BVMs for computing Sturm–Liouville symmetric potentials ☆

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ABSTRACT

The paper deals with the numerical solution of inverse Sturm–Liouville problems with unknown potential symmetric over the interval $[0, \pi]$. The proposed method is based on the use of a family of Boundary Value Methods, obtained as a generalization of the Numerov scheme, aimed to the computation of an approximation of the potential belonging to a suitable function space of finite dimension. The accuracy and stability properties of the resulting procedure for particular choices of such function space are investigated. The reported numerical experiments put into evidence the competitiveness of the new method.

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1. Introduction

Inverse Sturm–Liouville problems (SLPs) consist of recovering the potential $q(x) \in L^2[0, \pi]$ from

$$-y'' + q(x)y = \lambda y, \quad x \in [0, \pi], \tag{1}$$

$$a_1 y(0) - a_2 y'(0) = 0, \quad |a_1| + |a_2| \neq 0, \tag{2}$$

$$b_1 y(\pi) - b_2 y'(\pi) = 0, \quad |b_1| + |b_2| \neq 0, \tag{3}$$

and the knowledge of suitable spectral data. They play an important role in several areas such as geophysics, engineering and mathematical-physics. The research concerning the development of numerical techniques for the approximation of their solution represents therefore a very active and interesting field of investigation.

The existence and uniqueness of the solution of an inverse SLP has been proved for several formulations of it among which we quote:

- The *two-spectrum* problem characterized by the knowledge of two sets of eigenvalues $\{\lambda_k^{(j)}\}_{k=1}^{\infty}$, $j = 1, 2$, corresponding to two SLPs sharing the first boundary condition (2) (BC in the sequel) and differing for the second one (3), [1];
- The *spectral function data* problem where the input consists of one spectrum $\{\lambda_k\}_{k=1}^{\infty}$ and the ratios $\{\|y_k\|_2^2/y_k^2(0)\}_{k=1}^{\infty}$ or $\{\|y_k\|_2^2/(y_k'(0))^2\}_{k=1}^{\infty}$ in the case $a_2 \neq 0$ or $a_2 = 0$, respectively. Here y_k denotes the eigenfunction corresponding to λ_k, [2];
- The *endpoint data* problem occurring when the spectrum of the SLP subject to Dirichlet BCs is known together with the terminal velocities $\kappa_k = \log(|y_k'(\pi)|/|y_k'(0)|)$, $k = 1, 2, \ldots$, [3];
- The *symmetric* problem for which a potential q satisfying

$$q(x) = q(\pi - x), \tag{4}$$

for all $x \in [0, \pi]$, has to be reconstructed from the knowledge of one spectrum corresponding to symmetric BCs (i.e. $a_1 b_2 + a_2 b_1 = 0$), [1].

The latter is the problem that we shall consider in this paper. It is known that, if $q \in L^2[0, \pi]$, the kth eigenvalue of (1)–(3) behaves asymptotically as

$$\lambda_k = \lambda_k(q) = \mu_k + \overline{q} + \delta_k(q), \tag{5}$$

where $\mu_k = O(k^2)$ depends only on the BCs of the SLP, $\overline{q} = \frac{1}{\pi} \int_0^\pi q(x)dx$ and $\{\delta_k(q)\}_{k=1}^\infty \in \ell^2$, [4]. This implies that, in addition to (4), the information concerning the variation of q for the symmetric problem are contained in the small terms $\delta_k(q)$.

Obviously, in the practice, the set of known eigenvalues is finite and usually consists of the first M ones. The matrix methods are therefore well-suited for the solution of inverse SLPs and among them the three-point scheme and the Numerov method are the most popular ones. In general, the matrix methods are based on the use of finite difference or finite element methods for the solution of ODEs over an assigned partition of $[0, \pi]$ frequently composed by:

$$x_i = ih, \quad i = 0, 1, \ldots, N+1, \quad h = \frac{\pi}{N+1}. \tag{6}$$

When applied for solving direct SLPs, such methods replace the continuous problem with a generalized matrix eigenvalue one of the form

$$A(q)\mathbf{y}^{(h)} = \lambda^{(h)}S(q)\mathbf{y}^{(h)}. \tag{7}$$

Here $\lambda^{(h)}$ is the approximation of one of the exact eigenvalues, $\mathbf{y}^{(h)}$ the corresponding numerical eigenfunction and the square matrices $A(q)$ and $S(q)$, besides the potential q, depend on the particular method and on the BCs of the SLP. As well-known the accuracy of the approximation $\lambda_k^{(h)}$ of λ_k deteriorates significantly for increasing values of the index k so that the discretization error of a matrix method inevitably swamps the term $\delta_k(q)$ in (5) with the exception of the first few indices. The application of the asymptotic (or algebraic) correction technique, introduced in [5,6] for the three-point formula and in [7–9] for the Numerov method, allows to greatly improve such eigenvalue estimates. It is based on the observation that the leading term in the discretization error is independent of the potential q. This has suggested to correct the estimate $\lambda_k^{(h)}$ by adding to it the term $\epsilon_k^{(h)} = \lambda_{k,0} - \lambda_{k,0}^{(h)}$ where $\lambda_{k,0}$ and $\lambda_{k,0}^{(h)}$ are the kth exact and numerical eigenvalues corresponding to the potential $q(x) \equiv 0$, respectively.

Among the first successful algorithms for the solution of symmetric inverse SLPs subject to Dirichlet BCs (DBCs from now on) we mention the ones proposed in [10–12]. In particular, the method in [12] used the three-point scheme for which the coefficient matrix $A(q)$ in (7) is symmetric and tridiagonal while $S(q)$ is the identity matrix. The number of meshpoints N in (6) was set equal to the number M of known eigenvalues so that $A(q)$ was of size M. An inverse matrix eigenvalue problem for a centrosymmetric $A(q)$ was then solved with the very important shrewdness, derived from the asymptotic correction technique, of taking $\lambda_k - \epsilon_k^{(h)}$ as kth reference eigenvalue instead of simply λ_k for each k. From the knowledge of $A(q)$ an approximation $\mathbf{q}_{in}^{(h)}$ of $\mathbf{q}_{in} = (q(x_1), q(x_2), \ldots, q(x_N))^T$ was then easily computed. The defect of this method, however, was the use of the entire numerical spectrum which even after the application of the asymptotic correction presents discretization error of order $O(1)$ in the largest eigenvalues.

A more reliable method for the same type of inverse SLP was then proposed in [13] which still used the three-point formula but involved only the first half of the computed numerical eigenvalues. In this case, in fact, N was set equal to $2M$ and the approximation $\mathbf{q}_{in}^{(h)}$ of $\mathbf{q}_{in}$ was computed by solving the system of nonlinear equations

$$\lambda_k^{(h)} - \lambda_k + \epsilon_k^{(h)} = 0, \quad k = 1, 2, \ldots, M, \tag{8}$$

where $\lambda_k^{(h)} = \lambda_k^{(h)}(q) = \lambda_k^{(h)}\left(\mathbf{q}_{in}^{(h)}\right)$ represents the kth eigenvalue of $A(q)$. By virtue of the symmetry condition (4), the constraint $\mathbf{q}_{in}^{(h)} = \widehat{J}\mathbf{q}_{in}^{(h)}$ was imposed on $\mathbf{q}_{in}^{(h)}$ where $\widehat{J}$ denotes the anti-identity matrix. The unknowns in (8) were therefore the first M entries of $\mathbf{q}_{in}^{(h)}$ and a modified Newton method was used for solving such system. The convergence properties of the latter method were also studied in details in [13] for q "sufficiently" close to a constant.

A similar approach for solving symmetric inverse SLPs has been considered in [14,15] where the Numerov method has been used in place of the three-point formula. Moreover, in [15] the treatment of the Neumann boundary conditions (NBCs in the sequel) has been discussed. It must be said that while this extension is straightforward for the three-point method, the same definitely does not happen for the Numerov one.

As final reference for the currently available numerical techniques for the problem under consideration, we mention the one recently proposed in [16]. In this case the continuous problem is reformulated as a system of first order ODEs and a family of Boundary Value Methods (BVMs) obtained from the Obrechkoff formulas in conjunction with the asymptotic correction technique is applied for the solution of the direct problem (see also [17,18]). The resulting generalized eigenvalue problem (7) has size $4M - 4$ with $N = 2M - 3$ and the Newton method is used for solving (8).

In this paper, for the solution of the symmetric inverse problem, we consider the application of the BVMs introduced in [19,20] for the direct one. These schemes are obtained as a generalization of the Numerov method and provide competitive results with respect to the latter improved with the asymptotic correction technique. Moreover, in [20] a compact formulation of the corresponding generalized eigenvalue problem (7) is given which covers all possible types of BCs (2) and (3). With respect to the methods in [13–16], a relevant difference of our procedure is constituted by the fact that we look for an approximation of the unknown potential of the form $q^{(h)}(x) = \phi(x, \mathbf{c}^{(h)})$ where, for any $\mathbf{c} = (c_1, c_2, \ldots, c_L)^T$, $\phi(x, \mathbf{c}) = \sum_{j=1}^L c_j \phi_j(x)$ being $\{\phi_j(x)\}_{j=1}^L$ a set of symmetric linearly independent functions. The chosen value of L usually depends on

the number of known eigenvalues while the number of meshpoints N in (6) is left free. A system of nonlinear equations analogous to (8) is formulated where now $\lambda_k^{(h)} = \lambda_k^{(h)}(\phi(\cdot, \mathbf{c}))$. This is solved by means of a Newton type method if $L = M$ or in the least-square sense if $L < M$, i.e. $\mathbf{c}^{(h)}$ is determined so that $\sum_{k=1}^{M} \left(\lambda_k^{(h)}(\phi(\cdot, \mathbf{c})) - \lambda_k + \epsilon_k^{(h)} \right)^2$ is minimized. We observe that the previous summation represents a numerical version of the functional introduced by Röhrl in [21] and already used in [22].

The paper is organized as follows. In Section 2 we recall the main facts concerning the BVMs introduced in [19,20] for the solution of direct SLPs with general BCs. In Section 3 the procedure for the reconstruction of the unknown potential is described and the properties of the method used with $M = L$ are discussed for some function spaces. In Section 4 an upper bound for the error $\|q - q^{(h)}\|_2$ is derived which separates the contribute due to the discretization operated through the BVMs from the one due to the function space used. Finally, in Section 5 some numerical results are reported which proves the effectiveness of the new method.

2. Boundary value methods for the direct problem

Recently a family of BVMs has been proposed for the approximation of the eigenvalues of regular SLPs subject to general BCs [19,20]. According to the usual structure of BVMs, the considered $2v$-step ($v \geqslant 1$) scheme approximates a second order differential equation of special type

$$y'' = f(x, y), \quad x \in [0, \pi],$$

over the mesh (6) by using the following set of Linear Multistep Formulas

$$\frac{y_{s-1} - 2y_s + y_{s+1}}{h^2} = \sum_{i=0}^{2v} \beta_i^{(s)} f_i, \quad s = 1, 2, \ldots, v - 1, \tag{9}$$

$$\frac{y_{n-1} - 2y_n + y_{n+1}}{h^2} = \sum_{i=0}^{2v} \beta_i^{(v)} f_{n+i-v}, \quad n = v, v + 1, \ldots, N + 1 - v, \tag{10}$$

$$\frac{y_{m-1} - 2y_m + y_{m+1}}{h^2} = \sum_{i=0}^{2v} \beta_i^{(s)} f_{m-s+i}, \quad s = v + 1, \ldots, 2v - 1, \quad m = N + 1 + s - 2v, \tag{11}$$

where $y_i \approx y(x_i)$ and $f_i = f(x_i, y_i)$. The formula in (10) is named *main method* while those in (9) and (11) are called *initial* and *final additional methods*, respectively, [17]. For each $s = 1, 2, \ldots, 2v - 1$, the coefficients $\beta_i^{(s)}$ are uniquely determined by imposing the sth formula to have order at least $2v + 1$. As proved in [19], the so-obtained composite scheme (9)–(11) turns out to be symmetric, namely $\beta_i^{(s)} = \beta_{2v-i}^{(2v-s)}, i = 0, 1, \ldots, 2v, s = 1, 2, \ldots, v$. In particular, the main formula, which is the one corresponding to $s = v$, is a symmetric Linear Multistep Formula and this implies that its order of accuracy is actually $p = 2v + 2$ since it must be even and not less than $2v + 1$ by construction. In the sequel, when speaking about the order of the composite scheme we will refer to the order p of its main formula. It is important to remark that when $v = 1$ the proposed scheme reduces to the Numerov method.

When applied to (1), the Eqs. (9)–(11) can be written in matrix form as

$$\widetilde{A}(q)\tilde{\mathbf{y}}^{(h)} \equiv \left(-\frac{1}{h^2} \widetilde{T} + \widetilde{B}^{(v)} \widetilde{Q} \right) \tilde{\mathbf{y}}^{(h)} = \lambda^{(h)} \widetilde{B}^{(v)} \tilde{\mathbf{y}}^{(h)}, \tag{12}$$

where $\lambda^{(h)}$ represents the approximation of an exact eigenvalue, $\tilde{\mathbf{y}}^{(h)} = (y_0, y_1, \ldots, y_{N+1})^T$ and, by denoting with $\widehat{J}$ the anti-identity matrix of size N, with $\mathbf{e}_1^{(N)}$ the first unit vector in $\mathbb{R}^N$ and by posing $q_i = q(x_i)$ for each i, the matrices $\widetilde{T}$ and $\widetilde{Q}$ are given by:

$$\widetilde{T} = \left(\mathbf{e}_1^{(N)} \middle|\, T \,\middle| \widehat{J}\mathbf{e}_1^{(N)} \right) = \begin{pmatrix} 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 & 1 \end{pmatrix} \in \mathbb{R}^{N \times (N+2)},$$

$$\widetilde{Q} = \begin{pmatrix} q_0 & & \\ & Q & \\ & & q_{N+1} \end{pmatrix}, \quad Q = \text{diag}(q_1, \ldots, q_N).$$

Finally, the matrix $\widetilde{B}^{(v)}$ is defined as

$$\widetilde{B}^{(v)} = \left(\boldsymbol{\beta}_0^{(v)} \middle| B^{(v)} \middle| \widehat{J}\boldsymbol{\beta}_0^{(v)} \right) \in \mathbb{R}^{N \times (N+2)}, \quad \boldsymbol{\beta}_0^{(v)} \in \mathbb{R}^N,$$

with

$$\boldsymbol{\beta}_0^{(v)} = \left(\beta_0^{(1)}, \beta_0^{(2)}, \ldots, \beta_0^{(v)}, 0, \ldots, 0\right)^T \in \mathbb{R}^N,$$

$$B^{(v)} = \begin{pmatrix}
\beta_1^{(1)} & \cdots & \beta_v^{(1)} & \cdots & \beta_{2v-1}^{(1)} & \beta_{2v}^{(1)} \\
\vdots & & \vdots & & \vdots & \vdots \\
\beta_1^{(v-1)} & \cdots & \beta_v^{(v-1)} & \cdots & \beta_{2v-1}^{(v-1)} & \beta_{2v}^{(v-1)} \\
\beta_1^{(v)} & \cdots & \beta_v^{(v)} & \cdots & \beta_1^{(v)} & \beta_0^{(v)} \\
\beta_0^{(v)} & \beta_1^{(v)} & \cdots & \beta_v^{(v)} & \cdots & \beta_1^{(v)} & \beta_0^{(v)} \\
& \ddots & \ddots & & \ddots & & \ddots & \ddots \\
& & \beta_0^{(v)} & \beta_1^{(v)} & \cdots & \beta_v^{(v)} & \cdots & \beta_1^{(v)} & \beta_0^{(v)} \\
& & & \beta_0^{(v)} & \beta_1^{(v)} & \cdots & \beta_v^{(v)} & \cdots & \beta_1^{(v)} \\
& & & \beta_{2v}^{(v-1)} & \beta_{2v-1}^{(v-1)} & \cdots & \beta_v^{(v-1)} & \cdots & \beta_1^{(v-1)} \\
& & & \vdots & \vdots & & \vdots & & \vdots \\
& & & \beta_{2v}^{(1)} & \beta_{2v-1}^{(1)} & \cdots & \beta_v^{(1)} & \cdots & \beta_1^{(1)}
\end{pmatrix}_{N \times N}.$$

Concerning the discretization of the BC (2), the $(2v + 2)$-step Forward Differentiation Formula of order $2v + 2$ and coefficients $\{\alpha_i\}_{i=0}^{2v+2}$ is used for the approximation of $y'(0)$, i.e.

$$\sum_{i=0}^{2v+2} \alpha_i y(x_i) = hy'(0) + \tau_L, \quad \tau_L = O\left(h^{2v+3}\right).$$

By neglecting τ_L, the following approximation of the first BC is therefore obtained

$$a_2 \sum_{i=0}^{2v+2} \alpha_i y_i = ha_1 y_0 \iff y_0 = \frac{a_2}{ha_1 - a_2\alpha_0} \sum_{i=1}^{2v+2} \alpha_i y_i = \gamma_L \boldsymbol{\alpha}^T \mathbf{y}^{(h)}, \tag{13}$$

where $\mathbf{y}^{(h)} = (y_1, y_2, \ldots, y_N)^T$,

$$\gamma_L = \frac{a_2}{ha_1 - a_2\alpha_0} \quad \text{and} \quad \boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_{2v+2}, 0, \ldots, 0)^T \in \mathbb{R}^N.$$

Similarly, the $(2v + 2)$-step Backward Differentiation Formula of order $2v + 2$ and coefficients $\hat{\alpha}_i = -\alpha_{2v+2-i}, i = 0, 1, \ldots, 2v + 2$, is applied for discretizing the BC (3) thus getting

$$y_{N+1} = -\gamma_R \left(\boldsymbol{\alpha}^T \widehat{J}\right) \mathbf{y}^{(h)}, \quad \gamma_R = \frac{b_2}{hb_1 + b_2\alpha_0}. \tag{14}$$

Now, combining (12) with (13) and (14), after some computation one obtains that the coefficient matrices $A(q)$ and $S(q) = S$ of the generalized eigenvalue problem (7) the considered BVM generates for the solution of the direct SLP (1)–(3) are given by:

$$A(q) = -\frac{1}{h^2} T + B^{(v)} Q + \gamma_L \left(-\frac{1}{h^2} \mathbf{e}_1^{(N)} + q_0 \boldsymbol{\beta}_0^{(v)}\right) \boldsymbol{\alpha}^T - \gamma_R \widehat{J} \left(-\frac{1}{h^2} \mathbf{e}_1^{(N)} + q_{N+1} \boldsymbol{\beta}_0^{(v)}\right) \boldsymbol{\alpha}^T \widehat{J}, \tag{15}$$

$$S = B^{(v)} + \gamma_L \boldsymbol{\beta}_0^{(v)} \boldsymbol{\alpha}^T - \gamma_R \widehat{J} \boldsymbol{\beta}_0^{(v)} \boldsymbol{\alpha}^T \widehat{J}, \tag{16}$$

respectively. Concerning the convergence of the so-obtained approximations for the kth eigenvalue, in [19,20] it has been proved that if kh is "sufficiently" small and $v > 1$ one has

$$|\lambda_k - \lambda_k^{(h)}| \sim O\left(k^{p+1} h^{p-\frac{1}{2}}\right) + O(k^{p+2} h^p), \quad p = 2v + 2. \tag{17}$$

By virtue of this result the proposed BVMs are able to provide substantially more accurate estimates of the eigenvalues λ_k with respect to those given by the corrected Numerov method at least for the lowest indexes k. Moreover, there is numerical evidence that the asymptotic correction is successful in improving the eigenvalue approximations provided by the former methods and this extends the range of values of k for which they are competitive with the latter one.

In the sequel, in order to better emphasize the dependence of λ_k, $\lambda_k^{(h)}$ and of $\mathbf{y}_k^{(h)}$ on the potential q, we shall denote them as $\lambda_k(q)$, $\lambda_k^{(h)}(q)$ and $\mathbf{y}_k^{(h)}(q)$, respectively.

Remark 1. For later reference, we observe that if the potential is shifted by a constant ϑ, i.e. $q(x)$ is replaced with $q(x) + \vartheta$, the matrix S does not vary while $A(q(x) + \vartheta) = A(q(x)) + \vartheta S$. This implies that, analogously to the continuous problem, $\lambda_k^{(h)}(q(x) + \vartheta) = \lambda_k^{(h)}(q(x)) + \vartheta$ with the same corresponding eigenvector, see (7).

Remark 2. A drawback of the proposed schemes is the fact that when the order p of the method increases the spectrum of the matrix pencil $(A(q), S)$ may contain some few couples of complex conjugate eigenvalues. This is in contrast with the peculiarity of a regular SLP with a real-valued potential q of having a real spectrum. A possible strategy for overcoming such inconsistency is that of taking a finer mesh near the extremes of the interval of integration, namely in discretizing the interval $[0, \pi]$ as follows:

$$x_0 = 0, \quad x_i = x_{i-1} + h_i, \quad i = 1, 2, \ldots, N+1, \quad x_{N+1} = \pi,$$

where

$$\begin{cases} h_1 \leqslant h_2 \leqslant \cdots \leqslant h_\eta, \\ h_i = h_\eta, & i = \eta + 1, \ldots, N - \eta + 1, \\ h_i = h_{N-i+2}, & i = N - \eta + 2, \ldots, N + 1. \end{cases}$$

The choice of the nonuniformly distributed nodes can be made in several ways. For example, they can be derived starting from the zeros of suitable orthogonal polynomials of degree $2\eta + 1$, or arranged with a geometric progression distribution (see [19,20] for further details).

3. Reconstruction of symmetric potentials

The first step of the numerical procedure we have studied for solving the inverse SLP (1)–(3) consists in selecting a subspace Φ of $L^2[0, \pi]$ composed by symmetric functions and of finite dimension L inside of which we look for an approximation of the exact potential $q(x)$. In particular, Φ is chosen so that the constant functions belong to it since a reasonable basic property a "good" method for inverse SLPs must satisfy is that of allowing the exact reconstruction of constant potentials. As a matter of fact, all matrix methods improved with the asymptotic correction technique solve exactly direct SLPs with such potentials.

The outline of our method is the following. Let us denote with

$$\Lambda = (\lambda_1, \lambda_2, \ldots, \lambda_M)^T,$$

the vector containing the input data of the problem and, for each $\phi \in \Phi$, let us collect into

$$\Lambda(\phi) = (\lambda_1(\phi), \lambda_2(\phi), \ldots, \lambda_M(\phi))^T, \tag{18}$$

the exact eigenvalues of the SLP (1)–(3) with potential ϕ and into

$$\Lambda^{(h)}(\phi) = \left(\lambda_1^{(h)}(\phi), \lambda_2^{(h)}(\phi), \ldots, \lambda_M^{(h)}(\phi) \right)^T, \tag{19}$$

the corresponding numerical approximations provided by the (2ν)-step BVM with ν a priori fixed. In addition, let $E^{(h)} = \left(\epsilon_1^{(h)}, \epsilon_2^{(h)}, \ldots, \epsilon_M^{(h)} \right)^T$ be the vector containing the correction terms in (8) associated to the selected BVM and to the BCs of the SLP. We then take as approximation of the exact potential the function $q^{(h)} \in \Phi$ for which the corresponding corrected numerical eigenvalues better approximate in the least-square sense the reference ones, i.e.

$$q^{(h)}(x) = \arg\min_{\phi \in \Phi} G^{(h)}(\phi),$$

where $G^{(h)}(\phi) = \|\Lambda^{(h)}(\phi) - \Lambda + E^{(h)}\|_2^2$. We observe that, as $h \searrow 0$, $G^{(h)}(\phi)$ approaches the Röhrl functional $\|\Lambda(\phi) - \Lambda\|_2^2$ introduced and analyzed in [21].

By considering that the function space Φ is chosen of finite dimension L, in practice we fix a suitable basis for Φ, say

$$\mathcal{B} = \{\phi_1(x), \phi_2(x), \ldots, \phi_L(x)\}, \tag{20}$$

with $\Phi = \text{span}(\mathcal{B})$, and we compute the coefficients of the representation of $q^{(h)}(x)$ with respect to such basis. This means that if we define

$$\phi(x, \mathbf{c}) = \sum_{j=1}^{L} c_j \phi_j(x),$$

$$F^{(h)}(\mathbf{c}, \Omega) = \Lambda^{(h)}(\phi(x, \mathbf{c})) - \Omega, \tag{21}$$

for each $\mathbf{c} = (c_1, c_2, \ldots, c_L)^T$ and each $\Omega \in \mathbb{R}^M$, then

$$q^{(h)}(x) = \phi(x, \mathbf{c}^{(h)}), \tag{22}$$

where $\mathbf{c}^{(h)}$ solves in the least-square sense the system of M nonlinear equations, analogous to that in (8),

$$F^{(h)}\left(\mathbf{c}, \Lambda - E^{(h)} \right) = \Lambda^{(h)}(\phi(x, \mathbf{c})) - \Lambda + E^{(h)} = \mathbf{0}, \tag{23}$$

being from now on $\mathbf{0}$ the zero vector of suitable size depending on the context.

Remark 3. If the SLP is subject to DBCs the method in [14] is a particular instance of our procedure corresponding to the following choices: $p = 4$, $N = 2M$, $L = M$, and for each $i, j = 1,2,\ldots,L$, $\phi_j(x)$ is such that $\phi_j(x_i) = 1$ if $i = j$, $N + 1 - j$, and $\phi_j(x_i) = 0$ otherwise. In this setting, the approach is that of solving (23) exactly since the number of unknowns M of such system equals the number L of its nonlinear equations. Similar correspondences can be found with the methods in [13,16] via some suitable adjustments.

Concerning the effective computation of $\mathbf{c}^{(h)}$ standard nonlinear optimization methods like the Gauss–Newton or the Levenberg–Marquardt methods with line search can be used [23–25].

Alternatively, when $M = L$, the classical Newton method can be applied for solving (23). Nevertheless, in order to reduce the computational cost of the procedure, the use of the modified Newton method is frequently preferred which has good convergence properties if the potential is assumed to be "sufficiently" close to a constant, [13–15]. The corresponding recurrence relation is given by:

$$\mathbf{c}_{r+1}^{(h)} = \mathbf{c}_r^{(h)} - \left(J^{(h)}(\mathbf{0})\right)^{-1} F^{(h)}\left(\mathbf{c}_r^{(h)}, \Lambda - E^{(h)}\right), \quad r = 0, 1, 2, \ldots, \tag{24}$$

with $\mathbf{c}_0^{(h)}$ a suitable initial approximation and $J^{(h)}(\mathbf{0})$ the Jacobian matrix

$$J^{(h)}(\mathbf{c}) = \frac{\partial F^{(h)}\left(\mathbf{c}, \Lambda - E^{(h)}\right)}{\partial \mathbf{c}} = \frac{\partial \Lambda^{(h)}(\phi(x,\mathbf{c}))}{\partial \mathbf{c}}, \tag{25}$$

evaluated at $\mathbf{c} = \mathbf{0}$. Clearly, the iteration (24) is well defined provided $J^{(h)}(\mathbf{0})$ is nonsingular. Now, if we assume that the coefficient matrix S in (16), which is constant with respect to $\mathbf{c}$, is nonsingular, $\lambda_k^{(h)}(\phi(x,\mathbf{c}))$ is the kth eigenvalue of $S^{-1}A(\phi(x,\mathbf{c}))$, see (7), where the matrix $A(\phi(x,\mathbf{c}))$ in (15) can be decomposed as

$$A(\phi(x,\mathbf{c})) = A_0 + \sum_{j=1}^{L} c_j A_j,$$

with $A_0 = -h^{-2}\left(T + \gamma_L \mathbf{e}_1^{(N)} \boldsymbol{\alpha}^T - \gamma_R \widehat{J} \mathbf{e}_1^{(N)} \boldsymbol{\alpha}^T \widehat{J}\right)$ and

$$A_j = B^{(v)}\begin{pmatrix} \phi_j(x_1) & & \\ & \ddots & \\ & & \phi_j(x_N) \end{pmatrix} + \gamma_L \phi_j(x_0)\boldsymbol{\beta}^{(v)}\boldsymbol{\alpha}^T - \gamma_R \phi_j(x_{N+1})\widehat{J}\boldsymbol{\beta}^{(v)}\boldsymbol{\alpha}^T \widehat{J}.$$

As a consequence, see (19), it is not difficult to verify that, for any M and L, the entries of the Jacobian (25) are given by the classical formula

$$\left(J^{(h)}(\mathbf{c})\right)_{kj} = \frac{\left\langle \mathbf{v}_k^{(h)}(\phi(x,\mathbf{c})), S^{-1}A_j\mathbf{y}_k^{(h)}(\phi(x,\mathbf{c}))\right\rangle}{\left\langle \mathbf{v}_k^{(h)}(\phi(x,\mathbf{c})), \mathbf{y}_k^{(h)}(\phi(x,\mathbf{c}))\right\rangle},$$

being $\langle \cdot, \cdot \rangle$ the standard scalar product and $\mathbf{y}_k^{(h)}(\phi(x,\mathbf{c}))$ and $\mathbf{v}_k^{(h)}(\phi(x,\mathbf{c}))$ right and left eigenvectors of $S^{-1}A(\phi(x,\mathbf{c}))$ corresponding to $\lambda_k^{(h)}(\phi(x,\mathbf{c}))$, respectively.

Some considerations have to be made at this point concerning the choice of the function space Φ and of its set of basis functions $\mathcal{B}$. With reference to the former choice, standard arguments from the approximation theory, like the regularity and the flexibility of the approximating functions, have been adopted and the accuracy of the approximation $q^{(h)}(x) \approx q(x)$ obtained clearly depends on this choice. In determining the performance of the overall procedure, however, the selection of $\mathcal{B}$ turns out to be of no minor relevance. The Jacobian $J^{(h)}(\mathbf{c})$, in fact, depends on $\mathcal{B}$ and the properties of such matrix determine the stability of the method with respect to perturbations on the input data or perturbations due to the use of the finite precision arithmetic. A general discussion of such properties, however, is rather difficult. Nevertheless, if we assume from now on that the potential to be reconstructed is "sufficiently" close in some norm to a constant then $J^{(h)}(\mathbf{0})$ represents a "good" model for carrying out an analysis of the stability of the method (observe that if $\phi(x,\tilde{\mathbf{c}})$ is constant then from Remark 1 one deduces $\mathbf{y}_k^{(h)}(\phi(x,\tilde{\mathbf{c}})) = \mathbf{y}_k^{(h)}(\phi(x,\mathbf{0}))$, $\mathbf{v}_k^{(h)}(\phi(x,\tilde{\mathbf{c}})) = \mathbf{v}_k^{(h)}(\phi(x,\mathbf{0}))$ and, consequently, $J^{(h)}(\tilde{\mathbf{c}}) = J^{(h)}(\mathbf{0})$). In addition, when $M = L$ the convergence properties of the iterative method used for solving (23) like, for instance, the modified Newton one are strictly related to the conditioning of $J^{(h)}(\mathbf{0})$.

As the notation used underline, the previous matrix depends on the discretization stepsize h of the BVM. Nevertheless, unlike the methods in [13–16], in our case we have the freedom of choosing h arbitrarily small independently of the number M of known eigenvalues. We observe that $\Lambda^{(h)}(\phi(x,\mathbf{c}))$ converges to $\Lambda(\phi(x,\mathbf{c}))$ as $h \searrow 0$ for any $\mathbf{c}$ and from now on we shall assume that

$$\lim_{h\to 0} J^{(h)}(\mathbf{0}) = \lim_{h\to 0} \frac{\partial \Lambda^{(h)}(\phi(x,\mathbf{c}))}{\partial \mathbf{c}} = \left.\frac{\partial \Lambda(\phi(x,\mathbf{c}))}{\partial \mathbf{c}}\right|_{\mathbf{c}=\mathbf{0}} \equiv J(\mathbf{0}), \tag{26}$$

whose entries are given by Röhrl [21]

$$(J(\mathbf{0}))_{kj} = \frac{\int_0^\pi y_k^2(x)\phi_j(x)dx}{\int_0^\pi y_k^2(x)dx}, \quad k = 1, \ldots, M, \quad j = 1, \ldots, L, \tag{27}$$

being $y_k(x)$ the kth exact eigenfunction for the SLP with zero potential and the same BCs. This assumption is supported by the results of some numerical experiments we have conducted with the function spaces Φ described in the following subsections. In the sequel, we will therefore refer to the limit Jacobian $J(\mathbf{0})$ when talking about the stability of the method.

Before proceeding, we mention that similar function spaces have been used also in [26].

3.1. Trigonometric polynomials

It is known that the asymptotic estimates (5) for the Dirichlet eigenvalues for large k specify to, see [3],

$$\lambda_k(q) = k^2 + \bar{q} - \frac{1}{\pi}\int_0^\pi q(x)\cos(2kx)dx + O(1/k) \equiv \xi_k^{(D)}(q) + O(1/k), \tag{28}$$

so that, as discussed in [13], the informations in them contained are related to the coefficients of the Fourier cosine series of q. In addition, in [15], the following eigenvalue estimates

$$\lambda_k(q) \sim (k-1)^2 + \bar{q} + \frac{1}{\pi}\int_0^\pi q(x)\cos(2(k-1)x)dx = \xi_k^{(N)}(q) \tag{29}$$

are given for large k when talking about the solution of symmetric inverse SLPs with NBCs. In the same paper, it is therefore argued that also such eigenvalues give an approximation to the truncated Fourier cosine series of q.

The previous two estimates suggest to consider the space Φ constituted by the symmetric trigonometric polynomials with coordinate functions given by:

$$\phi_j(x) = \cos(2(j-1)x), \quad j = 1, 2, \ldots, L, \tag{30}$$

which have been already successfully used in the derivation of the methods proposed in [10,27].

Clearly, in this case the best approximation in L_2-norm of q that we can obtain is represented by its truncated Fourier cosine series.

The limit Jacobian (26) associated to (30) have a very simple structure if the SLP is subject to DBCs or to NBCs. In more details, the eigenfunctions for the former conditions and $q(x) \equiv 0$ are $y_k(x) = \sin(kx)$, $k = 1, 2, \ldots$, so that from (27) after some computations one verifies that the only nonzero entries of $J(\mathbf{0})$ are given by:

$$(J(\mathbf{0}))_{k1} = 1, \quad k = 1, 2, \ldots, M,$$
$$(J(\mathbf{0}))_{j-1j} = -\frac{1}{2}, \quad j = 2, 3, \ldots, \min\{L, M+1\}. \tag{31}$$

For the NBCs and zero potential, instead, the eigenfunctions are known to be $y_k(x) = \cos((k-1)x)$, $k = 1, 2, \ldots$, and the Jacobian $J(\mathbf{0})$ corresponding to (30) is lower triangular with nonzero entries given by:

$$(J(\mathbf{0}))_{k1} = 1, \quad k = 1, 2, \ldots, M, \quad (J(\mathbf{0}))_{jj} = \frac{1}{2}, \quad j = 2, 3, \ldots, \min\{L, M\}. \tag{32}$$

In both the previous cases, when $M = L$ there is numerical evidence that $J^{(h)}(\mathbf{0})$ rapidly approaches $J(\mathbf{0})$ as h goes to zero and the same happens for their inverses. For the computation of the coefficient vector $\mathbf{c}^{(h)}$ in (22) the very simple structure of the limit matrix $J(\mathbf{0})$ suggests therefore to apply the modified Newton method in (24) with $J^{(h)}(\mathbf{0})$ replaced by $J(\mathbf{0})$. The convergence properties of the so-obtained iterative procedure turn out to be very satisfactory in all our experiments. Moreover, it is not difficult to verify that the spectral condition number of $J(\mathbf{0})$, say $\kappa(J(\mathbf{0}))$, grows linearly with respect to M.

Finally, it is worth to mention that for SLPs subject to more general BCs, the limit Jacobian $J(\mathbf{0})$ corresponding to (30) is not known in closed form since the same holds for the exact eigenfunctions. Nevertheless, when $M = L$, the behaviour of $\kappa(J^{(h)}(\mathbf{0}))$ observed is still $O(M)$.

3.2. Algebraic polynomials

A second function space to be considered is surely represented by the algebraic polynomials symmetric with respect to $\frac{\pi}{2}$ and, actually, this has been our first choice in chronological order. At the time being, however, the results obtained with this choice are definitely negative in terms of stability properties of the numerical procedure. When $M = L$, in fact, the condition number of the limit Jacobian (26) associated to different sets of basis functions, like the shifted and scaled Legendre and Chebyschev polynomials of even degree, grows very quickly with M.

In this situation, it is evident that with this function space if we set $L = M$ then we may get an accurate approximation of the unknown potential only if the first few eigenvalues contain almost all the information about it and the given input eigenvalues M is very small. Alternatively, one may set $L \ll M$ and solve (23) in the least-square sense.

Anyway, it must be said that we cannot exclude that there exists a set of basis functions, which we have not yet considered, such that the stability properties of the method becomes acceptable, say a linear or at most quadratical growth with

respect to M of the conditioning of the limit Jacobian (26) when $M = L$. In our opinion, however, the cause of its instability is intrinsic to the function space since the use of polynomials of very high degree is usually not recommended. This is the motivation which has led us to consider the function space described in the following subsection.

3.3. Cubic spline functions

It is well-known that many of the most well established methods for function approximations are based on the use of cubic spline functions [28]. This is due to their peculiarity of combining flexibility with almost always sufficient smoothness properties. By virtue of this fact, the third function space we have considered is constituted by the cubic spline functions symmetric with respect to $\pi/2$. In this context, the most natural choice is surely represented by the ones defined over a uniform partition Δ of $[0, \pi]$ with a set of symmetric basis functions derived from the B-spline basis.

In more details, the first choice of spline function space of size L that we have considered is the following. The partition Δ has been fixed as

$$\Delta : 0 = t_0 < t_1 < \cdots < t_{2L-4} = \pi;$$
$$t_i = t_0 + ih_t, \quad i = 0, 1, \ldots, 2L - 4, \quad h_t = \frac{t_{2L-4} - t_0}{2L - 4}, \tag{33}$$

and, by denoting with $\{\psi_i(x)\}_{i=1}^{2L-1}$ the B-spline basis of order four for the knot sequence $t_i = t_0 + ih_t$, $i = -3, -2, \ldots, 2L-1$, the basis functions in (20) are set as

$$\phi_i(x) = \frac{\hat{\phi}_i(x)}{\int_0^\pi \hat{\phi}_i(x) dx}, \quad \hat{\phi}_i(x) = \psi_i(x) + \psi_{2L-i}(x), \quad i = 1, 2, \ldots, L. \tag{34}$$

Unfortunately, this straightforward approach does not give positive results from the point of view of the stability of the obtained method. When $M = L$, in fact, the condition number of $J(\mathbf{0})$ grows as $O(M^4)$ for DBCs and as $O(M^2)$ for NBCs. This behaviour has been observed experimentally and the obtained estimates for the rate of growth of $\kappa(J(\mathbf{0}))$ have been reported in Table 1 where this method has been called "type 1 method". A direct inspection of the entries of $J(\mathbf{0})$ and of its inverse shows that such negative results are mainly caused by the first two basis functions in (34) which have a smaller support with respect to the others. This implies that the corresponding coefficients in (22) are kept less under control since the computed approximation of the unknown potential depends on them only in small intervals near the extremes of $[0, \pi]$. In addition, an explanation of the worse results for the DBCs relies on the fact that the corresponding eigenfunctions are close to zero near $x = 0, \pi$ so that the entries in the first columns of the limit Jacobian (26) have a much smaller magnitude with respect to those corresponding to the NBCs.

A possible remedy for improving the stability of the procedure is therefore that of enlarging the support of the first basis spline functions. In particular, the approach that we have considered is the following. For a function space Φ of size L, the first knot in (33) is taken strictly positive, that is $t_0 > 0$ and, consequently, $t_{2L-4} = \pi - t_0 < \pi$. In the subinterval $[t_0, t_{2L-4}] \subsetneq [0, \pi]$ the symmetric cubic splines $\hat{\phi}_i(x)$ in (34) are defined in the same way as just described while in $[0, t_0]$ and $[t_{2L-4}, \pi]$ they are obtained by extending the corresponding polynomials in $[t_0, t_1]$ and $[t_{2L-5}, t_{2L-4}]$, respectively. In more details, for each j, $\hat{\phi}_j(x)|_{[0, t_0]}$ and $\hat{\phi}_j(x)|_{[t_{2L-4}, \pi]}$ are taken to be the cubic polynomials $\hat{\phi}_j(x)|_{[t_0, t_1]}$ and $\hat{\phi}_j(x)|_{[t_{2L-5}, t_{2L-4}]}$, respectively. The basis functions ϕ_j are finally computed by applying the normalization given in the left formula in (34). It is not difficult to realize that the so-obtained functions are symmetric not-a-knot splines with respect to the partition composed by the $2L - 2$ knots

$$\Delta' : 0 < t_0 < t_1 < \cdots < t_{2L-4} < \pi. \tag{35}$$

Table 1
Conditioning of the limit Jacobian $J(\mathbf{0})$ for some spline function spaces.

M	Type 1 method		Type 2 method		Type 3 method	
	$\kappa(J(\mathbf{0}))$	Rate	$\kappa(J(\mathbf{0}))$	Rate	$\kappa(J(\mathbf{0}))$	Rate
Dirichlet boundary conditions						
10	8.5509e+02	–	5.1626e+01	–	4.2834e+01	–
20	1.5130e+04	–	1.8275e+02	–	5.8132e+01	–
40	2.7125e+05	4.1642	7.0508e+02	1.9940	8.0754e+01	0.5644
80	4.6571e+06	4.0980	2.8023e+03	2.0054	1.1320e+02	0.5203
160	7.7424e+07	4.0524	1.1219e+04	2.0048	1.5939e+02	0.5094
320	1.2636e+09	4.0269	4.4948e+04	2.0027	2.2493e+02	0.5046
Neumann boundary conditions						
10	8.4090e+01	–	2.0469e+01	–	4.5433e+01	–
20	2.9168e+02	–	3.4011e+01	–	9.7890e+01	–
40	1.1214e+03	1.9989	6.3836e+01	1.1392	2.3777e+02	1.4149
80	4.4429e+03	2.0011	1.2417e+02	1.0164	6.0989e+02	1.4117
160	1.7739e+04	2.0011	2.4516e+02	1.0038	1.6266e+03	1.4501
320	7.0943e+04	2.0006	4.8724e+02	1.0007	4.4515e+03	1.4742

In this general setting, the question to be addressed is the choice of the first knot t_0 and to this regard the adopted criterion has been that of finding a good compromise between the accuracy of the best approximation in L_2-norm of q over Φ and the stability of the method for inverse SLPs. The first natural attempt is therefore that of taking (35) to be a uniform partition of $[0, \pi]$ and this choice turns out to be successful in improving the stability of the method which we have called "*type 2 method*." As shown in Table 1, in fact, when $M = L$, $\kappa(J(\mathbf{0}))$ now grows quadratically with respect to M for DBCs and linearly for NBCs. Nevertheless, for the former conditions we consider the behaviour of $\kappa(J(\mathbf{0}))$ still not satisfactory so that a further enlargement of the subinterval $[0, t_0]$ is operated. In particular, when $M = L$, a noticeable improvement of the stability of the method for DBCs is obtained by taking t_0 so that $t_0 = 2(t_1 - t_0)$ and $t_i - t_{i-1} = (t_1 - t_0)$ for each $i = 2, 3, \ldots, 2L - 4$, see the data in Table 1 corresponding to the "*type 3 method*". For completeness, in the same table we have also reported the values of $\kappa(J(\mathbf{0}))$ for such method applied to problems with NBCs. As one can see, in this case the use of the type 3 method is not convenient.

In the case of symmetric inverse SLP subject to general BCs not of Dirichlet type the most appropriate method to be used seems to be the "*type 2 method*". This is because, like in the Neumann case, the value of the corresponding eigenfunctions is surely different from zero for $x = 0, \pi$.

By virtue of these results, in the sequel when talking about the use of the spline functions for solving the inverse SLP (1)–(3) we will refer to the "*type 3 method*" for DBCs and to the "*type 2 method*" otherwise.

Remark 4. We would like to underline the fact that with the spline functions the behaviour of $\kappa(J(\mathbf{0}))$ with respect to M coincides with that of the methods in [13,15]. Moreover, for later reference, we mention that with the normalization (34) it results $\|(J(\mathbf{0}))^{-1}\|_2 = O(1)$.

4. Error analysis

The error in the approximation of the unknown potential $q(x)$ through the described methods is here analyzed and discussed. We will assume that $q(x)$ is "sufficiently" close to a constant and consider only the case where $L = M$ and the coefficient vector $\mathbf{c}^{(h)}$ of the computed approximation $q^{(h)}(x) = \phi(x, \mathbf{c}^{(h)})$, see (22), solves exactly the system of nonlinear equations (23). Moreover, we will concentrate on the case of inverse problems subject to DBCs and to NBCs. In our opinion, however, the results obtained for the latter conditions hold also for problems subject to more general BCs not of Dirichlet type.

As we are going to see, the error in the approximation $q^{(h)}(x) \approx q(x)$ can be splitted in three terms all depending on the function space Φ used and consequently on the number M of known eigenvalues since its size L is set equal to M. The error due to the discretization of the SLP operated by applying the described BVMs is present instead in only one term of such decomposition.

If we denote with $\phi(x, \mathbf{c}^*)$ the best approximation in L_2-norm of the unknown potential over Φ, namely

$$\mathbf{c}^* = \left(c_1^*, c_2^*, \ldots, c_M^* \right)^T = \arg \min_{\mathbf{c} \in \mathbb{R}^M} \| q - \phi(\cdot, \mathbf{c}) \|_2, \tag{36}$$

then we get

$$\left\| q - q^{(h)} \right\|_2 \leqslant \| q - \phi(\cdot, \mathbf{c}^*) \|_2 + \left\| \phi(\cdot, \mathbf{c}^*) - \phi(\cdot, \mathbf{c}^{(h)}) \right\|_2 \leqslant \| q - \phi(\cdot, \mathbf{c}^*) \|_2 + \sum_{j=1}^{M} \left| c_j^* - c_j^{(h)} \right| \|\phi_j\|_2$$

$$\leqslant \| q - \phi(\cdot, \mathbf{c}^*) \|_2 + \left(\max_{j=1,2,\ldots,M} \|\phi_j\|_2 \right) \| \mathbf{c}^* - \mathbf{c}^{(h)} \|_1. \tag{37}$$

In order to find an estimate of $\| q - q^{(h)} \|_2$ we therefore need to study the behaviour of $\| \mathbf{c}^* - \mathbf{c}^{(h)} \|_1$. From (21) and (19), one immediately deduces that for each h

$$F^{(h)} \left(\mathbf{c}^*, \Lambda^{(h)}(\phi(x, \mathbf{c}^*)) \right) = \mathbf{0},$$

whereas under the assumption we have made

$$F^{(h)} \left(\mathbf{c}^{(h)}, \Lambda - E^{(h)} \right) = \mathbf{0}.$$

It follows that a first order approximation of $\mathbf{c}^* - \mathbf{c}^{(h)}$ is given by:

$$\mathbf{c}^* - \mathbf{c}^{(h)} \simeq \left(J^{(h)}(\mathbf{c}^*) \right)^{-1} \left(\Lambda^{(h)}(\phi(x, \mathbf{c}^*)) - \Lambda + E^{(h)} \right),$$

where $J^{(h)}(\mathbf{c}^*)$ is the Jacobian in (25). Consequently

$$\| \mathbf{c}^* - \mathbf{c}^{(h)} \|_1 \lessapprox \left\| \left(J^{(h)}(\mathbf{c}^*) \right)^{-1} \right\|_1 (\|\Delta\Lambda_1\|_1 + \|\Delta\Lambda_2\|_1), \tag{38}$$

with, see (18),

$$\Delta \Lambda_1 = \Lambda^{(h)}(\phi(x, \mathbf{c}^*)) - \Lambda(\phi(x, \mathbf{c}^*)) + E^{(h)},$$
$$\Delta \Lambda_2 = \Lambda(\phi(x, \mathbf{c}^*)) - \Lambda. \tag{39}$$

With reference to the behaviour of $\|(J^{(h)}(\mathbf{c}^*))^{-1}\|_1$, we shall assume that, if h is small enough then there exists a coefficient $\omega = \omega(q)$ independent of M and h such that

$$\left\| \left(J^{(h)}(\mathbf{c}^*) \right)^{-1} \right\|_1 \leqslant \omega \left\| (J(\mathbf{0}))^{-1} \right\|_1 \tag{40}$$

where $J(\mathbf{0})$ is the limit Jacobian in (26). This assumption is based on the fact that q is supposed to be "sufficiently" close to a constant so that the eigenfunctions of the corresponding SLP are close to those for the zero potential even for the first indices k. The numerically observed values of ω are always of moderate size. For example, for $q(x) = \sin(x)$, $q(x) = |x - \pi/2|$ and $q(x) = x(\pi - x)$ it results $\omega \approx 1$ for DBCs and $\omega \leqslant 2.5$ for NBCs for both the trigonometric polynomials and the spline functions.

By setting

$$\chi(M) = \omega \left(\max_{j=1,2,\ldots,M} \|\phi_j\|_2 \right) \left\| (J(\mathbf{0}))^{-1} \right\|_1, \tag{41}$$

from (37), (38) and (40) we therefore obtain

$$\|q - q^{(h)}\|_2 \leqslant \|q - \phi(\cdot, \mathbf{c}^*)\|_2 + \chi(M)(\|\Delta \Lambda_1\|_1 + \|\Delta \Lambda_2\|_1). \tag{42}$$

Concerning the behaviour of $\|\Delta \Lambda_1\|_1$, from (39), (18) and (19) it is evident that $\Delta \Lambda_1$ represents the discretization error in the numerical approximations of the eigenvalues of the SLP (1)–(3) with potential $\phi(x, \mathbf{c}^*)$ when the selected BVM improved with the asymptotic correction technique is applied. As already underlined in Section 3, such error can be arbitrarily reduced since the choice of the stepsize h is left free. More precisely, from (17) it follows that (at least) $\|\Delta \Lambda_1\|_1 = O(h^{p-1/2})$ being p the order of accuracy of the BVM.

The terms $\chi(M)$ and $\|\Delta \Lambda_2\|_1$ in (42) closely depend on the function space Φ used and, in particular, for the trigonometric polynomials and the spline functions the following are the behaviours with respect to M that we have observed for them.

- *Trigonometric polynomials:* It is immediate to verify that $\chi(M) = O(M)$ for this function space. In fact, from (30)–(32) one deduces that $\max_{j=1,2,\ldots,M} \|\phi_j\|_2 = \sqrt{\pi}$ and $\|(J(\mathbf{0}))^{-1}\|_1 = O(M)$.
  Concerning the vector $\Delta \Lambda_2$ defined in (39), it contains the differences between the first M exact eigenvalues of the SLP (1)–(3) with potential $\phi(x, \mathbf{c}^*)$ and $q(x)$. It is well-known that regular SLPs are well-conditioned with respect to perturbations on their coefficients and a first estimate of $\|\Delta \Lambda_2\|_1$ can be obtained by applying Theorem 2.8 in [29] which gives $\|\Delta \Lambda_2\|_1 \leqslant M\|q - \phi(\cdot, \mathbf{c}^*)\|_\infty$. In all our experiments, however, such upper bound turns out to be definitely crude and a sharper estimate for the trigonometric polynomials is given by:

$$\|\Delta \Lambda_2\|_1 \leqslant \sigma(M)\|q - \phi(\cdot, \mathbf{c}^*)\|_2, \tag{43}$$

  where $\sigma(M)$ is a suitable coefficient independent of the potential q whose behaviour is $\sigma(M) = O(M^{-1/2})$ and $\sigma(M) = o(M^{-1})$ if the SLP is subject to DBCs or to NBCs, respectively. These results can be explained by considering (28) and (29). It is in fact clear that the terms $\xi_k^{(D)}$ and $\xi_k^{(N)}$ in such equations coincide for q and its Fourier cosine series. Therefore, since $\phi(x, \mathbf{c}^*)$ represents such series truncated to the Mth harmonic we have $\xi_k^{(D)}(q) = \xi_k^{(D)}(\phi(\cdot, \mathbf{c}^*))$ with $k = 1, \ldots, M-1$ and $\xi_k^{(N)}(q) = \xi_k^{(N)}(\phi(\cdot, \mathbf{c}^*))$ for $k = 1, \ldots, M$.
- *Spline functions:* In this case, after some computations, one obtains that with the normalization (34) $\max_{j=1,2,\ldots,M} \|\phi_j\|_2 = O(\sqrt{M})$. Concerning the behaviour of $\|(J(\mathbf{0}))^{-1}\|_1$, from Remark 4 we deduce that it grows at most as $O(\sqrt{M})$. Nevertheless, the numerically computed values of $\|(J(\mathbf{0}))^{-1}\|_1$ for $M \leqslant 1500$ suggest that such quantity has actually an horizontal asymptote. From the previous arguments, see (41), we therefore get that $\chi(M) = O(\sqrt{M})$.
  With reference to $\|\Delta \Lambda_2\|_1$ the estimate obtained from Theorem 2.8 in [29] is considerably not sharp also for this function space. In fact, the experiments indicate that

$$\|\Delta \Lambda_2\|_1 \leqslant \sigma(M)\|q - \phi(\cdot, \mathbf{c}^*)\|_2 \tag{44}$$

for a suitable coefficient $\sigma(M) = O(\sqrt{M})$ which is independent of the potential q.

By collecting all the previous considerations, from (42)–(44) we finally get

$$\|q - q^{(h)}\|_2 \leqslant (1 + \sigma(M)\chi(M))\|q - \phi(\cdot, \mathbf{c}^*)\|_2 + \chi(M)\|\Delta \Lambda_1\|_1, \tag{45}$$

where for the trigonometric polynomials, $\chi(M) = O(M)$ while $\sigma(M) = O(M^{-1/2})$ and $\sigma(M) = o(M^{-1})$ for SLPs with DBCs and NBCs, respectively. For the spline functions, instead, $\chi(M) = O(\sqrt{M})$ and $\sigma(M) = O(\sqrt{M})$.

The obtained upper bound for $\|q - q^{(h)}\|_2$ put into evidence that the convergence properties of our procedure for the solution of symmetric inverse SLPs are closely related to the behaviour of $\|q - \phi(\cdot, \mathbf{c}^*)\|_2$ which, in turn, depends on the regularity of q, on the number of known eigenvalues and on the function space used. In this context, the following is an important consideration.

Remark 5. If the unknown potential belongs to the function space used, our procedure allows to reconstruct it with arbitrarily high accuracy. This happens even if a fixed and not necessarily large number M of known eigenvalues is given.

More generally, when q is "sufficiently" regular, the results obtained with the spline functions are usually more accurate than those obtained with the trigonometric polynomials in spite of the faster growth of the coefficient $\sigma(M)\chi(M)$ in (45) for the former space. The well-known flexibility of the spline functions, in fact, usually allows the best spline approximation $\phi(\cdot, \mathbf{c}^*)$ to be much closer to q than its truncated Fourier cosine series is. In particular, this clearly happens if $q'(0)$ and $q'(\pi)$ are different from zero since in such case the accuracy of the approximation obtained with the trigonometric polynomials inevitably deteriorates near the extremes of $[0, \pi]$. On the other hand, the trigonometric polynomials are simpler to be manipulated and, obviously, they are the functions to be used when the interest is devoted to the knowledge of the harmonics of q instead of to its global behaviour.

Before concluding, we must say that even though many of the arguments used in this section are purely experimental, we think that our approach for the analysis of the error is valid since it allows to isolate the term due the discretization operated by the matrix methods used. Moreover, many of the papers currently available in the literature concerning the solution of inverse SLP, like [13–16], do not treat this aspect and are mainly interested on the analysis of the convergence properties of the iterative procedure used for solving the system of nonlinear Eq. (8).

5. Numerical examples

In this section some numerical results obtained with the proposed procedure, always used with $L = M$ (see Section 3), are reported which put into evidence its competitiveness with respect to other classical methods. In particular, the numerical experiments we have conducted suggest that if the potential $q(x)$ to be recovered is at least continuous then the approximation provided by our method is globally more accurate than the one provided by the Numerov method used as described in [15]. On the other hand, if $q(x)$ is discontinuous then the results given by the two methods are very similar. This can be explained by considering that in the previous case the main term in the decomposition of the error (45) is the one involving $\|q - \phi(\cdot, \mathbf{c}^*)\|_2$ i.e. the one associated to the projection of the unknown potential over the function space Φ.

Finally, the last example is aimed to confirm what observed in Remark 5.

Before proceeding, we mention that in all the following examples the required reference eigenvalues have been computed by using the MATSLISE software package [30] while the numerical eigenvalues have been computed with the routine EIG of MATLAB.

Example 1. Let us consider the SLP (1) with $q(x) = 10\sin(x)$ subject to DBCs. For solving the corresponding inverse problem we have used the cubic spline functions defined according to the "*type 3 method*" described in Section 3. The involved direct problems have been solved by applying the BVM of order $p = 8$ defined over $N = 6M$ uniformly distributed meshpoints being M the number of known eigenvalues. The obtained results have been reported in Fig. 1 where the two subplots correspond to $M = 5$ and $M = 10$, respectively. More precisely, the error $|q(x) - q^{(h)}(x)|, x \in [0, \pi]$, for the cubic spline functions is plotted and compared with the error of the pointwise approximation given by the Numerov method [15].

It is evident that our procedure provides definitely more accurate approximations than the one given by the Numerov method and that, with respect to it, the gain in accuracy of our method as M increases is larger.

Example 2. In this second example we have solved the inverse SLP subject to NBCs with exact potential $q(x) = |x - \frac{\pi}{2}|$. We have applied the BVM of order $p = 8$ defined over a nonuniform mesh with geometrically distributed stepsize as described in Remark 2 and the function space Φ used is constituted by the cubic spline functions defined according to the "*type 2 method*". The problem has been solved with $M = 10$ and $M = 20$ known eigenvalues and $N = 6M$ meshpoints for the BVM. The corresponding errors have been reported in Fig. 2 where we have also compared our results with that provided by the Numerov method labeled as *Method 1* in [15, Section 3].

As one may expect, in a neighbourhood of $x = \frac{\pi}{2}$, where the exact potential is only continuous, the two errors are quite similar. In the remaining part of the interval of integration, however, our procedure gives a significantly more accurate approximation of the unknown potential. In particular, this happens near the extremes $x = 0, \pi$ where the accuracy of the approximation provided by the Numerov method rapidly deteriorates.

Example 3. The potential to be reconstructed in this example is the step-function

$$q(x) = \begin{cases} 1 & \text{if } \frac{\pi}{4} < x < \frac{3\pi}{4}, \\ -1 & \text{if } 0 \leqslant x \leqslant \frac{\pi}{4}, \ \frac{3\pi}{4} \leqslant x \leqslant \pi, \end{cases} \tag{46}$$

starting from the knowledge of the corresponding Neumann spectrum. In the first three subplots of Fig. 3, together with the exact potential, the approximations obtained by using the trigonometric polynomials, the BVM of order $p = 6$ with $N = 6M$ geometrically distributed meshpoints and $M = 16, 32, 48$ known eigenvalues have been reported, respectively. As one can see at first sight such approximation improves for increasing values of M; actually, the reconstructed potential $q^{(h)}$ more
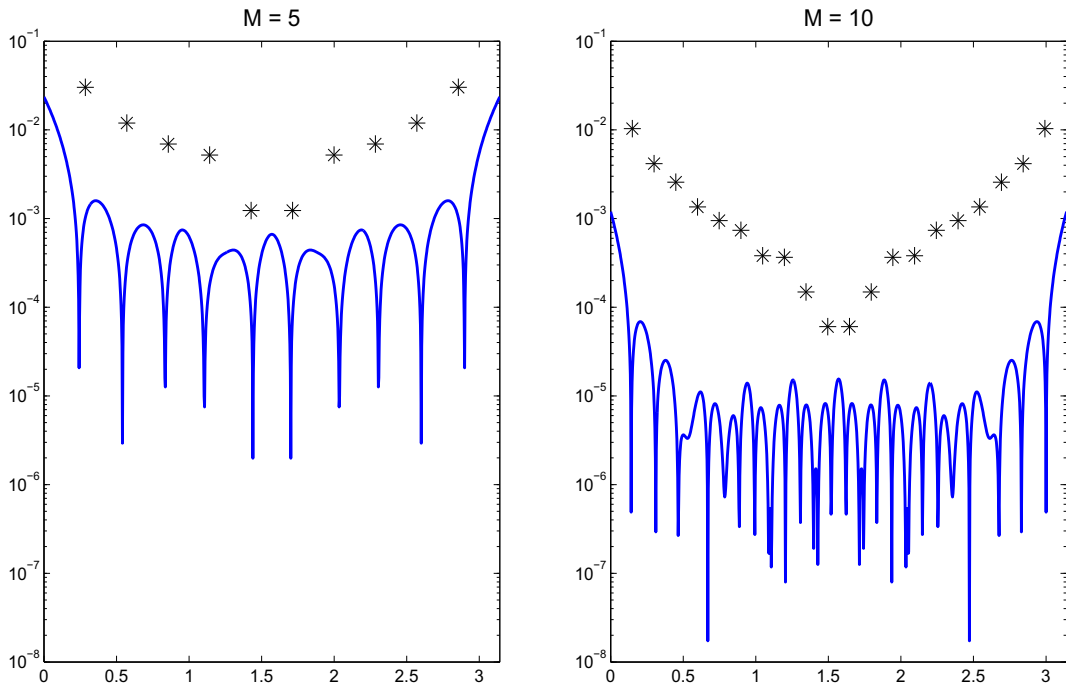
Fig. 1. Error in the reconstruction of $q(x) = 10 \sin(x)$ for the spline functions (solid line) and the Numerov method (*).
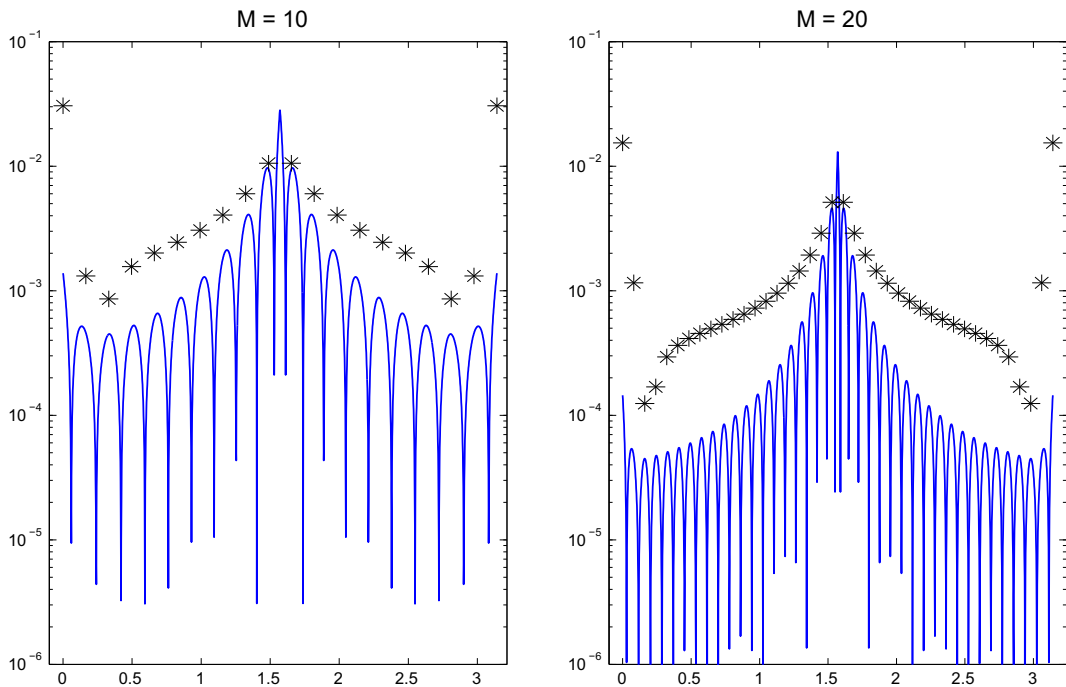

Fig. 2. Error in the reconstruction of $q(x) = |x - \frac{\pi}{2}|$ for the spline functions (solid line) and the Numerov method (*).

closely constitutes an approximation of the truncated Fourier cosine series of q limited to the Mth harmonic. This is shown in the last subplot of Fig. 3 where the errors $\|q - q^{(h)}\|_2$ (solid line) and, see (36), $\|\phi(\cdot, \mathbf{c}^*) - q^{(h)}\|_2$ (dashed line) computed with M even have been reported. This result perfectly agrees with the error analysis carried out in Section 4 and we mention that a similar comparison had been done in [13].
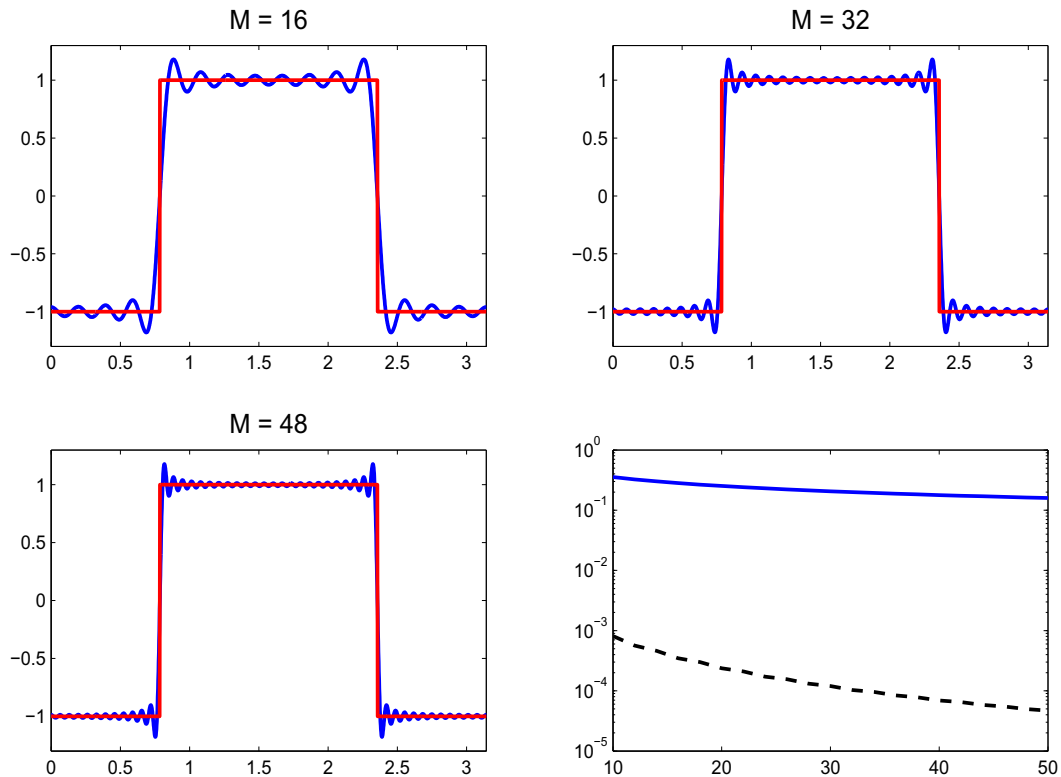
Fig. 3. Reconstruction of the discontinuous potential (46) with trigonometric polynomials and corresponding error in the approximation.

Table 2
L_2-norm of the errors in the reconstruction of $q(x) = \cos(6x)$ with trigonometric polynomials, $M = 8$ Dirichlet and Neumann known eigenvalues and increasing number N of meshpoints.

N	Dirichlet BC		Neumann BC	
	Order 6	Order 8	Order 6	Order 8
25	6.5937e−03	2.4742e−03	1.0136e−03	2.0918e−04
50	9.3910e−05	2.3805e−06	3.5753e−05	6.4272e−06
75	9.3355e−06	5.6048e−07	2.7278e−06	2.6838e−07
100	1.4209e−06	5.9983e−08	3.8299e−07	2.1873e−08
125	3.1333e−07	8.9742e−09	8.0664e−08	2.9519e−09
150	8.9623e−08	1.7998e−09	2.2294e−08	5.6213e−10

Example 4. In this last example the trigonometric polynomials are used for the reconstruction of $q(x) = \cos(6x)$ with the aim of confirming what observed in Remark 5. In particular, in Table 2, for the corresponding inverse SLPs with DBCs and NBCs, we have listed the errors $\|q - q^{(h)}\|_2$ obtained with $M = 8$ by applying the BVMs of order $p = 6, 8$ with geometrically distributed variable stepsize for increasing number N of meshpoints. It is evident that such errors approach zero and that the accuracy increases with the order of the method.

6. Conclusions

The procedure proposed for the solution of symmetric inverse SLPs have provided positive results. The accuracy of the obtained approximation is closely related to the regularity of the unknown potential q. In particular, when q is sufficiently smooth, our method turns out to be very competitive with respect to the Numerov method used as described in [15]. By virtue of this fact, an interesting topic for future investigation is the application of the adopted approach for solving nonsymmetric inverse SLPs.

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