Moshinsky Atom as a Test for FEM on Hypercubes

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June 23-25, 2025, Moscow

6th International Conference
“Computer Algebra”

Outline

- Motivation
- The statement of the problem
- FEM scheme with on hyperparallelepipedal elements
- Tests
  - Moshinsky atom
  - Hyperellipsoid
- Conclusion

Motivation: 6D BVP

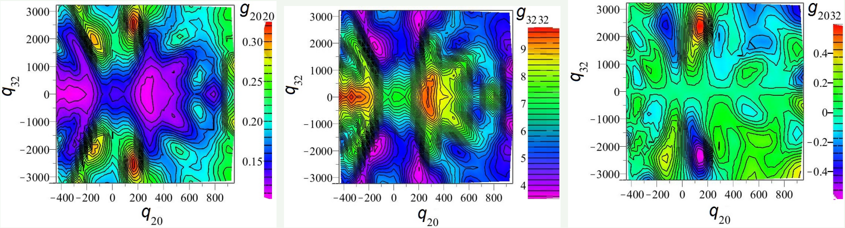
A realistic and quantized quadrupole-octupole-vibrational collective Hamiltonian

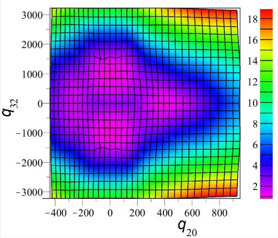
$$H_{\text{coll}}=-\frac{\hbar^2}{2}\left\{\frac{1}{\det B_2}\sum_{\nu,\nu'=0,2}\frac{\partial}{\partial\alpha_{2\nu}}\sqrt{\det B_2}[B_2^{-1}]^{\nu\nu'}\frac{\partial}{\partial\alpha_{2\nu'}}+\frac{1}{\det B_3}\sum_{\nu,\nu'=0}^{3}\frac{\partial}{\partial\alpha_{3\nu}}\sqrt{\det B_3}[B_3^{-1}]^{\nu\nu'}\frac{\partial}{\partial\alpha_{3\nu'}}\right\}$$
$$+V(\alpha_{20},\alpha_{22},\alpha_{30},\alpha_{31},\alpha_{32},\alpha_{33})$$

α_{20}, α_{22}, α_{30}, α_{31}, α_{32}, α_{33} quadrupole and octupole collective variables with metrics; $B_2 \equiv B_2(\alpha_{20}, \alpha_{22})$, $B_3 \equiv B_3(\alpha_{30}, \alpha_{31}, \alpha_{32}, \alpha_{33})$ denote the quadrupole and octupole microscopic mass tensor

A. Dobrowolski, K. Mazurek, and A. Góźdź, Consistent quadrupole-octupole collective model. Phys. Rev. C 94, p. 054322 (2016)
A. Dobrowolski, K. Mazurek, and A. Góźdź, Rotational bands in the quadrupole-octupole collective model. Phys. Rev. C 97, p. 024321 (2018)
A.A. Gusev et al, Finite Element Method for Solving the Collective Nuclear Model with Tetrahedral Symmetry. Acta Physica Polonica B Proceedings Supplement 12, p. 589–594 (2019).

Example: reduced 2D model ^{156}Dy nucleus





The coefficients $g_{ij}(x)$ and the potential energy $V(x_1, x_2)$ of ^{156}Dy nucleus given in variables (q_{20}, q_{32}) in units $10^{-5}\hbar^2/(\text{MeV fm}^5)$.

A. Dobrowolski, K. Mazurek, and A. Góźdź, Rotational bands in the quadrupole-octupole collective model. Phys. Rev. C 97, p. 024321 (2018)

A.A. Gusev et al, Finite Element Method for Solving the Collective Nuclear Model with Tetrahedral Symmetry. Acta Physica Polonica B Proceedings Supplement 12, p. 589–594 (2019).

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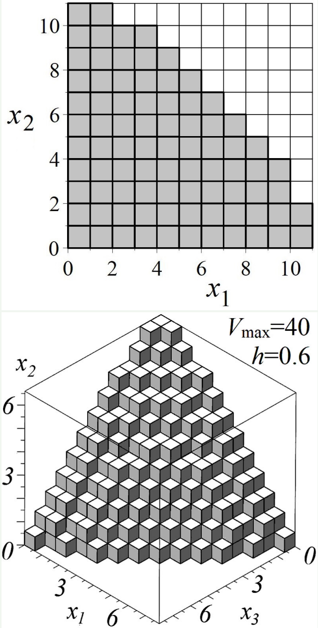
- ...

Features

- The mixed derivatives are present
- The calculation of the tabulated coefficients of differential equations with even relatively low accuracy takes quite a long time
  - ⇒ The problem of constructing optimal unstructured grids does not arise
  - ⇒ It is sufficient to limit ourselves to constructing the FEM schemes on hyperparallelepipedal grids
- To save computer resources, the BVP is solved on a reduced complex domain composed of parallelepipeds and reduced set of basis functions

Examples of 2D and 3D grids



The statement of the discrete spectrum boundary value problem (BVP)

A self-adjoint elliptic PDE in the region $z=(z_1,...,z_d)\in\Omega\subset\mathcal{R}^d$ (Ω is polyhedra)

$$\left(-\frac{1}{g_0(z)}\sum_{ij=1}^{d}\frac{\partial}{\partial z_i}g_{ij}(z)\frac{\partial}{\partial z_j}+V(z)-E\right)\Phi(z)=0,\quad g_0(z)>0,\quad g_{ji}(z)=g_{ij}(z).$$

Boundary conditions

$$\Phi(z)|_S=0,$$

$$\left.\frac{\partial\Phi(z)}{\partial n_D}\right|_S=0,\ \frac{\partial\Phi(z)}{\partial n_D}=\sum_{ij=1}^{d}(\hat{n},\hat{e}_i)g_{ij}(z)\frac{\partial\Phi(z)}{\partial z_j},$$ derivative along the conormal

$\hat{n}$ is the outer normal to the boundary of the domain $\partial\Omega$.

+ Conditions of normalization and orthogonality

Ladyzhenskaya, O. A., The Boundary Value Problems of Mathematical Physics, Applied Mathematical Sciences, 49, (Berlin, Springer, 1985).
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Finite Element Method

BVP $\to$ problem of determination of stationary points of the variational functional

$$\int_\Omega \left(\sum_{ij=1}^{d} \frac{\partial \Phi(z)}{\partial z_i} g_{ij}(z) \frac{\partial \Phi(z)}{\partial z_j} + g_0(z)\Phi(z)(V(z)-E)\Phi(z) \right) dz$$

Expansion of solutions in the form of a finite sum over the basis of local functions $N_\mu^g(z)$

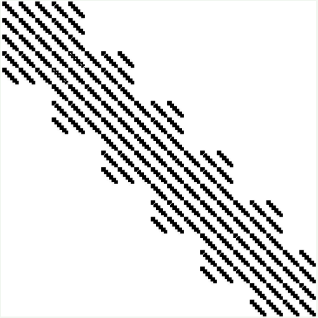
$$\Phi(z) = \sum_{l=1}^{L} \Phi_l^h N_l^g(z). \qquad (*)$$

After substituting (*) into a variational functional and minimizing it, we obtain the generalized algebraic eigenvalue problem

$$\mathbf{A}^p \boldsymbol{\xi}^h = \varepsilon^h \mathbf{B}^p \boldsymbol{\xi}^h.$$

Here $\mathbf{A}^p$ is the stiffness matrix; $\mathbf{B}^p$ is the positive definite mass matrix;

Structure of matrix at $d = 2$



Construction of basis of one dimensional local functions $N^g_\mu(z)$

A non-uniform Finite Element grid on interval $\Omega = [z_{\min} \equiv z_0, z_{\max} \equiv z_{q^{\max}}]$

$$\Delta_q = [z_{q-1}, z_q], \quad q = 1, ..., q^{\max}, \quad \Omega = \bigcup_{q=1}^{q^{\max}} \Delta_q$$

Shape functions

are one-dimensional LIPs or HIPs $\varphi_{rq}(x) \equiv \varphi^{\kappa_{r'}}_{r'q}(x)$, $r = 1, ..., r^{\max}$ with nodes $r' = 0, ..., \rho$ of different multiplicities $\kappa^{\max}_{r'}$ satisfying the relations

$$\varphi^{\kappa}_{r'q}(x_{r''}) = \delta_{r'r''}\delta_{\kappa 0}, \quad \left.\frac{d^{\kappa'}\varphi^{\kappa}_{r'q}(x)}{dx^{\kappa'}}\right|_{x=x_{r''}} = \delta_{r'r''}\delta_{\kappa\kappa'}$$

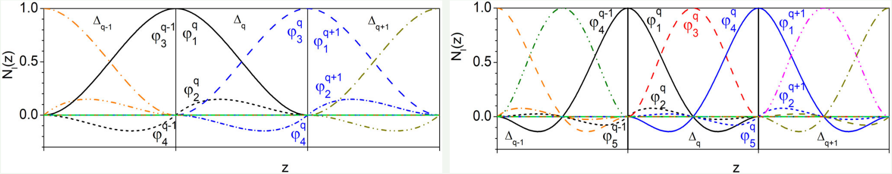
and ordered by r', and for equal r' by κ.

In our implementation of the FEM $\kappa^{\max}_0 = \kappa^{\max}_\rho$ and there is a number s such that $\varphi_{rq}(x) \equiv \varphi^{\kappa_{r'}}_{0q}(x)$, $\varphi_{r+sq}(x) \equiv \varphi^{\kappa_{r'}}_{\rho q}(x)$.

Construction of basis of one dimensional local functions $N^g_\mu(z)$

The local functions $N^g_\mu(z)$ are obtained by matching of shape functions

$$N_l(x) = \sum_{s'=0,1} \{\varphi_{r+ss',q-s'}(z), x \in \Delta_{q-s'}\}.$$



The set of local functions $N^g_\mu(z)$ constructed by matching of 3rd and 4th -order shape functions.

Construction of basis of multidimensional local functions $N^g_\mu(z)$

A non-uniform Finite Element grid with rectangular cells in a complex domain

$$\Delta_q \equiv \Delta_{q_1,\ldots,q_d} = [x_{1;q_1-1}, x_{1;q_1}] \otimes \cdots \otimes [x_{d;q_d-1}, x_{d;q_d}], \quad q_i = 1, \ldots, q_i^{\max},$$

$$q \equiv q(q_1, \ldots, q_d), \quad \text{is global number of the FE}$$

Shape functions are products of one-dimensional LIPs or HIPs

$$\varphi_{rq}(x) \equiv \varphi_{r_1\ldots r_d q_1\ldots q_d}(x) = \varphi_{r_1 q_1}(x_1) \times \ldots \times \varphi_{r_d q_d}(x_d) = \varphi^{\kappa_{r'_1}}_{r'_1 q_1}(x_1) \times \ldots \times \varphi^{\kappa_{r'_d}}_{r'_d q_d}(x_d)$$

The local functions $N^g_\mu(z)$

$$N_l(x) = \sum_{s_1,\ldots,s_d=0,1}^{\prime} \{\varphi_{r_1+ss_1\ldots r_d+ss_d, q_1-s_1\ldots q_d-s_d}(x), x \in \Delta_{q_1-s_1\ldots q_d-s_d}\}$$

where the summation is taken over those $s_1, \ldots, s_d$ for which the shape functions $\varphi_{r_1\ldots r_d q_1\ldots q_d}(x)$ and the cell $\Delta_{q_1-s_1\ldots q_d-s_d} \subset \Delta$ are defined.

To reduce the dim of AEP we drop $N_l(x)$ with $\kappa_{r'_1} + \ldots + \kappa_{r'_d} \geq \breve{\kappa}$

Test 1: The Moshinsky atom

(system of $A \geq 3$ identical particles with pair oscillatory interaction)

The BVP of the relative motion in the c.m.s. in symmetrized coordinates X

$$\left(\sum_{i=1}^{A-1}\left(-\frac{\partial^2}{\partial X_i^2}+X_i^2\right)-E_n^{\mathrm{S,A}}\right)\Phi_n^{\mathrm{S,A}}(X)=0,\quad X=(X_1,...,X_d)\in\mathcal{R}^d,\quad d=A-1$$

the nonrectangular domain is bounded by planes

$$\frac{2-\sqrt{A}}{\sqrt{A}-1}X_1+\frac{1}{\sqrt{A}-1}\sum_{i=2}^{A-1}X_i=0,\quad X_{j-1}-X_j=0,\quad j=2,...,A-1.$$

To construct states that are symmetric (S) or antisymmetric (A) w.r.t. permutations of pairs of particles, the Dirichlet or Neumann BCs, should be applied.

The degenerate spectrum

$$E_n^{\mathrm{S}}=A-1, A+3, A+5, A+7, A+9, ...,\quad E_n^{\mathrm{A}}=A^2-1, A^2+3, A^2+5, A^2+7, A^2+9, ...$$

A.A. Gusev, S.I. Vinitsky, O. Chuluunbaatar, L.L. Hai, V.L. Derbov and P.M. Krassovitskiy, Resonant tunneling of the few bound particles through repulsive barriers, Physics of Atomic Nuclei 77, 389 (2014).

The Moshinsky atom

Affine coordinates $z=(z_1,...,z_d)\in\mathcal{R}^d$, $d=A-1$

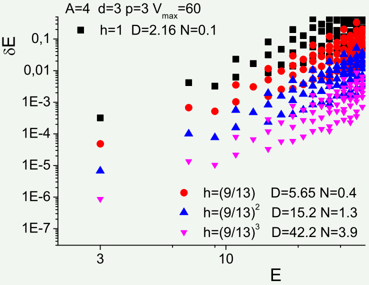
$$z_1 = \frac{2-\sqrt{A}}{\sqrt{A}-1}X_1 + \frac{1}{\sqrt{A}-1}\sum_{i=2}^{A-1} X_i, \quad z_j = X_{j-1} - X_j, \quad j = 2, ..., A-1,$$

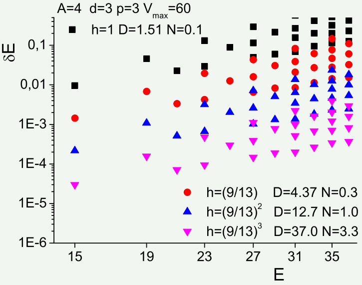
The BVP in a rectangular domain $\Omega(z) = \{z \in \mathcal{R}^d_+\}$

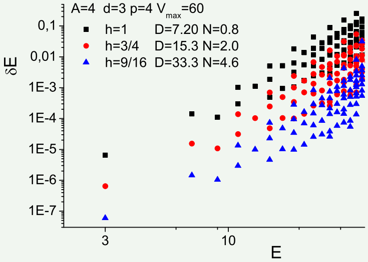
$$\left(-\frac{1}{g_0(z)} \sum_{ij=1}^{d} \frac{\partial}{\partial z_i} g_{ij}(z) \frac{\partial}{\partial z_j} + V(z) - E \right) \Phi(z) = 0,$$

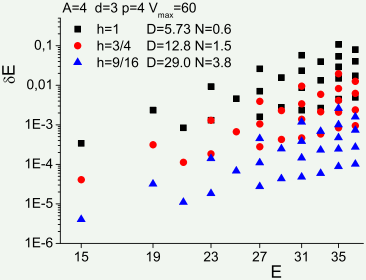
$$g_0(z) = 1, \quad g_{ij}(z) = \{2, i=j; -1, i=j\pm 1; 0 \text{ otherwise}\}, \quad i,j = 1, ..., A-1$$

The Moshinsky atom

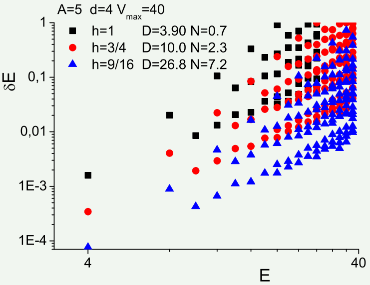


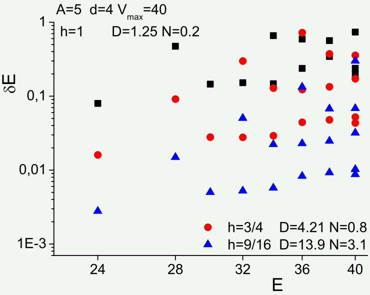


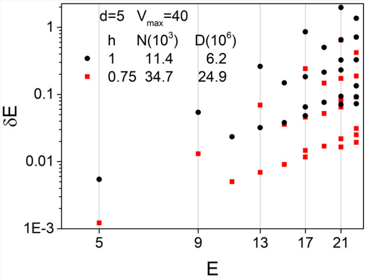


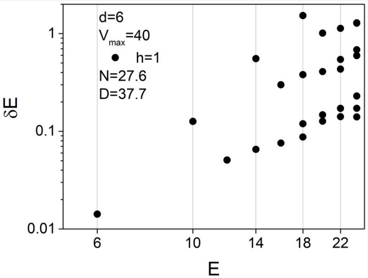


The Moshinsky atom









Test 2: the Helmholtz problem on hyperellipsoid

The BVP with Dirichlet BCs

$$\left(-\sum_{i=1}^{d} \frac{\partial^2}{\partial X_i^2} - E\right)\Phi = 0, \quad \Omega = \left\{(X_1, ..., X_d) \in \mathcal{R}^d \,\middle|\, \sum_{i=1}^{d} \frac{X_i^2}{a_i^2} < 1\right\}$$

The non-orthogonal coordinates $z_1 = r$, $z_k = \theta_{k-1}$, $k = 2, ..., d$

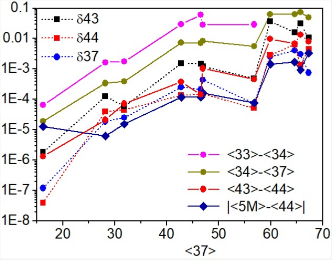
$$X_1 = a_1 r \sin\theta_{d-1} \ldots \sin\theta_2 \sin\theta_1,$$
$$X_k = a_k r \sin\theta_{d-1} \ldots \sin\theta_k \cos\theta_{k-1}, \quad k = 2, ..., d-1$$
$$X_d = a_d r \cos\theta_{d-1}$$
$$r \in [0, +\infty), \quad \theta_1 \in [0, +2\pi], \quad \theta_{k-1} \in [0, +\pi], \quad k = 3, ..., d-1, \quad \theta_{d-1} \in [0, +\pi].$$

The coefficients $g_0(x)$ and $g_{ij}(x)$ of BVP at $d = 3$

$$g_0(z) = r^2 \sin\theta_1, \qquad V(z) = 0,$$
$$g_{11}(z) = r^2 \sin\theta_2((a_1^{-2}\sin^2\theta_1 + a_2^{-2}\cos^2\theta_1)\sin^2\theta_2 + a_3^{-2}\cos^2\theta_2), \qquad g_{12}(z) = \cos\theta_1 \sin\theta_1 \cos\theta_2 (a_1^{-2} - a_2^{-2}),$$
$$g_{22}(z) = (a_1^{-2}\cos^2\theta_1 + a_2^{-2}\sin^2\theta_1)/\sin\theta_2, \qquad g_{13}(z) = -r\cos\theta_2 \sin^2\theta_2 \cos\theta_2 (a_1^{-2}\sin^2\theta_1 + a_2^{-2}\cos^2\theta_1 - a_3^{-2})$$
$$g_{33}(z) = \sin\theta_2((a_1^{-2}\cos^2\theta_1 + a_2^{-2}\sin^2\theta_1)\cos^2\theta_2 + a_3^{-2}\sin^2\theta_2), \qquad g_{23}(z) = \cos\theta_1 \sin\theta_1 \cos\theta_2 (a_1^{-2} - a_2^{-2})$$

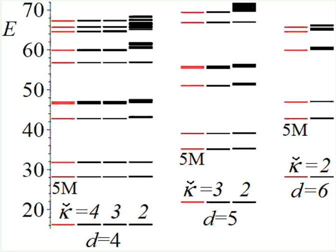
Helmholtz problem on hyperspheroid a_i=0.84, a_j=1, j=1, ..., d, $j \neq i$

4D Hyperspheroid



$< pN > \equiv E_j^{pN}$ and δpN means the mean value and difference between the upper and lower calculated eigenvalues from the level. Here $\check{\kappa} = 3$.

(p, N)	(3,3)	(3,4)	(3,7)	(4,3)	(4,4)
D^S	2368	6000	41472	11326	30672
$N^S, 10^6$	0.48	1.45	12.81	5.97	18.60
D^A	1600	4450	34816	9034	25826
$N^A, 10^6$	0.27	0.97	10.31	4.19	14.38



d	4	5	6
D^S	432	1539	5346
$N^S, 10^6$	0.03	0.32	3.01

Here $p = 3$, $\check{\kappa} = 2$,
grid $\{0(\frac{1}{3})1\} \otimes \{0, \frac{\pi}{4}, \frac{\pi}{2}\}^{d-1}$

Grid $\{0(1/N)1\} \otimes \{0(\pi/N)\pi\}^{d-1}$ with Dirichlet BCs at $r = 1$ and $\theta_1 = 0, \pi$ for antysymmetric states and Neumann otherwise.
KANTBP 5M (by Kantorovich method 28 eqs) for 5th-order HIPs [2,1,1,2], grid: $\{0, 0.01, 0.03, 0.06, 0.1(0.1), 0.9, 0.94, 0.97, 0.99, 1\}$ at d<6 and $\{0.01, ..., 1\}$ at d=6.

Resume

- When solving multidimensional boundary value problems, the main problem with increasing dimension is the exponential increase in both the dimension of the algebraic boundary value problem and, to a greater extent, the number of nonzero elements.
- To restrain such an increase, we use complex rectangular grids and the exclusion of functions with large multiplicity of the grid nodes from the piecewise polynomial basis functions were used.
- Available on PCs: to solve AEP of dimension ~ 30000, the number of nonzero elements is ~ 20 million.
  - This enough to solve with good accuracy the 2D, 3D and 4D BVPs, and with low accuracy 5D and 6D BVPs.
- The expectations to solve with appropriate accuracy 6D BVPs: dimension of AEP 100000, the number of nonzero elements being 150 million.
- In addition, it is possible to reduce memory, for example, by eliminating small non-diagonal matrix elements, which allows solving problems of describing quadrupole-octupole deformations on a personal computer to be reported in our further papers.

THANK YOU FOR YOUR ATTENTION