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Inverse eigenvalue problem for the discrete three-diagonal Sturm–Liouville operator and the continuum limit

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Abstract

The self-contained derivation of the inverse eigenvalue problem is given using a discrete approximation of the Sturm–Liouville operator on a bounded interval. Within this approximation, the Hamiltonian is treated as a finite three-diagonal symmetric Jacobi matrix. This derivation is more correct in comparison with previous works which used only single-diagonal matrix. It is demonstrated that the inverse problem procedure is nothing but the well-known Gram–Schmidt orthonormalization in Euclidean space for special vectors numbered by the space coordinate index. All the results of the usual inverse problem with continuous coordinate are reobtained by employing a limiting procedure, including the Goursat problem—the equation in partial derivatives for the solutions of the inversion integral equation.

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1. Introduction

There is much literature on the inverse scattering problem. It suffices to mention the classical monographs [1–5], see also [6]. This theory has multiple applications and is still developing [7]. In parallel with its renovation, attempts to give a clear and obvious treatment were undertaken [8–10] using a finite-difference approach which reduces the problem to solving relatively simple algebraic equations. Passage to the limit of the continuous variable allows one to obtain the classical results of the inverse problem. Thus, the finite-difference version represents a valuable tool for reproducing all the results of the inversion procedure at a more accessible level of understanding. This is not only of pedagogical interest. The aim of science is, among others, to supply the maximum compact and clear knowledge free from superfluous and often obscure details.

The authors of [8–10] restricted their consideration to the finite-difference matrix Hamiltonian with potential coefficients only on the main diagonal of the operator. So, there

appears a disparity in the numbers of interaction parameters and spectral data (see discussion below). As a result, we need either to impose some restrictions on spectral parameters or to introduce additional nonlocal potentials, as is done in the present paper. This problem was not considered in [8–10], which led to an 'erroneous' final result for the potential in the continuum limit: there must be an additional factor 2 (missed in the papers mentioned) in front of the derivative of the solution to the inverse problem integral equation (see equation (37)). This oversight was partially compensated in [11] by Berryman and Green, where the authors introduced nonlocal potentials which are needed for correct final results in the continuum limit. However, in respect of their methods, one can mention an insufficiently grounded introduction of the off-diagonal elements of the matrix Hamiltonian in the difference approximation proposed by the authors.

At the same time, the inverse eigenvalue problem for the discrete analogue of the Sturm–Liouville operator is now well developed. There is a sufficiently large number of papers on this subject, see [12], where one can find most of the references. There are different variants of the inverse problem in the discrete approximation. All of them deal with a matrix (finite or infinite) with several diagonals which may differ in number and are recovered from given (spectral) parameters. For the Gel'fand–Levitan–Marchenko analogue, which is the most known inversion variant, the central theorem is valid: given the set of eigenvalues of a three-diagonal Jacobi matrix and the first components of the associated orthonormal eigenvectors, there exists a unique Jacobi matrix corresponding to these data, see, e.g., [12, 13] and references therein. The usual proof of this theorem is performed using orthogonal polynomials [12].

Thus, we have the continuous and discrete variants, where the inversion procedure is well established. However, considerably less was done to link them both. Presumably, the problem is that the recovery procedures in discrete and continuum cases outwardly have little in common. In the continuum version, the inversion procedure (by Gel'fand–Levitan–Marchenko) is built as a transition from a certain known system (free motion, as a rule) to the system with known spectral data but with the unknown potential to be restored. The aim of this paper is to give such a derivation of the inverse eigenvalue problem from its discrete variant which would be free from the previous errors.

In the discrete variant, we have to develop, in a more explicit form, a structure similar to that in the continuum case. In doing so, we have to use a general criterion which would strongly specify whether our development is correct. The orthogonal polynomials method gives such a hint. This is the orthonormality relation (in a special spectral measure) which is valid for any system. As is well known, the Gram–Schmidt method is essential in constructing these polynomials. So the central idea of the present paper is to employ this method in order to restore the set of eigenvectors orthonormalized in the initial spectral measure when the last is changed in a given way. We shall construct some 'prototype' of the transformation procedure that realizes the restoration of the potential of the regular Schrödinger operator in the continuum case.

We begin, in section 2, with several results consisting of some preliminary constructions which appear as intermediate steps in the course of the methods discussed. First of all, we give the discrete statement of the Sturm–Liouville problem on a bounded interval with zero boundary conditions which is equivalent to consideration of a three-diagonal symmetric Jacobi matrix. In the continuum limit, these diagonals merge in a single diagonal (local potential). Then we pose the inverse eigenvalue problem in terms of eigenvalues and associated spectral weight factors, first components of the orthonormalized eigenvectors. Introducing the so-called regular solutions admits the explicit presentation of these parameters which serve as a spectral measure (of bounded support) entering in the Parseval relation for eigenvectors. That measure

allows us to represent this equality as an orthonormality condition for the same vectors but from a different standpoint when the energies represent components, and the discrete coordinate numbers the vectors. The next step is the application of the Gram–Schmidt technique to obtain a new orthonormal set of eigenvectors (in the sense mentioned) corresponding to the new measure. We shall see that the procedure indeed reproduces prototypes for equations of the inverse problem in the continuum limit. The proof is given that such an orthogonalization is the only possible development. Next, we use the new eigenvectors to recover the potential coefficients on three diagonals of the Jacobi matrix (discrete Sturm–Liouville operator) by using the completeness relation for the new eigenvectors.

In section 3, we pass to the continuum limit. We demonstrate how all the discrete equations-prototypes go over into the classical equations of the inverse Sturm–Liouville problem: Gel'fand–Levitan equations, expression for the potential, classical Goursat problem, etc. That accomplishes our programme.

2. Discrete version of the inverse problem on finite interval

2.1. Preliminary notation

It is most easy to demonstrate the essence of the inverse eigenvalue problem by the example of finite-difference Schrödinger equation in the discrete variable $x_n, n \in \mathbb{Z}$ with the mesh width Δ:

$$-\frac{\Psi(x_{n+1}, E) - 2\Psi(x_n, E) + \Psi(x_{n-1}, E)}{\Delta^2} + V(x_n)\Psi(x_n, E) + u(x_n)\Psi(x_{n+1}, E) + u(x_{n-1})\Psi(x_{n-1}, E) = E\Psi(x_n, E), \tag{1}$$

where $V(x_n)$ and $u(x_n)$ are real, as this problem is reduced to linear algebraic equations. The first three terms in this equation represent the finite-difference operator of the second derivative, i.e., kinetic energy. Note the existence, in the Schrödinger equation, of terms $u(x_n)$ corresponding to a 'minimally nonlocal' interaction. We shall soon come back to them and their introduction will turn out to be justified.

Let us consider the bounded interval $[0, \pi]$ with a finite number N of points inside: $x_0 = 0$; $x_{N+1} = \pi$, so that $\Delta = x_{n+1} - x_n = \pi/(N+1)$. Let us supplement equation (1) by the Dirichlet boundary conditions:

$$\Psi(x_0, E) = \Psi(x_{N+1}, E) = 0. \tag{2}$$

These zero boundary conditions have the well-known physical interpretation that the movement of a particle is restricted by the infinitely tall walls at the points x_0 and x_{N+1} (the infinite rectangular potential well).

The spectrum of the problem (1) and (2) is a ladder of discrete energy levels $\{E_\nu\}_{\nu=1}^{N}$ for bound states representing the unit vectors $\Psi_\nu(x_n) \equiv \Psi(x_n, E_\nu)$,

$$\sum_{n=0}^{N+1} \Delta\Psi_\mu(x_n)\Psi_\nu(x_n) = \delta_{\mu\nu}.$$

The Sturm–Liouville problem (1) and (2) can be rewritten in a more visible form by using the symmetric tridiagonal (Jacobi) matrix $(N \times N)$

$$\hat{H} = \hat{T} + \hat{J},$$

$$\hat{T} = \begin{pmatrix} 2/\Delta^2 & -1/\Delta^2 & 0 & 0 & \cdot & \cdot & \cdot \\ -1/\Delta^2 & 2/\Delta^2 & -1/\Delta^2 & 0 & \cdot & \cdot & \cdot \\ 0 & -1/\Delta^2 & 2/\Delta^2 & -1/\Delta^2 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 0 & -1/\Delta^2 & 2/\Delta^2 \end{pmatrix},$$

$$\hat{J} = \begin{pmatrix} V(x_1) & u(x_1) & 0 & 0 & \cdot & \cdot & \cdot \\ u(x_1) & V(x_2) & u(x_2) & 0 & \cdot & \cdot & \cdot \\ 0 & u(x_2) & V(x_3) & u(x_3) & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 0 & u(x_{N-1}) & V(x_N) \end{pmatrix}, \tag{3}$$

which acts on the vector-column $\Psi_\nu \in \mathbb{R}^N$:

$$\hat{H}\Psi_\nu = E_\nu \Psi_\nu, \qquad \Psi_\nu = \begin{pmatrix} \Psi(x_1, E_\nu) \\ \Psi(x_2, E_\nu) \\ \cdot \\ \cdot \\ \cdot \\ \Psi(x_N, E_\nu) \end{pmatrix}.$$

This explicit form elucidates why the $u(x_n)$ stands in front of $\Psi(x_{n+1}, E)$: this is because of the upper u-diagonal in $\hat{J}$ which is one element shorter than the main V-diagonal and contains $N - 1$ elements. The same coefficients form up the lower diagonal (thanks to the matrix symmetry). Let us specially note that homogeneous boundary conditions being generally different from (2) would require some modification of the matrix representation (3). In passing to the continuum limit $\Delta \to 0$, it will be impossible to distinguish between the u- and V-diagonals, i.e., the resulting interaction will be simply the sum of limiting values for us and Vs. A paragraph later, we shall give the motivation for the appearance of the additional diagonals in the interaction matrix $\hat{J}$.

Besides the energy levels, let us introduce additional fundamental spectral parameters, namely, norming constants or spectral weight factors. By definition, these are the coefficients c_ν of proportionality between the normalized eigenstates $\Psi_\nu(x_n)$ and so-called *regular solutions* $\varphi(x_n, E_\nu)$ at the eigenvalue energy, $\varphi(0, E) = 0, \varphi(x_1, E) = \Delta$ (i.e., the derivative is equal to 1), $\varphi_\nu(x_n) \equiv \varphi(x_n, E_\nu)$:

$$\Psi_\nu(x_n) = c_\nu \varphi_\nu(x_n). \tag{4}$$

The continuum analogue of the regular solution satisfies $\varphi(0, E) = 0, \varphi'(x, E)|_{x=0} = 1$. The continuum generalization of the spectral weight factors introduced is obvious. In the classical inverse Sturm–Liouville problem (continuous coordinate), it is well known that the double set of the spectral parameters $\{E_\nu, c_\nu\}$ uniquely specifies the potential.

2.2. The inversion procedure as the Gram–Schmidt reorthogonalization

Now our task is to pose such a discrete version of the inverse Sturm–Liouville problem that, in passing to the continuum limit, as direct reproduction of all the results of the continuum

version as possible may be feasible. So, the problem within which it seems logical to work is posed as follows: given the set $\{E_\nu, c_\nu\}$ with c_ν in (4), the potential matrix $\hat{J}$ with the coefficients $V(x_n)$ and $u(x_n)$ must be recovered completely. In principle, a question may arise whether the three-diagonal Hamiltonian with the 'nonlocal' u-coefficients is consistent with the uniqueness of the potential recovery from the set $\{E_\nu, c_\nu\}$. What forces extra us? As has already been mentioned in the introduction, any set $\{E_\nu, c_\nu\}$ can occur for a unique three-diagonal $\hat{H}$. Moreover, there is an extension of that result. It is the theorem by Gladwell and Willms [13] in which the statement was proved that a symmetric p-band matrix (a matrix with $2p + 1$ bands, p bands below the diagonal) may be uniquely constructed (apart from certain sign ambiguities) from its eigenvalues and the first p components of its normalized eigenvectors. Hence, once we know all E_νs and the first eigenvector components (by virtue of equation (4) these are Δc_ν in our problem) we can uniquely restore 1-band, i.e., three-diagonal Hamiltonian (3). That also accounts for the us.

Let us give an additional 'half-heuristic' explanation of this fact. If we have only a local potential $V(x_n)$ with N values at N points, the number N of free parameters $\{V(x_n)\}_{n=1}^N$ equals exactly the number of eigenvalues E_ν. To the point, the corresponding inverse problem has no complete solution. If we introduce both spectral parameters, E_ν and c_ν, while the single-diagonal $\hat{J}$ persists, we shall really face a problem of overdetermination of the set $\{E_\nu, c_\nu\}$ of two $N - 1$ free parameters. In fact, there are N levels E_ν and $N - 1$ parameters c_ν by virtue of the relation $\sum_{\nu=1}^N c_\nu^2 = 1/\Delta^3$ that follows from (6) for $n = m = 1$, while $V(x_n)$ contains only N ones. It is introduction of $N - 1$ coefficients $u(x_n), n = 1, \ldots, N - 1$ into equation (1) (or additional diagonals in (3)) that ensures the equality of numbers of spectral data and interaction parameters. In the case of continuous coordinate, the overfilling of the set of spectral parameters reveals itself only in many-dimensional $D \geqslant 2$ problems, so we shall manage to recover the one-dimensional local potential from the complete spectral set (see (37)).

The functions $\varphi_\nu(x_n)$ can be considered as vectors in special Hilbert (Euclidean, to be precise) space, in which the coordinate x_n numbers the eigenvectors while energy index ν is only used to denote the νth vector component. The inner product in that space is determined by the measure given by the spectral weight factors c_ν. In fact, the Parseval's completeness relation

$$\sum_{\nu=1}^{N} \Psi_\nu(x_m)\Psi_\nu(x_n) = \delta_{mn}/\Delta \tag{5}$$

can be rewritten using equation (4) as

$$\sum_{\nu=1}^{N} c_\nu^2 \varphi_\nu(x_m)\varphi_\nu(x_n) = \delta_{mn}/\Delta. \tag{6}$$

Let us consider this expression as an orthogonality relation for the vectors $\varphi_\nu(x_m)$ and $\varphi_\nu(x_n)$ (in the limit $\Delta \to 0$, the 'numbers' $x_{m,n}$ of the vectors become the continuous variable x). Here, the inner product is given by not simply a sum over energy index ν but also by a sum with a weight (measure) c_ν^2.

Different potentials correspond to different weight factors determining the metrics of our 'energy space', but the relation (6) holds true for any potential. In the classical variant, the inverse problem can be treated as a transition to the sought potential $\overset{\circ}{V}(x_n) \to V(x_n)$ from a certain 'initial' (in what follows we shall use the symbol '$\circ$' to denote everything related to the initial system) potential $\overset{\circ}{V}(x_n)$, for which all the solutions $\overset{\circ}{\varphi}_\nu(x_n)$ and the whole spectral

set $\{\overset{\circ}{E}_\nu, \overset{\circ}{c}_\nu\}$ are known, and the relation (6) is valid:

$$\sum_{\nu=1}^{N} \overset{\circ}{c}{}_\nu^2 \; \overset{\circ}{\varphi}_\nu(x_m)\, \overset{\circ}{\varphi}_\nu(x_n) = \delta_{mn}/\Delta. \tag{7}$$

All this gives us a hint for deriving new solutions corresponding to the given spectral set $\{E_\nu, c_\nu\}_{\nu=1}^N$. Although we do not yet know the sought potential matrix $\hat{J}$, we know beforehand that the regular solutions $\varphi_\nu(x_n)$ to this matrix must satisfy the orthogonality relation (6) with the new c_ν. We shall catch at this fact and use the orthogonality relation as a central criterion in finding new eigenvectors (solutions $\varphi_\nu(x_n)$). Changing the metrics of Euclidean space in replacing $\overset{\circ}{c}_\nu \to c_\nu$ results in that the 'old' unit vectors $\overset{\circ}{\varphi}_\nu(x_n)$ are no longer orthogonal. So the idea is as follows: once new unit vectors must satisfy equation (6), we could obtain them, e.g., orthogonalizing the $\overset{\circ}{\varphi}_\nu(x_n)$ with the new weight c_ν^2 by using the Gram–Schmidt scheme. In other words, the new vectors obtained in that way and satisfying (6) with the weight multipliers c_ν^2 will be the solutions to the new potentials Vs and us. Indubitably, this makes sense only when the procedure really gives the desired vectors, i.e., it is unique (see the proof further on).

For simplicity, we shall at first think $\overset{\circ}{E}_\nu = E_\nu$. Let us recall this standard orthogonalization procedure by the example of two initially nonorthogonal (in a sense of new weight function) vectors (i.e., when $N = 2$) $\overset{\circ}{\varphi}_\nu(x_1)$, $\overset{\circ}{\varphi}_\nu(x_2)$, $\nu = 1, 2$. As the first unit vector $\varphi_\nu(x_1)$ of the new system, we take the unchanged unit vector $\overset{\circ}{\varphi}_\nu(x_1)$, and the second unit vector is constructed from the second unaltered one, only we have to subtract everything superfluous (parallel to $\overset{\circ}{\varphi}_\nu(x_1)$) for the orthogonality with the new measure:

$$\varphi_\nu(x_1) = \overset{\circ}{\varphi}_\nu(x_1); \qquad \varphi_\nu(x_2) = \overset{\circ}{\varphi}_\nu(x_2) + \Delta K(x_2, x_1)\, \overset{\circ}{\varphi}_\nu(x_1).$$

The coefficient $K(x_2, x_1)$ is derived from the condition of orthogonality of the new vectors with the new weight c_ν:

$$\varphi_\nu(x_2) \perp \varphi_\nu(x_1) \equiv \overset{\circ}{\varphi}_\nu(x_1).$$

We have

$$\sum_{\nu=1}^{2} c_\nu^2 \, \overset{\circ}{\varphi}_\nu(x_1)\, \overset{\circ}{\varphi}_\nu(x_2) + \Delta \sum_{\nu=1}^{2} c_\nu^2 K(x_2, x_1)\, \overset{\circ}{\varphi}{}_\nu^2(x_1) = 0 \Longrightarrow K(x_2, x_1)$$
$$+ \sum_{\nu=1}^{2} c_\nu^2 \, \overset{\circ}{\varphi}_\nu(x_1)\, \overset{\circ}{\varphi}_\nu(x_2) + \Delta K(x_2, x_1) \sum_{\nu=1}^{2} \left(c_\nu^2 - \overset{\circ}{c}{}_\nu^2\right) \overset{\circ}{\varphi}{}_\nu^2(x_1) = 0, \tag{8}$$

where we add and subtract the term $\overset{\circ}{c}{}_\nu^2$ from the multiplier c_ν^2 and, furthermore, use equation (7). We can rewrite the last equality in the form as follows (extremely simplified two-dimensional 'prototype' of the inverse problem equation):

$$K(x_2, x_1) + Q(x_2, x_1) + \Delta K(x_2, x_1) Q(x_1, x_1) = 0, \tag{9}$$

where

$$Q(x_m, x_n) = \sum_{\nu=1}^{N=2} c_\nu^2 \, \overset{\circ}{\varphi}_\nu(x_m)\, \overset{\circ}{\varphi}_\nu(x_n) - \sum_{\mu=1}^{N=2} \overset{\circ}{c}{}_\mu^2 \, \overset{\circ}{\varphi}_\mu(x_m)\, \overset{\circ}{\varphi}_\mu(x_n); \qquad m, n = 1, 2. \tag{10}$$

In the general case of N-dimensional Euclidean space we shall follow the same scheme. In doing so, it is possible to take into account the case when the levels change: $\overset{\circ}{E}_\nu \neq E_\nu$. We must

orthogonalize N vectors in the measure c_ν^2: $\overset{\circ}{\varphi}(x_m, E_\nu)$, $(m = 1, 2, \ldots, N, \nu = 1, 2, \ldots, N)$. Consequently, for the new solutions we have

$$\varphi(x_m, E_\nu) = \overset{\circ}{\varphi}(x_m, E_\nu) + \sum_{n=1}^{m-1} \Delta K(x_m, x_n)\, \overset{\circ}{\varphi}(x_n, E_\nu), \tag{11}$$

where the coefficients K (the kernel of the transformation operator (11)) follow from the conditions of orthogonality of the new vectors (in measure c_ν^2) $\varphi(x_m, E_\nu)(m = 1, 2, \ldots, N)$:

$$\varphi(x_{m>n}, E_\nu) \perp \varphi(x_n, E_\nu),$$

which lead to the system of algebraic equations for K-discrete analogue of the central equations of the inverse problem:

$$K(x_m, x_n) + Q(x_m, x_n) + \sum_{p=1}^{m-1} \Delta K(x_m, x_p) Q(x_p, x_n) = 0; \qquad m > n, \tag{12}$$

where $Q(x_n, x_m)$ is determined as in (10), only the values m and n are no longer restricted to 1 and 2, and the indices μ and ν number solutions at the initial and shifted energy levels, respectively.

$$Q(x_m, x_n) = \sum_{\nu=1}^{N} c_\nu^2\, \overset{\circ}{\varphi}(x_m, E_\nu)\, \overset{\circ}{\varphi}(x_n, E_\nu) - \sum_{\mu=1}^{N} \overset{\circ}{c}{}_\mu^2\, \overset{\circ}{\varphi}(x_m, \overset{\circ}{E}_\mu)\, \overset{\circ}{\varphi}(x_n, \overset{\circ}{E}_\mu). \tag{13}$$

Let us note that the form (11) ensures the desired boundary condition for the regular solution: $\varphi(x_0, E_\nu) = 0$; $\varphi(x_1, E_\nu) = \Delta$. The system (12) of the recurrence computation of Ks provides them uniquely. We can formally introduce the diagonal terms $K(x_n, x_n)$ (bearing no relation to $\varphi(x, E_\nu)$) such that $K(x_{n+1}, x_n) - K(x_n, x_n) \sim O(\Delta)$ which will be useful in what follows.

The following is very important and will be used in the subsequent derivations. When the first $m + 1$ unit vectors $\overset{\circ}{\varphi}(x_i, E_\nu)$, $i = 1, \ldots, m + 1$ are orthogonalized, this corresponds to an intermediate submatrix–block transformation of the initial Jacobi-like operator (3) so that

$$\hat{J} = \begin{pmatrix} \hat{J}_m & \mathbf{0} \\ \mathbf{0} & \hat{\overset{\circ}{J}}_{N-m} \end{pmatrix},$$

$$\hat{J}_m = \begin{pmatrix} V(x_1) & u(x_1) & 0 & 0 & \cdot & \cdot & \cdot \\ u(x_1) & V(x_2) & u(x_2) & 0 & \cdot & \cdot & \cdot \\ 0 & u(x_2) & V(x_3) & u(x_3) & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & 0 & u(x_{m-1}) & V(x_m) & \overset{\circ}{u}(x_m) \end{pmatrix}, \tag{14}$$

$$\hat{\overset{\circ}{J}}_{N-m} = \begin{pmatrix} \overset{\circ}{u}(x_m) & \overset{\circ}{V}(x_{m+1}) & \overset{\circ}{u}(x_{m+1}) & 0 & \cdot & \cdot & \cdot \\ 0 & \overset{\circ}{u}(x_{m+1}) & \overset{\circ}{V}(x_{m+2}) & \overset{\circ}{u}(x_{m+2}) & 0 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & 0 & \overset{\circ}{u}(x_{N-1}) & \overset{\circ}{V}(x_N) \end{pmatrix},$$

where the symbols $\mathbf{0}$ in the top-right and bottom-left corners of the $\hat{J}$ matrix denote zero $(m \times N - m - 1)$ and $(N - m \times m - 1)$ matrices, respectively. The submatrix $\hat{J}_m$ is formed up by the perturbed coefficients while the $\hat{\overset{\circ}{J}}_{N-m}$ is not yet affected by the transformation

associated with the reorthogonalization. Note that the last row of the submatrix $\hat{J}_m$ contains only two transformed elements, $u(x_{m-1})$ and $V(x_m)$, apart from the $\overset{\circ}{u}(x_m)$. This is because only the $(m \times m)$ *quadratic* submatrix was transformed which contains, in its last row, two nonzero elements mentioned. The coefficients of that intermediate transformation block may be found from formulae (20) and (21) where one should substitute $\overset{\circ}{u}(x_m)$ for $u(x_m)$. See also the subsequent discussion after the formulae (20) and (21).

2.3. The theorem of uniqueness for the Gram–Schmidt scheme

Now we are ready to give the proof that the above procedure is unique.

Theorem. *For the spectral set $\{E_\mu, c_\mu\}_{\mu=1}^N$ to the Sturm–Liouville problems (1) and (2), there is a unique regular solution to (1) at eigenvalue E_ν given by the decomposition (11) with the mth summand $\overset{\circ}{\varphi}(x_m, E_\nu)$.*

Proof. Let us carry it out by induction. Suppose that the desired transformed vectors (11) (being numbered by m) are uniquely given by equation (11) for $m \leqslant \bar{N}$, $\bar{N} < N$ for a certain $\bar{N}$ being the integer. For $\bar{N} = 1$, this is verified trivially. Let us show that formula (11) holds true at the point $x_{\bar{N}+1}$. Indeed, $\varphi(x_{\bar{N}+1}, E_\nu)$, being orthogonal to all $\varphi(x_m, E_\nu)$, $m \leqslant \bar{N}$, can be sought, in principle, as a combination of the initial $\overset{\circ}{\varphi}(x_n, E_\nu)$ for all n. The coefficients of such a hypothetical combination (there are N pieces of them in all) have to be determined from the condition of orthogonality of $\varphi(x_{\bar{N}+1}, E_\nu)$ to both $\varphi(x_m, E_\nu)$, $m = 1, \ldots, \bar{N}$ and certain $N - \bar{N}$ unknown vectors from the new orthogonal set (6). For ascertaining what we shall do now, we involve the Schrödinger equation (1), which is a recurrence procedure of the step-by-step computation of $\varphi(x_n, E_\nu)$. As N vectors are obtained, we mean the block operator $\hat{J}_{\bar{N}}$ in (14), the last row:

$$-\frac{\varphi(x_{\bar{N}+1}, E_\nu) - 2\varphi(x_{\bar{N}}, E_\nu) + \varphi(x_{\bar{N}-1}, E_\nu)}{\Delta^2} + V(x_{\bar{N}})\varphi(x_{\bar{N}}, E_\nu)$$
$$+ \overset{\circ}{u}(x_{\bar{N}})\varphi(x_{\bar{N}+1}, E_\nu) + u(x_{\bar{N}-1})\varphi(x_{\bar{N}-1}, E_\nu) = E_\nu\varphi(x_{\bar{N}}, E_\nu).$$

It is seen that $(\overset{\circ}{u}(x_{\bar{N}}) - 1/\Delta^2)\varphi(x_{\bar{N}+1}, E_\nu)$ is a linear combination of $(u(x_{\bar{N}-1}) - 1/\Delta^2)\varphi(x_{\bar{N}-1}, E_\nu)$, $(V(x_{\bar{N}}) + 2/\Delta^2)\varphi(x_{\bar{N}}, E_\nu)$ and $E_\nu\varphi(x_{\bar{N}}, E_\nu)$. Consequently, by the assumptions of the validity of (11) for $m \leqslant \bar{N}$, $(\overset{\circ}{u}(x_{\bar{N}}) - 1/\Delta^2)\varphi(x_{\bar{N}+1}, E_\nu)$ can only be represented in terms of $(V(x_{\bar{N}}) + 2/\Delta^2)K(x_{\bar{N}}, x_m)\,\overset{\circ}{\varphi}(x_m, E_\nu)$, $m = 1, \ldots, \bar{N} - 1$; $(V(x_{\bar{N}}) + 2/\Delta^2)\,\overset{\circ}{\varphi}(x_{\bar{N}}, E_\nu)$; $(u(x_{\bar{N}-1}) - 1/\Delta^2)K(x_{\bar{N}-1}, x_m)\,\overset{\circ}{\varphi}(x_m, E_\nu)$, $m = 1, \ldots, \bar{N} - 2$; $(u(x_{\bar{N}-1}) - 1/\Delta^2)\,\overset{\circ}{\varphi}(x_{\bar{N}-1}, E_\nu)$; $K(x_{\bar{N}-1}, x_m)E_\nu\,\overset{\circ}{\varphi}(x_m, E_\nu)$, $m = 1, \ldots, \bar{N}-1$ and $E_\nu\,\overset{\circ}{\varphi}(x_{\bar{N}}, E_\nu)$. For the last term, we find from the non-perturbed Schrödinger equation that $E_\nu\,\overset{\circ}{\varphi}(x_{\bar{N}}, E_\nu)$ is expressed in terms of $(\overset{\circ}{u}(x_{\bar{N}}) - 1/\Delta^2)\,\overset{\circ}{\varphi}(x_{\bar{N}+1}, E_\nu)$, $(\overset{\circ}{V}(x_{\bar{N}}) + 2/\Delta^2)\,\overset{\circ}{\varphi}(x_{\bar{N}}, E_\nu)$, $(\overset{\circ}{u}(x_{\bar{N}-1}) - 1/\Delta^2)\,\overset{\circ}{\varphi}(x_{\bar{N}-1}, E_\nu)$ (and similarly for other $E_\nu\,\overset{\circ}{\varphi}(x_m, E_\nu)$) and, finally, the $\varphi(x_{\bar{N}+1}, E_\nu)$ must be sought as a linear combination of $\overset{\circ}{\varphi}(x_m, E_\nu)$, $m = 1, \ldots, \bar{N} + 1$. In other words, $\varphi(x_{\bar{N}+1}, E_\nu) \in \operatorname{span}\{\overset{\circ}{\varphi}(x_m, E_\nu)\}_{m=1}^{\bar{N}+1}$, besides that $\varphi(x_{\bar{N}+1}, E_\nu) \perp \operatorname{span}\{\overset{\circ}{\varphi}(x_m, E_\nu)\}_{m=1}^{\bar{N}} = \operatorname{span}\{\varphi(x_m, E_\nu)\}_{m=1}^{\bar{N}}$. It is well known that the Gram–Schmidt orthogonalization enables a unique solution satisfying these two conditions. Note that the $(\bar{N}+1)$th term $(\overset{\circ}{u}(x_{\bar{N}}) - 1/\Delta^2)\varphi(x_{\bar{N}+1}, E_\nu)$ is a combination of the summand $(\overset{\circ}{u}(x_{\bar{N}}) - 1/\Delta^2)\,\overset{\circ}{\varphi}(x_{\bar{N}+1}, E_\nu)$ and other terms with $m \leqslant \bar{N}$. In other words, in the decomposition of $\varphi(x_{\bar{N}+1}, E_\nu)$, we have the term $\overset{\circ}{\varphi}(x_{\bar{N}+1}, E_\nu)$ with the unit factor. Consequently, $\varphi(x_{\bar{N}+1}, E_\nu)$ is represented in the form (11) again. □

2.4. Solutions to the recovered potential and its derivation

It should be noted that formula (11) is also valid for solutions at energies E lying between the levels E_ν where the regular solutions, being the Cauchy problem solutions, are defined (though nonphysical). Do not confuse 'running' energy values at which the solutions $\varphi(x_m, E)$ are defined with the energies occurring in the inverse problem equations (13). Indeed, let us decompose $\varphi(x_m, E)$ into the complete set of solutions $\varphi(x_m, E_\nu)$ (in a sense of the usual inner product $\sum_{m=1}^{N} \Delta c_\nu c_\mu \varphi(x_m, E_\nu)\varphi(x_m, E_\mu)$):

$$\varphi(x_m, E) = \sum_{\nu=1}^{N} \xi(E, E_\nu)\varphi(x_m, E_\nu); \qquad \xi(E, E_\nu) = \sum_{m=1}^{N} \Delta c_\nu \varphi(x_m, E_\nu)\varphi(x_m, E). \tag{15}$$

Since $\varphi(x_m, E_\nu)$s are expressed, in accordance with (11), in terms of the unperturbed $\overset{\circ}{\varphi}(x_m, E_\nu)$, we shall expand them, too, in a complete set of old solutions $\overset{\circ}{\varphi}(x_m, \overset{\circ}{E}_\mu)$:

$$\begin{aligned} \overset{\circ}{\varphi}(x_m, E_\nu) &= \sum_{\mu=1}^{N} \zeta(E_\nu, \overset{\circ}{E}_\mu)\, \overset{\circ}{\varphi}(x_m, \overset{\circ}{E}_\mu); \\ \zeta(E_\nu, \overset{\circ}{E}_\mu) &= \sum_{m=1}^{N} \Delta\, \overset{\circ}{c}_\mu \overset{\circ}{\varphi}(x_m, E_\nu)\, \overset{\circ}{\varphi}(x_m, \overset{\circ}{E}_\mu). \end{aligned} \tag{16}$$

Combining (11), (15) and (16), we get the following expression for the new solutions at arbitrary E:

$$\begin{aligned} \varphi(x_m, E) = \sum_{\mu,\nu} A(E, E_\nu, \overset{\circ}{E}_\mu)\, \overset{\circ}{\varphi}(x_m, \overset{\circ}{E}_\mu) + \sum_{\mu,\nu} \sum_{n=1}^{m-1} \Delta K(x_m, x_n) \\ \times A(E, E_\nu, \overset{\circ}{E}_\mu)\, \overset{\circ}{\varphi}(x_n, \overset{\circ}{E}_\mu); \qquad A(E, E_\nu, \overset{\circ}{E}_\mu) = \xi(E, E_\nu)\zeta(E_\nu, \overset{\circ}{E}_\mu). \end{aligned} \tag{17}$$

In the limit when the new and old spectral parameters coincide, K vanishes and, hence, $\varphi(x_m, E)$ turn into the unperturbed solution

$$\overset{\circ}{\varphi}(x_m, E) = \sum_{\mu,\nu} A(E, \overset{\circ}{E}_\nu, \overset{\circ}{E}_\mu)\, \overset{\circ}{\varphi}(x_m, \overset{\circ}{E}_\mu).$$

On the other hand, putting $m = 1$ in this equality and formula (17) we have ($\overset{\circ}{\varphi}(x_1, E) = \varphi(x_1, E) = \Delta$)

$$\sum_{\mu,\nu} A(E, \overset{\circ}{E}_\nu, \overset{\circ}{E}_\mu)\Delta = \sum_{\mu,\nu} A(E, E_\nu, \overset{\circ}{E}_\mu)\Delta,$$

or

$$\overset{\circ}{\varphi}(x_1, E) = \sum_{\mu,\nu} A(E, \overset{\circ}{E}_\nu, \overset{\circ}{E}_\mu)\, \overset{\circ}{\varphi}(x_1, \overset{\circ}{E}_\mu) = \sum_{\mu,\nu} A(E, E_\nu, \overset{\circ}{E}_\mu)\, \overset{\circ}{\varphi}(x_1, \overset{\circ}{E}_\mu).$$

By virtue of the uniqueness of the decomposition of $\overset{\circ}{\varphi}(x_m, E)$ in terms of $\overset{\circ}{\varphi}(x_m, \overset{\circ}{E}_\mu)$, the last equality holds true at any m:

$$\overset{\circ}{\varphi}(x_m, E) = \sum_{\mu,\nu} A(E, E_\nu, \overset{\circ}{E}_\mu)\, \overset{\circ}{\varphi}(x_m, \overset{\circ}{E}_\mu).$$

Substituting this expression in (17), we get

$$\varphi(x_m, E) = \overset{\circ}{\varphi}(x_m, E) + \sum_{n=1}^{m-1} \Delta K(x_m, x_n)\, \overset{\circ}{\varphi}(x_n, E). \tag{18}$$

Let us stress here that K is independent of energy E. Formulae (18), (12) and (13) give the expression for K in the form of the sum of products of the old and transformed solutions:

$$K(x_m, x_n) = -\sum_{\nu}^{N} c_\nu^2 \varphi(x_m, E_\nu)\, \mathring{\varphi}(x_n, E_\nu) + \sum_{\mu}^{N} \mathring{c}_\mu^2 \varphi(x_m, \mathring{E}_\mu)\, \mathring{\varphi}(x_n, \mathring{E}_\mu). \tag{19}$$

It remains to obtain equations for the transformed potentials V and u. We already know the solutions of equation (1) with the unknown potentials $V(x_n)$ and $u(x_n)$ (see formulae (11) and (12)), i.e., eigenvectors of the new Hamiltonian plus associated eigenvalues E_ν. As has been mentioned, by virtue of the theorem by Gladwell and Willms [13], this is enough for recovering the three-diagonal Hamiltonian matrix (with off-diagonal elements). These authors used the block Lanczos algorithm. However, we shall apply an outwardly different method pursuing the aim of reproducing final formulae in the continuum limit. Let us multiply both parts of the Schrödinger equation (1) for the solutions $\varphi(x_m, \mathring{E}_\mu)$ (equation (18)) and $\mathring{\varphi}(x_n, \mathring{E}_\mu)$ by $\mathring{\varphi}(x_n, \mathring{E}_\mu)$ and $\varphi(x_m, \mathring{E}_\mu)$, respectively, sum over μ with weight $\mathring{c}_\mu^2$ and subtract from each other the resulting expressions. At fixed m, we perform this procedure for $n = m, m-1, \ldots$. In calculating sums (over μ) one should take into account relation (7). As a result, we get the following equations for V and u:

$$\begin{aligned}
&\{V(x_m) - \mathring{V}(x_n)\}K(x_m, x_n) + u(x_m)K(x_{m+1}, x_n) - \mathring{u}(x_n) \\
&\qquad \times K(x_m, x_{n+1}) + u(x_{m-1})K(x_{m-1}, x_n) - \mathring{u}(x_{n-1})K(x_m, x_{n-1}) \\
&\qquad = \frac{K(x_{m+1}, x_n) - 2K(x_m, x_n) + K(x_{m-1}, x_n)}{\Delta^2} \\
&\qquad - \frac{K(x_m, x_{n+1}) - 2K(x_m, x_n) + K(x_m, x_{n-1})}{\Delta^2}; \qquad n \leqslant m-2,
\end{aligned} \tag{20}$$

and for $n = m, m-1$

$$\begin{cases}
\dfrac{u(x_{m-1}) - \mathring{u}(x_{m-1})}{\Delta} = \dfrac{K(x_{m+1}, x_{m-1}) - K(x_m, x_{m-2})}{\Delta^2} \\
-V(x_m)K(x_m, x_{m-1}) + \mathring{V}(x_{m-1})K(x_m, x_{m-1}) \\
-u(x_m)K(x_{m+1}, x_{m-1}) + \mathring{u}(x_{m-2})K(x_m, x_{m-2}); \qquad n = m-1 \\
\dfrac{V(x_m) - \mathring{V}(x_m)}{\Delta} = \dfrac{K(x_{m+1}, x_m) - K(x_m, x_{m-1})}{\Delta^2} \\
-u(x_m)K(x_{m+1}, x_m) + K(x_m, x_{m-1})\, \mathring{u}(x_{m-1}); \qquad n = m,
\end{cases} \tag{21}$$

where the terms $K(x_m, x_n)$ for which $m, n > N$ or $m, n < 1$ are omitted. But for $n = m+1$ we obtain that $u(x_m) = \mathring{u}(x_m)$. There is nothing strange in this because the summation is carried out for the term $\mathring{\varphi}(x_{m+1}, \mathring{E}_\mu)$ that is *orthogonal* to all $\mathring{\varphi}(x_n, \mathring{E}_\mu), n < m+1$. The kernel K containing all the information about the new solutions just stands at these summands, see formula (18) for $n = m+1$. In other words, for the case $n = m+1$ the summation expunges everything that bears a relation to the new system under construction. Indeed, from the Schrödinger equation for $\mathring{\varphi}(x_{m+1}, \mathring{E}_\mu)$ multiplied by $\varphi(x_m, \mathring{E}_\mu)$ and summed over μ with the weight $\mathring{c}_\mu^2$ we have

$$\sum_{\mu=1}^{N} \mathring{c}_\mu^2\, \mathring{E}_\mu\, \varphi(x_m, \mathring{E}_\mu)\, \mathring{\varphi}(x_{m+1}, \mathring{E}_\mu) = \frac{\mathring{u}(x_m)}{\Delta} - \frac{1}{\Delta^3}.$$

How should one treat this? One variant is that $u(x_m) = \overset{\circ}{u}(x_m)$, which corresponds to restoration of a $m \times m$ submatrix for which the element $\overset{\circ}{u}(x_m)$ is an outer one, see (14). This can also serve as a proof of (14). The other interpretation is that $u(x_m) \neq \overset{\circ}{u}(x_m)$ (but not for $m = N$), nevertheless (i.e., the above procedure does not work). This takes place for the whole $\hat{J}$-matrix transformed but equations (21) alone do not allow the computation of $u(x_m)$. How then to uniquely restore $\hat{J}$ will be discussed a bit later, but now we must ascertain how it is possible that the same solution $\varphi(x_m, E)$ may satisfy the Schrödinger equation (1) with *different* potential coefficients $\overset{\circ}{u}(x_m)$ and $u(x_m)$ at x_{m+1}. The matter is that we deal with (finite-difference) nonlocal potential and this ambiguity is just characteristic of it. Indeed, let $\varphi(x_m, E)$ satisfy the Schrödinger equations with both $\{u_1(x_{m-1}), V_1(x_m), u_1(x_m)\}$ and $\{u_2(x_{m-1}), V_2(x_m), u_2(x_m)\}$. Subtracting these equations from each other we have

$$[V_1(x_m) - V_2(x_m)]\varphi(x_m, E) + [u_1(x_m) - u_2(x_m)]\varphi(x_{m+1}, E) + [u_1(x_{m-1}) - u_2(x_{m-1})]\varphi(x_{m-1}, E) = 0.$$

Thus, we can see that, for several nonlocal potential coefficients coupling neighbouring x points, this equation clearly demonstrates that $V_1(x_m) - V_2(x_m)$ and other potential differences may all be nonzero. Summing up this discussion, we have elucidated that the procedure used for derivation of (20) and (21) cannot distinguish all the variants of the $u(x_m)$-coefficient determination proceeding from a general incapability of giving a unique nonlocal interaction associated with a certain solution of the Schrödinger equation.

However, for the whole vector $\varphi(x_m, E_\nu)$, i.e., the solution defined at *all* the points $x_m, m = 1, \ldots, N$, we are able to uniquely derive the quadratic potential matrix $\hat{J}$ whose eigenvectors are $\varphi(x_m, E_\nu)$. Taking $m = N$ we first find $u(x_{N-1})$, $V(x_N)$ and $u(x_N)$. Of course, this requires the knowledge of $u(x_N)$. However, we have no more equations for determining the potential coefficient $u(x_N)$. We can see that $u(x_N)$ is a continuation of the last Nth row of the matrix $\hat{J}$. This resembles the case with the unfinished restoration of $\hat{J}$, see (14), i.e., the potential perturbation (in the form of a quadratic matrix) never reached $u(x_N)$. That is, the $u(x_N)$ is independent of the transformation generated by K-coefficients. Then, taking $\{E_\nu, c_\nu\} = \{\overset{\circ}{E}_\nu, \overset{\circ}{c}_\nu\}$, we can see that $K = 0$ and $u(x_N)$ exactly corresponds to the reference potential. Thus, we have $u(x_N) = \overset{\circ}{u}(x_N)$. Next, at the point x_N we have, instead of (21), the following system of equations:

$$\begin{cases} \dfrac{u(x_{N-1}) - \overset{\circ}{u}(x_{N-1})}{\Delta} = \dfrac{\sum_{\mu=1}^{N} \overset{\circ}{c}{}_\mu^2 \varphi(x_{N+1}, \overset{\circ}{E}_\mu)\, \overset{\circ}{\varphi}(x_{N-1}, \overset{\circ}{E}_\mu) - K(x_N, x_{N-2})}{\Delta^2} \\ -V(x_N)K(x_N, x_{N-1}) + \overset{\circ}{V}(x_{N-1})K(x_N, x_{N-1}) \\ -u(x_N)\displaystyle\sum_{\mu=1}^{N} \overset{\circ}{c}{}_\mu^2 \varphi(x_{N+1}, \overset{\circ}{E}_\mu)\overset{\circ}{\varphi}(x_{N-1}, \overset{\circ}{E}_\mu) + \overset{\circ}{u}(x_{N-2})K(x_N, x_{N-2}), \\ \dfrac{V(x_N) - \overset{\circ}{V}(x_N)}{\Delta} = \dfrac{\sum_{\mu=1}^{N} \overset{\circ}{c}{}_\mu^2 \varphi(x_{N+1}, \overset{\circ}{E}_\mu)\overset{\circ}{\varphi}(x_N, \overset{\circ}{E}_\mu) - K(x_N, x_{N-1})}{\Delta^2} \\ -u(x_N)\displaystyle\sum_{\mu=1}^{N} \overset{\circ}{c}{}_\mu^2 \varphi(x_{N+1}, \overset{\circ}{E}_\mu)\overset{\circ}{\varphi}(x_N, \overset{\circ}{E}_\mu) + K(x_N, x_{N-1})\, \overset{\circ}{u}(x_{N-1}), \end{cases} \tag{22}$$

where $\varphi(x_{N+1}, \overset{\circ}{E}_\mu)$ is found from the Schrödinger equation (1):

$$\varphi(x_{N+1}, \overset{\circ}{E}_\mu) = \frac{\Delta^2}{1-\Delta^2 u(x_N)}[u(x_{N-1})\varphi(x_{N-1}, \overset{\circ}{E}_\mu) + V(x_N)\varphi(x_N, \overset{\circ}{E}_\mu) - \overset{\circ}{E}_\mu \varphi(x_N, \overset{\circ}{E}_\mu)] - \frac{-2\varphi(x_N, \overset{\circ}{E}_\mu) + \varphi(x_{N-1}, \overset{\circ}{E}_\mu)}{1-\Delta^2 u(x_N)}, \tag{23}$$

where $\varphi(x_n, \overset{\circ}{E}_\mu)$ is given by (18) and $u(x_N) = \overset{\circ}{u}(x_N)$. From (22) and (23), we obtain $V(x_N)$ and $u(x_{N-1})$. We then substitute the value $u(x_{N-1})$ (by virtue of the symmetry of the potential matrix) into equations (20) for $m = N-1; n = m-2, m-3$ from which we find, in turn, $V(x_{N-1})$ and $u(x_{N-2})$. Afterward, we substitute this last coefficient into equation (20) for $m = N-2; n = m-2, m-3$ and get $V(x_{N-2})$ and $u(x_{N-3})$ and so on. Thus, these equations allow the computation of V and u via the solutions of the inverse problem equation (12)—the coefficients $K(x_m, x_n), m > n$ (plus an additional requirement concerning $u(x_N)$). For any finite N, these linear equations are uniquely solved.

However, with the N being sufficiently large, the numerical instability increases, we mean the well-known problem of the ill-posed inversion procedure. Of course, the difference scheme itself can be treated as a regularization of the continuum inverse problem, but a concrete recipe depends on a specific problem under consideration. Most generally, the essence of these algorithms is that we need to change concordantly the regularization parameter (i.e, the mesh width Δ) and the estimation precision $\delta\{E_\nu, c_\nu\}$ so that the errors in the potential under restoration and the corresponding solutions may not exceed (in a certain norm) the limits consistent with the errors in spectral data. Explicitly, there exists a function $\Delta(\delta\{E_\nu, c_\nu\})$ such that for any $\varepsilon > 0$ one can find the number $\delta(\varepsilon)$ such that if $\rho_S(\{E_\nu, c_\nu\}, \{E_\nu, c_\nu\} + \delta\{E_\nu, c_\nu\}) \leqslant \delta(\varepsilon)$ then $\rho_V(\{V^{(1)}(x_i), u^{(1)}(x_i)\}, \{V^{(2)}(x_i), u^{(2)}(x_i)\}) < \varepsilon$, where ρ_S and ρ_V denote metrics functions for the spaces $\{E_\nu, c_\nu\} \subseteq \mathbb{R}^{2N-1}$ and $\{V(x_i), u(x_i)\} \subseteq \mathbb{R}^{2N-1}$, respectively.

3. Continuum limit

3.1. Preliminary remarks

In this section, we shall pass to the limit of the continuous variable x, i.e., to the limit $\Delta \to 0$ ($N \to \infty$) so that $\Delta N = \pi N/(N+1) \to \pi, x_m \to x$ in formulae (11), (12), (20) and (21). There are known (sufficient) conditions for the convergence of the difference scheme. This scheme must be numerically stable, unique and approximate the continuum problem. All the derivations below mainly concern approximation aspects. However, we need the theorem of numerical stability. The *regularization* technique resolves this problem in the following way: we must decrease the mesh width Δ and make the estimation of the spectral data more precise in a concordant manner. As an example, we can recall the standard difference approximation of the first-order differentiation operator

$$\frac{f(x_n) - f(x_{n-1})}{\Delta} \to \frac{\mathrm{d}f}{\mathrm{d}x}, \tag{24}$$

which is ill-posed but has the continuum limit. Let us give here the standard rules of the transitions from other finite-difference operators to their continuum counterparts:

$$\sum \Delta \to \int \mathrm{d}x, \tag{25}$$

$$\frac{f(x_{n+1}) - 2f(x_n) + f(x_{n-1})}{\Delta^2} \to \frac{\mathrm{d}^2 f}{\mathrm{d}x^2}. \tag{26}$$

Thus, the existence of the continuum limit may be substantiated by the hypothesis (based on the regularization possibilities) that we can choose (a very subtle fit) the mesh $\{x_0, x_1, \ldots, x_n, \ldots, x_{N+1}\}$ that would satisfy regularization properties (see above). As $\delta\{E_\nu, c_\nu\} \to 0$ and $\Delta(\delta\{E_\nu, c_\nu\}) \to 0$, our (difference) regularized approximate solutions tend in metrics ρ_V to the exact solutions of the continuous problem. In what follows, we shall mean, by the terms 'go over into ...', etc, the convergence in this metrics (or similar metrics for the solutions to the potential to recover). The metrics itself may be chosen, e.g., as follows: $\rho(x, y) = \sqrt{\sum_{k=1}^{2N-1}(y_k - x_k)^2}$. Most likely, however, a *uniform convergence* is valid. But this needs to be carefully examined (open problem).

Now let us look at the Parseval relation that takes, in the continuum limit, its usual form for the infinite-dimensional (Hilbert) space

$$\sum_{\mu=1}^{\infty} \overset{\circ}{c}{}_\mu^2 \, \overset{\circ}{\varphi}(x, \overset{\circ}{E}_\mu) \, \overset{\circ}{\varphi}(y, \overset{\circ}{E}_\mu) = \delta(x - y), \tag{27}$$

and the same is for the new regular solutions $\varphi(x, E)$.

In the continuum case, we have $\varphi(0, E) = 0$, $\varphi'(0, E) = 1$. Spectral weight factors are in this case, too, the coefficients of proportionality between normalized eigenfunctions and regular solutions. That is why they are also referred to as norming constants since the multiplication by $c_\nu = 1 \Big/ \int_0^\pi \varphi^2(x, E_\nu)\,\mathrm{d}x$ turns a regular solution (at $E = E_\nu$) into the normalized one,

$$\Psi'(x, E_\nu)|_{x=0} = c_\nu.$$

3.2. Passage to the continuum limit for the solutions and the potential

The expression for the transformed regular solutions has now the following form (using (25)):

$$\varphi(x, E_\nu) = \overset{\circ}{\varphi}(x, E_\nu) + \int_0^x K(x, y) \, \overset{\circ}{\varphi}(y, E_\nu)\,\mathrm{d}y, \tag{28}$$

and similarly

$$\varphi(x, E) = \overset{\circ}{\varphi}(x, E) + \int_0^x K(x, y) \, \overset{\circ}{\varphi}(y, E)\,\mathrm{d}y, \tag{29}$$

where $x \in [0, \pi]$. These formulae have just demonstrated the passage to the limit $\Delta \to 0$. For the kernel K of the operator (28) which transforms the solutions to the initial potential into the solutions to the new one (generalized shift operator), we have the continuum analogue of equation (12)—the inverse problem equation proper:

$$K(x, y) + Q(x, y) + \int_0^x K(x, z) Q(z, y)\,\mathrm{d}z = 0, \tag{30}$$

where the kernel Q is constructed from the unperturbed functions with the old and new spectral parameters (as in equation (10)):

$$Q(x, y) = \sum_\nu c_\nu^2 \, \overset{\circ}{\varphi}(x, E_\nu) \, \overset{\circ}{\varphi}(y, E_\nu) - \sum_\mu \overset{\circ}{c}{}_\mu^2 \, \overset{\circ}{\varphi}(x, \overset{\circ}{E}_\mu) \, \overset{\circ}{\varphi}(y, \overset{\circ}{E}_\mu). \tag{31}$$

For the continuous coordinate, expression (19) for K has a similar form

$$K(x, y) = -\sum_\nu c_\nu^2 \varphi(x, E_\nu) \, \overset{\circ}{\varphi}(y, E_\nu) + \sum_\mu \overset{\circ}{c}{}_\mu^2 \varphi(x, \overset{\circ}{E}_\mu) \, \overset{\circ}{\varphi}(y, \overset{\circ}{E}_\mu). \tag{32}$$

As we have carried out the passage to the continuum limit in solutions (11), one can also proceed to such a limit for the potential. In fact, the expressions for the potential coefficients

(20) and (21) were secondary with respect to (11), i.e., we can always derive them from the Schrödinger equation using the information about its solutions (see the section above). As has been shown, this procedure is substantially based upon the completeness relation which stands good for *any* Δ, including the continuum case. Moreover, we might use the continuum solution (29) and the Parseval relation (27) for the continuum potential to be derived. However, we choose the way of continuum passage in (20) and (21). Another point is that the continuum potential is *local*. Indeed, the us and V in each row of the discrete Sturm–Liouville operator are specified at the very neighbouring points x_n and x_{n+1} that merge if we pass to the continuum limit, which entails, in turn, superimposing the potential coefficients at one point: $V+2u$. The distinct feature of the local potential is that the limiting equation must determine it uniquely in contrast to (20) and (21) which could not uniquely specify us and Vs by reason of the 'nonlocal' interaction in the discrete case (we remember that there was required additional knowledge of $u(x_N)$ at the boundary of the interval for the uniqueness). But for the Schrödinger equation with a local potential, it is well known that the potential always occurs for the unique solution (with given boundary conditions) and vice versa. Thus, we can anticipate beforehand an expression for a unique specification of the local potential in the continuum case.

We shall now prove that, as $\Delta \to 0$, equations (20) and (21) go over, respectively, into

$$\{V_d(x) - \mathring{V}_d(y) + 2[u_d(x) - \mathring{u}_d(y)]\}K(x,y) = \frac{\partial^2}{\partial x^2}K(x,y) - \frac{\partial^2}{\partial y^2}K(x,y), \tag{33}$$

and

$$\begin{cases} \tilde{V}_d(x) - \mathring{V}_d(x) + \tilde{u}_d(x) - \mathring{u}_d(x) = 2\frac{\mathrm{d}}{\mathrm{d}x}K(x,x) \\ \{\tilde{V}_d(x) - \mathring{V}_d(x) + \tilde{u}_d(x) - \mathring{u}_d(x)\}K(x,x) \\ = \frac{\partial^2}{\partial x^2}K(x,y)\big|_{y=x} - \frac{\partial^2}{\partial y^2}K(x,y)\big|_{y=x}, \end{cases} \tag{34}$$

where $V_d(x) \equiv \lim_{\substack{\Delta\to 0 \\ m\to\infty}} V(x_m)$ and, analogously, $u_d(x) \equiv \lim_{\substack{\Delta\to 0 \\ m\to\infty}} u(x_m)$. The tilde sign stands for the potentials obtained in passing to the limit of the continuous coordinate in the solutions of equations (21).

In developing these equalities, it is useful to employ the diagonal terms $K(x_n, x_n)$ such that $K(x_{n+1}, x_n) - K(x_n, x_n) \sim O(\Delta)$. First of all, let us consider the term $(K(x_{m+1}, x_{m-1}) - K(x_m, x_{m-2}))/\Delta^2$ in (21). We add to and subtract from the expression in the numerator the term $K(x_{m-1}, x_{m-1}) - K(x_m, x_m)$. Then

$$\frac{K(x_{m+1}, x_{m-1}) - K(x_m, x_{m-2})}{\Delta^2} = \frac{K(x_{m+1}, x_{m-1}) + K(x_{m-1}, x_{m-1})}{\Delta^2} - \frac{K(x_m, x_m) + K(x_{m-1}, x_{m-1}) - K(x_m, x_m) + K(x_m, x_{m-2})}{\Delta^2} = \zeta.$$

Next, let us again add to and subtract from the new expression in the numerator the term $2K(x_m, x_{m-1})$:

$$\zeta = \frac{K(x_{m+1}, x_{m-1}) - 2K(x_m, x_{m-1}) + K(x_{m-1}, x_{m-1})}{\Delta^2} - \frac{K(x_m, x_m) - 2K(x_m, x_{m-1}) + K(x_m, x_{m-2})}{\Delta^2} + \frac{K(x_m, x_m) - K(x_{m-1}, x_{m-1})}{\Delta^2}.$$

The first two lines in this expression are the second derivatives with respect to the first and second arguments of $K(x, y)$ (see (26)). Hence, in the continuum limit they become

$$\frac{\partial^2}{\partial x^2}K(x,y)\bigg|_{y=x} - \frac{\partial^2}{\partial y^2}K(x,y)\bigg|_{y=x}.$$

The third fraction diverges as $\Delta \to 0$: $\Delta^{-1}\,\mathrm{d}K(x,x)/\mathrm{d}x$. As a result, we have

$$\frac{K(x_{m+1},x_{m-1})-K(x_m,x_{m-2})}{\Delta^2} \longrightarrow \frac{\partial^2}{\partial x^2}K(x,y)\bigg|_{y=x} - \frac{\partial^2}{\partial y^2}K(x,y)\bigg|_{y=x} + \Delta^{-1}\frac{\mathrm{d}}{\mathrm{d}x}K(x,x). \tag{35}$$

Likewise, it is not difficult to obtain that

$$\frac{K(x_{m+1},x_m)-K(x_m,x_{m-1})}{\Delta^2} = \frac{K(x_{m+1},x_m)-K(x_m,x_m)+K(x_m,x_m)-K(x_m,x_{m-1})}{\Delta^2}$$
$$\longrightarrow \Delta^{-1}\frac{\mathrm{d}}{\mathrm{d}x}K(x,x); \qquad \Delta \to 0. \tag{36}$$

In equation (20) we can see the finite-difference second derivative in an explicit form. So in the continuum case this equation becomes (33). If we introduce $V(x) \equiv V_d(x) + 2u_d(x)$ the term in front of $K(x,y)$ is simply the difference $V(x) - \overset{\circ}{V}(y)$. It is obvious that we introduced a local limiting potential which results from the limiting merging of V-diagonal and nearby u-diagonals.

Now let us multiply both sides of equations (21) for $n = m-1$ and $n = m$ by Δ. We sum the resulting equations and pass to the continuum limit. Then, by virtue of (35) and (36), we get the first equation in (34) valid to within $O(\Delta)$ (the multiplication by Δ has removed the divergence associated with Δ^{-1}).

The last equation in (34) is not obvious. Indeed, one would think that the term $u(x_m)$ must first be derived from the recurrence procedure (20) and (21) and only afterwards can the passage to the limit $\Delta \to 0$ be carried out—the procedure of a prodigious complexity. However, we have a way out: we simply take the sum of non-diverging terms (taking into account expression (35)) in the right-hand side of equation (21), $n = m-1$ to be zero in the continuum limit, i.e., we get the last equation in (34). This by no means contradicts the uniqueness of the sought limiting potential. First, this provides the limiting equation for $K(x,y)$ for the case $x = y$ which must exist, obviously. Second, by continuity, the factor $V_d(x) - \overset{\circ}{V}_d(y) + 2[u_d(x) - \overset{\circ}{u}_d(y)]$ in front of $K(x,y)$ must coincide with $\tilde{V}_d(x) - \overset{\circ}{V}_d(x) + \tilde{u}_d(x) - \overset{\circ}{u}_d(x)$ when $x = y$. In other words, that means that $V(x) = V_d(x) + 2u_d(x) = \tilde{V}_d(x) + \tilde{u}_d(x) + \overset{\circ}{u}_d(x)$, i.e., the solutions of (21) go over, in the limit $\Delta \to 0$, into *the same* local potential $V(x)$, which was clear beforehand. Hence, with the new definition for $V(x)$, we have from (33) and (34):

$$V(x) = \overset{\circ}{V}(x) + 2\frac{\mathrm{d}}{\mathrm{d}x}K(x,x). \tag{37}$$

This is the known result of recovering potential in the continuum case, which only now has become reproducible from a discrete mathematics.

Equations (33) and (34) can now be rewritten as

$$\begin{cases} \{V(x) - \overset{\circ}{V}(y)\}K(x,y) \\ = \frac{\partial^2}{\partial x^2}K(x,y) - \frac{\partial^2}{\partial y^2}K(x,y), \\ V(x) - \overset{\circ}{V}(x) = 2\frac{\mathrm{d}}{\mathrm{d}x}K(x,x). \end{cases} \tag{38}$$

This system (added by $K(0,0) = 0$) represents the classical Goursat problem (for determining $K(x,y)$) and its solvability follows from the well-known theorems.

The orthogonalization can also be started from the last vector $\varphi(\pi)$ with 'number' $x = \pi$ at the right boundary of the interval $[0,\pi]$. Then, instead of the solutions $\varphi(x)$, the solutions $f(x)$ will be used such that $f(\pi) = 0$, $f'(\pi) = 1$. The corresponding inverse problem equations, which can be associated with the orthogonalization 'from the right to the left', have

an analogous form as equations (28), (30), (31) and (37), only with other integration limits and a different sign in front of the derivative in the expression for $V(x)$:

$$f(x, E) = \overset{\circ}{f}(x, E) + \int_x^\pi K(x, y)\overset{\circ}{f}(y, E)\,\mathrm{d}y, \tag{39}$$

$$K(x, y) + Q(x, y) + \int_x^\pi K(x, z)\,Q(z, y)\,\mathrm{d}z = 0, \tag{40}$$

$$Q(x, y) = \sum_\nu \gamma_\nu^2 \overset{\circ}{f}(x, E_\nu)\overset{\circ}{f}(y, E_\nu) - \sum_\mu \overset{\circ}{\gamma}{}_\mu^2 \overset{\circ}{f}(x, \overset{\circ}{E}_\mu)\overset{\circ}{f}(y, \overset{\circ}{E}_\mu), \tag{41}$$

$$V(x) = \overset{\circ}{V}(x) - 2\frac{\mathrm{d}}{\mathrm{d}x}K(x, x). \tag{42}$$

Here, the symbol γ_ν stands for the spectral weight factor which is an analogue of c_ν. The only discrepancy is that γ_ν characterizes the behaviour of the νth eigenfunction at the right boundary

$$\Psi(x, E_\nu) = \gamma_\nu f(x, E_\nu); \qquad \gamma_\nu = \frac{\mathrm{d}}{\mathrm{d}x}\Psi(x, E_\nu)\bigg|_{x=\pi}.$$

Finally, let us mention about the eigenvalue inverse problem for the Schrödinger equation added by boundary conditions of arbitrary kind:

$$\Psi'(0) - g\Psi(0) = 0, \qquad \Psi'(\pi) + G\Psi(\pi) = 0. \tag{43}$$

Here, we also have analogous inversion equations, and as spectral weight factors there appear values of the corresponding eigenfunctions at the interval edges: $c_\nu = \Psi(0, E_\nu)$ or $\gamma_\nu = \Psi(\pi, E_\nu)$.

4. Conclusions

In the present paper, we carried out the derivation of main formulae of the inverse eigenvalue problem on the basis of its discrete approximation. Several statements of that problem have been developed by now; we selected such a statement in which it is possible to reproduce in a straightforward way the future structure of the limiting inversion procedure: the transition from a known system to the system with given spectral data (eigenvalues plus norming constants) but with unknown potential to be restored. The off-diagonal elements are introduced into the matrix Sturm–Liouville operator (three-diagonal matrix), which is consistent (in contrast to the previous works) with the problem statement involving this double set of spectral parameters. Finally, in comparison with the usual derivation of the continuum inversion equations, our development seems to be no more complicated. At the same time, the reader acquires the ability to track additional aspects of the formalism in more detail, in particular to look upon the operator transformation realizing the recovering procedure as the orthonormalization of the operator eigenvectors.

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