Solving Sturm-Liouville problems by piecewise perturbation methods, revisited

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Solving Sturm-Liouville problems by piecewise perturbation methods, revisited

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Abstract

We present the extension of the successful Constant Perturbation Method (CPM) for Schrödinger problems to the more general class of Sturm-Liouville eigenvalue problems. Whereas the orginal CPM can only be applied to Sturm-Liouville problems after a Liouville transformation, the more general CPM presented here solves the Sturm-Liouville problem directly. This enlarges the range of applicability of the CPM to a wider variety of problems and allows a more efficient solution of many problems. The CPMs are closely related to the second-order coefficient approximation method underlying the SLEDGE software package, but provide for higher order approximations. These higher order approximations can also be obtained by applying a modified Neumann method. The CPM approach, however, leads to simpler formulae in a more convenient form.

Key words: Sturm-Liouville, CPM, eigenvalue, shooting

1 Introduction

In this paper we are concerned with differential equation eigenvalue problems that can be put in the general form of the classical Sturm-Liouville (SL) problem

$$-(p(x)y'(x))' + q(x)y(x) = Ew(x)y(x) \tag{1}$$

defined on an interval $a < x < b$ with boundary conditions at the ends as appropriate. A value of the eigenparameter E for which there is a non-trivial solution subject to the boundary conditions, is called an eigenvalue, and the

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solution y is the corresponding eigenfunction. For regular problems the eigenvalues can be ordered as an increasing sequence tending to infinity

$$E_0 < E_1 < E_2 < \dots \tag{2}$$

and with this labelling the eigenfunction y_k, corresponding to E_k and unique up to a normalizing constant, has exactly k zeros on the open interval (a, b). The calculation of the eigenvalues E and eigenfunctions y of (1) is of great importance both in classical physics and in quantum physics. Since most of the eigenvalue problems can not be solved analytically, good numerical approximation methods are essential. Finding the eigenvalues of a SL problem can, however, be a computationally challenging task. It is well known that as E grows, the solutions of (1) become increasingly oscillatory. In fact, as $E \to +\infty$ the solution "wave length" approaches $2\pi/\sqrt{E}$. This highly oscillatory character of the solution is the reason why standard numerical methods for ODEs encounter difficulties in efficiently estimating the higher eigenvalues: naive integrators will be forced to take increasingly smaller steps, thereby rendering them exceedingly expensive. By taking into account the characteristic features of the SL problem, one can however construct specialized numerical algorithms having some crucial advantages over general-purpose codes.

An important class of methods for the numerical solution of SL problems is based on coefficient approximation (CA). The basic idea here is to replace the coefficient functions $p(x)$, $q(x)$, $w(x)$ of the SL equation piecewisely by low degree polynomials so that the resulting equation can be solved analytically. The idea dates back at least to Gordon [1] and Canosa and De Oliveira [2] and was studied also by Ixaru [3], Paine and de Hoog [4] and Smooke [5], but the standard reference is due to Pruess [6,7]. He constructed a convergence and error analysis of methods based on piecewise polynomial CA. The simplest CA method (often called the Pruess method, e.g. by Pryce in [8]) is based on piecewise constant (midpoint) approximation. With $a = x_0 < x_1 < x_2 < \dots < x_n = b$ the partition of the integration interval, the functions p, q and w then have constant values $\bar{p}$, $\bar{q}$, $\bar{w}$ in the ith interval (x_{i-1}, x_i), $i = 1, \dots, n$ with step size $h = x_i - x_{i-1}$:

$$-(\bar{p}y'(x))' + \bar{q}y(x) = E\bar{w}y(x). \tag{3}$$

The solution y of this approximating problem over $[x_{i-1}, x_i]$ is then advanced by the relation

$$\begin{pmatrix} y(x_i) \\ p(x_i)y'(x_i) \end{pmatrix} = \begin{pmatrix} \xi(Z) & h\eta_0(Z)/\bar{p} \\ \bar{p}Z\eta_0(Z)/h & \xi(Z) \end{pmatrix} \begin{pmatrix} y(x_{i-1}) \\ p(x_{i-1})y'(x_{i-1}) \end{pmatrix} \tag{4}$$

with $Z = h^2(\bar{q} - \lambda\bar{w})/\bar{p}$ and the functions ξ and η_0 as introduced in [9]:

$$\xi(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z \leq 0\,, \\ \cosh(Z^{1/2}) & \text{if } Z > 0\,, \end{cases} \qquad \eta_0(Z) = \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0\,, \\ 1 & \text{if } Z = 0\,, \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0\,, \end{cases}$$

One can also propagate the solution from x_i to x_{i-1}, by taking the inverse of the transfer matrix in (4), which is just the result of replacing h by $-h$ in this matrix. This gives us a method for explicitly integrating (y, py') over the x range, and to use a shooting method. This is done e.g. in the Fortran SL solver SLEDGE and combined with the ideas based on the Prüfer substitution to be able to home in on a particular eigenvalue (see [10]). An important advantage of the Pruess method, is that the step size is not restricted by the oscillations in the solution. A drawback of this simple CA method based on piecewise constant approximation is the difficulty in obtaining higher order methods. It is clear that the step sizes must be sufficiently small such that the error introduced by the approximation by piecewise constants is not too large. This means that for problems with strongly varying coefficient functions the number of intervals in a mesh can be quite large. To obtain higher order CA methods, piecewise polynomial approximations of higher degree should be used. However only piecewise constant polynomials were used in practical software packages as SLEDGE for a long time, because for these eq. (1) is easily integrated analytically.

More recently some approaches were suggested to construct higher-order CA methods and thus to realize the approximation of the coefficient functions by higher order polynomials while still retaining the nice property of the Pruess method that the solution of the approximating problem is integrated explicitly in terms of trigonometric/hyperbolic functions. The so-called Constant (reference potential) Perturbation Methods (CPM) were specially devised for the solution of Schrödinger problems of the form

$$y'' = (q(x) - E)y. \tag{5}$$

These methods use a perturbation technique to construct some correction terms that are added to the known solution of the approximating problem with a piecewise-constant potential q. In this way methods up to order 16 were constructed (see [11,12]) which can efficiently compute the eigenvalues of regular Schrödinger problems. The CPM were extended to the more general SL problem (1) using the Liouville transformation and were implemented in the Fortran code SLCPM12 [13] and the Matlab package MATSLISE [14]. The Liouville transformation converts a SL problem in a Schrödinger problem with the same eigenvalues. However, this transformation is rather expensive due to the quadrature which is needed for the conversion between old and new

variables. Moreover the transformation can only be realized for sufficiently well-behaved (and non-singular) p, q and w functions (see [8]): q must be continuous and p and w should have a continuous second order derivative (users of the SLCPM12 package even have to give the expressions of the derivatives as input). As a consequence the software packages based on CPM still have a smaller range of applicability in comparison with e.g. SLEDGE, which applies the Pruess method directly to a SL problem. In order to really outperform the software packages based on the second-order Pruess method, higher order CA methods must be constructed for general SL problems.

In [15] it was shown that the piecewise perturbation approach for regular Schrödinger problems may be viewed as the application of a modified Neumann method where in fact each extra CPM correction term is an extra term in the Neumann series. In [16] we described how a modified Neumann series method can be applied directly to the general SL problem (1). This modified Neumann method forms the first higher-order CA method for SL equations which are not necessarily in the Schrödinger form. In the present paper we will reconsider this construction of higher-order CA methods for SL problems, and use now a piecewise perturbation approach. This will lead to formulae which are less sensitive to near-cancellation effects and which directly reduce to the CPM schemes for the Schrödinger problem. In this way, we realize the generalization of the CPM to a broad class of SL problems. In section 2 we briefly discuss the CPM for Schrödinger problems as they were presented in [9,17]. In section 3, we show that a very similar procedure can be used to construct formulae for general SL problems. We show in section 4 that the obtained formulae are equivalent with the application of a modified Neumann method.

2 CPM for Schrödinger problems

The Piecewise Perturbation Methods (PPM) are based on an idea from mathematical physics: the perturbation approximation. These PPM are CA methods, in the sense that the original differential equation is replaced piecewisely by another differential equation, called the reference equation by Ixaru in [9], which can be solved exactly. Some perturbation corrections are then added to the solution of the reference equation, which gives a more accurate approximation to the solution of the original equation. The PPM are identified by the type of piecewise approximation: if the coefficients are approximated by piecewise constants the method is referred to as a constant perturbation method (CPM) while if piecewise lines are used the method is called a line perturbation method (LPM) (see [18,19]). The first systematic description of both the CPM and LPM technique is due to Ixaru in [9]. The CPM are generally considered to be more convenient for applications than the LPM. We

will discuss here this CPM algorithm in short. For the full details we refer the reader to [17,11].

Consider the initial value problem for the Schrödinger equation,

$$y'' = (q(x) - E)y\,, \quad x \in [a,b]\,, \quad y(a) = \alpha, \quad y'(a) = \beta\,, \tag{6}$$

where $q(x)$ is supposed to be a well behaved function. On the current mesh interval $[x_{i-1}, x_i]$ the solution is advanced by the algorithm

$$\begin{pmatrix} y(x_i) \\ y'(x_i) \end{pmatrix} = \begin{pmatrix} u(h) & v(h) \\ u'(h) & v'(h) \end{pmatrix} \begin{pmatrix} y(x_{i-1}) \\ y'(x_{i-1}) \end{pmatrix}, \quad h = x_i - x_{i-1}. \tag{7}$$

The functions $u(\delta)$ and $v(\delta)$ are two linear independent solutions of the local problem

$$y''(\delta) = (q(x_{i-1} + \delta) - E)y(\delta)\,, \quad \delta \in [0,h] \tag{8}$$

with the initial values $y(0) = 1, y'(0) = 0$, for u and $y(0) = 0, y'(0) = 1$ for v. The inverse propagation algorithm reads

$$\begin{pmatrix} y(x_{i-1}) \\ y'(x_{i-1}) \end{pmatrix} = \begin{pmatrix} v'(h) & -v(h) \\ -u'(h) & u(h) \end{pmatrix} \begin{pmatrix} y(x_i) \\ y'(x_i) \end{pmatrix}. \tag{9}$$

The knowledge of the "propagators" u and v and their first derivatives is thus sufficient to advance the solution in both directions. However, analytic forms of these u and v are known only for a restricted number of expressions for the function $q(x)$, let such functions be denoted by $\bar{q}(x)$. The idea is to replace $q(x)$ piecewisely by a $\bar{q}(x)$. The propagators corresponding to this approximating problem are called the reference propagators and denoted by $\bar{u}$ and $\bar{v}$. To further improve the accuracy, some extra correction terms, which are derived from the perturbation $\Delta_q = q(x) - \bar{q}(x)$, are added to $\bar{u}$ and $\bar{v}$. The CPM schemes use piecewise constant values $\bar{q}$ as approximation for the potential. As seen in section 1, problems with a piecewise constant potential function have a nice analytic form for $\bar{u}$ and $\bar{v}$ which can be expressed in terms of the functions ξ and η_0. In [9,17] the following theorem was derived:

Theorem 2.1 CPM algorithm for the Schrödinger problem. *The solution of* (8) *with the initial conditions* $y(x_{i-1}) = \alpha$ *and* $y'(x_{i-1}) = \beta$ *can be written as*

$$\begin{pmatrix} y(x_{i-1} + \delta) \\ y'(x_{i-1} + \delta) \end{pmatrix} = \begin{pmatrix} u(\delta) & v(\delta) \\ u'(\delta) & v'(\delta) \end{pmatrix} \begin{pmatrix} y(x_{i-1}) \\ y'(x_{i-1}) \end{pmatrix}$$

where u *and* v *are written as perturbation series:*

$$u(\delta) = \sum_{k=0}^{\infty} u_k(\delta), \; v(\delta) = \sum_{k=0}^{\infty} v_k(\delta). \tag{10}$$

The zeroth order propagators are exactly the reference propagators: $u_0(\delta) = \bar{u}(\delta) = \xi(Z(\delta))$, $v_0(\delta) = \bar{v}(\delta) = \delta\eta_0(Z(\delta))$, $u_0'(\delta) = \bar{u}'(\delta) = Z(\delta)\eta_0(Z(\delta))/\delta$ *and* $v_0'(\delta) = \bar{v}'(\delta) = \xi(Z(\delta))$, *with* $Z(\delta) = (\bar{q} - E)\delta^2$. *The correction terms* ($z = u, v$, *k=1,2,...*) *are computed as follows:*

$$z_k'' = (\bar{q} - E)z_k + \Delta_q(\delta)z_{k-1}\,, \quad z_k(0) = z_k'(0) = 0\,. \tag{11}$$

For the construction of the perturbation corrections, some additional functions have to be defined first (denoted as $\bar{\eta}_m(Z)$ in [9]):

$$\eta_1(Z) = [\xi(Z) - \eta_0(Z)]/Z, \tag{12}$$
$$\eta_m(Z) = [\eta_{m-2}(Z) - (2m-1)\eta_{m-1}(Z)]/Z, \quad m = 2, 3, \ldots. \tag{13}$$

For negative Z the function $\eta_m(Z)$ is an oscillating function whose amplitude damps out when $Z \to -\infty$. For positive Z however, all these functions increase exponentially with Z.

Theorem 2.2 *(from [9,17]) If the potential function* $q(\delta)$ *is a polynomial in* δ, *then the k'th correction* z_k *for the propagator* $z = u, v$ *is of the form*

$$z_k(\delta) = \sum_{m=0} C_m(\delta)\delta^{2m+1}\eta_m(Z(\delta)), \tag{14}$$
$$z_k'(\delta) = C_0(\delta)\xi(Z(\delta)) + \sum_{m=0}[C_m'(\delta) + \delta C_{m+1}(\delta)]\delta^{2m+1}\eta_m(Z(\delta) \tag{15}$$

with a finite number of terms. This means that the product $\Delta_q z_{k-1}$ *is of the form*

$$\Delta_q(\delta)z_{k-1}(\delta) = G(\delta)\xi(Z(\delta)) + \sum_{m=0} S_m(\delta)\delta^{2m+1}\eta_m(Z(\delta)), \tag{16}$$

and the coefficients $C_0(\delta), C_1(\delta), \ldots$ *are then polynomials in* δ *which are given by quadrature*

$$C_0(\delta) = \frac{1}{2}\int_0^\delta G(\delta_1)d\delta_1, \tag{17}$$
$$C_m(\delta) = \frac{1}{2}\delta^{-m}\int_0^\delta \delta_1^{m-1}[S_{m-1}(\delta_1) - C_{m-1}''(\delta_1)]d\delta_1, \quad m = 1, 2, \ldots \tag{18}$$

The starting functions in $\Delta_q u_0(\delta)$ *are* $G(\delta) = \Delta_q(\delta), S_0(\delta) = S_1(\delta) = \cdots = 0$, *while for* v_0 *they are* $G(\delta) = 0, S_0(\delta) = \Delta_q(\delta), S_1(\delta) = S_2(\delta) = \cdots = 0$.

There is an intermediate stage in the procedure in which $q(x_{i-1}+\delta)$ is approximated by a polynomial in δ. This ensures that the system (11) has an analytic solution which can be computed by the procedure described in Theorem 2.2. More specificially, the potential function $q(x)$ is approximated (piecewisely) by a series over shifted Legendre polynomials:

$$q(x_{i-1} + \delta) \approx \sum_{n=0}^{\nu-1} Q_n h_i^n P_n^*(\delta/h_i), \quad \delta = x - x_{i-1}. \tag{19}$$

The expressions of the first shifted Legendre polynomials $P_s^*(\gamma), \gamma \in [0,1]$ are

$$P_0^*(\gamma) = 1, \quad P_1^*(\gamma) = -1 + 2\gamma, \quad P_2^*(\gamma) = 1 - 6\gamma + 6\gamma^2. \tag{20}$$

By the method of least squares the expressions for the coefficients Q_n are obtained:

$$Q_n = \frac{(2n+1)}{h_i^{n+1}} \int_0^h q(x_{i-1} + \delta) P_n^*(\delta/h_i) d\delta. \tag{21}$$

We then take $\bar{q} = Q_0$ and $\Delta_q(\delta) \approx \sum_{n=1}^{\nu-1} Q_n h_i^n P_n^*(\delta/h_i)$. To compute the integrals (21) Gauss-Legendre quadrature, requiring ν function evaluations of q, is used.

Depending on the degree of the approximating polynomial and the number of perturbation corrections included, CPM versions of different order were constructed.

3 CPM for Sturm-Liouville problems

Let us now follow an analogous procedure for the SL problem. We focus on the initial value problem over the current interval $[x_{i-1}, x_i]$ with step length h

$$-[p(x_{i-1} + \delta) y'(x_{i-1} + \delta)]' + q(x_{i-1} + \delta) y(x_{i-1} + \delta) = E w(x_{i-1} + \delta) y(x_{i-1} + \delta), \tag{22}$$

with given initial conditions in x_{i-1} and $\delta \in [0, h]$. We consider two particular solutions $u(\delta)$ and $v(\delta)$ which satisfy the initial conditions

$$u(0) = 1, \; p(x_{i-1}) u'(0) = 0,$$

and

$$v(0) = 0, \; p(x_{i-1}) v'(0) = 1.$$

Since the functions u and v are linearly independent, a general solution of (22) has the form

$$y(x_{i-1} + \delta) = c_1 u(\delta) + c_2 v(\delta).$$

From the initial conditions for u and v we know that $c_1 = y(x_{i-1})$ and $c_2 = p(x_{i-1}) y'(x_{i-1})$. The solution can thus be written in matrix form as

$$\begin{pmatrix} y(x_{i-1} + \delta) \\ p(x_{i-1} + \delta) y'(x_{i-1} + \delta) \end{pmatrix} = \begin{pmatrix} u(\delta) & v(\delta) \\ p(x_{i-1} + \delta) u'(\delta) & p(x_{i-1} + \delta) v'(\delta) \end{pmatrix} \begin{pmatrix} y(x_{i-1}) \\ p(x_{i-1}) y'(x_{i-1}) \end{pmatrix}.$$

The determinant $D(\delta) = p(x_{i-1} + \delta) \left(u(\delta) v'(\delta) - u'(\delta) v(\delta) \right)$ of the transfer matrix equals one, since its derivative equals zero and $D(0) = 1$. Taking the

inverse of the propagation formula, we thus obtain

$$\begin{pmatrix} y(x_{i-1}) \\ p(x_{i-1})y'(x_{i-1}) \end{pmatrix} = \begin{pmatrix} p(x_{i-1}+\delta)v'(\delta) & -v(\delta) \\ -p(x_{i-1}+\delta)u'(\delta) & u(\delta) \end{pmatrix} \begin{pmatrix} y(x_{i-1}+\delta) \\ p(x_{i-1}+\delta)y'(x_{i-1}+\delta) \end{pmatrix}.$$

To compute $u(\delta)$, $v(\delta)$, $p(\delta)u'(\delta)$ and $p(\delta)v'(\delta)$, we generalise the Schrödinger CP approach. This means that we write the coefficient functions as $P(x) = 1/p(x) = \bar{P} + \Delta_P(x)$, $q(x) = \bar{q} + \Delta_q(x)$ and $w(x) = \bar{w} + \Delta_w(x)$, and we define $Z(\delta) = \bar{P}(\bar{q} - E\bar{w})\delta^2$. Note that, as in [16], we replace the P function by a piecewise polynomial rather than its inverse p. This ensures that the perturbation corrections will have a closed analytic form.

The reference equation is then defined as follows

$$-\Big(y'(x)/\bar{P}\Big)' + \bar{q}y(x) = E\bar{w}y(x). \tag{23}$$

The reference propagators $\bar{u} = \xi(Z(\delta))$, $\bar{v} = \bar{P}\delta\eta_0(Z(\delta))$, $\bar{u}' = Z(\delta)\eta_0(Z(\delta))/\delta$ and $\bar{v}' = \bar{P}\xi(Z(\delta))$ corresponding to this equation, form the zeroth order propagators in our perturbation method. Corrections of different order can be added in order to approximate the unknown propagators more accurately. When no corrections are added, one obtains the second order Pruess method.

3.1 The perturbation corrections

We introduce the parameter dependent functions F_P, F_q and F_w

$$F_P(\delta;\gamma) = \bar{P} + \gamma\Delta_P(\delta),\ F_q(\delta;\gamma) = \bar{q} + \gamma\Delta_q(\delta),\ F_w(\delta;\gamma) = \bar{w} + \gamma\Delta_w(\delta),$$

with $\gamma \in [0,1]$. These functions reproduce the original functions P, q, w and the reference functions $\bar{P}, \bar{q}, \bar{w}$ when γ takes its extreme values 1, resp. 0. Let us now define $u(\delta;\gamma)$ and $v(\delta;\gamma)$, generically denoted by $z(\delta;\gamma)$ as

$$z(\delta;\gamma) = \sum_{k=0}^{\infty} z_k(\delta)\gamma^k, \tag{24}$$

where $z = u$ if $z(0;\gamma) = 1, z'(0;\gamma) = 0$ and $z = v$ if $z(0;\gamma) = 0, z'(0;\gamma) = P(x_{i-1})$. To calculate z_k we introduce $z(\delta;\gamma)$ into the differential equation:

$$-\Big(\frac{z'(\delta;\gamma)}{\bar{P} + \gamma\Delta_P(\delta)}\Big)' + \Big(\bar{q} + \gamma\Delta_q(\delta)\Big)z(\delta;\gamma) = E\Big(\bar{w} + \gamma\Delta_w(\delta)\Big)z(\delta;\gamma) \tag{25}$$

and organize the terms in Eq. (25) in powers of γ. To simplify the expressions we first define

$$\rho(\delta) = \frac{z'(\delta)}{P(x_{i-1}+\delta)}, \quad \rho(\delta;\gamma) = \sum_{k=0}^{\infty} \rho_k(\delta)\gamma^k, \tag{26}$$

and $\bar{r} = \bar{q} - E\bar{w}$ and $\Delta_r = \Delta_q - E\Delta_w$. Eq. (25) can then be written as

$$-\Big(\sum_{k=0}^{\infty} \rho_k \gamma^k\Big)' + (\bar{r} + \gamma\Delta_r) \sum_{k=0}^{\infty} z_k \gamma^k = 0 \tag{27}$$

where the δ-dependence is omitted for brevity reasons. Since (27) has to be satisfied for every $\gamma \in [0,1]$, the δ dependent weights of γ^m must vanish for any $k = 0, 1, \ldots,$ i.e.

$$\rho_0' = \bar{r} z_0 \tag{28}$$

$$\rho_k' = \bar{r} z_k + \Delta_r z_{k-1}, \quad k = 1, 2, \ldots. \tag{29}$$

Note that these equations reduce to Eq. (11) for the Schrödinger problem. From (26), we can deduce that

$$\bar{P} \sum_{k=0}^{\infty} \rho_k \gamma^k = \frac{\sum_{k=0}^{\infty} z_k' \gamma^k}{1 + \gamma \frac{\Delta_P}{\bar{P}}} \tag{30}$$

$$= \left(\sum_{k=0}^{\infty} z_k' \gamma^k\right) \sum_{s=0}^{\infty} (-\gamma)^s \left(\frac{\Delta_P}{\bar{P}}\right)^s \tag{31}$$

$$= \sum_{k=0}^{\infty} \sum_{s=0}^{k} \left(\frac{-\Delta_P}{\bar{P}}\right)^{k-s} z_s' \gamma^k, \tag{32}$$

which leads us to expressions for the perturbations $\rho_k(\delta), k = 1, 2, \ldots$:

$$\rho_k = \frac{1}{\bar{P}} \sum_{s=0}^{k} \left(\frac{-\Delta_P}{\bar{P}}\right)^{k-s} z_s' \tag{33}$$

$$= \frac{z_k'}{\bar{P}} - \frac{\rho_{k-1}\Delta_P}{\bar{P}}, \tag{34}$$

and $\rho_0 = z_0'/\bar{P}$.

From (24) we can derive that $z(\delta;0) = z_0(\delta)$. On the other hand, we know that $z(\delta;0) = \bar{z}(\delta)$, so we get $z_0(\delta) = \bar{z}(\delta)$. Since the initial values for $z(\delta;\gamma)$ are the same as for $\bar{z}(\delta)$, the difference $z(0;\gamma) - z_0(0)$ vanishes:

$$\sum_{k=1}^{\infty} z_k(0)\gamma^k = 0 \quad \gamma \in [0,1]. \tag{35}$$

Analogously the initial values for $\rho(\delta;\gamma)$ equal the ones for $\rho_0(\delta) = \bar{z}'(\delta)/\bar{P}$,

and we have

$$\sum_{k=1}^{\infty} \rho_k(0)\gamma^k = 0 \quad \gamma \in [0,1]. \tag{36}$$

This means that

$$z_k(0) = \rho_k(0) = 0, \quad k = 1, 2, 3, \ldots. \tag{37}$$

In short, we then have the following results:

Theorem 3.1 CPM algorithm for SL problems. *The solution of* (22) *with initial conditions* $y(x_{i-1}) = \alpha$ *and* $p(x_{i-1})y'(x_{i-1}) = \beta$ *can be written as*

$$\begin{pmatrix} y(x_{i-1}+\delta) \\ p(x_{i-1}+\delta)y'(x_{i-1}+\delta) \end{pmatrix} = \begin{pmatrix} u(\delta) & v(\delta) \\ \mu(\delta) & \nu(\delta) \end{pmatrix} \begin{pmatrix} y(x_{i-1}) \\ p(x_{i-1})y'(x_{i-1}) \end{pmatrix}$$

where the propagators u, v, μ *and* ν *are written as perturbation series:*

$$u(\delta) = \sum_{k=0}^{\infty} u_k(\delta),\ v(\delta) = \sum_{k=0}^{\infty} v_k(\delta),\ \mu(\delta) = \sum_{k=0}^{\infty} \mu_k(\delta),\ \nu(\delta) = \sum_{k=0}^{\infty} \nu_k(\delta). \tag{38}$$

The zeroth order propagators are exactly the reference propagators: $u_0(\delta) = \bar{u}(\delta) = \xi(Z(\delta))$, $v_0(\delta) = \bar{v}(\delta) = \bar{P}\delta\eta_0(Z(\delta))$, $\mu_0(\delta) = \bar{u}'(\delta)/\bar{P} = Z(\delta)\eta_0(Z(\delta))/(\delta\bar{P})$ *and* $\nu_0(\delta) = \bar{v}'(\delta)/\bar{P} = \xi(Z(\delta))$. *The correction terms* ($k = 1, 2, \ldots$) *satisfy the following relations:*

$$\mu_k' = \bar{r}u_k + \Delta_r u_{k-1}, \tag{39}$$
$$\nu_k' = \bar{r}v_k + \Delta_r v_{k-1}, \tag{40}$$
$$\bar{P}\mu_k = u_k' - \mu_{k-1}\Delta_P, \tag{41}$$
$$\bar{P}\nu_k = v_k' - \nu_{k-1}\Delta_P, \tag{42}$$

with initial conditions

$$u_k(0) = v_k(0) = \mu_k(0) = \nu_k(0) = 0. \tag{43}$$

3.2 The construction of the perturbation corrections

To construct the kth correction z_k with $z = u, v$ and $\rho = \mu, \nu$, we first rewrite (39)-(40) using (41)-(42) to obtain:

$$\frac{z_k''}{\bar{P}} = \bar{r}z_k + \Delta_r z_{k-1} + \frac{\Delta_P'\rho_{k-1}}{\bar{P}} + \frac{\Delta_P\rho_{k-1}'}{\bar{P}}. \tag{44}$$

We assume that the inhomogeneous term in (44) can be expressed in terms of the functions ξ and $\delta\eta_0, \delta^3\eta_1, ..., \delta^{2M+1}\eta_M$, as follows:

$$\Delta_r z_{k-1} + \frac{(\Delta_P \rho_{k-1})'}{\bar{P}} = G(\delta)\xi(Z(\delta)) + \sum_{m=0}^{M} S_m(\delta)\delta^{2m+1}\eta_m(Z(\delta)) \tag{45}$$

where $G, S_0, S_1, ...$ are polynomials in δ. Now we search for z_k of the form

$$z_k(\delta) = \sum_{m=0}^{+\infty} C_m(\delta)\delta^{2m+1}\eta_m(Z(\delta)) \ . \tag{46}$$

We will see that the sum in (46) has a finite number of terms and that the coefficients $C_m(\delta)$ are polynomials in δ. We differentiate (46) with respect to δ and use the differentiation properties of the ξ and η functions

$$\frac{\partial\xi(Z(\delta))}{\partial\delta} = Z(\delta)\eta_0(Z(\delta))/\delta, \quad \frac{\partial\delta\eta_0(Z(\delta))}{\partial\delta} = \xi(Z(\delta)), \tag{47}$$

$$\frac{\partial\delta^{2m+1}\eta_m(Z(\delta))}{\partial\delta} = \delta^{2m}\eta_{m-1}(Z(\delta)), \quad m = 1, 2, \cdots , \tag{48}$$

to obtain

$$z_k'(\delta) = C_0\xi(Z) + [C_0' + \delta C_1]\delta\eta_0(Z) + \cdots + [C_m' + \delta C_{m+1}]\delta^{2m+1}\eta_m(Z) + \ldots \tag{49}$$

Differentiating this again with respect to δ and using (47)-(48), gives us

$$\begin{aligned} z_k''(\delta) = (2C_0' + \delta C_1)\xi(Z) + [C_0'' + C_0 Z/\delta^2 + C_1 + 2C_1'\delta + \delta^2 C_2]\delta\eta_0(Z) \\ + \cdots + [C_m'' + C_{m+1} + 2C_{m+1}'\delta + \delta^2 C_{m+2}]\delta^{2m+1}\eta_m(Z) + \ldots \end{aligned} \tag{50}$$

One can then construct an expression for $\frac{z_k''(\delta)}{\bar{P}} - \bar{r}z_k(\delta)$:

$$\begin{aligned} \frac{z_k''(\delta)}{\bar{P}} - \bar{r}z_k(\delta) &= \frac{z_k''(\delta)}{\bar{P}} - \frac{Z z_k(\delta)}{\bar{P}\delta^2} \\ &= \frac{2C_0'\xi}{\bar{P}} + \frac{1}{\bar{P}}[C_0'' + 2C_1 + 2C_1'\delta]\delta\eta_0 + \ldots \\ &\quad + \frac{1}{\bar{P}}[C_m'' + 2(m+1)C_{m+1} + 2\delta C_{m+1}']\delta^{2m+1}\eta_m + \ldots \end{aligned} \tag{51}$$

where we used relations (12)-(13). From (39), we know that (51) should be equal to $\Delta_r z_{k-1} + \frac{\Delta_P \rho_{k-1}'}{\bar{P}} + \frac{\Delta_P' \rho_{k-1}}{\bar{P}}$. Then, upon identifying the coefficients of

$\xi, \eta_0, \eta_1, ...$ of the expressions (45) and (51), one gets

$$
\begin{aligned}
2C_0'(\delta) &= \bar{P}G(\delta) \\
C_m''(\delta) + 2[\delta C_{m+1}'(\delta) + (m+1)C_{m+1}(\delta)] &= \bar{P}S_m(\delta), \quad m = 1, 2, \ldots, M \\
C_m''(\delta) + 2[\delta C_{m+1}'(\delta) + (m+1)C_{m+1}(\delta)] &= 0, \qquad\qquad m = M+1, M+2, \ldots.
\end{aligned}
$$

These equations can be solved iteratively; for C_0 the following formula is obtained

$$
C_0(\delta) = \frac{\bar{P}}{2}\int_0^\delta G(\delta_1)d\delta_1 + \beta, \quad \beta = z_k'(0), \tag{52}
$$

while for $C_1(\delta), C_2(\delta), ...$ we get

$$
C_m(\delta) = \frac{1}{2}\delta^{-m}\int_0^\delta \delta_1^{m-1}H_{m-1}(\delta_1)d\delta_1, \tag{53}
$$

where

$$
H_m(\delta) = \begin{cases} \bar{P}S_m(\delta) - C_m''(\delta) & \text{if } m = 0, 1, 2, ..., M \\ -C_m''(\delta) & \text{if } m = M+1, M+2, ... \end{cases} \tag{54}
$$

Since, from (34), $z_k'(0) = \bar{P}\rho_k(0) + \rho_{k-1}(0)\Delta_P(0)$, and $\mu_k(0) = 0$ for $k = 0, 1, \ldots$ and $\nu_0(0) = 1, \nu_k(0) = 0$ for $k = 1, 2, \ldots$, the constant $\beta = z_k'(0)$ in (52) is nonzero only for $z_k = v_1$, in which case we have $\beta = \Delta_P(0)$.

Let us denote the degree of a polynomial P by $d(P)$. Eqs. (52) and (54) imply that H_0 is a polynomial with maximal degree $d(H_0) = \max(d(S_0), d(C_0'')) = \max(d(S_0), d(G) - 1)$, so that C_1 which results from eq. (53) is a polynomial of the same degree. Also for higher m-values, the degree of C_m is equal to the degree of H_{m-1} and $d(H_{m-1}) = \max(d(S_{m-1}), d(C_{m-1}'')) = \max(d(S_{m-1}), d(C_{m-1}) - 2)$ for $m \leq M+1$, but $d(H_{m-1}) = d(C_{m-1}'') = d(C_{m-1}) - 2$ for $m > M+1$. It follows that $d(C_{M+2}) = d(C_{M+1}) - 2$, $d(C_{M+3}) = d(C_{M+1}) - 4$ and so on. Thus, upon denoting the integer part of $d(C_{M+1})/2$ by $\bar{M}$, it results that $C_m(\delta) = 0$ for any $m > M + \bar{M} + 1$, i.e. the last term in the sum (46) is $C_{M+\bar{M}+1}(\delta)\eta_{M+\bar{M}+1}(\delta)$. Upon this we have shown that if $\Delta_r z_{k-1} + \frac{\Delta_P \rho_{k-1}'}{\bar{P}} + \frac{\Delta_P' \rho_{k-1}}{\bar{P}}$ can be written as (45) then $z_k(\delta)$ results in the form (46) with a finite number of terms, and also that the coefficients are polynomials in δ which can be calculated by Eqs. (52)-(54). The only remaining question is whether the assumed form for (45) is valid. The answer is positive provided Δ_r and Δ_P are polynomials in δ. In fact, for $k = 1$, the expression in the right handside of (45) consists of two terms: the first term with $G(\delta) = \Delta_r(\delta) + \frac{\bar{r}\Delta_P(\delta)}{\bar{P}}$ for $z = u$, $G(\delta) = \frac{\Delta_P'(\delta)}{\bar{P}}$ for $z = v$, and the second term $S_0(\delta) = \frac{\bar{r}\Delta_P'(\delta)}{\bar{P}}$ for $z = u$, $S_0(\delta) = \Delta_r(\delta)\bar{P} + \bar{r}\Delta_P(\delta)$ for $z = v$. This guarantees that z_1 will be of the form (46). In turn, since $\rho_1 = \frac{z_1'}{\bar{P}} - \frac{\rho_0 \Delta_P}{\bar{P}}$, $\rho_0 = z_0'/\bar{P}$ and $\rho_1' = \bar{r}z_1 + \Delta_r z_0$, the expression $\Delta_r z_1 + \frac{\Delta_P \rho_1'}{\bar{P}} + \frac{\Delta_P' \rho_1}{\bar{P}}$ will also be of the form (45), and so on.

We can summarize the previous in the following theorem:

Theorem 3.2 *If the functions p, q, w are polynomials in δ, then the k'th ($k = 1, 2, \dots$) correction z_k for the propagator z ($z = u, v$) is of the form*

$$z_k(\delta) = \sum_{m=0} C_m(\delta)\delta^{2m+1}\eta_m(Z(\delta)) \ , \tag{55}$$

$$z_k'(\delta) = C_0(\delta)\xi(Z(\delta)) + \sum_{m=0}[C_m'(\delta) + \delta C_{m+1}(\delta)]\delta^{2m+1}\eta_m(Z(\delta)) \tag{56}$$

with a finite number of terms. This means that $\Delta_r z_{k-1} + \frac{\Delta_P \rho_{k-1}'}{\bar{P}} + \frac{\Delta_P' \rho_{k-1}}{\bar{P}}$ is of the form

$$G(\delta)\xi(Z(\delta)) + \sum_{m=0} S_m(\delta)\delta^{2m+1}\eta_m(Z(\delta)), \tag{57}$$

and the coefficients $C_m(\delta)$ are polynomials in δ which are given by quadrature

$$C_0(\delta) = \frac{\bar{P}}{2}\int_0^\delta G(\delta_1)d\delta_1 + \beta, \tag{58}$$

$$C_m(\delta) = \frac{1}{2}\delta^{-m}\int_0^\delta \delta_1^{m-1}[\bar{P}S_{m-1}(\delta_1) - C_{m-1}''(\delta_1)]d\delta_1, \quad m = 1, 2, \dots. \tag{59}$$

The k'th correction for $\rho = \mu, \nu$ is given by

$$\rho_k = \frac{z_k'}{\bar{P}} - \frac{\rho_{k-1}\Delta_P}{\bar{P}}, \tag{60}$$

$$\rho_k' = \bar{r}z_k + \Delta_r z_{k-1}. \tag{61}$$

The starting functions in $\Delta_r u_0 + \frac{\Delta_P \mu_0'}{\bar{P}} + \frac{\Delta_P' \mu_0}{\bar{P}}$ are $G(\delta) = \Delta_r(\delta) + \frac{\bar{r}\Delta_P(\delta)}{\bar{P}}$, $S_0(\delta) = \frac{\bar{r}\Delta_P'(\delta)}{\bar{P}}$, $S_1(\delta) = S_2(\delta) = \cdots = 0$, while for $\Delta_r v_0 + \frac{\Delta_P \nu_0'}{\bar{P}} + \frac{\Delta_P' \nu_0}{\bar{P}}$ they are $G(\delta) = \frac{\Delta_P'(\delta)}{\bar{P}}$, $S_0(\delta) = \Delta_r(\delta)\bar{P} + \bar{r}\Delta_P(\delta)$, $S_1(\delta) = S_2(\delta) = \cdots = 0$. The constant β is nonzero only for $z_k = v_1$, viz. $\beta = \Delta_P(0)$.

3.3 A pilot reference equation

Theorem 3.2 assumes that the functions P, q and w are polynomials in δ. Also the integrals in (58)–(59) are difficult to deal with when Δ_P and Δ_r are not of the polynomial form. Therefore, we add an extra stage to the procedure in which we approximate the functions $P(x_{i-1} + \delta)$, $q(x_{i-1} + \delta)$ and $w(x_{i-1} + \delta)$ by polynomials in δ, as was also described for the Schrödinger CPM schemes in Section 2. Each coefficient function $f = q, w, P$ is approximated by

$$f(x_{i-1} + \delta) \approx \sum_{s=0}^{\nu-1} F_s h_i^s P_s^*(\delta/h_i), \quad \delta \in [0, h_i]. \tag{62}$$

where the coefficients $F_s(F = Q, W, P)$ are given by:

$$F_s = \frac{(2s+1)}{h_i^{s+1}} \int_0^{h_i} f(x_{i-1} + \delta) P_s^*(\delta/h_i) d\delta, \quad m = 0, 1, 2, \ldots. \tag{63}$$

The reference coefficient functions can then be taken as follows: $\bar{q} = Q_0, \bar{P} = P_0, \bar{w} = W_0$. As we will see in section 5, the value of ν can be chosen in such a way (i.e. high enough) that the differences between the coefficients functions and their approximations do not affect the accuracy of the method.

4 The CPM as modified Neumann method

Let us rewrite the SL problem (1) in matrix form as

$$\mathbf{y}'(x) = A(x)\mathbf{y}(\mathbf{x}), \quad \mathbf{y}(\mathbf{a}) = \mathbf{y_0}, \tag{64}$$

with

$$A(x) = \begin{pmatrix} 0 & 1/p(x) \\ q(x) - Ew(x) & 0 \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} y(x) \\ p(x)y'(x) \end{pmatrix}. \tag{65}$$

There is an emerging family of numerical methods based on integral series representation of ODE solutions which can be applied on systems of the form (64) (see [20,21]). The Neumann series is an example of such an integral series. When the solution of a linear system $\mathbf{y}' = A(x)\mathbf{y}$ oscillates rapidly, a Neumann method should not be applied directly to the problem but modified schemes should be used, as recommended in [15,22,23]. Here we show that the application of a modified Neumann method to the SL problem is in fact theoretically equivalent to the CPM approach discussed in the previous section.

Suppose that we have already computed $\mathbf{y}_{i-1} \approx \mathbf{y}(x_{i-1})$ and that we wish to advance the numerical solution to $x_i = x_{i-1} + h$. The first step in the modified Neumann scheme is to change the variables locally

$$\mathbf{y}(x) = e^{(x-x_{i-1})\bar{A}}\mathbf{u}(x - x_{i-1}), \quad x_{i-1} \le x \le x_i \tag{66}$$

where $\bar{A}(E)$ is a (piecewise) constant approximation of the matrix function A

$$\bar{A}(E) = \begin{pmatrix} 0 & \bar{P} \\ \bar{r} & 0 \end{pmatrix}, \quad P(x) = 1/p(x). \tag{67}$$

We treat $\mathbf{u}$ as our new unknown which itself obeys the equation

$$\mathbf{u}'(\delta) = B(\delta, E)\mathbf{u}(\delta), \quad \delta \in [0, h], \quad \mathbf{u}(0) = \mathbf{y}_{i-1} \tag{68}$$

where

$$B(\delta, E) = e^{-\delta\bar{A}}\left(A(x_{i-1}+\delta) - \bar{A}\right)e^{\delta\bar{A}} = e^{-\delta\bar{A}}\Delta_A(\delta)e^{\delta\bar{A}}. \tag{69}$$

Over each interval $[x_{i-1}, x_i]$, we apply a Neumann method to the modified equation $\mathbf{u}'(\delta) = B(\delta)\mathbf{u}(\delta), \mathbf{u}(0) = \mathbf{y}_{i-1}$. This gives

$$\mathbf{u}_i = \mathbf{y}_{i-1} + \int_0^h B(x)dx\mathbf{y}_{i-1} + \int_0^h \int_0^{x_1} B(x_1)B(x_2)dx_2dx_1\mathbf{y}_{i-1} + \dots \tag{70}$$

The solution $\mathbf{y}$ in $x = x_i$ of the original system is then obtained from $\mathbf{y}(E, x_i) = e^{h\bar{A}}\mathbf{u}(h)$, where $e^{h\bar{A}}$ is given by

$$e^{h\bar{A}} = \begin{pmatrix} \xi(Z(h)) & h\bar{P}\eta_0(Z(h)) \\ \dfrac{Z(h)\eta_0(Z(h))}{h\bar{P}} & \xi(Z(h)) \end{pmatrix}. \tag{71}$$

When only the first term in the Neumann series (70) is retained, one has exactly the second-order Pruess method. In [16] we constructed some higher order methods by including more Neumann terms. Each such Neumann term corresponds to a CPM correction term. This can be seen as follows. Applying a modified Neumann method, the fundamental solution Y on the ith interval is constructed as the limit of the series

$$Y(E, x, x_{i-1}) = T_0(x) + T_1(x) + T_2(x) + \dots, x \in [x_{i-1}, x_i], \tag{72}$$

where

$$T_0(x) = e^{(x-x_{i-1})\bar{A}} \tag{73}$$

and

$$T_1(x) = T_0(x)\int_0^\delta B(s)ds, \quad \delta = x - x_{i-1}. \tag{74}$$

$$T_k(x) = T_0(x)\int_0^\delta B(s_1)\int_0^{s_1} B(s_2)\dots\int_0^{s_{k-1}} B(s_k)ds_k\dots ds_2ds_1, \quad k = 2, 3, \dots.$$

Equivalently,

$$T_k(x) = T_0(x)\int_0^\delta T_0^{-1}(s)\Delta_A(s)T_{k-1}(s)ds, \quad k = 1, 2, \dots, \tag{75}$$

or

$$\frac{d}{dx}\left[T_0^{-1}(x)T_k(x)\right] = T_0^{-1}(x)\Delta_A(x)T_{k-1}(x), \quad k = 1, 2, \dots. \tag{76}$$

With (73), this can also be written as

$$T_k'(x) = \bar{A}T_k(x) + \Delta_A(x)T_{k-1}(x), \quad T_k(x_{i-1}) = 0, \quad k = 1, 2, \dots. \tag{77}$$

For the four entries in the matrix function T_k we have (where we now use k

as the superscript instead of subscript)

$$T_{11}^{k\,\prime} = \bar{P}T_{21}^{k} + \Delta_P T_{21}^{k-1}, \qquad T_{12}^{k\,\prime} = \bar{P}T_{22}^{k} + \Delta_P T_{22}^{k-1}, \tag{78}$$

$$T_{21}^{k\,\prime} = \bar{r}T_{11}^{k} + \Delta_r T_{11}^{k-1}, \qquad T_{22}^{k\,\prime} = \bar{r}T_{12}^{k} + \Delta_r T_{12}^{k-1}. \tag{79}$$

With $u = T_{11}$, $v = T_{12}$, $\mu = T_{21}$ and $\nu = T_{22}$, these equations correspond exactly to Eqs. (39)–(42).

In [16], practical Neumann algorithms were constructed by truncating the Neumann series and applying a Filon-Legendre approach to approximate the oscillating integrals in the modified scheme (70). The Filon method, in fact, fits a polynomial to the nonoscillatory part of the integrand and solves the resulting integral analytically. That is, the functions $q, w, P = 1/p$ were replaced by interpolating polynomials written as series over shifted Legendre polynomials, in the exact same way as for the CPM in section 3.3.

5 The CPM[N,K]: CPM versions of different order

The formulae in Theorem 3.2 allow us to obtain the analytic form of the corrections (with the help of a symbolic software package). Depending on the number of corrections and the degree of the approximating polynomials, different CPM versions can be formulated. Ixaru introduced the notation CPM[N,K] in [9] for a Schrödinger CPM with N the degree of the polynomial approximating the potential function q, and K the number of perturbation corrections retained in the algorithm. Let us use here the same notation to identify the different versions. We also introduce some extra notations (for $m = 1, ..., N$):

$$\hat{P}_m = P_m h^{m+2}, \quad \hat{R}_m = (Q_m - EW_m)h^{m+2}. \tag{80}$$

and

$$U_m = \hat{R}_m \bar{P} - \hat{P}_m \bar{r}, \quad V_m = \hat{R}_m \bar{P} + \hat{P}_m \bar{r}. \tag{81}$$

5.1 CPM[0,0]: a method of order 2

The CPM[0,0] method is the simplest version, in which P, q and w are approximated by piecewise constants and no correction term is introduced. In this case the propagators are approximated as follows ($Z = Z(h)$):

$$u(h) \approx \xi(Z), \;\; v(h) \approx \bar{P}h\eta_0(Z), \tag{82}$$

$$\mu(h) \approx Z\eta_0(Z)/(h\bar{P}), \;\; \nu(h) \approx \xi(Z). \tag{83}$$

5.2 CPM[1,1]: a method of order 4

Taking linear pilot reference functions and one correction term, we obtain:

$$u(h) \approx \xi(Z) - \frac{U_1}{2}\eta_1(Z) \tag{84}$$

$$v(h) \approx \bar{P}h\eta_0(Z) \tag{85}$$

$$h\bar{P}\mu(h) \approx Z\eta_0(Z) \tag{86}$$

$$\nu(h) \approx \xi(Z) + \frac{U_1}{2}\eta_1(Z). \tag{87}$$

This scheme is theoretically equivalent to the Neumann method with one integral term and first degree approximating polynomials (see [16]), and is thus also fourth order. Note that although the procedure is a bit complicated, surprisingly simple formulae are obtained in the end. For comparison, the fourth order Neumann method presented in [16] reads

$$\begin{pmatrix} y(x_i) \\ p(x_i)y'(x_i) \end{pmatrix} = T(h) \begin{pmatrix} y(x_{i-1}) \\ p(x_{i-1})y'(x_{i-1}) \end{pmatrix}$$

where the elements of $T(h) = e^{h\bar{A}}(I + N_1)$, with I the identity matrix and N_1 the approximation of the first Neumann integral, are given by

$$u(h) = T_{11}(h) = \xi(Z)(1 + I_1) - h\eta_0(Z)\frac{I_2}{2} \tag{88}$$

$$v(h) = T_{12}(h) = \xi(Z)\frac{I_2}{2\bar{r}} + h\bar{P}\eta_0(Z)(1 - I_1) \tag{89}$$

$$\mu(h) = T_{21}(h) = \bar{r}h\eta_0(Z)(1 + I_1) - \xi(Z)\frac{I_2}{2\bar{P}} \tag{90}$$

$$\nu(h) = T_{22}(h) = h\eta_0(Z)\frac{I_2}{2} + \xi(Z)(1 - I_1) \tag{91}$$

with

$$I_1 = \frac{2\hat{\eta}_0 - 1 - \hat{\xi}}{4Z}U_1, \quad I_2 = -\frac{2Z\hat{\eta}_0 + 1 - \hat{\xi}}{2hZ}U_1,$$

and

$$\hat{\xi} = \xi(\hat{Z}) = 2\xi(Z)^2 - 1, \quad \hat{\eta}_0 = \eta_0(\hat{Z}) = \eta_0(Z)\xi(Z), \quad \hat{Z} = 4Z.$$

The Neumann approach of truncating the Neumann series and using a Filon-type method to approximate the integrals, led us to expressions which are not linear in $\xi(Z)$ and $\eta_0(Z)$, in contrast to the CPM formulae (84)-(87). By rearranging the terms in (88)-(91), introducing the set of functions $\eta_1, \eta_2, \ldots,$ and using the trigonometric and hyperbolic identities, the formulae (88)-(91) can be proven to be equal to (84)-(87). For higher order methods it is not so

obvious to reduce formulae obtained by the Neumann method to the CPM ones, and a CPM approach which directly expresses the formulae in terms of the $\xi, \eta_0, \eta_1, \ldots$ functions should be prefered.

Another observation is that the formulae (84)-(87) reduce to the formulae for the Schrödinger CPM[1,1] method when $p = w = 1$:

$$\begin{aligned} u(h) &\approx \xi(Z) - \frac{\hat{Q}_1}{2}\eta_1(Z) \\ v(h) &\approx h\eta_0(Z) \\ hu'(h) &\approx Z(h)\eta_0(Z) \\ v'(h) &\approx \xi(Z) + \frac{\hat{Q}_1}{2}\eta_1(Z). \end{aligned}$$

5.3 CPM[2,2]: a method of order 6

As for the sixth order Neumann scheme [16], a sixth order CPM scheme is constructed by taking second degree approximating polynomials and two correction terms. With $\widetilde{P}_1 = (\hat{P}_1\bar{r})/Z = \hat{P}_1/(h^2\bar{P})$, $\widetilde{P}_2 = \hat{P}_2/(h^2\bar{P})$ we obtain

$$\begin{aligned} u(h) \approx & \xi(Z) + \left[\frac{U_1\widetilde{P}_1}{12} + \frac{U_2\widetilde{P}_2}{20}\right]\eta_0(Z) + \left[-\frac{U_1}{2} - \frac{\widetilde{P}_1(V_2+U_1) + \widetilde{P}_2V_1}{4}\right]\eta_1(Z) \\ & + \left[\frac{3\widetilde{P}_1V_2 + \widetilde{P}_2(7V_1 - 3U_2)}{4} - \frac{U_2V_2}{40} - \frac{U_1V_1}{24}\right]\eta_2(Z) \\ & + \frac{5V_1(U_2+2V_2) + V_2(5U_1 - 3U_2)}{40}\eta_3(Z) \\ \frac{v(h)}{hP_0} \approx & \left[1 - \frac{\widetilde{P}_1^2}{2} + \widetilde{P}_2\right]\eta_0(Z) + \left[\frac{3(\widetilde{P}_1^2 + \widetilde{P}_2^2)}{2} - 3\widetilde{P}_2 + \frac{\widetilde{P}_1(U_1+V_1)}{12} + \frac{\widetilde{P}_2(U_2+V_2)}{20}\right]\eta_1(Z) \\ & - \left[\frac{V_2}{2} + \frac{15\widetilde{P}_2^2}{2} + \frac{\widetilde{P}_1(U_1+V_1)}{6} + \frac{\widetilde{P}_2(2U_2+7V_2)}{10}\right]\eta_2(Z) \\ & + \left[-\frac{V_2^2}{40} - \frac{V_1^2}{24} + \frac{\widetilde{P}_2(9U_2+24V_2)}{10}\right]\eta_3(Z) + \frac{9V_2^2}{40}\eta_4(Z) \end{aligned}$$

$$\begin{aligned} h\bar{P}\mu(h) \approx & \left[\frac{\widetilde{P}_1U_1}{12} + \frac{\widetilde{P}_2U_2}{20}\right]\xi(h) + \left[Z(h) + \frac{U_2}{2} + \frac{\widetilde{P}_2(V_2 - U_2 + U_1)}{4} + \frac{\widetilde{P}_1(V_1 - U_2)}{4}\right]\eta_0(Z) \\ & + \left[-\frac{3U_2}{2} - \frac{U_2V_2}{40} - \frac{U_1V_1}{24} - \frac{3\widetilde{P}_2(3V_2 - U_2 + U_1)}{4} - \frac{\widetilde{P}_1(3V_1 + U_1 - 3U_2)}{4}\right]\eta_1(Z) \\ & - \left[\frac{U_1V_1}{6} + \frac{U_2V_2}{40} + \frac{U_1V_2 - U_2V_1 + V_1^2 + V_2^2}{8} + \frac{3\widetilde{P}_2(U_2 - 10V_2)}{4}\right]\eta_2(Z) \\ & + \left[\frac{V_2(30V_2 + 27U_2)}{40}\right]\eta_3(Z) \end{aligned}$$

$$
\begin{aligned}
\nu(h) \approx & \left[1+\frac{\widetilde{P}_1(\widetilde{P}_1+2\widetilde{P}_2-2)}{2}\right]\xi(Z) \\
& + \left[(1-4\widetilde{P}_2)\widetilde{P}_1+\frac{(V_1+U_1)\widetilde{P}_1}{12}+\frac{(V_2+U_2)\widetilde{P}_2}{20}-\frac{\widetilde{P}_1^2-3\widetilde{P}_2^2}{2}\right]\eta_0(Z) \\
& + \left[\frac{(1-\widetilde{P}_1)V_1}{2}-\frac{9\widetilde{P}_2(\widetilde{P}_2-2\widetilde{P}_1)}{2}+\frac{\widetilde{P}_1V_2+\widetilde{P}_2U_1}{2}\right]\eta_1(Z) \\
& - \left[\frac{3\widetilde{P}_2(V_2+2V_1)}{2}+\frac{\widetilde{P}_1(V_2+3U_2)}{2}+\frac{V_2^2}{40}+\frac{V_1^2}{24}\right]\eta_2(Z)-\frac{V_2(3V_2+20V_1)}{40}\eta_3(Z)
\end{aligned}
$$

Again these formulae reduce to the corresponding Schrödinger CPM formulae (see e.g. the formulae mentioned in Appendix B of [11]) when $p = w = 1$, i.e. when all terms in $\widetilde{P}_1$ and $\widetilde{P}_2$ are dropped, and U_1, V_1 and U_2, V_2 are replaced by $\hat{Q}_1$ and $\hat{Q}_2$, respectively.

As for the fourth order method, we can remark that in contrast to the expressions for the sixth order Neumann method from [16], these CPM formulae are expressed in terms of the functions $\xi, \eta_0, \eta_1, \ldots$. The CPM approach generates corrections which are linear in ξ and η_0. The Neumann approach however led to equations which are cubic in ξ and η_0. This means that the CPM formulae are less sensitive to the numerical effect of near cancellation of large terms. Similar arguments were used in [9] (p. 233) to explain the reduced sensitivity of the piecewise perturbation methods over Gordon's approach.

As for the Neumann schemes from [16], the (absolute) error of the CPM behaves asymptotically (i.e. for $Z(h) \ll 0$) like $O(E)$ for a SL problem not in the Schrödinger form, while for a Schrödinger problem the error is $O(E^{-1/2})$ for $Z(h) \ll 0$ (see [17]). Consequently, for some well-behaved regular Sturm-Liouville problems, on which the Liouville's transformation can be applied and is not too expensive, it is still a good idea to transform the problem to the Schrödinger problem, since larger stepsizes can then be taken as the (index of the) eigenvalue increases or one and the same E-independent mesh can be used to compute all eigenvalues required.

6 Eigenvalue computations

To locate the eigenvalues of the boundary value problem we can use a shooting procedure. The CPM algorithms presented here are well suited for the repeated solution of the initial value problems appearing in this shooting procedure. Shooting procedures were described for the Schrödinger problem in [24] and for the Neumann schemes in [16]. The same Prüfer-based procedure as described in [16] can be used to count the oscillations in the solution as to home in on a particular eigenvalue. Many data can be computed before the actual shooting,

as e.g. the values of $\bar{q}$, $\bar{w}$, $\bar{P}$, $\hat{Q}_m$, $\hat{P}_m$, $\hat{W}_m$. This means that no further function evaluations of the coefficient functions are needed during shooting.

7 Some numerical experiments

The first test problem was also used as test problem for the SLCPM12 package in [13]. The problem has the coefficient functions

$$p(x) = (\gamma + x)^3, \quad q(x) = 4(\gamma + x), \quad w(x) = (\gamma + x)^5, \quad \gamma = \sqrt{0.2} \tag{92}$$

and is defined over the integration interval $[a, b]$ with $a = 0$ and $b = -\gamma + \sqrt{\gamma^2 + 2\pi}$ and $y(a) = y(b) = 0$. We call this problem the Paine problem, since by the Liouville transformation it can be transformed to a Schrödinger problem introduced by Paine in [25]:

$$p(x) = 1, \quad q(x) = 1/(x + 0.1)^2, \quad w(x) = 1, \quad y(0) = y(\pi) = 0. \tag{93}$$

The second test problem is the Collatz problem [26]

$$y'' + \frac{3}{4x^2} y = -\frac{1}{x^6} E y \quad y(1) = y(2) = 0. \tag{94}$$

This problem can be solved in closed form. The solutions are

$$E_k = \frac{64}{9} k^2 \pi^2, \quad y_k = \frac{3}{8k\pi} x^{3/2} \sin \frac{4k\pi}{3} \left(1 - \frac{1}{x^2}\right), \quad k = 1, 2, 3, \ldots. \tag{95}$$

Some numerical results for these test problems are given in the double logarithmic plot in Figure 1. The CPMs of order two, four and six were used to propagate y from a with starting values $y(a) = 0, y'(a) = 1$ to b. The methods were applied with constant step sizes h. The plots confirm the order of the different schemes numerically. Table 1 shows some eigenvalue computations.

In Figure 2, the E dependence of the error is illustrated for both a Schrödinger problem and a SL problem. We used two problems with the same eigenvalues: the Paine Schrödinger problem (93) and the Paine SL problem (92). Where the error increases with E for the SL problem, this is not the case for the Schrödinger problem: the error even slightly decreases. It is clear that when for a regular SL problem with sufficiently well-behaved p, q, w, a large batch of eigenvalues, or just particularly large eigenvalues are computed, it is a good idea to transform the problem to the Schrödinger form before a CPM is applied. For some problems however, the Liouville transformation may be difficult or expensive to realize and in this case applying a CPM directly to the SL problem forms a way out. Let us consider a SL problem on which both

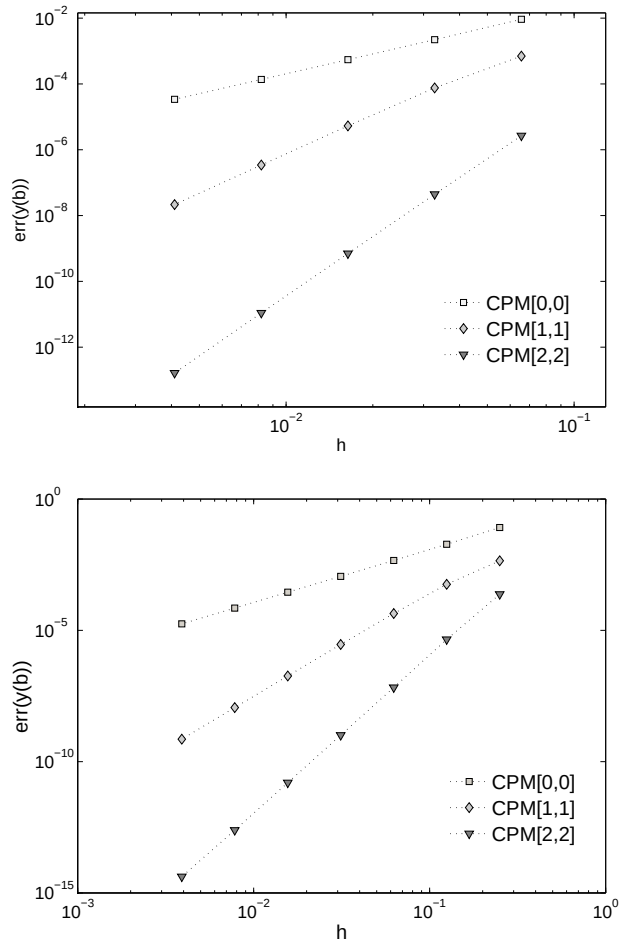

Fig. 1. Application of different CPM schemes on the Paine (upper figure) and the Collatz problem (lower figure). The absolute error in $y(b)$ is shown as a function of h for $E = E_9 = 102.42498839825$ (Paine) and $E = E_0 = 64\pi^2/9$ (Collatz).

Table 1
The relative errors in some eigenvalue computations for the Collatz problem and the Paine problem, computed by the sixth order CPM[2,2]. *nsteps* is the number of mesh intervals in the equidistant mesh and the notation $a(-b)$ stands for $a\,10^{-b}$.

	Collatz (nsteps= 128)		Paine (nsteps=192)	
k	E_k	rel. err.	E_k	rel. err.
0	70.1836836876	4.6(-13)	1.5198658211	3.0(-13)
10	47444.18579306	7.7(-11)	37.9644258619	5.3(-11)
20	182548.2030025	3.6(-10)	123.4977068009	1.9(-10)
30	405381.9379249	1.2(-9)	443.8529598352	4.2(-10)
40	715945.489746	4.6(-9)	963.9644462621	7.3(-10)
50	1114238.858465	3.2(-9)	1684.0120143379	1.1(-9)

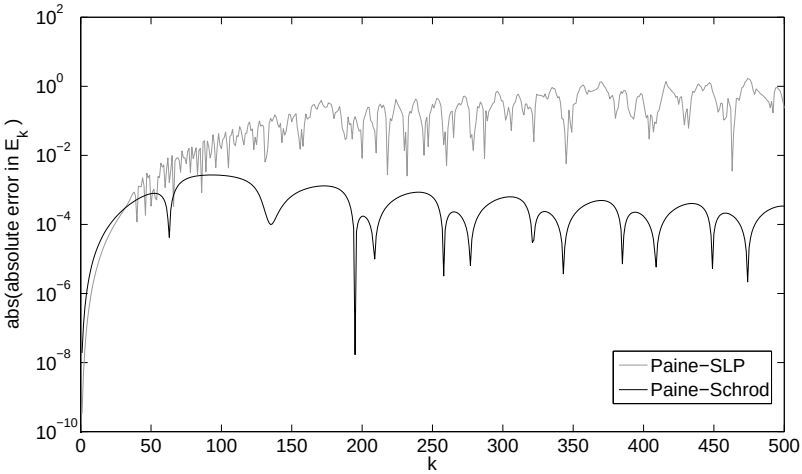

Fig. 2. The absolute value of the (absolute) errors in the eigenvalue approximations obtained with the sixth order CPM[2,2] for the Paine problem in the Schödinger form (Paine-Schrod) and the Paine problem in the Sturm-Liouville form (Paine-SLP) computed over a mesh with 64 equidistant mesh intervals.

Table 2
Error in the eigenvalues of the Pruess-Fulton problem 123, computed by CPM[2,2] on the mesh shown in Figure 3. E_k denotes the values of the two eigenvalues mentioned in [27]. *err* is the relative error between E_k and the computed eigenvalues.

k	E_k	*err*
1	9.139761599	7.2(-8)
9	714.36156162	7.8(-8)

SLCPM12 and MATSLISE fail:

$$p(x) = 1+x^{0.5}, \quad q(x) = 0, \quad w(x) = 1+(1-x)^{0.2}, \quad py'(0) = py'(1) = 0. \quad (96)$$

The problem is listed, as problem 123, in the Pruess-Fulton test set which was used to test SLEDGE [27]. The problem (96) is a regular SL problem. Applying Liouville's transformation, however, leads to a Schrödinger problem with singularities in both endpoints. In Figure 3, the potential function q of this Schrödinger problem is shown, as well as the coefficient functions p and w of the SL problem (96). Where the functions p and w are regular and well-defined over the interval [0,1], the derivatives of w are singular in 1 and the derivatives of p are singular in 0, causing the singularities in the Schrödinger q function. By applying a CPM directly to the SL problem (96), the difficulties associated with the singularities in the Schrödinger problem are avoided. Table 2 shows the eigenvalues we obtained by applying the sixth order CPM to (96). The same mesh selection procedure was used as in the MATSLEMN package, which implements the sixth order Neumann method [16], to obtain a mesh with 69 mesh points. The mesh is shown in Figure 3.

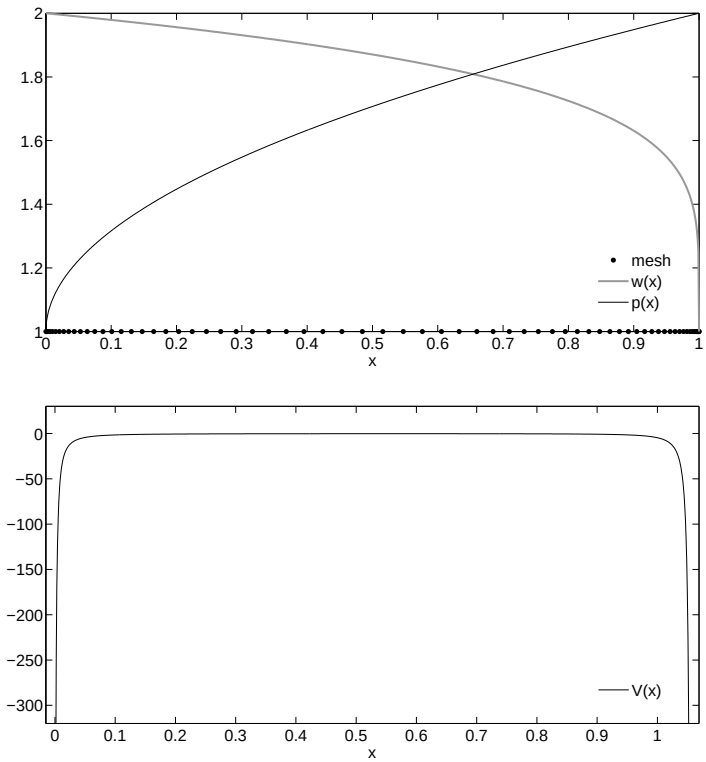

Fig. 3. Problem 123 in the Pruess-Fulton test set. In the upper plot the functions p and w of the SL problem and the mesh on which the results from Table 2 were computed, are shown. The lower figure contains a plot of the potential function of the Schrödinger problem which is obtained after applying Liouville's transformation.

The Collatz problem, the Paine problem and problem 123 from the Pruess-Fulton test set are regular problems. The CPM can, however, also be used to solve singular problems, i.e. problems defined on an infinite integration interval and problems with singular endpoints. These singular problems require a special numerical treatment: an interval truncation procedure must be adopted. As shown in [16] higher order CA methods (CPM or Neumann-based) preserve the interesting advantage of the Pruess methods that they allow a very simple truncation algorithm for singular problems. Evaluating the coefficient functions only at the Legendre nodes effectively regularizes the problem. A suitable (variable) mesh can be constructed in a very similar way as for the algorithm in SLEDGE or as described in [16] for the Neumann methods. We consider here a singular problem originating from mass and heat transfer studies as described by Dranoff in [28]. The problem is also listed, as problem 9, in the Pruess-Fulton test set [27]. The problem has the following form:

$$p = x,\ q = 0,\ w = 4x(1-x^2), \quad a = 0, b = 1, \quad py'(a) = py'(b) = 0. \tag{97}$$

Table 3 shows some eigenvalues computed with the sixth order CPM. Again, the same mesh selection procedure was applied as in MATSLEMN. The eigenvalues obtained here agree with the first approximations Dranoff computed

with little accuracy (6 digits) in [28] and the ones mentioned in [27].

Table 3
Some eigenvalues of the Dranoff problem, computed by the sixth order CPM.

k	E_k
1	6.41990300049
9	347.2056119022
19	1493.549086178

8 Conclusion

The CPM family was originally devised as a class of methods for the solution of one-dimensional, as well as multichannel and multidimensional Schrödinger equations (see e.g. [29,30]). These CPM exhibit the very important advantage that with them the energy dependence of the error is bounded. As a direct consequence, the step widths are unusually big and the computation is fast. Where until now the CPM could only be applied on general Sturm-Liouville (SL) problems after a Liouville transformation, we presented here new CPM formulae which can be applied directly on the SL problem. The new, more general formulae, allow us to also efficiently solve problems where a Liouville transformation is problematic or expensive. We showed that the CPM procedure is (theoretically) equivalent to applying a modified Neumann method. The CPM approach, however, leads to algorithms which are easy to construct and brings the formulae in a more convenient form. The formulae for a method upto order six were derived, but the procedure presented can be used to construct more correction terms and thus to realize higher order methods, forming equivalents to the high order CPM for Schrödinger problems.
We presented some numerical experiments illustrating the power of the CPM algorithms to solve a wide class of SL problems efficiently. Combined with automatic meshsize selection and error control, the CPM algorithms can form the basis for a new general-purpose Sturm-Liouville software package which outperforms the other codes. A substantial enhancement in efficiency can be expected from flexible programs which combine different techniques and deploy them adaptively on the fly. For problems of the Schrödinger type, the orginal CPM for Schrödinger problems are the most efficient. Without question, a Liouville's transformation can be a good idea for regular well-behaved SL problems, since it transforms the SL problem into a Schrödinger problem for which CPM have the best error behaviour, i.e. the error decreases with E. But the general CPM algorithms introduced in this paper are the best option for SL problems with discontinuities, singularities, or just strongly varying coefficient functions or with no second order derivatives of p and w available.

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