

Criticality in the Interacting Boson Model with configuration mixing

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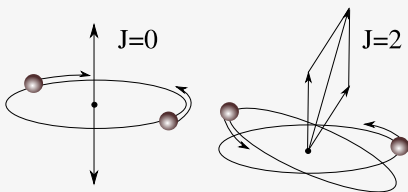
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Outline

- 1 The interacting boson model (IBM)
- 2 U(5)-QQ mixing
- 3 QQ-QQ mixing
- 4 Conclusions and outlook

The interacting boson model

Basic building blocks



Nucleon pairs coupled to $J = 0$ and $J = 2$ are approximately treated as s and d bosons. These are the basic building blocks of the IBM.

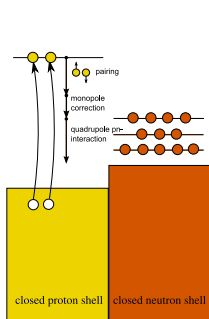
The Hamiltonian is 'generated' by group theory

$$\hat{H}_{\text{cwf}} = \varepsilon \hat{n}_d + \kappa \hat{Q}(\chi) \cdot \hat{Q}(\chi)$$

Three symmetry limits in which the Hamiltonian is analytically solvable

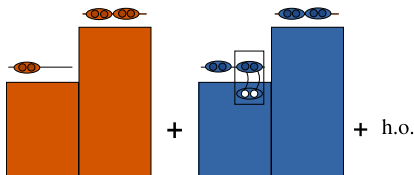
- ▶ **U(5)-limit** : $\kappa = 0$
- ▶ **SU(3)-limit** : $\varepsilon = 0$ and $\chi = \pm\sqrt{7}/2$
- ▶ **O(6)-limit** : $\varepsilon = 0$ and $\chi = 0$

The interacting boson model with configuration mixing



If particle-hole configurations out of a closed shell are sufficiently lowered in energy, **configuration mixing** occurs.

K. Heyde et al., Nucl. Phys. A466, 189 (1987)



The IBM Hamiltonian can be extended to include particle-hole configurations

$$\hat{H} = \hat{P}_N^\dagger \hat{H}_{\text{cqf}}^N \hat{P}_N + \hat{P}_{N+2}^\dagger \left(\hat{H}_{\text{cqf}}^{N+2} + \Delta^{N+2} \right) \hat{P}_{N+2} + \hat{V}_{\text{mix}}^{N, N+2} + \text{h.o.}$$

Δ^{N+2} takes corrected excitation energy of 2p-2h configuration into account

Geometry of the IBM

A single configuration

J. N. Ginocchio *et al.*, Phys. Rev. Lett. 44, 1744 (1980)

IBM

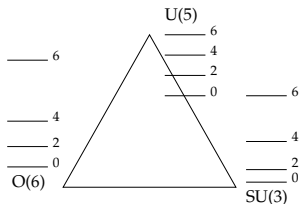
calculate expectation value



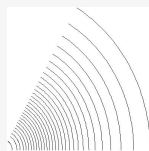
energy surface in β and γ

in intrinsic state

$$E^N(\beta, \gamma; \varepsilon, \kappa, \chi) = \varepsilon N \frac{\beta^2}{1 + \beta^2} + \kappa \left[\frac{N [5 + (1 + \chi^2)\beta^2]}{1 + \beta^2} + \frac{N(N-1)}{(1 + \beta^2)^2} \left(\frac{2}{7} \chi^2 \beta^4 - 4\sqrt{\frac{2}{7}} \chi \beta^3 \cos(3\gamma) + 4\beta^2 \right) \right]$$



U(5): vibrational



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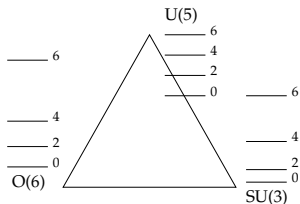
calculate expectation value



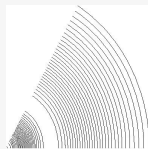
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$$E^N(\beta, \gamma; \varepsilon, \kappa, \chi) = \varepsilon N \frac{\beta^2}{1 + \beta^2} + \kappa \left[\frac{N [5 + (1 + \chi^2)\beta^2]}{1 + \beta^2} + \frac{N(N-1)}{(1 + \beta^2)^2} \left(\frac{2}{7} \chi^2 \beta^4 - 4\sqrt{\frac{2}{7}} \chi \beta^3 \cos(3\gamma) + 4\beta^2 \right) \right]$$



O(6): γ -unstable rotor



Geometry of the IBM

A single configuration

J. N. Ginocchio *et al.*, Phys. Rev. Lett. **44**, 1744 (1980)

IBM

calculate expectation value



energy surface in β and γ

in intrinsic state

$$E^N(\beta, \gamma; \varepsilon, \kappa, \chi) = \varepsilon N \frac{\beta^2}{1 + \beta^2} + \kappa \left[\frac{N [5 + (1 + \chi^2)\beta^2]}{1 + \beta^2} + \frac{N(N-1)}{(1 + \beta^2)^2} \left(\frac{2}{7} \chi^2 \beta^4 - 4\sqrt{\frac{2}{7}} \chi \beta^3 \cos(3\gamma) + 4\beta^2 \right) \right]$$

Mixing between two configurations

A. Frank *et al.*, Phys. Rev. C **69**, 034323 (2004)

IBM with configuration mixing



energy surface in β and γ

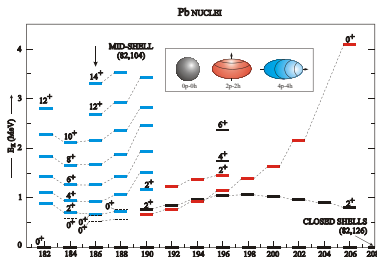
energies are the eigenvalues of

energy surface is lowest eigenvalue of

$$\begin{pmatrix} H_{\text{cwf}}^N & V_{\text{mix}}^{N, N+2} \\ \tilde{V}_{\text{mix}}^{N, N+2} & H_{\text{cwf}}^{N+2} + \Delta \end{pmatrix}$$

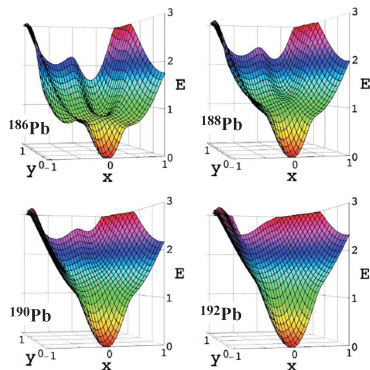
$$\begin{pmatrix} E^N(\beta, \gamma; \varepsilon_1, \kappa_1, \chi_1) & \omega(\beta) \\ \omega(\beta) & E^{N+2}(\beta, \gamma; \varepsilon_2, \kappa_2, \chi_2) + \Delta \end{pmatrix}$$

Motivation



- ▶ $Z=82$ is a magic number
- ▶ systematic lowering of two collective bands when proceeding towards neutron midshell
- ▶ these collective bands are understood as arising from $2p-2h$ and $4p-4h$ excitations across the closed $Z=82$ shell

Geometric interpretation of the IBM



A. Frank *et al.*, Phys. Rev. C 69, 034323 (2004)

Critical changes of the energy surface

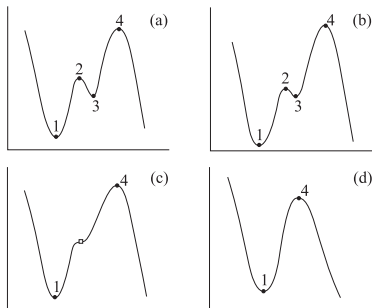
Question

How does the qualitative behaviour of a family of functions $F(x_1, \dots, x_n; a_1, \dots, a_k)$ change as a function of the parameters (a_1, \dots, a_k) ?

A one-dimensional example

For the function $f(x; a_1, \dots, a_k)$, the degenerate critical points are determined by

$$\frac{\partial f}{\partial x} = 0 \quad \text{and} \quad \frac{\partial^2 f}{\partial x^2} = 0$$



Critical changes of the energy surface

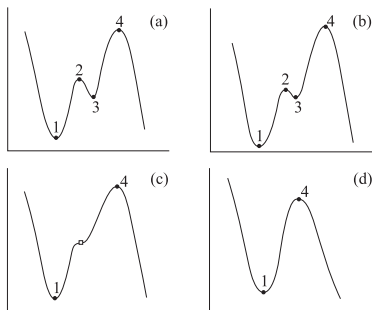
Answer

Degenerate critical points mark out the regions where qualitative behaviour of $F(x_1, \dots, x_n; a_1, \dots, a_k)$ remains unaltered

A one-dimensional example

For the function $f(x; a_1, \dots, a_k)$, the degenerate critical points are determined by

$$\frac{\partial f}{\partial x} = 0 \quad \text{and} \quad \frac{\partial^2 f}{\partial x^2} = 0$$

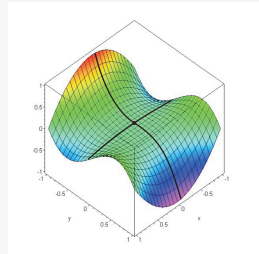


An energy surface associated with the IBM-CM

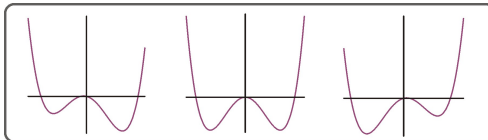
For $E_-(\beta, \gamma; \varepsilon_1, \varepsilon_2, \kappa_1, \kappa_2, \chi_1, \chi_2, \omega, \Delta, N)$, the degenerate critical points are determined by

$$\frac{\partial E_-}{\partial \beta} = 0, \quad \frac{\partial E_-}{\partial \gamma} = 0,$$

$$\det(\mathcal{S}) = \begin{pmatrix} \frac{\partial^2 E_-}{\partial \beta^2} & \frac{\partial^2 E_-}{\partial \beta \partial \gamma} \\ \frac{\partial^2 E_-}{\partial \gamma \partial \beta} & \frac{\partial^2 E_-}{\partial \gamma^2} \end{pmatrix} = 0$$



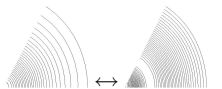
In regions where the energy surface has several minima, it is of interest to know **the Maxwell points**



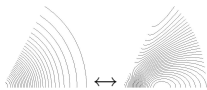
Criticality in the IBM with two-configuration mixing

A study of the full phase space $(\varepsilon_1, \varepsilon_2, \kappa_1, \kappa_2, \chi_1, \chi_2, \omega, \Delta, N)$ of the energy surface $E_-(\beta, \gamma; \varepsilon_1, \varepsilon_2, \kappa_1, \kappa_2, \chi_1, \chi_2, \omega, \Delta, N)$ is a tremendous, if not impossible, task. Therefore, we focus on mixing cases between **the dynamical symmetry limits** which are the benchmarks of the model.

$$1. U(5) - \hat{Q}(\chi) \cdot \hat{Q}(\chi) \text{ mixing} \longrightarrow U(5) - O(6):$$



$$\longrightarrow U(5) - SU(3):$$



$$2. \hat{Q}(\chi_1) \cdot \hat{Q}(\chi_1) - \hat{Q}(\chi_2) \cdot \hat{Q}(\chi_2) \text{ mixing}$$

\longrightarrow encompasses mixing between the $SU(3)$, the $\overline{SU}(3)$, and the $O(6)$ limit



$U(5) - \hat{Q}(\chi) \cdot \hat{Q}(\chi)$ mixing

The energy surface is given as

$$\begin{aligned}
 E_- = & \frac{|\kappa|}{2(1+\beta^2)^2} \left(\left[\epsilon' N - (N+2)(1+\chi^2) - \frac{2}{7}(N+2)(N+1)\chi^2 + \Delta' \right] \beta^4 \right. \\
 & + \left[\epsilon' N - (N+2)(6+\chi^2) - 4(N+2)(N+1) + 2\Delta' \right] \beta^2 \\
 & + \frac{4}{7}(N+2)(N+1)\sqrt{14}\chi\beta^3 \cos(3\gamma) - 5(N+2) + \Delta' \\
 & - \left[\left[\epsilon' N + (N+2)(1+\chi^2) + \frac{2}{7}(N+2)(N+1)\chi^2 - \Delta' \right] \beta^4 \right. \\
 & + \left[\epsilon' N + (N+2)(6+\chi^2) + 4(N+2)(N+1) - 2\Delta' \right] \beta^2 \\
 & \left. - \frac{4}{7}(N+2)(N+1)\sqrt{14}\chi\beta^3 \cos(3\gamma) + 5(N+2) - \Delta' \right]^2 \\
 & \left. + \omega'^2(1+\beta^2)^4 \right)^{\frac{1}{2}}
 \end{aligned}$$

The parameters

- ▶ N number of bosons
- ▶ χ parameter in quadrupole operator (prolate, oblate, or γ -unstable rotor)
- ▶ κ strength of quadrupole interaction
- ▶ $\epsilon' = \epsilon/|\kappa|$ scaled strength of vibrational contribution
- ▶ $\omega' = 2\omega/|\kappa|$ scaled mixing strength
- ▶ $\Delta' = \Delta/|\kappa|$ scaled excitation energy of intruders

An **analytical solution** to the criticality conditions is obtained from a Taylor expansion in $(\beta, \gamma) = (0, n\pi/3)$

$$E_- = t_{00} + \frac{1}{2!}t_{20}\beta^2 + \frac{1}{3!}t_{30}\beta^3 + \frac{1}{4!}t_{40}\beta^4 + \frac{1}{5!}t_{50}\beta^5 + \dots$$

$$\blacktriangleright t_{20}=0 \Rightarrow \varepsilon'_c = -\frac{(N+2)(4N+\chi^2)}{N} \frac{5(N+2)-\Delta'+\sqrt{(5(N+2)-\Delta')^2+\omega_c'^2}}{5(N+2)-\Delta'-\sqrt{(5(N+2)-\Delta')^2+\omega_c'^2}}$$

χ is part of a scaling factor

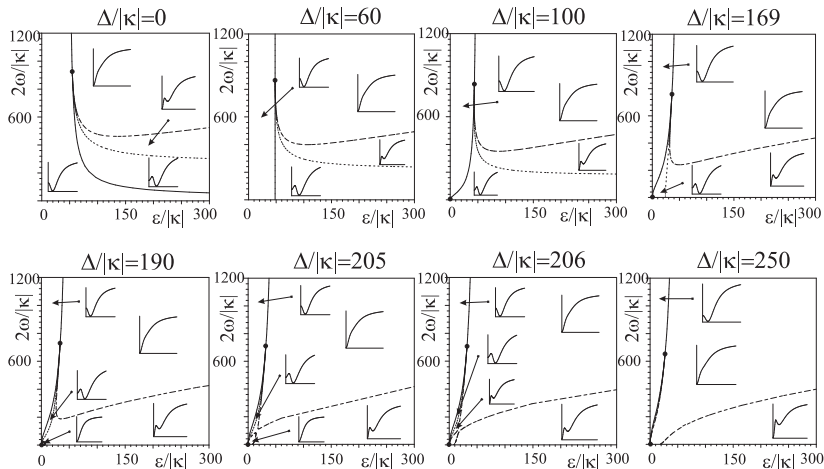
triple point?

$$t_{30} = \frac{24}{7}(N+2)(N+1)\sqrt{14}\chi \cos(n\pi) \frac{5(N+2)-\Delta'+\sqrt{(5(N+2)-\Delta')^2+\omega'^2}}{\sqrt{(5(N+2)-\Delta')^2+\omega'^2}}$$

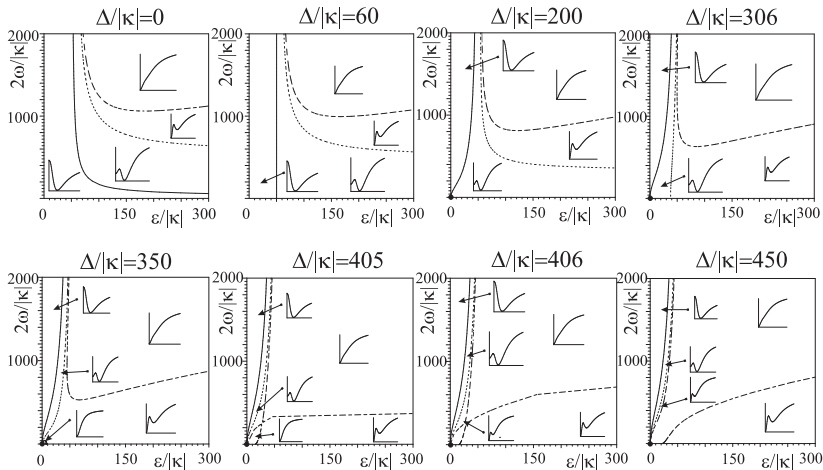
\Rightarrow only in case of $U(5)$ - $O(6)$ mixing

\Rightarrow triple point is obtained from $t_{20} = t_{40} = 0$

Phase diagram for U(5)-O(6) mixing



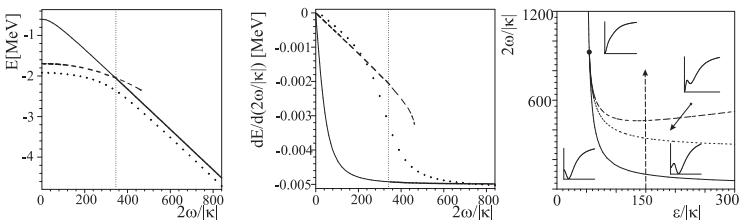
Phase diagram for U(5)-SU(3) mixing



Phase transitions for U(5)-O(6) mixing

In analogy to the Ehrenfest classification for thermodynamical phase transition, an analogous classification for **quantum phase transitions** can be proposed

- ▶ 1st order : discontinuity in first derivative of the energy of the global minimum



- ▶ 2nd order : discontinuity in second derivative of the energy of the global minimum

In the transition **from a spherical to a deformed minimum** in case of $U(5) - O(6)$ mixing, the deformation β_0 exhibits **powerlaw behaviour**.

From the condition that $\partial E_- / \partial \beta = 0$, we derive

$$\omega'_{\pm} = \pm \frac{4\sqrt{-(1+\beta^2)\varepsilon'N(N+2)[(N+2)\beta^2 - N]}}{(1+\beta^2)^2([\varepsilon'N + 4(N+2)^2]\beta^2 + N[\varepsilon' - 4(N+2)])} \\ \times \left([\varepsilon'N - 4(N+2) + \zeta]\beta^4 + [\varepsilon'N + 4N(N+2) + 2\zeta]\beta^2 + \zeta \right)$$

where $\zeta = -\Delta' + 5(N+2)$.

Powerlaw at the degenerate critical points

the deformation of the global minimum in the vicinity of the degenerate critical points

$$\beta_0 = \sqrt{\frac{\zeta N}{2\varepsilon'_c [4N^2(N+2) + \zeta(N+1) - \varepsilon'_c N^2]}} (\varepsilon'_c - \varepsilon')^{1/2}$$

for $\omega'_c > \omega'_t$ and $\varepsilon' < \varepsilon'_c$

In the transition **from a spherical to a deformed minimum** in case of $U(5) - O(6)$ mixing, the deformation β_0 exhibits **powerlaw behaviour**.

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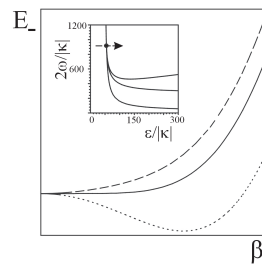
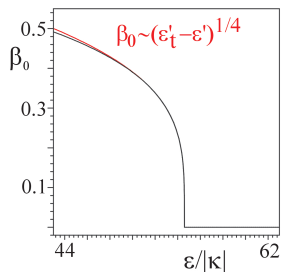
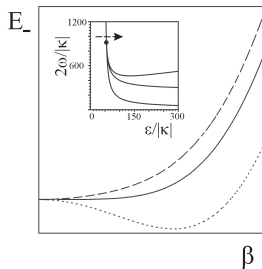
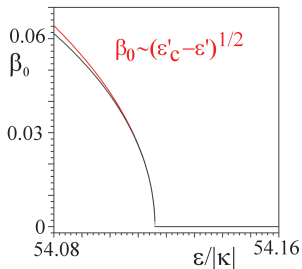
where $\zeta = -\Delta' + 5(N+2)$.

Powerlaw at the triple point

the deformation of the global minimum in the vicinity of the triple point

$$\beta_0 = \left(\frac{N^4}{3(N+1)^2[4N^2(N+2) + \zeta(N+1)]} \right)^{1/4} (\varepsilon'_t - \varepsilon')^{1/4}$$

Phase transitions for U(5)-O(6) mixing



- powerlaw behaviour fingerprint for 2nd order phase transitions

$\hat{Q}(\chi_1) \cdot \hat{Q}(\chi_1) - \hat{Q}(\chi_2) \cdot \hat{Q}(\chi_2)$ mixing

The energy surface is given as

$$E_- = \frac{|\kappa|}{2(1+\beta^2)^2} \left[a_1 \beta^4 + a_2 \beta^2 + a_3 \beta^3 \cos(3\gamma) - 5(N + |\sigma'|)(N+2) + \Delta' \right. \\ \left. - \left[(b_1 \beta^4 + b_2 \beta^2 + b_3 \beta^3 \cos(3\gamma) - 5(N - |\sigma'|)(N+2) - \Delta' \right)^2 \right. \\ \left. + \omega'^2 (1 + \beta^2)^4 \right]^{1/2}$$

with

$$a_1 = -N \left(1 + \frac{1}{7} (2N+5) \chi_1^2 \right) - |\sigma'| (N+2) \left(1 + \frac{1}{7} (2N+9) \chi_2^2 \right) + \Delta',$$

$$a_2 = -N (\chi_1^2 + 2(2N+1)) - |\sigma'| (N+2) (\chi_2^2 + 2(2N+5)) + 2\Delta',$$

$$a_3 = \frac{4}{7} \sqrt{14} (N(N-1) \chi_1 + |\sigma'| (N+1)(N+2) \chi_2),$$

$$b_1 = -N \left(1 + \frac{1}{7} (2N+5) \chi_1^2 \right) + |\sigma'| (N+2) \left(1 + \frac{1}{7} (2N+9) \chi_2^2 \right) - \Delta',$$

$$b_2 = -N (\chi_1^2 + 2(2N+1)) + |\sigma'| (N+2) (\chi_2^2 + 2(2N+5)) - 2\Delta',$$

$$b_3 = \frac{4}{7} \sqrt{14} (N(N-1) \chi_1 - |\sigma'| (N+1)(N+2) \chi_2)$$

The parameters

- ▶ N number of bosons
- ▶ χ_1 and χ_2 parameter in quadrupole operator (prolate, oblate, or γ -unstable rotor)
- ▶ κ strength of quadrupole interaction for the regular configuration
- ▶ $|\sigma'| = |\sigma|/|\kappa|$ scaled strength of quadrupole interaction for the intruder configuration
- ▶ $\omega' = 2\omega/|\kappa|$ scaled mixing strength
- ▶ $\Delta' = \Delta/|\kappa|$ scaled excitation energy of intruders

Two classes of solutions

From the condition $\frac{\partial E_-}{\partial \gamma} = 0$, it follows that γ can be frozen $n\pi/3$ such that the other criticality conditions reduce to

$$\frac{\partial E_-}{\partial \beta} \Big|_{\gamma=n\pi/3} = 0, \quad \det \begin{pmatrix} \frac{\partial^2 E_-}{\partial \beta^2} \Big|_{\gamma=n\pi/3} & 0 \\ 0 & \frac{\partial^2 E_-}{\partial \gamma^2} \Big|_{\gamma=n\pi/3} \end{pmatrix} = 0$$

Hence, there are **two classes** of solutions to the criticality conditions :

1. degenerate critical points indicating changes in the number of extrema in the β -direction
2. degenerate critical points indicating changes in the number of extrema in the γ -direction

Prolate-oblate coexistence?

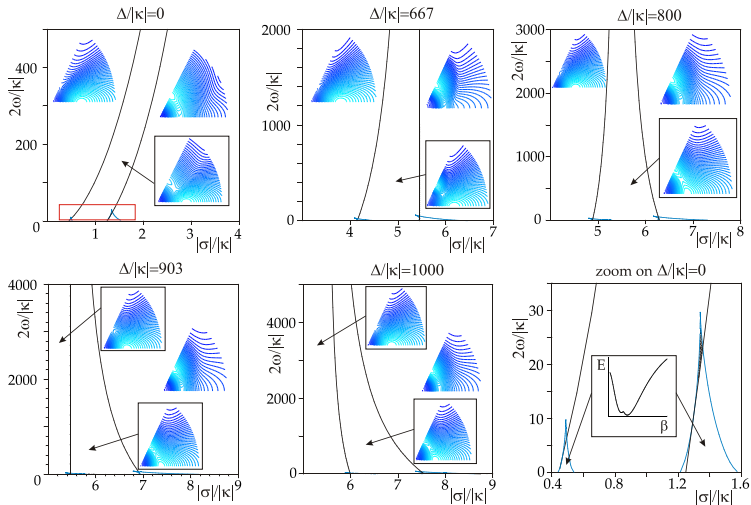
From the condition $\left. \frac{\partial^2 E_-}{\partial \gamma^2} \right|_{\gamma=n\pi/3} = 0$, we derive

$$\omega' = \pm \sqrt{(b_3 - a_3)(b_3 + a_3)} \frac{b_1 \beta^4 + b_2 \beta^2 + b_3 \beta^3 - 5(N - |\sigma'|)(N + 2) - \Delta'}{a_3(1 + \beta^2)^2}$$

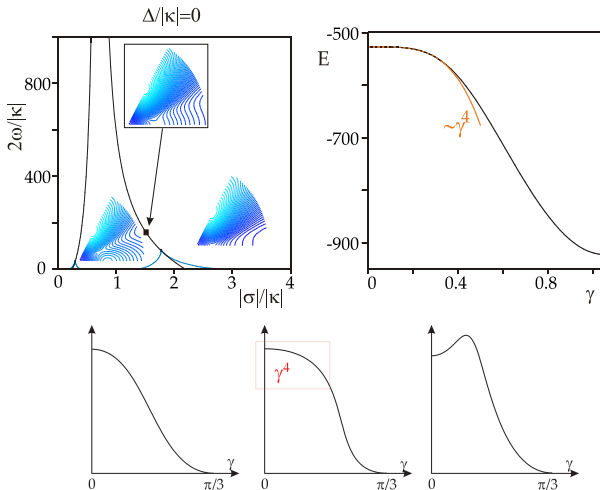
with

$$\sqrt{(b_3 - a_3)(b_3 + a_3)} = \frac{8}{7} \sqrt{-14|\sigma'|(N - 1)N(N + 1)(N + 2)\chi_1\chi_2}$$

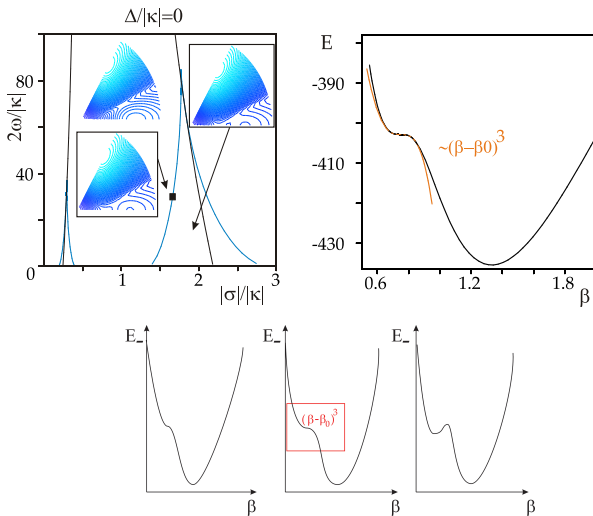
⇒ Prolate-oblate shape coexistence only occurs if χ_1 and χ_2 have opposite sign.

Phase diagram for $SU_-(3)-\hat{Q}(\chi_2)\hat{Q}(\chi_2)$ mixing ($\chi_2 = \sqrt{7}/16$)

By means of a Taylor expansion, the behaviour in the degenerate critical point can be derived



By means of a Taylor expansion, the behaviour in the degenerate critical point can be derived



Conclusions and outlook

- ▶ An extensive region of shape coexistence is found for various excitation energies of the intruder configuration in the phase diagrams for the IBM with configuration mixing. This makes shape coexistence an important aspect of the IBM with configuration mixing.
- ▶ In case of mixing between two deformed configurations, shape coexistence between a prolate and an oblate minimum can only arise if χ_1 and χ_2 have opposite sign
- ▶ Future perspectives :
 - ▶ calculation of the Maxwell points in case of mixing between two deformed configurations and possibility of first-order shape phase transitions?
 - ▶ study of the energy surface associated with configuration mixing in less schematic cases
 - ▶ ...