Abstract

We present here a novel numerical solution to the linear Boltzmann equation. The method is based on reducing the linear Boltzmann equation to a matrix partial differential equation rather than a partial integro-differential equation. A method for calculating the evolution using a complex generalised eigenfunction method is present for two simple example cases. The generalisation of this method follows straightforwardly.

1 Introduction

We are interested in the following equation

\[-i \frac{\partial I}{\partial t} = i \cos \theta \frac{\partial I}{\partial x} + i \chi(0,\infty) \int_0^{2\pi} S(\theta, \theta') I(\theta) d\theta, \tag{1}\]

where \( \chi \) is the characteristic function, for \( I(x,t,\theta), -\infty < x < \infty, 0 < t < \infty, \) and \( 0 < \theta < 2\pi \) subject to the initial conditions

\[ I(x,0,\theta) = I_0(x,\theta). \]

This equation governs a wide variety of scattering phenomenon from neutron scattering to wave scattering in the marginal ice zone.

More specifically we wish to construct a numerical solution method to the equation. We assume that the scattering kernel \( S(\theta, \theta') \) is sufficiently smooth that the integral operator is compact. We also assume that \( S > 0 \) and that \( S(\theta, \theta') = S(\theta', \theta) \) so that the integral operator is positive and self adjoint. We can use the eigenfunctions of the operator to transform the operator to a discrete (infinite dimensional) matrix operator. For example, if the scattering kernel is of the form \( S(\theta - \theta') \) then the integral operator commutes with translation by \( 2n\pi \) and so the eigenfunctions will be exponentials \( e^{in\theta} \). For numerical reasons we do not wish to deal with infinite dimensional matrices and hence we will truncate the matrix to the first \( m \) dimensions. In practice there may be other approximations to that by the eigenfunctions of the integral operator which are preferred. All that we will assume is that the compact operator is replaced by a finite dimensional one (a matrix) which is positive and self adjoint. Therefore equation (1) becomes

\[-i \frac{\partial I}{\partial t} = iD \frac{\partial I}{\partial x} + i\chi(0,\infty)MI \tag{2}\]

where \( I(x,t) \) is an \( m \) dimensional vector whose elements are functions of \( x \) and \( t, -\infty < x < \infty, 0 < t < \infty, \) \( D \) is a diagonal matrix which is not positive but is self adjoint, and \( M \) is a positive self adjoint matrix. Equation 2 is subject to the initial conditions

\[ I(x,0) = I_0(x). \]

In what follows we will use the notation

\[-i \frac{\partial I}{\partial t} = A + iB^2 \]
where
\[ A = i \cos \theta \frac{\partial I}{\partial x} \quad \text{or} \quad iD \frac{\partial I}{\partial x} \]
and
\[ iB^2 = i\chi \Delta \int_0^{2\pi} S(\theta, \theta') I(\theta) d\theta \quad \text{or} \quad i\chi \Delta M I. \]
Formally we can then say that the solution to equations (1) and (2) are given by
\[ I(t) = T(t)I_0 \]
where \( T(t) \) are dissipative operators which form a strongly continuous semigroup of contractions generated by \( i(A + iB^2) \), i.e.
\[ T(t) = e^{it(A+iB^2)}. \]

The essential property which makes this a semigroup is the fact that \( T(t_1)T(t_2) = T(t_1 + t_2) \). In this paper we will begin with an example of equation (2) where \( m = 2 \), i.e. the vector \( I \) is only 2 dimensional. In this cases we can write the solutions explicitly which will obviously not be possible in the cases when \( m \) is larger. Then we will consider a second example where \( m = 4 \) and finally we will briefly discuss how these methods can be generalised to equations with \( m > 2 \). First of all we will briefly discuss a simple time marching method which may be used to solve these equations. This will be primarily for checking our solution although it may be of interest in itself.

2 Time Marching Solution method

Equations (1) and (2) can be solved by a very simple time marching method. This method may be thought of in the following way. If the operators \( C \) and \( D \) commute then \( e^{C+D} = e^C e^D \). This is clearly not the case if the operators do not commute. However if the norm of \( e^C \) and \( e^D \) is small (of order \( \varepsilon \) say) then the difference between \( e^{C+D} \) and \( e^C e^D \) will be small. Therefore for small time steps \( \Delta t \) we can approximate \( T(\Delta t) \), from equation 3, as follows
\[ T(\Delta t) \approx e^{iA\Delta t} e^{-B^2\Delta t}. \]
The action of these two operators is trivial. \( e^{iA} \) is simply a shift
\[ e^{iA\Delta t} = e^{i\cos \theta \Delta t} \Delta f(x, \theta) = f(x - \cos \theta \Delta t, \theta), \]
likewise for the discrete case. \( e^{-B^2} \) can be calculated from the eigenfunctions of \( B^2 \), i.e. if \( u_i \) are the eigenfunctions with eigenvalue \( \lambda_i \) then we can calculate \( e^{-B^2} \) as
\[ e^{-B^2\Delta t} = |u_i\rangle e^{-\lambda_i \Delta t} \langle u_i|. \]
We will use the time marching method to provide us with a check on our numerics. This is especially important since there are no known analytic solutions.
3 Example A

The first example we will consider is the following equation

\[
-i \frac{\partial I}{\partial t} = \left[ i \frac{\partial}{\partial x} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + i \chi_{(0,\infty)} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \right] I \\
= (A + iB^2) I \\
= \Lambda I,
\]

where

\[
A = i \frac{\partial}{\partial x} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad B = \chi_{(0,\infty)} \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix},
\]

subject to the boundary conditions

\[I |_{t=0} = I_0.\]

The dissipative operator \(T(t)\) we will denote by

\[T(t) = e^{i\Lambda t}.\]

This operators acts in the space

\[
\begin{pmatrix} L_2(-\infty, \infty) \\ L_2(-\infty, \infty) \end{pmatrix}.
\]

We will refer to the subspace

\[
\begin{pmatrix} L_2(-\infty, \infty) \\ 0 \end{pmatrix}
\]

as the top channel and the subspace

\[
\begin{pmatrix} 0 \\ L_2(-\infty, \infty) \end{pmatrix}
\]

as the bottom channel. The top channel evolves to the right and the bottom channel to the left in the absence of scattering. Since the scatterer occupies the region \((0, \infty)\) we refer to

\[
\begin{pmatrix} L_2(-\infty, 0) \\ 0 \end{pmatrix}
\]

as the incoming channel and

\[
\begin{pmatrix} 0 \\ L_2(-\infty, 0) \end{pmatrix}
\]

as the outgoing channel.
3.1 Numerical Time Marching Solution method

A numerical solution method for Example A can be developed as described in section 2. We know that

\[ T(t + \Delta t)I_0 = T(\Delta t)T(t)I_0 \]

and we can approximate

\[ T(\Delta t) \approx e^{i(\lambda + iB^2)\Delta t}e^{-B^2\Delta t}. \]

The last approximation is valid for small \( \Delta t \). \( e^{i\lambda\Delta t} \) is

\[ e^{i\lambda\Delta t}\begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} = \begin{pmatrix} f_1(x - \Delta t) \\ f_2(x + \Delta t) \end{pmatrix}, \]

i.e. \( e^{i\lambda\Delta t} \) is the shift operator, and \( e^{-B^2\Delta t} \) is

\[ e^{-B^2\Delta t} = \begin{pmatrix} \frac{1}{\Delta t} & \frac{1}{\Delta t} \\ \frac{1}{\Delta t} & -\frac{1}{\Delta t} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & e^{-2\Delta t} \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \]

\[ = \begin{pmatrix} 1 & \Delta t \\ \Delta t & 1 - \Delta t \end{pmatrix}, \]

i.e. \( e^{-B^2\Delta t} \) removes \( \Delta t \) from channel one and adds \( \Delta t \) to channel two etc. This is the physical interpretation of the operators, \( e^{i\lambda\Delta t} \) shifts the solution in each channel and \( e^{-B^2\Delta t} \) mixes the solutions between the channels.

3.2 Example of a solution by the time marching method

Figures 1 to 4 show evolutions of the initial data

\[ I_0 = \begin{pmatrix} H(x + 1) - H(x + \frac{1}{2}) \\ 0 \end{pmatrix}, \quad (4) \]

where \( H \) is the Heaviside function.

3.3 Generalised eigenfunctions of the operator

We want to determine the generalised eigenfunctions of the operator \( \Lambda \). They will allow us to construct a change of basis in which \( \Lambda \) will become a multiplicative operator. The equation which the generalised eigenfunctions must satisfy is the following

\[ \left[ i \frac{\partial}{\partial x} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + i\chi_{(0,\infty)} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \right] I(\lambda, x) = \lambda I(\lambda, x). \quad (5) \]
Figure 1: The spatial evolution in the top channel of $I_0 = H(x+1) - H(x + \frac{1}{2})$ for the times shown.
Figure 2: The spatial evolution in the bottom channel of $I_0 = H(x+1) - H(x+\frac{1}{2})$ for the times shown.
Figure 3: The temporal evolution in the top channel of $I_0 = H(x+1) - H(x+\frac{1}{2})$ for the positions shown.
Figure 4: The temporal evolution in the bottom channel of $I_0 = H(x + 1) - H(x + \frac{1}{2})$ for the positions shown.
We also impose appropriate boundary conditions on $I(\lambda, x)$. We know that the
generalised eigenfunctions will not be in the space
\[
\begin{pmatrix}
L_2 (-\infty, \infty) \\
L_2 (-\infty, \infty)
\end{pmatrix}
\]
but that the inner product, which is what defines the change of basis, with any
function must be less than infinity, i.e.
\[
\langle I(\lambda, x), f(x) \rangle < \infty \quad \text{forall } f \in \begin{pmatrix}
L_2 (-\infty, \infty) \\
L_2 (-\infty, \infty)
\end{pmatrix}.
\]
This is essentially the boundary condition for the generalised eigenfunctions. Of
course we expect oscillatory exponentials exactly as in Fourier theory. To solve
equation 5 we break the problem into two regions. If $x \notin (0, \infty)$ then
\[
I(\lambda, x) = \begin{pmatrix}
e^{-i\lambda x} & 0 \\
0 & e^{i\lambda x}
\end{pmatrix} I(\lambda, 0), \quad x < 0.
\]
If $x \in (0, \infty)$ then
\[
\frac{\partial}{\partial x} I(\lambda, x) = -i \begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}^{-1} \left( \lambda \begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix} - i \begin{pmatrix}
1 & -1 \\
-1 & 1
\end{pmatrix} \right) I(\lambda, x)
\]
\[
= \begin{pmatrix}
-i\lambda - 1 & 1 \\
-1 & i\lambda + 1
\end{pmatrix} I(\lambda, x)
\]
which has solution
\[
I(\lambda, x) = a \begin{pmatrix}
i\lambda + 1 - i\mu \\
1
\end{pmatrix} e^{ix\mu} + b \begin{pmatrix}
i\lambda + 1 + i\mu \\
1
\end{pmatrix} e^{-ix\mu},
\]
where
\[
i\mu = \sqrt{-\lambda^2 + 2i\lambda}.
\]
We will always assume that the square root have positive real part.

Consider the matrix $M(\lambda)$
\[
M(\lambda) = \begin{pmatrix}
-i\lambda - 1 & 1 \\
-1 & i\lambda + 1
\end{pmatrix}.
\]
We have already seen that this matrix plays a distinguished role in the derivation
of the generalised eigenfunctions. Under the restrictions outlined in section 1
the real axis will always lie in the spectrum of the operator. We will refer to
this spectrum as the “real” spectrum. The part of the spectrum with non-zero
imaginary part will be determined by the characteristic polynomial of the matrix
$M(\lambda)$. It is best to think of the characteristic equation of $M(\lambda)$ as defining an
algebraic variety in $\mathbb{C}^2$. In our simple example the characteristic polynomial (in
$i\mu$) of $M(\lambda)$ is $(i\mu)^2 + \lambda^2 - 2i\lambda$. If we set this polynomial to zero we obtain the
following algebraic variety in $\mathbb{C}^2$
\[
(i\mu)^2 + \lambda^2 - 2i\lambda = 0.
\]
The part of the spectrum with non-zero imaginary part is given by the intersection of this algebraic variety with the plane \( \text{Im}\mu = 0 \). We will refer to this spectrum as the “complex” spectrum. It is apparent that we can solve for this surface, which will be a one dimensional manifold, by setting \( \mu \in \mathcal{R} \) and solving equation 10 for \( \lambda \). This will give two solutions for \( \lambda \) since equation 10 is quadratic which we will refer to as the two branches of the “complex” spectrum. It is important to realise that for each \( \mu \in \mathcal{R} \) there corresponds two values of \( \lambda \), the spectral parameter, one on each “complex” branch.

For the “real” spectrum \( \lambda \in \mathcal{R} \) and the generalised eigenfunctions are, assuming that \( \text{Re}\mu > 0 \),

\[
I^> (\lambda, x) = \begin{cases} 
\begin{pmatrix} 1 \\ i\lambda + 1 - i\mu \\
0 
\end{pmatrix} e^{-ix\mu}, & x > 0, \\
\begin{pmatrix} 1 \\ 0 
\end{pmatrix} e^{-ix\lambda} + \begin{pmatrix} 0 \\ i\lambda + 1 - i\mu 
\end{pmatrix} e^{ix\lambda}, & x < 0.
\end{cases}
\]  

(8)

For the “complex” spectrum \( \mu \in \mathcal{R} \) and the generalised eigenfunctions are

\[
I^+_{1,2} (\mu, x) = \begin{cases} 
\begin{pmatrix} i\lambda_{1,2} + 1 - i\mu \\
1 
\end{pmatrix} e^{ix\mu} - \begin{pmatrix} i\lambda_{1,2} + 1 + i\mu \\
1 
\end{pmatrix} e^{-ix\mu}, & x > 0, \\
\begin{pmatrix} -2i\mu \\
0 
\end{pmatrix} e^{-ix\lambda_{1,2}}, & x < 0.
\end{cases}
\]  

(9)

The subscript \( 1,2 \) refers to the two branches of solution for \( \lambda \) for a given \( \mu \in \mathcal{R} \) (from equation 10),

\[
\lambda_1 = i + \sqrt{\mu^2 - 1} \quad \text{and} \quad \lambda_2 = i - \sqrt{\mu^2 - 1}.
\]  

(10)

It is important to realise that although we express the generalised eigenfunctions corresponding to the complex spectrum with respect to the parameter \( \mu \) the eigenvalue is \( \lambda \). \( \mu \) may be thought of as a function of \( \lambda \) from equation 10 or \( \lambda \) may be thought of as a function of \( \mu \) from equation 10.

\( I^+ (\mu, x) = -I^+ (-\mu, x) \) which means that only for \( \mu \in \mathcal{R}^+ \) do we have independent generalised eigenfunctions. Also for every \( \mu \in \mathcal{R}^+ \) we have two solutions for \( \lambda \), namely \( \lambda_1 \) and \( \lambda_2 \).

It follows from equation 6 that \( \lambda = i \pm \sqrt{\mu^2 - 1} \) so that if \( \mu \in \mathcal{R}^+ \) then the spectrum is the following subset of the complex plane \( \{ z \in \mathbb{C} : \text{Im} \, z = 1 \text{ or } \text{Re} \, z \in [0,2] \} \).

The total spectrum is this set and the real axis (the spectrum corresponding to the generalised eigenfunctions \( I^> (\lambda, x) \)) and is shown in shown in figure 5.

3.4 Generalised eigenfunctions of the adjoint operator

We require the generalised eigenfunctions of the adjoint \( \Lambda^* \) to construct a biorthogonal system. The adjoint operator \( \Lambda^* \) is given by

\[
\Lambda^* I = \left[ i \frac{\partial}{\partial x} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - i\chi(0,\infty) \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \right] I = (A - iB^2) I.
\]
Figure 5: The spectrum of the operator in $\mathcal{C}$. 
We find the generalised eigenfunctions, $\hat{I}(\lambda, x)$, of $\Lambda^*$ exactly as in subsection 3.3. If $x \in (0, \infty)$ then
\[
\frac{\partial}{\partial x} \hat{I}(\lambda, x) = -i \left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right) \left( \lambda \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) + i \left( \begin{array}{cc} 1 & -1 \\ -1 & 1 \end{array} \right) \right) \hat{I}(\lambda, x)
\]
\[
= \left( \begin{array}{cc} -i\lambda + 1 & -1 \\ 1 & i\lambda - 1 \end{array} \right) \hat{I}(\lambda, x)
\]
which has solution
\[
a \left( \begin{array}{c} \frac{1}{-i\lambda + 1 - i\hat{\mu}} \\ \frac{1}{-i\lambda + 1 + i\hat{\mu}} \end{array} \right) e^{ix\hat{\mu}} + b \left( \begin{array}{c} \frac{1}{-i\lambda + 1 + i\hat{\mu}} \\ \frac{1}{-i\lambda + 1 - i\hat{\mu}} \end{array} \right) e^{-ix\hat{\mu}},
\]
where $i\hat{\mu} = \sqrt{-\lambda^2 - 2i\lambda}$. Two possibilities, either $\hat{\mu} \in \mathcal{R}^+$ or $\lambda \in \mathcal{R}$. If $
abla \in \mathcal{R}$ then the eigenfunctions are of the form (assuming that $Re\hat{\mu} > 0$)
\[
\hat{I}^>(\lambda, x) = \left\{ \begin{array}{ll} 
\left( \frac{-i\lambda + 1 - i\hat{\mu}}{1} \right) e^{-ix\hat{\mu}}, & x > 0, \\
\left( \frac{-i\lambda + 1 - i\hat{\mu}}{0} \right) e^{-ix\lambda} + \left( \frac{0}{1} \right) e^{ix\lambda}, & x < 0.
\end{array} \right.
\]
If $\hat{\mu} \in \mathcal{R}^+$ then the eigenfunctions are of the form
\[
\hat{I}^+_{1,2}(\hat{\mu}, x) = \left\{ \begin{array}{ll} 
\left( \frac{1}{-i\lambda_{1,2} + 1 - i\hat{\mu}} \right) e^{ix\hat{\mu}} - \left( \frac{1}{-i\lambda_{1,2} + 1 + i\hat{\mu}} \right) e^{-ix\hat{\mu}}, & x > 0, \\
\left( \frac{0}{-2i\hat{\mu}} \right) e^{ix\lambda_{1,2}}, & x < 0,
\end{array} \right.
\]
where $\lambda_1 = -i + \sqrt{\hat{\mu}^2 - 1}$ and $\lambda_2 = -i - \sqrt{\hat{\mu}^2 - 1}$.

3.5 Normalising the Biorthogonal System

Hilbert space theory tells us that the generalised eigenfunctions of the operators $\Lambda$ and $\Lambda^*$ must form a biorthogonal system. Calculation of their inner products is accomplished in appendix 5 and we obtain the results that
\[
\left\langle \hat{I}^>(\lambda, x), \hat{I}^>(\lambda', x) \right\rangle = 2\pi S(\lambda)\delta(\lambda - \lambda'),
\]
where
\[
S(\lambda) = i\lambda + 1 - \sqrt{-\lambda^2 + 2i\lambda}, \tag{12}
\]
\[
\left\langle \hat{I}^+_{1}(\mu, x), \hat{I}^+_{1}(\hat{\mu}, x) \right\rangle = 2\pi (2i\lambda_1 + 2) \delta(\mu - \hat{\mu}), \tag{13}
\]
and
\[
\left\langle \hat{I}^+_{2}(\mu, x), \hat{I}^+_{2}(\hat{\mu}, x) \right\rangle = 2\pi (2i\lambda_2 + 2) \delta(\mu - \hat{\mu}). \tag{14}
\]
Obviously
\[
\left\langle \hat{I}^+_{1}(\mu, x), \hat{I}^+_{2}(\hat{\mu}, x) \right\rangle = \left\langle \hat{I}^+_{2}(\mu, x), \hat{I}^+_{1}(\hat{\mu}, x) \right\rangle = 0 \tag{15}
\]
since these generalised eigenfunctions correspond to different values of spectral parameter $\lambda$. 

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3.6 Using the generalised eigenfunctions to construct a change of basis

Consider the operator $\Gamma$,

$$\Gamma : \begin{pmatrix} L_2 (-\infty, \infty) \\ L_2 (-\infty, \infty) \end{pmatrix} \rightarrow \begin{pmatrix} L_2 (-\infty, \infty) \\ L_2 (0, \infty) \end{pmatrix},$$

which acts as follows

$$\Gamma (I (x)) = \begin{pmatrix} h^> (\lambda) \\ h_1^+ (\mu) \\ h_2^+ (\mu) \end{pmatrix},$$

where

$$h^> (\lambda) = \frac{\langle I_0 (x), \hat{I}^> (\lambda, x) \rangle}{2\pi S (\lambda)}.$$ 

which is the contribution from the “real” spectrum and

$$h_1^+ (\mu) = \frac{\langle I_0 (x), \hat{I}_1^+ (\mu, x) \rangle}{2\pi (2i\lambda_1 + 2)}$$ and $$h_2^+ (\mu) = \frac{\langle I_0 (x), \hat{I}_2^+ (\mu, x) \rangle}{2\pi (2i\lambda_2 + 2)}$$

which are the contributions from the “complex” spectrum. From the biorthogonality condition the inverse of this operator is given by

$$\Gamma^{-1} \begin{pmatrix} h^> (\lambda) \\ h_1^+ (\mu) \\ h_2^+ (\mu) \end{pmatrix} = \int_{-\infty}^{\infty} h^> (\lambda) I^> (\lambda, x) d\lambda + \int_0^{\infty} h_1^+ (\mu) I_1^+ (\mu, x) d\mu + \int_0^{\infty} h_2^+ (\mu) I_2^+ (\mu, x) d\mu.$$ 

Consider the operator $\Lambda$. We can use operators $\Gamma$ and $\Gamma^{-1}$ to construct a change of basis, i.e.

$$\Lambda I (x) = \Gamma^{-1} \hat{\Lambda} \Gamma I (x)$$

where the operator $\hat{\Lambda}$ is the operator $\Lambda$ acting w.r.t. the new basis. $\hat{\Lambda}$ is given by

$$\hat{\Lambda} \begin{pmatrix} h^> (\lambda) \\ h_1^+ (\mu) \\ h_2^+ (\mu) \end{pmatrix} = \begin{pmatrix} \lambda h^> (\lambda) \\ \lambda_1 (\mu) h_1^+ (\mu) \\ \lambda_2 (\mu) h_2^+ (\mu) \end{pmatrix},$$

where $\lambda_1 (\mu) = i + \sqrt{\mu^2 - 1}$ and $\lambda_2 (\mu) = i - \sqrt{\mu^2 - 1}$. Consider now the semigroup operator $T(t)$.

$$T(t) I_0 (x) = \Gamma^{-1} \hat{T}(t) \Gamma,$$

where the operator $\hat{T}(t)$ is given by

$$\hat{T} (t) \begin{pmatrix} h^> (\lambda) \\ h_1^+ (\mu) \\ h_2^+ (\mu) \end{pmatrix} = \begin{pmatrix} e^{i\lambda t} h^> (\lambda) \\ e^{i\lambda_1 (\mu) t} h_1^+ (\mu) \\ e^{i\lambda_2 (\mu) t} h_2^+ (\mu) \end{pmatrix},$$
This is of course exactly the change of basis we have been seeking in which the transformed operator $\hat{A}$ is a multiplicative operator and hence the transformed semigroup operator generated by $\hat{A}$, $\hat{T}(t) = e^{i\hat{A}t}$ is also a multiplicative operator.

### 3.7 A Scattering Theory

We can use this change of basis to develop a scattering theory. This scattering theory will only allow us to solve for the evolution of an input which is initially zero in the scattering region, i.e. $I_0(x) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ for $x \in (0, \infty)$. We will denote the incoming and outgoing channels by $\mathcal{D}_-$ and $\mathcal{D}_+$ respectively, i.e.

$$\mathcal{D}_- = \begin{pmatrix} \mathbb{L}_2(-\infty,0) \\ 0 \end{pmatrix}$$

and

$$\mathcal{D}_+ = \begin{pmatrix} 0 \\ \mathbb{L}_2(-\infty,0) \end{pmatrix}.$$  

We know that initial data in the outgoing channel will simply evolve by the shift operator and is hence trivial. Therefore we will developing a theory for the evolution of an initial data which is non-zero only in the incoming channel. If $I_0 \in \mathcal{D}_-$ then $I_0$ can be written as

$$I_0 = \begin{pmatrix} f(x) \\ 0 \end{pmatrix}, \quad f(x) = 0, \quad x > 0.$$  

The generalised eigenfunctions of $\Lambda^*$ which correspond to the “complex” spectrum, $\hat{E}_1^+(\mu,x)$ and $\hat{E}_2^+(\mu,x)$ both vanish in the incoming channel so it follows using the change of basis operator $\Gamma$ defined in equation 16 that

$$\Gamma I_0 = \begin{pmatrix} \langle I_0(x), \hat{E}^>(\lambda,x) \rangle \\ \frac{1}{2\pi S(\lambda)} \end{pmatrix}.$$  

Therefore the semigroup operator $T(t)$ is given by

\begin{equation}
T(t)I_0 = \Gamma^{-1} \hat{T}(t) \Gamma I_0 = \Gamma^{-1} \begin{pmatrix} e^{i\lambda t} \langle I_0(x), \hat{E}^>(\lambda,x) \rangle \\ \frac{S(\lambda)}{0} \end{pmatrix}.
\end{equation}

We know that

$$\frac{\langle I_0(x), \hat{E}^>(\lambda,x) \rangle}{2\pi S(\lambda)} = \frac{1}{2\pi S(\lambda)} \int_{-\infty}^{0} S(\lambda)e^{i\lambda x} f(x) \, dx = F(\lambda)$$

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and follows from equation 17 and 20 that

\[ T(t)I_0 (x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\lambda} F(\lambda) I^>(\lambda, x) d\lambda. \]  

(21)

This expression allows us to construct a scattering theory. The generalised eigenfunction \( I^>(\lambda, x) \) shows how exponentials in the incoming channel are mapped to exponentials in the outgoing channel. The operator which performs such a map is called a scattering operator. Since

\[ P_D^- I^>(\lambda, x) = e^{i\lambda x} \]

and

\[ P_D^+ I^>(\lambda, x) = S(\lambda) e^{-i\lambda x} \]

it follows that the scattering operator is \( S(\lambda) \).

We now separately consider the projections onto the subspaces \( D_-, D_+ \) and \( K = \mathcal{H} \odot (D_- \oplus D_+) \) of \( T(t)I_0 (x) \) using equation 21. The projection onto the subspace \( D_- \) is

\[ P_{D_-}T(t)I_0 = \begin{cases} \int_{-\infty}^{\infty} e^{-i\lambda(x-\theta)} F(\lambda) d\lambda, & x < 0, \\ 0, & x > 0, \\ 0 & 0 \end{cases} \]  

(22)

which is simply the shift operator. The projection onto the subspace \( D_+ \) is

\[ P_{D_+}T(t)I_0 = \begin{cases} \int_{-\infty}^{\infty} e^{i\lambda(x+\theta)} S(\lambda)F(\lambda) d\lambda, & x < 0, \\ 0, & x > 0. \end{cases} \]  

(23)

The projection onto the subspace \( K \) is

\[ P_K T(t)f (x) = \int_{-\infty}^{\infty} \left( \frac{1}{S(\lambda)} \right) \hat{f}(\lambda) e^{i\lambda} e^{-\sqrt{-\lambda^2+2ix\lambda}} d\lambda, \]  

(24)

where as always the root with positive real part is taken.

A brief mention of the relation between this scattering theory and the classical scattering theory of Lax and Philips (1989) is worthwhile. Where as their scattering matrix is singular (or zero depending on your definition) at the points of complex spectrum our scattering matrix has non-analytic branches, or more precisely branches over which scattering matrix can not be extended analytically at the branches of continuous complex spectrum. This non-analyticity is caused by the square root operator in equation 12 and the fact that we always take the branch with positive real part. There is almost certainly a new branch of scattering theory which could be developed here, however this is not the purpose of the present paper.
Figure 6: The temporal evolution in the bottom channel of $I_0 = H(x + 1) - H(x + \frac{1}{2})$ in the top channel calculated by the scattering and time marching methods for $x = 0$.

3.8 Numerical calculation of evolutions using scattering theory.

We present here some results. The numerical calculation of the projections given in equations 23 and 24 is via the fast Fourier transform (FFT). We consider the same initial input as in subsection 3.2, i.e.

$$I_0 = \begin{pmatrix} H(x + 1) - H(x + \frac{1}{2}) \\ 0 \end{pmatrix}$$

and calculate the intensity $I$ at various positions by the spectral (equations 23 and 24) and time marching solution method (subsection 3.1). The purpose of the time marching solution method is to give us a check that our numerics are indeed correct. It is obvious from Figures 6, 7, and 8 that these two methods give the same results.
Figure 7: The temporal evolution in the top channel of $L_0 = H(x+1) - H \left( x + \frac{1}{2} \right)$ in the top channel calculated by the scattering and time marching methods for $x = 1$. 
Figure 8: The temporal evolution in the bottom channel of $I_0 = H(x + 1) - H\left(x + \frac{1}{2}\right)$ in the top channel calculated by the scattering and time marching methods for $x = 1$. 
3.9 Solving for an initial data, $I_0$, in the scattering space $K$

The semigroup operator $T(t)$ is given by

$$T(t)I_0 = \Gamma^{-1} \tilde{T}(t) \Gamma I_0$$

$$= \Gamma^{-1} \begin{pmatrix}
    e^{i\lambda_1 (\mu)} h_1^+(\mu) \\
    e^{i\lambda_2 (\mu)} h_2^+(\mu)
\end{pmatrix}. \quad (25)$$

It follows from equation 17 that

$$T(t)I_0 = \int_{-\infty}^{\infty} \hat{h}^+(\lambda) \hat{I}^+(\lambda, x)e^{i\lambda x} d\lambda + \int_{0}^{\infty} h^+_1(\mu) I^+_1(\mu, x)e^{i\mu x} d\mu + \int_{0}^{\infty} h^+_2(\mu) I^+_2(\mu, x)e^{i\mu x} d\mu.$$

Of course

$$\hat{h}^+(\lambda) = \frac{\langle I_0(x), \hat{I}^+(\lambda, x) \rangle}{2\pi S(\lambda)}$$

and

$$h^+_1(\mu) = \frac{\langle I_0(x), \hat{I}^+_1(\mu, x) \rangle}{2\pi (2i\lambda_1 + 2)} \quad \text{and} \quad h^+_2(\mu) = \frac{\langle I_0(x), \hat{I}^+_2(\mu, x) \rangle}{2\pi (2i\lambda_2 + 2)}.$$

We are only interested in $I_0(x) \in K$ since we already know how to deal with $I_0(x) \in D_+$ or $I_0(x) \in D_-$ using the scattering theory of subsection 3.7.

3.10 Test problem

The initial input we will solve for is the following

$$I_0(x) = \begin{pmatrix} H(x-1) - H(x-2) \\ 0 \end{pmatrix}$$

where again $H$ is the Heavyside function.

3.10.1 Projections

Therefore (recalling that $i\mu = \sqrt{-\lambda^2 - 2i\lambda}$ and we always take the square root with positive real part) we obtain

$$\hat{h}^+(\lambda) = \frac{e^{-i\mu} - e^{-2i\mu}}{2\pi i\mu}$$

and

$$h^+_1(\mu) = \frac{i(\cos 2\mu - \cos \mu)}{2\pi \mu (i\lambda_i + 1)}.$$
The projections onto $\mathcal{D}_-$ is

$$
P_{D_-} T(t) I_0(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\mu} - e^{-2i\mu}}{i\mu} \ e^{-i\lambda x} e^{i\lambda t} d\lambda 
- \frac{1}{2\pi} \int_{0}^{\infty} \frac{i(\cos 2\mu - \cos \mu)}{(i\lambda_1 + 1)} 2ie^{-i\lambda_1(\mu)} e^{i\lambda_1(\mu)} d\mu 
- \frac{1}{2\pi} \int_{0}^{\infty} \frac{i(\cos 2\mu - \cos \mu)}{(i\lambda_2 + 1)} 2ie^{-i\lambda_2(\mu)} e^{i\lambda_2(\mu)} d\mu.
$$

The projection onto $\mathcal{D}_+$ is

$$
P_{D_+} T(t) I_0(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\mu} - e^{-2i\mu}}{i\mu} (i\lambda + 1 - i\mu) e^{i\lambda x} e^{i\lambda t} d\lambda.
$$

The projection onto $\mathcal{K}$ is

$$
P_{\mathcal{K}} T(t) I_0(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\mu} - e^{-2i\mu}}{i\mu} (i\lambda + 1 - i\mu) e^{i\lambda x} e^{i\lambda t} d\lambda 
+ \frac{1}{2\pi} \int_{0}^{\infty} \frac{i(\cos 2\mu - \cos \mu)}{\mu(i\lambda_1 + 1)} \left( \frac{e^{-i\mu}}{e^{i\mu} - e^{-i\mu}} \right) e^{i\lambda_1(\mu)} d\mu 
+ \frac{1}{2\pi} \int_{0}^{\infty} \frac{i(\cos 2\mu - \cos \mu)}{\mu(i\lambda_2 + 1)} \left( \frac{e^{-i\mu}}{e^{i\mu} - e^{-i\mu}} \right) e^{i\lambda_2(\mu)} d\mu.
$$

3.10.2 Numerical Calculation of the Projections

We present here numerical calculations of the projections of subsection 3.10.3.10.1. The simplest result to calculate numerically is the solution in the outgoing channel

$$
P_{D_+} T(t) I_0^+(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\mu} - e^{-2i\mu}}{i\mu} (i\lambda + 1 - i\mu) e^{i\lambda x} e^{i\lambda t} d\lambda
$$

which is accomplished using the FFT algorithm. Figure 9 shows the results calculated by the time marching solution method and the spectral method.

Although we know that the evolution in the incoming channel must be zero we can determine separately the projections due to the "real" and "complex" spectrum which we denote $I_0^-(x)$ and $I_0^+(x)$ respectively. The separate projections are

$$
P_{D_-} T(t) I_0^-(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{-i\mu} - e^{-2i\mu}}{i\mu} e^{i\lambda x} e^{i\lambda t} d\lambda,
$$

which can be done by the FFT algorithm, and

$$
P_{D_-} T(t) I_0^+(x) = \frac{i}{\pi} \int_{0}^{\infty} \frac{(\cos \mu - \cos 2\mu)}{\sqrt{\mu^2 - 1}} \left( e^{i(t-x)\lambda_1} - e^{i(t-x)\lambda_2} \right) d\mu,
$$

which is computed by integration. Figure 10 shows the calculation of $P_{D_-} I_0^-(x)$ and $P_{D_-} I_0^+(x)$. It is clear that the sum will be zero within numerical error. Note the appearance of the familiar "ringing" in the spectral solution due to
Figure 9: The temporal evolution of $I_0(x) = H(x - 1) - H(x - 2)$ in the top channel in the outgoing channel $D_+$ calculated by the scattering and time marching methods.
Figure 10: The spatial evolution in the incoming channel of $I_0(x) = H(x-1) - H(x-2)$ in the top channel calculated separately for the “real” and “complex” spectrum, $t = 0$. 
the Gibb's phenomenon. Of course this could be removed in the standard way by smoothing the initial condition \( I_0(x) \).

The projection in the subspace \( \mathcal{K} \), the scattering region, is calculated in the same manner as the projection in the incoming channel. As before we consider separately the projections due to the "real" and "complex" spectrum since the numerical methods used to evaluate them are different. The first projection is

\[
P_{\mathcal{K}T}(t) I_0^+ (x) = \frac{1}{2\pi} \int \frac{e^{-i\mu} - e^{-2i\mu}}{i\mu} \left( \frac{e^{-i\mu x}}{i\lambda + 1 - i\mu} e^{-i\mu x} \right) e^{i\lambda t} d\lambda,
\]

which is evaluated by the FFT. The second projection is

\[
P_{\mathcal{K}T}(t) I_0^- (x) = \frac{1}{2\pi} \int \frac{(\cos 2\mu - \cos \mu)}{\mu \sqrt{\mu^2 - 1}} \left( \frac{(i\lambda_1 + 1 - i\mu) e^{i\mu x} - (i\lambda_1 + 1 + i\mu) e^{-i\mu x}}{e^{i\mu x} - e^{-i\mu x}} \right) e^{i\lambda_2 t} d\mu
\]

\[
- \frac{1}{2\pi} \int \frac{(\cos 2\mu - \cos \mu)}{\mu \sqrt{\mu^2 - 1}} \left( \frac{(i\lambda_2 + 1 - i\mu) e^{i\mu x} - (i\lambda_2 + 1 + i\mu) e^{-i\mu x}}{e^{i\mu x} - e^{-i\mu x}} \right) e^{i\lambda_2 t} d\mu,
\]

which is evaluated by integration.

The results for the top and bottom channels are shown in Figures 11 and 12. It is interesting to consider the projections \( P_{\mathcal{K}T}(t) I_0^+ \) and \( P_{\mathcal{K}T}(t) I_0^- \) separately as shown in Figures 13 and 14.

4 Example B

We consider a four dimensional problem, i.e. \( m = 4 \). This problem shows how the methods presented can be generalised for large \( m \). Consider the following equation

\[
-\imath \partial I = \begin{bmatrix} \frac{\partial}{\partial t} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} + \imath \chi_{(0,\infty)} \begin{pmatrix} 3 & -1 & -1 & -1 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ -1 & -1 & -1 & 3 \end{pmatrix} \end{bmatrix} I
\]

\[
= \Lambda I,
\]

subject to the boundary conditions

\[ I_{t=0} = I_0(x). \]

This example lies between the case when \( m \) is too large for any analytic methods and the case when no numerical method is required. We will refer to the subspaces

\[
\begin{pmatrix} L_2(-\infty, \infty) \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ L_2(-\infty, \infty) \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ L_2(-\infty, \infty) \\ 0 \end{pmatrix}, \quad \text{and} \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ L_2(-\infty, \infty) \end{pmatrix}
\]

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Figure 11: The temporal evolution in the top channel of $I_0(x) = H(x - 1) - H(x - 2)$ in the top channel calculated by the scattering and time marching methods for $x = 1.5$. 
Figure 12: The temporal evolution in the bottom channel of $I_0(x) = H(x - 1) - H(x - 2)$ in the top channel calculated by the scattering and time marching methods for $x = 1.5$. 
Figure 13: The temporal evolution in the top channel of $I_0(x) = H(x - 1) - H(x - 2)$ in the top channel calculated separately for the “real” and “complex” spectrum for $x = 1.5$. 
Figure 14: The temporal evolution in the bottom channel of $I_0(x) = H(x - 1) - H(x - 2)$ in the top channel calculated separately for the “real” and “complex” spectrum for $x = 1.5$. 
as the first, second, third, and fourth channels respectively. The incoming and outgoing channels, $D_-$ and $D_+$ respectively, are

$$
D_- = \begin{pmatrix}
L_2(-\infty,0) \\
L_2(-\infty,0) \\
0 \\
0
\end{pmatrix}
$$

and

$$
D_+ = \begin{pmatrix}
0 \\
0 \\
L_2(-\infty,0) \\
L_2(-\infty,0)
\end{pmatrix}
$$

We must again determine the generalised eigenfunctions of $\Lambda$.

### 4.1 The spectrum of $\Lambda$

As before we consider the equation for the generalised eigenfunctions

$$
\left[ i \frac{\partial}{\partial x} \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{2} & 0 & 0 \\
0 & 0 & -\frac{1}{2} & 0 \\
0 & 0 & 0 & -1
\end{pmatrix} + i\chi(0,\infty) \begin{pmatrix}
3 & -1 & -1 & -1 \\
-1 & 3 & -1 & -1 \\
-1 & -1 & -1 & 3 \\
-1 & -1 & -1 & 3
\end{pmatrix} \right] I(\lambda,x) = \lambda I(\lambda,x).
$$

We solve equation 28 by breaking the problem into two regions. If $x \notin (0,\infty)$ then

$$
I(\lambda,x) = \begin{pmatrix}
e^{-i\lambda x} & 0 & 0 & 0 \\
0 & e^{-2i\lambda x} & 0 & 0 \\
0 & 0 & e^{2i\lambda x} & 0 \\
0 & 0 & 0 & e^{i\lambda x}
\end{pmatrix} I(\lambda,0), \quad x < 0.
$$

If $x \in (0,\infty)$ then

$$
\frac{\partial}{\partial x} I(\lambda,x) = -i \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{1}{2} & 0 & 0 \\
0 & 0 & -\frac{1}{2} & 0 \\
0 & 0 & 0 & -1
\end{pmatrix}^{-1} \begin{pmatrix}
3 & -1 & -1 & -1 \\
-1 & 3 & -1 & -1 \\
-1 & -1 & 3 & -1 \\
-1 & -1 & -1 & 3
\end{pmatrix} I(\lambda,x)
$$

$$
= \begin{pmatrix}
-2 & -2 & 2i\lambda + 6 & 2 \\
-2 & -2 & 2i\lambda + 6 & 2 \\
-1 & -1 & -1 & i\lambda + 3
\end{pmatrix} I(\lambda,x).
$$

We will call this matrix $M(\lambda)$, i.e.

$$
M(\lambda) = \begin{pmatrix}
-2 & -2 & 2i\lambda + 6 & 2 \\
-2 & -2 & 2i\lambda + 6 & 2 \\
-1 & -1 & -1 & i\lambda + 3
\end{pmatrix}.
$$
The solution of equation 29 is

\[ I(\lambda, x) = c_1 u_1 e^{i\mu_1 x} + c_2 u_2 e^{i\mu_2 x} + c_3 \bar{u}_1 e^{-i\mu_1 x} + c_4 \bar{u}_2 e^{-i\mu_2 x}, \]

where \( u_1, u_2, \bar{u}_1 \) and \( \bar{u}_2 \) are the eigenvectors of \( M(\lambda) \) and \( \pm i\mu_1 \) and \( \pm i\mu_2 \) are the eigenvalues of \( M(\lambda) \). We use the overbar to denote a reversal of the elements of the vector. What are the conditions under which we will have generalised eigenfunctions? As before either \( \lambda \in \mathbb{R} \) or \( \mu_1 \in \mathbb{R} \), or \( \mu_2 \in \mathbb{R} \). Since the characteristic polynomial of \( M(\lambda) \), in \( i\mu \), is

\[ f(\mu, \lambda) = 4\lambda^4 - 48i\lambda^3 + \left(5(i\mu)^2 - 192\right) \lambda^2 \]
\[ + \left(-30i(i\mu)^2 + 256i\right) \lambda - 40(i\mu)^2 + (i\mu)^4. \]

The spectrum with non trivial complex part must be given by the intersection of the algebraic variety

\[ 4\lambda^4 - 48i\lambda^3 + \left(5(i\mu)^2 - 192\right) \lambda^2 \]
\[ + \left(-30i(i\mu)^2 + 256i\right) \lambda - 40(i\mu)^2 + (i\mu)^4 = 0 \]

and the plane \( \text{Im} \mu = 0 \). Again since the eigenvalues of \( M(\lambda) \) occur in \( \pm \) pairs the generalised eigenfunctions corresponding to \( i\mu \) and \(-i\mu\) are not independent. To find the spectral points we set \( \mu \in \mathbb{R}^+ \) and solve for \( \lambda \). Since the equation is fourth order we will obtain four solutions for \( \lambda \) which we will denote by \( \lambda_1, \lambda_2, \lambda_3 \), and \( \lambda_4 \). The complex spectrum of \( \Lambda \) will therefore consist of four branches. The total spectrum for \( \Lambda \) is shown in Figure 15 and the four branches are shown in Figure 16.

4.2 Generalised Eigenfunctions of \( \Lambda \) and \( \Lambda^* \)

The derivation of the generalised eigenfunctions is exactly as for example \( \Lambda \). Because there are two incoming channels the generalised eigenfunctions corresponding to the “real” spectrum, \( \lambda \in \mathbb{R} \), have multiplicity two and we define two distinguished generalised eigenfunctions for each \( \lambda \in \mathbb{R} \),

\[ I_1^+(\lambda, x) = \begin{pmatrix} e^{-i\lambda x} \\ S_{21}(\lambda) e^{2i\lambda x} \\ S_{11}(\lambda) e^{i\lambda x} \end{pmatrix} \quad x < 0 \text{ or } u_1 e^{i\mu_1 x} + u_2 e^{i\mu_2 x}, \quad x > 0, \]

and

\[ I_2^+(\lambda, x) = \begin{pmatrix} 0 \\ S_{22}(\lambda) e^{2i\lambda x} \\ S_{12}(\lambda) e^{i\lambda x} \end{pmatrix} \quad x < 0 \text{ or } u'_1 e^{i\mu_1 x} + u'_2 e^{i\mu_2 x}, \quad x > 0, \]
Figure 15: The spectrum for example B.

Figure 16: The four branches of the complex spectrum for example B.
where we assume that \( \mu_1 \) and \( \mu_2 \) are the eigenvalues of \( M(\lambda) \) with positive imaginary part and \( u_1 \) and \( u_2 \) or \( u'_1 \) and \( u'_2 \) are the corresponding eigenvectors. They obviously satisfy

\[
\begin{pmatrix}
1 & 0 \\
S_{21}(\lambda) & S_{11}(\lambda)
\end{pmatrix}
\quad \text{and} \quad
\begin{pmatrix}
0 & 1 \\
S_{22}(\lambda) & S_{12}(\lambda)
\end{pmatrix}
\]

The scattering matrix, \( S(\lambda) \), is given by

\[
S(\lambda) = \begin{pmatrix}
S_{11}(\lambda) & S_{12}(\lambda) \\
S_{21}(\lambda) & S_{22}(\lambda)
\end{pmatrix}
\]

so that \( S(\lambda) \) is now a \( 2 \times 2 \) matrix as expected since there are two incoming and outgoing channels. The generalised eigenfunctions of the adjoint operator \( \Lambda^* \) are given by

\[
\hat{I}_{1}^\gamma (\lambda', x) = \begin{pmatrix}
S_{11}(\lambda) e^{-i\lambda x} \\
S_{21}(\lambda) e^{-2i\lambda x} \\
e^{i\lambda x}
\end{pmatrix}, \quad x < 0 \quad \text{or} \quad \hat{u}_1^* e^{i\mu_1 x} + \hat{u}_2^* e^{i\mu_2 x}, \quad x > 0,
\]

where the overbar denotes reversal of the elements, and

\[
\hat{I}_{2}^\gamma (\lambda', x) = \begin{pmatrix}
S_{12}(\lambda) e^{-i\lambda x} \\
S_{22}(\lambda) e^{-2i\lambda x} \\
e^{i\lambda x}
\end{pmatrix}, \quad x < 0 \quad \text{or} \quad \hat{u}_3^* e^{i\mu_1 x} + \hat{u}_4^* e^{i\mu_2 x}, \quad x > 0.
\]

The inner products can be deduced exactly as we did for example A (appendix 1). It follows that

\[
\left\langle \hat{I}_{1}^\gamma (\lambda, x), \hat{I}_{1}^\gamma (\lambda', x) \right\rangle = 2\pi S_{11}(\lambda) \delta(\lambda - \lambda'),
\]

\[
\left\langle \hat{I}_{2}^\gamma (\lambda, x), \hat{I}_{2}^\gamma (\lambda', x) \right\rangle = \pi S_{22}(\lambda) \delta(\lambda - \lambda'),
\]

and

\[
\left\langle \hat{I}_{1}^\gamma (\lambda, x), \hat{I}_{2}^\gamma (\lambda', x) \right\rangle = \pi \left( \frac{1}{2} S_{21}(\lambda) + S_{12}(\lambda) \right) = 2\pi S_{12},
\]

\[
\left\langle \hat{I}_{2}^\gamma (\lambda, x), \hat{I}_{1}^\gamma (\lambda', x) \right\rangle = \pi \left( \frac{1}{2} S_{21}(\lambda) + S_{12}(\lambda) \right) = 2\pi S_{12}.
\]

Our biorthogonal system is therefore

\[
\hat{I}_{1}^\gamma, \hat{I}_{2}^\gamma, \Omega_1 \text{ and } \Omega_2,
\]

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where
\[
\Omega_1 (\lambda, x) = S_{22} (\lambda) \tilde{I}_1^\gamma (\lambda, x) - S_{21} (\lambda) \tilde{I}_2^\gamma (\lambda, x) \\
= \begin{pmatrix}
(S_{22} (\lambda) S_{11} (\lambda) - S_{12} (\lambda) S_{21} (\lambda)) e^{-i \lambda x} \\
0 \\
-S_{21} (\lambda) e^{2i \lambda x} \\
S_{22} (\lambda) e^{i \lambda x}
\end{pmatrix}
\]
and
\[
\Omega_2 (\lambda, x) = S_{11} (\lambda) \tilde{I}_2^\gamma (\lambda, x) - S_{12} (\lambda) \tilde{I}_1^\gamma (\lambda, x) \\
= \begin{pmatrix}
0 \\
(S_{22} (\lambda) S_{11} (\lambda) - S_{12} (\lambda) S_{21} (\lambda)) e^{-i \lambda x/2} \\
S_{11} (\lambda) e^{2i \lambda x} \\
-S_{12} (\lambda) e^{i \lambda x}
\end{pmatrix}
\]
Therefore
\[
\langle I_1^\gamma (\lambda, x), \Omega_1 (\lambda', x) \rangle = 2\pi \delta (\lambda - \lambda') (S_{22} (\lambda) S_{11} (\lambda) - S_{21} (\lambda) S_{12} (\lambda)) \\
= 2\pi \delta (\lambda - \lambda') |S (\lambda)|,
\]
\[
\langle I_2^\gamma (\lambda, x), \Omega_2 (\lambda', x) \rangle = \pi \delta (\lambda - \lambda') (S_{22} (\lambda) S_{11} (\lambda) - S_{21} (\lambda) S_{12} (\lambda)) \\
= \pi \delta (\lambda - \lambda') |S (\lambda)|,
\]
and
\[
\langle I_1^\gamma (\lambda, x), \Omega_2 (\lambda', x) \rangle = \langle I_2^\gamma (\lambda, x), \Omega_1 (\lambda', x) \rangle = 0.
\]
To find the generalised eigenfunctions for the “complex” spectrum we solve equation 30 for each value of \( \mu \in \mathbb{R}^+ \). Since equation 30 is forth order we obtain four solutions for \( \lambda \), which must be grouped by branch. The generalised eigenfunctions for the “complex” spectrum are given by
\[
I_i^+ (\mu, x) = \begin{cases}
\begin{pmatrix}
v_1 (\mu, i) e^{i\mu x} + v_2 (\mu, i) e^{-i\mu x} + v_3 (\mu, i) e^{i\kappa x}, \ x > 0,
\end{pmatrix} \\
\begin{pmatrix}
0 \\
0 \\
v_1 (\mu, i) e^{2i\lambda x} \\
v_2 (\mu, i) e^{i\lambda x}
\end{pmatrix}, \ x > 0,
\end{cases}
\]
where \( v_1 (\mu, i), v_2 (\mu, i) \) and \( v_3 (\mu, i) \) are eigenvectors of \( M (\lambda_i) \) for the corresponding eigenvalue \( \lambda_i \), \( \text{Re} \kappa < 0 \),
\[
v_1 (\mu, i) + v_2 (\mu, i) + v_3 (\mu, i) = \begin{pmatrix}
0 \\
0 \\
v_1 (\mu, i) \\
v_2 (\mu, i)
\end{pmatrix},
\]
and \( i \) denotes the corresponding spectral branch. The generalised eigenfunctions of the adjoint operator are
\[
\hat{I}_i^+ (\mu, x) = \begin{cases} \\
\varphi_1^* (\mu, i) e^{-i\mu x} + \varphi_2^* (\mu, i) e^{i\mu x} + \varphi_3^* (\mu, i) e^{i\lambda x}, x > 0, \\
\frac{\mu_0 (\mu, i) e^{-i\lambda x}}{2}, x > 0.
\end{cases}
\]

Again the inner products can be calculated as in appendix 1 and it follows that
\[
\langle \hat{I}_i^+ (\mu, x), \hat{I}_j^+ (\mu', x) \rangle = 2\pi \langle \varphi_1 (\mu, i), \varphi_2 (\mu', j) \rangle \delta (\mu - \mu') \delta_{ij},
\]

where \(\delta_{ij}\) is the Kronecker delta.

### 4.3 Using the generalised eigenfunctions to construct a change of basis

Consider the operator \(\Gamma\),
\[
\Gamma : \begin{pmatrix} L_2 (-\infty, \infty) \\ L_2 (-\infty, \infty) \\ L_2 (-\infty, \infty) \\ L_2 (-\infty, \infty) \end{pmatrix} \rightarrow \begin{pmatrix} L_2 (-\infty, \infty) \\ L_2 (0, \infty) \\ L_2 (0, \infty) \\ L_2 (0, \infty) \end{pmatrix},
\]
which acts as follows
\[
\Gamma (I(x)) = \begin{pmatrix} h_1^\gamma (\lambda) \\ h_2^\gamma (\lambda) \\ h_3^\gamma (\mu) \\ h_4^\gamma (\mu) \end{pmatrix},
\]
where
\[
h_1^\gamma (\lambda) = \frac{\langle I_0 (x), \Omega_1 (\lambda', x) \rangle}{2\pi \| S (\lambda) \|}, 
\]
\[
h_2^\gamma (\lambda) = \frac{\langle I_0 (x), \Omega_2 (\lambda', x) \rangle}{\pi \| S (\lambda) \|},
\]
\[
h_j^\mu (\mu) = \frac{\langle I_0 (x), \hat{I}_j^+ (\mu, x) \rangle}{2\pi \langle \varphi_1 (\mu, j), \varphi_2 (\mu', j) \rangle}.
\]

From the biorthogonality condition the inverse of this operator is given by
\[
\Gamma^{-1} = \sum_{i=1}^2 \int_{-\infty}^\infty h_i^\gamma (\lambda) I_i^\gamma (\lambda, x) d\lambda + \sum_{j=1}^4 \int_0^\infty h_j^\mu (\mu) I_j^+ (\mu, x) d\mu.
\]

(32)
Consider the operator \( \tilde{\Lambda} \) given by

\[
\Lambda I(x) = \Gamma^{-1} \tilde{\Lambda} \Gamma I(x).
\]

\( \tilde{\Lambda} \) is given by

\[
\tilde{\Lambda} = \begin{pmatrix} h_1^\gamma(\lambda) \\
                      h_2^\gamma(\lambda) \\
                      h_1^\mu(\mu) \\
                      h_2^\mu(\mu) \\
                      h_3^\mu(\mu) \\
                      h_4^\mu(\mu) \\
\end{pmatrix} = \begin{pmatrix} \lambda h_1^\gamma(\lambda) \\
                           \lambda h_2^\gamma(\lambda) \\
                           \lambda_1(\mu) h_1^\mu(\mu) \\
                           \lambda_2(\mu) h_2^\mu(\mu) \\
                           \lambda_3(\mu) h_3^\mu(\mu) \\
                           \lambda_4(\mu) h_4^\mu(\mu) \\
\end{pmatrix}, \quad (33)
\]

where \( \lambda_i(\mu) \) is the solution of \( \lambda \) for \( \mu \) on the \( i \)th branch. Consider now the semigroup operator \( T(t) \),

\[
T(t) I_0(x) = \Gamma^{-1} \tilde{T}(t) \Gamma,
\]

where the operator \( \tilde{T}(t) \) is given by

\[
\tilde{T}(t) = \begin{pmatrix} h_1^\gamma(\lambda) \\
                           h_2^\gamma(\lambda) \\
                           h_1^\mu(\mu) \\
                           h_2^\mu(\mu) \\
                           h_3^\mu(\mu) \\
                           h_4^\mu(\mu) \\
\end{pmatrix} = \begin{pmatrix} e^{i\lambda t} h_1^\gamma(\lambda) \\
                           e^{i\lambda t} h_2^\gamma(\lambda) \\
                           e^{i\lambda_1(\mu) t} h_1^\mu(\mu) \\
                           e^{i\lambda_2(\mu) t} h_2^\mu(\mu) \\
                           e^{i\lambda_3(\mu) t} h_3^\mu(\mu) \\
                           e^{i\lambda_4(\mu) t} h_4^\mu(\mu) \\
\end{pmatrix}, \quad (34)
\]

Again in this basis the transformed operator \( \tilde{\Lambda} \) is multiplicative and hence the transformed semigroup operator generated by \( \tilde{\Lambda} \), \( \tilde{T}(t) = e^{i\tilde{\Lambda} t} \), is also multiplicative.

### 4.4 A Scattering Theory

We can develop a scattering theory equivalent to section 3.7. We assume that \( I_0 \in D_- \) and is of the form

\[
I_0 = \begin{pmatrix} f_1(x) \\
                      f_2(x) \\
                      0 \\
                      0 \\
\end{pmatrix}, \quad x < 0.
\]

The generalised eigenfunctions of \( \Lambda^* \) which correspond to the “complex” spectrum vanish in the incoming channel so it follows that

\[
\Gamma I_0 = \begin{pmatrix} \langle I_0(x), \Omega_1(x') \rangle \\
                           \frac{2\pi i S(\lambda)}{\sqrt{2\pi i S(\lambda)}} \langle I_0(x), \Omega_2(x') \rangle \\
                           0 \\
                           0 \\
\end{pmatrix}.\]

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Therefore the semigroup operator $T(t)$ is given by

$$T(t)I_0 = \Gamma^{-1}\mathcal{F}(t)\Gamma I_0$$

$$= \Gamma^{-1}\begin{pmatrix}
\langle I_0(x)\Omega_1(x)\rangle e^{i\lambda t} \\
\langle I_0(x)\Omega_2(x)\rangle e^{i\lambda t} \\
\pi \rho |S(\lambda)| \\
0 \\
0 \\
0 \\
0
\end{pmatrix}. \quad (35)$$

We know that

$$\frac{\langle I_0(x), \Omega_k(x') \rangle}{2\pi |S(\lambda)|} = \frac{1}{2\pi |S(\lambda)|} \int_0^\infty |S(\lambda)| e^{i\lambda x} f_i(x) dx = F_i(\lambda)$$

and follows that

$$T(t)I_0(x) = \sum_{i=1}^2 \frac{1}{2\pi} \int_{-\infty}^\infty e^{i\lambda t} F_i(\lambda) I_0^\wedge(\lambda, x) d\lambda.$$  \quad (36)

The projection of the solution in the outgoing channel is therefore

$$P_{D_+} T(t)I_0 = \begin{pmatrix}
0 \\
0 \\
\int_{-\infty}^\infty e^{i\lambda(x+t)} \begin{pmatrix}
S_{21}(\lambda) & S_{22}(\lambda) \\
S_{11}(\lambda) & S_{12}(\lambda)
\end{pmatrix} \begin{pmatrix}
F_1(\lambda) \\
F_2(\lambda)
\end{pmatrix} d\lambda, \ x < 0, \\
0, \ x > 0.
\end{pmatrix}$$

Note that the swapping of the rows of the matrix is due simply to the fact that we have associated the first and fourth channels and the second and third channels. This is because they are the channels which propagate with the same speed. Figure 17 shows the output for the initial condition

$$I_0 = \begin{pmatrix}
H(x+2) - H(x+1) \\
0 \\
0 \\
0
\end{pmatrix}. \quad (37)$$

in the fourth channel and Figure 18 shows the output in the third channel, calculated by the scattering and time marching methods.

Again it is obvious that the scattering and time marching methods give the same result. The staircase structure in the time marching method is an artifact of the numerical method which could be easily removed by smoothing.
Figure 17: The temporal evolution in the fourth channel of $I_0 = H(x + 2) - H(x + 1)$ in the first channel calculated by the scattering and time marching methods for $x = 0$. 
Figure 18: The temporal evolution in the third channel of $I_0 = H(x+2) - H(x+1)$ in the first channel calculated by the scattering and time marching methods for $x = 0$. 
4.5 Evolution of an input in $K$

We know that the semigroup operator $T(t)$ is given by

$$ T(t)I_0(x) = \Gamma^{-1}\tilde{T}(t) $$

Since the generalised eigenfunctions corresponding to the “complex” spectrum are zero in the incoming channels we can calculate the evolution in the outgoing channel by only integrating over the real channel, i.e.,

$$ \mathcal{P}_D T(t)I_0 = \sum_{i=1}^{2} \int_{-\infty}^{\infty} e^{i\lambda h_i^+ (\lambda)} I_i^+ (\lambda, x) d\lambda $$

We consider an initial input similar to that of section 3.10

$$ I_0 = \begin{pmatrix} H(x-1) - H(x-2) \\ 0 \\ 0 \\ 0 \end{pmatrix} $$

The calculation of the integrals in equation 39 is by the FFT algorithm and the results are shown in figures 19 and 20 as well as the same evolutions calculated by the time marching solution method. It is obvious that the two methods agree.

The evolution in $K$ is given by

$$ \mathcal{P}_K T(t)I_0 = \sum_{i=1}^{2} \int_{-\infty}^{\infty} e^{i\lambda h_i^+ (\lambda)} I_i^+ (\lambda, x) d\lambda + \sum_{j=1}^{4} \int_{0}^{\infty} e^{i\lambda_0 (\mu) h_j^+ (\mu)} I_j^+ (\mu, x) d\mu. $$

The numerical results for the evolution given by equation 41 for the initial input of equation 40 are shown in figures 21 and 21, where the results are again also calculated using the time marching method for comparison. It is clear from these figures that the two methods give the same answers.

5 Conclusions

Although we began by considering equation 2,

$$ -i\frac{\partial I}{\partial t} = iD \frac{\partial I}{\partial x} + i\chi(0, \infty)MI, $$

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Figure 19: The temporal evolution in the fourth channel of $I_0 = H(x - 1) - H(x - 2)$ in the first channel calculated by the scattering and time marching solution methods for $x = 0$. 
Figure 20: The temporal evolution in the third channel of $I_0 = H(x - 1) - H(x - 2)$ in the first channel calculated by the scattering and time marching solution methods for $x = 0$. 
Figure 21: The temporal evolution in the first channel of $I_0 = H(x-1) - H(x-2)$ in the first channel calculated by the scattering and time marching solution methods for $x = 1.5$. 

Example B, Scattering method $(\kappa T(t)I_0)$, $x = 1.5$, first channel

Example B, Time marching method $(\phi T(t)I_0)$, $x = 1.5$, first channel
Figure 22: The temporal evolution in the fourth channel of $J_0 = H(x - 1) - H(x - 2)$ in the first channel calculated by the scattering and time marching solution methods for $x = 1.5$. 
all that has been presented is a solution for two very simple subcases of this equation. We should now consider equation 2 once more. While we have not presented a solution method to equation 2 it should be apparent that the solution method which we have presented for our simple examples could easily be generalised. The spectrum of the operator would consist of the real axis and several complex branches. The branches of “complex” spectrum will be determined as the intersection of an algebraic variety derived from the characteristic polynomial of some matrix and the hypersurface where the imaginary part of one of the variables is zero. Once the spectrum has been found the generalised eigenfunctions can be determined. The normalisation of the generalised eigenvectors could be computed using the appropriate coefficients of the purely imaginary exponentials. The generalised eigenfunctions of the operator would permit a change of basis in which the operator becomes multiplicative. This would allow us to solve for the evolution numerically using spectral theory.

References


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Appendix 1: Determining the coefficients in the biorthogonal expansion

The generalised eigenfunctions of $\Lambda$ are, assuming that $\text{Re}i\mu > 0$,

$$I^>(\lambda, x) = \begin{cases} \left( \begin{array}{c} 1 \\ i\lambda + 1 - i\mu \\
1 & e^{-ix\lambda} + \left( \begin{array}{cc} 0 \\ i\lambda + 1 - i\mu \end{array} \right) e^{ix\lambda}, \quad x < 0, \end{array} \right), \quad x > 0, \\
0 \end{cases}$$

and

$$I^+_{1,2}(\mu, x) = \begin{cases} \left( \begin{array}{c} i\lambda_{1,2} + 1 - i\mu \\ 1 \\
-2i\mu \\
0 \end{array} \right) e^{-ix\lambda_{1,2}}, \quad x < 0, \end{cases}$$

$$e^{ix\mu}, \quad x > 0,$$
where \( \lambda_1 = i + \sqrt{\mu^2 - 1} \) and \( \lambda_2 = i - \sqrt{\mu^2 - 1} \). The generalised eigenfunctions \( \hat{I}_\lambda \) of the adjoint operator \( \Lambda^* \) are, assuming that \( \text{Re} i\mu > 0 \),

\[
\hat{I}^> (\lambda, x) = \begin{cases} 
    \left( -i\lambda + 1 - i\mu \right) e^{-ix\mu}, & x > 0, \\
    \left( -i\lambda + 1 - i\mu \right) e^{-ix\lambda} + \left( \frac{1}{1} \right) e^{ix\lambda}, & x < 0,
\end{cases}
\]

and

\[
\hat{I}^<_{1,2} (\mu, x) = \begin{cases} 
    \frac{1}{\lambda_{1,2} + 1 - i\mu} e^{ix\mu} - \left( -i\lambda_{1,2} + 1 + i\mu \right) e^{-ix\mu}, & x > 0, \\
    0, \quad & x < 0,
\end{cases}
\]

where \( \lambda_1 = -i + \sqrt{\mu^2 - 1} \) and \( \lambda_2 = -i - \sqrt{\mu^2 - 1} \). We know from Hilbert space theory that the generalised eigenfunctions of \( \Lambda \) and \( \Lambda^* \) must form a biorthogonal system but we must determine the normalisation.

Let us now take the inner product

\[
\langle \hat{I}^> (\lambda, x), \hat{I}^> (\lambda', x) \rangle = \int_{-\infty}^{\infty} e^{-ix\mu} (i\lambda + 1 - i\mu) e^{i\lambda' x} dx + \int_{0}^{\infty} e^{-ix\mu} (i\lambda' + 1 + i\mu^*) e^{i\lambda x} dx
\]

\[
+ \int_{-\infty}^{0} (i\lambda + 1 - i\mu) e^{i\lambda x} e^{-i\lambda' x} dx + \int_{-\infty}^{0} e^{-ix\mu} (i\lambda' + 1 + i\mu^*) e^{i\lambda' x} dx
\]

\[
= \int_{-\infty}^{\infty} (i\lambda + 1 - i\mu) e^{i\lambda x} e^{-i\lambda' x} dx + \int_{0}^{\infty} (i\lambda' + 1 + i\mu^* - i\lambda - 1 + i\mu) e^{i\lambda x} e^{-i\lambda' x} dx
\]

\[
+ \int_{0}^{\infty} (i\lambda + 2 - i\mu + i\lambda' + i\mu^*) e^{-i\lambda x} e^{i\lambda' x} dx
\]

\[
= 2\pi (i\lambda + 1 - i\mu) \delta (\lambda - \lambda') + \frac{1}{i\lambda' - i\lambda} \left( i\lambda' + i\mu^* - i\lambda + i\mu \right)
\]

\[
+ \frac{1}{i\mu - i\mu^*} (i\lambda + 2 - i\mu + i\lambda' + i\mu^*)
\]

\[
= 2\pi (i\lambda + 1 - i\mu) \delta (\lambda - \lambda')
\]

\[
+ \frac{1}{(i\mu - i\mu^*)(i\lambda' - i\lambda)} [(i\mu - i\mu^*) (i\lambda' + i\mu^* - i\lambda + i\mu)
\]

\[
+ (i\lambda' - i\lambda) (i\lambda + 2 - i\mu + i\lambda' + i\mu^*)]
\]

\[
= 2\pi (i\lambda + 1 - i\mu) \delta (\lambda - \lambda') + \frac{\lambda'^2 - \mu^2 - \lambda^2 + 2i\lambda' + \lambda^2 - 2i\lambda}{(i\mu - i\mu^*) (i\lambda' - i\lambda)}
\]

\[
= 2\pi (i\lambda + 1 - i\mu) \delta (\lambda - \lambda')
\]

\[
+ 2\pi S(\lambda) \delta (\lambda - \lambda'),
\]

and

\[
\langle \hat{I}^+_{1} (\mu, x), \hat{I}^+_{1} (\mu, x) \rangle = \int_{0}^{\infty} (e^{i\lambda x} - e^{-i\lambda x}) ((i\lambda + 1 + i\mu) e^{-i\lambda x} - (i\lambda + 1 - i\mu) e^{i\lambda x}) dx
\]
\[ + \int_{0}^{\infty} \left( (i\lambda_1 + 1 - i\mu) e^{ix\mu} - (i\lambda_1 + 1 + i\mu) e^{-ix\mu} \right) \left( e^{-ij\mu x} - e^{ij\mu x} \right) dx \]
\[ = \int_{0}^{\infty} e^{ix\mu} e^{-ij\mu x} \left( (i\lambda'_1 + 1 + i\hat{\mu}) + (i\lambda_1 + 1 - i\mu) \right) dx \]
\[ + \int_{0}^{\infty} e^{-ix\mu} e^{ij\mu x} \left( (i\lambda'_1 + 1 - i\hat{\mu}) + (i\lambda_1 + 1 + i\mu) \right) dx \]
\[ + \int_{0}^{\infty} e^{ij\mu x} e^{ij\mu x} \left( - (i\lambda'_1 + 1 - i\hat{\mu}) - (i\lambda_1 + 1 - i\mu) \right) dx \]
\[ + \int_{0}^{\infty} e^{-ij\mu x} e^{-ij\mu x} \left( - (i\lambda'_1 + 1 + i\hat{\mu}) - (i\lambda_1 + 1 + i\mu) \right) dx \]
\[ = \int_{-\infty}^{\infty} e^{ix\mu} e^{-ij\mu x} \left( (i\lambda'_1 + 1) + (i\lambda_1 + 1) \right) dx \]
\[ = 2\pi \left( 2i\lambda_1 + 2 \right) \delta (\mu - \hat{\mu}). \]

Likewise
\[ \left\langle \hat{I}_2^+(\mu, x), \hat{I}_2^+(\hat{\mu}, x) \right\rangle = 2\pi \left( 2i\lambda_2 + 2 \right) \delta (\mu - \hat{\mu}). \]