Inverse Problem for the Two-Dimensional Discrete Schrödinger Equation in Square

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The potential of the two-dimensional discrete Schrödinger equation can be reconstructed from a part of spectrum and prescribed symmetry conditions of the basis eigenfunctions. The discrete potential along with the missing eigenvalues is found by solving a polynomial system of equations, which is derived and solved using the REDUCE computer algebra system. To ensure the convergence of the iterative process implemented in the Numeric package in REDUCE, proper initial data must be specified. The prescribed eigenvalues are perturbed original eigenvalues corresponding to zero discrete potential. The original eigenvalues provide the natural initial data for the corresponding missing eigenvalues. In the case of square there are many multiple eigenvalues among the original eigenvalues. The direct application of the variant of the Newton method implemented in the Numeric package in REDUCE is impossible in the case of multiple initial data. In [1] a modification of the method proposed earlier [2] for calculating the discrete potential of the two-dimensional discrete Schrödinger equation in a square is illustrated by a concrete example. The problem under study is reduced to the matrix inverse problem. Under the prescribed symmetry conditions the basis eigenvectors have the odd-even structure. This leads to decompositing the spectrum into disjoint sets. Respectively the polynomial system of equations is decomposed into subsystems that are solved one after another. When solving the next system, the initial data are found using the results obtained by solving the preceding systems.

Further a concrete example of calculating the discrete potential of the two-dimensional discrete Schrödinger equation in a square is discussed:

$$-(\psi_{i+1,j} - 2\psi_{i,j} + \psi_{i-1,j})h_x^{-2} - (\psi_{i,j+1} - 2\psi_{i,j} + \psi_{i,j-1})h_y^{-2} + p_{i,j}\psi_{i,j} = \lambda\psi_{i,j},$$

for $1 \leq i \leq M$, and $1 \leq j \leq N$, with the zero boundary conditions: $\psi_{0,j} = \psi_{M+1,j} = \psi_{i,0} = \psi_{i,N+1} = 0$. It ts assumed that the basis discrete eigenfunctions satisfy the prescribed symmetry conditions (see the theorem in [1]) that ensure a smooth continuation of the basis eigenfunctions from the rectangle to the entire plane. Below we consider the case $h_x = h_y = 1$, $M = N = 7$. We want to determine the discrete potential $p_{i,j}$ given the perturbed original (corresponding to $p_{i,j} = 0$) eigenvalues and some prescribed symmetry conditions for the basis eigenfunctions. The solution of this inverse problem is reduced to the reconstruction of the persymmetric block three-diagonal matrix C of order 49:

$$C = \begin{bmatrix} A_1 & -I & O & O & O & O & O \\ -I & A_2 & -I & O & O & O & O \\ O & -I & A_3 & -I & O & O & O \\ O & O & -I & A_4 & -I & O & O \\ O & O & O & -I & A_3 & -I & O \\ O & O & O & O & -I & A_2 & -I \\ O & O & O & O & O & -I & A_1 \end{bmatrix}, \ A_i = 4I + \begin{bmatrix} \theta_1^i & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & \theta_2^i & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & \theta_3^i & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & \theta_4^i & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & \theta_3^i & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & \theta_2^i & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & \theta_1^i \end{bmatrix},$$

here I is the identity matrix of order 7 and O is the zero matrix of order 7. Such a matrix has 16 distinct diagonal entries and it can be reconstructed from 16 given perturbed eigenvalues. The inverse matrix problem is reduced [1] to solving a polynomial system of equations, which derived and solved using REDUCE, version 3.7 [3]. In the derivation of the polynomial set of equations, a series of analytical recurrent computations with polynomial matrices is performed (see formula (11) in [2]). REDUCE provides convenient tools for such calculations. Moreover REDUCE includes the Numeric package, which proved to be effective in solving polynomial systems of equations. We need this package to numerically solve the derived system of equations.

The eigenvalues of the original matrix (the matrix C with $\theta^i_j = 0$) satisfy the equation $det[(A-\lambda I)((A-\lambda I)^2 - 2I)((A-\lambda I)^4 - 4(A-\lambda I)^2 + 2I)] = 0$. Here A are diagonal blocks of the original matrix. Therefore the seven eigenvalues of the original matrix are eigenvalues of the block A. These eigenvalues are associated with the basis eigenvectors

$$E = [t, 0, -t, 0, \mp t, 0, \pm t]', \quad (A - \lambda I)t = 0.$$

Below we assume that the eigenvalues of A_1 are eigenvalues of the unknown perturbed matrix and the corresponding basis eigenvectors have the form

$E = [t, 0, -t, 0, \mp t, 0, \pm t]', \quad (A_1 - \lambda I)t = 0.$

This implies that the first and the third diagonal blocks are identical $A_1 = A_3$. The matrix to be found has 12 distinct diagonal entries. It can be reconstructed from 12 given perturbed eigenvalues.

We present the found discrete potential

$$||p_{i,j}|| = \begin{bmatrix} -0.0034... & -0.0115... & 0.0034... & -0.0021... & 0.0034... & -0.0115... & -0.0034... \\ 0.1013... & 0.0092... & 0.0500... & -0.1675... & 0.0500... & 0.0092... & 0.1013... \\ -0.0034... & -0.0115... & 0.0034... & -0.0021... & 0.0034... & -0.0115... & -0.0034... \\ -0.1073... & 0.1915... & -0.0695... & -0.0280... & -0.0695... & 0.1915... & -0.1073... \\ -0.0034... & -0.0115... & 0.0034... & -0.0021... & 0.0034... & -0.0115... & -0.0034... \\ 0.1013... & 0.0092... & 0.0500... & -0.1675... & 0.0500... & 0.0092... & 0.1013... \\ -0.0034... & -0.0115... & 0.0034... & -0.0021... & 0.0034... & -0.0115... & -0.0034... \end{bmatrix}$$

The discrete potential was reconstructed using 12 given perturbed eigenvalues. The elements of this potential along with the missing eigenvalues were found by solving the system of 49 polynomial equations which were derived and solved using REDUCE. The maximum deviation of the missing eigenvalues from the corresponding original eigenvalues is value of the same order of magnitude as the deviation of the prescribed perturbed eigenvalues from the original ones.

References

[1] S.I.Serdyukova // Programming and Computer Software, 2007,v.33,No.2,pp.117-119.

[2] S.I.Serdyukova //Dokl.Math. 2006, v.73, pp.121-124.

[3] Hearn A.C. - *REDUCE User's and Contributed Packages Manuel, Version 3.7.* Santa Monica, CA and Codemist Ltd, February 1999. p.488.