Analyticity properties of the scattering matrix for discrete matrix Schrödinger operators

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Quasi-$1d$ discrete Schrödinger (Jacobi matrix)

$$(H\,u)(n) \;=\; u(n+1) \;+\; V(n)u(n) \;+\; u(n-1) \qquad , \qquad n \in \mathbb{Z}$$

for $u : \mathbb{Z} \to \mathbb{C}^{L\times L}$ matrix-valued and with $V(n) = V(n)^* \in \mathbb{C}^{L\times L}$

View H as bounded selfadjoint operator on $\ell^2(\mathbb{Z}, \mathbb{C}^L)$

Here: $V(n) \neq 0$ for only finitely many $n \in [K_- + 1, K_+]$

H finite rank perturbation of discrete Laplacian $H_0 = H - V$

Weyl essential spectrum theorem: $\sigma_{\text{ess}}(H) = [-2, 2] = \sigma(H_0)$

Many contributions on scattering theory, e.g.:

Scalar half-space case: Hinton, Klaus and Shaw (1991)

Matrix Schrödinger: Klaus (1988) Aktosun, Klaus, Weder (2013 - 2020)

Discrete half-space case: Aktosun et al, Nuygen et al (2019)

Aims

- Analyticity of scattering matrix and time delay in complex energy E or rather z defined by $E = z + z^{-1}$, including thresholds
- Unitarity relation of scattering matrix extended to $z \in \mathbb{C}$
- Main tool: analyticity, $\mathcal{J}$-unitarity and multiplicativity of

  plane wave transfer matrices

- Plane wave versus standard transfer matrices of Jacobi operators
- Application: Levinson-like theorem
  (equality of total time delay to number of bound/half-bound states)
- Elementary algebraic proofs of the main results
  (suited for an introductory course to quantum scattering theory)

Free solutions

Two free solutions u_0^z and $u_0^{1/z}$ of $H_0 u = Eu$ are

$$u_0^z(n) \;=\; z^n\,\mathbf{1} \qquad , \qquad u_0^{1/z}(n) \;=\; z^{-n}\,\mathbf{1}$$

where $\mathbf{1} \in \mathbb{C}^{L\times L}$ identity and $z, z^{-1} \in \mathbb{C}$ given by

$$E \;=\; z \,+\, z^{-1}$$

NB: map $z \mapsto E$ two-to-one with $\mathbb{S}^1 \mapsto [-2,2]$ and $\mathbb{R} \mapsto \mathbb{R}\backslash(-2,2)$

For $E \notin [-2,2]$, free solutions exponentially increasing or decreasing

For $z \in \mathbb{S}^1\backslash\{-1,1\}$ plane wave, so of constant modulo in n

For $z = \pm 1$, namely band edges $E = \pm 2$, only one free solutions $u_0^{\pm 1}$

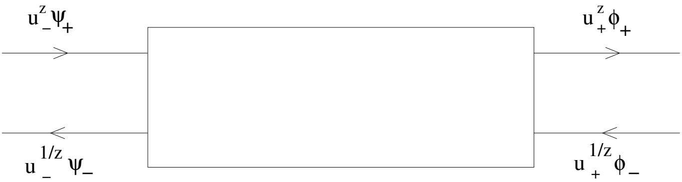
Second solution $v_0^{\pm 1}$ of $H_0 u = \pm 2u$ given by $v_0^{\pm 1} = (\pm 1)^n\, n$

Jost solutions and plane wave transfer matrix

Jost solutions $u^z_\pm$ of perturbed $Hu = Eu$ with $E = z + z^{-1}$ fixed by

$$u^z_+(n) = u^z_0(n) \quad , \quad u^z_-(-n) = u^z_0(-n) \quad , \quad n > |K_\pm|$$

Solutions $u^z_\pm$ called outgoing/incoming if increasing/decreasing at $\pm\infty$



$(u^z_\pm, u^{1/z}_\pm)$ both fundamental solutions for all $z \in \mathbb{C}\backslash\{-1, 0, 1\}$

Plane wave transfer matrix $\mathcal{M}^z \in \mathbb{C}^{2L\times 2L}$ is defined by

$$\left(u^z_-, u^{1/z}_-\right) = \left(u^z_+, u^{1/z}_+\right) \mathcal{M}^z$$

Scattering matrix

The $L \times L$ entries of transfer matrix are denoted by

$$\mathcal{M}^z = \begin{pmatrix} M_-^{1/z} & N_-^z \\ N_-^{1/z} & M_-^z \end{pmatrix}$$

Defining relation: $u_-^z = u_+^z M_-^{1/z} + u_+^{1/z} N_-^{1/z}$ and $u_-^{1/z} = u_+^z N_-^z + u_+^{1/z} M_-^z$

If M_-^z invertible, rewrite to $u_+^{1/z} = u_+^z N_-^z (M_-^z)^{-1} - u_-^{1/z} (M_-^z)^{-1}$

For $z \in \mathbb{C}_0 = \{z \in \mathbb{C} \backslash \{-1, 0, 1\} \ : \ M_-^{1/z}$ and M_-^z invertible$\}$ set

$$(u_-^z, u_+^{1/z}) = (u_+^z, u_-^{1/z}) \, \mathcal{S}^z$$

Expresses incoming in terms of outgoing Jost solutions

$L \times L$ entries are transmission and reflection coefficients

$$\mathcal{S}^z = \begin{pmatrix} T_+^z & R_-^z \\ R_+^z & T_-^z \end{pmatrix} = \begin{pmatrix} ((M_-^{\overline{z}})^*)^{-1} & -N_-^z (M_-^z)^{-1} \\ (M_-^z)^{-1} N_-^{1/z} & (M_-^z)^{-1} \end{pmatrix}$$

Left versus right action of $\mathcal{S}^z$ and $\mathcal{M}^z$

In solid state physics literature rather action from left!

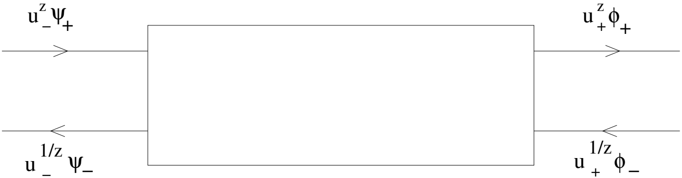
Connection: incoming solutions $u_-^z\psi_+$ and $u_+^{1/z}\phi_-$ via $\psi_+, \phi_- \in \mathbb{C}^L$

Outgoing solutions $u_-^{1/z}\psi_-$ and $u_+^z\phi_+$ given by $\psi_-, \phi_+ \in \mathbb{C}^L$. Then

$$\left(u_-^z, u_+^{1/z}\right)\begin{pmatrix}\psi_+\\ \phi_-\end{pmatrix} = \left(u_+^z, u_-^{1/z}\right)\mathcal{S}^z\begin{pmatrix}\psi_+\\ \phi_-\end{pmatrix} = \left(u_+^z, u_-^{1/z}\right)\begin{pmatrix}\phi_+\\ \psi_-\end{pmatrix}$$

namely

$$\mathcal{S}^z\begin{pmatrix}\psi_+\\ \phi_-\end{pmatrix} = \begin{pmatrix}\phi_+\\ \psi_-\end{pmatrix} \quad\Longleftrightarrow\quad \mathcal{M}^z\begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix} = \begin{pmatrix}\phi_+\\ \phi_-\end{pmatrix}$$



Basic algebraic facts

$$\mathcal{K} = \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix} \quad , \quad \mathcal{I} = \begin{pmatrix} 0 & -\mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix} \quad , \quad \mathcal{J} = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}$$

- Plane wave transfer matrix satisfies for $z \in \mathbb{C} \setminus \{-1, 0, 1\}$

$$(\mathcal{M}^{1/\overline{z}})^* \, \mathcal{J} \, \mathcal{M}^z = \mathcal{J} \qquad , \qquad \mathcal{M}^z \, \mathcal{J} \, (\mathcal{M}^{1/\overline{z}})^* = \mathcal{J}$$

  $\mathcal{J}$-unitarity relation $(\mathcal{M}^z)^* \mathcal{J} \mathcal{M}^z = \mathcal{J}$ for $z \in \mathbb{S}^1 \setminus \{-1, 1\}$

- For $z \in \mathbb{R}$ so that $E \in \mathbb{R} \setminus (-2, 2)$, $\mathcal{M}^z$ is $\mathcal{I}$-unitary

$$(\mathcal{M}^z)^* \, \mathcal{I} \, \mathcal{M}^z = \mathcal{I}$$

- $\mathcal{S}^z$ unitary for $z \in \mathbb{S}^1 \setminus \{-1, 1\}$. Extended relation for $z \in \mathbb{C}_0$:

$$(\mathcal{S}^{1/\overline{z}})^* \, \mathcal{S}^z = \mathbf{1} \qquad , \qquad \mathcal{S}^{\overline{z}} = \mathcal{K} \, (\mathcal{S}^z)^* \, \mathcal{K}$$

- If $V = 0$, one has $\mathcal{M}^z = \mathbf{1}$ and $\mathcal{S}^z = \mathbf{1}$ for $z \in \mathbb{C}_0$
- Both $\mathcal{M}^z$ and $\mathcal{S}^z$ are meromorphic on $\mathbb{C}$

Passage from $\mathcal{M}^z$ to $\mathcal{S}^z$

Proposition

The set of $\mathcal{J}$-unitaries $\{\mathcal{M} \in \mathbb{C}^{2L\times 2L} \,:\, \mathcal{M}^*\mathcal{J}\mathcal{M} = \mathcal{J}\}$ bijectively mapped by $\mathcal{V}$ to unitaries from $\mathrm{U}(2L)$ with invertible diagonals:

$$\mathcal{M} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad \mapsto \quad \mathcal{V}(\mathcal{M}) = \begin{pmatrix} (A^*)^{-1} & -BD^{-1} \\ B^*(A^*)^{-1} & D^{-1} \end{pmatrix}$$

$\mathcal{V}(\mathcal{M})$ is the phase of Lagrangian graph of $\mathcal{M}$. It satisfies

$$\mathcal{V}(\mathcal{M}) = \mathcal{V}(\mathcal{M}^{-1})^* = \mathcal{J}\,\mathcal{V}(\mathcal{M}^*)^*\mathcal{J}$$

Here for $z \in \mathbb{S}^1 \backslash \{-1, 0, 1\}$,

$$\mathcal{V}(\mathcal{M}^z) = \mathcal{S}^z$$

This relation is extended analytically away from $\mathbb{S}^1$

Analytic properties of matrix entry M_-^z

Recall

$$\mathcal{M}^z = \begin{pmatrix} M_-^{1/z} & N_-^z \\ N_-^{1/z} & M_-^z \end{pmatrix}$$

- M_-^z invertible for $|z| \leqslant 1$ except when

  $z = \pm 1$ or z roots z_j of $E_j = z + z^1 \in \sigma(H)$ with $j = 1, \ldots, J_b$
- Zeros of $z \mapsto \det(M_-^z)$ at z_j of order of eigenvalue E_j (difficult!)
- High energy asymptotics $\lim_{z\to 0} M_-^z = \mathbf{1}$
- $\det(M_-^z)$ has poles at ± 1 of order $L - J_h^{\pm}$ where

  $J_h^{\pm}$ dimension of (half-) bounded solutions of $Hu = \pm 2u$
- If $\mathbb{S}_r^1$ circle of radius r and $J_h = J_h^+ + J_h^-$, then argument principle

$$\oint_{\mathbb{S}^1_{1-\epsilon}} \frac{dz}{2\pi i}\,\partial_z \log \det(M_-^z) = J_b \quad , \quad \oint_{\mathbb{S}^1_{1+\epsilon}} \frac{dz}{2\pi i}\,\partial_z \log \det(M_-^z) = J_b + J_h$$

Main results

Theorem

The scattering matrix extends analytically from $\mathbb{C}_0$ to $\{-1, 1\}$

It has poles at z_j for $j = 1, \ldots, J_b$ in the diagonal entries

It has a pole at $z = 0$ in the off-diagonal entries

Theorem (Levinson-type theorem)

The number of bound states J_b and half-bound states J_h satisfy

$$J_b + \tfrac{1}{2} J_h - L = \int_{-2}^{2} \frac{dE}{2\pi i} \operatorname{Tr}\big((\mathcal{S}^E)^* \partial_E \mathcal{S}^E\big)$$

where $\mathcal{S}^E = \mathcal{S}^z$ if $E = z + z^{-1}$ and $\Im m(z) > 0$

Based on:

$$\operatorname{Tr}\big((\mathcal{S}^{1/\bar{z}})^* \partial_z \mathcal{S}^z\big) = \partial_z \log \det(M_-^{1/z}) - \partial_z \log \det(M_-^z)$$

Standard transfer matrix

$$\mathcal{T}^E(n) = \begin{pmatrix} E - V(n) & -\mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}$$

over several sites

$$\mathcal{T}^E(n,m) = \mathcal{T}^E(n)\cdots\mathcal{T}^E(m+1) \qquad , \qquad n > m$$

Also $\mathcal{T}^E(n,n) = \mathbf{1}_{2L}$ and $\mathcal{T}^E(m,n) = \mathcal{T}^E(n,m)^{-1}$. Then $\mathcal{I}$-unitarity

$$\mathcal{T}^{\overline{E}}(n,m)^* \mathcal{I}\,\mathcal{T}^E(n,m) = \mathcal{I}$$

For solution u of $Hu = Eu$, set

$$\Phi(n) = \begin{pmatrix} u(n+1) \\ u(n) \end{pmatrix}$$

Then

$$\Phi(n) = \mathcal{T}^E(n)\,\Phi(n-1) = \mathcal{T}^E(n,m)\,\Phi(m)$$

Plane wave versus standard transfer matrix

$$\mathcal{M}^z(n) \;=\; \begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{1} \end{pmatrix} + i\,\nu^z \begin{pmatrix} V(n) & z^{-2n}V(n) \\ -z^{2n}V(n) & -V(n) \end{pmatrix} \quad , \quad \nu^z = \frac{i}{z - z^{-1}}$$

Note $\mathcal{M}^z(n) = \mathbf{1}$ if $V(n) = 0$, hence adapted to perturbation theory

Proposition

$$\mathcal{M}^z(n) \;=\; \left(\mathcal{C}^z\mathcal{D}^z(n)\right)^{-1} \mathcal{T}^E(n)\left(\mathcal{C}^z\mathcal{D}^z(n-1)\right)$$

where $E = z + z^{-1}$ *and*

$$\mathcal{C}^z \;=\; \begin{pmatrix} z\,\mathbf{1} & z^{-1}\,\mathbf{1} \\ \mathbf{1} & \mathbf{1} \end{pmatrix} \quad , \quad \mathcal{D}^z(n) \;=\; \begin{pmatrix} z^n\mathbf{1} & 0 \\ 0 & z^{-n}\mathbf{1} \end{pmatrix}$$

One has $\mathcal{M}^{1/\overline{z}}(n)^*\mathcal{J}\mathcal{M}^z(n) = \mathcal{J}$*, hence* $\mathcal{J}$*-unitarity for* $z \in \mathbb{S}^1$

Generalized Cayley transform passing from $\mathcal{I}$- to $\mathcal{J}$-unitaries

Multiplicativity of plane wave transfer matrices

As above, set $\mathcal{M}^z(n,n) = \mathbf{1}$ and

$$\mathcal{M}^z(n,m) \;=\; \mathcal{M}^z(n)\cdots\mathcal{M}^z(m+1) \qquad , \qquad n > m$$

Then

$$\mathcal{M}^{1/\overline{z}}(n,m)^*\,\mathcal{J}\,\mathcal{M}^z(n,m) \;=\; \mathcal{J}$$

Proposition

Plane wave transfer matrix $\mathcal{M}^z$ of scattering theory is

$$\mathcal{M}^z \;=\; \mathcal{M}^z(K_+,K_-)$$

Thus

$$\mathcal{M}^z \;=\; \big(\mathcal{C}^z\mathcal{D}^z(K_+)\big)^{-1}\,\mathcal{T}^E(K_+,K_-)\,\big(\mathcal{C}^z\mathcal{D}^z(K_-)\big)$$

Due to different $\mathcal{D}^z$-factors **not** just change of representation

Other potential application: perturbation theory for Lyapunov exponent

Application: analyticity issues

$$\mathcal{M}^z \;=\; \prod_{n=K_-+1}^{K_+} \left[\begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{1} \end{pmatrix} \;+\; i\,\nu^z \begin{pmatrix} V(n) & z^{-2n} V(n) \\ -z^{2n} V(n) & -V(n) \end{pmatrix} \right]$$

At band edge $z \to \pm 1$ one has $\nu^z = \frac{i}{z - z^{-1}} \to \infty$. Very singular? No:

Proposition

With analytic $\mathcal{G}^z$ in neighborhood of $z = \pm 1$,

$$\mathcal{M}^z \;=\; \mathcal{G}^z \;+\; \nu^z\,\mathcal{F}$$

Matrix $\mathcal{F}$ contains all information at band edges, determines $L - J_h^\pm$

In spite of singular factors, algebraic (semigroup) structure shows for lower right entry M_-^z of $\mathcal{M}^z$ that

Proposition

$\lim_{z \to 0} M_-^z \;=\; \mathbf{1}$

Link to Green matrix

For $n, m \in \mathbb{Z}$ and $E \notin \sigma(H)$,

$$G^E(n,m) \;=\; \pi_n\,(H-E)^{-1}\,(\pi_m)^* \;\in\; \mathbb{C}^{L\times L}\;,$$

where $\pi_n : \ell^2(\mathbb{Z},\mathbb{C}^L) \to \mathbb{C}^L$ restriction to site n

Well-known link of Green matrices to entries of transfer matrices:

Proposition

M^z_- invertible for $E = z + z^{-1} \notin \sigma(H)$ with $|z| < 1$ and

$$M^z_- \;=\; \frac{z^{K_+ - K_-}}{z - z^{-1}}\, G^E(K_-,K_+)^{-1}$$

Moreover:

$$\mathcal{S}^z = \frac{z^{K_- - K_+}}{z - z^{-1}} \begin{pmatrix} G^E(K_+,K_-) & -z^{-K_+ - K_-}(G^E(K_+,K_+) + i\nu^z) \\ -z^{K_+ + K_-}(G^E(K_-,K_-) + i\nu^z) & G^E(K_-,K_+) \end{pmatrix}$$

Outlook: Extension to short range potentials

General procedure applies. Alternative: make sense out of

$$\mathcal{M}^z = \prod_{n=-\infty}^{\infty} \left[\begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{1} \end{pmatrix} + i\,\nu^z \begin{pmatrix} V(n) & z^{-2n} V(n) \\ -z^{2n} V(n) & -V(n) \end{pmatrix} \right]$$

Use

$$\|\mathcal{M}^z(n) - \mathbf{1}\| \leqslant 4\,|\nu^z|\,\|V(n)\|$$

Slight extension of Wedderburn (1934):

Proposition

If

$$\sum_{n=-\infty}^{\infty} \|V(n)\| < \infty$$

then infinite product $\mathcal{M}^z$ converges and analytic in $z \in \mathbb{C}\backslash\{-1, 0, 1\}$

Then $\mathcal{S}^z$ obtained after same algebraic passage