FINITE ELEMENT METHOD FOR SOLVING THE COLLECTIVE NUCLEAR MODEL WITH TETRAHEDRAL SYMMETRY*

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We apply a new calculation scheme of a finite element method (FEM) for solving an elliptic boundary-value problem describing a quadrupole vibration collective nuclear model with tetrahedral symmetry. We use shape functions constructed with interpolation Lagrange polynomials on a triangle finite element grid and compare the FEM results with those obtained earlier by a finite difference method.

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1. Introduction

In recent papers, the consistent approach to quadrupole–octupole collective vibrations coupled with the rotational motion was presented to find and/or verify some fingerprints of possible high-rank symmetries (*e.g.*, tetrahedral, octahedral, ...) in the recent experimental data of nuclear collective bands [1, 2]. A realistic collective Hamiltonian with variable mass-parameter tensor and potential obtained through the macroscopic–microscopic Strutinsky-like method with particle-number-projected BCS approach in full vibrational and rotational, nine-dimensional collective space was diagonalized in the basis of projected harmonic oscillator eigensolutions. In this approach, the symmetrized orthogonal basis of zero-, one-, two- and three-phonon oscillator-like functions in vibrational part, coupled with the cor-

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responding Wigner function have been applied for solving the boundary value problem (BVP) in 6D domain [3]. The algorithms for construction of the symmetrized basis were considered in [4, 5] w.r.t. symmetrization group [6–8]. In Ref. [9], the BVP in 2D domain describing the above quadrupole vibration collective nuclear model of ^{156}Dy nucleus with tetrahedral symmetry [10] has been solved by a finite difference method (FDM) that was a part of the BVP in 6D domain. However, the FDM approach did not obtain further generalization on the above multi-dimensional domain.

In this paper, we consider the alternative approach which is applicable for solving the BVP in the multi-dimensional domain of d-dimensional Euclidean space divided into the $d!$ simplexes in the framework of a finite element method (FEM) with Lagrangian elements and PI-type Gauss quadrature formulas in the simplexes [11–13].

An efficiency of the applied finite element calculation scheme is shown by the benchmark calculations of the above BVP in the 2D domain. We apply shape functions on triangle finite element grid using the interpolation Lagrange polynomials of two variables with quadrature rules in triangle [14] and compare our FEM results with those obtained earlier by the FDM [9].

2. The setting of the problem

Consider a self-adjoint boundary-value problem for the elliptic differential equation of the second order [11, 13]

$$(D-E)\Phi(x) \equiv \left(-\frac{1}{g_0(x)} \sum_{ij=1}^{d} \frac{\partial}{\partial x_i} g_{ij}(x) \frac{\partial}{\partial x_j} + V(x) - E \right) \Phi(x) = 0\,. \quad (1)$$

It is also assumed that $g_0(x) > 0$, $g_{ji}(x) = g_{ij}(x)$ and $V(x)$ are real-valued functions, continuous together with their generalized derivatives to a given order in the domain of $x \in \bar{\Omega} = \Omega \cup \partial\Omega$ with the piecewise continuous boundary $S = \partial\Omega$, which provides the existence of nontrivial solutions obeying the boundary conditions of the first kind (I) or the second kind (II)

$$\text{(I)}\ \Phi(x)\Big|_S = 0\,, \quad \text{(II)}\ \frac{\partial\Phi(x)}{\partial n_D}\Big|_S = 0\,, \quad \frac{\partial\Phi(x)}{\partial n_D} = \sum_{ij=1}^{d} (\hat{n}, \hat{e}_i) g_{ij}(x) \frac{\partial\Phi(x)}{\partial x_j}\,. \quad (2)$$

Here, $\frac{\partial\Phi_m(x)}{\partial n_D}$ is the derivative along the conormal direction, $\hat{n}$ is the outer normal to the boundary of the domain $S = \partial\Omega$, $\hat{e}_i$ is the unit vector of $x = \sum_{i=1}^{d} \hat{e}_i x_i$, and $(\hat{n}, \hat{e}_i)$ is the scalar product in $\mathcal{R}^d$.

For a discrete spectrum problem, the functions $\Phi_m(x)$ from the Sobolev space $H_2^{s\geq 1}(\Omega)$, $\Phi_m(x) \in H_2^{s\geq 1}(\Omega)$, corresponding to the real eigenvalues E: $E_1 \leq E_2 \leq \ldots \leq E_m \leq \ldots$ satisfy the conditions of normalization and orthogonality

$$\langle \Phi_m(x)|\Phi_{m'}(x)\rangle = \int\limits_{\Omega} \mathrm{d}x g_0(x)\Phi_m(x)\Phi_{m'}(x) = \delta_{mm'}\,, \quad \mathrm{d}x = \mathrm{d}x_1 \ldots \mathrm{d}x_d\,. \tag{3}$$

The FEM solution of the boundary-value problems (1)–(3) is reduced to the determination of stationary points of the variational functional [11, 13]

$$\Xi(\Phi_m, E_m) \equiv \int\limits_{\Omega} \mathrm{d}x g_0(x)\Phi_m(x)\left(D - E_m\right)\Phi(x) = \Pi(\Phi_m, E_m)\,, \tag{4}$$

where $\Pi(\Phi, E)$ is the symmetric quadratic functional

$$\Pi(\Phi, E) = \int\limits_{\Omega} \mathrm{d}x \left[\sum_{ij=1}^{d} g_{ij}(x)\frac{\partial\Phi(x)}{\partial x_i}\frac{\partial\Phi(x)}{\partial x_j} + g_0(x)\Phi(x)(V(x) - E)\Phi(x)\right].$$

3. Quadrupole–octupole-vibrational collective model

Below, we solve the BVP (1)–(3) in the 2D domain $d = 2$ that describe the quadrupole–octupole-vibrational collective model of ^{156}Dy nucleus [9] with the coefficients $g_0(x)$ and $g_{ij}(x)$ determined by the expressions $i, j = 1, 2$

$$\begin{aligned} g_0(x_1, x_2) &= \frac{2}{\hbar^2}\sqrt{\det B(x_1, x_2)}\,, \\ g_{ij}(x_1, x_2) &= \sqrt{\det B(x_1, x_2)}\left[B^{-1}(x_1, x_2)\right]_{ij}\,. \end{aligned} \tag{5}$$

The coefficients $B_{ij}(x_1, x_2)$ have been calculated [9] in terms of the average nuclear deformations $x = (x_1, x_2) = (q_{20}, q_{32})$ determined in [15], and shown in Fig. 1 (a)–(d). The potential energy function $V(x_1, x_2)$ has been calculated in the terms of the nuclear deformations $x = (x_1, x_2) = (\alpha_{20}, \alpha_{32})$ [9] and shown in these coordinates as well as in coordinates $x = (x_1, x_2) = (q_{20}, q_{32})$ in Fig. 2 (a), (b).

Table I shows a low part of the spectrum of $v = 1, \ldots, 10$ states of ^{156}Dy counted from minimum of potential energy ($V_{\min}(\alpha_{20}, \alpha_{32}) = 0.685$ MeV). Second column shows eigenenergies E_v^{FDM} calculated by the FDM code of the second order [9]. The remaining columns show the eigenvalues $E_v^{\mathrm{FEM}}(p)$ of the BVP (1)–(5) in $\Omega(q_{20}, q_{32})$ with coefficients $g_{ij}(q_{20}, q_{32})$ determined by formulas (5) and the potential energy functions $V(q_{20}, q_{32})$ calculated in the present paper by the FEM code with the Gaussian quadratures PI type till the eighth order [14]. Calculations have been carried out with the second type (II) boundary conditions (2) and orthonormalization condition (3) with triangular Lagrange elements of the order of $p = 1, 2, 3, 4$ in the finite element grid $\Omega(q_{20}, q_{32})$. Discrepancy $E_v^{\mathrm{FDM}} - E_v^{\mathrm{FEM}}(p)$ between the results

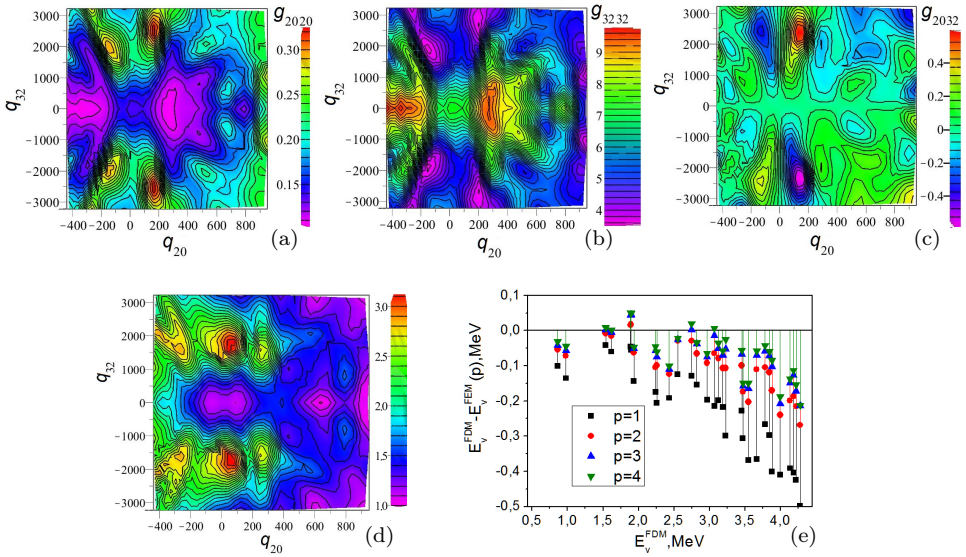

Fig. 1. The coefficients $g_{ij}(x)$ from (5) given in variables (q_{20}, q_{32}) (a), (b), (c). Square root of the determinant $g_0(x) = \sqrt{\det B(q_{20}, q_{32})}$ constructed out of collective inertia parameters in units $10^{-5}\hbar^2/(\text{MeV fm}^5)$ (d). The differences $E_v^{\text{FDM}} - E_v^{\text{FEM}}(p)$ between eigenvalues of E_v^{FDM} of ^{156}Dy nucleus calculated by the FDM [9] and $E_v^{\text{FEM}}(p)$ calculated in the present paper by FEM with triangular Lagrange elements of the order of $p = 1, 2, 3, 4$ for 30 lowest states of the BVP (1)–(5) in variables (q_{20}, q_{32}) (e).

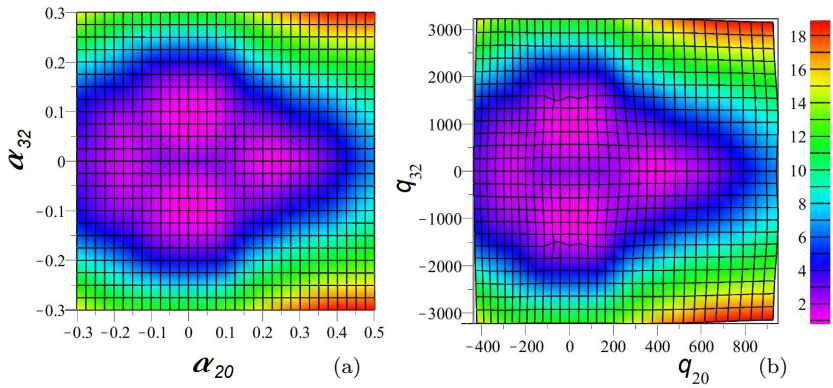

Fig. 2. The potential energy $V(x_1, x_2)$ of ^{156}Dy nucleus given in variables $(\alpha_{20}, \alpha_{32})$ (a) and in variables (q_{20}, q_{32}) (b). The nodal points of finite element grid are intersection points of horizontal and vertical lines.

TABLE I

The low part of the spectrum of 10 lowest states of ^{156}Dy nucleus counted from minimum of potential energy ($V_{\min}(\alpha_{20}, \alpha_{32}) = 0.685$ MeV). E_v^{FDM} calculated by FDM of the second order [9] and $E_v^{\mathrm{FEM}}(p)$ calculated by FEM with triangular Lagrange elements of the order of $p = 1, 2, 3, 4$ in the present paper.

v	E_v^{FDM}	$E_v^{\mathrm{FEM}}(1)$	$E_v^{\mathrm{FEM}}(2)$	$E_v^{\mathrm{FEM}}(3)$	$E_v^{\mathrm{FEM}}(4)$
1	0.85988	0.96000	0.91329	0.90234	0.89065
2	0.97588	1.11144	1.04808	1.03297	1.02068
3	1.53669	1.57813	1.54403	1.53371	1.52776
4	1.61774	1.67776	1.63332	1.62287	1.61571
5	1.88907	1.93560	1.87335	1.84504	1.83794
6	1.89469	1.94932	1.87706	1.84925	1.84631
7	1.93369	2.07731	1.99714	1.98486	1.98032
8	2.23907	2.41405	2.34335	2.29594	2.28444
9	2.25778	2.46383	2.35681	2.33287	2.31778
10	2.43288	2.62454	2.55679	2.54278	2.53388

of FDM and FEM calculations in dependence of the order of $p = 1, 2, 3, 4$ of the FEM approximation is shown in Fig. 1 (e). One can see that in increasing the order of the FEM approximation the discrepancy is decreased till 1%. Figure 3 displays the corresponding eigenfunctions $\Phi_v(q_{20}, q_{32})$ in the finite element grid $\Omega(q_{20}, q_{32})$. The eigenfunctions of the ground and first excited states are in good agreement with the eigenfunctions calculated in domain $\Omega(\alpha_{20}, \alpha_{32})$ by the FDM [9]. The third eigenfunction has one node line in direction α_{20} in contrast with the third FDM eigenfunction that has no nodes. Meanwhile, the forth function has two node lines in the direction of α_{20} and qualitatively coincides with the forth FDM eigenfunction. We

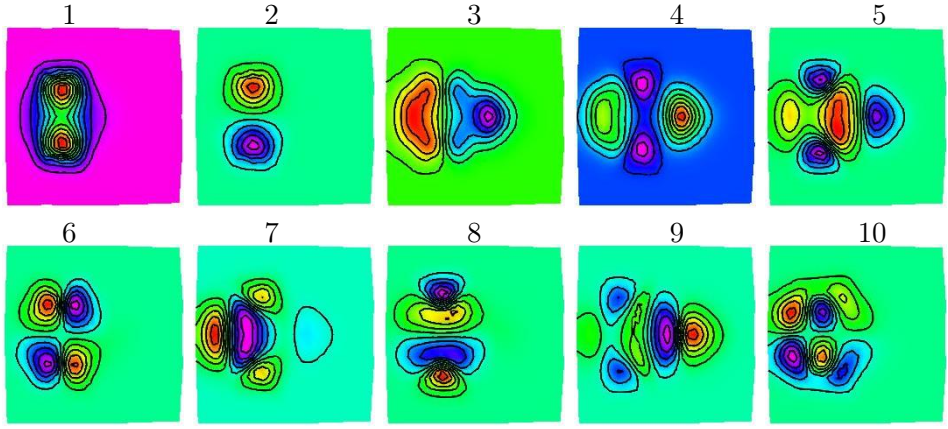

Fig. 3. The first ten eigenfunctions of ^{156}Dy nucleus in the plane (q_{20}, q_{32}).

can suppose that the revivable distinctions are a consequence of approximation of table values of $V(\alpha_{20}, \alpha_{32})$ on the FEM grid $\Omega(q_{20}, q_{32})$ instead of approximation of derivatives of table values of $g_{ij}(q_{20}, q_{32})$ on the FDM grid $\Omega(\alpha_{20}, \alpha_{32})$ accepted in [9].

4. Conclusion

We applied the new calculation schemes in the framework of FEM with the triangular Lagrange elements and Gaussian quadratures for analysis of the quadrupole vibration collective nuclear model with tetrahedral symmetry. We constructed shape functions on triangle finite element grid and compared our FEM results with the obtained earlier by FDM and found that they are in a good agreement. This approach is directly generalized for the solving BVP in multidimensional domain by using the algorithms and their program realization [12, 13]. We will apply the proposed FEM for solving the BVP in the six dimensional domain describing the above quadrupole–octupole collective vibration model in our further papers.

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