

FEM SOLVER FOR CONFINED QUANTUM SYSTEM

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New FEM schemes for solving boundary-value problems (BVPs) of elliptic PDEs in d-dimensional domain or systems of coupled PDEs are presented. The smooth FEM basis functions composed matching multivariate Hermitian interpolated polynomials (HIPs) preserved mixed continuous derivatives up to a given order of required solutions on boundaries of joint finite elements are applied. The FEM schemes are implemented in Wolfram Mathematica and FORTRAN by GCMFEM-8 or GCMFEM-9 programs are elaborated and approbated up to $d = 6$ in a personal computer. Benchmark calculations of BVPs for PDEs or system PDEs for quantum dots describing Helmholtz problem on 3D ellipsoid domain, hydrogen atom and ion in magnetic field, and Dirac oscillator are confirmed robustness of the elaborated schemes and programs, that is also applicable to a wide class of the quantum confined systems.

1. INTRODUCTION

The spectral characteristics of hydrogen-like atoms and ions in a magnetic field are the subject of theoretical and experimental studies from atomic and molecular physics, plasma physics and astrophysics, to technological applications in the form of artificial atoms - quantum dots in LEDs and other quantum nanostructures [1].

A magnetically compressed hydrogen atom or ion have axial symmetry, meaning that a 3-dimensional boundary value problem (BVP) for a fixed magnetic quantum number is reduced to a 2-dimensional BVP for the elliptic partial differential equations(PDEs) with non-separable variables in the spherical, cylindrical, parabolic or spheroidal coordinate systems, respectively. At small of magnetic field strength they look as Coulomb system while at large values they look similar to oscillator systems studied in semiconductor quantum dots, well and wires [1,2]. It means that for small values of the radial or quasiradial variable, the Coulomb interaction predominates, while for large values, the potential energy of interaction with the magnetic

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field predominates. Accordingly, the energy eigenvalues are characterized by spherical quantum numbers at small magnetic fields while cylindrical or parabolic quantum numbers at large magnetic fields, see Fig.1. Therefore, solving the problem using the Galerkin method requires introducing a composite basis taking into account these properties, that are revealed in the corresponding coordinate systems, respectively, as well as stitching them together, which is cumbersome procedure. Thus, the solving of the 2D BVP by finite element method is more relevant. Here it's demonstrated by calculating the eigenvalues and eigenfunctions of a lower part of the energy spectra of ellipsoidal quantum dot, Hydrogen atom and ion in uniform magnetic field and Dirac oscillator by means of author's programs GCMFEM 8 and GCMFEM 9 for solving up to six dimensional BVPs for systems of PDEs [3, 4] that is also applicable to a wide class of the quantum confined systems.

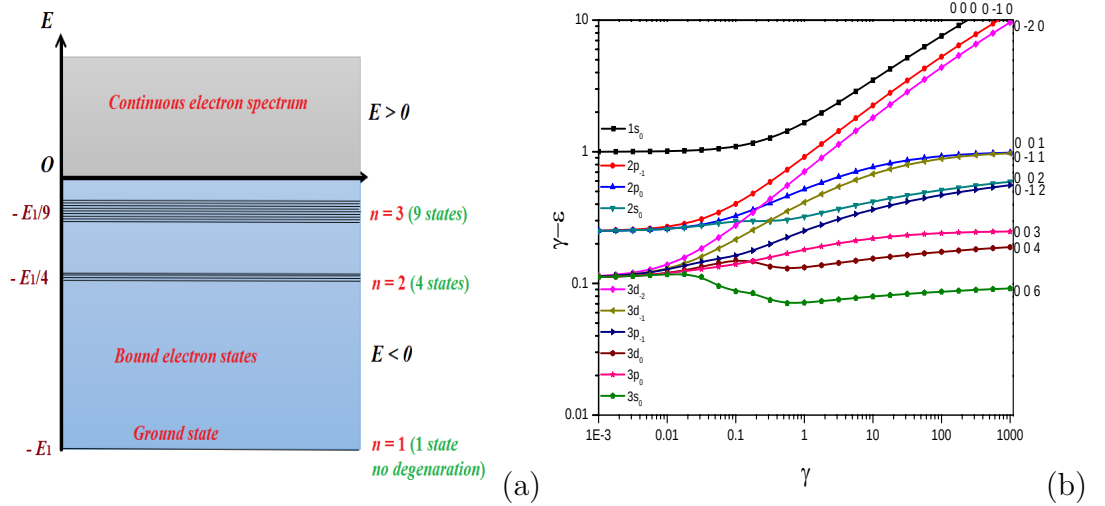


Fig. 1. The energy eigenvalues $E_n^{(0)} = E_{nlm}^{(0)} = -Z^2/(2n^2)$ (in a.u.) are independent of n , l , and m . All $n^2 = 4, 9, \dots$ states with the same $n = 2, 3, \dots$ have the same energy $E_2^{(0)} = -1/(2(2)^2)$, $E_3^{(0)} = -1/(2(3)^2)$, ..., i.e., they are degenerate. b. The first ten levels of double the binding energy $\mathcal{E}_i = \gamma - \epsilon_i$ (Ry = 2 a.u.) for $m \leq 0$ depending on the value of a dimensionless parameter $\gamma = B/B_0$ of magnetic field strength $B_0 = m_e^2 c(e/\hbar)^3 \cong 2.35 \times 10^9 G = 2.35 \times 10^5 T$. The rule of correspondence $(Nlm) \rightarrow (N_\rho m N_z)$ of quantum numbers in spherical and cylindrical coordinates.

2. FEM SCHEMES FOR SOLVING BVPs OF SYSTEMS PDEs

We consider self-adjoint d -dimensional BVP for $\mathcal{N}$ coupled elliptic PDEs

$$\left(\mathbf{I}T(x) + \mathbf{Q}(x)\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\mathbf{Q}(x) + \mathbf{V}(x) - E_v\mathbf{I} \right) \Phi_v(x) = 0, \quad (1)$$

$$T(x) = -\frac{1}{g_0(x)} \sum_{i,j=1}^d \frac{\partial}{\partial x_i} g_{ij}(x) \frac{\partial}{\partial x_j}$$

$$\mathbf{Q}(x)\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\mathbf{Q}(x) = \sum_{i=1}^d \frac{1}{g_0(x)} \mathbf{Q}^{(i)}(x) \frac{\partial}{\partial x_i} + \sum_{i=1}^d \frac{1}{g_0(x)} \frac{\partial}{\partial x_i} \mathbf{Q}^{(i)}(x)$$

in the appropriate domain $x = (x_1, \dots, x_d) \in \bar{\Omega} = \Omega \cup \partial\Omega \subset \mathbb{R}^d$ with the Dirichlet or Neumann boundary conditions (BCs) on their boundary $S = \partial\Omega$.

It is also assumed that $g_0(x) > 0$, $g_{ji}(x) = g_{ij}(x)$, $\mathbf{I}$ is a unit matrix of dimension $\mathcal{N} \times \mathcal{N}$, $\mathbf{V}(x) = \{V_{kn}(x)\}_{k,n=1}^{\mathcal{N}}$, $\mathbf{Q}^{(i)} = \{Q_{kn}^{(i)}(x)\}_{k,n=1}^{\mathcal{N}}$ are symmetric and skew-symmetric real-valued matrix functions, providing the existence of nontrivial eigenfunctions $\Phi_v(x) = (\Phi_{1v}(x), \dots, \Phi_{\mathcal{N}v}(x))^T$, where T means the matrix transposition, and the corresponding eigenvalues E_v .

The BVP is reduced to the stationary points of variation functional:

$$\int_{\Omega} \sum_{ij=1}^d \left(g_{ij} \frac{\partial \Phi^T}{\partial x_i} \frac{\partial \Phi}{\partial x_j} + \Phi^T \mathbf{Q}^{(i)} \frac{\partial \Phi}{\partial x_i} - \frac{\partial \Phi^T}{\partial x_i} \mathbf{Q}^{(i)} \Phi + g_0 (\Phi^T \mathbf{V} \Phi - E \Phi^T \Phi) \right) d^d x.$$

The FEM reduction of the considered BVP for Eqs. (1), using the piecewise polynomial functions $N_l(x) \in C^{\kappa^c}$ constructed from the p -order Hermite interpolation polynomials (HIPs),

$$\Phi(x) = \sum_{l=1}^{\mathcal{N}} \Phi_{n(l)}^h N_{n(l)}(x) \quad (2)$$

leads to the generalized algebraic eigenvalue problem

$$(\mathbf{A} - E_v^h \mathbf{B}) \Phi_v^h = (\mathbf{A}^{(1)} + \mathbf{A}^{(2)} + \mathbf{A}^{(3)} - E_v^h \mathbf{B}) \Phi_v^h = 0, \quad (\Phi_v^h)^T \mathbf{B} \Phi_v^h = \mathbf{I}. \quad (3)$$

The elements of the symmetric matrices $\mathbf{A}^{(1)} = (A_{ll'}^{(1)})$, $\mathbf{A}^{(2)} = (A_{ll'}^{(2)})$, $\mathbf{A}^{(3)} = (A_{ll'}^{(3)})$, and $\mathbf{B} = (B_{ll'})$ of dimension $L \times L$ are expressed through the integrals

$$A_{ll'}^{(1)} = \int_{\Omega} \sum_{i,j=1}^d \frac{\partial N_l}{\partial x_i} g_{ij} \frac{dN_{l'}}{dx_j} dx, \quad (4)$$

$$A_{ll'}^{(2)} = \int_{\Omega} \left[\sum_{i=1}^d \left[N_l Q_{k(l)n(l')}^{(i)} \frac{\partial N_{l'}}{\partial x_i} - \frac{\partial N_l}{\partial x_i} Q_{k(l)n(l')}^{(i)} N_{l'} \right] dx \right],$$

$$A_{ll'}^{(3)} = \int_{\Omega} N_{k(l)} g_0 V_{k(l)n(l')} N_{l'} dx, \quad B_{ll'} = \int_{\Omega} N_l g_0 N_{l'} dx,$$

where $dx = dx_1 \times \dots \times dx_d$ and the argument x of functions is omitted.

Integrals (4) are calculated at Gaussian nodes and quadratures of the order $p+1$. The deviation of the approximate solution $E_v^h, \Phi_v^h(x) \in \mathcal{H}_2^{\kappa^c+1 \geq 1}(\Omega_h)$ from the exact one $E_v, \Phi_v(x) \in \mathcal{H}_2^2(\Omega)$ is estimated in [3] as follows

$$|E_v - E_v^h| \leq c_1 h^{2p}, \quad \|\Phi_v(x) - \Phi_v^h(x)\|_0 \leq c_2 h^{p+1}, \quad (5)$$

where h is the maximal size of the finite element Δ_q , p is the FEM scheme order, $c_1 > 0$ and $c_2 > 0$ are coefficients independent of h , and $\|\dots\|_0$ is norm

$$\|\Phi_v(x)\|_0^2 = \int_{\Omega} g_0(x) \Phi_v^T(x) \Phi_v(x) dx. \quad (6)$$

3. TWO AND THREE -DIMENSIONAL BVPs

3.1. Quantum dots [5, 6]: the Helmholtz problem on hyperellipsoid

We consider a BVP for the Helmholtz equation on d dimensional domain $\Omega \subset \mathbb{R}^d$ of a hyperellipsoid with semiaxes $a_1, \dots, a_d$

$$\left(- \sum_{i=1}^d \frac{\partial^2}{\partial \hat{x}_i^2} - E'_v \right) \Psi_{v'}(\hat{x}) = 0, \quad \Omega = \left\{ (\hat{x}_1, \dots, \hat{x}_d) \in \mathcal{R}^d \left| \sum_{i=1}^d \frac{\hat{x}_i^2}{a_i^2} < 1 \right. \right\} \quad (7)$$

with Dirichlet boundary conditions on its boundary $\partial\Omega$ in generalized hyper-spherical coordinates x related to the original ones $\hat{x}$ by the formulas

$$\begin{aligned} x_1 &= \theta_1 \in [0, +2\pi], \quad x_k = \theta_{k-1} \in [0, +\pi], \quad k = 2, \dots, d-1, \quad x_d = r, \\ \hat{x}_1 &= a_1 r \sin \theta_{d-1} \dots \sin \theta_2 \sin \theta_1, \quad r = \sqrt{\frac{\hat{x}_1^2}{a_1^2} + \dots + \frac{\hat{x}_d^2}{a_d^2}}, \\ \hat{x}_k &= a_k r \sin \theta_{d-1} \dots \sin \theta_k \cos \theta_{k-1}, \quad k = 2, \dots, d-1, \quad \hat{x}_d = a_d r \cos \theta_{d-1}. \end{aligned}$$

Taking symmetry into account, the BVP (7) has 2^d classes of solutions $\Psi_{v'}^{t_1 \dots t_d}(\hat{x}_1, \dots, \hat{x}_d)$, specified by $t_i = e$ or $t_i = o$, meaning that the solution is symmetric or antisymmetric with respect to $\hat{x}_i = 0$.

As a test we seek a solution $\Psi_{v'}(x, z)$ in the form of the Kantorovich expansion with unknown coefficient functions $\Phi_{nv'}(x) \equiv \Phi_{nv}(x_1, \dots, x_{d-1})$

$$\Psi_{v'}(x, z) = \sum_{n=1}^{\mathcal{N}} B_n(z; x) \Phi_{nv'}(x).$$

Here two-parameter basis functions $B_n(z; x) \equiv B_n(z; \theta_1, \dots, \theta_{d-2}, r)$ of the independent variable $z = \hat{x}_d$ on the interval $z \in (z_{\min}, z_{\max})$, where $z_{\max} = -z_{\min} = a_d \sqrt{1 - r^2}$ and the corresponding eigenvalues $E_n(x)$ are known in analytical form and depend only on the parameter $x_{d-1} = r = \sqrt{\hat{x}_1^2 + \dots + \hat{x}_{d-1}^2}$:

$$B_n(z; x) = \frac{\sin \left(\frac{(z + a_d \sqrt{1 - r^2}) \pi n}{2 a_d \sqrt{1 - r^2}} \right)}{\sqrt{a_d \sqrt{1 - r^2}}}, \quad E_n(x) = \frac{\pi^2 n^2}{4 a_d^2 (1 - r^2)}. \quad (8)$$

Integrating of (7) over $B_n(z, x)$ by $z \in (z_{\min}, z_{\max})$, we arrive at a system of PDEs (1) for $\Phi_{v'}^{t_1, \dots, t_d}(x)$ in the reduced domain $\Omega'_{d-1}(x) \subset \mathbb{R}^{d-1}$ with appropriate BCs and matrix elements $V_{nn'}(x)$ and $Q_{nn'}^{(i)}(x)$, $i = 1, \dots, d-1$, given by formulas:

$$\begin{aligned} V_{nn'}(x) &= E_n(x) \delta_{nn'} + H_{nn'}(x), \\ H_{nn}(x) &= \frac{g_{d-1d-1}(x)}{g_0(x)} \frac{\pi^2 n^2 + 3}{12} \frac{r^2}{(1 - r^2)^2} \delta_{nn'} \\ &+ \frac{g_{d-1d-1}(x)}{g_0(x)} \frac{2n'n(n^2 + n'^2)(1 + \cos(\pi n') \cos(\pi n))}{(n^2 - n'^2)^2} \frac{r^2}{(1 - r^2)^2} (1 - \delta_{nn'}), \\ Q_{nn'}^{(i)}(x) &= g_{d-1i}(x) \frac{n'n(1 + \cos(\pi n') \cos(\pi n))}{(n^2 - n'^2)} \frac{r}{(1 - r^2)} (1 - \delta_{nn'}). \end{aligned} \quad (9)$$

Table 1. The lower part of the spectrum $E_{v'}^{t_1 t_2 t_3} = E_{vm}^{t_1 t_2 t_3}$ of BVP (7) in three-dimensional ellipsoid calculated using the GCMFEM8 program with all correct digits (top), and the BVP (1) calculated using the GCMFEM9 program (bottom).

	E_{vm}^{eee}	$E_{vm}^{eoe}, E_{vm}^{oeo}$	$E_{vm}^{eee}, E_{vm}^{ooo}$	$E_{vm}^{eoe}, E_{vm}^{oeo}$
v	$m = 0$	$m = 1$	$m = 2$	$m = 3$
1	11.229170984 11.2292	21.84594348 21.8461	35.1501001 35.150	51.029602 51.030
2	37.7674466 37.768	55.878366 55.879	76.100923 76.10	98.47922 98.48
3	47.5391890 47.539	66.871385 66.872	89.39125 89.392	
4	77.969986 77.97		$m = 4$ $v = 1$	$m = 5$ $v = 1$
5	92.39580 92.40		69.410248 69.411	90.23847 90.240

At $d = 3$, the BVP for system of $\mathcal{N} = 28$ PDEs (1), (9) for parameters $a_1 = a_2 = 1$ and $a_3 = 0.84$ were solved on $\Omega'_{\theta_1, r} = \{0(\pi/16)\pi/2\} \otimes \{0(0.16)0.8, 0.88, 0.96, 1.00\}$ with 4-order HIPs using program GCMFEM9 implemented in Mathematica on the PC. The eigenvalues $E_{v'}^{t_1 t_2 t_3} = E_{vm}^{t_1 t_2 t_3}$ classified by additional quantum number m and z -parity $\sigma = (-1)^n$ are given in Table 1 for $\sigma = +1$ with accuracy of up to 4 significant digits and agree with the etalon ones for BVP (7) on grid $\Omega'_{\theta_1, \theta_2, r} = \{0(\frac{\pi}{12})\frac{\pi}{2}\} \otimes \{0(\frac{\pi}{12})\frac{\pi}{2}\} \otimes \{0(\frac{1}{12})1\}$ using program GCMFEM8, with an accuracy of about 10^{-3} .

Table 2. The binding energies $\mathcal{E} = (\gamma - 2E)/2$ of the $\mathcal{E}_{Nlm}$ (in a.u.) of Hydrogen atom in magnetic field strength $\gamma = B/B_0$ of states classified by spherical quantum number (Nlm): $\mathcal{E}_{100} = \mathcal{E}(1s0)$ and $\mathcal{E}_{200} = \mathcal{E}(2s0)$ for $m = 0, \sigma = +1$. The first row contains the results of the FEM solution of the two-dimensional boundary value problem (10)-(11) using the GCMFEM 8 (G 8) [3] program on the grid $\Omega(r, \theta) = \{0(0.5)4, 4.75, 5.5, 6.5, 7.5, 8.75, 10, 12.5, 15, 20, 25, 32.5, 40, 52.5, 65, 82.5, 100\} \otimes \{0(\pi/8)\pi/2\}$. The results of DKV [8] and KLJ [7] are given in the second and third rows for each value of γ .

γ		$E(1s0)$	$E(2s0)$	$E(2p0)$	$E(3p0)$
0.000	G 8	0.499 999 999 999(1)	0.125 000 000 0(1)	0.125 000 000 0(1)	0.055 555 555 5(1)
	DKV	0.500 000 000 00(2)	0.124 999 999 99(7)	0.125 000 000 000(1)	0.055 555 555 55(07)
	KLJ	-	-	-	-
0.001	G 8	0.500 499 749 999(1)	0.125 496 500 1(1)	0.125 498 500 0(1)	0.056 046 559 0(1)
	DKV	0.500 499 749 9(62)	0.125 496 500 1(54)	0.125 498 500 0(40)	0.056 046 559 08(18)
	KLJ	0.500 499 750 000(1)	0.125 496 500 159(1)	0.125 498 500 042(1)	0.056 046 559 1(1)
0.5	G 8	0.697 210 538 46(1)	0.150 807 6(1)	0.224 760 3(1)	0.083 38(1)
	DKV	0.697 210 538 4(15)	0.150 807 855 7(68)	0.224 760 340 7(72)	0.083 390 113 0(17)
	KLJ	0.697 210 538 458(1)	0.150 807 855 777(1)	0.224 760 340 776(1)	0.083 390 113 0(1)
2.0	G 8	1.022 213 907 1(1)	0.173 857(1)	0.297 707 2(1)	0.094 77(1)
	DKV	1.022 213 907(57)	0.173 944 705 9(52)	0.297 710 972 3(77)	0.096 854 600 9(92)
	KLJ	1.022 213 907 665(1)	0.173 944 705 973(1)	0.297 710 972 385(1)	0.096 854 601 0(1)

3.2. Hydrogen atom in uniform magnetic field

Two-dimensional boundary value problem for the hydrogen atom H at $Z = 1$ in an axially symmetric uniform magnetic field $\mathbf{B} = (B_x, B_y, B_z) = (0, 0, B)$, directed along the z axis of the Cartesian coordinate system $\{x, y, z\}$, for the wave function $\Psi_m(r, \theta, \varphi) = \Psi_m(r, \theta) \frac{\exp(im\varphi)}{\sqrt{2\pi}}$ in spherical coordinates (r, θ, φ) :

$$x = r \sin \theta \cos \varphi, \quad y = r \sin \theta \sin \varphi, \quad z = r \cos \theta,$$

has the form

$$\begin{aligned} & \left(-\frac{1}{g_{00}(r, \theta)} \left(\frac{\partial}{\partial r} g_{11}(r, \theta) \frac{\partial}{\partial r} + \frac{\partial}{\partial \theta} g_{22}(r, \theta) \frac{\partial}{\partial \theta} \right) + V(r, \theta) - \epsilon_t \right) \Psi_t(r, \theta) = 0, \\ & g_{00}(r, \theta) = g_{11}(r, \theta) = r^2 \sin \theta, \quad g_{22}(r, \theta) = \sin \theta, \\ & V(r, \theta) = \frac{m^2}{r^2 \sin^2 \theta} + \gamma m + \frac{1}{4} \gamma^2 r^2 \sin^2 \theta - \frac{2Z}{r}, \end{aligned} \quad (10)$$

where $m = 0, \pm 1, \dots$ is the magnetic quantum number, $\gamma = B/B_0$, $B_0 = m_e^2 e^3 c \hbar^{-3} \cong 2.35 \times 10^9 G = 2.35 \times 10^5 T$ is a dimensionless parameter determining the field strength B , and atomic units (au) $\hbar = m_e = e = 1$ are used under the assumption of an infinite mass of a nucleus with charge Z . In these expressions, $\epsilon_t = 2E_t$ is the doubled energy (in Rydbergs, $1\text{Ry} = (1/2) \text{AU} = 27.211385/2 \text{ eV}$) of the bound state $|t\rangle = |vm\sigma\rangle$ for fixed values of m and z -parity ($z \rightarrow -z$); $\sigma = \pm 1$; $\Psi_t \equiv \Psi_{vm\sigma}(r, \theta) = (\Psi_{vm}(r, \theta) + \sigma \Psi_{vm}(r, \pi - \theta))/\sqrt{2}$ is the corresponding wave function, $v = 1, 2, \dots$. Here, the sign of the z -parity $\sigma = (-1)^{N_\theta}$ is determined by the number (even or odd) of nodes $N_\theta \equiv N_\eta$ in the solution Ψ_t with respect to the angular variable θ in the interval $0 < \theta < \pi$ or $-1 < \eta = \cos \theta < 1$.

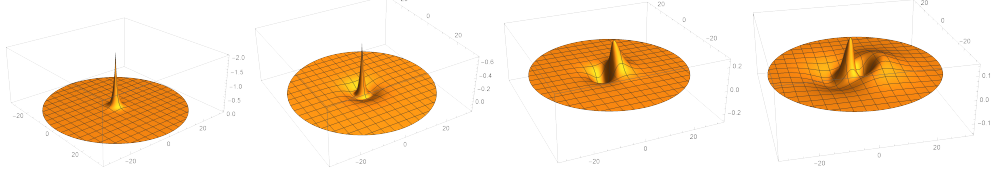


Fig. 2. Wave functions of the hydrogen atom $\Psi_{v=1,2}^{\sigma=+1,m=0}(x, y = 0, z; \gamma)$, $\Psi_{v=1,2}^{\sigma=-1,m=0}(x, y = 0, z; \gamma)$ in the absence of a magnetic field $\gamma = 0$

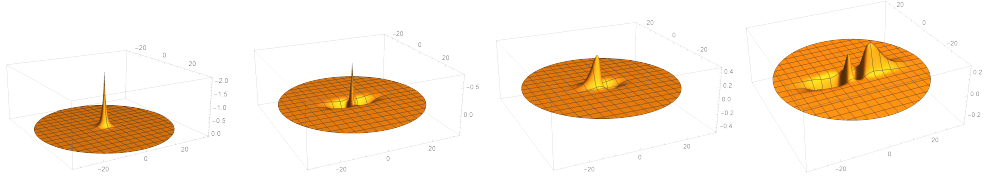


Fig. 3. Wave functions of the hydrogen atom $\Psi_{v=1,2}^{\sigma=+1,m=0}(x, y = 0, z; \gamma)$, $\Psi_{v=1,2}^{\sigma=-1,m=0}(x, y = 0, z; \gamma)$ in a magnetic field $\gamma = 0.5$

Boundary conditions

$$\begin{aligned} \lim_{\theta \rightarrow 0, \pi} \sin \theta \frac{\partial \Psi_t}{\partial \theta}(r, \theta) &= 0, \quad \text{at } m = 0, \quad \Psi_t(r, 0) = \Psi_t(r, \pi) = 0, \quad \text{at } m \neq 0, \\ \lim_{r \rightarrow 0} r^2 \frac{\partial \Psi_t}{\partial r}(r, \theta) &= 0, \quad \Psi_t(r_{\max}, \theta) = 0 \quad \lim_{r \rightarrow r_{\max}} r^2 \frac{\partial \Psi_t}{\partial r}(r, \theta) = 0, \end{aligned}$$

Orthonormalization condition

$$\int_0^{r_{\max}} dr \int_0^\pi d\theta g_{00}(r, \theta) \Psi_t(r, \theta) \Psi_{t'}(r, \theta) = \delta_{tt'}. \quad (11)$$

The wave functions of the hydrogen atom $\Psi_{v=1,2}^{\sigma=+1,m=0}(x, y = 0, z; \gamma)$, $\Psi_{v=1,2}^{\sigma=-1,m=0}(x, y = 0, z; \gamma)$ calculated as eigenfunctions of the two-dimensional boundary-value FEM problem with positive $\sigma = +1$ and negative $\sigma = -1$ parity for the magnetic number $m = 0$ are shown in Figs 2 and 3, and the binding energies in Table 2 are compared with alternative results.

3.3. Hydrogen ion in a uniform magnetic field

Two-dimensional boundary value problem for the hydrogen ion H_2^+ for $Z_a = Z_b = 1$ in an axially symmetric uniform magnetic field $\mathbf{B} = (B_x, B_y, B_z) = (0, 0, B)$, directed along the z axis of the Cartesian coordinate system $\{x, y, z\}$, with respect to the energy eigenvalue $E_t = \epsilon_t/2$ in (a.u.=2 Ry) and the wave function $\Psi_m(r, \theta, \varphi) = \Psi_m(r, \theta) \frac{\exp(im\varphi)}{\sqrt{2\pi}}$ in spheroidal coordinates (ξ, η, φ) :

$$\begin{aligned} x &= (R/2)\sqrt{(\xi^2 - 1)(1 - \eta^2)} \cos \varphi, \\ y &= (R/2)\sqrt{(\xi^2 - 1)(1 - \eta^2)} \sin \varphi, \\ z &= (R/2)\xi\eta \end{aligned}$$

has the form

$$\begin{aligned} &\left(-\frac{1}{g_{00}(\xi, \eta)} \left(\frac{\partial}{\partial \xi} g_{11}(\xi, \eta) \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} g_{22}(\xi, \eta) \frac{\partial}{\partial \eta} \right) + V(\xi, \eta) - E_t \right) \Psi_t(\xi, \eta; R) = 0, \\ g_{00}(\xi, \eta) &= \frac{R^3}{8}(\xi^2 - \eta^2), \quad g_{11}(\xi, \eta) = \frac{R}{4}(\xi^2 - 1), \\ g_{22}(\xi, \eta) &= \frac{R}{4}(1 - \eta^2), \\ V(\xi, \eta) &= \frac{2}{R} \frac{(Z_a + Z_b)\xi + (Z_b - Z_a)\eta}{\xi^2 - \eta^2} - \frac{2}{R^2} \frac{m^2}{(\xi^2 - 1)(1 - \eta^2)} \\ &\quad - \frac{1}{2}\gamma m - \frac{R^2}{32}\gamma^2(\xi^2 - 1)(1 - \eta^2). \end{aligned} \tag{12}$$

Boundary conditions

$$\begin{aligned} \lim_{\xi \rightarrow 1} g_{11}(\xi, \eta) \frac{\partial \Psi_t}{\partial \xi}(\xi, \eta; R) &= 0, \quad \lim_{\eta \rightarrow \pm 1} g_{22}(\xi, \eta) \frac{\partial \Psi_t}{\partial \eta}(\xi, \eta; R) = 0, \\ \lim_{\xi \rightarrow \xi_{\max}} g_{11}(\xi, \eta) \Psi_t(\xi, \eta; R) &= 0, \quad \text{or} \quad \lim_{\xi \rightarrow \xi_{\max}} g_{11}(\xi, \eta) \frac{\partial \Psi_t}{\partial \xi}(\xi, \eta; R) = 0 \end{aligned} \tag{13}$$

Orthonormalization condition

$$\int g_{00}(\xi, \eta) d\xi d\eta \Psi_t(\xi, \eta; R) \Psi_{t'}(\xi, \eta; R) = \delta_{tt'}. \tag{14}$$

These problems are solved by the finite-elements method, which makes it possible to find eigenvalues for E_a and $E_I(R)$ and the eigenfunctions $\psi_a(r, \theta)$ and $\psi_I(\xi, \eta; R)$ to the given degree of exactness which in this paper amounts to $10^{-6} \div 10^{-8}$. Having used the above-mentioned method, we present in Table 3 results of our calculations of the ground-state energy E_a , of the atom and the molecular hydrogen ion $E_I(R_0)$ for certain values of the $0.425 \leq \gamma \leq 0.425 \times 10^5$ dimensionless parameter. The calculations was performed by GCMFEM8 on grid $(\xi, \eta) \in \{x_1 = 1, x_i = x_{i-1} + h_i, h_i = \{0.2, x_{i-1} \leq 3; 1.2h_{i-1}\}, i = 2, \dots, 30\} \otimes \{0(0.05)1\}$. These results correspond to $10^9 \leq H \leq 10^{14}$ G field strengths. {In point R, the total energy $W_0 = 2(E(R_0) + 1/R_0)$ of the hydrogen molecular ion is at a minimum.} In addition, Table 3 also

Table 3. The ground-state energy E_a (Ry) and $E_I(R_0)$ (a.u.=2Ry) of the Hydrogen atom and molecular ion in a magnetic field strength B (in G), dimensionless parameter $\gamma = B/B_0$, $B_0 = m_e^2 c(e/\hbar)^3 \cong 2.35 \times 10^9 G = 2.35 \times 10^5 T$) calculated in point R (in a.u.), where the total energy $W_0 = 2(E(R_0) + 1/R_0)$ (in Ry) of the hydrogen molecular ion is at a minimum. Binding energy of molecular hydrogen ion $E_B = W_0 - E_a$ counted on the energy of hydrogen atom E_a (in Ry). First row contains results calculated by the GCMFEM 8, second row contains results [9]. (remaining characteristics are described in the text)

$B(\text{gauss})$ γ	R_0	$E_I(R_0)$	W_0	E_a	E_B	E_{osc}
10^9	1.923424	-1.095269	-1.150725	-0.9208328	-0.2298922	
0.4255022	1.9	-1.10139	-1.15015	-0.92078	-0.22937	
5×10^9	1.502400	-0.840410	-0.349616	0.0427881	-0.392404	
2.127511	1.7	-0.75771	-0.33894	0.04946	-0.38840	
10^{10}	1.246470	-0.257223	1.090086	1.639947	-0.549861	
4.255022	1.2	-0.28699	1.09269	1.64034	-0.54765	
5×10^{10}	0.747055	6.405318	15.48781	16.75002	-1.26221	
21.27511	0.8	6.50247	15.50494	16.7544	-1.24943	
10^{11}	0.593285	15.83437	35.03980	36.83099	-1.79119	
42.55022	0.6	15.87009	35.67352	36.84789	-1.17437	
5×10^{11}	0.351413	96.78749	199.2663	203.1402	-3.8739	
212.7511	0.354	96.95319	199.5561	203.54342	-3.98732	
10^{12}	0.283098	200.6501	408.3650	414.3859	-6.0209	
425.5022	0.287	201.1893	409.3473	416.43125	-7.08395	429.19
5×10^{12}	0.172503	1043.763	2099.119	2156.870	-57.751	
2127.511	0.181	1049.031	2109.111	2151.7669	-42.655	2164.92
10^{13}	0.137696	2103.544	4221.613	4396.525	-174.912	
4255.022	0.15	2115.95	4245.234	4323.2055	-77.97	4337.22
5×10^{13}	0.080233	10612.84	21250.61	23830.63	-2580.02	
21275.11	0.104	10678.75	21376.72	21928.05	-551.33	21948.30
10^{14}	0.063268	21266.10	42563.81	52515.30	-9951.49	
42550.22	0.086	21402.58	42828.41	45396.85	-2568.44	45404.33

presents values for the total energy $W_0 = W(R_0)$ and energy of molecular hydrogen ion binding $E_B = W_0 - E_a$ which is calculated in relation to the E_a , energy of the hydrogen atom's ground state in a corresponding magnetic field. If one puts zero of charge value $Z_b = 0$ of second Coulomb center, then we have eigenenergy E_a of Hydrogen atom in magnetic field from BVP in spheroidal coordinates so it is also calculated by solving the BVP in the same grid

By way of comparison, the last column in Table 3 presents energy E_{osc} , values for the ground state of the anisotropic oscillator. As the intensity of the H field increases, the corresponding E_a , values of the hydrogen atom's ground state gravitate toward these values. For example, then, for $B = 10^{14}\text{G}$, $E_{\text{osc}} - E_a \approx 7.5\text{Ry}$, which represents $\approx 0.02\%$ of the corresponding value of the anisotropic oscillator energy.

Note, derivative of $E_t(R) = dE_t(R)/dr$ by R needed for calculation minimum $d(E(R) + Z_a Z_b / R) / dR = 0$ at $R = R_0$ are calculated by Eq. (22) of Algorithm from Appendix. If for calculation of integrals with $\Psi_t(\xi, \eta; R)$ and its derivative of $\partial\Psi_t(\xi, \eta; R) / \partial R$ is needed for solving the 3D BVP of a three-body problem by the Kantorovich method, then it is composed from Eq. (2) using Φ_t^h obtained by solving nonhomogeneous algebraic equations Eqs.(25) and (26) from Appendix.

3.4. The Dirac Oscillator

The Dirac oscillator equation were produced by M. Moshinsky [12, 13]

$$-\imath \frac{\partial \psi}{\partial x^0} = (\alpha \cdot (\mathbf{p} - \imath \omega \mathbf{r} \beta) + \beta) \psi, \quad \psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \exp(-\imath E x^0), \quad (15)$$

where ω is oscillator frequency, $\mathbf{r} = \{x_i\}$ and $\mathbf{p}$ is the ordinary three-dimensional momentum, i.e. $p_i = -\imath \frac{\partial}{\partial x_i}$, $i = 1, 2, 3$ and α and β are the 4×4 matrices

$$\alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \quad (16)$$

with σ being the vector whose components σ_i , $i = 1, 2, 3$ are the 2×2 Pauli spin matrices and I is a unit matrix.

Equation (15) for positive energy E and corresponded large and small two dimensional components $\psi_1 = (\phi_1, \phi_2)^T$ and $\psi_2 = (\phi_3, \phi_4)^T$ of the wave function ψ takes the form:

$$\begin{aligned} (E - 1)\psi_1 &= \boldsymbol{\sigma} \cdot (\mathbf{p} + \imath \omega \mathbf{r}) \psi_2, \\ (E + 1)\psi_2 &= \boldsymbol{\sigma} \cdot (\mathbf{p} - \imath \omega \mathbf{r}) \psi_1 \end{aligned} \quad (17)$$

Multiplying the first equation (17) by $(E + 1)$ and using the second one we arrive that ψ_1 satisfies

$$(E^2 - 1)\psi_1 = (\mathbf{p}^2 + \omega^2 r^2 - 3\omega - 4\omega \mathbf{L} \cdot \mathbf{S})\psi_1, \quad \mathbf{L} = \mathbf{r} \times \mathbf{p}, \quad \mathbf{S} = \frac{\boldsymbol{\sigma}}{2}$$

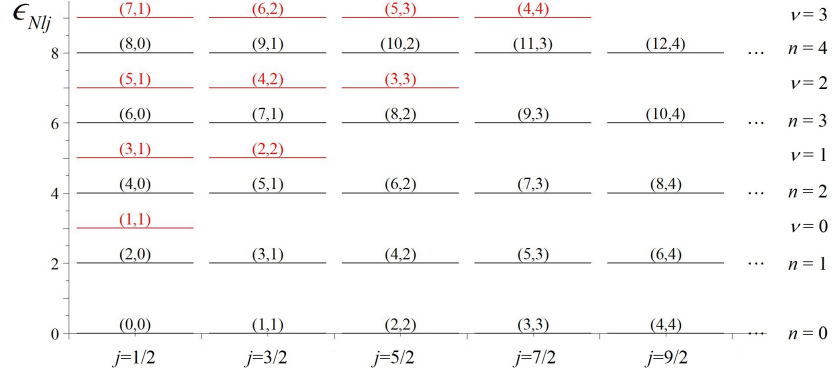


Fig. 4. Energy spectrum ϵ_{Nlj} of the Dirac oscillator. The abscissa corresponds to the total angular momentum j and the ordinate $\epsilon_{Nlj} = \epsilon_\nu = (2\omega)^{-1}(E_{N,j+1/2,j}^2 - 1) = 2\nu + 3$; $\nu = \frac{1}{2}(N + j - \frac{3}{2})$, $l = j + 1/2$, $\nu = 0, 1, 2, \dots$ and $\epsilon_{Nlj} = \epsilon_n = (2\omega)^{-1}(E_{N,j-1/2,j}^2 - 1) = 2n$; $n = \frac{1}{2}(N - j + \frac{1}{2})$, $l = j - 1/2$, $n = 0, 1, 2, \dots$. The values (N, l) are given above the levels.

where $\mathbf{L}$ and $\mathbf{S}$ are the orbital and spin angular momenta.

Taking into account relations $\mathbf{L} \cdot \mathbf{S} = \frac{1}{2}(J^2 - L^2 - S^2)$ and $N = 2n + l$ spectrum has of the form [12] (a low part of the spectrum is shown in Fig. 4):

$$E_{Nlj}^2 = 1 + \omega \begin{cases} (2(N - j) + 1) & \text{if } l = j - \frac{1}{2}, \\ (2(N - j) + 3) & \text{if } l = j + \frac{1}{2}. \end{cases}$$

The Dirac oscillator equation in spherical coordinates

$$x_1 = r \sin \theta \cos \varphi, \quad x_2 = r \sin \theta \sin \varphi, \quad x_3 = r \cos \theta$$

reduced to system of two coupled equations for large component

$$\psi_1 = \begin{pmatrix} \phi_1 = \phi_1(r, \theta) \exp(im\varphi) \\ \phi_2 = \phi_2(r, \theta) \exp(i(m+1)\varphi) \end{pmatrix}$$

at integer $m = 0, 1, 2, \dots$, which was used in the benchmark calculations:

$$\begin{aligned} \mathcal{L}\phi_1 + V_{11}\phi_1 + V_{12}\phi_2 &+ \frac{g_{22}}{g_{00}}Q_{12}^\theta \partial_\theta \phi_2 + \frac{1}{g_{00}}\partial_\theta(g_{22}Q_{12}^\theta)\phi_2 = (E^2 - 1)\phi_1, \\ \mathcal{L}\phi_2 + V_{22}\phi_2 + V_{12}\phi_1 &- \frac{g_{22}}{g_{00}}Q_{12}^\theta \partial_\theta \phi_1 - \frac{1}{g_{00}}\partial_\theta(g_{22}Q_{12}^\theta)\phi_1 = (E^2 - 1)\phi_2, \end{aligned}$$

where operator $\mathcal{L}$ has of the form

$$\mathcal{L} = -\frac{1}{g_{00}}[\partial_r(g_{11}\partial_r) + \partial_\theta(g_{22}\partial_\theta)]$$

, metric and potential coefficients read as

$$\begin{aligned} g_{00} &= r^2 \sin \theta, \quad g_{11} = r^2 \sin \theta, \quad g_{22} = \sin \theta, \\ V_{11} &= \frac{m^2}{r^2 \sin^2 \theta} + \omega^2 r^2 - 2\omega m - 3\omega, \quad V_{12} = \omega(2m+1)\frac{\cos \theta}{\sin \theta}, \\ V_{22} &= \frac{(m+1)^2}{r^2 \sin^2 \theta} + \omega^2 r^2 + 2\omega(m+1) - 3\omega, \quad Q_{12}^\theta = \omega r^2. \end{aligned}$$

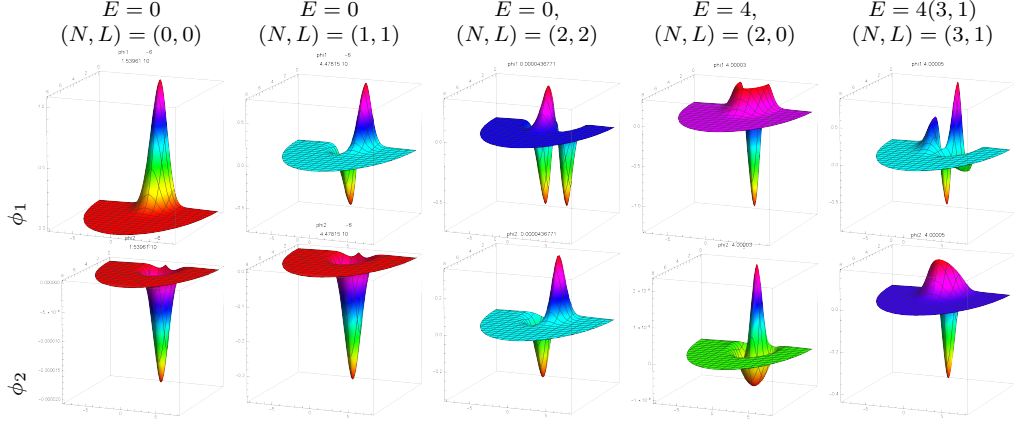


Fig. 5. The wave functions of a low part of the infinite degeneracy spectrum.

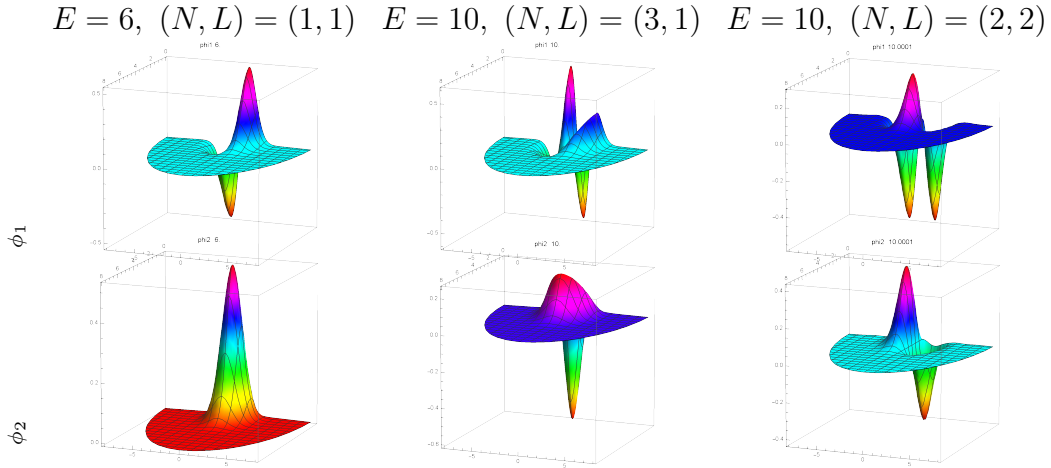


Fig. 6. The wave functions of a low part of the finite degeneracy spectrum.

The eigenfunctions $\phi_{1v}(r, \theta)$ and $\phi_{2v}(r, \theta)$, corresponding to the eigenvalues $\mathcal{E}_v = E_v^2 - 1$, $v = 1, 2, \dots$, subject to suitable boundary conditions of the first and second kind and the intermediate orthonormalization condition

$$\int_0^{r_{max}} \int_0^\pi g_{00}(r, \theta) [\phi_{1v}(r, \theta) \phi_{1v'}(r, \theta) + \phi_{1v}(r, \theta) \phi_{1v'}(r, \theta)] = \delta_{vv'}. \quad (18)$$

Small components are calculated by substituting the values of the major components into the last two equations of the original system of four first-order differential equations and calculating the normalization coefficients for both the major and minor components and the conditions for their joint normalization. Note that there is an $m \rightarrow -m-1$ symmetry, so it is sufficient to consider the equation for positive $m = 0, 1, 2, \dots$

Specification and results. Spin-orbit coupling via V_{12} , conormal derivatives on boundary, exact accidental degeneracy of spectrum, a low part of it is shown in Fig. 4. Note that, the eigenfunctions of the infinite degenerate spectrum (see fig. 5): $\epsilon_{Nlj} = \epsilon_\nu = (2\omega)^{-1}(E_{N,j+1/2,j}^2 - 1) = 2\nu + 3$; $\nu = \frac{1}{2}(N + j - \frac{3}{2})$, $l = j + 1/2$, $\nu = 0, 1, 2, \dots$ corresponds to representation of group $SO(3, 1)$ while the eigenfunctions of the finite degenerate spectrum (see fig. 6): $\epsilon_{Nlj} = \epsilon_n = (2\omega)^{-1}(E_{N,j-1/2,j}^2 - 1) = 2n$; $n = \frac{1}{2}(N - j + \frac{1}{2})$, $l = j - 1/2$, $n = 0, 1, 2, \dots$ corresponds to representation of group $SO(4)$ [14]

The low part of the spectrum was calculated by program GCMFEM 9 with six significant digits and components with three significant digits. (see figs. 5,6 The calculations was performed on the FEM mesh $\{0(\pi/6)\pi\} \otimes \{0(0.4)10\}$ with third-order IHPs.

CONCLUSION

The above FEM schemes for solving BVPs of systems of multidimensional coupled elliptic PDEs with smooth FEM basis functions composed matching multivariate Hermitian interpolated polynomials (HIPs) preserved mixed continuous derivatives up to a given order of required solutions on boundaries of joint finite elements were elaborated and implemented in Wolfram Mathematica and FORTRAN by GCMFEM-8 and GCMFEM-9 programs on modern personal computers (e.g., Intel Core i7, 16 GB RAM), for solving BVPs of PDEs and a systems of PDEs, respectively . Benchmark calculations of BVPs for PDEs or systems PDEs quantum dots describing Helmholtz problem on 3D ellipsoid domain, hydrogen atom and ion in magnetic field, and Dirac oscillator are confirmed declared order and robotises of the elaborated FEM schemes and programs, that is also applicable to a wide class of the quantum confined systems , for example, in external fields [2,15].

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CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

4. APPENDIX. ALGORITHM OF CALCULATION OF PARAMETRIC DERIVATIVE OF ALGEBRAIC EIGENVALUE PROBLEM

Let $\mathbf{c}^{(0)} \equiv \{\mathbf{c}_j(R)\}_{j=1}^{j_{max}} \equiv \{\{\{c_s(R)\}_s^{s_{max}}\}_j\}_{j=1}^{j_{max}}$ and $\lambda^{(0)} \equiv \{\lambda_j(R)\}_{j=1}^{j_{max}}$ are eigensolutions of an generalized algebraic eigenvalue problem depended on continuous parameter R :

$$\mathbf{A}^{(0)}\mathbf{c}^{(0)} - \mathbf{B}^{(0)}\mathbf{c}^{(0)}\lambda^{(0)} = 0, \quad (19)$$

with normalization and orthogonality conditions

$$\mathbf{c}^{(0)T}\mathbf{B}^{(0)}\mathbf{c}^{(0)} = \mathbf{I}, \quad \mathbf{c}_i^{(0)T}\mathbf{B}^{(0)}\mathbf{c}_j^{(0)} = \delta_{ij}, \quad (20)$$

unit matrix I and symmetric matrix $\mathbf{A}^{(0)} \equiv \mathbf{A}^{(0)}(R)$ and $\mathbf{B}^{(0)} \equiv \mathbf{B}^{(0)}(R)$ of dimension $s_{max} \times s_{max}$ determined in (3) following (12).

Step 1. As follows from (19), we should solve the following linear set of algebraic equations

$$\begin{aligned} \mathbf{A}^{(0)}\mathbf{c}^{(1)} - \mathbf{B}^{(0)}\mathbf{c}^{(1)}\lambda^{(0)} &= -(\mathbf{A}^{(1)}\mathbf{c}^{(0)} - \mathbf{B}^{(1)}\mathbf{c}^{(0)}\lambda^{(0)} - \mathbf{B}^{(0)}\mathbf{c}^{(0)}\lambda^{(1)}), \\ \mathbf{A}^{(1)} &\equiv \frac{d\mathbf{A}^{(0)}}{dR}, \quad \mathbf{B}^{(1)} \equiv \frac{d\mathbf{B}^{(0)}}{dR}, \end{aligned} \quad (21)$$

where $\mathbf{c}^{(0)} \equiv \mathbf{c}_j$, $\lambda^{(0)} \equiv \lambda_j$, $\mathbf{c}^{(1)} \equiv \mathbf{c}_j^{(1)} \equiv d\mathbf{c}_j^{(0)}/dR$ and $\lambda^{(1)} \equiv d\lambda_j/dR$.

Step 2. Taking account that $\lambda^{(0)}$ is eigenvalue of operator (19), problem (21) has solution iff, when w.h.s. is orthogonal eigenfunction $\mathbf{c}^{(0)}$. Multiplaying (21) by $(\mathbf{c}^{(0)})^T$ and using normalization condition (20), one gets expression for $\lambda^{(1)}$

$$\lambda^{(1)} = (\mathbf{c}^{(0)})^T \mathbf{A}^{(1)} \mathbf{c}^{(0)} - (\mathbf{c}^{(0)})^T \mathbf{B}^{(1)} \mathbf{c}^{(0)} \lambda^{(0)}, \quad (22)$$

and a set of inhomogeneous algebraic equations for unknown vector $\mathbf{c}^{(1)}$

$$\mathbf{K} \equiv \mathbf{A}^{(0)}\mathbf{c}^{(1)} - \mathbf{B}^{(0)}\mathbf{c}^{(1)}\lambda^{(0)} = \mathbf{b}^{(1)}, \quad (23)$$

$$\mathbf{b}^{(1)} = -\mathbf{A}^{(1)}\mathbf{c}^{(0)} + \mathbf{B}^{(1)}\mathbf{c}^{(0)}\lambda^{(0)}$$

Now the problem (23) has a solution, but it is not unique. From the normalization condition (20) we obtain the required additional equality

$$(\mathbf{c}^{(1)})^T \mathbf{B}^{(0)} \mathbf{c}^{(0)} = 0, \quad (24)$$

providing the uniqueness of the solution (23). Since $\lambda^{(0)}$ is an eigenvalue of (19), the matrix $\mathbf{K}$ in (23) is degenerate.

Note, if matrix $\mathbf{A}^{(0)}$ is diagonal one, then solution of system (23)–(24) are calculated in analytical form.

Algorithm of numerical solving (23) in the case of a degenerated nondiagonal matrix $\mathbf{A}^{(0)}$ in distinction of [8] is formulated as following.

Step 3. Calculate solution $\mathbf{c}^{(1)}$ of the modified nonhomogenous algebraic equations

$$\bar{\mathbf{K}}\mathbf{c}^{(1)} = \bar{\mathbf{b}}^{(1)} \quad (25)$$

with the nondegenerated matrix $\bar{\mathbf{K}}$ of dimension $s_{max} \times s_{max}$, which includes in an explicit form orthogonality conditions(24): $(\mathbf{c}^{(1)})^T \mathbf{c}^{(0)} = 0$, and with a modified w.h.s. $\bar{\mathbf{b}}^{(1)}$ which is vector of dimension s_{max} :

$$\bar{K}_{ss'} = \begin{cases} K_{ss'}, & s \neq S, \\ c_{s'}^{(0)}, & s = S, \end{cases} \quad (26)$$

$$\bar{b}_s^{(1)} = \begin{cases} b_s^{(1)}, & s \neq S, \\ 0, & s = S, \end{cases} \quad (27)$$

where S is number of maximum by module element $c_S^{(0)}$ of eigenvector $\mathbf{c}^{(0)} \equiv \mathbf{c}_j$ of dimension s_{max} of algebraic eigenvalue problem (19).

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