Hohenberg Kohn theorem

Bijection:
density ↔ energy ↔ ground state wave function

(non degenerate)

Consequence: the energy is a (unknown) functional of the density

$$F[n] = T_{\mathrm{s}}[n] + U[n] + E_{\mathrm{xc}}[n]$$

kinetic energy

direct term

$$U[n] = \frac{1}{2}\int \mathrm{d}^3r \int \mathrm{d}^3r' \, \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

exchange-correlation energy
form unknown

2. Minimization of the energy with respect to all N-electron densities

$$E = \min_n E_v[n]$$
$$= \min_n \left\{ F[n] + \int \mathrm{d}^3 r \, v(\mathbf{r}) n(\mathbf{r}) \right\}$$

The density is determined through the Kohn Sham equation:

$$(-\frac{\hbar^2}{2m}\Delta + u([n];\vec{r}) + v_{xc}([n];\vec{r}))\psi_\alpha(\vec{r}) = \epsilon_\alpha \psi_\alpha(\vec{r})$$

obtained by variation of *E* with respect to *n*
fictitious one-particle Shrödinger equation.

It looks like HF but is not HF!

All correlations in the interaction?

- There should be according to the DFT!
- BUT: form of the functional is unknown
- Double counting problem if correlations are added

  to a density functional

- It is better to avoid in the density functional correlations which vary rapidly with A
- Physical interpretations could be more obvious if beyond mean-field correlations are explicitly treated

  (rotational and vibrational correlations)
- Spectra, transition probabilities?

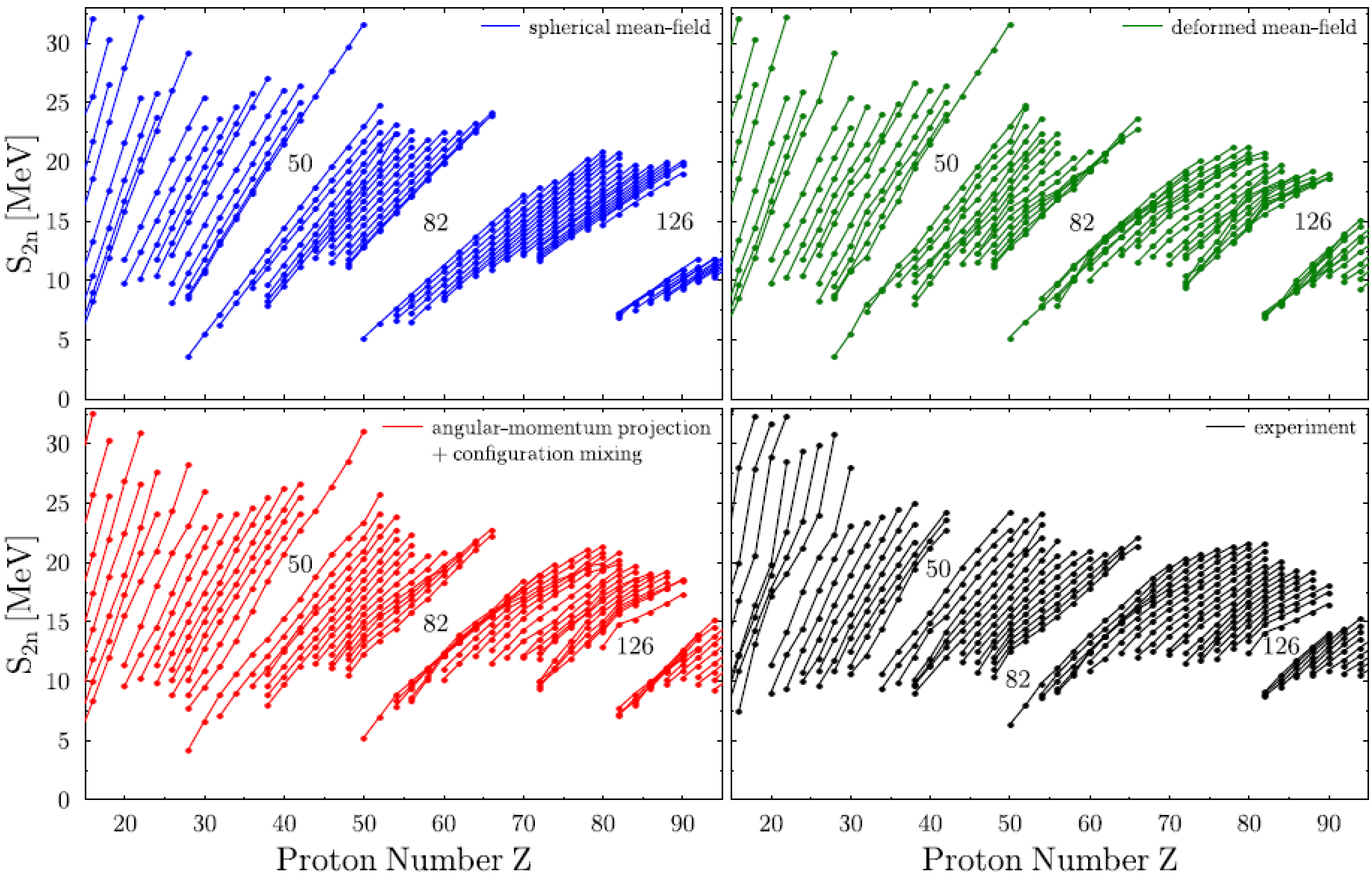
Example: shell effects far from stability

- How do shell effects evolve with N and Z far from stability
- Quenching of shell effects far from stability?
- Coupling between the continuum and the bound sp states?

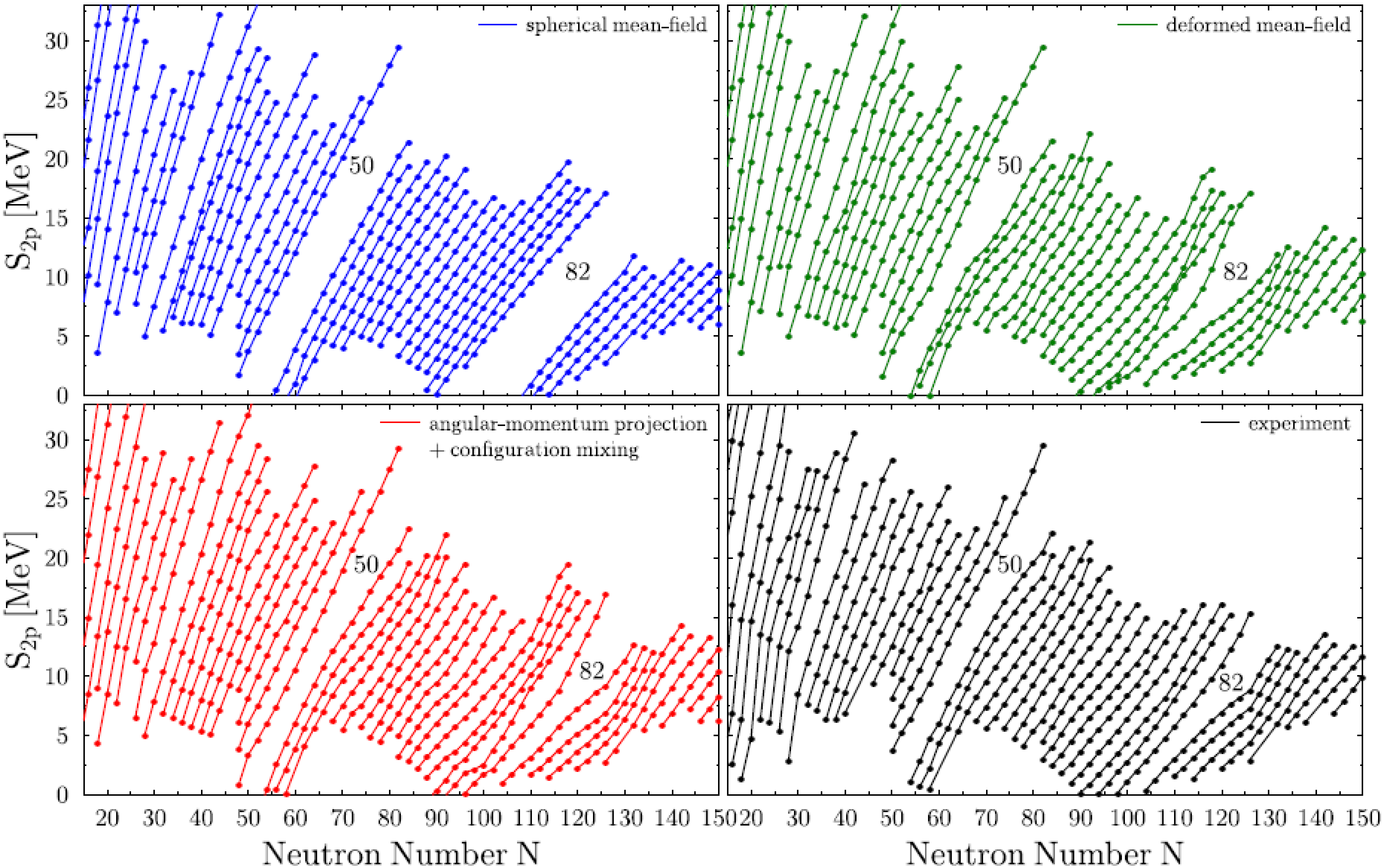
- M. Bender, G. Bertsch, P.-H. Heenen:

Calculation of the ground state of all e-e nuclei including correlations due to symmetry restorations

configuration mixing



spherical mean-field
deformed mean-field
angular-momentum projection
+ configuration mixing
experiment
50
82
126
S_{2n} [MeV]
Proton Number Z
0
5
10
15
20
25
30
20
30
40
50
60
70
80
90



spherical mean-field
deformed mean-field
angular-momentum projection
+ configuration mixing
experiment
50
82
S_{2p} [MeV]
Neutron Number N

Shell closures at N=32 and 34

T. Rodriguez and J. Egido, PRL 99, 062501 (2007)

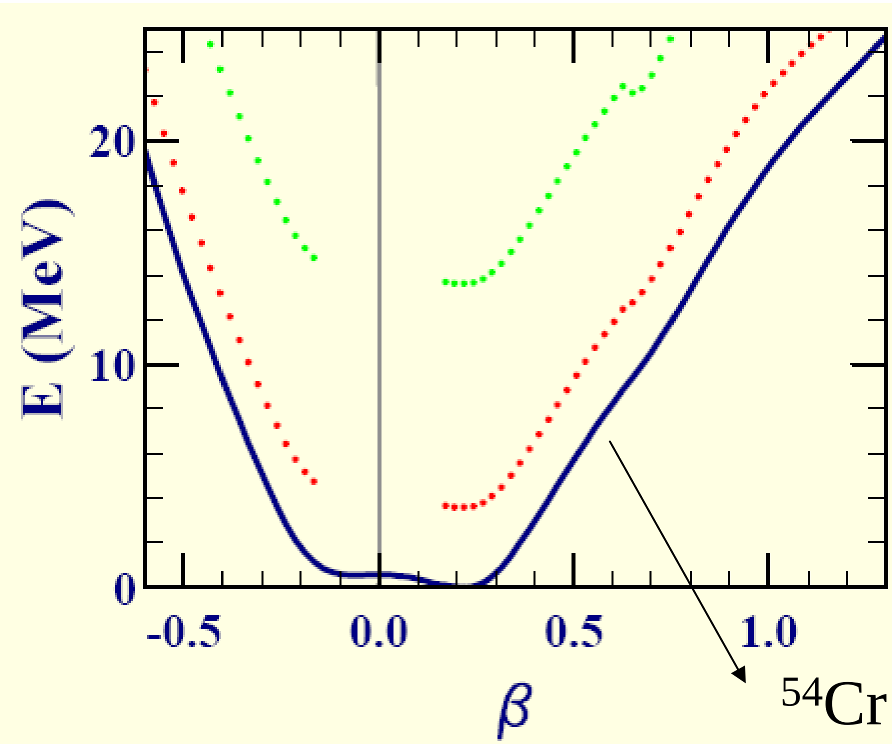
Method: configuration mixing of projected mean-field wave functions

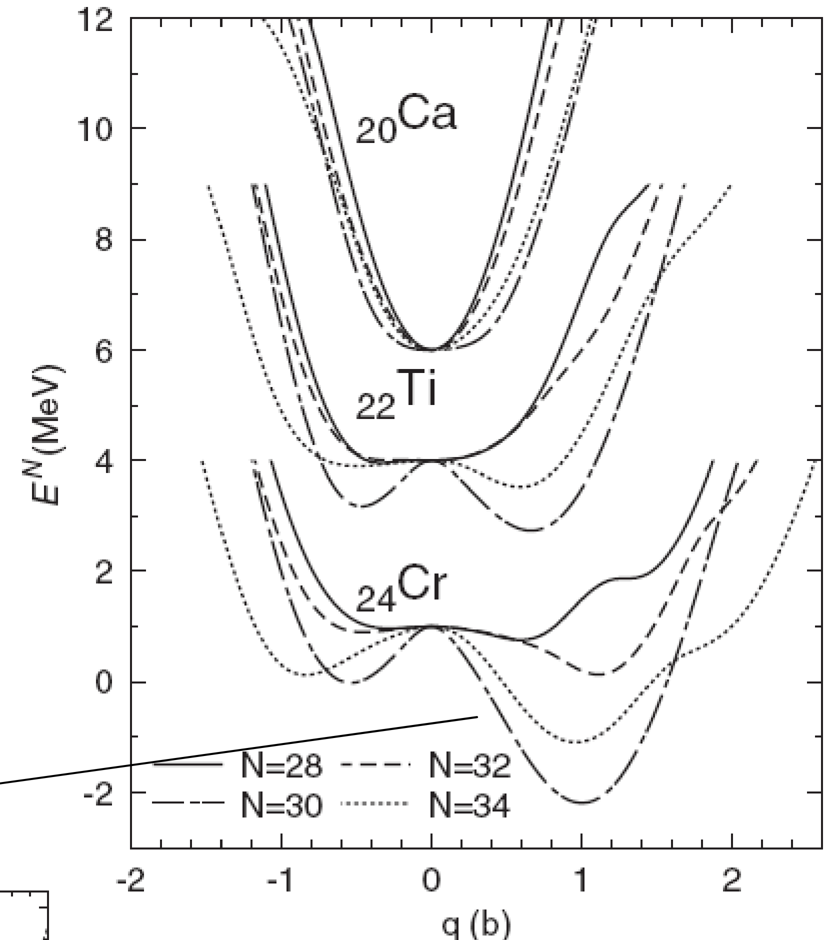
BUT: projection on particle number before to vary the mean-field

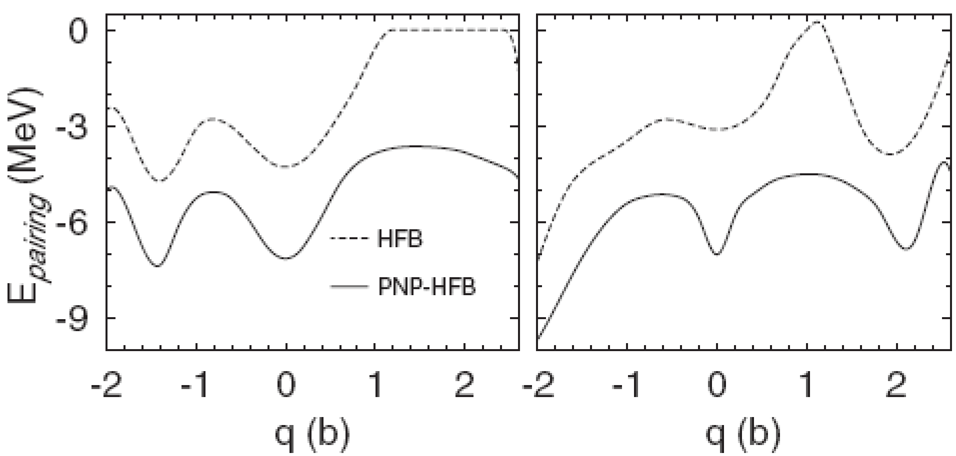
$$|J0q\rangle = \frac{1}{\mathcal{N}_{J0q}} \hat{P}^{J}_{00} \underbrace{\hat{P}_{Z} \hat{P}_{N} |q\rangle}_{\text{performed at the mf level}},$$

It does exactly what is approximated by the Lipkin Nogami prescription

HFB (Bruyeres)







HFB+ VAP

(Rodriguez and Egido)

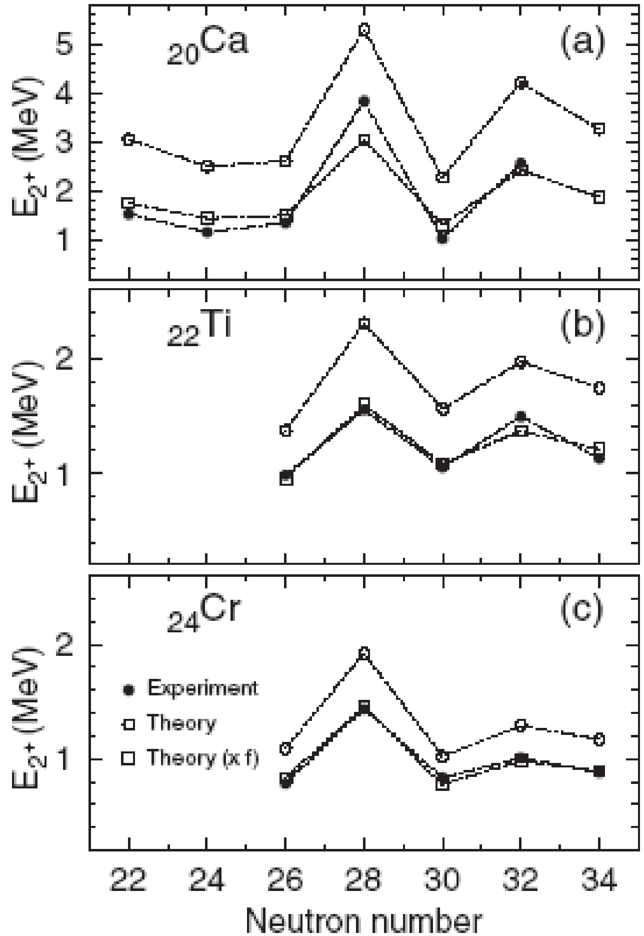


FIG. 4. Excitation energies of the 2_1^+ states for the Ca, Ti, and Cr isotopes; the experimental data are taken from [2] (Ca), [3–6] (Ti), and [7,8] (Cr). The values of the factor f are: 0.58 (Ca), 0.69 (Ti), and 0.76 (Cr).

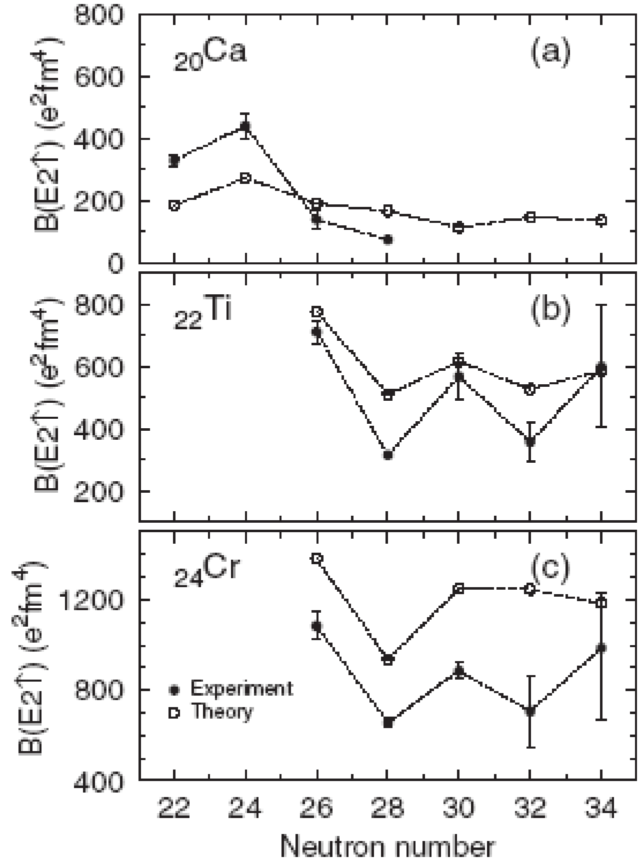


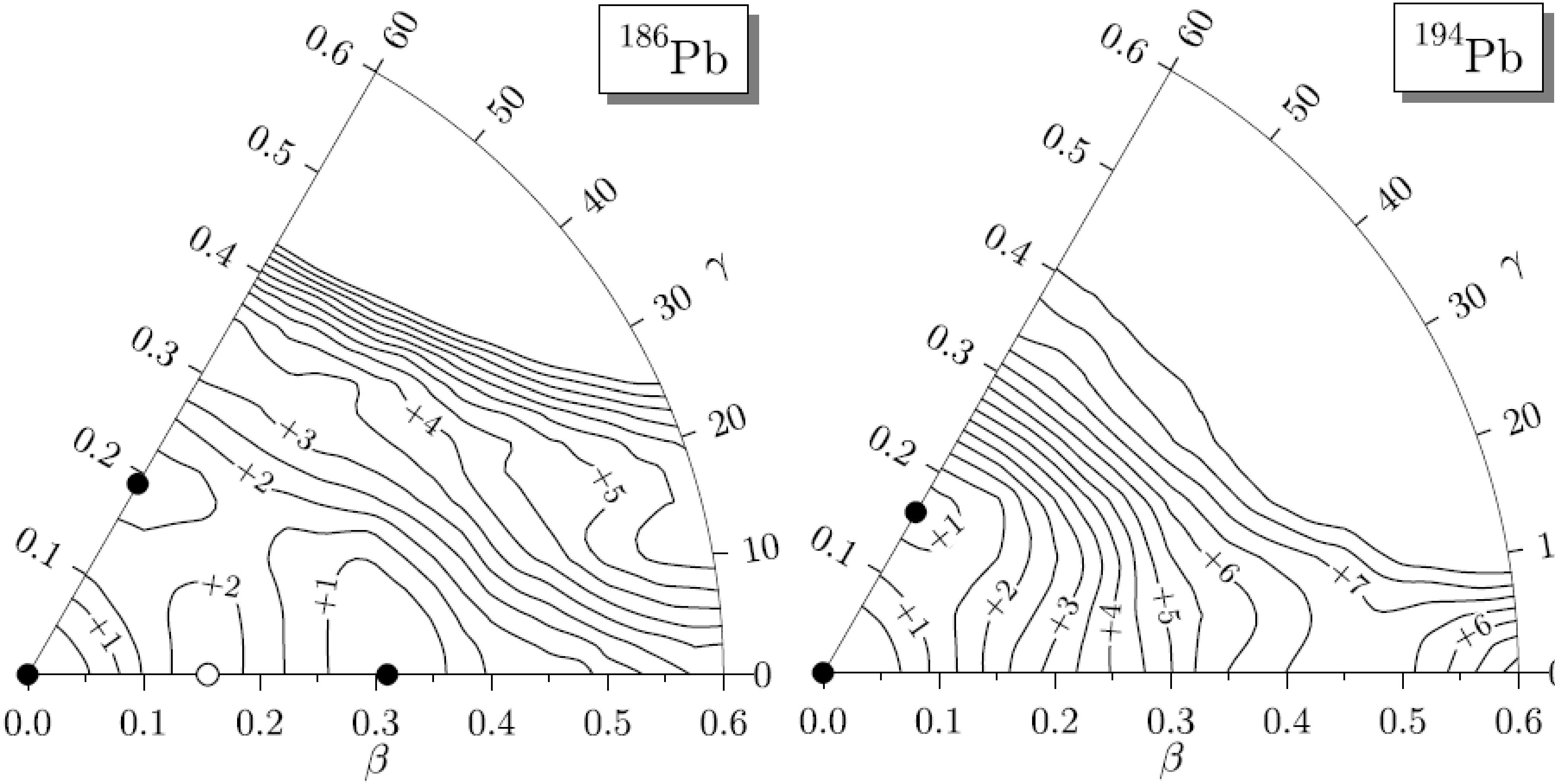
FIG. 5. $E2$ transition probabilities for the Ca, Ti, and Cr isotopes. The experimental data are taken from Ti [9] and Cr [10].

Up to now: restrictions to axial deformations

Why to include triaxiality?

1. Many axial extrema are saddle points
2. Some evidence that optimal path from prolate to oblate through triaxiality
3. overestimation of excitation energies (cure by triaxiality?)
4. breaking of time-reversal invariance:
   - cranking wave functions
   - odd nuclei
   - 2qp excitations

Triaxial deformations of Pb isotopes



Mean-field wave-functions generated by a double constraint:

$$
\begin{aligned}
q_1 &= Q_0 \cos(\gamma) - \frac{1}{\sqrt{3}} Q_0 \sin(\gamma) \\
q_2 &= \frac{2}{\sqrt{3}} Q_0 \sin(\gamma) \,.
\end{aligned}
$$

$$
\beta_2 = \sqrt{\frac{5}{16\pi}}\, \frac{4\pi Q_0}{3R^2 A}
$$

and projected on good angular momentum with the projector:

$$
\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2} \int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \, \sin(\beta) \int_0^{2\pi} d\gamma \, \mathcal{D}^{J\,*}_{MK} \, \hat{R}
$$

projected also on N and Z

Three steps:

1. Projection on N, Z, J, K and M of the mean-field wave functions

$$|JMKq\rangle = \hat{P}^J_{MK}\,\hat{P}^Z\hat{P}^N|q\rangle$$

after projection, *q* is a label (reminder) of the mean-field state
Non orthogonal basis as a function of *q* before and after projection!

2. K-mixing:

$$|JM\kappa q\rangle = \sum_{K=-J}^{+J} f^J_\kappa(K)\,|JMKq\rangle$$

3. Selection of the relevant states (truncation on κ) and mixing on the deformation:

$$|JM\nu\rangle = \sum_q \sum_{\kappa=1}^{\kappa^{J,q}_m} F^J_\nu(\kappa,q)\,|JM\kappa q\rangle$$

(cut-off in κ in J and q)

The coefficients *F* are determined by minimizing the energy:

$$\frac{\delta}{\delta F_\nu^{J\,*}(K,q)} \frac{\langle JM\nu|\hat{H}|JM\nu\rangle}{\langle JM\nu|JM\nu\rangle} = 0$$

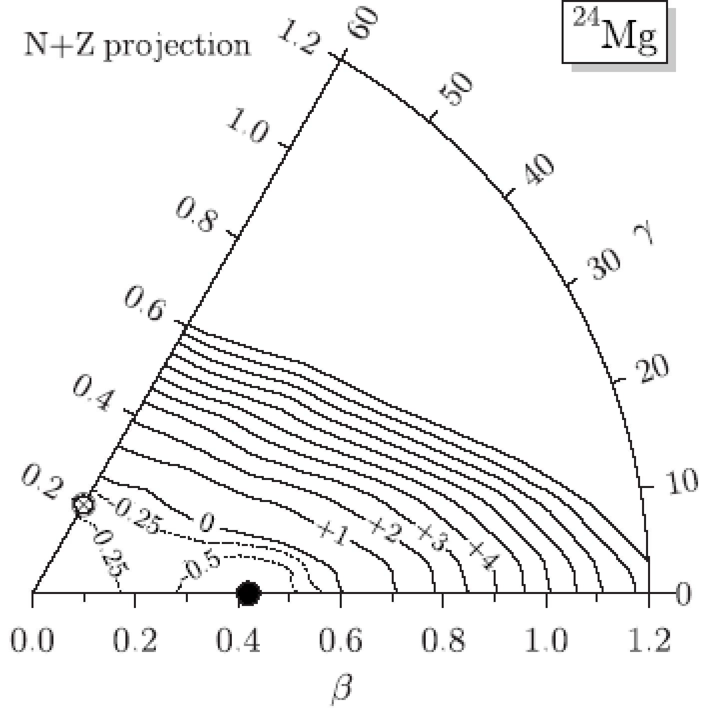
and are obtained by solving the HWG equation:

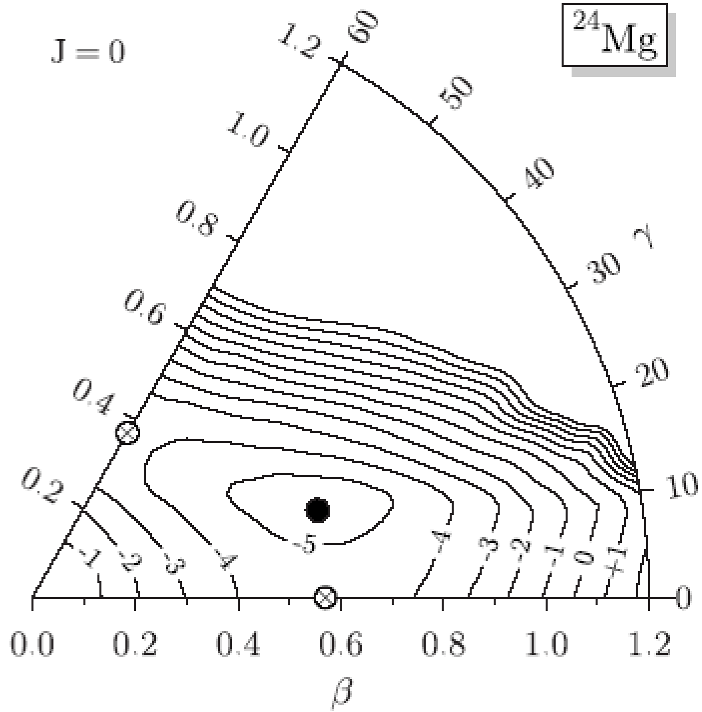
$$\sum_{q'} \sum_{\kappa'=1}^{\kappa_m^{J,q}} \left[\mathcal{H}_J(\kappa,q;\kappa',q') \quad - E_\nu^J \mathcal{I}_J(\kappa,q;\kappa',q')\right] F_\nu^J(\kappa',q') = 0$$

Core of the problem: determination of the kernels:

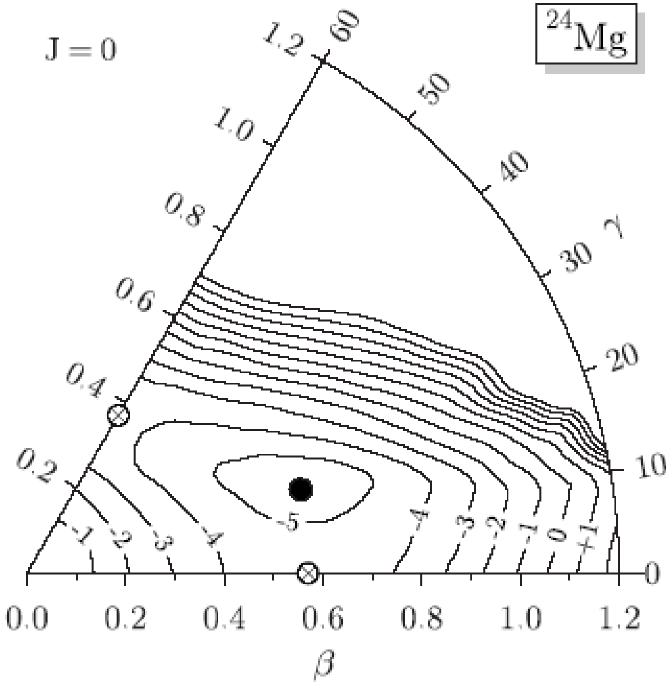
$$\begin{aligned}\mathcal{H}^J(\kappa,q;\kappa',q') &= \langle JM\kappa q|\hat{H}|JM\kappa' q'\rangle \\ \mathcal{I}^J(q,\kappa;q',\kappa') &= \langle JM\kappa q|JM\kappa' q'\rangle\,.\end{aligned}$$

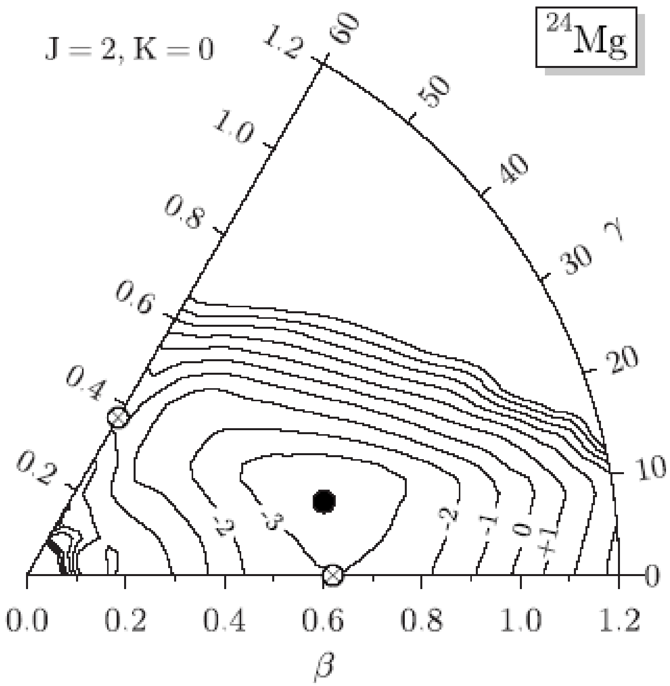
Projection of triaxial map:





Triaxial minimum?
lost of the meaning of *q* after projection!
no orthogonality of wave functions!





z=symmetry axis

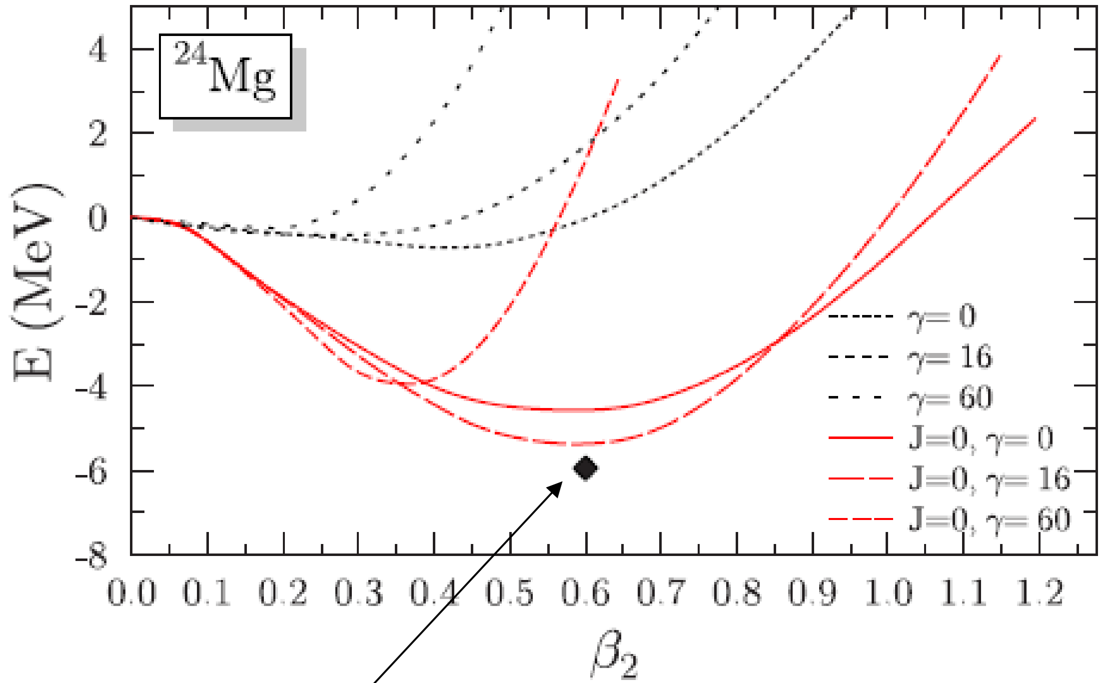
the maps for the other orientations have no simple interpretations

Configuration mixing:

comparison between different bases:

1. purely prolate
2. axial
3. purely triaxial
4. triaxial + a few prolate configurations

Cut in the Q,γ plane: and GCM calculations



All the GCM calculations: axial (prolate+oblate)

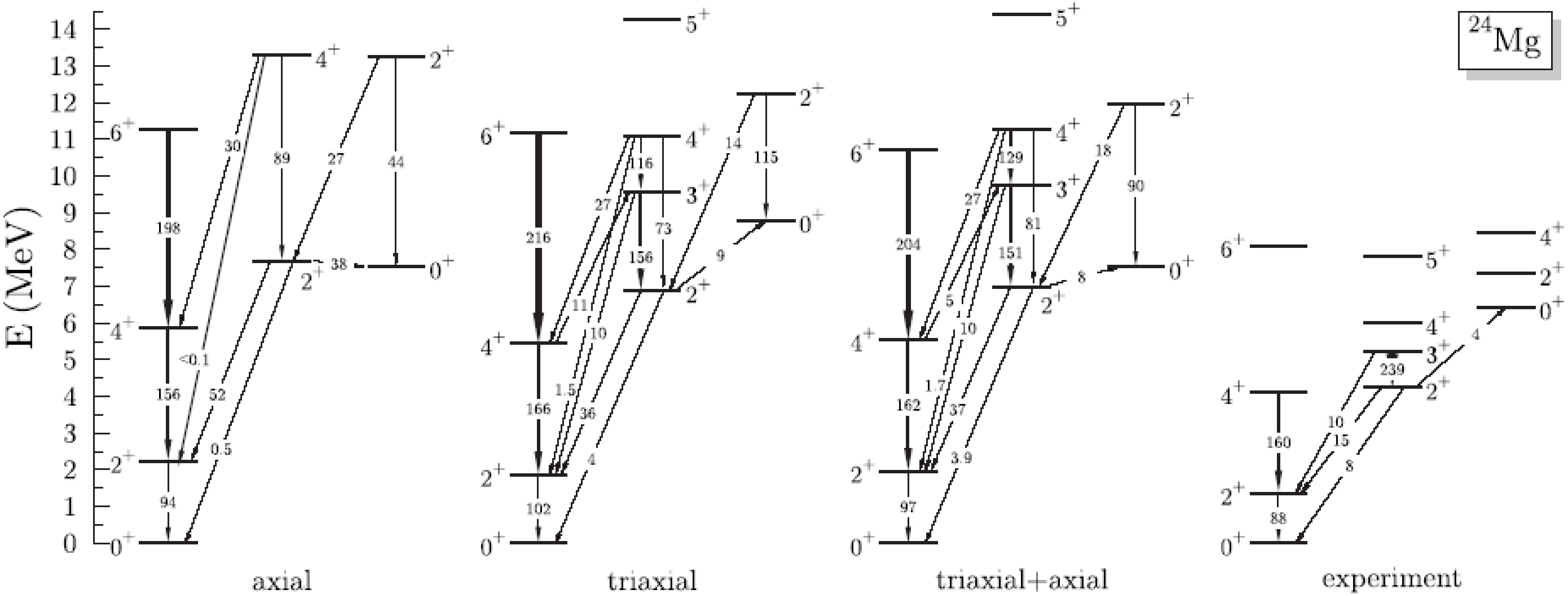
purely triaxial (35 keV lower than axial)

triaxial + prolate (160 keV lower than triaxial)

Triaxial correlations described by configuration mixing of axial configurations!

Spectra in 3 bases

No vectors in common!



increase of energy for excited states
due to the correlations in the ground state!

TABLE III: Comparison of calculated excitation energies in MeV and spectroscopic quadrupole moments in units of e fm^2 with experimental values taken from Ref. [82].

level	E_{ex}				Q_s			
	ax	triax	compl	Expt.	ax	triax	compl	Expt.
2_1^+	2.24	1.87	1.97	1.37	−17.1	−19.6	−19.4	−16.6 (6)
4_1^+	5.88	5.44	5.57	4.12	−25.1	−26.1	−26.0	
2_2^+	7.69	6.88	6.99	4.24	9.9	17.1	16.6	
3_1^+	—	9.59	9.74	5.24	—	−0.1	−0.1	
4_2^+	13.29	11.12	11.28	6.01	9.0	−7.3	−7.4	
0_2^+	7.53	8.79	7.520	6.42	0.0	0.0	0.0	0.0

Remaining error eliminated by breaking time reversal invariance? (cranking)

	triaxial		full	
	prolate	axial	prolate	axial
	0.97	0.99	097	0.99
$J = 0$	0.89	0.94	0.96	0.97
	0.16	0.93	-	0.96
	097	0.98	0.97	0.98
$J = 2$	0.21	0.86	0.23	0.88
	0.88^*	0.82	0.88^*	0.81

Weight of the eigenstates of triaxial and triaxial+prolate GCM in the prolate and prolate+oblate GCM

The future

- Breaking of time reversal invariance (in principle ready, phase problem?)
- Projection of cranked states optimized for the J-value on which they are projected
- Odd nuclei = 1qp states
- Interaction problems
- Test of models…