Unitarity Theorem and Bound States Description in Multichannel Scattering for the Schrödinger Equation on a Line with Closed Channels

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Setup

We consider the matrix Shrodinger equation on the line

$$[\partial_z g_{ij}(z)\partial_z + V_{ij}(z;\lambda)]u_j(z) = 0, \quad z \in \mathbb{R}, \qquad i,j \in \{1,\dots,N\}, \tag{1}$$

Where $V_{ij}(z;\lambda) = V_{ij}(z) - \lambda g_{ij}(z)$, and λ is an auxiliary parameter.

$g(z)$ and $V(z)$ are real and symmetric. $g(z)$ is positive definite and $g_{ij}(z)$ are once piecewise continuously differentiable functions. $V_{ij}(z)$ are piecewise continuous functions.

We also assume that there exists $L > 0$ such that

$$\begin{cases} g_{ij}(z)\Big|_{z>L} = g^+_{ij}, & V_{ij}(z)\Big|_{z>L} = V^+_{ij}, \\ g_{ij}(z)\Big|_{z<-L} = g^-_{ij}, & V_{ij}(z)\Big|_{z<-L} = V^-_{ij}. \end{cases} \tag{2}$$

Historical review

- **Single channel** scattering problem for one-dimensional Shrodinger equation on the line was solved by Fadeev (1964) [1,2]
- The proof of unitarity of the S-matrix in the presence of closed scattering channels on **semi-axis** is given by Newton (1982) [3]
- Some scattering and analytical properties for **two-channel** Hamiltonians were revealed by Melgaard (2001) [4,5]
- Multichannel scattering problem on the line for the one-dimensional Shrodinger equation on the line was investigated mostly by Aktosun (2001) [6-9], however the **unitarity was not proved.**

To our knowledge, the description of properties of the S-matrix, of the Jost solutions, and of the bound states in the general case of multichannel scattering on a line with different thresholds at both left and right infinities is absent in the literature.

Jost solutions

By definition, the Jost solutions to Eq. (1) have the asymptotics

$$(F_{\pm}^{+})_{is}\,(z;\lambda) \xrightarrow[z\to+\infty]{} (f_{+})_{is'}\left(e^{\pm iK_{+}z}\right)_{s's}, \qquad (F_{\pm}^{-})_{is}\,(z;\lambda) \xrightarrow[z\to-\infty]{} (f_{-})_{is'}\left(e^{\pm iK_{-}z}\right)_{s's}. \quad (3)$$

where $$(K_{\pm}\,)_{ss'} = \delta_{ss'}\sqrt{\Lambda_{s}^{\pm}-\lambda}, \qquad g_{ij}^{\pm}f_{js}^{\pm}\Lambda_{s}^{\pm} = V_{ij}^{\pm}f_{js}^{\pm}, \qquad (f^{\pm})^{T}g^{\pm}f^{\pm} = 1, \quad (4)$$

The Jost solutions $F_{\pm}^{+}$ and $F_{\pm}^{-}$ constitute bases in the space of solutions of Eq. (1). Consequently,

$$\begin{aligned} F_{+}^{+} &= F_{+}^{-}\Phi_{+} + F_{-}^{-}\Psi_{+}, \\ F_{-}^{+} &= F_{+}^{-}\Psi_{-} + F_{-}^{-}\Phi_{-}. \end{aligned} \quad (5)$$

It is clear, that the Wronskian,

$$\omega[\varphi,\psi] \coloneqq \varphi^{T}(z)g(z)\partial_{z}\psi(z) - \partial_{z}\varphi^{T}(z)g(z)\psi(z), \quad (6)$$

of two solutions $\varphi(z)$, and $\psi(z)$, of Eq. (1) is independent of z and defines a skew-symmetric scalar product on the space of solutions of Eq. (1). The Wronskian generates identities in space of solutions of Eq. (1).

Main identities

Let us introduce the transmission matrices $t_{(1,2)}$ and the reflection matrices $r_{(1,2)}$

$$F_+^+ t_{(1)} = F_+^- + F_-^- r_{(1)}, \qquad F_-^- t_{(2)} = F_-^+ + F_+^+ r_{(2)}, \tag{7}$$

Define the S-matrix as

$$S \coloneqq \begin{bmatrix} t_{(1)} & r_{(2)} \\ r_{(1)} & t_{(2)} \end{bmatrix}. \tag{8}$$

Then the S-matrix possesses the symmetries

$$\begin{bmatrix} 0 & K_- \\ K_+ & 0 \end{bmatrix} S = S^T \begin{bmatrix} 0 & K_+ \\ K_- & 0 \end{bmatrix}, \qquad \begin{bmatrix} 0 & K_- \\ K_+ & 0 \end{bmatrix} \overline{S} = \overline{S}^T \begin{bmatrix} 0 & K_+ \\ K_- & 0 \end{bmatrix},$$

$$\overline{S}^T \begin{bmatrix} K_+ & 0 \\ 0 & K_- \end{bmatrix} S = \begin{bmatrix} K_- & 0 \\ 0 & K_+ \end{bmatrix}. \tag{9}$$

$\overline{\Phi}_\pm \coloneqq \Phi_\mp,$

$\overline{\Psi}_\pm \coloneqq \Psi_\mp.$

The case when all scattering channels are open

Theorem 1. *If λ belongs to none of the cuts of the functions $(K_\pm)_s, s \in \{1, \dots, N\}$, i.e., when all the scattering channels are open, the S-matrix is unitary*

$$S^\dagger \begin{bmatrix} K_+ & 0 \\ 0 & K_- \end{bmatrix} S = \begin{bmatrix} K_- & 0 \\ 0 & K_+ \end{bmatrix}, \qquad (10)$$

Remark. *Introducing the notation*

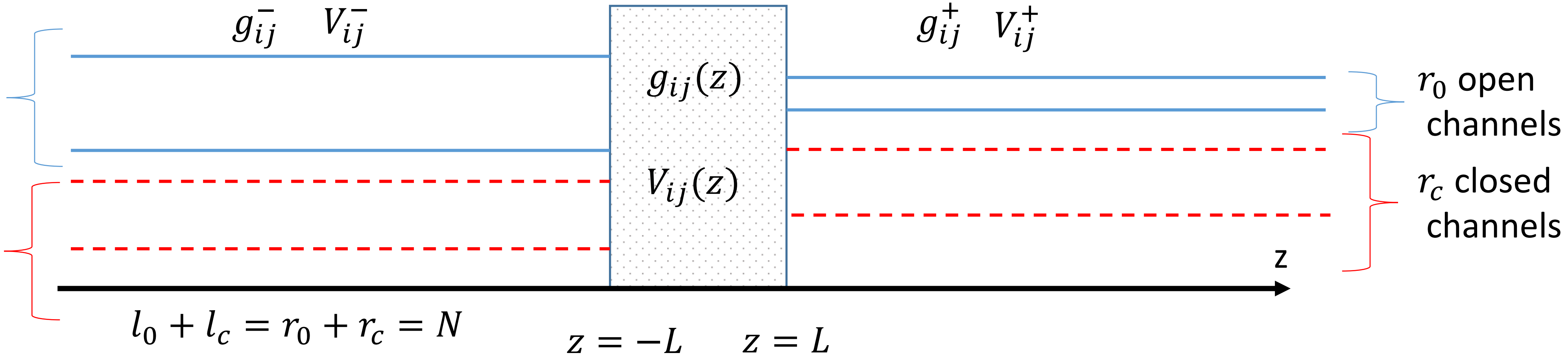
$$\widetilde{\Phi}_\pm := K_-^{\frac{1}{2}} \Phi_\pm K_+^{-\frac{1}{2}}, \quad \tilde{\psi}_\pm := K_-^{\frac{1}{2}} \Psi_\pm K_+^{-\frac{1}{2}}, \qquad (11)$$

One can reduce (9) to the standard form $\tilde{S}^\dagger \tilde{S} = 1$.

Proposition 1. *If all scattering channels are open, there are no bound states.*

The case with closed scattering channels

Fig. 1



We split the relations (7) into blocks with respect to the indices s, s' in accordance with splitting into open and closed channels,

$$\begin{aligned}
&(F_+^+)_o t_{(1)oo} + (F_+^+)_c t_{(1)co} = (F_+^-)_o + (F_-^-)_o r_{(1)oo} + (F_-^-)_c r_{(1)co},\\
&(F_+^+)_o t_{(1)oc} + (F_+^+)_c t_{(1)cc} = (F_+^-)_c + (F_-^-)_o r_{(1)oc} + (F_-^-)_c r_{(1)cc},\\
&(F_-^-)_o t_{(2)oo} + (F_-^-)_c t_{(2)co} = (F_-^+)_o + (F_+^+)_o r_{(2)oo} + (F_+^+)_c r_{(2)co},\\
&(F_-^-)_o t_{(2)oc} + (F_-^-)_c t_{(2)cc} = (F_-^+)_c + (F_+^+)_o r_{(2)oc} + (F_+^+)_c r_{(2)cc}.
\end{aligned} \tag{12}$$

Where, for example,

$$t_{(1)} = \begin{bmatrix} t_{(1)oo} & t_{(1)oc} \\ t_{(1)co} & t_{(1)cc} \end{bmatrix}, \qquad F_\pm^+ = [(F_\pm^+)_o \quad (F_\pm^+)_c]. \tag{13}$$

Identities in the subspace of open channels

Theorem 2. The S*-matrix in the subspace of open channels is unitary:*

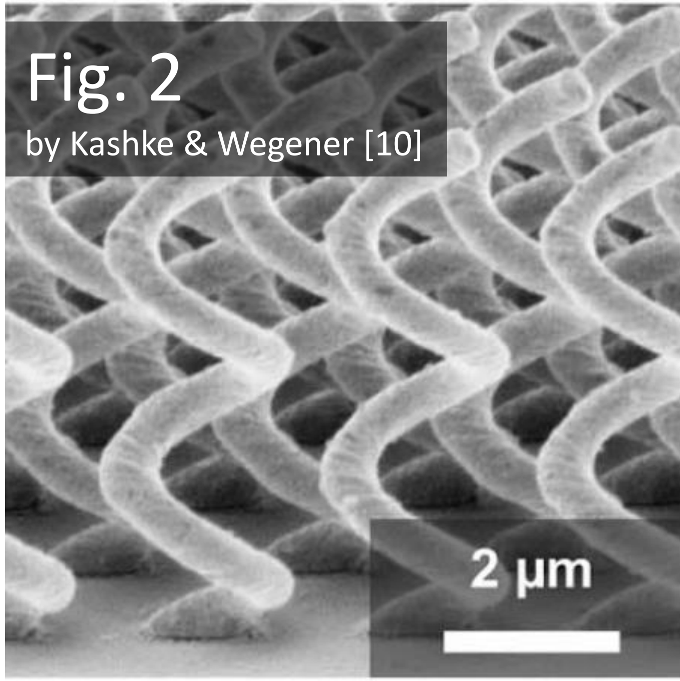
$$
\begin{aligned}
t^{\dagger}_{(2)oo}(K_-)_0 r_{(1)oo} M + r^{\dagger}_{(2)oo}(K_+)_0 t_{(1)oo} &= 0, \\
t^{\dagger}_{(1)oo}(K_+)_0 t_{(1)oo} + r^{\dagger}_{(1)oo}(K_-)_0 r_{(1)oo} &= (K_-)_0. \\
r^{\dagger}_{(1)oo}(K_-)_0 t_{(2)oo} + t^{\dagger}_{(1)oo}(K_+)_0 r_{(2)oo} &= 0, \\
t^{\dagger}_{(2)oo}(K_-)_0 t_{(2)oo} + r^{\dagger}_{(2)oo}(K_+)_0 r_{(2)oo} &= 1.
\end{aligned}
\qquad (14)
$$

Where $M \coloneqq t^{\vee}_{(1)oo} t_{(1)oo} = t_{(2)oo} t^{\vee}_{(2)oo}$, and $A^{\vee}$ - pseudo inverse matrix.

Theorem 3. The following condition $\det \Phi_+(\lambda) = 0, \quad \lambda \in \mathbb{R},$ (15)

is a necessary and sufficient condition for the existence of bound states of Eq. (1).

An electrodynamic example: helical wired metamaterial



The kernel of the non-local effective permittivity tensor $\hat{\varepsilon}_{ij}$ in a helical wire metamaterial reads as

$$K_{ij}(k_0;\boldsymbol{x},\boldsymbol{x}') = \varepsilon_h\left(\delta_{ij} - \tau_i(z)\frac{\omega_p^2}{\omega_0^2 - v^2(\boldsymbol{\tau}(z)\widehat{\boldsymbol{k}})^2}\tau_j(z')\right)\delta(\boldsymbol{x}-\boldsymbol{x}'), \quad (16)$$

where

$$\boldsymbol{\tau}(z) = (\sin\alpha\sin qz\ ,\sin\alpha\cos qz\,,\cos\alpha),\ \ \omega_0 = \varepsilon_h^{1/2}\mathrm{k}_0,\ \ \hat{k}_i = -i\frac{\partial}{\partial x_i}. \quad (17)$$

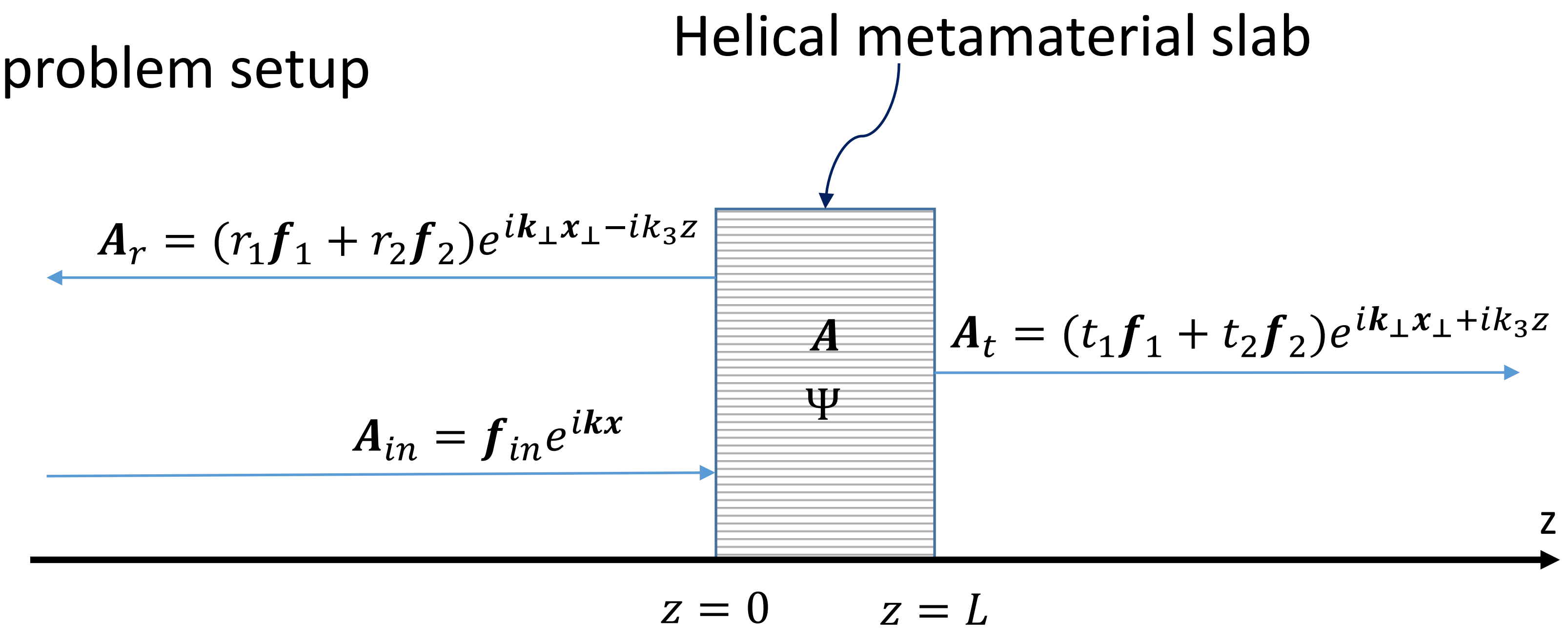
The Maxwell equations in a dispersive medium take the form

We can get rid of nonlocality in the Maxwell equations with the permittivity tensor $\hat{\varepsilon}_{ij}$ by introducing the additional scalar field Ψ obeying certain boundary conditions.

$$\left(\mathrm{rot}_{ij}^2 - k_0^2\hat{\varepsilon}_{ij}\right)A_j = 0. \quad \sim \quad \begin{aligned} (\omega_0^2 - v^2(\boldsymbol{\tau}(z)\widehat{\boldsymbol{k}})^2)\Psi + \omega_0\omega_p\,(\boldsymbol{\tau}\boldsymbol{A}) &= 0, \\ (\omega_0^2 - \mathrm{rot}^2)\,\boldsymbol{A} + \omega_0\omega_p\Psi\boldsymbol{\tau} &= 0. \end{aligned} \quad (18)$$

An electrodynamic example: helical wired metamaterial

Scattering problem setup



Boundary conditions

$$[\boldsymbol{A}_\perp]_{z=0} = [\boldsymbol{A}_\perp]_{z=L} = 0, \qquad [rot\boldsymbol{A}_\perp]_{z=0} = [rot\boldsymbol{A}_\perp]_{z=L} = 0, \qquad \boxed{\Psi_{z=0} = \Psi_{z=L} = 0.} \qquad (19)$$

An electrodynamic example: helical wired metamaterial

The system of Maxwell's equations reduces to the matrix Schrödinger equation

$$[\partial_z g_{ij}(z)\partial_z + V_{ij}(z)]u_j(z) = 0, \tag{20}$$

where

$$g_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & v\cos\alpha \end{bmatrix}, \quad V_{ij}(z) = \begin{bmatrix} \omega_0^2 & 0 & \frac{\omega_p}{\sqrt{2}}\omega_0 \sin\alpha\, e^{i\,q\,z} \\ 0 & \omega_0^2 & \frac{\omega_p}{\sqrt{2}}\omega_0 \sin\alpha\, e^{-i\,q\,z} \\ \frac{\omega_p}{\sqrt{2}}\omega_0 \sin\alpha\, e^{-i\,q\,z} & \frac{\omega_p}{\sqrt{2}}\omega_0 \sin\alpha\, e^{i\,q\,z} & \omega_0^2 - \omega_p^2\cos^2\alpha \end{bmatrix}, \quad u_j(z) = \begin{bmatrix} a_+ \\ a_- \\ \tilde{\Psi} \end{bmatrix} := \begin{bmatrix} A_1 + iA_2 \\ A_1 - iA_2 \\ \sqrt{2}\Psi \end{bmatrix}, \tag{21}$$

This system of equations turns out to be exactly solvable

$$a_\pm = -\frac{\omega_p\omega_0 \sin\alpha}{\sqrt{2}(\omega_0^2 - (k_3 \pm q)^2)} e^{i\,(k_3 \pm q)z}, \qquad \tilde{\Psi} = e^{i\,k_3 z}, \tag{22}$$

where the momentum k_3 is found from the solution of the dispersion equation

$$\omega_0^2\omega_p^2 \sin^2\alpha\,(\omega_0^2 - q^2 - k_3^2) - (\omega_0^2 - (k_3+q)^2)(\omega_0^2 - (k_3-q)^2)\big(\omega_0^2 - \big(\omega_p^2 + v^2k_3^2\big)\cos^2\alpha\big) = 0. \tag{23}$$

Unitarity relation holds!

$$|r_1|^2 + |r_2|^2 + |t_1|^2 + |t_2|^2 = 1. \tag{24}$$

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