The time-dependent Schrödinger equation with piecewise constant potential

Bernard Deconinck

Department of Applied Mathematics
University of Washington

bernard@amath.washington.edu

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Exact solutions of interface problems using the method of Fokas

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Department of Applied Mathematics
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bernard@amath.washington.edu

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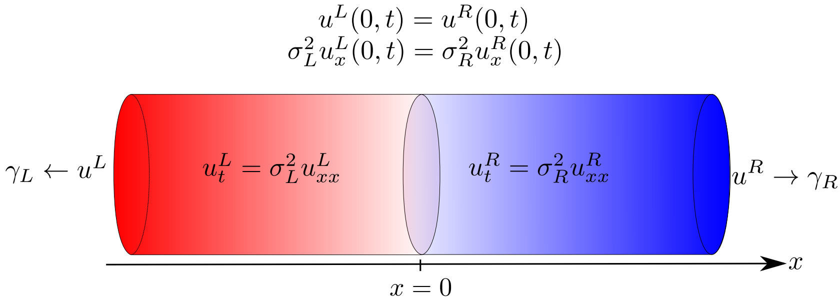
Interface Problems

- "Classical" BVPs: prescribed domain, prescribed boundary functions

Interface Problems

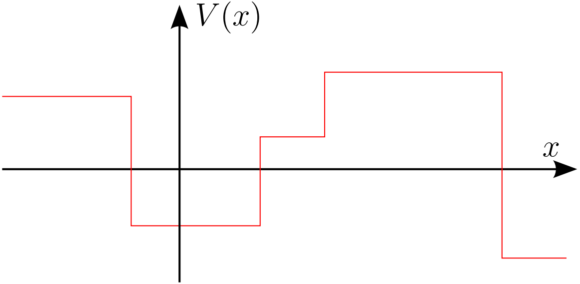
- "Classical" BVPs: prescribed domain, prescribed boundary functions
- What if the boundary functions or the location of the boundary are not directly known?

Example 1. The heat equation in a composite rod



- The domain is known.
- No functions are known at the boundary, all depend on the solution of the problem.
- The boundary is a material interface.

Example 2. The Schrödinger equation with piecewise constant potential



$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\psi_{xx} + V(x)\psi,$$

with ψ and ψ_x continuous across the jumps.

The Method of Fokas

Let's see how the Method of Fokas is used to solve the following problem:

$$
\begin{aligned}
iv_t &= v_{xx}, && x > 0, t > 0, \\
v(x,0) &= v_0(x), && x > 0, \\
v(0,t) &= f(t), && t > 0.
\end{aligned}
$$

1. Local relation

The PDE is equivalent to

$$\frac{\partial}{\partial t}(e^{-ikx+\omega t}v) - \frac{\partial}{\partial x}(e^{-ikx+\omega t}(kv - iv_x)) = 0,$$

with

$$\omega(k) = -ik^2.$$

2. Global relation

We integrate the local relation over the domain where the equation is defined, up to t:

$$\hat{v}_0(k) - e^{\omega t}\hat{v}(k,t) - kg_0(\omega,t) + ig_1(\omega,t) = 0,$$

which is valid in the lower half k plane.

$$\hat{v}_0(k) - e^{\omega t}\hat{v}(k,t) - kg_0(\omega,t) + ig_1(\omega,t) = 0,$$

Here

$$\begin{aligned}
\hat{v}_0(k) &= \int_0^\infty e^{-ikx} v_0(x)dx, \\
\hat{v}(k,t) &= \int_0^\infty e^{-ikx} v(x,t)dx, \\
g_0(\omega,t) &= \int_0^t e^{\omega s} v(0,s)ds, \\
g_1(\omega,t) &= \int_0^t e^{\omega s} v_x(0,s)ds.
\end{aligned}$$

3. "Solution" formula

From the global relation

$$\begin{aligned} v(x,t) =& \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega t}\hat{v}_0(k)dk + \\ & \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega t}(ig_1(\omega,t) - kg_0(\omega,t))dk. \end{aligned}$$

3. "Solution" formula

From the global relation

$$v(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega t}\hat{v}_0(k)dk + \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega t}(ig_1(\omega,t) - kg_0(\omega,t))dk.$$

Unfortunately, we do not know $g_1(\omega,t)\ldots$

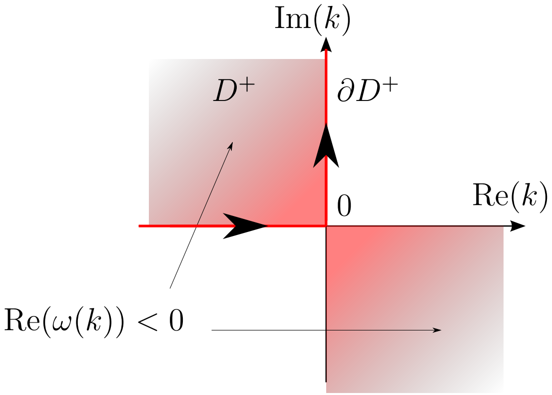
4. Deformed "solution" formula

The solution formula is rewritten as

$$\begin{aligned} v(x,t) = &\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega t}\hat{v}_0(k)dk + \\ &\frac{1}{2\pi}\int_{\partial D^+} e^{ikx-\omega t}(ig_1(\omega,t) - kg_0(\omega,t))dk, \end{aligned}$$

where

$$D^+ = \{k \in \mathbb{C} : \mathrm{Im}(k) > 0 \text{ and } \mathrm{Re}(\omega(k)) < 0\}.$$



Im(k)
D+
∂D+
0
Re(k)
Re(ω(k)) < 0

5. Symmetries of $\omega(k)$

The dispersion relation $\omega(k)$ is unchanged under the transformation $k \to -k$. Applying this to the global relation,

$$\hat{v}_0(-k) - e^{\omega t}\hat{v}(-k,t) + kg_0(\omega,t) + ig_1(\omega,t) = 0,$$

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which is valid in the upper half plane.

This equation is solved for the unknown boundary function:

$$ig_1(\omega,t) = e^{\omega t}\hat{v}(-k,t) - \hat{v}_0(-k) - kg_0(\omega,t).$$

6. Solution

$$
\begin{aligned}
v(x,t) =& \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega t}(\hat{v}_0(k) - \hat{v}_0(-k))dk + \\
& \frac{1}{2\pi}\int_{\partial D^+} e^{ikx}\hat{v}(-k,t)dk - \frac{1}{\pi}\int_{\partial D^+} e^{ikx-\omega t} k g_0(\omega,t)dk.
\end{aligned}
$$

6. Solution

$$v(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega t}(\hat{v}_0(k) - \hat{v}_0(-k))dk + \frac{1}{2\pi}\int_{\partial D^+} e^{ikx}\hat{v}(-k,t)dk - \frac{1}{\pi}\int_{\partial D^+} e^{ikx-\omega t} k g_0(\omega,t)dk.$$

The term in red is shown to vanish, by closing over D^+. Thus

$$v(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega t}(\hat{v}_0(k) - \hat{v}_0(-k))dk + - \frac{1}{\pi}\int_{\partial D^+} e^{ikx-\omega t} k g_0(\omega,t)dk.$$

Summary

- Local relation, dispersion relation $\omega(k)$
- Global relation
- Solution reconstruction, with deformed contour
- Extra global relations, using symmetries of $\omega(k)$
- Solution, after eliminating unknown boundary conditions

An interface problem: the linear Schrödinger equation

Consider

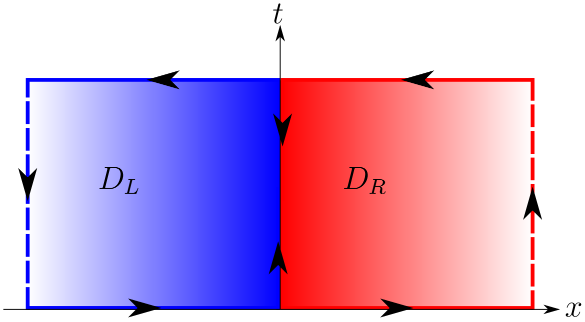
$$
\begin{aligned}
iq_t^L &= \sigma_L q_{xx}^L, && -\infty < x < 0,\ t > 0,\\
iq_t^R &= \sigma_R q_{xx}^R, && 0 < x < \infty,\ t > 0,
\end{aligned}
$$

with initial conditions

$$
\begin{aligned}
q^L(x,0) =& q_0^L(x), && -\infty < x < 0,\\
q^R(x,0) =& q_0^R(x), && 0 < x < \infty,
\end{aligned}
$$

and interface conditions

$$
\begin{aligned}
q^L(0,t) =& q^R(0,t), && t > 0,\\
\beta_L q_x^L(0,t) =& \beta_R q_x^R(0,t), && t > 0.
\end{aligned}
$$



t
D_L
D_R
x

1. Local relations

$$\left(e^{-ikx+\omega_L t}v^L\right)_t = \left(\sigma_L e^{-ikx+\omega_L t}(kv^L - iv_x^L)\right)_x, \quad -\infty < x < 0,$$
$$\left(e^{-ikx+\omega_R t}v^R\right)_t = \left(\sigma_R e^{-ikx+\omega_R t}(kv^R - iv_x^R)\right)_x, \quad 0 < x < \infty,$$

with $\omega_L = -i\sigma_L k^2$, $\omega_R = -i\sigma_R k^2$.

2. Global relations

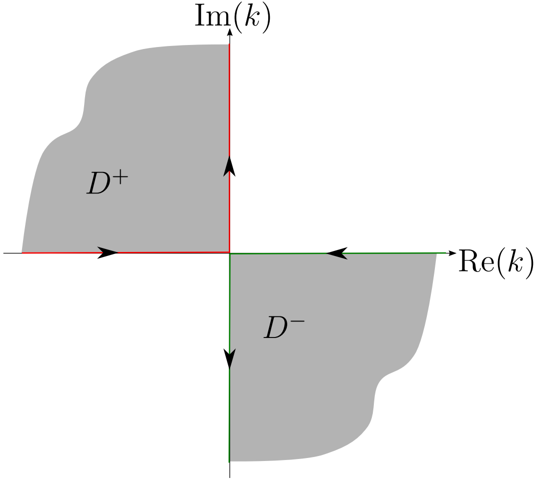
$$0 = \hat{v}_0^L(k) - e^{\omega_L t}\hat{v}^L(k,t) + k\sigma_L g_0(\omega_L,t) - i\sigma_L g_1(\omega_L,t),$$
$$0 = \hat{v}_0^R(k) - e^{\omega_R t}\hat{v}^R(k,t) - k\sigma_R g_0(\omega_R,t) + \frac{i\sigma_R\beta_L}{\beta_R} g_1(\omega_R,t),$$

with

$$g_0(\omega,t) = \int_0^t e^{\omega s} v^L(0,s)\,\mathrm{d}s = \int_0^t e^{\omega s} v^R(0,s)\,\mathrm{d}s,$$
$$g_1(\omega,t) = \int_0^t e^{\omega s} v_x^L(0,s)\,\mathrm{d}s = \frac{\beta_R}{\beta_L}\int_0^t e^{\omega s} v_x^R(0,s)\,\mathrm{d}s,$$
$$\hat{v}^L(k,t) = \int_{-\infty}^0 e^{-ikx} v^L(x,t)\,\mathrm{d}x, \qquad \hat{v}_0^L(k) = \int_{-\infty}^0 e^{-ikx} v_0^L(x)\,\mathrm{d}x,$$
$$\hat{v}^R(k,t) = \int_0^\infty e^{-ikx} v^R(x,t)\,\mathrm{d}x, \qquad \hat{v}_0^R(k) = \int_0^\infty e^{-ikx} v_0^R(x)\,\mathrm{d}x.$$

3-4. Deformed "solution" formulae

$$
\begin{aligned}
v^L(x,t) =& \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega_L t}\hat{v}_0^L(k)\,\mathrm{d}k + \\
& - \frac{\sigma_L}{2\pi}\int_{\partial D^-} e^{ikx-\omega_L t}(kg_0(\omega_L,t) - ig_1(\omega_L,t))\,\mathrm{d}k, \\
v^R(x,t) =& \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega_R t}\hat{v}_0^R(k)\,\mathrm{d}k + \\
& + \frac{\sigma_R}{2\pi}\int_{\partial D^+} e^{ikx-\omega_R t}\left(-kg_0(\omega_R,t) + \frac{i\beta_L}{\beta_R}g_1(\omega_R,t)\right)\mathrm{d}k.
\end{aligned}
$$



$\rightarrow$ We don't know g_0 or g_1...

5. Symmetries of $\{\omega_L(k), \omega_R(k)\}$

The set $\{\omega_L(k), \omega_R(k)\}$ is invariant under

$$k \to -k, \quad k \to k\sqrt{\sigma_L/\sigma_R}.$$

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- Using these symmetries results in new global relations with the same unknowns.
- The new global relations are solved for the unknown boundary functions.
- The dependence on $\hat{v}^L(-k,t)$, $\hat{v}^R(-k,t)$, $\hat{v}^L(k\sqrt{\sigma_R/\sigma_L}, t)$, $\hat{v}^R(k\sqrt{\sigma_L/\sigma_R}, t)$ vanishes, using Jordan's lemma.

6. Solutions

$$
\begin{aligned}
q^L(x,t) =& \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega_L t}\hat{v}_0^L(k)\,\mathrm{d}k \\
&+ \frac{\beta_R\sigma_L - \beta_L\sqrt{\sigma_L\sigma_R}}{2\pi(\beta_R\sigma_L + \beta_L\sqrt{\sigma_L\sigma_R})}\int_{\partial D^-} e^{ikx-\omega_L t}\hat{v}_0^L(-k)\,\mathrm{d}k \\
&- \frac{\beta_R\sigma_L}{\pi(\beta_L\sigma_R + \beta_R\sqrt{\sigma_L\sigma_R})}\int_{\partial D^-} e^{ikx-\omega_L t}\hat{v}_0^R\left(k\sqrt{\frac{\sigma_L}{\sigma_R}}\right)\,\mathrm{d}k, \\
q^R(x,t) =& \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega_R t}\hat{v}_0^R(k)\,\mathrm{d}k \\
&+ \frac{\beta_L\sigma_R}{\pi\left(\beta_R\sigma_L + \beta_L\sqrt{\sigma_R\sigma_L}\right)}\int_{\partial D^+} e^{ikx-\omega_R t}\hat{v}_0^L\left(k\sqrt{\frac{\sigma_R}{\sigma_L}}\right)\,\mathrm{d}k \\
&+ \frac{\beta_R\sigma_L - \beta_L\sqrt{\sigma_L\sigma_R}}{2\pi\left(\beta_R\sigma_L + \beta_L\sqrt{\sigma_R\sigma_L}\right)}\int_{\partial D^+} e^{ikx-\omega_R t}\hat{v}_0^R(-k)\,\mathrm{d}k.
\end{aligned}
$$

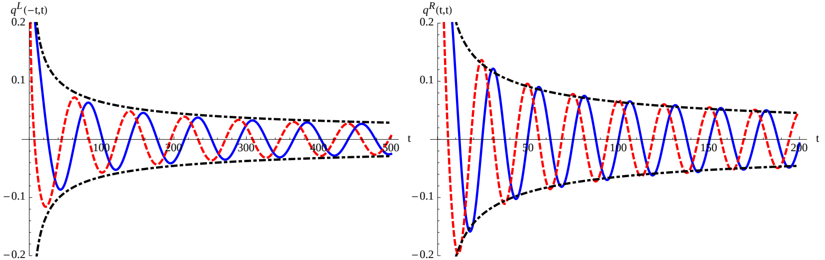
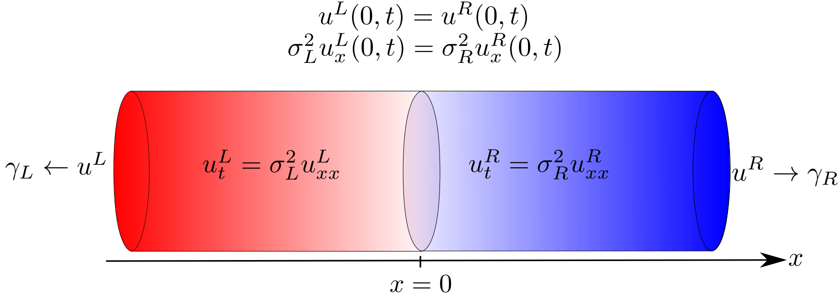


Figure: Leading order behavior of $q^L(-t,t)$ and $q^R(t,t)$, $\beta_L = 4, \beta_R = 1, \sigma_L = 3$, and $\sigma_R = 1$ with $q_0^L(x) = (1+\beta_R x)e^{-x^2}$ and $q_0^R(x) = (1+\beta_L x)e^{-x^2}$.

The heat equation in a composite rod



Steps of the solution process are the same, leading to

$$u^L(x,t) = \gamma^L + \frac{\sigma_R(\gamma^R - \gamma^L)}{\sigma_L + \sigma_R}\,\mathrm{erfc}\left(\frac{x}{2\sqrt{\sigma_L^2 t}}\right) +$$

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-(\sigma_L k)^2 t}\hat{v}_0^L(k)\,\mathrm{d}k +$$

$$+\int_{\partial D^-} e^{ikx-(\sigma_L k)^2 t}\left(\frac{\sigma_R - \sigma_L}{2\pi(\sigma_L + \sigma_R)}\hat{v}_0^L(-k) - \frac{\sigma_L}{\pi(\sigma_L + \sigma_R)}\hat{v}_0^R\left(\frac{k\sigma_L}{\sigma_R}\right)\right)\mathrm{d}k,$$

$$u^R(x,t) = \gamma^R + \frac{\sigma_L(\gamma^L - \gamma^R)}{\sigma_L + \sigma_R}\,\mathrm{erfc}\left(\frac{x}{2\sqrt{\sigma_R^2 t}}\right) +$$

$$+\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-(\sigma_R k)^2 t}\hat{v}_0^R(k)\,\mathrm{d}k +$$

$$+\int_{\partial D^+} e^{ikx-(\sigma_R k)^2 t}\left(\frac{\sigma_R - \sigma_L}{2\pi(\sigma_L + \sigma_R)}v_0^R(-k) + \frac{\sigma_R}{\pi(\sigma_L + \sigma_R)}v_0^L\left(\frac{k\sigma_R}{\sigma_L}\right)\right)\mathrm{d}k.$$

Initial condition $\to$ interface value maps

- Using the same ideas used to construct Dirichlet $\to$ Neumann maps using the Method of Fokas, one can construct maps from the initial data to data at the interface.

Initial condition $\rightarrow$ interface value maps

- Using the same ideas used to construct Dirichlet $\rightarrow$ Neumann maps using the Method of Fokas, one can construct maps from the initial data to data at the interface.
- Once the interface data is constructed, the solution can be found using a standard BVP.

Example: Initial condition → Dirichlet interface data

$$
\begin{aligned}
u(0,t) =& \frac{1}{2\pi}\int_{\partial D^+}\int_{-\infty}^{0} e^{-ikx-\sigma_1^2k^2t}u_0^{(1)}(x)\,\mathrm{d}x\,\mathrm{d}k \\
&- \frac{1}{2\pi}\int_{\partial D^-}\int_{0}^{\infty} e^{-ikx-\sigma_2^2k^2t}u_0^{(2)}(x)\,\mathrm{d}x\,\mathrm{d}k.
\end{aligned}
$$

A similar formula may be derived for the flux interface data.

The time-dependent Schrödinger eqn with piecewise constant potential

$$i\psi_t = -\psi_{xx} + \alpha(x)\psi, \qquad x \in \mathbb{R}, t > 0,$$

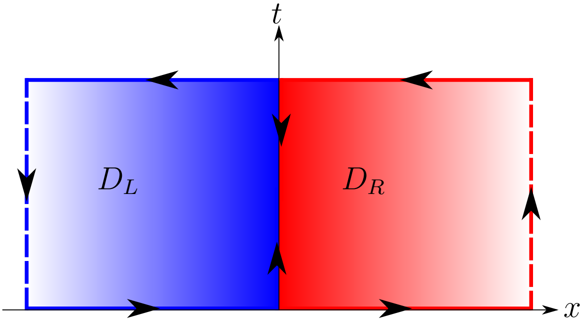
$$\alpha(x) = \begin{cases} \alpha_1, & x < 0, \\ \alpha_2, & x > 0, \end{cases},$$

or

$$\begin{aligned} i\psi_t^{(1)} &= -\psi_{xx}^{(1)} + \alpha_1 \psi^{(1)}, && x < 0,\ t > 0, \\ i\psi_t^{(2)} &= -\psi_{xx}^{(2)} + \alpha_2 \psi^{(2)}, && x > 0,\ t > 0, \\ \psi^{(1)}(x,0) &= \psi_0^{(1)}(x), && x < 0, \\ \psi^{(2)}(x,0) &= \psi_0^{(2)}(x), && x > 0. \end{aligned}$$

We impose the interface conditions

$$\psi^{(1)}(0,t) = \psi^{(2)}(0,t), \quad \psi_x^{(1)}(0,t) = \psi_x^{(2)}(0,t).$$



t
x
D_L
D_R

1. Local relations

$$\left(e^{-ikx+\omega_1 t}\psi^{(1)}\right)_t = \left(e^{-ikx+\omega_1 t}(-k\psi^{(1)} + i\psi_x^{(1)})\right)_x, \quad -\infty < x < 0,$$
$$\left(e^{-ikx+\omega_2 t}\psi^{(2)}\right)_t = \left(e^{-ikx+\omega_2 t}(-k\psi^{(2)} + i\psi_x^{(2)})\right)_x, \quad 0 < x < \infty,$$

with $\omega_j = i(\alpha_j + k^2)$, $j = 1, 2$.

2. Global relations

$$
\begin{aligned}
\hat{\psi}^{(1)}(k,t) =& e^{-\omega_1 t}\left(\hat{\psi}_0^{(1)}(k) - k g_0(\omega_1,t) + i g_1(\omega_1,t)\right),\\
\hat{\psi}^{(2)}(k,t) =& e^{-\omega_2 t}\left(\hat{\psi}_0^{(2)}(k) - k g_0(\omega_2,t) + i g_1(\omega_2,t)\right),
\end{aligned}
$$

with

$$
\begin{aligned}
g_0(\omega,t) &= \int_0^t e^{\omega s}\psi^{(1)}(0,s)\,\mathrm{d}s = \int_0^t e^{\omega s}\psi^{(2)}(0,s)\,\mathrm{d}s,\\
g_1(\omega,t) &= \int_0^t e^{\omega s}\psi_x^{(1)}(0,s)\,\mathrm{d}s = \int_0^t e^{\omega s}\psi_x^{(2)}(0,s)\,\mathrm{d}s,\\
\hat{\psi}^{(1)}(k,t) &= \int_{-\infty}^0 e^{-ikx}\psi^{(1)}(x,t)\,\mathrm{d}x, \quad \hat{\psi^{(1)}}_0(k) = \int_{-\infty}^0 e^{-ikx}\psi_0^{(1)}(x)\,\mathrm{d}x,\\
\hat{\psi}^{(2)}(k,t) &= \int_0^\infty e^{-ikx}\psi^{(2)}(x,t)\,\mathrm{d}x, \quad \hat{\psi^{(2)}}_0(k) = \int_0^\infty e^{-ikx}\psi_0^{(2)}(x)\,\mathrm{d}x.
\end{aligned}
$$

3. “Solution” formulae

From the global relations:

$$
\begin{aligned}
\psi^{(1)}(x,t) =& \frac{1}{2\pi}\int_{\infty}^{\infty} e^{ikx-\omega_1 t}\hat{\psi}_0^{(1)}(k)\,\mathrm{d}k + \\
& \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega_1 t}(ig_1(\omega_1,t) - kg_0(\omega_1,t))\,\mathrm{d}k, \\
\psi^{(2)}(x,t) =& \frac{1}{2\pi}\int_{\infty}^{\infty} e^{ikx-\omega_2 t}\hat{\psi}_0^{(2)}(k)\,\mathrm{d}k + \\
& \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-\omega_2 t}(ig_1(\omega_2,t) - kg_0(\omega_2,t))\,\mathrm{d}k,
\end{aligned}
$$

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From the global relations:

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It would be convenient if the unknowns g_1 and g_0 depended on the same arguments.

To this end, let

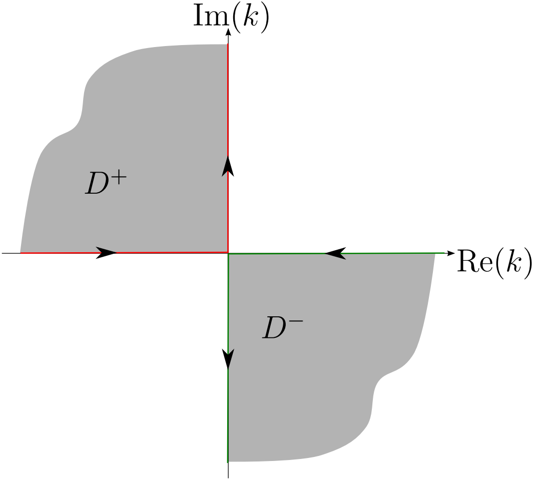
$$\nu^{(j)}(k) = ik\sqrt{1 + \frac{\alpha_j}{k^2}},$$

with the argument of the square root in $(-\pi, \pi)$. Then

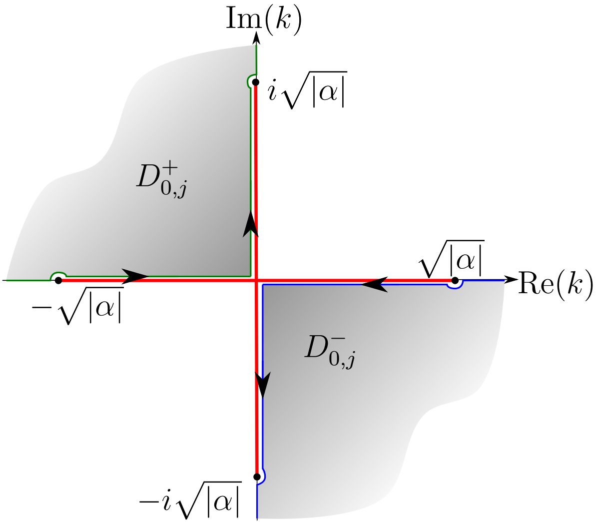
$$\omega_j(\nu^{(j)}(k)) = -ik^2.$$

Let $\alpha = \max_j |\alpha_j|$.

Initially, we have



The Domains D^+ and D^-.



The deformed contours of integration, avoiding branch singularities.

4. Deformed "solution" formulae

$$\psi^{(1)}(x,t) = \frac{1}{2\pi}\int_{\infty}^{\infty} e^{ikx-\omega_1 t}\hat{\psi}_0^{(1)}(k)\,\mathrm{d}k +$$
$$-\frac{1}{2\pi}\int_{\partial D_0^-} e^{i\nu^{(1)}(-k)x+ik^2t}\left(\frac{1}{\sqrt{1+\frac{\alpha_1}{k^2}}}g_1(-ik^2,t)+kg_0(-ik^2,t)\right)\,\mathrm{d}k,$$
$$\psi^{(2)}(x,t) = \frac{1}{2\pi}\int_{\infty}^{\infty} e^{ikx-\omega_1 t}\hat{\psi}_0^{(2)}(k)\,\mathrm{d}k +$$
$$-\frac{1}{2\pi}\int_{\partial D_0^-} e^{i\nu^{(2)}(k)x+ik^2t}\left(\frac{-1}{\sqrt{1+\frac{\alpha_1}{k^2}}}g_1(-ik^2,t)+kg_0(-ik^2,t)\right)\,\mathrm{d}k.$$

5. Symmetries of the dispersion relation

- After our transformations, the only dispersion relation in play is $\omega = -ik^2$.
- The only symmetry is $k \to -k$
- This results in new global relations, allowing us to eliminate $g_0(\omega, t)$ and $g_1(\omega, t)$ in terms of the initial condition and the solution evaluated at a transformed argument.
- The contributions of the latter vanish, using Jordan's lemma.

6. Solution formulae

$$\psi^{(1)}(x,t) = \frac{1}{2\pi}\int_{\infty}^{\infty} e^{ikx-\omega_1 t}\hat{\psi}_0^{(1)}(k)\,\mathrm{d}k +$$

$$-\int_{\partial D_0^-}\frac{e^{i\nu^{(1)}(-k)x+ik^2t}}{\Delta_1(k)}\left(\sqrt{1+\frac{\alpha_1}{k^2}}-\sqrt{1+\frac{\alpha_2}{k^2}}\right)\hat{\psi}_0^{(1)}(\nu^{(1)}(k))\,\mathrm{d}k$$

$$-2\int_{\partial D_0^-}\frac{e^{i\nu^{(1)}(-k)x+ik^2t}}{\Delta_1(k)}\sqrt{1+\frac{\alpha_1}{k^2}}\hat{\psi}_0^{(2)}(\nu^{(2)}(-k))\,\mathrm{d}k,$$

for $x<0$, and a similar formula for $\psi^{(2)}$. Here

$$\Delta_1(k) = 2\pi i\sqrt{1+\frac{\alpha_1}{k^2}}\left(\sqrt{1+\frac{\alpha_1}{k^2}}+\sqrt{1+\frac{\alpha_2}{k^2}}\right).$$

Conclusion

- The **Method of Fokas** or the **Unified Transform Method** is a powerful method for solving many BVPs that are not solvable using classical methods.
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- It may be used to solve **interface problems** that are not solvable using classical methods.

- The **heat equation** (on semi-infinite and finite domains, on the ring, on graphs)
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- The free **linear Schrödinger equation** (on semi-infinite and finite domains)
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- The **linear Schrödinger equation with piecewise constant potential**
    - N.E. Sheils and B. Deconinck. “The time-dependent Schrödinger equation with piecewise constant potentials.” (In preparation) (2015).
- The **linear KdV equation** on two semi-infinite domains
    - N.E. Sheils, D. A. Smith and B. Deconinck. “Well posedness of linear third-order equations with interfaces.” (In preparation) (2015).