ON THE DYNAMICS OF SHOOTING METHODS FOR SOLVING STURM-LIOUVILLE PROBLEMS

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Abstract. It is shown that simple shooting and a standard iterative technique, e.g. Newton’s method, applied to a regular elliptic Sturm-Liouville boundary value problem form a chaotic dynamical system. We then develop and apply an action-angle modification of the Prüfer substitution based on a Hamiltonian formalism which, when applied to the transformed Sturm-Liouville system, eliminates the chaotic set and ensures convergence of the Newton iterates.

A further generalization of the Prüfer modified transformation leads to a class of higher order heuristic methods for integrating Sturm-Liouville equations.

1. Introduction

Regular Sturm-Liouville two-point boundary value problems have the form,

\begin{align*}
-(p(x)u')' + q(x)u &= \lambda r(x)u \\
\alpha u(a) - \alpha' p(a)u'(a) &= 0 \\
\beta u(b) + \beta' p(b)u'(b) &= 0
\end{align*}

where

\[ \alpha, \alpha', \beta, \beta' \geq 0, \quad \alpha + \alpha' \neq 0, \quad \beta + \beta' \neq 0, \]

\[ p(x), r(x) > 0 \ \forall x \in [a, b], \quad q, r \in C[a, b], \quad p \in C^1[a, b]. \]

For regular Sturm-Liouville problems, there exists an infinite number of real eigenvalues \( \{\lambda_k\}_{k=1}^\infty \) which can be ordered \( 0 < \lambda_1 < \lambda_2 < ... < \lambda_k \to \infty \) and for each \( \lambda_k \) the corresponding eigenfunction oscillates and has \( (k - 1) \) zeros in \( (a, b) \) [7]. Despite the fact that there is a rich and well developed theory for Sturm-Liouville problems (see for example [18]), there remain both regular and singular Sturm-Liouville equations for which no adequate numerical solutions have been computed [11]. Currently, several groups are working on developing software specifically designed to solve Sturm-Liouville problems [3], [4], [12], [15]. In this paper we analyze the

1991 Mathematics Subject Classification. Primary 34B24, 65L10; Secondary 58F05, 58F13.
dynamics of shooting methods for solving regular problems. By focusing on relatively straightforward techniques and problems we provide a fresh point of view and some new ideas which we believe can be used to improve more sophisticated methods to compute difficult singular problems.

For a fixed value of $\lambda$ the phase portrait of a Sturm-Liouville problem is composed of elliptic, linear, or hyperbolic curves depending on the sign of the coefficients in equation (1.1). This observation motivates the following definitions.

**Definition 1.** For a fixed value of $\lambda$ an elliptic interval for a Sturm-Liouville problem is an open interval $(a^*, b^*) \subseteq [a, b]$ such that for all $x \in (a^*, b^*)$, $\lambda r(x) - q(x) > 0$.

**Definition 2.** For a fixed value of $\lambda$ a hyperbolic interval for a Sturm-Liouville problem is an open interval $(a^*, b^*) \subseteq [a, b]$ such that for all $x \in (a^*, b^*)$, $\lambda r(x) - q(x) < 0$.

The trivial case of a subinterval on which $\lambda r(x) - q(x) = 0$ will be call a linear interval. We will call a Sturm-Liouville problem an elliptic problem if there exists a $\delta_0 < \lambda_1$ (where $\lambda_1$ is the smallest eigenvalue) such that $(a, b)$ is an elliptic interval for all $\lambda > \delta_0$. A Sturm-Liouville problem containing both elliptic intervals and hyperbolic intervals will be called a mixed-type problem.

An example of an elliptic problem is the harmonic oscillator,

\begin{align}
(1.4) \quad u'' + \lambda u &= 0 \\
       u(0) = u(1) &= 0
\end{align}

while an example of a mixed-type problem is the Coffey-Evans equation which is one of the more difficult test problems in the literature [17],

\begin{align}
(1.5) \quad u'' + [\lambda r(x) - q(x)]u &= 0 \\
       u(\pi/2) = u(\pi/2) &= 0
\end{align}

where $r(x) = 1$ and $q(x) = -2 \beta \cos 2x + \beta^2 \sin 2x$.

We will show that fundamental differences in the dynamics and stability properties of elliptic intervals and of hyperbolic intervals indicate that it may be advantageous to develop separate numerical strategies for each case. These strategies can then be combined to produce a successful method for solving mixed-type problems.
**STURM-LIOUVILLE PROBLEMS**

**Numerical shooting.** A standard technique for solving a Sturm-Liouville problem numerically is to use single (or simple) shooting which we will refer to as shooting. The strategy is to fix an initial value of $\lambda$ and then solve the initial value problem using an integrator such as a Runge-Kutta method. In order to guarantee a unique solution to the initial value problem, the initial conditions are normalized as follows:

$$u(a) = \begin{cases} \frac{\alpha'}{\alpha} & \alpha \neq 0 \\ 1 & \alpha = 0 \end{cases} \quad \text{and} \quad (p u')(a) = \begin{cases} 1 & \alpha \neq 0 \\ 0 & \alpha = 0. \end{cases}$$

The solution to the initial value problem depends on both $\lambda$ and $x$, and will be denoted by $(u(\lambda, x), u'(\lambda, x))$. Then $(u(\lambda, x), u'(\lambda, x))$ is a solution to the boundary value problem if it solves the initial value problem and satisfies the boundary condition

$$\psi(\lambda) \overset{\text{def}}{=} \beta u(\lambda, b) + \beta' p(b) u'(\lambda, b) = 0.$$  

(1.6)

Roots of this nonlinear equation correspond to eigenvalues of the Sturm-Liouville system. Newton’s method,

$$\lambda_{n+1} = N_{\psi}(\lambda_n) \overset{\text{def}}{=} \lambda_n - \frac{\psi(\lambda_n)}{\partial \psi / \partial \lambda}(\lambda_n),$$

(1.7)

can be used to determine a sequence of iterates which, it is hoped, will converge to the desired eigenvalue. The partial, $\partial \psi / \partial \lambda$ is a continuous function of $\lambda$ ([9], p. 95) and is determined by solving an associated variational equation [10].

**Prüfer transformation.** The polar coordinate substitution known as the Prüfer transformation makes it possible to specify the eigenvalue to be computed. This technique first appeared in a 1923 paper [16]. There the change of variables was used to develop oscillation and comparison theorems. The Prüfer transformation is

$$u(x) = R(x) \sin \theta(x)$$
$$p(x) u'(x) = R(x) \cos \theta(x).$$

(1.8)

When (1.8) is substituted into (1.1) the second order differential equation is decoupled into two first order equations.

$$\theta'(x) = \frac{1}{p(x)} \cos^2 \theta(x) + (\lambda r(x) - q(x)) \sin^2 \theta(x)$$

(1.9)
$$R'(x) = \left[\frac{1}{p(x)} - (\lambda r(x) - q(x))\right] \sin \theta(x) \cos \theta(x) R(x)$$

(1.10)

with corresponding boundary conditions

$$\theta(a) = \tan^{-1} \left( \frac{\alpha'}{\alpha} \right), \quad 0 \leq \theta(a) < \pi$$

(1.11)
$$\theta(b) = \tan^{-1} \left( \frac{-\beta'}{\beta} \right) + k \pi, \quad 0 < \theta(b) \leq \pi$$

(1.12)
where \( k \) depends on the eigenvalue to be determined. This boundary value problem can be solved by finding solutions to the initial value problem (1.9), (1.11) which satisfy the nonlinear equation,

\[
\phi(\lambda) \overset{\text{def}}{=} \theta(\lambda, b) - \tan^{-1} \left( \frac{\theta(\lambda, a)}{u(\lambda, a)} \right) - k \pi = 0.
\]

Once \( \lambda \) and \( \theta(\lambda, x) \) are known, \( R(x) \) can be determined by quadrature

\[
R(x) = R(a) \exp \int_a^x \left[ \frac{1}{p(t)} - (\lambda r(t) - q(t)) \right] \sin \theta(t) \cos \theta(t) \, dt.
\]

**Numerical methods.** Several variants of the Prüfer transformation have been developed and used in implementations of the shooting method for solving Sturm-Liouville problems. Bailey [2] developed the modified Prüfer method

\[
\begin{align*}
\phi(x) &= S^{-1/2} R(x) \sin \theta(x) \\
p(x) u'(x) &= S^{1/2} R(x) \cos \theta(x),
\end{align*}
\]

where the scaling constant \( S \) was chosen by the rule, \( S = k\pi/U \) and \( k \) is the eigenvalue index and \( U \) is approximately the length of the interval on which \( \lambda r - q \) is positive. This rule was implemented in the SLEIGN code [5]. Recently, the software has been extended to solve both regular and singular problems [3], [4].

Pryce [17] implemented another modified Prüfer substitution of the form (1.14) where \( S \) is a positive piecewise linear function chosen so that both \( S/p - |q|/S \) and \( S'/S \) are kept small. Shooting is performed from each end-point of the interval \([a, b]\) to a central point. Roots of the resulting “miss-distance” function are then computed. This method is implemented in the NAG library as D02KDF.

Another strategy is to replace the coefficient functions of the Sturm-Liouville equation by piecewise polynomial approximations. Banks and Kurowski [6], Canosa and DeOliveira [8], and Paine and de Hoog [13] analyzed the case of piecewise constant coefficient approximations. The standard reference for convergence in the piecewise polynomial case is Pruess [14]. This strategy has been implemented for the piecewise constant coefficient case by Pruess and Fulton in the code SLEDGE [15]. Their code is intended to solve both regular and singular problems by using global error estimates.

Marletta and Pryce [12] have developed a method which combines ideas based on the Prüfer substitution with the technique of replacing the coefficient functions by piecewise constant functions and then solving the simplified problems exactly. Currently, they are working on implementing this method for singular problems.

In this article we develop a new modification of the Prüfer transformation and compare its global performance with some of the above techniques from the point of view of differentiable
dynamical systems. Within the context of shooting the eigenvalues are roots of a nonlinear equation. In general, an iterative method is required to determine these eigenvalues, e.g. Newton’s method.

In the next section we show that the iterates of Newton’s method applied to this nonlinear equation are chaotic for regular elliptic problems. In §3 the symplectic geometry inherent in Hamiltonian systems is used to develop a modification of the Prüfer transformation based on action-angle variables. We prove in §4 that when shooting is applied to this transformed Sturm-Liouville system, the chaotic set is eliminated and Newton’s method converges globally for regular elliptic problems. In §5 the action-angle Prüfer substitution is extended to include mixed-type problems and a class of numerical methods using this extension is introduced. In §6 we describe the Hamiltonian dynamics of Sturm-Liouville problems with piecewise constant coefficients in order to isolate and illuminate the potential numerical problems associated with mixed-type problems.

2. Existence of a chaotic set of Newton iterates for elliptic problems

We now analyze the dynamics of the system determined by iteration of Newton’s method applied to regular elliptic Sturm-Liouville problems. Using theory developed by Saari and Urenko [19] we prove that the iterates of Newton’s method applied to \( \psi(\lambda) = \beta u(\lambda, b) + \beta' p(b) u'(\lambda, b) \) are chaotic.

First we review some definitions and notation from [19]. For a smooth function \( f \) define the set of roots of \( f \) on a given set \( \Lambda \) to be, \( Z(f) \overset{\text{def}}{=} \{ \lambda \in \Lambda : f(\lambda) = 0 \} \). The forward iterates of Newton’s method applied to \( f \), that is \( N_f^m(\lambda) \), either converge to a root of \( f \), diverge by landing in \( Z(f') \), or neither converge nor diverge. These three sets are denoted respectively by

\[
\begin{align*}
S_1 & \overset{\text{def}}{=} \{ \lambda \in \mathbb{R} : N_f^m(\lambda) \to Z(f) \text{ as } n \to \infty \} \\
S_2 & \overset{\text{def}}{=} \{ \lambda \in \mathbb{R} : \exists m \text{ such that } N_f^m(\lambda) \in Z(f') \} \\
S_3 & \overset{\text{def}}{=} \mathbb{R} \sim (S_1 \cup S_2)
\end{align*}
\]

and are invariant sets under iteration of \( N_f \).

**Definition 3.** A function \( f \) will be called oscillatory if it satisfies all of the following conditions:

1. The zeros of \( f \) separate or are equal to the zeros of \( f' \).
2. The zeros of \( f' \) separate or are equal to the zeros of \( f'' \).
3. \( Z(f), Z(f') \) consist of isolated points.
(4) If $Z(f)$ is finite then $Z(f')$ is contained within the interval defined by the extreme points of $Z(f)$; also, $Z(f'')$ is contained within the interval defined by the extreme points of $Z(f')$.

A typical oscillatory function is illustrated in Figure 1. Figure 2 depicts one step of Newton’s method applied to $\psi(\lambda)$. Roots of $\psi$ correspond to fixed points of $N_\psi$. The essential property of $N_\psi(\lambda)$ which allows Newton’s method to admit chaotic behavior is that $N_\psi(\lambda)$ approaches infinity as $\lambda$ approaches $\gamma$. To describe the dynamics of the Newton map, a symbolic representation is needed. Label the bounded intervals of $\mathbb{R} \sim Z(f')$ by $\ldots, a_{-1}, a_0, a_1, a_2, \ldots$ and let $\mathcal{A}$ be the set of these labels. Let $\mathbf{b} = (b_0, b_1, \ldots)$, where $b_i \in \mathcal{A}$, be an ordered sequence listing the future for some Newton sequence. For a given sequence $\mathbf{b}$ we wish to find some point $p$ which lies in the interval corresponding to $b_0$ such that $N^i(p)$ lies in the interval $b_i$ for all $i$. The set of all possible sequences $\mathbf{b}$ is given by $D = \mathcal{A}^I$ where $I$ is the set of nonnegative integers. In order to link the dynamics of iteration for Newton’s method applied to a function $f$ and the symbolic dynamics, define the shift map $T$ by $T(b_0, b_1, b_2, \ldots) = (b_1, b_2, \ldots)$. We seek a point $p$ so that $N^i(p)$ will lie in the interval associated with $T^i(\mathbf{b}), i = 0, 1, 2, \ldots$. The following lemma states when this is possible.

**Lemma 2.1.** (Saari, Urenko [19]) Let $f$ be a smooth oscillatory function where $f'$ has at least 3 distinct zeros. Let $S_3$ have the subspace topology inherited from $\mathbb{R}$. Then there is a continuous surjective map $h : S_3 \rightarrow D$ such that the diagram below commutes. In addition, corresponding to any periodic sequence in $D$ (with the exception of the constant sequences), there is a periodic orbit of $N$ with the same period. For every constant sequence in $D$, there is a pair of period two points in the indicated interval.

\[
\begin{array}{c}
S_3 \\
N \\
S_3 \\
\end{array}
\begin{array}{c}
h \\
\uparrow \\
h \\
\end{array}
\begin{array}{c}
D \\
T \\
D \\
\end{array}
\]

The point $p$ in the interval $b_0$ is mapped to $h(p) = (b_0, b_1, \ldots)$ and $N(p)$ is mapped to $h(N(p)) = T(b_0, b_1, \ldots) = (b_1, \ldots)$ and therefore $N(p)$ is in the interval $b_1$. Intuitively, the surjectivity of $h$ implies that all possible types of random behavior can occur. In particular, the
Figure 1. $\psi(\lambda)$ for the harmonic oscillator

Figure 2. One step of Newton’s method applied to $\psi(\lambda)$
lemma states that is is possible to find a periodic orbit of any order which can travel through any prescribed ordering of intervals in $\mathcal{A}$. In this paper we will refer to the iterates of a function $f$ on a set $S$ which satisfy Lemma 2.1 as **chaotic iterates**. Furthermore the set of points on which Newton’s method produces chaotic iterates is perfect.

**Lemma 2.2.** (Saari, Urenko [19]) Define $CS = S_3$ if $Z(f)$ is bounded and $S_2 \cup S_3$ otherwise. With the assumptions of Lemma 2.1, $CS$ is a perfect set (i.e., it is closed and every point is an accumulation point of the set).

The oscillatory motion of $\psi(\lambda)$ for the harmonic oscillator in Figure 1 is typical of the behavior for regular elliptic Sturm-Liouville problems. We will apply Lemma 2.1 to $\psi(\lambda)$ to prove that for all regular elliptic Sturm-Liouville problems there exists a set of initial values of $\lambda$ on which Newton’s method applied to $\psi(\lambda)$ produces chaotic iterates. To satisfy the hypotheses of Lemma 2.1, $\psi(\lambda)$ must be shown to be an oscillatory function. Because $\psi(\lambda)$ cannot be determined explicitly, we must first approximate the coefficients by piecewise constant functions and show that the corresponding $\psi(\lambda)$ for any such approximation is oscillatory. Then we will use these approximations to prove that $\psi(\lambda)$ is oscillatory for all regular elliptic Sturm-Liouville problems.

**Piecewise constant coefficient approximation of a Sturm-Liouville problem.** Following [14], on each interval $(x_{j-1}, x_j]$ of a mesh

$$\pi \overset{def}{=} \{a = x_0 < x_1 < \cdots < x_n = b\},$$

chosen to be of uniform size $h$ for simplicity, the coefficients of the Sturm-Liouville equation can be approximated by

$$p_j = p(x_j) \quad r_j = r(x_j) \quad q_j = q(x_j).$$

The approximate Sturm-Liouville problem is

$$-(p_j \hat{\alpha}_j')' + q_j \hat{\alpha}_j = \lambda r_j \hat{\alpha}_j$$

(2.3)

$$\alpha \hat{\alpha}_1(a) - \alpha' p_1 \hat{\alpha}_1'(a) = 0$$

(2.4)

$$\beta \hat{\alpha}_n(b) + \beta' p_n \hat{\alpha}_n'(b) = 0,$$

(2.5)

where $p_j$, $q_j$ and $r_j$ are constant on each interval $(x_{j-1}, x_j]$. Appropriate normalizing conditions are chosen as in (1.6) to ensure a unique solution to the initial value problem given a value of $\lambda$. In each interval $(x_{j-1}, x_j]$ a solution to the initial value problem (2.3) (2.4) has the form

$$\hat{\alpha}_j(\lambda, x) = c_j \eta_j(\lambda, x) + d_j \zeta_j(\lambda, x),$$

(2.6)
where \( \eta_j \) and \( \zeta_j \) are fundamental solutions of \( \hat{u}'' = -\mu_j \hat{u} \) and \( \mu_j = (\lambda x_j - q_j)/p_j \). The functions, \( \eta_j \) and \( \zeta_j \), are defined as

\[
\eta_j(\lambda, x) = \begin{cases} 
\cos(\sqrt{\mu_j}(x - x_{j-1})) & \mu_j > 0 \\
1 & \mu_j = 0 \\
\cosh(\sqrt{-\mu_j}(x - x_{j-1})) & \mu_j < 0 
\end{cases}
\]

\[
\zeta_j(\lambda, x) = \begin{cases} 
\sin(\sqrt{\mu_j}(x - x_{j-1}))/\left(p_j \sqrt{\mu_j}\right) & \mu_j > 0 \\
(x - x_{j-1})/(p_j \sqrt{-\mu_j}) & \mu_j = 0 \\
\sinh(\sqrt{-\mu_j}(x - x_{j-1}))/\left(p_j \sqrt{-\mu_j}\right) & \mu_j < 0 
\end{cases}
\]

and at each of the mesh points the solutions are matched so that \( \hat{u} \) and \( \hat{u}' \) are continuous. Therefore at each \( x_j \), \( j = 1, \ldots, n \), we need the condition

\[
(2.7) \quad \begin{pmatrix} p_j \hat{u}'_j \\ \hat{u}'_{j-1} \end{pmatrix}(\lambda, x_j) = P \begin{pmatrix} p_j \hat{u}'_{j-1} \\ \hat{u}'_{j-1} \end{pmatrix}(\lambda, x_j)
\]

where the matrix \( P \) is given by

\[
(2.8) \quad P = \begin{pmatrix} p_j \hat{\zeta}_j & p_j \eta_j \\ \zeta_j & \eta_j \end{pmatrix}(\lambda, x_j)
\]

\[
= \begin{cases} 
\begin{pmatrix} \cos(\sqrt{\mu_j}h) & -p_j \sqrt{\mu_j}\sin(\sqrt{\mu_j}h) \\
\frac{1}{p_j \sqrt{\mu_j}}\sinh(\sqrt{\mu_j}h) & \cos(\sqrt{\mu_j}h) \end{pmatrix} & \text{when } \mu_j > 0 \\
\begin{pmatrix} \cosh(\sqrt{\mu_j}h) & p_j \sqrt{\mu_j}\sinh(\sqrt{\mu_j}h) \\
\frac{1}{p_j \sqrt{\mu_j}}\sinh(\sqrt{\mu_j}h) & \cosh(\sqrt{\mu_j}h) \end{pmatrix} & \text{when } \mu_j < 0 \\
\begin{pmatrix} 1 & 0 \\
1 & 1 \end{pmatrix} & \text{when } \mu_j = 0 
\end{cases}
\]

where \( h = x_j - x_{j-1} \) for all \( j \).

Using this approximation the following lemma, which will be proved in §5, is true.

**Lemma 2.3.** For every piecewise constant coefficient approximation (2.2) of a regular elliptic Sturm-Liouville problem, when \((\hat{u}(\lambda, b), \hat{u}'(\lambda, b))\) is a solution of the initial value problem (2.3), (2.4) the function

\[
(2.9) \quad \dot{\psi}(\lambda) \overset{d_e}{=} \beta\hat{u}(\lambda, b) + \beta'p(b)\hat{u}'(\lambda, b)
\]

is an oscillatory function of \( \lambda \) for all \( \lambda > \delta_0 \) (where \( \delta_0 \) is given in Definition 1).

Now by utilizing work by Prüss [14] on the uniform convergence of a numerical method which approximates the coefficients of Sturm-Liouville problems by piecewise polynomial approximations, we can show that \( \psi(\lambda) \) is a oscillatory function for all regular elliptic Sturm-Liouville problems. We will only state Prüss’ results for piecewise constant coefficients, although he has proved a more general result for piecewise polynomial approximations.
Lemma 2.4. (Prüss[14]) If $p, q, r \in C^1[a, b]$, then for piecewise constant approximate problems (2.3), for $h$ sufficiently small, $\| u_k - \hat{u}_k \| = O(h)$ and $\| p_k u'_k - p_k \hat{u}'_k \| = O(h)$ for each $k$.

Thus, the solution to the initial value problem (1.1), (1.2) is uniformly approximated by the solution of the approximate initial value problem (2.3). The following lemma follows directly from Lemma 2.3 and Lemma 2.4 when $h$ is chosen to be sufficiently small.

Lemma 2.5. The function $\psi(\lambda) \overset{def}{=} \beta u(\lambda, b) + \beta' p(b) u'(\lambda, b)$ where $u$ and $u'$ are solutions to the elliptic initial value problem (1.1), (1.2) is an oscillatory function of $\lambda$.

Finally, Lemmas 2.1, 2.2, and 2.5 can be combined to produce the main result of this section.

Theorem 2.6. When shooting is applied to a regular elliptic Sturm-Liouville problem (1.1), (1.2), (1.3) then there exists a perfect set of initial values of $\lambda$ on which the iterates of Newton’s method applied to $\psi(\lambda)$, defined by (1.6), are chaotic.

3. A modification of shooting

We now develop a modification of the Prüss transformation which eliminates the chaotic set of Newton iterates described above in Theorem 2.6. A Sturm-Liouville equation is a Hamiltonian system with Hamiltonian

$$(3.1) \quad H(u, u') = \frac{(u')^2}{2p(x)} + (\lambda r(x) - q(x)) \frac{u^2}{2} = \kappa(x).$$

We will utilize the underlying symplectic geometry of Hamiltonian systems to develop this modification.

The canonical variables for a completely integrable Hamiltonian system are action-angle variables. Usually, action-angle variables are difficult to compute explicitly. Further, a regular Sturm-Liouville system with nonconstant coefficients is not integrable and its Hamiltonian is not necessarily identically equal to a constant. Action-angle variables cannot be applied directly to such systems. However, when shooting is applied to a Sturm-Liouville system modified by a Prüss transformation, Newton’s method is applied to the nonlinear equation (1.13). Thus the properties of action-angle variables are only required at the point $x = b$. Although we cannot transform a Sturm-Liouville system into action-angle variables, we can create a change of variables which causes the transformed system to behave like action-angle variables at precisely the point $x = b$ and it turns out that this is sufficient.
Action-angle variables. Below we outline the construction of action-angle variables. A more complete discussion of symplectic geometry and action-angle variables can be found in [1].

**Definition 4.** [1] In general, a transformation \( S : \mathbb{R}^{2n} \to \mathbb{R}^{2n} \) is symplectic if and only if it is linear and canonical, i.e., preserves the differential 2-form \( \omega^2 = dp_1 \wedge dq_1 + \cdots + dp_n \wedge dq_n \).

We note that in \( \mathbb{R}^2 \) a linear transformation is symplectic if and only if its determinant is 1.

The strategy for constructing action-angle variables is to find symplectic coordinates \((I, \varphi)\) such that the first integral \( F \) depends only on \( I \), and \( \varphi \) is an angular coordinate on the torus, \( M_a = \{ x : F(x) = a \} \). For the system

\[
\begin{align*}
\dot{q} &= \frac{\partial H}{\partial p} \\
\dot{p} &= -\frac{\partial H}{\partial q}
\end{align*}
\]

with Hamiltonian \( H(p, q) \), under the hypotheses of Liouville’s theorem [1], there is a canonical transformation \((p, q) \to (I, \varphi)\) so that the solution of the differential equation takes the form

\[
\begin{align*}
\frac{dI}{dx} &= 0 \\
\frac{d\varphi}{dx} &= \omega(I) = \frac{\partial H}{\partial I}
\end{align*}
\]

**Action-angle modified Prüfer transformation.** To motivate our modification of the Prüfer transformation we will compute the action-angle variables for an example which is slightly more general than the harmonic oscillator. Specifically, we consider the following regular elliptic Sturm-Liouville problem with constant coefficients:

\[
(3.2) \quad (pu'(x))' + (\lambda r - q)u(x) = 0 \\
u(a) = u(b) = 0
\]

where \( p, q, r \) are constants such that \( p, r > 0 \). In this example, the Hamiltonian is constant and action-angle variables can be computed explicitly,

\[
(3.3) \quad H(u, u') \overset{df}{=} \frac{(u')^2}{2p} + (\lambda r - q)\frac{u^2}{2} = \kappa.
\]

The action is,

\[
(3.4) \quad I(\kappa) = \frac{1}{2\pi} \int_{M_a} u' \, du = \frac{2}{\pi} \frac{1}{\sqrt{2\kappa[\lambda r - q]}} \int_0^{\sqrt{2\kappa[\lambda r - q]}} \sqrt{2p\kappa - \omega^2 u^2} \, du = \frac{\kappa}{\sqrt{\mu}}
\]
where $\mu = (\lambda r - q)/p$ and $\omega = \sqrt{p(\lambda r - q)}$. This implies that $\kappa(I) = \sqrt{p}I$. Now a generating function

$$S(I, u) = \int_0^u \sqrt{2\omega I - \omega^2 u_1^2} \, du_1$$

can be used to determine the angle,

$$\theta(I, u) = \frac{\partial S}{\partial I}(I, u)$$

(3.5)

$$= \frac{\partial H}{\partial I} \int_0^u \frac{du_1}{\sqrt{2\omega I - \omega^2 u_1^2}}$$

$$= \sqrt{\mu} x.$$

Hence, the equations (3.4), (3.5) produce the desired change of variables necessary to transform the system to action-angle coordinates

$$\begin{pmatrix} u \\ u' \end{pmatrix} = \begin{pmatrix} \omega^{-1/2} & 0 \\ 0 & \omega^{1/2} \end{pmatrix} \begin{pmatrix} \sqrt{2I} \sin \theta \\ \sqrt{2I} \cos \theta \end{pmatrix}.$$

Note that for $x = b$ the angle is an increasing concave function of $\lambda$. This is exactly the property which we want to retain when this transformation is extended to include all regular elliptic Sturm-Liouville equations.

The transformation which we will refer to as the action-angle modification of the Prüfer transformation is

(3.6)

$$\begin{pmatrix} u(x) \\ p(x)u'(x) \end{pmatrix} = \begin{pmatrix} \omega^{-1/2} & 0 \\ 0 & \omega^{1/2} \end{pmatrix} \begin{pmatrix} R(x) \sin \theta(x) \\ R(x) \cos \theta(x) \end{pmatrix}$$

where $\omega = \sqrt{(\lambda r(b) - q(b))/p(b)}$. Note that the system has not been transformed to action-angle variables. Instead, a polar symplectic transformation which retains the properties of action-angle variables at the point $x = b$ has been generated. This results in the following boundary value problem for $\theta$

(3.7)

$$\theta' = \frac{\omega}{p(x)} \cos^2(\theta) + \frac{(\lambda r(x) - q(x))}{\omega} \sin^2(\theta).$$

(3.8)

$$\theta(a) = \tan^{-1} \left( \frac{\omega \alpha'}{\alpha} \right)$$

(3.9)

$$\theta(b) = \tan^{-1} \left( \frac{-\omega \beta'}{\beta} \right) + k\pi,$$

and

(3.10)

$$\phi(\lambda, b) \overset{def}{=} \theta(\lambda, b) - \tan^{-1} \left( \frac{-\omega \beta'}{\beta} \right) - k\pi.$$

Extensive numerical tests indicate that the behavior illustrated by the harmonic oscillator (1.4) is typical of the behavior exhibited for general elliptic Sturm-Liouville problems. In what follows we present illustrations of that case. Figures 3 and 4 depict $\phi(\lambda)$ and $N_\phi(\lambda)$ respectively.
when the unmodified Prüfer method (1.8) is applied to the harmonic oscillator. Although \( \phi(\lambda) \) is monotone increasing, without any modification the small ripples in \( \phi(\lambda) \) cause the Newton function to have high frequency oscillations. These oscillations become increasingly pronounced as \( \lambda \) increases as shown in Figure 4. It is likely that the high frequency oscillations in the right-hand portion of the graph are due to numerical errors.

Figures 5 and 6 depict \( \phi(\lambda) \) and \( N_\phi(\lambda) \) for a modified Prüfer method (1.14). This modification dampens the oscillations, but does not eliminate them completely. Test results show that for larger values of \( k \) (corresponding to larger eigenvalues) these oscillations become more pronounced.

Figures 7 and 8 illustrate the behavior of \( \phi(\lambda) \) and \( N_\phi(\lambda) \) when the action-angle modified Prüfer method (3.6) is applied to the harmonic oscillator. Our action-angle modified system retains exactly those symplectic properties which are needed to make \( \phi(\lambda) \) an increasing and concave function. Therefore, it is plausible that a proof for the convergence of the Newton iterates is possible in the context of our action-angle modification.

4. Global convergence of Newton’s method

We utilize piecewise constant coefficient approximations to prove that when the action-angle modified Prüfer method is applied to a regular elliptic Sturm-Liouville problem, Newton’s method converges globally. In order to do this we will show that the conditions of the following lemma, which is a corollary of a standard convergence result for Newton’s method [20], are satisfied.

**Lemma 4.1.** Let \( f(x) \) be twice continuously differentiable on \( [a, b] \) and let the following conditions be satisfied:

(i) \( f(a)f(b) < 0 \)

(ii) \( f'(x) \neq 0, \, x \in [a, b] \)

(iii) \( f''(x) \) is either \( \geq 0 \) or \( \leq 0 \) \( \forall x \in [a, b] \)

(iv) at the endpoints \( \left| f(a) \right| / | f'(a) | < b - a \) and \( \left| f(b) \right| / | f'(b) | < b - a \).

Then Newton’s method applied to \( f(x) \) converges to a unique root of \( f(x) = 0 \) on \( [a, b] \).

We first prove some preparatory lemmas for piecewise constant coefficient approximations of the Sturm-Liouville problem. When the action-angle modified Prüfer substitution,

\[
\hat{u}_j = \omega_j^{-1/2} \hat{R}_j \sin \hat{\theta}_j \\
p_j \hat{a}_j = \omega_j^{1/2} \hat{R}_j \cos \hat{\theta}_j
\]
Figure 3. Typical example of $\phi(\lambda)$ using unmodified Prüfer

Figure 4. Typical example of $N_\phi(\lambda)$ using unmodified Prüfer
Figure 5. Typical example of $\phi(\lambda)$ using Bailey’s modified Prüfer

Figure 6. Typical example of $N_\phi(\lambda)$ using Bailey’s modified Prüfer
Figure 7. Typical example of $\phi(\lambda)$ using action-angle modified Prüfer

Figure 8. Typical example of $N_\phi(\lambda)$ using action-angle modified Prüfer
where $\omega_j = [(\lambda r_j - q_j)p_j]^{1/2}$, is applied to the approximate problem (2.3) on each interval $[x_{j-1}, x_j]$, the differential equation for $\hat{\theta}$ is

$$
(4.2) \quad \hat{\theta}_j = \frac{\omega_j}{p_j} \cos^2 \hat{\theta}_j + \frac{\lambda r_j - q_j}{\omega_j} \sin^2 \hat{\theta}_j \equiv \sqrt{\hat{\mu}_j}
$$

$$
(4.3) \quad \hat{\theta}_1(a) = \tan^{-1} \left( \frac{\omega_1 \alpha'}{\alpha} \right)
$$

when $\alpha \neq 0$ and where $\hat{\mu}_j = (\lambda r_j - q_j)/p_j$. When $\alpha = 0$ $\hat{\theta}_1(a) = \pi(2k + 1)/2$ and proofs are omitted for this straightforward case.

The general solution on $(x_{j-1}, x_j)$, is

$$
(4.4) \quad \hat{\theta}_j(\lambda, x) = \sqrt{\hat{\mu}_j}(x - x_{j-1}) + \sum_{i=1}^{j-1} \sqrt{\hat{\mu}_i} h + \tan^{-1} \left( \frac{\omega_i \alpha'}{\alpha} \right)
$$

At the point $x = b$, the solution is

$$
(4.5) \quad \hat{\theta}(\lambda, b) \overset{def}{=} \hat{\theta}_n(\lambda, b) = \sum_{i=1}^{n} \sqrt{\hat{\mu}_i} h + \tan^{-1} \left( \frac{\omega_n \alpha'}{\alpha} \right)
$$

and

$$
(4.6) \quad \hat{\phi}(\lambda) \overset{def}{=} \hat{\theta}(\lambda, b) - \tan^{-1} \left( -\frac{\beta \omega_n}{\beta} \right) - k\pi
$$

where $\hat{\theta}(\lambda, b)$ is a solution of the initial value problem (4.2),(4.3).

**Lemma 4.2.** $\hat{\theta}(\lambda, b)$ as defined by (4.5) is a strictly increasing, concave function of $\lambda$ (where it is assumed that $\lambda > \delta_0$) for regular elliptic Sturm-Liouville problems.

**Proof.** From equation (4.5), the first and second derivatives of $\hat{\theta}$ with respect to $\lambda$ can be computed exactly. By hypothesis, $\omega_j, r_j, p_j, \alpha_j, \alpha'_j > 0 \; \forall \; j = 1 \ldots n$, so

$$
(4.7) \quad \frac{\partial \hat{\theta}}{\partial \lambda}(\lambda, b) = \sum_{j=1}^{n} \frac{r_j h}{2\omega_j} + \frac{\alpha' r_1 p_1}{2\alpha\omega_1 \zeta_1} > 0
$$

$$
(4.8) \quad \frac{\partial^2 \hat{\theta}}{\partial \lambda^2}(\lambda, b) = -\sum_{j=1}^{n} \frac{h r_j^2 p_j}{4\omega_j^3} - \frac{\alpha'}{2\alpha} \left[ \frac{r_1 p_1}{\omega_1 \zeta_1} \right]^2 \left[ \left( \frac{\alpha'}{\alpha} \right)^2 \omega_1 + \frac{\zeta_1}{2\omega_1} \right] < 0
$$

for all $\lambda > 0$ where $\zeta_1 \overset{def}{=} (\omega_1 \alpha'/\alpha)^2 + 1$. \hfill \square

**Lemma 4.3.** The function $\hat{\phi}(\lambda)$ (4.6) is an increasing, concave function of $\lambda$ for all $\lambda > \delta_0$. 

**Proof.** We have defined \( \hat{\phi}(\lambda) = \hat{\theta}(\lambda, b) + \tan^{-1} \left( \frac{\beta'}{\omega_n \beta} \right) - k \pi \). By Lemma 4.2, \( \partial \hat{\theta} / \partial \lambda > 0 \) and \( \partial^2 \hat{\theta} / \partial \lambda^2 < 0 \) for all \( \lambda > \delta_0 \) and by hypothesis \( \omega_n, r_n, p_n, \beta, \beta' > 0 \). Thus

\[
\frac{\partial \hat{\phi}}{\partial \lambda}(\lambda) = \frac{\partial \hat{\theta}}{\partial \lambda}(\lambda, b) + \frac{\beta' r_n p_n}{2 \beta \omega_n \zeta_2} > 0
\]

\[
\frac{\partial^2 \hat{\phi}}{\partial \lambda^2}(\lambda) = \frac{\partial^2 \hat{\theta}}{\partial \lambda^2}(\lambda, b) - \frac{\beta'}{2 \beta^2} \left[ \frac{r_n p_n}{\omega_n \zeta_2} \right] \left[ \left( \frac{\beta'}{\beta} \right)^2 \omega_n + \frac{\zeta_2}{2 \omega_1} \right] < 0
\]

where \( \zeta_2 \stackrel{def}{=} (\omega_n \beta' / \beta)^2 + 1 \). \qed

Now Lemma 2.3 from Chapter 2 can be proved easily by using Lemma 4.3.

**Proof of Lemma 2.3:** We now prove that the function,

\[ \hat{\psi}(\lambda) = \beta \hat{u}(\lambda, b) + \beta' p(b) \hat{u}'(\lambda, b) \]

is an oscillatory function of \( \lambda \) for all \( \lambda > \delta_0 \) where \( \hat{u} \) and \( \hat{u}' \) are solutions of the initial value problem (2.3), (2.4).

Substituting the action-angle modified Prüfer transformation into equation (2.9), \( \hat{\psi}(\lambda) \) becomes,

\[
\hat{\psi}(\lambda) = \beta \omega^{-1/2} \hat{R} \sin \hat{\theta} + \beta' \omega^{1/2} \hat{R} \cos \hat{\theta} = A \sin \left( \hat{\theta} + \xi \right)
\]

where \( \xi = \tan^{-1} \left( \frac{\omega_n \beta'}{\beta} \right) \) and \( A = \hat{R} [\beta^2 / \omega_n + (\beta')^2 \omega_n]^{1/2} \). The functions \( A, \hat{\theta}, \) and \( \xi \) are all strictly increasing functions of \( \lambda \); therefore, \( \hat{\psi}(\lambda) \) must be an oscillatory function of \( \lambda \) for all \( \lambda > \delta_0 \). \qed

It is also true that \( \phi(\lambda) \) is uniformly approximated by \( \hat{\phi}(\lambda) \).

**Lemma 4.4.** If \( p, q, r \in C^1[a, b] \) and \( \theta(\lambda, b) \) is the solution of the initial value problem (3.7), (3.8), and \( \hat{\theta}(\lambda, b) \) is the solution of the initial value problem (4.2), (4.3) then for \( h \) sufficiently small,

\[ \| \phi_j - \hat{\phi}_j \| = O(h) \]

for each \( j = 1 \ldots n \).

**Proof.** Since \( \phi(\lambda) - \hat{\phi}(\lambda) = \theta(\lambda, b) - \hat{\theta}(\lambda, b) \), the function

\[ \theta(\lambda, b) = \tan^{-1} \left[ \frac{\omega_n (\lambda, b)}{p u' (\lambda, b)} \right] + k \pi \]

is a continuous, strictly increasing function of \( \lambda \). By Lemma 2.4, \( u \) and \( u' \) are uniformly approximated by \( \hat{u} \) and \( \hat{u}' \), so \( \theta \) is also uniformly approximated by \( \hat{\theta} \). \qed

Lemma 4.3 combined with Lemma 4.4 gives us the following result:
Lemma 4.5. The function, $\phi(\lambda) = \theta(\lambda, b) - \tan^{-1}(\omega_{1}a'/\alpha)$, where $\theta(\lambda, b)$ is a solution of the initial value problem (3.7), (3.8) is a strictly increasing, concave function of $\lambda$ for all $\lambda > \delta_{0}$.

Finally, using Lemma 4.5, the conditions for Lemma 4.1 can be satisfied to obtain the following main result of this section.

Theorem 4.6. Newton’s method applied to the shooting function $\phi(\lambda)$ defined by (3.10) for regular elliptic Sturm-Liouville problems transformed by the action-angle modification of the Prüfer substitution (3.7), (3.8), (3.9) converges for all $\lambda > \delta_{0}$.

5. A GENERAL MODIFIED PRÜFER TRANSFORMATION FOR MIXED-TYPE PROBLEMS

In this section we present a generalization of the action-angle modified Prüfer substitution which encompasses the elliptic and hyperbolic cases. Using the more general approach we can establish a heuristic class of numerical methods for solving Sturm-Liouville problems which we believe have interest in their own right. This general transformation is applicable when $\lambda r(b) - q(b) \neq 0$.

The general transformation is

$$
\begin{pmatrix}
u(x) \\
p(x)u'(x)
\end{pmatrix} =
\begin{pmatrix}
(\zeta\omega)^{-1/2}\zeta^{-1} & 0 \\
0 & (\zeta\omega)^{1/2}
\end{pmatrix}
\begin{pmatrix}
R\sin(\zeta\theta(x)) \\
R\cos(\zeta\theta(x))
\end{pmatrix}
$$

where

$$
\omega = \sqrt{(\lambda r(b) - q(b))p(b)}
$$

$$
\zeta = \frac{\omega}{|\omega|} = \begin{cases}
1 & \text{if } \lambda r(b) - q(b) > 0 \\
i & \text{if } \lambda r(b) - q(b) < 0
\end{cases}
$$

The resulting differential equation is

$$
\theta'(x) = \frac{\zeta\omega}{p(x)}\cos^{2}(\zeta\theta(x)) + \frac{(\lambda r(x) - q(x))}{\zeta^{3}\omega}\sin^{2}(\zeta\theta(x))
$$

$$
R'(x) = R'\sin(\zeta\theta(x))\cos(\zeta\theta(x))\left(\frac{\zeta^{2}\omega}{p(x)} - \frac{\lambda r(x) - q(x)}{\zeta^{2}\omega}\right).
$$

When $\lambda r(b) - q(b) > 0$, (5.1) is identical to (3.6). However, when $\lambda r(b) - q(b) < 0$, the action-angle modified Prüfer transformation is

$$
\begin{pmatrix}
u(x) \\
p(x)u'(x)
\end{pmatrix} =
\begin{pmatrix}
(\hat{\omega})^{-1/2} & 0 \\
0 & (\hat{\omega})^{1/2}
\end{pmatrix}
\begin{pmatrix}
R\sinh(\hat{\omega}\theta(x)) \\
R\cosh(\hat{\omega}\theta(x))
\end{pmatrix}
$$

while the differential equation for $\theta$ is

$$
\theta'(x) = \frac{\hat{\omega}}{p(x)}\cosh^{2}(\theta(x)) + \frac{(\lambda r(x) - q(x))}{\hat{\omega}}\sinh^{2}(\theta(x))
$$

where $\hat{\omega} \overset{\text{def}}{=} \omega = \sqrt{-\frac{(\lambda r(b) - q(b))p(b)}{\lambda r(b) - q(b)}}$ is real-valued.
Now, using this general transformation a class of numerical integration methods can be derived. The strategy is to combine the change of variables just developed with implicit integrators to construct a family of higher order integration methods. Indeed, we show that when the general action-angle modified Prüfer transformation is used the implicit dependence drops out.

On each subinterval \([x_{j-1}, x_j]\) of the mesh \(\pi\) the differential equation is

\[
\theta_j'(x) = \frac{\zeta_j \omega_j}{p(x)} \cos^2(\zeta_j \theta_j(x)) + \frac{(\lambda r(x) - q(x))}{\zeta_j^2 \omega_j} \sin^2(\zeta_j \theta_j(x)) = f(x, \theta_j(x))
\]

where \(\omega_j = \sqrt{(\lambda r(x_j) - q(x_j)) p(x_j)}\) and \(\zeta_j = \omega_j / |\omega_j|\) (and where we assume for technical convenience that \(|\omega_j| > \epsilon\) for some \(\epsilon > 0\) [12]). In order to ensure continuity at the mesh points we require the compatibility conditions

\[
\begin{align*}
  u_{j-1}(x_j) &= u_j(x_j) \\
  p(x) u_{j-1}'(x_j) &= p(x) u_j'(x_j)
\end{align*}
\]

\[
\frac{\tan(\zeta_{j-1} \theta_{j-1}(x_j))}{\zeta_{j-1}^2 \omega_{j-1}} = \frac{\tan(\zeta_j \theta_j(x_j))}{\zeta_j^2 \omega_j} \\
\Rightarrow \quad \theta_j(x_j) &= \frac{1}{\zeta_j} \tan^{-1} \left( \frac{\zeta_j \omega_j}{\zeta_{j-1}^2 \omega_{j-1} \tan(\zeta_{j-1} \theta_{j-1}(x_j))} \right) + k \pi.
\]

If we now use an implicit method to compute \(\theta_j(x_j)\), for example an implicit Euler’s method,

\[
\frac{\theta_j(x_j) - \theta_j(x_{j-1})}{h} \approx f(x_j, \theta_j(x_j)),
\]

we obtain

\[
\begin{align*}
\theta_j(x_j) &\approx \theta_j(x_{j-1}) + h f(x_j, \theta_j(x_j)) \\
= &\begin{cases} 
\theta_j(x_{j-1}) + h \left( \frac{\omega_j}{p(x_j)} \cos^2(\theta_j(x_j)) + \frac{(\lambda r(x_j) - q(x_j))}{\omega_j} \sin^2(\theta_j(x_j)) \right) & \text{if } \mu_j > 0 \\
\theta_j(x_{j-1}) + h \left( \frac{\omega_j}{p(x_j)} \cos^2(\theta_j(x_j)) + \frac{(\lambda r(x_j) - q(x_j))}{\omega_j} \sinh^2(\theta_j(x_j)) \right) & \text{if } \mu_j < 0.
\end{cases}
\end{align*}
\]

\[
\begin{align*}
= &\begin{cases} 
\theta_j(x_{j-1}) + h \mu_j^{1/2} & \text{if } \mu_j > 0 \\
\theta_j(x_{j-1}) + h \mu_j^{1/2} & \text{if } \mu_j < 0.
\end{cases}
\end{align*}
\]

\[
= \theta_j(x_{j-1}) + h \zeta_j \mu_j^{1/2}
\]

where \(\omega_j = \sqrt{(\lambda r(x_j) - q(x_j)) p(x_j)}\), \(\hat{\omega}_j = \omega_j\) and \(\mu_j = [\lambda r(x_j) - q(x_j)] / p(x_j)\), \(\hat{\mu}_j = -\mu_j\).

Because of our choice of transformation, i.e., the action-angle modified Prüfer substitution, the implicit dependence on \(\theta\) has disappeared. Let us note that in this case, when the implicit method is Euler’s method, we recover the approach implemented by Marletta and Pryce in [12].
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Our approach is quite general. As a further example, if an implicit trapezoid method is used, we obtain the following higher order scheme.

\[
\theta_j(x_j) \approx \theta_j(x_{j-1}) + \frac{h}{2} [f(x_{j-1}, \theta_j(x_{j-1})) + f(x_j, \theta_j(x_j))] \\
= \theta_j(x_{j-1}) + \frac{h}{2} \left[ \frac{\zeta_j \omega_j}{p(x_{j-1})} \cos^2(\zeta_j \theta_j(x_{j-1})) \\
+ \frac{\lambda r(x_{j-1}) - q(x_{j-1})}{\zeta_j^2 \omega_j} \sin^2(\zeta_j \theta_j(x_{j-1})) + \zeta_j \mu_j^{1/2} \right]
\]

Again, as in the case of the implicit Euler example, the \( \theta_j(x_j) \) terms drop out of the right hand side of the differential equation and the resulting difference step is explicit. In general, since the expression, \( f(x_j, \theta_j(x_j)) = \zeta_j \mu_j^{1/2} \), can be computed explicitly, the implicit term drops out for higher order implicit methods such as the Adams-Moulton implicit \( m \)-step methods and therefore the method becomes explicit.

6. THE HAMILTONIAN DYNAMICS OF PIECEWISE CONSTANT COEFFICIENT MIXED-TYPE PROBLEMS

In the previous sections we have analyzed shooting applied to regular elliptic Sturm-Liouville problems. Our approach has been to use a Hamiltonian formalism. In this section we provide a heuristic description of the dynamics of mixed-type problems in order to delineate some of the potential numerical difficulties from the same Hamiltonian point of view and to link our work to current research on numerical techniques for solving singular Sturm-Liouville problems which utilize piecewise constant coefficient approximations.

As was shown in §2 when the coefficients of a Sturm-Liouville equation are piecewise constants the problem is an integrable Hamiltonian system which can be solved exactly. Its local piecewise constant Hamiltonian is,

\[
H(\dot{u}_j, \dot{u}'_j) = \frac{(\dot{u}'_j)^2}{2p_j} + (\lambda r_j - q_j) \frac{\dot{u}_j^2}{2} \equiv \tilde{\kappa}_j,
\]

for \( j = 1, \ldots n \). For each \( j \) there is a dense set of phase space orbits which are either elliptic, linear or hyperbolic depending on whether \( \mu_j \) is positive, zero or negative. Continuity of \( u \) and \( u' \) ensure continuity of the phase space orbits.

For example, let us consider the phase space trajectory for a piecewise constant problem in which \( j = 2 \) and \( \mu_1 > 0, \mu_2 < 0 \). As illustrated in Figure 9, when \( x \) moves through the elliptic interval \( (x_0, x_1) \), the corresponding phase space solution curve traverses an elliptic path; then as \( x \) moves through the adjacent hyperbolic interval \( (x_1, x_2) \) the corresponding phase space solution curve traverses a hyperbolic path.
Heuristically, the elliptic and linear orbits are stable while the hyperbolic orbits are unstable. Thus, numerically, small errors in elliptic and linear regions of the solution should cause no difficulties, while small errors in hyperbolic intervals are expected to be amplified.

Potential difficulties are illustrated in the Coffey-Evans equation (1.5) which contains several elliptic and hyperbolic intervals. It is viewed as one of the more challenging software test problems in the literature [17] and [15]. Figures 10 through 13 illustrate some of the numerical difficulties of following solution curves which transit hyperbolic intervals. A conclusion to be drawn from these figures is that solution curves in such regions clearly exhibit sensitivity to mesh size because mesh spacing determines the accuracy of the approximation to the coefficients and in hyperbolic regions any errors in the coefficients are readily amplified.

Further, given a good approximation to an eigenvalue, Figure 11 shows the values of the the piecewise constant coefficient approximation to \( \lambda r(x) - q(x) \) for a mesh width of 0.1. The solution curve in Figure 10 begins at the origin, then follows an elliptic path to the right, then transits a hyperbolic path, which connects to another elliptic arc. Without any computational errors the solution curve would be expected to follow another hyperbolic path, and then an elliptic path back to the origin, and hence solve the boundary value problem. However, due to small numerical errors the orbit actually intersects a hyperbolic path which causes it to be thrown away from the origin. Figures 12 and 13 show that, as expected, the solution curve improves as the mesh width is decreased to 0.0375. Of course as \( h \to 0 \) the solution to the piecewise constant coefficient approximate problem will converge to the true solution of the
Figure 10. Phase orbit for Coffey-Evans equation using mesh in Figure 11 with $\beta = 10$ and $\lambda \approx 37.805900$

Figure 11. Piecewise constant approximation of $\lambda r(x) - q(x)$ for Coffey-Evans equation when $\beta = 10$ and $\lambda \approx 37.805900$
Figure 12. Phase orbit for Coffey-Evans equation using mesh in Figure 13 with $\beta = 10$ and $\lambda \approx 37.805900$.

Figure 13. Piecewise constant approximation of $\lambda r(x) - q(x)$ for Coffey-Evans equation when $\beta = 10$ and $\lambda \approx 37.805900$. 
boundary value problem. However, based on additional numerical experiments on problems of this type, we find that it is necessary to use a very small mesh width in order to adequately approximate the true solution. Based on these heuristics, we believe that because of the distinct differences in the dynamics of elliptic and hyperbolic intervals, a successful numerical strategy for solving mixed-type problems must address both the oscillatory behavior of the elliptic intervals and the stability problems of the hyperbolic intervals.

Acknowledgement

The authors wish to thank Richard McGehee of the School of Mathematics at the University of Minnesota for providing them with many valuable insights during his visit to the University of Colorado in 1990-91.
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