic et al., Comp. Phys. Commun. 276, 108367 (2022)

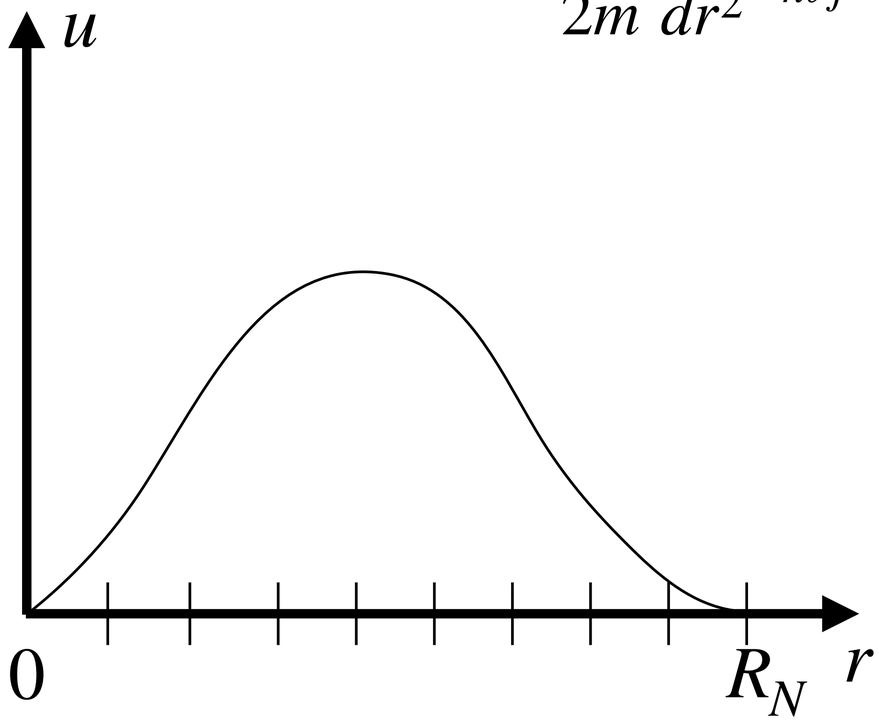
HOODD HFB in 3D HO basis

Schunck et al., Comp. Phys. Commun. 216, 145 (2017)



Exercise and Homework

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u_{n\ell j}(r)+\left(V_{\rm WS}(r)+\frac{\hbar^2\ell(\ell+1)}{2mr^2}\right)u_{n\ell j}(r)=\varepsilon_{n\ell j}u_{n\ell j}(r)$$



$$hu=-B\begin{pmatrix}-2+\star & 1 & 0 & \cdots & 0\\ 1 & -2+\star & 1 & \cdots & 0\\ 0 & 1 & -2+\star & \ddots & \vdots\\ \vdots & \ddots & \ddots & \ddots & 1\\ 0 & \cdots & 0 & 1 & -2+\star\end{pmatrix}\begin{pmatrix}u_2\\ u_3\\ u_4\\ \vdots\\ u_{N-1}\end{pmatrix}$$

include the spin–orbit potential

$$[\ell\cdot sW(r)]u_{nlj}=\frac{1}{2}\left[j(j+1)-\ell(\ell+1)-\frac{3}{4}\right]W(r)u_{nlj}$$

$$V_{\rm WS}(r)=-V_0\frac{1}{1+\exp[(r-R)/a]}=-V_0 f_{\rm WS}$$

$$W(r)=V_{\rm so}r_0^2\frac{1}{r}\frac{df_{\rm WS}}{dr}$$

+: proton
-: neutron

$$V_0=-51\pm 33\frac{N-Z}{A}\,\text{MeV},\ a=0.67\,\text{fm},\ V_{so}=22\pm 14\frac{N-Z}{A}\,\text{MeV}$$

$r(i)=r_i=i\times\Delta,$
$i=0,1,\cdots N_r$

Δ: radial mesh size

N_r: number of mesh points

Homework

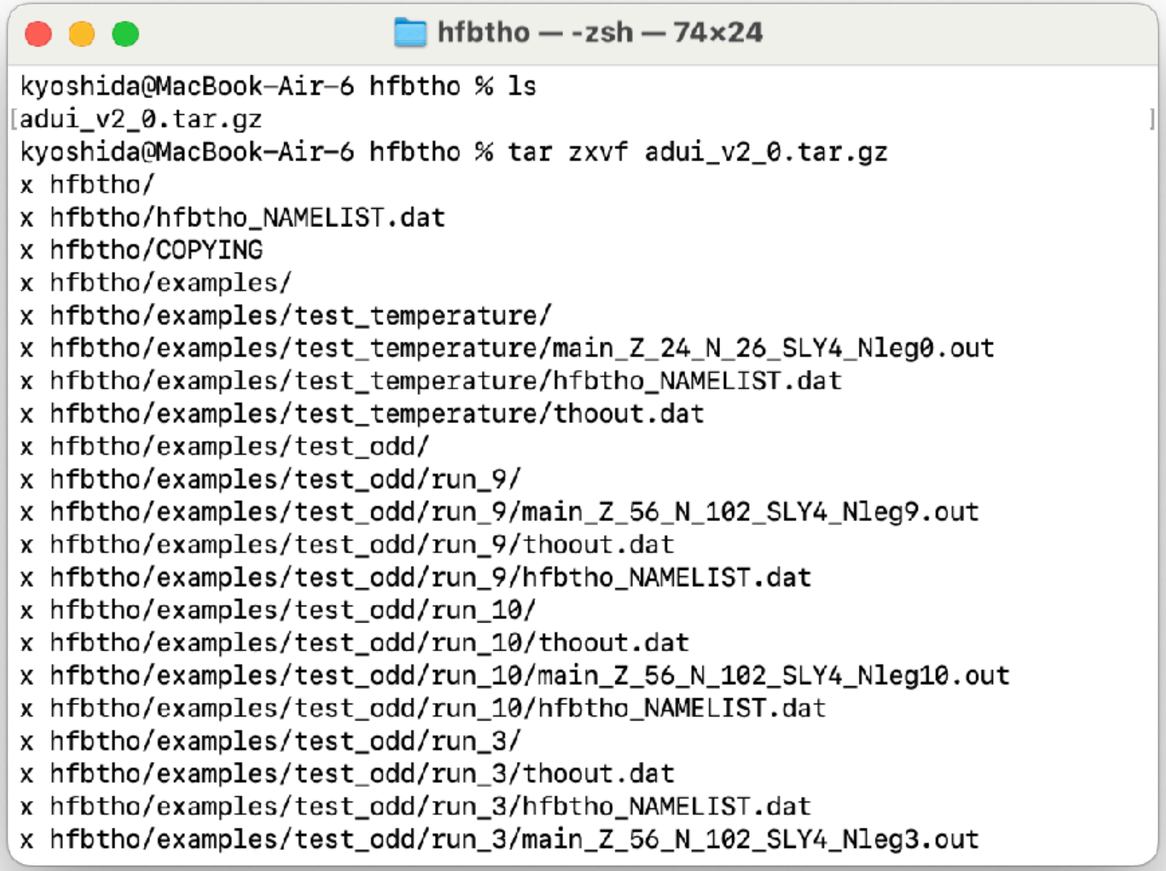
HFBTHO axially-symmetric transformed HO (THO) basis

v2.00d: Stoitsov et al., Comp. Phys. Commun. 184, 1592 (2013)

this is not the latest version, but you can enjoy the physics

https://data.mendeley.com/datasets/f8n37xtbmg/1

tar zxvf adui_v2_0.tar.gz



Let’s try the HFB calculation by using HFBTHO

```
hfbtho — -zsh — 72×6
[kyoshida@MacBook-Air-6 hfbtho % cd hfbtho
[kyoshida@MacBook-Air-6 hfbtho % ls
COPYING                 blas.f                  hfbtho_v200d.f90
Makefile                examples                lapack.f
README                  hfbtho_NAMELIST.dat     main_v200d.f90
[kyoshida@MacBook-Air-6 hfbtho % vim Makefile
```

one can find the source files (codes) in ”hfbtho” directory

including libraries such as lapack and blas

```
hfbtho — vim Makefile — 88×31
44
45 SHELL := /bin/bash
46
47 # Names
48 VERSION         = 200d
49 HFBTHO_EXE      = main
50 HFBTHO_SOURCE   = main_v$(VERSION).f90
51 HFBTHO_OBJ      = main_v$(VERSION).o
52
53 # Makefile Options
54 COMPILER        = GFORTRAN
55 FORTRAN         = gfortran
56 DEBUG           = FALSE
57 ACML_LIBRARY    = FALSE
58 STATIC_LIB      = FALSE
59
60 # Preprocessor options
61 hide_openmp     = 1
62
63 # BLAS and LACPACK libraries
64 ifeq ($(ACML_LIBRARY),TRUE)
65       LAPACK_OBJ =
66       BLAS_OBJ   =
67       ACML       = -L$(HOME)/lib/lapack-3.4.1 -llapack_LINUX -lblas_LINUX
68 else
69       LAPACK_OBJ = lapack.o
70       BLAS_OBJ   = blas.o
71       ACML       =
72 endif
73
```

Open the Makefile

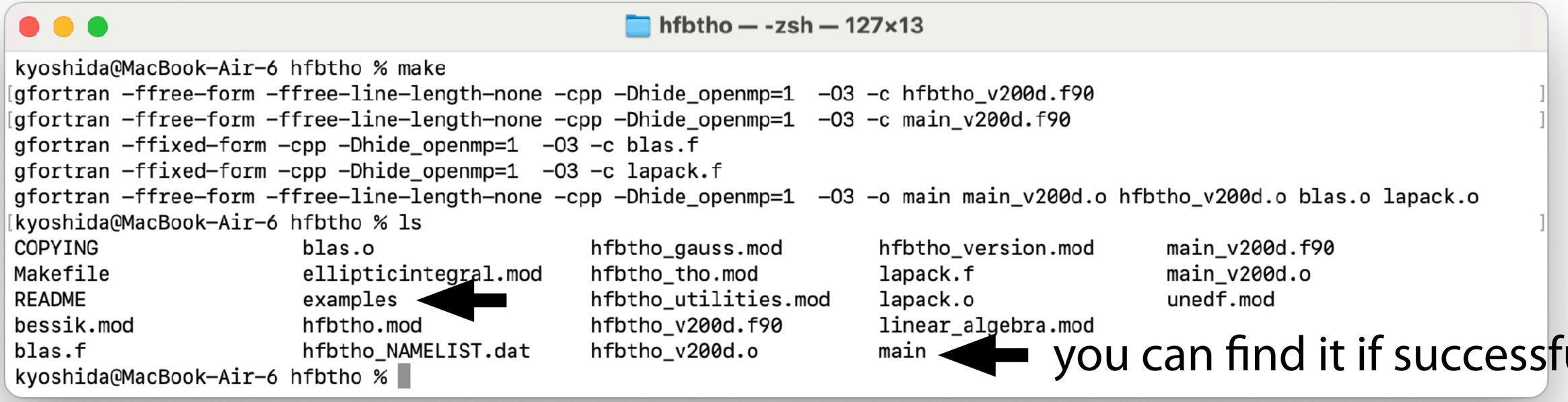
ACML_LIBRARY = TRUE

↓

FALSE

Let’s try the HFB calculation by using HFBTHO

then, make to prepare the executable file “main”



you can find some examples in the “examples” directory

Let's try the HFB calculation by using HFBTHO

an example examples/test_spherical/run_0

input file: hfbtho_NAMELIST.dat

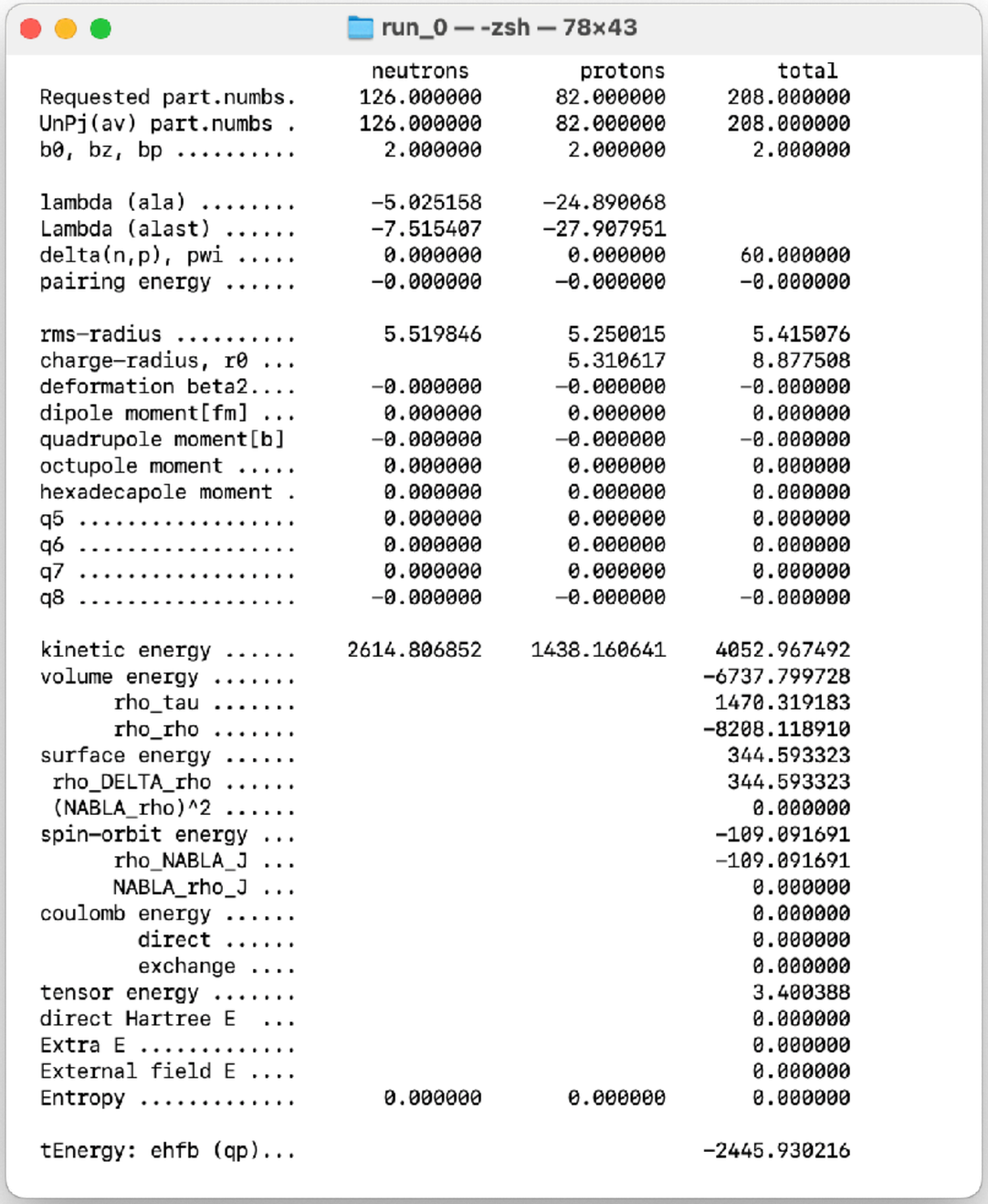
you can execute the job: ./main

run_0 — vim hfbtho_NAMELIST.dat — 78×29

```
 1 &HFBTHO_GENERAL
 2  number_of_shells = 16,
 3  oscillator_length = 2.0,
 4  basis_deformation = 0.0,
 5  proton_number = 82, neutron_number = 126, type_of_calculation = 1 /
 6 &HFBTHO_ITERATIONS
 7  number_iterations = 100, accuracy = 1.E-9, restart_file = -1 /
 8 &HFBTHO_FUNCTIONAL
 9  functional = 'SLY5', add_initial_pairing = F,
10  type_of_coulomb = 0/
11 &HFBTHO_PAIRING
12  user_pairing = T, vpair_n = -300.0, vpair_p = -300.0,
13  pairing_cutoff = 60.0, pairing_feature = 0.5 /
14 &HFBTHO_CONSTRAINTS
15  lambda_values = 1, 2, 3, 4, 5, 6, 7, 8,
16  lambda_active = 0, 0, 0, 0, 0, 0, 0, 0,
17  expectation_values = 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0 /
18 &HFBTHO_BLOCKING
19  proton_blocking = 0, 0, 0, 0, 0, neutron_blocking = 0, 0, 0, 0, 0 /
20 &HFBTHO_PROJECTION
21  switch_to_THO = 0, projection_is_on = 0,
22  gauge_points = 1, delta_Z = 0, delta_N = 0 /
23 &HFBTHO_TEMPERATURE
24  set_temperature = F, temperature = 0.0 /
25 &HFBTHO_DEBUG
26  number_Gauss = 40, number_Laguerre = 40, number_Legendre = 80,
27  compatibility_HFODD = T, number_states = 969, force_parity = T,
28  print_time = 0 /
```

^{208}Pb(Z=82, N=126)

Skyrme SLy5 interaction



one will obtain

lambda: chemical potential
pairing gap and pairing energy

radius, charge radius, and moments

breakdown of the energy

total energy：$-B$

Let’s try the HFB calculation by using HFBTHO

154Sm (Z=62, N=92)

away from the magic numbers

modify the input file: hfbtho_NAMELIST.dat

proton_number = 62

neutron_number = 92

functional = SKM*

often used in the structure calculations

Question: is this nucleus deformed? what is the deformation?

deformation beta2

quadrupole moment