

Full Solution of Nuclear Quadrupole-Octupole Model for Odd- A Nuclei

M. Strecker¹, **N. Minkov**^{1,2}, **H. Lenske**¹

¹Institut für Theoretische Physik der Justus-Liebig-Universität, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany

²Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Tzarigrad Road 72, BG-1784 Sofia, Bulgaria

Abstract. A collective model of nuclear quadrupole-octupole vibrations and rotations, originally restricted to a coherent interplay between quadrupole and octupole modes, is now developed for application to odd- A nuclei beyond this restriction. The eigenvalue problem is solved by diagonalizing the unrestricted Hamiltonian in the basis of the analytic solution obtained in the case of the coherent-mode assumption. Within this scheme the yrast split parity-doublet band is constructed by the pairs of lowest eigenvalues with positive and negative parity obtained for the different angular momenta. Additionally we include the calculation of transition probabilities which are fitted together with the energy levels. As a result we obtain a unique set of model parameters which unambiguously determine the shape of the quadrupole-octupole potential. From the resulting wave functions quadrupole and octupole deformation expectation values can be calculated. The approach is tested on the yrast parity-doublet band of the nucleus ²⁴³Am.

1 Introduction

We consider both quadrupole and octupole deformations in nuclei which lead to interesting spectra with parity effects. In the case of simultaneous quadrupole and octupole deformations the theory provides vibrational, rotational and transitional structures. In [1]- [5] Minkov *et al.* applied a coherent quadrupole-octupole motion (CQOM) model to various regions of even-even and odd- A nuclei. This model is solved analytically after imposing equal frequencies for the quadrupole and octupole motion (coherent mode). The solution is shortly presented below.

The purpose of the present work, in continuation to the previous papers [6] and [7], is to develop the model approach to odd- A nuclei beyond the coherent-mode assumption. The structure of the spectrum of odd- A nuclei is characterized by the coupling between the reflection asymmetric even-even core and the motion of the unpaired particle and typically leads to a split parity-doublet structure.

The inclusion of transition probabilities into the fitting procedure leads to a unique determination of the model parameters, which are adjusted so as to reproduce the experimental values in the best way possible. As a consequence, the model potentials and the resulting wave functions are obtained unambiguously, as in case of even-even nuclei, and allow a prediction of the quadrupole and octupole deformations by calculating the corresponding expectation values.

2 Two-dimensional Coherent Quadrupole-Octupole Model

2.1 General Hamiltonian

The starting point is a vibration-rotation Hamiltonian formulated in the collective axial quadrupole and octupole deformation variables β_2 and β_3 [2, 3]

$$H_{qo} = -\frac{\hbar^2}{2B_2} \frac{\partial^2}{\partial \beta_2^2} - \frac{\hbar^2}{2B_3} \frac{\partial^2}{\partial \beta_3^2} + \frac{1}{2} C_2 \beta_2^2 + \frac{1}{2} C_3 \beta_3^2 + \frac{X(I, K, \pi a)}{d_2 \beta_2^2 + d_3 \beta_3^2}, \quad (1)$$

where for odd- A nuclei one has

$$X(I, K, \pi a) = \frac{1}{2} \left[d_0 + I(I+1) - K^2 + \pi a \delta_{K, \frac{1}{2}} (-1)^{I+1/2} \left(I + \frac{1}{2} \right) \right]. \quad (2)$$

B_2 and B_3 are mass parameters, C_2 and C_3 are stiffness parameters, d_2 and d_3 are moment of inertia parameters and d_0 determines the potential shape in the ground state. The decoupling parameter is denoted by a and π is the total intrinsic parity, given by the product of the parities of the unpaired single particle and the even-core wave function. K is the third angular momentum projection.

2.2 Coherent solution

The transition to ellipsoidal coordinates given by

$$\eta = \left[\frac{2(d_2 \beta_2^2 + d_3 \beta_3^2)}{d_2 + d_3} \right]^{\frac{1}{2}} \quad \text{and} \quad \phi = \arctan \left(\frac{\beta_3}{\beta_2} \sqrt{\frac{d_3}{d_2}} \right) \quad (3)$$

and the imposition of the relations

$$B := \frac{d}{d_2} B_2 = \frac{d}{d_3} B_3 \quad \text{and} \quad C := \frac{d}{d_2} C_2 = \frac{d}{d_3} C_3,$$

where $d = (d_2 + d_3)/2$, allows one to obtain the energy spectrum in the following closed formula [2, 3]

$$E_{n,k} = \hbar\omega \left[2n + 1 + \sqrt{k^2 + b \cdot X(I, K, \pi a)} \right], \quad (4)$$

Full Solution of Nuclear Quadrupole-Octupole Model for Odd-*A* Nuclei

where $\omega = \sqrt{C/B}$ and $b = 2B/\hbar^2 d$ are considered as fitting parameters. The model wave function has the form

$$\Psi_{nIMK}^\pi(\eta, \phi) = \sqrt{\frac{2I+1}{16\pi^2}} (D_{M,K}^I(\theta)\chi_K \pm (-1)^{I+K} D_{M,-K}^I(\theta)\chi_{-K}) \Phi_{nkI}^\pi(\eta, \phi), \quad (5)$$

where $D_{M,K}^I(\theta)$ is the Wigner rotation function, χ_K is the single-particle function and

$$\Phi_{nkI}^\pi(\eta, \phi) = \psi_{nk}^I(\eta)\varphi_k^\pi(\phi) \quad (6)$$

is the quadrupole-octupole vibration function. Here

$$\psi_{n,k}^I(\eta) = \sqrt{\frac{2c\Gamma(n+1)}{\Gamma(n+2s+1)}} e^{-c\eta^2/2} (c\eta^2)^s L_n^{2s}(c\eta^2) \quad (7)$$

is the ‘‘radial’’ part of $\Phi(\eta, \phi)$ with $c = \sqrt{BC}/\hbar$ and $s = \frac{1}{2}\sqrt{k^2 + bX(I, K, \pi a)}$ as well as

$$\varphi_k^+(\phi) = \sqrt{2/\pi} \cos(k\phi), \quad k = 1, 3, 5, \dots \quad (8)$$

$$\varphi_k^-(\phi) = \sqrt{2/\pi} \sin(k\phi), \quad k = 2, 4, 6, \dots \quad (9)$$

for the ‘‘angular’’ wave functions with either positive or negative parity.

For the quantum numbers $n = 0, 1, 2, \dots$ and $k = 1, 2, 3, \dots$ one chooses the lowest possible values to describe the yrast spectrum in the analytical model. This means one takes always $n = 0$ and $k = 1$ or $k = 2$. The choice of k leads to an up or down shift and thus generates the parity-doublets. As seen from the previous equations, the parity of the angular function, π_φ , depends on k and is always positive for $k = 1$ and negative for $k = 2$. k is chosen in such a way that the parity π_φ matches the parity of the considered energy level. Then, depending on the parity of the single-particle, π_χ , there is a shift upwards for levels with negative parity and a shift downwards for levels with positive parity, given a positive π_χ . The situation is just opposite in case of a negative π_χ . This means there is a shift downwards for levels with negative parity and a shift upwards for levels with positive parity.

The description of higher-lying (non-yrast) bands in the framework of the analytical model allows the involvement of larger values of the quantum numbers n and k [4, 5].

2.3 Numerical diagonalization

The details about the diagonalization procedure can be found in [6]. The CQOM basis functions $\Phi(\eta, \phi)$ have the advantage to automatically consider the boundary condition of the model, namely that the wave function must vanish along the β_3 -axis. An energy cutoff for the number of basis functions is applied and we consider only the lowest lying states for the diagonalization. The presented

calculation results are obtained with a basis size of 50 states. It is checked that this is enough to provide convergence of the results, *i.e.* the results do no longer change if more basis states are added. Furthermore the basis is optimized as explained in [6]. For the integration of the matrix elements we apply a formula which allows one to obtain the numerical values of the definite integrals quickly by means of a generalized hypergeometric function ${}_3F_2$. Then the eigenvalues and eigenvectors of the Hamiltonian matrix are calculated and we construct the model spectrum as described in [6].

2.4 Theory of transition operators

The basic theory about electromagnetic transitions in the coherent case can be found in [1]. We use the same transition theory as explained in [4] and [7]. This means we apply a generalization of the transition operators for a given fixed nuclear shape, which allows us to take into account the ‘‘overtones’’ related to the coherent collective oscillations of the system. The only difference is that while for even-even nuclei the projection K of the collective angular momentum on the principal symmetry axis is taken as zero, in the case of odd- A nuclei it is always nonzero (half-integer) and we take it equal to the value suggested by the experiment.

The fitting procedure for transitions also includes an effective charge e_{eff}^1 , which can have a value different from one, and is an adjustable parameter. We take into account transition probabilities related to the yrast band. As mentioned in [7], this is very important and necessary in order to obtain a set of parameters which is uniquely determined.

3 Application to ^{243}Am

Once the diagonalizations have been performed for all angular momenta, one obtains an yrast spectrum and is able to define a σ_{RMS} function which gives the root mean square deviation from the experimental levels. The transition probabilities are calculated and we construct an overall root mean square (RMS) deviation function including both energies and transitions. The transitions are included with weight factors providing the same order of magnitude for the fitting procedure. Then the model parameters $B_2, B_3, C_2, C_3, d_2, d_3, d_0$ and e_{eff}^1 can be adjusted so as to provide the best description of experimental data.

In order to test the numerical procedure described above we performed calculations for the nucleus ^{243}Am . The angular momentum on which the yrast parity-doublet band of this nucleus is built is $5/2^-$ and, therefore, the fit does not include a decoupling parameter. As an initial guess for the minimization we take the parameter values obtained from the CQOM model. As a result we obtain the theoretical energy levels and transition probabilities corresponding to the experimental data [8] available for the yrast split parity-doublet spectrum of ^{243}Am .

Full Solution of Nuclear Quadrupole-Octupole Model for Odd-A Nuclei

Table 1. Parameters of the model fits obtained by the coherent (analytical) and non-coherent (numerical) model solution for ^{243}Am . The parameters B_2 , B_3 are given in units of \hbar^2/MeV , C_2 and C_3 are given in units of MeV, d_2 and d_3 are given in $\hbar^2 \cdot \text{MeV}^{-1}$, d_0 is given in \hbar^2 and e_{eff}^1 is in units of elementary charge.

| Parameters | B_2 | B_3 | C_2 | C_3 | d_2 | d_3 | d_0 | e_{eff}^1 |
|--------------|-------|--------|-------|-------|--------|--------|-------|--------------------|
| coherent | 421.3 | 1856.5 | 4.48 | 19.75 | 1335.3 | 5883.4 | 6.84 | 0.531 |
| non-coherent | 12.02 | 71.96 | 20.38 | 2.433 | 781.7 | 499.7 | 26.20 | 0.297 |

The resulting optimal parameters are given in Table 1. The mass parameters B_2 and B_3 are fitted to quite small values in the non-coherent case compared to the coherent one. The stiffness parameters C_2 and C_3 show some change but remain in the region of 10 MeV. Also d_2 and d_3 are reduced in value in the non-coherent case. The non-coherent d_2 -value is half of the d_2 -value for the coherent case and in case of d_3 the non-coherent value is even less than 10 % of the coherent value. d_0 and e_{eff}^1 both change a bit, but not dramatically.

In Table 2 the energy values obtained in both, coherent and non-coherent cases are compared to experimental data. As we see, the overall agreement between theory and experiment is better in the non-coherent case. This is confirmed by the fact that the root mean square deviations between theory and experiment are $\sigma_{\text{RMS}} = 11.74$ keV for the coherent case (analytical solution) and $\sigma_{\text{RMS}} = 6.48$ keV for the full solution.

Table 2. Energies from the coherent (analytical) and the non-coherent (full numerical) solution of the model as well as experimental energies, in keV, for the yrast parity-doublet spectrum of ^{243}Am . The data is taken from [8].

| I^π | E (coherent) | E (non-coherent) | E (exp) |
|----------|--------------|------------------|---------|
| $5/2^+$ | 66.951 | 75.991 | 84.0 |
| $7/2^+$ | 107.196 | 108.640 | 109.2 |
| $9/2^+$ | 152.339 | 148.690 | 143.5 |
| $11/2^+$ | 200.747 | 194.981 | 189.3 |
| $13/2^+$ | 251.384 | 246.353 | 244.0 |
| $5/2^-$ | 0.000 | 0.000 | 0.000 |
| $7/2^-$ | 51.000 | 47.951 | 42.2 |
| $9/2^-$ | 104.455 | 103.243 | 96.4 |
| $11/2^-$ | 159.285 | 162.976 | 162.3 |
| $13/2^-$ | 214.952 | 225.038 | 238.0 |

The values of the transition probabilities in Weisskopf units are given in Table 3. The E2 transition value is fitted exactly by both the coherent and non-coherent model. This is a result of the fact that there is only 1 value to fit. The theoretical E1 transition values are reasonably close to the experiment.

Table 3. Theoretical (full solution) and experimental values of B(E1) and B(E2) transition probabilities in Weisskopf units (W.u.) for the yrast parity-doublet spectrum of ^{243}Am . The data is taken from [8].

| Mult | Transition | Exp [W.u.] | Theo [W.u.] | weight |
|------|---------------------------|---------------------|---------------------|-----------|
| E2 | $7/2^- \rightarrow 5/2^-$ | 574 | 574 | 10^{-1} |
| E1 | $5/2^+ \rightarrow 5/2^-$ | $9.7 \cdot 10^{-5}$ | $8.8 \cdot 10^{-5}$ | 10^5 |
| E1 | $5/2^+ \rightarrow 7/2^-$ | $2.6 \cdot 10^{-5}$ | $3.5 \cdot 10^{-5}$ | 10^5 |

We also calculate the corresponding wave function for the ground state angular momentum $I_0 = 5/2^-$ and the resulting quadrupole deformation expectation value given by

$$\langle \beta_2 \rangle = \int_{-\infty}^{\infty} \int_0^{\infty} \beta_2 \Phi(\beta_2, \beta_3)^2 d\beta_2 d\beta_3, \quad (10)$$

as well as the octupole deformation expectation value given by $\sqrt{\langle \beta_3^2 \rangle}$ where $\langle \beta_3^2 \rangle$ is given by

$$\langle \beta_3^2 \rangle = \int_{-\infty}^{\infty} \int_0^{\infty} \beta_3^2 \Phi(\beta_2, \beta_3)^2 d\beta_2 d\beta_3. \quad (11)$$

These values are obtained as $\langle \beta_2 \rangle = 0.298$ and $\sqrt{\langle \beta_3^2 \rangle} = 0.287$. The wave function at $I = I_0$ is plotted in Figure 1. According to [9] the β_2 deformation of ^{243}Am is 0.224 which is not too far away from the fitted value.

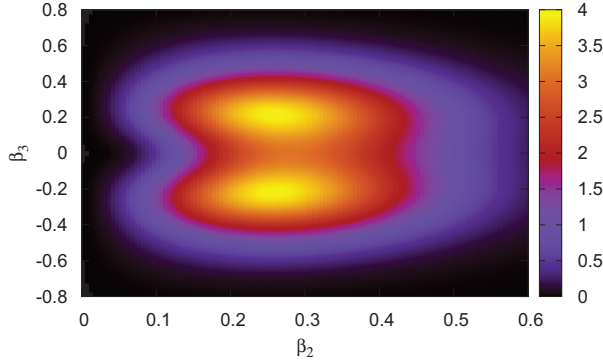


Figure 1. Wave function from the full model solution for ^{243}Am at angular momentum $I = 5/2^-$.

4 Discussion and Outlook

The numerical solution for the nucleus ^{243}Am leads to a better description of the yrast spectrum, and the RMS value for the energies could be improved by

a factor of about 2. At the same time the B(E1) transition probability values in Table 3 do not deviate too much from experimental data. The B(E1) values for the coherent case are $8.9 \cdot 10^{-5}$ W.u. instead of $8.8 \cdot 10^{-5}$ W.u. for the $5/2^+ \rightarrow 5/2^-$ transition which is almost the same, and $4.3 \cdot 10^{-5}$ W.u. instead of $3.5 \cdot 10^{-5}$ W.u. for the $5/2^+ \rightarrow 7/2^-$ transition which is a bit worse.

The B(E2) is exactly the same because we consider only one experimental value. All in all, the obtained results are in agreement with our expectation and experience from the calculations for even-even nuclei.

The obtained deformation expectation value for β_2 is quite reasonable while the octupole deformation expectation value seems to be too large. From the wave function it can be seen that due to the obtained parameters, the potential is of such a shape that the region of highest deformation probability is located at two symmetrically seated maxima, while the probability is a bit reduced along the β_2 -axis.

It should be kept in mind that the fitting algorithm finds a local minimum and it eventually could be that there is another minimum which provides an even better description. During the calculation of several other odd-A nuclei it turned out that when the coherent minimum is taken as initial guess for the fitting algorithm, the RMS deviation could only be improved very insignificantly.

This problem of escaping the given analytical minimum could be avoided by either choosing another guess or another algorithm (currently we use the Powell algorithm as described in [10]). Both of these ideas are currently under investigation.

Acknowledgements

This work is supported by DFG and HIC for FAIR.

References

- [1] N. Minkov, P. Yotov, S. Drenska, W. Scheid, D. Bonatsos, D. Lenis and D. Petrellis, *Phys. Rev. C* **73** (2006) 044315.
- [2] N. Minkov, S.B. Drenska, P. Yotov, D. Bonatsos, W. Scheid, *Physics of Atomic Nuclei* **70** (2007) 1470-1475.
- [3] N. Minkov, S. Drenska, P. Yotov, S. Lalkovski, D. Bonatsos and W. Scheid, *Phys. Rev. C* **76** (2007) 034324.
- [4] N. Minkov, S. Drenska, M. Strecker, W. Scheid and H. Lenske, *Phys. Rev. C* **85** (2012) 034306.
- [5] N. Minkov, S. Drenska, K. Drumev, M. Strecker, H. Lenske and W. Scheid, Description of Non-Yrast Split Parity-Doublet Bands in Odd-A Nuclei, *Nuclear Theory* **31**, Proceedings of the 31-st International Workshop on Nuclear Theory (Rila, Bulgaria 2012), eds. A.I. Georgieva and N. Minkov (Heron Press, Sofia, 2012) p. 35.
- [6] M. Strecker, N. Minkov and H. Lenske, Full solution of nuclear quadrupole-octupole model, *Nuclear Theory* **30**, Proceedings of the 30-th International Work-

- shop on Nuclear Theory (Rila, Bulgaria 2011), eds. A.I. Georgieva and N. Minkov (Heron Press, Sofia, 2011) p. 53.
- [7] M. Strecker, N. Minkov and H. Lenske, Energies and Transition Probabilities from the Full Solution of Nuclear Quadrupole-Octupole Model, *Nuclear Theory* **31**, Proceedings of the 31-st International Workshop on Nuclear Theory (Rila, Bulgaria 2012) eds. A.I. Georgieva and N. Minkov (Heron Press, Sofia, 2012) p. 47.
 - [8] http://www.nndc.bnl.gov/nudat2/indx_adopted.jsp.
 - [9] P. Möller, J.R. Nix, W.D. Myers and W.J. Swiatecki, *Atomic Data and Nuclear Data Tables* **59** (1995) 185-381.
 - [10] William H. Press, Brian P. Flannery, Saul A. Teukolsky, William T. Vetterling, *Numerical Recipes – The Art of Scientific Computing* (Cambridge University Press, New York, 1988).