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Configuration mixing of angular-momentum projected
triaxial relativistic mean-field wave functions

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25th, September, 2010



Outline

1 Introduction

- Low-lying states of exotic nuclei
- Beyond the self-consistent mean-field theory

2 The relativistic 3DAMP+GCM model

3 Application for nuclear low-lying states

- A well deformed nucleus Dysprosium
- Magnesium isotopes
- Carbon isotopes

4 Summary and perspective

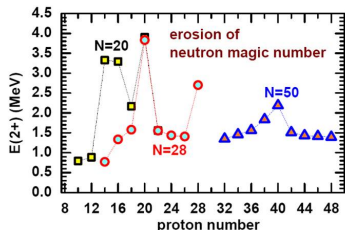
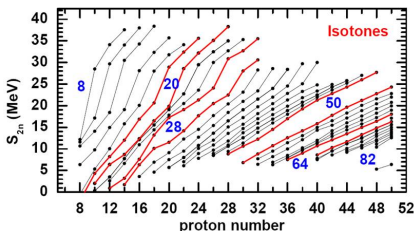
Low-lying states of exotic nuclei

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1 evolution of shell structure and collectivity



2 nuclear shape and shape phase transition

R. F. Casten, Nature Physics, 811 (2006); P. Cejnar, Rev. Mod. Phys. 82, 2155 (2010)

3 decoupling of neutrons and protons (in ^{16}C)

N. Imai et al., Phys. Rev. Lett. 92, 062501 (2004)

Beyond the SC mean-field approach for nuclear low-lying states

In the past decade, several **beyond SC mean-field models** have been developed that perform the **restoration of symmetries** broken by the static nuclear mean field, and take into account **fluctuations** around the mean-field minimum.

Restricted to axial shape

- PNP+1DAMP+GCM (HF with Skyrme force)
A. Valor, P.-H. Heenen, and P. Bonche, NPA671, 145(2000)
- PNP+1DAMP+GCM (HFB with Gogny force)
R. Rodriguez-Guzman, J. L. Egido, and L. M. Robledo, NPA709, 201(2002)
- PNP+1DAMP+GCM (RMF with point-coupling force)
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Applications for nuclear low-lying states

- low-spin normal-deformed and super-deformed collective states
Bender, Flocard & Heenen, PRC68, 044321 (2003)
- shape coexistence in Kr, Pb isotopes
Rodriguez-Guzman, Egido & Robledo, PRC 69, 054319 (2004);
Bender, Bonche & Heenen, PRC 74, 024312 (2006)
- shell closures at N=32 or 34?
Rodriguez & Egido, PRL 99, 062501 (2007)
- shape transition in Nd isotopes
Niksic, Vretenar, Lalazissis & Ring, PRL99, 092502 (2007);
Rodriguez & Egido, PLB 663, 49 (2008)

Beyond the self-consistent mean-field theory: Recent progress

Recently, the 1DAMP+GCM framework has been extended to the 3DAMP+GCM case, which makes it possible to study the nuclear low-lying states with the consideration of effects from

- 1 restoration of rotation symmetry in full 3D Euler space
- 2 shape fluctuation in full β - γ plane

Non-relativistic versions

- PNP+3DAMP+GCM (HFB with Skyrme force)
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Only illustrative calculations have been carried out in non-relativistic frameworks !

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Our relativistic 3DAMP+GCM model

starting from the RMF+BCS with point-coupling force

Yao, Meng, Ring & Pena Arteaga, PRC79, 044312 (2009);

Yao, Meng, Ring & Vretenar, PRC81, 044311 (2010)

- 1 framework of our relativistic 3DAMP+GCM model
- 2 its applications to the analysis of nuclear low-lying states in some interesting isotopes.

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Intrinsic states from the relativistic point-coupling calculations

The relativistic 3DAMP+GCM model

1. The relativistic point-coupling model+BCS calculations with constraints on quadrupole moments by minimizing the energy functional

$$E'[\rho_i, j_i^\mu] = E[\rho_i, j_i^\mu] - \sum_{\mu=0,2} \frac{C_\mu}{2} (\hat{Q}_{2\mu} - q_{2\mu})^2 \quad (1)$$

generate a large set of highly correlated **intrinsic deformed states** $|\Phi(q)\rangle$. The **pairing correlations**, for open-shell nuclei, are taken into account by augmenting the following pairing energy functional,

$$E[\kappa] = - \sum_{\tau} \int d\mathbf{r} \frac{V_{\tau}}{4} \kappa_{\tau}^*(\mathbf{r}) \kappa_{\tau}(\mathbf{r}) \quad (2)$$

with separately adjustable strengths $V_{p/n}$ for protons and neutrons.

PC-F1: Burvenich, Madland, Maruhn & Reinhard, PRC65, 044308 (2002).

DD-PC1: Niksic, Vretenar & Ring, PRC78, 034318 (2008).

PC-PK1: Zhao, Li, Yao & Meng, arXiv:1002.1789v1 [nucl-th].

Configuration of angular momentum projected triaxial states

The relativistic 3DAMP+GCM model

- The nuclear wavefunction with good angular momentum and shape fluctuation is obtained by projecting the intrinsic states $|\Phi(\beta, \gamma)\rangle$ onto good angular momentum (K-mixing) and performing GCM calculations (configuration mixing),

$$|\Psi_{\alpha}^{JM}\rangle = \int d\beta d\gamma \sum_{K \geq 0} f_{\alpha}^{JK}(\beta, \gamma) \underbrace{\frac{1}{(1 + \delta_{K0})} [\hat{P}_{MK}^J + (-1)^J \hat{P}_{M-K}^J]}_{(3)} |\Phi(\beta, \gamma)\rangle \quad (3)$$

The weight functions f_{α}^{JK} are determined from the solution of Hill-Wheeler-Griffin (HWG) integral equation: $q \equiv (\beta, \gamma)$

$$\int dq' \sum_{K' \geq 0} \left[\mathcal{H}_{KK'}^J(q, q') - E_{\alpha}^J \mathcal{N}_{KK'}^J(q, q') \right] f_{\alpha}^{JK'}(q') = 0, \quad (4)$$

where \mathcal{H} and \mathcal{N} are the angular-momentum **projected GCM kernel matrices** of the **Hamiltonian** and the **Norm**, respectively.

Electromagnetic moments and transition strengths

The relativistic 3DAMP+GCM model

3. The electromagnetic moments and transition strengths are evaluated with the nuclear wavefunction.
 - $E0$ and $E2$ transition strengths
 - g -factor: $\mu(J^\pi)/J$
 - Spectroscopic quadrupole moment: $Q^{\text{spec}}(J)$
 - ...

$$B(\sigma\lambda; J_i, \alpha_i \rightarrow J_f, \alpha_f) = \frac{e^2}{2J_i + 1} \sum_{M_i \mu M_f} \left| \langle J_f, M_f, \alpha_f | \hat{M}(\sigma\lambda\mu) | J_i, M_i, \alpha_i \rangle \right|^2 \quad (5)$$

The matrix elements are calculated in the full configuration space. **There is no need for effective charges.**

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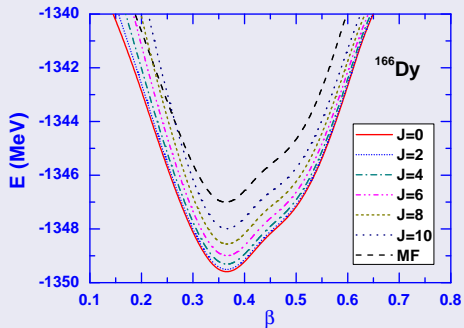
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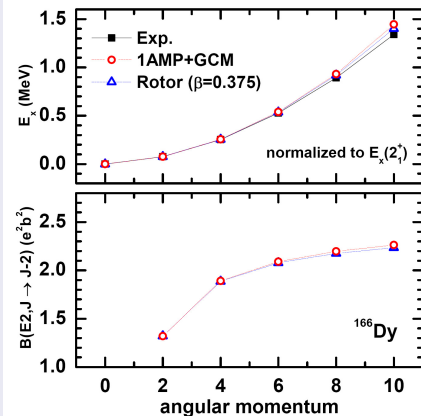
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Low-lying states in ^{166}Dy : AMP



- A pronounced minimum with $\beta = 0.350$ in the mean-field potential energy surface.
- After angular momentum projection, one obtains the projected PES with $J = 0, \dots, 10$.
- The projected PES with $J = 0$ has a minimum with $\beta = 0.375$.
- The energy gained from AMP is about 3 MeV.

Low-lying states in ^{166}Dy : comparison with a rigid rotor



- Good agreement has been found between the rigid rotor model and microscopic projected GCM calculations, both of which reproduce the data quite well.

Figure: The excitation energies [normalized to $E_x(2_1^+)$] and $B(E2)$ values of low-lying states as functions of angular momentum.

Low-lying states in magnesium isotopes: correlation energies

Total dynamical correlation energies E_{CORR} consists of two parts:

- 1 energy correction from the restoration of rotational symmetry

$$\Delta E_{J=0} = E_{J=0}(\beta_0) - E_{\text{MF}}(\beta_m), \quad (6)$$

- 2 the energy correlation from configuration mixing

$$\Delta E_{\text{GCM}} = E(0_1^+) - E_{J=0}(\beta_0). \quad (7)$$

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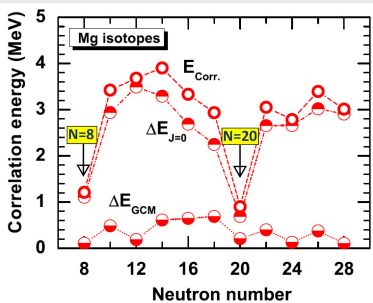
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- E_{CORR} shows a strong dependence on shape and shell structure.
- large for deformed mid-shell nuclei, with a maximum of ~ 4 MeV at $N = 14$, and is drastically reduced (~ 1 MeV) for the two isotopes with the neutron magic numbers $N = 8$ and $N = 20$.
- The rotational energy correction $\Delta E_{J=0}$ constitutes the dominant part. *Non-Rel. Cal.+GOA: Bender, Bertsch & Heenen, PRC73, 034322 (2006).*

Figure: Total ground-state dynamical correlation energies of Mg isotopes, as a function of the number of neutrons.

Low-lying states in magnesium isotopes: E2 transition strengths

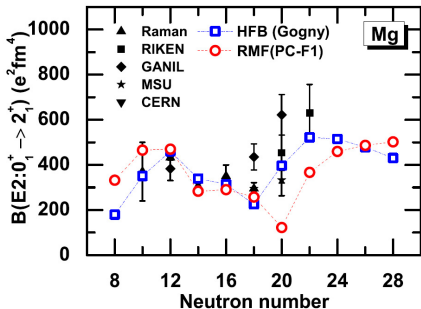
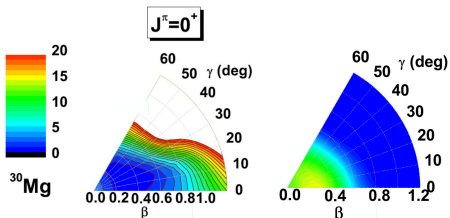


Figure: $B(E2; 0_1^+ \rightarrow 2_1^+)$ ($e^2 \text{fm}^4$) values in $^{20-40}\text{Mg}$, calculated using the 1DAMP+GCM model with the relativistic density functional PC-F1, are compared to available data and the results of the 1DAMP+GCM calculation based on the non-relativistic HFB framework with the Gogny force [Rodriguez-Guzman, Egido & Robledo, *NPA709, 201 (2002)*].

- Our calculations (PC-F1) yield results in reasonable agreement with data except, of course, at and in the neighborhood of the neutron number $N = 20$.
- A better adjustment of pairing strength parameters and eventually the inclusion of triaxiality, could improve the results for ^{32}Mg , giving $B(E2; 0_1^+ \rightarrow 2_1^+) = 330.1 e^2 \text{fm}^4$, much closer to the available data.

Effect of triaxiality in E0 transition of ^{30}Mg 

The projected PES ($J = 0$) and Probability distribution of 0_1^+ state in β - γ plane.

Table: Results from 1D and 3DAMP+GCM calculations with the relativistic PC-F1 force and non-relativistic Gogny force, compared to experimental values. Both the non-relativistic calculation results and experimental data are taken from Ref. [W. Schwerdtfeger et al., *PRL* 103, 012501 (2009)].

	$E_x(2_1^+)$ (MeV)	$E_x(0_2^+)$ (MeV)	$\rho_{21}^2(E0) \times 10^3$	$B(E2; 0_1^+ \rightarrow 2_1^+)$ ($e^2\text{fm}^4$)	$B(E2; 0_2^+ \rightarrow 2_1^+)$ ($e^2\text{fm}^4$)
Exp.	1.482	1.789	26.2 ± 7.5	241(31)	53(6)
3D(PC-F1)	1.713	2.864	24.72	277	68↑
1D(PC-F1)	1.905	3.275	15.56↓	257	47
1D(Gogny-D1S)	2.03	2.11	46↑	334.6	181.5↑

Excitation energies and BE2 values in Carbon isotopes

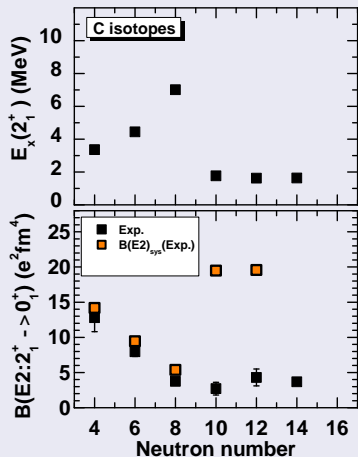


Figure: Excitation energies of 2_1^+ states $E_x(2_1^+)$ (MeV) and the $B(E2)$ values ($e^2 \text{fm}^4$) for even-even carbon isotopes.

- The experiment $B(E2)$ values are compared with the prediction by the empirical relation: *S. Raman et al., PRC37, 805 (1988)*

$$\begin{aligned}
 & B(E2 : 0_1^+ \rightarrow 2_1^+)_{\text{sys.}} \\
 &= 6.47 Z^2 A^{-0.69} E_x^{-1}(2_1^+). \quad (8)
 \end{aligned}$$

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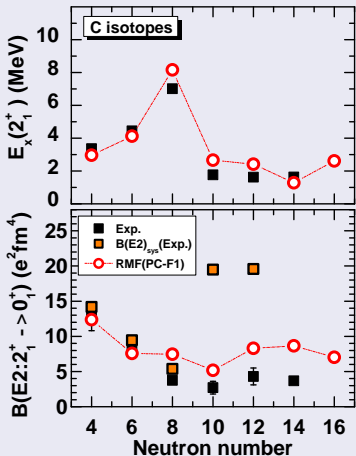


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- The systematics of both $E_x(2_1^+)$ and $B(E2 : 2_1^+ \rightarrow 0_1^+)$ are reproduced quite well
- The quenched $B(E2)$ values, combined with the very low $E_x(2_1^+)$ indicate that the decoupled structure of neutron and proton exist in $^{16-20}\text{C}$.

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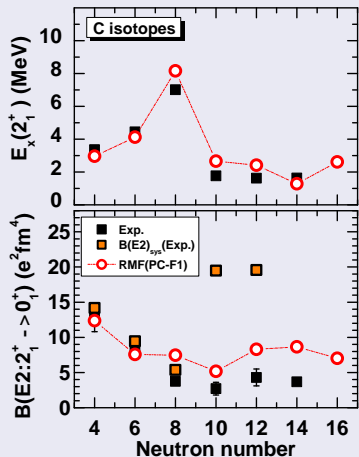


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- The large difference between neutron and proton deformations in $^{16-20}\text{C}$ is due to the special mp -2h configurations $\nu(1d_{5/2})^m \otimes \pi(1p_{3/2})^{-2}$, $m = 2, 4, 6$.

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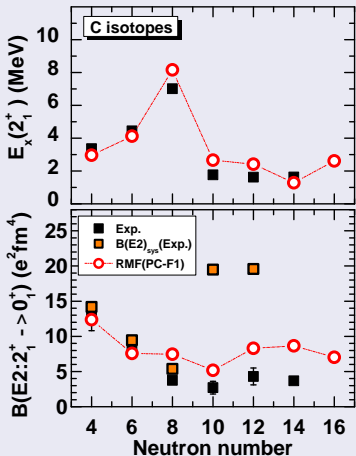


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- What about ^{22}C ? Neutron halo with $\nu(2s_{1/2})^2$? *K. Tanaka et al., PRL 104, 062701 (2010)*

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Summary

The relativistic version of 3DAMP+GCM approach and its applications

- The relativistic 3DAMP+GCM model has been developed that uses the generator coordinate method (GCM) to perform configuration mixing of three-dimensional angular-momentum projected (3DAMP) relativistic mean-field wave functions, generated by constrained self-consistent calculations for triaxial nuclear shapes.
- The relativistic 3DAMP+GCM model has been tested and compared with the rigid rotor model for the low-spin states in well deformed nucleus ^{166}Dy .
- The low-lying states of **magnesium** isotopes and **carbon** isotopes have been calculated. The spectroscopic properties, including excitation energy, $BE0$, $BE2$ transition strengths and g -factor, are studied. The effects of triaxiality and pair correlation are discussed.
- Triaxiality has been found to be important in ^{30}Mg .
- The quenched $B(E2)$ values, combined with the very low $E_x(2_1^+)$ indicate that the decoupled structure of neutron and proton exist in $^{16-20}\text{C}$.

Perspective

What can be done next?

- Using a **separable pairing force** in the pairing channel.
Tian, Ma & Ring, PLB676, 44 (2009).
- Comparing with the **same energy functional based Bohr Hamiltonian** calculation to examine the **Gaussian Overlap Approximation**.
Niksic, Li, Vretenar, Prochniak, Meng & Meng, PRC79, 034303 (2009)
- Including **two quasiparticle configurations** using the idea of projected shell model.
Hara & Sun, Int. J. Mod. Phys. E 4, 637-785 (1995)
- Augmenting the **particle number projection** and regularization
Lacroix, Duguet & Bender, PRC79, 044318 (2009).
Bender, Duguet & Lacroix, PRC79, 044319 (2009).
- ...

Acknowledgments

To my collaborators

Jie Meng

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Peter Ring, Daniel Pena Arteaga

TUM



Dario Vretenar

Zagreb Univ.



Kouichi Hagino

Tohoku Univ.



Thanks for Your attention!

Numerical details

- **Imposed symmetries:** parity, D_2 symmetry, and time reversal symmetry.
- **Basis expansion method:** a set of three-dimensional **isotropic** harmonic oscillator basis functions in Cartesian coordinates.
- **Modified Broyden's method** for accelerating convergence in self-consistent calculations *A. Baran et al., PRC 78, 014318 (2008)*
- The **Gaussian-Legendre quadrature** is used for integrals over the Euler angles ϕ, θ and ψ in the calculation of the norm and hamiltonian kernels.

Low-lying states in magnesium isotopes: g-factor

- g-factor: $g(J_\alpha^\pi) = \mu(J_\alpha^\pi)/J$, where the magnetic moment $\mu(J_\alpha^\pi)$ of excited state J_α^π can be calculated with the angular momentum projected wave function,

$$\mu(J_\alpha^\pi) = \langle J, M = J, \alpha | \hat{\mu}_{10} | J, M = J, \alpha \rangle \quad (9)$$

The magnetic moment vector $\hat{\mu}$ is related to effective electromagnetic current operator,

$$\hat{\mu}_k = \frac{1}{2} \int d^3 r [\mathbf{r} \times \mathbf{j}]_k, \quad k = x, y, z \quad (10)$$

that is determined by the effective EM current,

$$\hat{\mathbf{j}} = e\psi^\dagger \boldsymbol{\alpha} \psi + \frac{\kappa}{2M} \nabla \times [\psi^\dagger \boldsymbol{\beta} \boldsymbol{\Sigma} \psi], \quad (11)$$

where κ is the free anomalous gyromagnetic ratio of the nucleon: $\kappa^p = 1.793$ and $\kappa^n = -1.913$.

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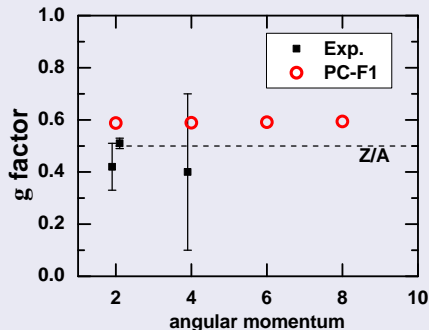


Figure: The g-factor as a function of angular momentum in ^{24}Mg .

Potential energy curves in Carbon isotopes

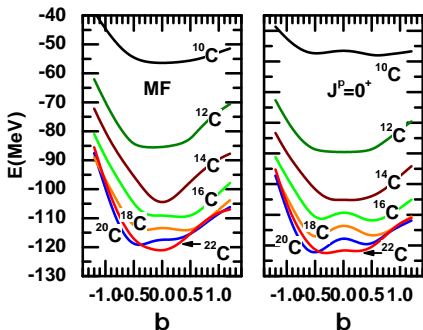


Figure: Self-consistent RMF+BCS mean-field (left panel), and angular-momentum projected 0^+ potential energy curves (right panel) of even-even magnesium isotopes, as functions of the axial deformation parameter β .

Potential energy curves in Carbon isotopes

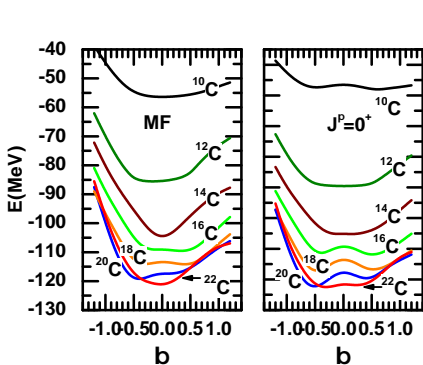


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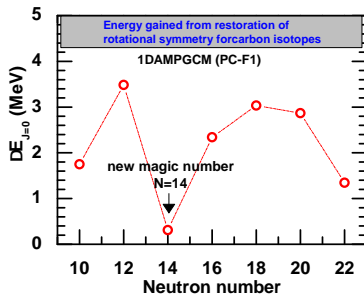


Figure: The rotational energy correction $\Delta E_{J=0}$ as a function of neutron number.

$$\Delta E_{J=0} = E_{J=0}(\beta_0) - E_{MF}(\beta_m), \quad (12)$$

where β_m and β_0 denote the axial deformation parameters at the minima of the mean-field and the ($J^\pi = 0^+$) angular-momentum projected PECs, respectively

probability

The solution of HWG equation determines both the energies E_α^J and the amplitudes $f_\alpha^{JK}(q)$ of collective states with good angular momentum $|\Psi_\alpha^{JM}\rangle$

$$f_\alpha^{JK}(q) = \sum_k \frac{g_k^{J\alpha}}{\sqrt{n_k^J}} u_k^J(i). \quad (13)$$

The weight functions $f_\alpha^{JK}(q)$ are not orthogonal and cannot be interpreted as collective wave functions for the deformation variables. The collective wave functions $g_\alpha^J(i)$ are calculated from the norm overlap eigenstates:

$$g_\alpha^J(i) = \sum_k g_k^{J\alpha} u_k^J(i), \quad (14)$$

The wave functions $g_\alpha^J(i)$ are orthonormal and, therefore, $|g_\alpha^J(i)|^2$ can be interpreted as a probability amplitude.