Dirichlet-Neumann bracketing for a class of banded Toeplitz matrices

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ABSTRACT. We consider boundary conditions of self-adjoint banded Toeplitz matrices. We ask if boundary conditions exist for banded self-adjoint Toeplitz matrices which satisfy operator inequalities of Dirichlet-Neumann bracketing type. For a special class of banded Toeplitz matrices including integer powers of the discrete Laplacian we find such boundary conditions. Moreover, for this class we give a lower bound on the spectral gap above the lowest eigenvalue.

1. Introduction and result

In this note we are concerned with self-adjoint banded Toeplitz matrices. Let $\mathbb{T} := \{0, 2\pi\}$ and $L \in \mathbb{N}$. We consider symbols of the form

$$f : \mathbb{T} \to \mathbb{R}, \quad f(x) = \sum_{k=-N}^{N} a_k e^{-ikx} \quad (1.1)$$

for some $N \in \mathbb{N}$, $a_k \in \mathbb{C}$ with $a_k = \overline{a_{-k}} \in \mathbb{C}$ for $k = -N, \ldots, N$. These give rise to self-adjoint banded Toeplitz matrices given by the sequence $\ldots, 0, a_{-N}, \ldots, a_{0}, \ldots, a_{N}, 0, \ldots$ and $T_{f,L}$ is the corresponding $L \times L$ Toeplitz matrix

$$T_{f,L} = \begin{pmatrix}
a_0 & a_1 & \cdots & a_N \\
& \ddots & \ddots & \vdots \\
& & a_{-N} & a_0 & \cdots & a_N \\
& & & \ddots & \vdots & \ddots \\
& & & & a_{-N} & \cdots & a_{-1} & a_0
\end{pmatrix}. \quad (1.2)$$

Throughout we assume that the matrix size $L$ is bigger than the band width $2N + 1$. Moreover, $T_f$ stands for the so-called Laurent or bi-infinite Toeplitz matrix

$$T_f : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z}), \quad (T_f b)_n := \sum_{m \in \mathbb{Z}} a_{m-n} b_m \quad (1.3)$$

where $b = (b_m)_{m \in \mathbb{Z}} \in \ell^2(\mathbb{Z})$ and $a_k = \frac{1}{2\pi} \int_{0}^{2\pi} dx f(x) e^{-ikx}$, $k \in \mathbb{Z}$. We write $(T_f)_{[a,b]}$ for the restriction of $T_f$ to $\ell^2([a,b]) \subseteq \ell^2(\mathbb{Z})$ for $a, b \in \mathbb{Z}$ with $a < b$. Then $T_{f,b-a+1}$ is the same matrix as $(T_f)_{[a,b]}$ and we use both notations interchangeably. For further reading about banded Toeplitz matrices we refer to [BG05].
We break $T_{f,L}$ into the direct sum of two Toeplitz matrices

$$T_{f,L_1} \oplus T_{f,L_2} = \begin{pmatrix} a_0 & \cdots & a_N & 0 \\ \vdots & \ddots & \vdots & \vdots \\ a_{-N} & \cdots & a_0 & 0 \\ 0 & \cdots & 0 & a_0 & \cdots & a_N \\ \vdots & \ddots & \ddots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & a_{-N} & \cdots & a_0 \end{pmatrix}$$

(1.4)

where $L_1, L_2 \in \mathbb{N}$ with $L_1 + L_2 = L$ and we assume for convenience that $L_1, L_2 \geq 2N + 1$. It is clear that the difference $T_{f,L} - T_{f,L_1} \oplus T_{f,L_2}$ is of no definite sign and therefore no operator inequality between the two operators $T_{f,L}$ and $T_{f,L_1} \oplus T_{f,L_2}$ holds.

We are interested in adding boundary conditions to $T_{f,L_1}$ and $T_{f,L_2}$ which overcome this lack of monotonicity. For a banded Toeplitz matrix with band size $2N+1$ boundary conditions refer to adding Hermitian $N \times N$ matrices at the corner of the respective boundary, i.e. a boundary condition $\star$ is given by a Hermitian $N \times N$ matrix $B_\star$ and

$$T_{f,L,\star}^0 := T_{f,L} + \begin{pmatrix} B_\star & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad T_{f,L,0}^\star := T_{f,L} + \begin{pmatrix} 0 & 0 \\ 0 & B_\star \end{pmatrix}$$

(1.5)

where $B_\star$ is the reflection of $B_\star$ along the anti-diagonal, i.e. $B_\star := U^* B_\star U$ with $U : \mathbb{C}^N \to \mathbb{C}^N$, $(Ux)_k := x_{N-k+1}$ for $x = (x_1, \ldots, x_N) \in \mathbb{C}^N$. The superscript 0 in the above indicates simple boundary condition at the respective endpoint which refers to no $N \times N$ matrix added. If simple boundary conditions are imposed at both endpoints we drop the 0 superscripts and note $T_{f,L,0}^0 = T_{f,L}$.

Our goal is to find boundary conditions $\mathcal{N}$ and $\mathcal{D}$ which give rise to a chain of operator inequalities of the form

$$T_{f,L,\mathcal{N}}^0 \oplus T_{f,L_2,\mathcal{D}} \leq T_{f,L} \leq T_{f,L_1,\mathcal{D}} \oplus T_{f,L_2,\mathcal{N}}$$

(1.6)

subject to the constraint

$$\inf f \leq T_{f,R}^{\mathcal{N},\mathcal{D}} \leq \sup f$$

(1.7)

where $R \in \{L_1, L_2\}$. Inequality (1.6) is easily satisfied for boundary conditions given by large multiples of the $N \times N$ identity however the non-trivial constraint is (1.7) which ensures that the spectra of the restricted operators are subsets of the spectrum of the corresponding infinite-volume operator (1.3). We address the question:

*Given a banded self-adjoint Toeplitz matrix, do boundary conditions in the sense of (1.5) exist such that inequalities (1.6) and (1.7) hold for all $L_1, L_2 \in \mathbb{N}$ with $L = L_1 + L_2$ and $L_1, L_2$ greater than the band width?*

Throughout we mainly focus on the boundary condition $\mathcal{N}$ and later on find boundary conditions $\mathcal{N}$ for a special class of banded Toeplitz matrices which satisfy the respective inequalities in (1.6) and (1.7). We don’t know if the answer to the above question remains yes for general banded self-adjoint Toeplitz matrices.

A chain of inequalities of the form (1.6) and (1.7) is referred to as Dirichlet-Neumann bracketing. This stems from the following: For the continuous negative
Laplace operator Dirichlet and Neumann boundary conditions naturally satisfy the operator inequality (1.6), see e.g. [RS78] Sec. XIII. Inspired by the continuous definition, this was later extended to the discrete Laplacian as well [Kir08, Sec. 5.2]. In both cases an inequality of the form (1.6) is by now a standard tool in mathematical physics and was, for example, used in the proof of Lifshitz tails for random Schrödinger operators [Sim85, Kir08, KM07] and Weyl asymptotics for continuum Schrödinger operators [RS78] Sec. XIII.

It might be tempting to think the natural Neumann boundary condition for \( T_{f,L} \) satisfies the first inequality in (1.6). This boundary condition, which we denote by the superscript \( N \), is given by the Toeplitz-plus-Hankel matrix

\[
T_{f,L}^{N,0} = T_{f,L} + \begin{pmatrix}
\alpha_1 & \cdots & \alpha_N & \cdots \\
\vdots & \ddots & \vdots & \ddots \\
\alpha_N & 0 & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots
\end{pmatrix},
\]

(1.8)

see e.g. [NCT99]. Here we abuse notation a little as the superscript \( N \) for Neumann boundary condition has nothing to do with the subscript \( N \) indicating the band width of the matrix. Except in the case of a self-adjoint 3-diagonal Toeplitz matrix this boundary condition does not satisfy \( T_{L,f}^{0,N} \oplus T_{L_0,f}^{N,0} \leq T_{L,f} \). To see this, we consider the square of the negative discrete Laplacian on \( \ell^2(\mathbb{Z}) \). Throughout, the negative discrete Laplacian \( -\Delta \) is the 3-diagonal Toeplitz matrix given by the rows \((-\cdots,0,-1,2,-1,0,\cdots)\) and therefore \((-\Delta)^2 = \Delta^2\) is 5-diagonal and given by \((-\cdots,0,1,-4,6,-4,1,0,\cdots)\). In that case a computation shows that

\[
(\Delta^2)_L - (\Delta^2)_L^{0,N} \oplus (\Delta^2)_L^{N,0} =
\begin{pmatrix}
0 & -1 & 0 & \ddots \\
-1 & 4 & -4 & 1 & \\
1 & -4 & 4 & -1 & \\
0 & 1 & -1 & 0 & \\
\ddots & \ddots & \ddots & \ddots & \ddots
\end{pmatrix}
\]

(1.9)

and 0 everywhere else. This matrix is not of definite sign and therefore the first inequality from the left in (1.6) does not hold.

In this note we introduce what we call modified Neumann boundary conditions \( \mathcal{N} \) which satisfy the first inequality in (1.6) and (1.7) for Toeplitz matrices given by symbols of the form

\[
f_{E_1,\cdots,E_n,\alpha_1,\cdots,\alpha_n}(x) := f_{E_1}^{a_1}(x) \cdots f_{E_n}^{a_n}(x) = \prod_{i=1}^n \left(2 - 2 \cos(x - E_i)\right)^{a_i},
\]

(1.10)

for \( x \in \mathbb{T} \) and some distinct \( E_1,\ldots,E_n \in \mathbb{T} \) and \( \alpha_1,\ldots,\alpha_n \in \mathbb{N} \). In the above, we have set \( f_{E}^{a}(x) := (2 - 2 \cos(x - E))^a \). Note that the minimum of \( f_{E_1,\cdots,E_n,\alpha_1,\cdots,\alpha_n} \) is 0 and it is attained at the points \( E_1,\ldots,E_n \).

We remark that \( T_{f_{E}}^{\mathcal{N}} \) is a 3-diagonal Laurent matrix given by rows \((-\cdots,0,e^{iE},2,e^{-iE},0,\cdots)\) which is unitarily equivalent to the discrete Laplacian \( -\Delta \)
and we set \(-\Delta_E := T_{\vec{f} \vec{E}}\). Using this notation, we can write

\[
T_{\vec{f}_{\alpha_1,\ldots,\alpha_n}} = \prod_{i=1}^n (-\Delta_E)^{\alpha_i}
\]  

(1.11)

which is a banded Laurent matrix with band width \(2N + 1\) where \(N = \sum_{i=1}^n \alpha_i\).

The main theorem regarding Dirichlet-Neumann bracketing for \(T_{\vec{f}_{\alpha_1,\ldots,\alpha_n}}\) is the following:

**Theorem 1.1.** Let \(n \in \mathbb{N}\), \(E_1,\ldots,E_n \in \mathbb{T}\) be distinct and \(\alpha_1,\ldots,\alpha_n \in \mathbb{N}\). Let \(g = f_{\vec{E}_1,\ldots,\vec{E}_n,\alpha_1,\ldots,\alpha_n}\) be of the form (1.10) and \(N = \sum_{i=1}^n \alpha_i\). Then there exist boundary conditions which we call modified Neumann and Dirichlet boundary conditions, \(\mathcal{N}\) and \(\mathcal{D}\), such that

\[
T_{g_1} \oplus T_{g_2} \leq T_{g_1} \oplus T_{g_2} \leq T_{g_1} \oplus T_{g_2}
\]  

(1.12)

and

\[
0 = \inf_g \left( T_{g_1} \oplus T_{g_2} \leq T_{g_1} \oplus T_{g_2} \right)
\]  

(1.13)

for all \(L_1, L_2 \in \mathbb{N}\) with \(L_1 + L_2 = L\) and \(L_1, L_2 \geq 2N + 1\). The boundary conditions \(\mathcal{N}\) and \(\mathcal{D}\) are given explicitly in Definition [2.2] below.

**Remarks 1.2.**

(i) For band width greater than 3 the boundary conditions \(\mathcal{N}\) and \(\mathcal{D}\) differ from the Neumann boundary \(N\) condition mentioned in (1.3) and the Dirichlet boundary condition used in e.g. [NCT99] which coincides with what we call simple boundary condition.

(ii) It would be desirable to have the inequality \(T_{f_1,f_2} \leq \sup_{f} T_{f_1,f_2}\) as well but our modified Dirichlet boundary condition \(\mathcal{D}\) defined in Definition [2.2] does not satisfy this. We obtain \(\mathcal{D}\) by a general principle that any inequality \(T_{g_1} \oplus T_{g_2} \leq T_{g_1} \oplus T_{g_2}\) induces modified Dirichlet boundary condition such that \(T_{g_1} \leq T_{g_1} \oplus T_{g_2}\) and vice versa, see Lemma [4.1].

(iii) The theorem holds for any integer power \((m \in \mathbb{N})\) of the discrete Laplacian as the symbol of \((-\Delta)^m : \ell^2(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})\) is

\[
g(x) = f_{0,m}(x) = (2 - 2\cos(x))^m, \quad x \in \mathbb{T}
\]  

(1.14)

and is of the form (1.10). In that case \(n = 1, E_1 = 0\) and \(\alpha_1 = m\).

Considering only symbols (1.10) seems very restrictive. But, for example, Theorem [4.1] gives Dirichlet-Neumann bracketing for a rather large class of 5-diagonal real-valued Toeplitz matrices:

**Corollary 1.3** (5-diagonal real-valued Toeplitz matrices). Let \(h : \mathbb{T} \rightarrow \mathbb{R}\) be the symbol

\[
h(x) = a_0 \mathrm{e}^{-2ix} + a_1 \mathrm{e}^{-ix} + a_2 \mathrm{e}^{ix} + a_3 \mathrm{e}^{2ix}
\]  

(1.15)

where \(a_0, a_1, a_2 \in \mathbb{R}\) with \(a_2 > 0\) and \(-4 \leq \frac{a_1}{a_2} \leq 4\). Then there exist modified Neumann and Dirichlet boundary conditions, \(\mathcal{N}\) and \(\mathcal{D}\), for the Toeplitz matrix \(T_{h,1}\) such that

\[
T_{h_1} \oplus T_{h_2} \leq T_{h_1} \oplus T_{h_2} \leq T_{h_1} \oplus T_{h_2}
\]  

(1.16)

and

\[
0 = \inf_h \left( T_{h_1} \oplus T_{h_2} \leq T_{h_1} \oplus T_{h_2} \right)
\]  

(1.17)
for all $L_1, L_2 \in \mathbb{N}$ with $L_1 + L_2 = L$ and $L_1, L_2 \geq 5$.

The upcoming paper [GRM] will heavily rely on the established Dirichlet-Neumann bracketing to prove Lifshitz tails of the integrated density of states for self-adjoint Toeplitz matrices with random diagonal perturbations. Fractional powers of Toeplitz matrices of the form (1.11) serve there as model operators. This is a continuation of our study of Lifshitz tails of randomly perturbed fractional Laplacians in [GRM20]. Generally, Dirichlet-Neumann bracketing is a common tool in proving Lifshitz tails, see e.g. [Kir08, Sec. 6]. Another main ingredient and of independent interest is a lower bound on the spectral gap above the ground state energy of Toeplitz matrices with modified Neumann boundary condition. We prove here:

**Proposition 1.4 (Spectral gap).** Let $n \in \mathbb{N}$, $E_1, \ldots, E_n \in \mathbb{T}$ be distinct and $\alpha_1, \ldots, \alpha_n \in \mathbb{N}$. Let $g = f_{E_1, \ldots, E_n, \alpha_1, \ldots, \alpha_n}$ be of the form (1.10) and $N = \sum_{i=1}^n \alpha_i$. We denote by $\lambda_1^L \leq \ldots \leq \lambda_N^L$ the eigenvalues of $T_{g, L}^{N,N}$ counting multiplicities and ordered increasingly. Then $\lambda_k^L = 0$ for $k = 1, \ldots, N$ and there exists $C > 0$ such that for all $L \geq 2N + 1$

$$\lambda_{N+1}^L \geq \frac{C}{L^{2\alpha_{\max}}}, \quad (1.18)$$

where $\alpha_{\max} := \max \{ \alpha_i : i = 1, \ldots, n \}$.

In the case of $T_{g, L}^{N,N}$, i.e. the Neumann boundary conditions defined in (1.8), the latter proposition follows rather directly from the explicit diagonalization of $T_{g, L}^{N,N}$, see [NCT99]. For the modified Neumann boundary conditions $T_{g, L}^{N', N'}$ it is more complicated as an explicit diagonalization of $T_{g, L}^{N', N'}$ is not known.

**2. Definition of boundary conditions $\mathcal{N}$ and $\mathcal{D}$**

The boundary conditions in Theorem 1.1 rely on a representation of self-adjoint Toeplitz matrices $T_{f_{E_1, \ldots, E_n, \alpha_1, \ldots, \alpha_n}}$ as a sum of rank-one operators. To see this we write for $E \in \mathbb{T}$

$$-\Delta_E = D_E^* D_E \quad (2.1)$$

where $D_E := T_{h_E} : \ell^2(Z) \to \ell^2(Z)$ is the Laurent matrix given by the symbol $h_E : \mathbb{T} \to \mathbb{C}$, $h_E(x) = 1 - e^{-iE} e^{-ix}$, i.e.

$$D_E = \begin{pmatrix}
\ddots & \ddots & \ddots \\
0 & 1 & e^{-iE}\\
0 & 1 & e^{-iE}\\
0 & 1 & e^{-iE}\\
\ddots & \ddots & \ddots
\end{pmatrix}. \quad (2.2)$$

Using this decomposition and (1.11), we write

$$T_{f_{E_1, \ldots, E_n, \alpha_1, \ldots, \alpha_n}} = \prod_{i=1}^n (D_{E_i}^* D_{E_i})^\alpha_i = \left( \prod_{i=1}^n D_{E_i}^* \right) \left( \prod_{i=1}^n D_{E_i} \right)^\alpha_i \quad (2.3)$$
where we used that all Laurent matrices commute. We denote by \((\delta_k)_{k \in \mathbb{Z}}\) the standard basis of \(\ell^2(\mathbb{Z})\). Inserting the identity \(1 = \sum_{k \in \mathbb{Z}} |\delta_k\rangle \langle \delta_k|\) in the above, we obtain
\[
T_{fE_1, \ldots, a_n} = \sum_{k \in \mathbb{Z}} \left| \prod_{i=1}^n D_{E_i}^{a_i} \delta_k \right| \left| \prod_{i=1}^n D_{E_i}^{a_i} \delta_0 \right|
\]
(2.4)
where the above series converge strongly. For \(k \in \mathbb{Z}\) we define the vector
\[
\psi_k^g := \prod_{i=1}^n D_{E_i}^{a_i} \delta_k = U_k \prod_{i=1}^n D_{E_i}^{a_i} \delta_0
\]
(2.5)
whose support satisfies \(\text{supp} \psi_k^g = [k, k+2] \subseteq \mathbb{Z}\) where \(\text{supp} \varphi = \{n \in \mathbb{Z} : \varphi(n) \neq 0\}\) for \(\varphi \in \ell^2(\mathbb{Z})\) and \(N = \sum_{i=1}^n a_i\). In the above \(U_k : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z}), (U_k x)_n = x_{n-k}\), is the right shift by \(k \in \mathbb{Z}\). Summarizing the above computation, we have proved the following:

**Proposition 2.1.** Let \(n \in \mathbb{N}, E_1, \ldots, E_n \in \mathbb{T}\) be distinct and \(\alpha_1, \ldots, \alpha_n \in \mathbb{N}\). Let \(g = f_{E_1, \ldots, a_n}\) be of the form (1.10). Then
\[
T_g = \sum_{k \in \mathbb{Z}} |\psi_k^g\rangle \langle \psi_k^g|
\]
(2.6)
with \(\psi_k^g \in \ell^2(\mathbb{Z})\) given by (2.5).

Now given Proposition 2.1 it is straightforward to define the boundary conditions \(\mathcal{N}\) and \(\mathcal{D}\) in the following way:

**Definition 2.2 (Boundary conditions \(\mathcal{N}\) and \(\mathcal{D}\)).** Let \(n \in \mathbb{N}, E_1, \ldots, E_n \in \mathbb{T}\) be distinct and \(\alpha_1, \ldots, \alpha_n \in \mathbb{N}\). Let \(g = f_{E_1, \ldots, a_n}\) be of the form (1.10), \(N = \sum_{i=1}^n a_i\) and \(\psi_k^g, k \in \mathbb{Z}\), be given in Proposition 2.1.

For \(a \in \mathbb{Z} \cup \{-\infty\}\) and \(b \in \mathbb{Z}\) with \(b - a > 2N + 1\) we define the restriction of \(T_g\) to \([a, b) \subseteq \mathbb{Z}\) with simple boundary conditions at \(a\) and

(i) boundary condition \(\mathcal{N}\) at \(b \in \mathbb{Z}\) by
\[
(T_g)_{[a,b)}^{\mathcal{N}} := \left( \sum_{k \in \mathbb{Z} : \langle k, b + N \rangle \subseteq (-\infty, b]} |\psi_k^g\rangle \langle \psi_k^g| \right)_{[a,b)} .
\]
(2.7)
To be precise, for \(a = -\infty\) the respective intervals are open at \(a\).

(ii) boundary condition \(\mathcal{D}\) at \(b \in \mathbb{Z}\) by
\[
(T_g)_{[a,b)}^{\mathcal{D}} := 2(T_g)_{[a,b)} - (T_g)_{[a,b)}^{\mathcal{N}} .
\]
(2.8)
Accordingly, we define \((T_g)_{[a,b]}^{\mathcal{N} \cap \mathcal{D}}\) by reflection along the anti-diagonal. In particular,

(iii) boundary conditions \(\mathcal{N}\) at both \(a, b \in \mathbb{Z}\) are given by
\[
(T_g)_{[a,b]}^{\mathcal{N} \cap \mathcal{D}} := \sum_{k \in \mathbb{Z} : \langle k, b + N \rangle \subseteq [a,b]} |\psi_k^g\rangle \langle \psi_k^g| .
\]
(2.9)

(iv) boundary conditions \(\mathcal{D}\) at both \(a, b \in \mathbb{Z}\) by
\[
(T_g)_{[a,b]}^{\mathcal{N} \cap \mathcal{D}} := 2(T_g)_{[a,b]} - (T_g)_{[a,b]}^{\mathcal{N} \cap \mathcal{D}} .
\]
(2.10)
Remarks 2.3. (i) From the definition of the boundary conditions \( \mathcal{N} \) and \( \mathcal{D} \) one notes that only the respective \( N \times N \) corner of \( (T_g)_{[a,b]} \) at the boundary is changed. More precisely,

\[
(T_g)_{[0,N]/\mathcal{D}} = (T_g)_{[a,b]} + \begin{pmatrix} 0 & 0 \\ 0 & \tilde{B}_{\mathcal{N}/\mathcal{D}} \end{pmatrix}
\]

with

\[
\tilde{B}_{\mathcal{N}} = - \sum_{k \in \mathbb{Z}, b+1 \in [k,k+N]} P |\psi_{g,k}^E \rangle \langle \psi_{g,k}^E | P \leq 0
\]

and

\[
\tilde{B}_{\mathcal{D}} = \sum_{k \in \mathbb{Z}, b+1 \in [k,k+N]} P |\psi_{g,k}^E \rangle \langle \psi_{g,k}^E | P \geq 0
\]

where \( P \) is the projection onto the \( N \)-dimensional space \( \ell^2([b-N+1,b]) \). Therefore \( \mathcal{N} \) and \( \mathcal{D} \) are boundary conditions in the sense of (1.5).

(ii) For functions \( g \) as in Theorem 1.1, the latter directly implies

\[
(T_g)_{[0,N]/\mathcal{D}} \leq (T_g)_{[a,b]} \leq (T_g)_{[0,D]/\mathcal{D}}
\]

3. An example

Example 3.1. Let \( E \in \mathbb{T} \). We consider the symbol

\[
g(x) = f_{0,E,1,1}(x) = (2-2\cos(x))(2-2\cos(x-E)), \quad x \in \mathbb{T}.
\]

The function \( g \) satisfies \( g \geq 0 \) and its minimal value is 0 and attained at \( x = 0 \) and \( x = E \). In the case \( E = 0 \) we have \( T_g = (-\Delta)^2 \) which was also discussed in the introduction, see (1.9). A short computation shows that \( T_g \) is the 5-diagonal Toeplitz matrix

\[
T_g = \begin{pmatrix}
\ddots & e^{-iE} & -2-2e^{-iE} & 4 + e^{-iE} + e^{iE} & -2 - 2e^{iE} & e^{iE} \\
& \ddots & \ddots & \ddots & \ddots & \ddots \\
& & \ddots & \ddots & \ddots & \ddots \\
& & & \ddots & \ddots & \ddots \\
& & & & \ddots & \ddots \\
& & & & & \ddots
\end{pmatrix}
\]

(3.2)

To define the Neumann boundary condition, we write using Proposition 2.1

\[
T_g = \sum_{k \in \mathbb{Z}} |\psi_k^g \rangle \langle \psi_k^g |
\]

(3.3)

where for \( k \in \mathbb{Z} \) we have \( \text{supp} \psi_k^g = [k,k+2] \). Moreover

\[
|\psi_k^g \rangle \langle \psi_k^g | = \begin{pmatrix}
\ddots & 1 & -1 - e^{iE} & e^{iE} \\
& -1 - e^{-iE} & 2 + e^{-iE} + e^{iE} & -1 - e^{iE} \\
& e^{-iE} & -1 - e^{-iE} & \ddots \\
& \ddots & \ddots & \ddots
\end{pmatrix}
\]

(3.4)
and 0 everywhere else. Then the boundary conditions $\mathcal{N}$ and $\mathcal{D}$ from Definition 2.2 are of the form

$$(T_R)_{a,b}^{\mathcal{N},0} = (T_R)_{a,b} - \begin{pmatrix} 3 + e^{iE} + e^{-iE} & -1 - e^{iE} & \cdots \\ -1 - e^{-iE} & 1 & \cdots \\ \vdots & \ddots & \ddots \end{pmatrix}$$

(3.5)

and

$$(T_R)_{a,b}^{\mathcal{D},0} = (T_R)_{a,b} + \begin{pmatrix} 3 + e^{iE} + e^{-iE} & -1 - e^{iE} & \cdots \\ -1 - e^{-iE} & 1 & \cdots \\ \vdots & \ddots & \ddots \end{pmatrix}$$

(3.6)

where the latter two matrices are 0 everywhere else. Here one clearly sees that the boundary conditions $\mathcal{N}$ and $\mathcal{D}$ consist of adding or subtracting a sign-definite $2 \times 2$ matrix in the respective corner of $(T_R)_{a,b}$. This is consistent with our definition of boundary conditions in the introduction.

4. Proof of Theorem 1.1 and Corollary 1.3

**Proof of Theorem 1.1** Let $L_1, L_2 \geq 2N + 1$ and $L_1 + L_2 = L$. The chain of inequalities

$$0 = \inf g \in T_{g,L}^N \subset T_{g,L}^{N,0} \subset T_{g,L}^{N',0} \subset T_{g,L}^{N',N} \subset T_{g,L}$$

(4.1)

follows directly from the definition of the boundary condition $\mathcal{N}$ as we drop in the definition of $\mathcal{N}$ non-negative rank-one projections from $T_{g,L}$. For the upper bound in the last inequality of (1.16) we note that

$$T_{g,L} = \begin{pmatrix} T_{g,L_1} & PT_{g,L}P^\perp \\ P^\perp T_{g,L}P & T_{g,L_2} \end{pmatrix} \geq \begin{pmatrix} T_{g,L_1}^{N,0} & 0 \\ 0 & T_{g,L_2}^{N,0} \end{pmatrix}$$

(4.2)

interpreted as an operator on $\ell^2([1,L_1]) \oplus \ell^2([L_1 + 1,L])$ and $P$ stands here for projection onto $\ell^2([L_1,1]) \oplus \{0\}$ and $P^\perp = 1 - P$. Now Lemma 4.1 below gives the result as the definition of the modified Dirichlet boundary condition in (2.8) is precisely of the form (4.3).

In the next lemma we show that any boundary condition satisfying the first inequality in (1.16) naturally induces a boundary condition satisfying the second inequality in (1.16).

**Lemma 4.1.** Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two possibly infinite-dimensional Hilbert spaces. Let $A : \mathcal{H}_1 \oplus \mathcal{H}_2 \to \mathcal{H}_1 \oplus \mathcal{H}_2$ be a bounded operator

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}. $$

(4.3)

Assume there exist $A_{11}^N : \mathcal{H}_1 \to \mathcal{H}_1$ and $A_{22}^N : \mathcal{H}_2 \to \mathcal{H}_2$ such that

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \geq \begin{pmatrix} A_{11}^N & 0 \\ 0 & A_{22}^N \end{pmatrix}. $$

(4.4)

Then

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \leq \begin{pmatrix} 2A_{11} - A_{11}^N & 0 \\ 0 & 2A_{22} - A_{22}^N \end{pmatrix}. $$

(4.5)
PROOF. We conjugate inequality (4.6) by the unitary \( U = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \). Hence (4.6) is equivalent to
\[
U^* AU \succeq U^* \begin{pmatrix} A_{11}^N & 0 \\ 0 & A_{22}^N \end{pmatrix} U = \begin{pmatrix} A_{11}^N & 0 \\ 0 & A_{22}^N \end{pmatrix}.
\]
(4.6)

We note that
\[
U^* AU = \begin{pmatrix} A_{11} & -A_{12} \\ -A_{21} & A_{22} \end{pmatrix}
\]
(4.7)
which together with (4.6) gives
\[
\begin{pmatrix} 2A_{11} & 0 \\ 0 & 2A_{22} \end{pmatrix} - \begin{pmatrix} A_{11} & -A_{12} \\ -A_{21} & A_{22} \end{pmatrix} \leq \begin{pmatrix} 2A_{11} & 0 \\ 0 & 2A_{22} \end{pmatrix} - \begin{pmatrix} A_{11}^N & 0 \\ 0 & A_{22}^N \end{pmatrix}
\]
(4.8)
which is the result.

PROOF OF COROLLARY 1.3 Let \( b \in \mathbb{T} \). We compute for \( x \in \mathbb{T} \)
\[
(2 - 2 \cos(x - b))(2 - 2 \cos(x + b))
\]
\[
= (2 - e^{ix} e^{-ib} - e^{-ix} e^{ib})(2 - e^{ix} e^{ib} - e^{-ix} e^{-ib})
\]
\[
= e^{-2ix} - 4 \cos(b) e^{ix} + 4 + 2 \cos(2b) - 4 \cos(b) e^{ix} + e^{2ix} =: w_b(x).
\]
(4.9)

Let \( h: \mathbb{T} \to \mathbb{R} \) be of the form as described in Corollary 1.3
\[
h(x) = a_2 e^{-2ix} + a_1 e^{-ix} + a_0 + a_1 e^{ix} + a_2 e^{2ix}
\]
(4.10)
where \( a_0, a_1, a_2 \in \mathbb{R} \) with \( a_2 > 0 \) and \(-4 \leq \frac{a_1}{a_2} \leq 4 \). We rewrite
\[
h(x) = a_2 \left( e^{-2ix} + \frac{a_1}{a_2} e^{-ix} + 1 \right) + a_1 e^{ix} + a_2 e^{2ix}
\]
(4.11)
As we assumed \(-4 \leq \frac{a_1}{a_2} \leq 4 \) there exists \( b \in \mathbb{T} \) such that \( 4 \cos(b) = \frac{a_1}{a_2} \) and hence using the definition of \( w_b \) in (4.9) we obtain
\[
h(x) = a_2 w_b(x) + c
\]
(4.12)
with \( c := a_0 - 4 - 2 \cos(2b) \). Theorem 1.1 implies there exists boundary conditions \( \mathcal{N} \) and \( \mathcal{D} \) such that
\[
0 = \inf_{\mathbb{T}} w_b \leq T_{w_b,L_1}^{\mathcal{N},0} \leq T_{w_b,L_2}^{\mathcal{N},0} \leq T_{w_b,L_1}^{\mathcal{D},0} \leq T_{w_b,L_2}^{\mathcal{D},0} \leq 2N + 1 \]
(4.13)
for all \( L_1, L_2 \in \mathbb{N} \) with \( L_1 + L_2 = L \) and \( L_1, L_2 \geq 2N + 1 \). Multiplying \( w_b \) with \( a_2 \geq 0 \) and adding \( c \) will not change the chain of operator inequalities (4.13) and the result follows.

5. Proof of Proposition 1.4

PROOF OF PROPOSITION 1.4 Fix \( g \) and \( N \) as in the assumptions and \( L \in \mathbb{N} \) with \( L \geq 2N + 1 \). We first prove that \( \lambda_k^L = 0 \) for all \( k = 1, \ldots, N \). To do so, we consider the \( N \) vectors
\[
\psi_{E_i}^k = (k^j e^{iE_i^k})_{k = 1, \ldots, L} = (1^j e^{iE_1^i}, \ldots, L^j e^{iE_L^i})^T \in \mathbb{C}^L = \ell^2([1, L])
\]
(5.1)
where \( i = 1, \ldots, n \) and \( j_i = 0, \ldots, \alpha_i - 1 \). A computation shows that for all \( k \in 1, \ldots, L - N \)
\[
\{ D_{E_i}^{a_i} \psi^{(i)}_{(l)} \}_k = 0
\]  
(5.2)
where we see \( D_{E_i}^{a_i} \) here as an operator \( D_{E_i}^{a_i} : \ell^2([1, L]) \to \ell^2([1, L]) \). Therefore by the definition of \( \psi^g_k \) in (2.5) we obtain for \( k \in 1, \ldots, L - N \)
\[
\langle \psi^g_k, \psi^{(i)}_{(l)} \rangle = 0
\]  
(5.3)
for all \( i = 1, \ldots, n \) and \( j_i = 0, \ldots, \alpha_i - 1 \). Recalling the definition of \( T_{g,L}^{N,N'} \) in (2.9), we obtain from the previous identity
\[
T_{g,L}^{N,N'} \psi^{(i)}_{(l)} = \sum_{m \in \mathbb{Z}, |k,k+N|\leq |1, L|} |\psi^g_k \rangle \langle \psi^g_k | \psi^{(i)}_{(l)} \rangle = 0
\]  
(5.4)
for \( i = 1, \ldots, n \) and \( j_i = 0, \ldots, \alpha_i - 1 \). Lemma 5.2 shows that the \( N \) vectors in (5.1) are linearly independent and therefore span a \( N \) dimensional space which implies \( \lambda^g_k = 0 \) for \( k = 1, \ldots, N \).

Next we prove the lower bound on \( \lambda^L_{N+1} = \lambda^L_{N+1}(T_{g,L}^{N,N'}) \), where we use the notation \( \lambda^L_{(\cdot)} \) if we want to emphasize to underlying operator. We consider first the \( L \times L \) restriction of \( T^g \) with periodic boundary conditions
\[
T^\text{per}_{g,L} := \left( \begin{array}{cccccc}
 a_0 & \cdots & a_N & a_{-N} & \cdots & a_{-1} \\
 \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
 a_{-N} & \cdots & a_0 & \cdots & a_{-N} & \cdots \\
 a_1 & \cdots & a_{N-1} & \cdots & a_{-N} & \cdots \\
 \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
 a_1 & \cdots & a_0 & \cdots & a_{N-1} & \cdots \\
 \end{array} \right).
\]  
(5.5)
For \( k = 1, \ldots, L \) we define the vector \( \psi^{(k)} = (\psi^{(k)}_1, \ldots, \psi^{(k)}_L)^T \in \mathbb{C}^L \)
\[
\psi^{(k)}_m := \frac{1}{\sqrt{L}} e^{\frac{2\pi km}{L}} \hbar, \quad m = 1, \ldots, L.
\]  
(5.6)
A computation shows for \( k = 1, \ldots, L \) that
\[
T^\text{per}_{g,L} \psi^{(k)} = g \left( \frac{2\pi k}{L} \right) \psi^{(k)}.
\]  
(5.7)
Therefore, the family of vectors \( (\psi^{(k)})_{k=1,\ldots,L} \) form an ONB of eigenvectors of \( T^\text{per}_{g,L} \) corresponding to the eigenvalues \( g \left( \frac{2\pi k}{L} \right) \), \( k = 1, \ldots, L \).

Using the definition of \( T_{g,L}^{N,N'} \) in (2.9), we observe that
\[
T^\text{per}_{g,L} T_{g,L}^{N,N'} = \sum_{k=L-N+1}^{L} \langle \psi^g_k | \psi^g_k \rangle
\]  
(5.8)
where for \( k = L - N + 1, \ldots, L \)
\[
\psi^g_k = (c_{L-k+1}, \ldots, c_N, 0, \cdots, 0, c_0, \cdots, c_{L-k})^T \in \mathbb{C}^L
\]  
(5.9)
with $c_k := (\psi_k^L)_k$ for $k = 0, ..., N$. Therefore, the difference in (5.8) is rank $N$. From the first part of the proof we know that $\lambda^1(T_{g,L}^{N',N}) = 0$ for $j = 1, ..., N$. Now the min-max principle implies the lower bound

$$\lambda^L_{N+1}(T_{g,L}^{N',N}) \geq \lambda^1_{N+1}(T_{g,L}^{N',N}) = \min_{k=1,\ldots,L} g\left(\frac{2\pi k}{L}\right)$$

(5.10)

and the last equality follows from (5.7). Next we define for $E \in \mathbb{T}$ the unitary $U_E: \mathbb{C}^L \to \mathbb{C}^L$, $(U_E b)_m = e^{-i E m_2} b_m$ for $b \in \mathbb{C}^L$ and $m = 1, \ldots, L$. Then, by the definition of $\psi_k^L$ the following identity holds

$$U_E T_{g,L}^{N',N} U_E^* = T_{g,E,L}^{N',N}$$

(5.11)

where $g_E(x) = g(x - E)$, $x \in \mathbb{T}$, and we extended $g$ here periodically such that $g(x - E)$ makes sense for any $x \in \mathbb{T}$ and $E \in \mathbb{T}$. As the spectrum does not change under conjugation by a unitary, we obtain

$$\lambda^L_{N+1}(T_{g,E,L}^{N',N}) = \lambda^L_{N+1}(T_{g,L}^{N',N})$$

(5.12)

for all $E \in \mathbb{T}$ and using the lower bound (5.10) we end up with

$$\lambda^L_{N+1}(T_{g,E,L}^{N',N}) = \max_{E \in \mathbb{T}} \min_{k=1,\ldots,L} g_E\left(\frac{2\pi k}{L}\right).$$

(5.13)

Given the distinct minima $E_1, \ldots, E_n \in \mathbb{T}$ of the function $g$, Lemma 5.1 below provides a constant $C_1 > 0$ such that for all $L > 2N + 1$ there exists $E \in \mathbb{T}$ such that

$$\frac{C_1}{L} \leq \min_{i=1,\ldots,n} \text{dist}(E_i, \left(\frac{2\pi k}{L} - \hat{E}\right) \text{mod} 2\pi : k = 1, \ldots, L) \leq \frac{\pi}{L}.$$  

(5.14)

We note that $C_1 > 0$ in the above is independent of $L$ and only depends on $n$. Since $E_1, \ldots, E_n$ are the minima of the function $g$, we obtain with the $E \in \mathbb{T}$ found above, inequality (5.14) and Taylor’s theorem the lower bound

$$\geq \min_{k=1,\ldots,L} g\left(\frac{2\pi k}{L} - \hat{E}\right)$$

$$\geq \frac{C_2}{L^{2a_{\text{aux}}}}$$

(5.15)

for some $C_2 > 0$ depending on $g$ but independently of $L$ which is the assertion. □

**Lemma 5.1.** Let $E_1, \ldots, E_n \in \mathbb{T}$ be $n \in \mathbb{N}$ distinct points and set $\mathcal{G}^{(n)} := \{E_i, i = 1, \ldots, n\}$. Then there exists $\hat{E} \in \mathbb{T}$ such that

$$\text{dist}(\mathcal{G}_{\hat{E}}, \mathcal{G}^{(n)}) \geq \frac{2\pi}{2\pi} \frac{1}{L}$$

(5.16)

where

$$\mathcal{G}_{\hat{E}} := \left\{\frac{2\pi k}{L} - \hat{E}\right\} \text{mod} 2\pi : k = 1, \ldots, L\right\}$$

(5.17)

and $\text{dist}(A, B) = \min \{|a - b| : a \in A, b \in B\}$ for $A, B \subset \mathbb{R}$.

**Proof.** We prove the lemma by induction on $n \in \mathbb{N}$.

For $n = 1$ let $\mathcal{G}^{(1)} = \{E_1\}$. Then we choose $\hat{E} = -E_1 + \frac{\pi}{L}$ and therefore (5.16) is true.
Assume the result is true for \( n - 1 \) distinct points \( E_1, \ldots, E_{n-1} \) and let \( E_n \) be a point distinct from the others. By assumption there exists \( \tilde{E} \) such that
\[
\text{dist}(\mathcal{S}_{\tilde{E}}, E^{(n-1)}) \geq \frac{2\pi}{2^{n-1} L}.
\] (5.18)
If \( \text{dist}(\mathcal{S}_{\tilde{E}}, E_n) \geq \frac{2\pi}{2^{n-1} L} \) we are done. If this is not the case we obtain by adding or subtracting \( \frac{2\pi}{2^{n-1} L} \) to \( \tilde{E} \) that there exists \( E \in \mathbb{T} \) such that
\[
\text{dist}(\mathcal{S}_E, E_n) \geq \frac{2\pi}{2^n L}.
\] (5.19)
Since \( |\tilde{E} - E| \leq \frac{2\pi}{2^n L} \) and \( \text{dist}(\mathcal{S}_E, E^{(n-1)}) \geq \frac{2\pi}{2^{n-1} L} \), we obtain
\[
\text{dist}(\mathcal{S}_E, E^{(n-1)}) \geq \frac{2\pi}{2^n L}
\] (5.20)
which is the assertion together with (5.19). \( \square \)

**Lemma 5.2.** Let \( n \in \mathbb{N} \), \( E_1, \ldots, E_n \in \mathbb{T} \) be distinct, \( \alpha_1, \ldots, \alpha_n \in \mathbb{N} \) and \( N = \sum_{i=1}^n \alpha_i \). Moreover, let \( L \in \mathbb{N} \) with \( L \geq N \). The \( N \) vectors
\[
\phi_{E_i}^l = (k^{ij} e^{iE_i})_{k=1,L} = \left(1^{ij} e^{iE_i}, \ldots, L^{ij} e^{iE_iL}\right)^T \in \mathbb{C}^L
\] (5.21)
where \( i = 1, \ldots, n \) and \( j = 0, \ldots, \alpha_i - 1 \) are linearly independent.

**Proof.** Let \( i \in \{1, \ldots, n\} \) and \( j \in \{0, \ldots, \alpha_i - 1\} \). We introduce the short-hand notation
\[
z_i := e^{iE_i} \text{ and define the truncation of } \phi_i^l \text{ to } \mathbb{C}^N
\]
\[
\hat{\phi}_i^l := (z_{i1}, 2^{ij} z_{i2}^2, \ldots, N^{ij} z_{iN}^N)^T \in \mathbb{C}^N.
\] (5.22)
This is just the truncation of \( \phi_i^l \) to the first \( N \) rows. Now
\[
\det(\hat{\phi}_1^{a_1-1}, \hat{\phi}_2^{a_2-1}, \ldots, \hat{\phi}_n^{a_n-1})
\]
is a confluent Vandermonde determinant which can be computed explicitly and evaluates to
\[
|\det(\hat{\phi}_1^{a_1-1}, \hat{\phi}_2^{a_2-1}, \ldots, \hat{\phi}_n^{a_n-1})| = \prod_{i=1}^n (\alpha_i - 1)! \prod_{1 \leq i < j \leq n} |z_i - z_j|^{|\alpha_i - \alpha_j|},
\] (5.23)
see e.g. [HG80, Thm. 1]. Since \( z_i \neq z_j \) for all \( i \neq j \), we obtain that the latter determinant is non-zero. Therefore, the \( N \) vectors \( \hat{\phi}_1^{a_1-1}, \hat{\phi}_2^{a_2-1}, \ldots, \hat{\phi}_n^{a_n-1} \) are linearly independent. This implies that the vectors \( \{\hat{\phi}_i^l : i = 1, \ldots, n, j_i = 0, \ldots, \alpha_i - 1\} \) are linearly independent as well. \( \square \)

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