MR-EDF calculations of odd-even nuclei

Benjamin Bally[1],

B. Avez[1], M. Bender[1] and P.-H. Heenen[2]

[1] Université Bordeaux 1; CNRS/IN2P3; Centre d'Etudes Nucléaires de Bordeaux Gradignan, UMR5797, Chemin du Solarium, BP120, F-33175 Gradignan, France
[2] Service de Physique Nucléaire Théorique, Université Libre de Bruxelles, C.P. 229, B-1050 Bruxelles, Belgium

Introduction

- Treatment of even-even and odd-even nuclei on the same footing.
- Particle number and angular momentum restored GCM of cranked triaxial quasiparticle states.
- Motivations :
  - Odd-A nuclei represent half of the chart of nuclides.
  - Coupling of single particle and shape degrees of freedom.
  - Analysis of signatures for shell structure (separation energies, g factors, spectroscopic quadrupole moments, ...).
  - Analysis of the interplay of pairing correlations and fluctuations in shape degrees of freedom for the odd-even mass staggering.
  - Study of coexistence phenomena (shape, single-particle levels).

Theoritical model

Philosophy of the approach

- Energy Density Functional : $\mathcal{E}[\rho, \kappa, \kappa^*]$

$$\rho_{ij}^{LR} = \frac{\langle \Psi_L | c_j^\dagger c_i | \Psi_R \rangle}{\langle \Psi_L | \Psi_R \rangle} \qquad \kappa_{ij}^{LR} = \frac{\langle \Psi_L | c_j c_i | \Psi_R \rangle}{\langle \Psi_L | \Psi_R \rangle} \qquad \kappa_{ij}^{*\,RL} = \frac{\langle \Psi_L | c_i^\dagger c_j^\dagger | \Psi_R \rangle}{\langle \Psi_L | \Psi_R \rangle}$$

- First step : Single-Reference EDF ("Self-consistent mean field", "HFB")

SR-EDF : "HFB" realization

- Minimization with constraint : $\delta(\mathcal{E} - \lambda\langle\hat{N}\rangle - \lambda_q\langle\hat{Q}\rangle) = 0$

  λ, λ_q : lagrange multipliers
  $\hat{N}$: particle number operator
  $\hat{Q}$: multipole operator

- "HFB" equations :

$$\begin{pmatrix} \hat{h} - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}^* + \lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix}$$

  $\hat{h} = \frac{\partial \mathcal{E}}{\partial \rho}$: particle-hole field $\quad \hat{\Delta} = \frac{\partial \mathcal{E}}{\partial \kappa^*}$: particle-particle field

  $\rho = V^* V^T \qquad \kappa = V^* U^T$

- Self-iterative blocking : $(U_{ki}, V_{ki}) \leftrightarrow ({V_{ki}}^*, {U_{ki}}^*)$

SR-EDF : "HFB+LN" realization

- Minimization with constraint : $\delta(\mathcal{E} - \lambda\langle\hat{N}\rangle - \lambda_2\langle\hat{N}^2\rangle - \lambda_q\langle\hat{Q}\rangle) = 0$

  λ_2 : not a lagrange multiplier
  λ, λ_q : lagrange multipliers
  $\hat{N}$: particle number operator
  $\hat{Q}$: multipole operator

- "HFB+LN" equations :

$$\begin{pmatrix} \hat{h} - \lambda & \hat{\Delta} \\ -\hat{\Delta}^* & -\hat{h}^* + \lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix}$$

$\hat{h} = \frac{\partial\mathcal{E}}{\partial\rho}$: particle-hole field $\quad \hat{\Delta} = \frac{\partial\mathcal{E}}{\partial\kappa^*}$: particle-particle field

$\rho = V^* V^T \qquad \kappa = V^* U^T$

- Self-iterative blocking : $(U_{ki}, V_{ki}) \leftrightarrow ({V_{ki}}^*, {U_{ki}}^*)$

SR-EDF : symmetries of the code

- Triaxial cranking code "CR8".

  P. Bonche, H. Flocard, P.-H. Heenen, S.J. Krieger and M.S. Weiss, Nucl. Phys. A 443 (1985) 39-63

- D_{2h}^{TD} subgroup { $\hat{R}_x$, $\hat{S}_y^T$, $\hat{P}$ } :

  X signature : $\hat{R}_x = e^{-i\pi \hat{J}_x}$.

  Y time-simplex : $\hat{S}_y^T = \hat{T}\hat{P}e^{-i\pi \hat{J}_y}$.

  Parity : $\hat{P}$.

SR-EDF : symmetries of the code

- Triaxial cranking code "CR8".

  P. Bonche, H. Flocard, P.-H. Heenen, S.J. Krieger and M.S. Weiss, Nucl. Phys. A 443 (1985) 39-63

- D_{2h}^{TD} subgroup $\{\ \hat{R}_x, \hat{S}_y^T, \hat{P}\ \}$:

  X signature : $\hat{R}_x = e^{-i\pi \hat{J}_x}$.

  Y time-simplex : $\hat{S}_y^T = \hat{T}\hat{P}e^{-i\pi \hat{J}_y}$.

  Parity : $\hat{P}$.

even-even vacua

$$\hat{R}_x|\Phi\rangle = |\Phi\rangle$$
$$\hat{P}|\Phi\rangle = |\Phi\rangle$$
$$\hat{S}_y^T|\Phi\rangle = |\Phi\rangle$$

SR-EDF : symmetries of the code

- Triaxial cranking code "CR8".

  P. Bonche, H. Flocard, P.-H. Heenen, S.J. Krieger and M.S. Weiss, Nucl. Phys. A 443 (1985) 39-63

- D_{2h}^{TD} subgroup { $\hat{R}_x$, $\hat{S}_y^T$, $\hat{P}$ } :

  X signature : $\hat{R}_x = e^{-i\pi \hat{J}_x}$.

  Y time-simplex : $\hat{S}_y^T = \hat{T}\hat{P}e^{-i\pi \hat{J}_y}$.

  Parity : $\hat{P}$.

even-even vacua

$$\hat{R}_x|\Phi\rangle = |\Phi\rangle$$
$$\hat{P}|\Phi\rangle = |\Phi\rangle$$
$$\hat{S}_y^T|\Phi\rangle = |\Phi\rangle$$

odd-even nuclei

$$\hat{R}_x|\Phi\rangle = \pm i\,|\Phi\rangle$$
$$\hat{P}|\Phi\rangle = \pm|\Phi\rangle$$
$$\hat{S}_y^T|\Phi\rangle = |\Phi\rangle$$

Philosophy of the approach

- Energy Density Functional : $\mathcal{E}[\rho, \kappa, \kappa^*]$

$$\rho_{ij}^{LR} = \frac{\langle \Psi_L | c_j^\dagger c_i | \Psi_R \rangle}{\langle \Psi_L | \Psi_R \rangle} \qquad \kappa_{ij}^{LR} = \frac{\langle \Psi_L | c_j c_i | \Psi_R \rangle}{\langle \Psi_L | \Psi_R \rangle} \qquad \kappa_{ij}^{*\,RL} = \frac{\langle \Psi_L | c_i^\dagger c_j^\dagger | \Psi_R \rangle}{\langle \Psi_L | \Psi_R \rangle}$$

- First step : Single-Reference EDF ("Self-consistent mean field", "HFB")

  ✔ takes into account static collective correlations.
  ✘ loss of quantum numbers and selection rules for transitions.

- Second step : Multi-Reference EDF ("Beyond mean field")

MR-EDF : symmetry restoration

Angular-momentum restoration operator :

$$\hat{P}^J_{MK} = \frac{2J+1}{8\pi^2} \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \, \sin(\beta) \int_0^{2\pi} d\gamma \, \underbrace{\mathcal{D}^{*J}_{MK}(\alpha,\beta,\gamma)}_{\text{Wigner function}} \, \overbrace{\hat{R}(\alpha,\beta,\gamma)}^{\text{rotation in real space}}$$

K is the z component of angular momentum in the body-fixed frame.

Projected states are given by

$$|JMq\kappa\rangle = \sum_{K=-J}^{+J} f_{J,\kappa}(K) \, \hat{P}^J_{MK} \, \hat{P}^Z \, \hat{P}^N \, |q\rangle = \sum_{K=-J}^{+J} f_{J,\kappa}(K) \, |JMKq\rangle$$

$f_{J,\kappa}(K)$ are the weights of the components K and determined variationally

MR-EDF : configuration mixing via the "Generator Coordinate Method"

Superposition of angular-momentum restored SR-EDF states

$$|JM\nu\rangle = \sum_q \sum_{K=-J}^{+J} f_{J\nu}(q,K)\,|JMKq\rangle \qquad \begin{cases} |JMKq\rangle & \text{projected mean-field state} \\ f_{J\nu}(q,K) & \text{weight function} \end{cases}$$

$$\frac{\delta}{\delta f^*_{J\nu}(q,K)} \frac{\langle JM\nu|\hat{H}|JM\nu\rangle}{\langle JM\nu|JM\nu\rangle} = 0 \quad \Rightarrow \quad \text{Hill-Wheeler-Griffin equation}$$

$$\sum_{q'} \sum_{K'=-J}^{+J} \left[\mathcal{H}_J(qK,q'K') - E_{J,\nu}\,\mathcal{I}_J(qK,q'K')\right] f_{J,\nu}(q',K') = 0$$

with

$$\begin{aligned} \mathcal{H}_J(qK,q'K') &= \langle JMKq|\hat{H}|JMK'q'\rangle & \text{energy kernel} \\ \mathcal{I}_J(qK,q'K') &= \langle JMKq|JMK'q'\rangle & \text{norm kernel} \end{aligned}$$

Angular-momentum projected GCM gives the

- correlated ground state for each value of J
- spectrum of excited states for each J

Philosophy of the approach

- Energy Density Functional : $\mathcal{E}[\rho, \kappa, \kappa^*]$

$$\rho_{ij}^{LR} = \frac{\langle \Psi_L | c_j^\dagger c_i | \Psi_R \rangle}{\langle \Psi_L | \Psi_R \rangle} \qquad \kappa_{ij}^{LR} = \frac{\langle \Psi_L | c_j c_i | \Psi_R \rangle}{\langle \Psi_L | \Psi_R \rangle} \qquad \kappa_{ij}^{*\,RL} = \frac{\langle \Psi_L | c_i^\dagger c_j^\dagger | \Psi_R \rangle}{\langle \Psi_L | \Psi_R \rangle}$$

- First step : Single-Reference EDF ("Self-consistent mean field", "HFB")

  ✔ takes into account static collective correlations.
  ✘ loss of quantum numbers and selection rules for transitions.

- Second step : Multi-Reference EDF ("Beyond mean field")

  ✔ takes into account fluctuations in collective degrees of freedom.
  ✔ restoration of quantum numbers and selection rules for transitions.

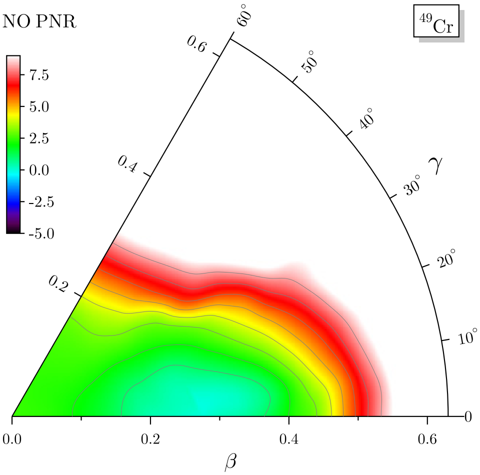
Preliminary results about ^{49}Cr

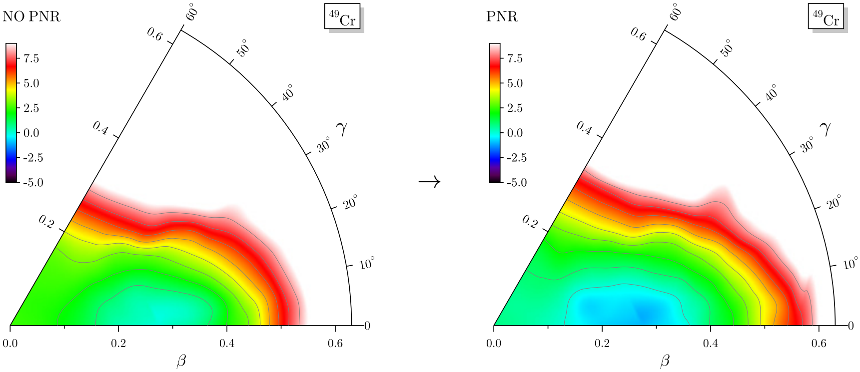
Choice of the functional

- Skyrme parametrization SIII.
- Delta force pairing
  (strength : 300 MeV for neutrons and protons).
- No coulomb exchange.
- Regularization of the functional to avoid the "pole problem".
  M. Bender, T. Duguet, P.-H. Heenen, D. Lacroix, Int. J. Mod. Phys. E 20 (2011) 259-269

Non-projected energy surface

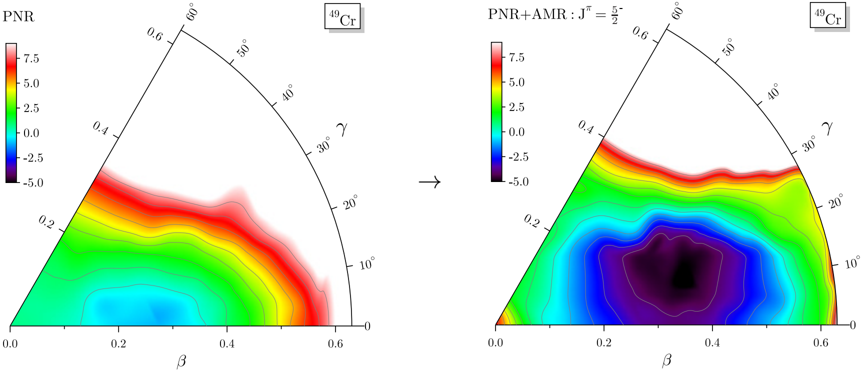
From the lowest quasiparticle with $\langle J_z \rangle^\pi \approx |2.5|^-$



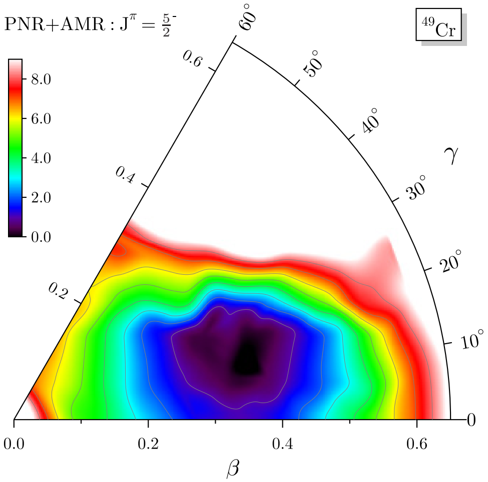


NO PNR
7.5
5.0
2.5
0.0
-2.5
-5.0
49Cr
60°
50°
40°
30°
20°
10°
0
γ
0.6
0.4
0.2
0.0
0.2
0.4
0.6
β
→
PNR
7.5
5.0
2.5
0.0
-2.5
-5.0
49Cr
60°
50°
40°
30°
20°
10°
0
γ
0.6
0.4
0.2
0.0
0.2
0.4
0.6
β

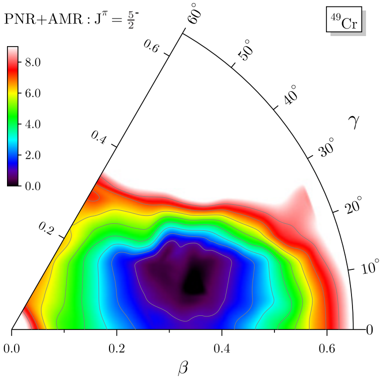
PNR → PNR+AMR : $J^\pi = \frac{5}{2}^-$ energy surface



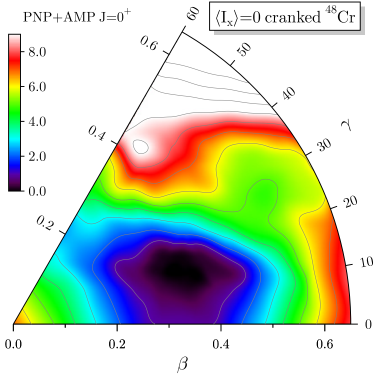
PNR+AMR : $J^\pi = \frac{5}{2}^-$ energy surface



^{49}Cr versus ^{48}Cr

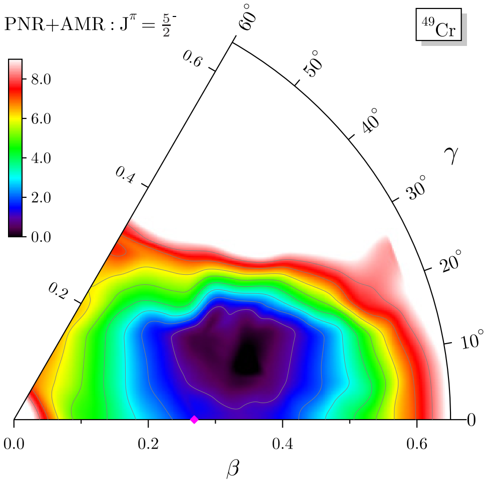


VS

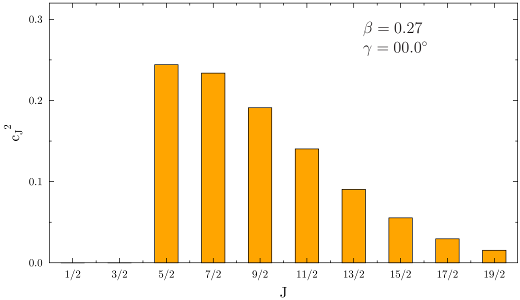


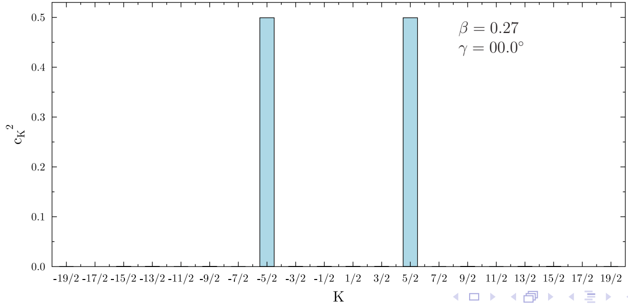
M. Bender, B. Avez, P.-H. Heenen, unpublished

PNR+AMR : $J^\pi = \frac{5}{2}^-$ energy surface

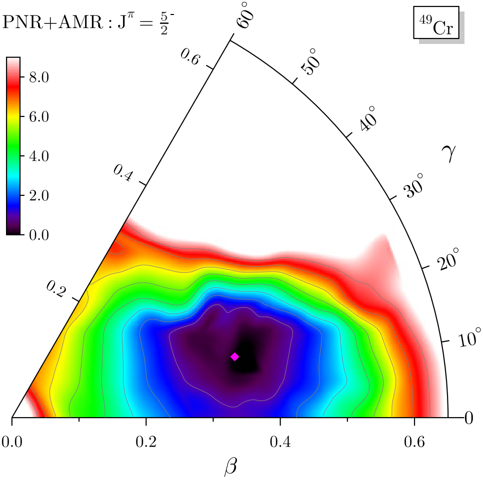


J and K decompositions

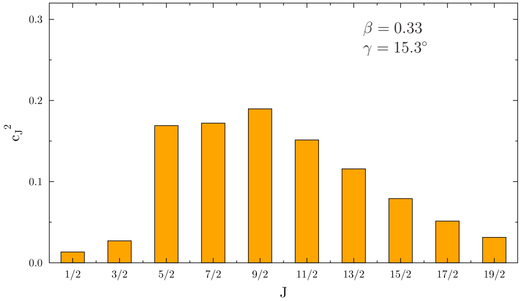


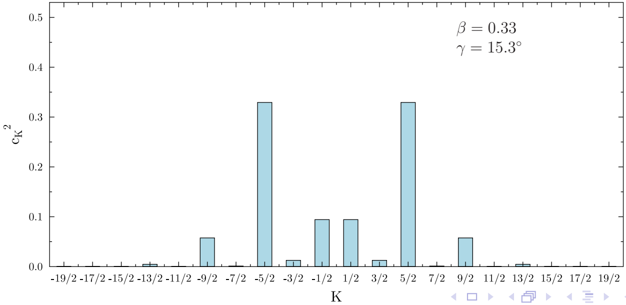


PNR+AMR : $J^\pi = \frac{5}{2}^-$ energy surface

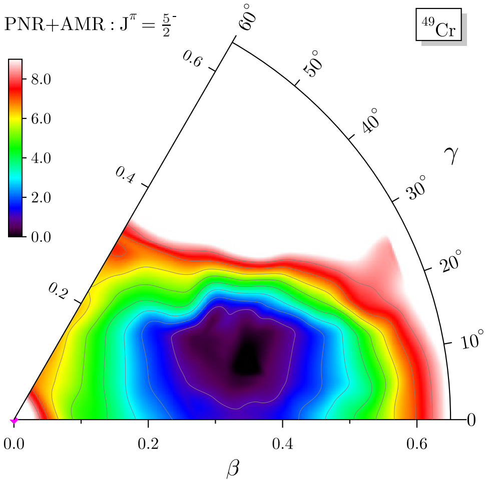


J and K decompositions

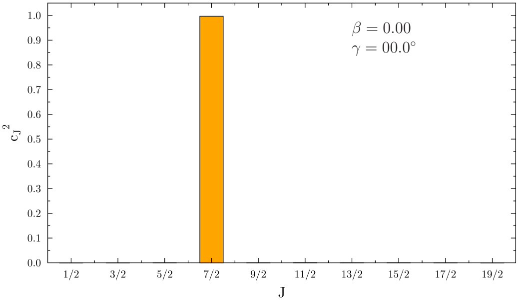


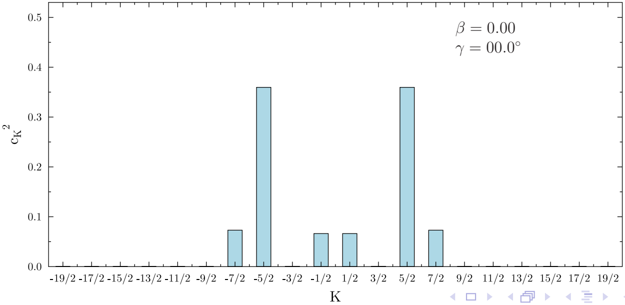


PNR+AMR : $J^\pi = \frac{5}{2}^-$ energy surface

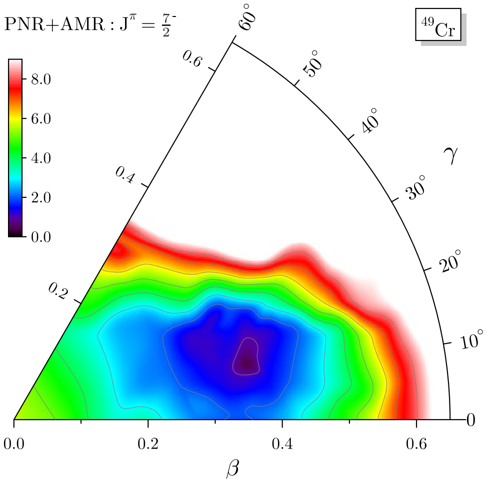


J and K decompositions

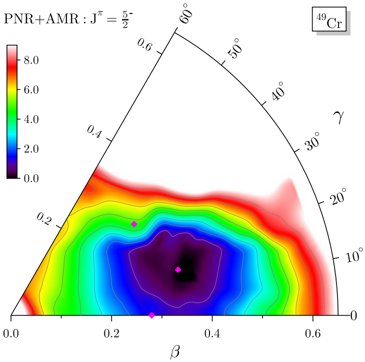




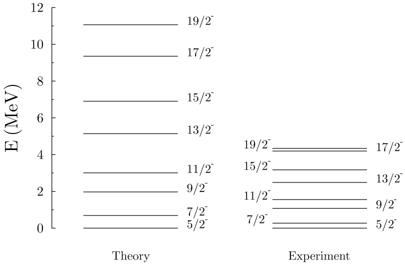
PNR+AMR : $J^\pi = \frac{7}{2}^-$ energy surface



Incomplete GCM (3 points)



→



Experiment : T.W. Burrows, Nuclear Data Sheets 109 (2008) 1879-2032

Cranking

- $\delta(\mathcal{E} - \lambda\langle\hat{N}\rangle - \lambda_2\langle\hat{N}^2\rangle - \lambda_q\langle\hat{Q}\rangle - \omega\langle\hat{J}_x\rangle) = 0$

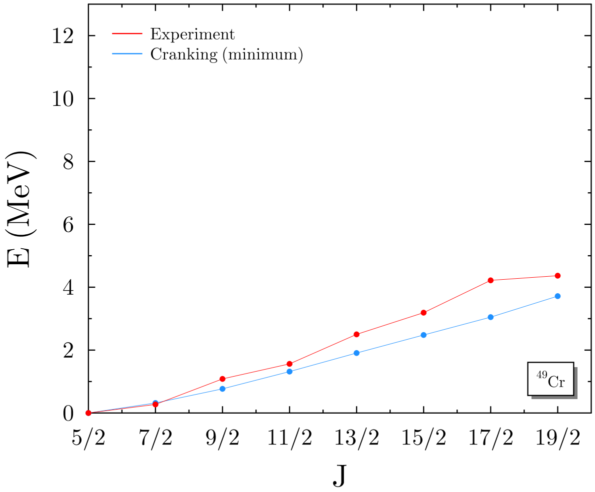
  ω : lagrange parameter

- $\langle\hat{J}_x\rangle = \sqrt{J^2 - K^2}$

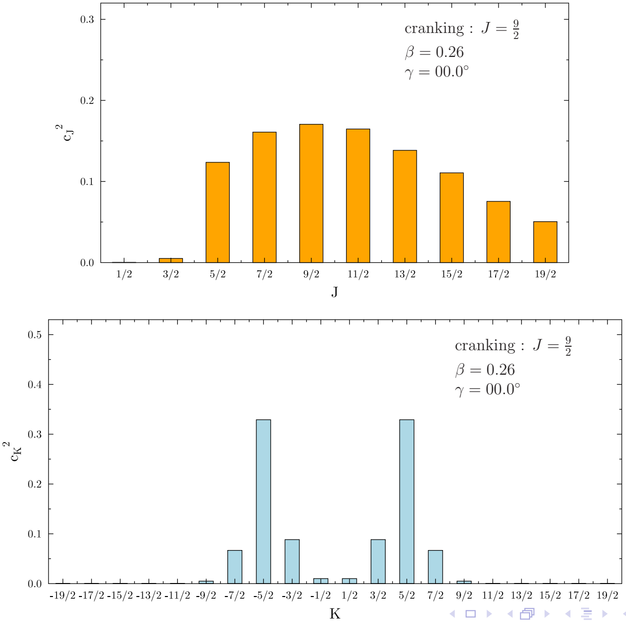
  $K = \frac{5}{2}$ ($\rightarrow$ see K decompositions)

- Projection of cranked states should improve the moments of inertia.

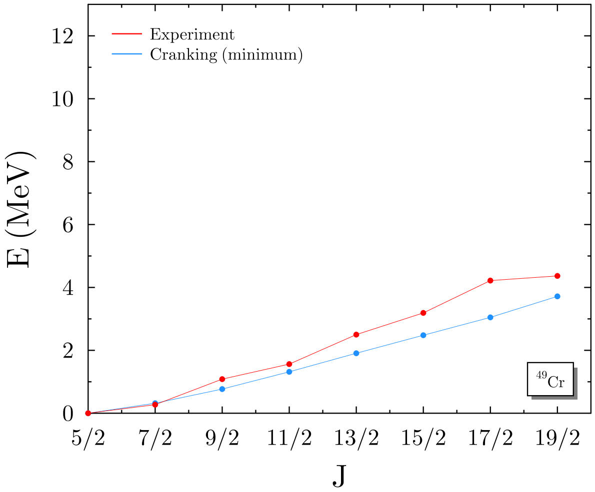
Experiment vs Cranking



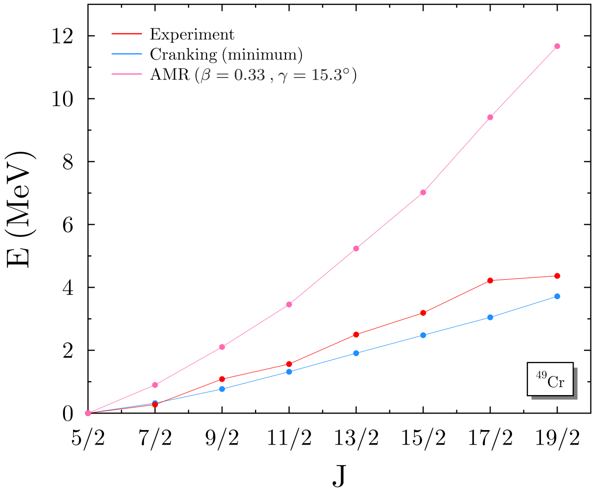
J and K decompositions (cranking) → arbitrary J assignement !



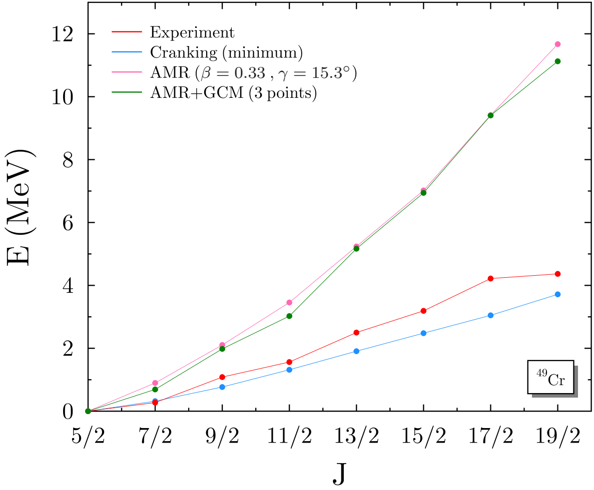
Experiment vs Cranking



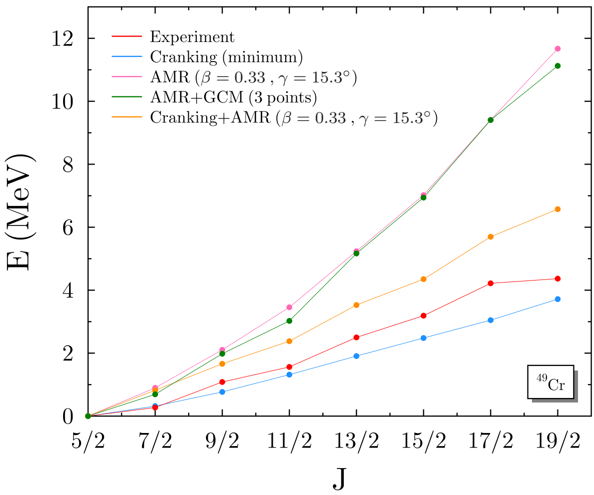
Experiment vs Cranking vs AMR



Experiment vs Cranking vs AMR vs AMR+GCM



Experiment vs Cranking vs AMR vs AMR+GCM vs Cranking+AMR



Conclusions

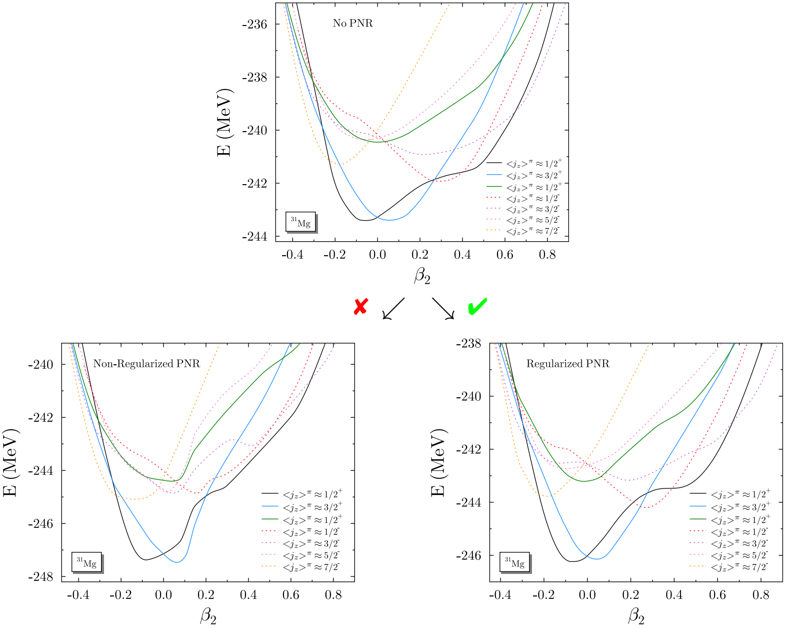
- Treatment of even-even and odd-even nuclei on the same footing !

  $\rightarrow$ Particle number and angular momentum restored GCM of cranked triaxial quasiparticle states.

- Preliminary results about ^{49}Cr.
  - $J^\pi = \frac{5}{2}^-$ triaxial minimum
  - Correct structure of the first rotational band.
  - Cranking+AMR improves a lot the moments of inertia.

- A lot remains to be learnt !

Backup slides


No PNR
Non-Regularized PNR
Regularized PNR
31Mg
E (MeV)
β2
<jz>π ≈ 1/2+
<jz>π ≈ 3/2+
<jz>π ≈ 1/2+
<jz>π ≈ 1/2-
<jz>π ≈ 3/2-
<jz>π ≈ 5/2-
<jz>π ≈ 7/2-

Deformation paramater : $\beta_2 = \sqrt{\frac{5}{16}} \frac{4\pi}{3R^2 A} \langle Q_2 \rangle$