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Solution of Boundary-Value Problems using Kantorovich Method

A.A. Gusev[1,a], L.L. Hai[1,2], O. Chuluunbaatar[1,3], S.I. Vinitsky[1,b], and V.L. Derbov[4]

[1] *Joint Institute for Nuclear Research, Dubna, Russia,*
[2] *Belgorod State University, Belgorod, Russia*
[3] *National University of Mongolia, UlaanBaatar, Mongolia*
[4] *Saratov State University, Saratov, Russia*

Abstract. We propose a computational scheme for solving the eigenvalue problem for an elliptic differential equation in a two-dimensional domain with Dirichlet boundary conditions. The solution is sought in the form of Kantorovich expansion over the basis functions of one of the independent variables with the second variable treated as a parameter. The basis functions are calculated as solutions of the parametric eigenvalue problem for an ordinary second-order differential equation. As a result, the initial problem is reduced to a boundary-value problem for a set of self-adjoint second-order differential equations for functions of the second independent variable. The discrete formulation of the problem is implemented using the finite element method with Hermite interpolation polynomials. The efficiency of the calculation scheme is shown by benchmark calculations for a square membrane with a degenerate spectrum.

1 Introduction

The calculation of spectral and optical properties of electronic states in axially symmetric quantum dots is reduced to the solution of two-dimensional boundary-value problems (BVP) for elliptic differential equations with nonseparable variables in a finite domain [1]. One of the ways to solve these problems is implemented as the set of programs ODPEVP-KANTBP [2, 3] based on the Kantorovich method that provides the reduction of the initial problem to a set of ordinary differential equations [4] with further use of the finite element method [5] with Lagrange interpolating polynomials. For the impurity states of quantum dots such BVPs are defined in domains of complicated geometry and involve piecewise-continuous potential functions. In this case it is necessary to preserve not only the continuity of the approximate solution, but also the continuity of its first derivative, which is most naturally achieved using the finite element method with Hermite interpolating polynomials [6, 7].

Testing such approach for the solution of two-dimensional BVPs is the aim of the present work. We present a computational scheme for solving the eigenvalue problem for an elliptic differential equation in a two-dimensional finite domain with Dirichlet boundary conditions. The solution is sought in the form of Kantorovich expansion over the basis functions of one of the independent variables with the second variable treated as a parameter. The basis functions are calculated as a solution

[a] e-mail: gooseff@jinr.ru
[b] e-mail: vinitsky@theor.jinr.ru

of the parametric eigenvalue problem for an ordinary second-order differential equation. Finally, the initial problem is reduced to a BVP for a set of self-adjoint second-order differential equations for functions of the second independent variable. The discretization of the problems is carried out using the finite element method with Hermite interpolation polynomials.

The result is used to formulate a generalized algebraic eigenvalue problem. For matrices of small dimension this problem is solved using Maple. For matrices of large dimension we use the symbolic algorithm to generate Fortran routines for numerical solution of the generalized algebraic eigenvalue problem. We demonstrate the efficiency of the programs generated in Maple and Fortran for 100×100 and higher-order matrices, respectively, in benchmark calculations for the exactly solvable eigenvalue problem of a square membrane with degenerate spectrum. This example is not trivial from the computational view point. It shows the applicability of the method, algorithms and program in solving the generalized algebraic eigenvalue problem with the higher-order matrices which has a quasidegenerate spectrum. The use of new coordinates that can be separated within the domain but not at the boundary allows the simulation of a potential function, depending upon two variables, and justifies the application of the Kantorovich method.

2 Kantorovich Method

Let us consider the 2D BVP in the two-dimensional domain $\Omega(x_f, x_s) \subset \mathbf{R}^2$:

$$\left(-\frac{\partial^2}{\partial x_s} - \frac{\partial^2}{\partial x_f} + V(x_f, x_s) - E\right)\Psi(x_f, x_s) = 0, \tag{1}$$

where $V(x_f, x_s)$ is a real-valued function and $\Psi(x_f, x_s)$ satisfies the Dirichlet condition at the boundary $\partial\Omega(x_f, x_s)$ of the domain $\Omega(x_f, x_s)$

$$\Psi(x_f, x_s)\Big|_{(x_f,x_s)\in\partial\Omega(x_f,x_s)} = 0. \tag{2}$$

The solution $\Psi(x_f, x_s) \in W_2^2(\Omega)$ of the BVP (1)–(2) is sought as a Kantorovich expansion [4]

$$\Psi_v(x_f, x_s) = \sum_{j=1}^{j_{\max}} \Phi_j(x_f; x_s)\chi_{jv}(x_s) \tag{3}$$

over the set of eigenfunctions $\Phi_j(x_f; x_s) \in \mathcal{F}_{x_s} \sim W_2^2(\Omega_{x_f}(x_s))$ of the parametric BVP

$$\left(-\frac{\partial^2}{\partial x_f} + V(x_f, x_s) - \epsilon_j(x_s)\right)\Phi(x_f; x_s) = 0, \tag{4}$$

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 boundary conditions

$$\Phi_j(x_f^{\min}(x_s); x_s) = 0, \quad \Phi_j(x_f^{\max}(x_s); x_s) = 0 \tag{5}$$

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 in the same interval $x_f \in \Omega_{x_f}(x_s)$:

$$\left\langle\Phi_i|\Phi_j\right\rangle = \int_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f; x_s)\Phi_j(x_f; x_s)\, dx_f = \delta_{ij}. \tag{6}$$

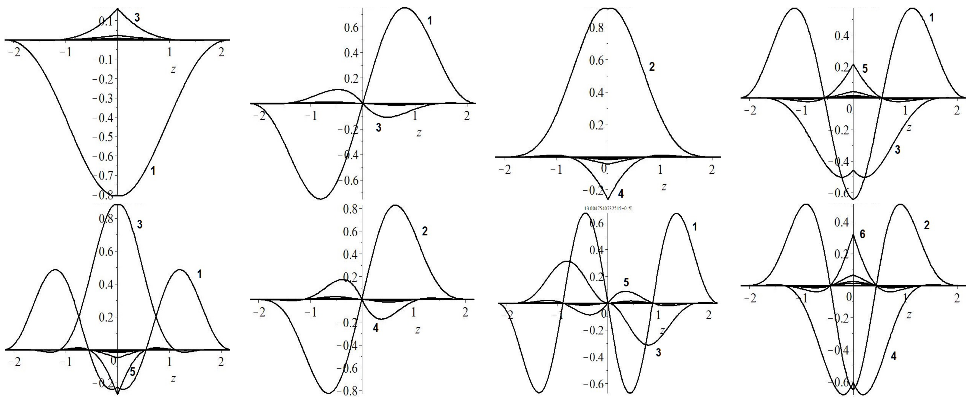

Figure 1. The components $\chi_{j\upsilon}(x_s)$ of the Kantorovich expansion (3) corresponding to the first eight eigenvalues

Here $\epsilon_1(x_s) < \cdots < \epsilon_{j_{\max}}(x_s) < \cdots$ is the desired set of real eigenvalues. If this parametric eigenvalue problem has no analytical solution, then it is solved numerically using the program ODPEVP [2].

Substituting (3) into (1) with (5) and (6) taken into account, we arrive at the set of self-adjoint ODEs for the unknown vector functions $\boldsymbol{\chi}_\upsilon(x_s, E) \equiv \boldsymbol{\chi}_\upsilon(x_s) = (\chi_{1\upsilon}(x_s), \ldots, \chi_{j_{\max}\upsilon}(x_s))^T \in W_2^2(\Omega_{x_s})$:

$$\left(-\mathbf{I}\frac{d^2}{dx_s^2} + \mathbf{U}(x_s) - 2E_\upsilon\,\mathbf{I} + \frac{d\mathbf{Q}(x_s)}{dx_s} + \mathbf{Q}(x_s)\frac{d}{dx_s}\right)\boldsymbol{\chi}_\upsilon(x_s) = 0. \tag{7}$$

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

$$\begin{aligned}
U_{ij}(x_s) &= \epsilon_i(x_s)\delta_{ij} + H_{ij}(x_s),\\
H_{ij}(x_s) &= H_{ji}(x_s) = \int_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \frac{\partial\Phi_i(x_f; x_s)}{\partial x_s}\frac{\partial\Phi_j(x_f; x_s)}{\partial x_s}\,dx_f,\\
Q_{ij}(x_s) &= -Q_{ji}(x_s) = -\int_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f; x_s)\frac{\partial\Phi_j(x_f; x_s)}{\partial x_s}\,dx_f.
\end{aligned} \tag{8}$$

The discrete spectrum solutions $E: E_1 < E_2 < \cdots < E_\upsilon < \cdots$ that obey the boundary conditions at the points $x_s^t = \{x_s^{\min}, x_s^{\max}\} = \partial\Omega_{x_s}$ located at the boundary of Ω_{x_s} and the orthonormality conditions

$$\boldsymbol{\chi}_\upsilon(x_s^t) = 0, \quad x_s^t = x_s^{\min}, x_s^{\max}, \quad \int_{x_s^{\min}}^{x_s^{\max}} (\boldsymbol{\chi}_\upsilon(x_s))^T \boldsymbol{\chi}_{\upsilon'}(x_s)\,dx_s = \delta_{\upsilon\upsilon'} \tag{9}$$

are calculated by means of the program KANTBP [3].

3 Benchmark calculation: rectangular membrane

As a benchmark example we consider the exactly solvable BVP for a rectangular membrane in conventional variables $(x, y) \in \Omega(x, y)$

$$\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - E\right)\Psi(x, y) = 0 \tag{10}$$

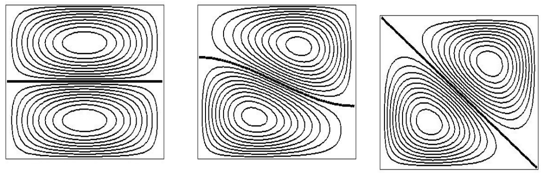

Figure 2. Profiles of the linear combinations of the eigenfunctions $\Psi_2(x_f, x_s)$ and $\Psi_3(x_f, x_s)$ corresponding to linear combinations of exact solutions u_{12} and u_{21}: u_{12}, $u_{12} + \sqrt{2/3}u_{21}$, $u_{12} + u_{21}$

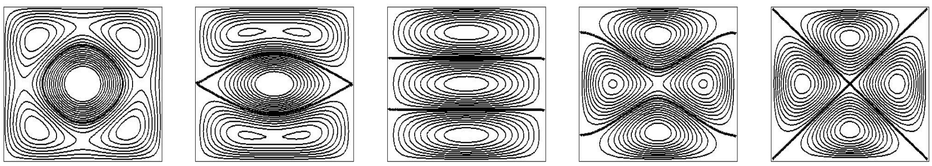

Figure 3. Profiles of the linear combinations of the eigenfunctions $\Psi_5(x_f, x_s)$ and $\Psi_6(x_f, x_s)$ corresponding to the linear combinations of the exact solutions u_{13} and u_{31}: $u_{13} + u_{31}$, $u_{13} + (1/3)u_{31}$, u_{13}, $u_{13} - (2/3)u_{31}$, $u_{13} - u_{31}$

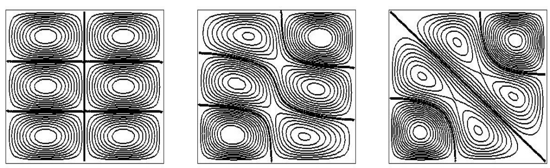

Figure 4. Profiles of the linear combinations of the eigenfunctions $\Psi_7(x_f, x_s)$ and $\Psi_8(x_f, x_s)$, corresponding to the linear combinations of the exact solutions u_{23} and u_{32}: u_{23}, $u_{23} + (1/3)u_{32}$, $u_{23} + u_{32}$

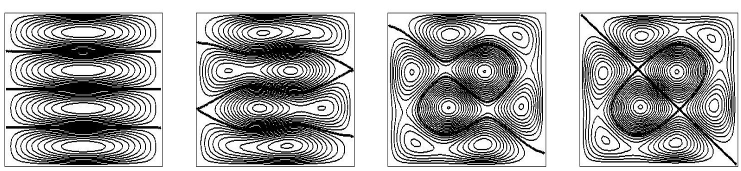

Figure 5. Profiles of the linear combinations of the eigenfunctions $\Psi_9(x_f, x_s)$ and $\Psi_{10}(x_f, x_s)$ corresponding to the linear combinations of the exact solutions u_{14} and u_{41}: u_{14}, $u_{14} + (1/3)\sqrt{2/3}u_{41}$, $u_{14} + \sqrt{2/3}u_{41}$, $u_{14} + u_{41}$

with the Dirichlet conditions for $\Psi(x, y)$ at the boundary $\partial\Omega(x, y)$ of the region $\Omega(x, y)$

$$\Psi(\pm a/2, y) = 0, \quad \Psi(x, \pm b/2) = 0. \tag{11}$$

We solve the BVP (1)–(2) for the rectangular membrane $x \in (-a/2, a/2)$, $y \in (-b/2, b/2)$, in the new variables x_f=$(x+y)/\sqrt{2}$, x_s=$(x-y)/\sqrt{2}$ with $V(x_f, x_s)$=0. The new variables can be separated within Ω but not at the boundary $\partial\Omega$, which simulates the presence of a potential $V(x_f, x_s) \neq 0$ and allows us to use the Kantorovich method and to seek for the approximate solution in the form (3). In the considered case the parametric eigenvalue problem (4)–(6) has an exact solution, i.e., the parametric eigenfunctions $\Phi_i\left(x_f;x_s\right)$ and the potential curves $\epsilon_i\left(x_s\right)$ are expressed in the analytical form

$$\epsilon_i\left(x_s\right)=\frac{\pi^2 i^2}{(x_f^{\max}(x_s)-x_f^{\min}(x_s))^2},\quad \Phi_i\left(x_f;x_s\right)=\frac{\sqrt{2}\sin\left(\dfrac{\pi i(x_f-x_f^{\min}(x_s))}{x_f^{\max}(x_s)-x_f^{\min}(x_s)}\right)}{\sqrt{x_f^{\max}(x_s)-x_f^{\min}(x_s)}}. \qquad (12)$$

With the basis functions (12), the integration in the effective potentials (8) can be carried out analytically. This yields the expressions

$$Q_{ij}(x_s)=-\frac{2ij}{i^2-j^2}\frac{\left((-1)^{i+j}\dfrac{dx_f^{\max}(x_s)}{dx_s}-\dfrac{dx_f^{\min}(x_s)}{dx_s}\right)}{x_f^{\max}(x_s)-x_f^{\min}(x_s)},\quad j\neq i,$$

$$H_{ij}(x_s)=-\frac{4ij(i^2+j^2)}{(i^2-j^2)^2}\frac{\left((-1)^{i+j}\dfrac{dx_f^{\max}(x_s)}{dx_s}-\dfrac{dx_f^{\min}(x_s)}{dx_s}\right)\left(\dfrac{dx_f^{\max}(x_s)}{dx_s}-\dfrac{dx_f^{\min}(x_s)}{dx_s}\right)}{(x_f^{\max}(x_s)-x_f^{\min}(x_s))^2}, \qquad (13)$$

$$H_{ii}(x_s)=\frac{\pi^2 i^2}{3}\frac{\left(\dfrac{dx_f^{\max}(x_s)}{dx_s}\right)^2+\left(\dfrac{dx_f^{\max}(x_s)}{dx_s}\right)\left(\dfrac{dx_f^{\min}(x_s)}{dx_s}\right)+\left(\dfrac{dx_f^{\min}(x_s)}{dx_s}\right)^2}{(x_f^{\max}(x_s)-x_f^{\min}(x_s))^2}$$

$$+\frac{1}{4}\frac{\left(\dfrac{dx_f^{\max}(x_s)}{dx_s}-\dfrac{dx_f^{\min}(x_s)}{dx_s}\right)^2}{(x_f^{\max}(x_s)-x_f^{\min}(x_s))^2}.$$

In the symmetric case $a=b$: $x_f^{\max}(x_s)=-x_f^{\min}(x_s)$ the matrix elements H_{ij} and Q_{ij} between even and odd indexes equal zero and one can solve the BVP for even (e) and odd (o) solutions separately.

Numerical calculations of the eigenvalue problem (7)–(9) were carried out for $j_{\max}=6$ using the program KANTBP4M implemented in Maple on the grid $\Omega_{x_s}=(-x_m(4)-7x_m/8(4)0(4)7x_m/8(4)x_m)$ at $x_m=\pi/\sqrt{2}-1/20$, where the number of finite elements in each subinterval is presented in parentheses. The finite-element local functions are constructed using the Hermite interpolation polynomials of the seventh order ($p'=\kappa^{\max}(p+1)-1=7$) with the multiplicity of the nodes $\kappa_r^{\max}=1$ and $p+1=8$ in each of the elements [7], which provides the accuracy $O(h^{p'+1})$ of the eigenfunctions and the eigenvalues, where h is the maximal element length. The dimension of the mass and stiffness matrices is 666×666 and their half-width is 48. The components $\chi_{jv}(x_s)$ of the corresponding eigenfunctions $\Psi_v(x_f,x_s)$ are shown in Fig. 1 that allows one to estimate the accuracy of the Kantorovich expansion (3) to be of the order of $4\cdot10^{-4}\div10^{-2}$ and the accuracy of the corresponding eigenvalues E_v^σ: 2.0004, 5.0004, 5.0017, 8.0050, 10.0042, 10.0016, 13.0034, 13.0153, 17.0050, 17.0053 of the order $4\cdot10^{-4}\div10^{-2}$, in comparison with the exact values E_v: 2, 5, 5, 8, 10, 10, 13, 13, 17, 17. For the number $j_{\max}$ of the parametric basis functions increased to 280, more RAM and computer time are needed. Here, we used the Fortran version of the program KANTBP4, which provides the accuracy $O(h^{p'+1})$ of the eigenfunctions and $O(h^{2p'})$ of the eigenvalues, and achieved the discrepancy $\delta E_v^\sigma=E_v^\sigma-E_v$ of the order of 10^{-8} for the eigenvalues that is shown in Table 1. One can see from the Table that the convergence rate of the Kantorovich expansion (3) is the order of $j_{\max}^{-3}$ which corresponds to the theoretical estimation given by the perturbation theory.

Table 1. The discrepancy $\delta E_v^\sigma = E_v^\sigma - E_v$, $\sigma = e, o$ vs a number of even (e) and odd (o) basis functions $j_{\max}$

$j_{\max}$	δE_1^e	δE_2^e	δE_3^o	δE_4^e	δE_5^e	δE_6^o	δE_7^e	δE_8^o
6	3.54(−4)	3.76(−4)	1.79(−3)	4.91(−3)	4.09(−3)	1.60(−3)	2.95(−3)	1.53(−2)
13	3.67(−5)	3.85(−5)	2.06(−4)	4.88(−4)	3.96(−4)	1.82(−4)	2.93(−4)	1.68(−3)
28	3.81(−6)	3.98(−6)	2.26(−5)	5.04(−5)	4.07(−5)	1.98(−5)	3.01(−5)	1.82(−4)
60	3.96(−7)	4.12(−7)	2.42(−6)	5.23(−6)	4.23(−6)	2.11(−6)	3.12(−6)	1.95(−5)
130	3.95(−8)	4.10(−8)	2.44(−7)	5.21(−7)	4.22(−7)	2.13(−7)	3.10(−7)	1.96(−6)
280	3.97(−9)	4.11(−9)	2.48(−8)	5.25(−8)	4.25(−8)	2.15(−8)	3.12(−8)	1.99(−7)
exact	E_1=2	E_2=5	E_3=5	E_4=8	E_5=10	E_6=10	E_7=13	E_8=13

The calculation time was about 100 sec. for $j_{\max} = 6$ in Maple and 80 sec. for $j_{\max} = 60$ in Fortran using a PC Intel Core i5 3.33GHz, 4Gb RAM, and a 64 bit Windows 7 as the operation system.

It is known that the eigenvalues of the rectangular membrane BVP may be degenerate. It is always the case, if the aspect ratio $a : b$ is a rational number, because in this case the equation $m^2/a^2 + n^2/b^2 = m'^2/a^2 + n'^2/b^2$ always has nontrivial integer solutions. For example, in the present case of a square membrane with $a = b = \pi$ such a solution is $m = n'$, $n = m'$. For the boundary condition $u = 0$ the corresponding fundamental functions are $\sin mx \sin ny$ and $\sin nx \sin my$. For any eigenvalue the degeneracy order is determined by the solution of the number theory problem of how many ways exist to represent an integer ν^2 as a sum of two squares: $\nu^2 = m^2 + n^2$ The nodal lines for the eigenfunctions $\sin nx \sin my$ are just straight lines parallel to the coordinate axes (x, y). However, with degenerate eigenvalues quite different nodal lines may appear, e.g., the square has a locus of points at which the function $\alpha \sin nx \sin my + \beta \sin mx \sin ny$ equals zero. In Figs. 2–5 some typical examples of profiles and nodal lines of linear combinations of the eigenfunctions are presented, corresponding to the exact doubly degenerate eigenvalues 5, 10, 13, and 17. In the captions the notation $u_{mn} = \sin mx \sin ny$ is used. The nodal lines of the eigenfunctions are shown by solid curves, which coincide with those presented in [8].

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