PARAMETRIC BASIS FUNCTIONS FOR COLLECTIVE NUCLEAR MODELS*

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We consider calculation schemes in the framework of the Kantorovich method — reduction of a elliptic boundary-value problem to a system of second order ordinary differential equations (ODEs) using the surface functions depending on the ODEs-independent variable as a parameter. We propose construction of the new parametric surface basis functions in an analytical form for solving the boundary-value problem of a quadrupole vibration collective nuclear model.

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1. Introduction

In a recent paper, the consistent approach to quadrupole–octupole collective vibrations coupled with the rotational motion was presented [1]. In this approach, the symmetrized orthogonal basis of zero-, one-, two- and three-phonon oscillator-like functions in vibrational part, coupled with the corresponding Wigner function has been applied for solving the boundary value problem (BVP) in the 6D domain [2]. The algorithms for construction of the symmetrized basis was considered in [3, 4] with respect to the symmetrization group [5]. In paper [6], the 2D BVP was solved by the finite difference method that was a part of the BVP in the 6D domain. However, this approach did not obtain generalization on the multidimensional domain.

In this paper, we consider the alternative approach for solving the BVP in a multidimensional domain in the framework of the Kantorovich method — reduction of an elliptic BVP to a system of second order ordinary differential equations (ODEs) using the surface functions depending on the

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ODE-independent variable as a parameter [7]. We propose construction of the new parametric surface basis functions in an analytical form for solving the BVP of a quadrupole vibration collective nuclear model using finite element method (FEM). The efficiency of calculation scheme is shown by a benchmark calculation of the 2D BVP.

2. Kantorovich method

Let us consider the BVP in the 2D domain $\Omega(x_f, x_s) \subset \mathbb{R}^2$

$$\begin{aligned} \left(-\frac{\partial^2}{\partial x_s^2} - \frac{\partial^2}{\partial x_f^2} + V\left(x_f, x_s\right) - E\right) \Psi\left(x_f, x_s\right) &= 0\,, \\ \Psi(x_f, x_s)\Big|_{\left(x_f, x_s\right) \in \partial\Omega} &= 0\,, \end{aligned} \tag{1}$$

where $V(x_f, x_s)$ is a real-valued function and $\Psi(x_f, x_s)$ satisfies the Dirichlet boundary condition (BC) at the boundary $\partial\Omega \equiv \partial\Omega(x_f, x_s)$ of the domain $\Omega(x_f, x_s)$. The solution $\Psi(x_f, x_s) \in W_2^2(\Omega)$ of the BVP (1) is sought in the form of Kantorovich expansion [7]

$$\Psi_i(x_f, x_s) = \sum_{j=1}^{j_{\max}} \Phi_j\left(x_f; x_s\right) \chi_{ji}(x_s)\,, \tag{2}$$

using the set of eigenfunctions of the parametric BVP

$$\left(-\frac{\partial^2}{\partial x_f} + V_0\left(x_f, x_s\right) - \epsilon_j(x_s)\right) \Phi_j(x_f; x_s) = 0 \tag{3}$$

defined in the interval $x_f \in (x_f^{\min}(x_s), x_f^{\max}(x_s)) = \Omega_{x_f}(x_s)$ and depending on the variable $x_s \in \Omega_{x_s}$ as a parameter. These functions obey the BCs

$$\Phi_j\left(x_f^{\min}(x_s); x_s\right) = 0\,, \qquad \Phi_j\left(x_f^{\max}(x_s); x_s\right) = 0 \tag{4}$$

at the boundary points $\{x_f^{\min}(x_s), x_f^{\max}(x_s)\} = \partial\Omega_{x_f}(x_s)$ of the interval $\Omega_{x_f}(x_s)$. The eigenfunctions satisfy the orthonormality condition

$$\langle \Phi_i | \Phi_j \rangle = \int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f; x_s) \Phi_j\left(x_f; x_s\right) \mathrm{d}x_f = \delta_{ij}\,. \tag{5}$$

Here, $\epsilon_1(x_s) < \ldots < \epsilon_{j_{\max}}(x_s) < \ldots$ is the desired set of real eigenvalues. If this parametric eigenvalue problem has no analytical solution, then it is solved numerically by the FEM using the program ODPEVP [8].

Substituting expansion (2) into Eq. (1) with Eqs. (4) and (5) taken into account, we arrive at the set of self-adjoint ODEs for the unknown vector functions $\boldsymbol{\chi}^{(i)}(x_s, E) \equiv \boldsymbol{\chi}^{(i)}(x_s) = (\chi_1^{(i)}(x_s), \ldots, \chi_{j_{\max}}^{(i)}(x_s))^T$

$$\left(-\mathbf{I}\frac{\mathrm{d}^2}{\mathrm{d}x_s^2} + \mathbf{U}(x_s) - 2E\,\mathbf{I} + \frac{\mathrm{d}\mathbf{Q}(x_s)}{\mathrm{d}x_s} + \mathbf{Q}(x_s)\frac{\mathrm{d}}{\mathrm{d}x_s}\right)\boldsymbol{\chi}^{(i)}(x_s) = 0\,. \tag{6}$$

Here $\mathbf{I}$, $\mathbf{U}(x_s)$ and $\mathbf{Q}(x_s)$ are matrices of the dimension $j_{\max} \times j_{\max}$

$$I_{ij} = \delta_{ij}\,, \qquad U_{ij}(x_s) = \epsilon_i(x_s)\delta_{ij} + H_{ij}(x_s) + V_{ij}(x_s)\,, \tag{7}$$

$$H_{ij}(x_s) = H_{ji}(x_s) = \int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \frac{\partial \Phi_i\,(x_f; x_s)}{\partial x_s}\frac{\partial \Phi_j\,(x_f; x_s)}{\partial x_s}\mathrm{d}x_f\,, \tag{8}$$

$$Q_{ij}(x_s) = -Q_{ji}(x_s) = -\int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i\,(x_f; x_s)\,\frac{\partial \Phi_j(x_f; x_s)}{\partial x_s}\mathrm{d}x_f\,, \tag{9}$$

$$V_{ij}(x_s) = V_{ji}(x_s) = \int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i\,(x_f; x_s)\,(V\,(x_f, x_s) - V_0\,(x_f, x_s))\,\Phi_j(x_f; x_s)\mathrm{d}x_f\,. \tag{10}$$

The solutions of the discrete spectrum $E : E_1 < E_2 < \ldots < E_v < \ldots$ that obey the BCs at the points $x_s^t = \{x_s^{\min}, x_s^{\max}\} = \partial\Omega_{x_s}$, bounding the interval Ω_{x_s} and satisfy the orthonormality conditions are

$$\boldsymbol{\chi}^{(p)}(x_s^t) = 0\,, \qquad x_s^t = x_s^{\min}, x_s^{\max}\,, \qquad \int\limits_{x_s^{\min}}^{x_s^{\max}} \left(\boldsymbol{\chi}^{(i)}(x_s)\right)^T \boldsymbol{\chi}^{(j)}(x_s)\mathrm{d}x_s = \delta_{ij}\,. \tag{11}$$

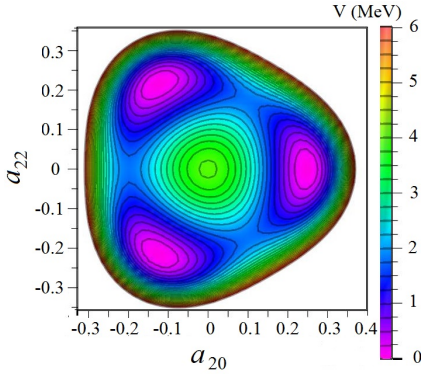
The quadrupole potential energy are approximated by quartic potential

$$V(a_{22}, a_{20}) = c_1\left(a_{22}^2 + a_{20}^2\right) + c_2\left(a_{22}^2 a_{20} - a_{20}^3/3\right) + c_3\left(a_{22}^2 + a_{20}^2\right)^2 + c_0\,. \tag{12}$$

We use a set of parameters $c_1 = -120$, $c_2 = 240$, $c_3 = 1200$, $c_0 = 65/16$ that are a crude approximated shape of ${}^{156}_{64}\mathrm{Gd}_{92}$ which has been fitted in the following points[1]: minima at $(a_{22}, a_{20}) = (0, 1/4)$, $V(0, 1/4) = 0$; maxima at $(a_{22}, a_{20}) = (0, 0)$, $V(0, 0) = 65/16$; and saddle points: $(a_{22}, a_{20}) =$

[1] This shape has been fitted in the following points in our parametrization connected with [1] by relations $a_{22} = \sqrt{2}\alpha_{22}, a_{20} = \alpha_{20}$.

$(0,-1/5)$, $V(0,-1/5) = 729/400$ (see Fig. 1). We choose the mass parameter $m = B_2 = 124$, thus there are ground and double degenerated excited states localized in three wells.



n	$\tilde{E}_n = 2mE_n$	E_n	irr.
1	381.754	1.53933	A1
2,3	387.240	1.56145	E
4,5	617.024	2.48800	E
6	667.104	2.68993	A2
7	695.166	2.80309	A1
8,9	785.680	3.16806	E
10	898.045	3.62115	A1
11,12	915.823	3.69283	E
13,14	993.158	4.00467	E
15	1063.73	4.28926	A1
16	1119.21	4.51296	A2
17,18	1174.71	4.73674	E

Fig. 1. The potential energy of quadrupole shape. The first energy levels E_n [MeV] of the problem at $N = 28$ parametric basis functions.

The solutions of the problem (1)–(12) have been calculated by the Kantorovich method using $N = 28$ parametric basis functions at $V_0(x_f, x_s) = V(x_f, x_s)$ with the help of the FEM program KANTBP 2 [9]. We solve the above eigenvalue problem on a domain $\sqrt{a_{20}^2 + a_{22}^2} < 1/2$ with the Dirichlet BCs at the boundary $\sqrt{a_{20}^2 + a_{22}^2} = 1/2$ by the scheme presented above. We perform calculations in the case of $(x_f, x_s) = (a_{22}, a_{20})$ as well as $(x_f, x_s) = (a_{20}, a_{22})$ on the finite element grid $\{-1/2(6)1/2\}$ with the Lagrange interpolation polynomials of the order of $p = 12$. The first 18 eigenvalues have been calculated with 10 significant digits and presented with 6 significant digits in table of Fig. 1. As it follows from the discrete symmetry C_{3v} of the problem (1), (12), we have four irreducible representations (irrs.) A1, A2, E1 and E2 for classification of solutions and besides the E-type, the states are double degeneracy [10, 11]. The first eigenfunctions for each irr. A1, A2, E1, E2 are presented in Fig. 2.

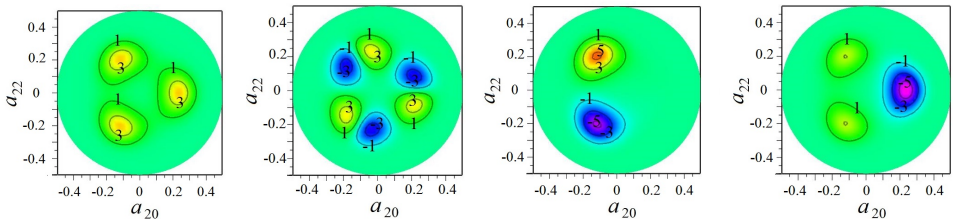


Fig. 2. Nondegenerated functions $\Psi_1(a_{22}, a_{20})$ (irr. A1) and $\Psi_6(a_{22}, a_{20})$ (irr. A2) and degenerated functions $\Psi_2(a_{22}, a_{20})$ (irr. E1) and $\Psi_3(a_{22}, a_{20})$ (irr. E2).

3. Parametric surface functions in analytical form

Let us consider the BVP for Eq. (3) with etalon potential $V_0(x_f, x_s)$

$$\left(-\frac{\partial^2}{\partial x_f^2} + V_0(x_f; x_s) - E\right)\Psi(x_f; x_s) = 0\,,$$
$$V_0\,(x_f, x_s) = V_0(x_s) + \omega^2(x_s)(x_f - z_0(x_s))^2\,. \tag{13}$$

In the considered case the parametric eigenvalue problem (3)–(5) has an exact solution, *i.e.*, the parametric eigenfunctions $\Phi_i(x_f; x_s)$ and potential curves $\epsilon_i(x_s)$ are expressed in the analytical form

$$\begin{aligned}
\epsilon_i\,(x_s) &= V_0(x_s) + \omega(x_s)(2(i-1)+1)\,,\\
\Phi_1\,(x_f; x_s) &= \frac{\omega^{1/4}(x_s)}{\pi^{1/4}}\exp\left(-\omega(x_s)(x_f - z_0(x_s))^2/2\right)\,,\\
\Phi_i\,(x_f; x_s) &= \frac{\sqrt{2}\sqrt{\omega(x_s)}(x_f - z_0(x_s))}{\sqrt{i-1}}\Phi_{i-1}\,(x_f; x_s) - \frac{\sqrt{i-2}}{\sqrt{i-1}}\Phi_{i-2}\,(x_f; x_s)\,.
\end{aligned} \tag{14}$$

The integration in the effective potentials (8)–(9) with the basis functions (14) is carried out analytically, which yields the expressions

$$Q_{ij}(x_s) = \mathrm{sign}(j-i)\left(\frac{\sqrt{2n\omega(x_s)}}{2}\frac{\mathrm{d}z_0(x_s)}{\mathrm{d}x_s}\delta_{|j-i|,1} - \frac{\sqrt{n(n-1)}}{4}\frac{\mathrm{d}\omega(x_s)}{\mathrm{d}x_s}\delta_{|j-i|,2}\right),$$

$$\begin{aligned}
H_{ij}(x_s) = &\left(\frac{n^2+n+1}{8\omega^2(x_s)}\delta_{j-i,0} - \frac{\sqrt{n(n-1)(n-2)(n-3)}}{16\omega^2(x_s)}\delta_{|j-i|,4}\right)\left(\frac{\mathrm{d}\omega(x_s)}{\mathrm{d}x_s}\right)^2\\
&+\left(\frac{\omega(x_s)(2n+1)}{2}\delta_{j-i,0} - \frac{\omega(x_s)\sqrt{n(n-1)}}{2}\delta_{|j-i|,2}\right)\left(\frac{\mathrm{d}z_0(x_s)}{\mathrm{d}x_s}\right)^2\\
&-\left(\frac{n\sqrt{2n}}{4\sqrt{\omega(x_s)}}\delta_{|j-i|,1} + \frac{\sqrt{2n(n-1)(n-2)}}{4\sqrt{\omega(x_s)}}\delta_{|j-i|,3}\right)\frac{\mathrm{d}z_0(x_s)}{\mathrm{d}x_s}\frac{\mathrm{d}\omega(x_s)}{\mathrm{d}x_s}\,,
\end{aligned}$$

where $n = \max(i,j) - 1$. The effective potentials (10) are calculated by integrating the difference $V(x_f, x_s) - V_0(x_f, x_s)$

$$V_{ij}(x_s) = \int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f; x_s)\left(V(x_f, x_s) - V_0(x_f, x_s)\right)\Phi_j(x_f; x_s)\mathrm{d}x_f\,. \quad (15)$$

During the simulation, the adiabatic parameters $V_0(x_s)$, $\omega(x_s)$, $z_0(x_s)$ of the etalon potential (13) are calculated from the conditions

$$\min_{V_0(x_s),\omega^2(x_s),z_0(x_s)} \int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \left(V(x_f, x_s) - V_0(x_f, x_s)\right)^2\mathrm{d}x_f\,. \quad (16)$$

For potential (12) from condition (16), we have

$$\begin{aligned}
\omega(x_s) &= \sqrt{2m}\sqrt{\frac{960}{7} + 240x_s + 2400x_s^2}\,, \qquad z_0(x_s) = 0\,,\\
\text{at } x_s &= a_{20}\,, x_f = a_{22}\,,\\
\omega(x_s) &= \sqrt{2m}\sqrt{\frac{960}{7} + 2400x_s^2}\,, \qquad z_0(x_s) = -\frac{7\left(20x_s^2 - 1\right)}{80\left(35x_s^2 + 2\right)}\,,\\
\text{at } x_s &= a_{22}\,, x_f = a_{20}\,.
\end{aligned}$$

We perform calculations for these parameters in the case of $(x_f, x_s) = (a_{22}, a_{20})$ as well as $(x_f, x_s) = (a_{20}, a_{22})$. The results coincide with calculations of previous sections with 10 significant digits.

4. Conclusion

We proposed a construction of parametric surface functions in an analytical form as eigenfunctions of the etalon equation (13) that provides a solution of the 2D BPV with given accuracy and reduce computer resources with respect to the conventional basis numerically calculated by the FEM. One can construct the parametric functions using a different type of etalon potentials, for example, two-center problem with harmonic oscillator potentials [12]. This approach is generalized for the BVP in multidimensional domain using, for example, the multistep Kantorovich method [7]. As follows from the analysis of the benchmark calculations, the Kantorovich and Galerkin method, using expansion of solution over the symmetrized basis of K-harmonics [13], can be also applied for solving N-dimensional BVPs describing rotational-vibrational nuclear models.

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