Free-Fermion entanglement and orthogonal polynomials

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Abstract

We present a simple construction for a tridiagonal matrix T that commutes with the hopping matrix for the entanglement Hamiltonian $\mathcal{H}$ of open finite free-Fermion chains associated with families of discrete orthogonal polynomials. It is based on the notion of algebraic Heun operator attached to bispectral problems, and the parallel between entanglement studies and the theory of time and band limiting. As examples, we consider Fermionic chains related to the Chebychev, Krawtchouk and dual Hahn polynomials. For the former case, which corresponds to a homogeneous chain, the outcome of our construction coincides with a recent result of Eisler and Peschel; the latter cases yield commuting operators for particular inhomogeneous chains. Since T is tridiagonal and non-degenerate, it can be readily diagonalized numerically, which in turn can be used to calculate the spectrum of $\mathcal{H}$, and therefore the entanglement entropy.

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1 Introduction

Entanglement, a distinctive feature of the quantum realm often quantified through entropies, is of fundamental relevance in black hole physics, information theory and many-body problems [1, 2, 3, 4]. It is hence actively studied in a variety of situations. This paper relates to entanglement in free-Fermion or solvable XX spin chains, a topic that is generating much attention on its own (for a review see for instance [5]). Basically, the question is the following: Suppose the whole chain is in the quantum (pure) state described by $|\Psi\rangle\!\rangle$, which we shall here take to be the ground state. We divide the chain in two spatial parts 1 and 2, and ask how are these parts coupled in $|\Psi\rangle\!\rangle$. Since all the properties of the subsystem 1 are provided by the reduced density matrix ρ_1 obtained by tracing $|\Psi\rangle\!\rangle\langle\!\langle\Psi|$ over part 2, therein will be all the entanglement information. For example, the von Neumann entropy is given by $S_1 = -\operatorname{tr}(\rho_1 \log \rho_1)$, which amounts to finding the eigenvalues of ρ_1.

In the following we shall take our subsystem 1 to consist of the first consecutive $l+1$ sites of the chain labelled by $n = 0, 1, ..., N$. Diagonalizing the $2^{l+1} \times 2^{l+1}$ reduced density matrix ρ_1 could become prohibitive as l grows. Fortunately, owing to the fact that the eigenstates of the chains considered are Slater determinants, it has been shown [6, 7] that ρ_1 in a chosen state can be obtained from the 1-particle correlation matrix C in that state, thus reducing the determination of the entanglement entropy to finding the eigenvalues of a $(l+1) \times (l+1)$ matrix. Furthermore, it was observed [7, 8] that as a consequence, ρ_1 must be of the thermodynamic form

$$\rho_1 = \kappa \, \exp(-\mathcal{H}) \,, \tag{1.1}$$

where $\mathcal{H}$, known as the *Entanglement Hamiltonian*, is also Fermionic (but is not the Hamiltonian of the subsystem). The constant κ simply ensures normalization, i.e. $\operatorname{tr} \rho_1 = 1$. The hopping matrix h that characterizes $\mathcal{H}$ [1] is hence a function of the correlation matrix C. It remains, however, that the eigenvalue problem for h or equivalently C becomes numerically quite difficult as l grows, because these are full matrices with closely spaced eigenvalues. As pointed out in [9] and stressed by Peschel and Eisler [10, 11, 12], classical results in signal processing (as well as in random matrix theory) can be brought to bear on the analysis of the entanglement properties of free-Fermion chains in certain instances. Since this is directly related to the main results that are reported in this paper, let us briefly offer here some relevant background.

In its initial form, the theory of *Time and Band Limiting* developed by Slepian, Landau and Pollack aims to determine an unknown function/signal with two kinds of limitations: (i) the duration of the transmission interval is finite and known, and (ii) only a piece of the function's Fourier transform, say over a certain band of frequencies, is available. The optimal use of this information requires finding the eigenfunctions of certain integral operators whose non-local character makes the numerical analysis almost intractable. Amazingly, Slepian et al. have circumvented this problem by finding a differential operator that commutes with the integral one, that thus shares with it common eigenfunctions, and that has eigenvalues that are nicely spread. The original work has been generalized in various directions and is

[1] We shall reserve the term "hopping matrix" for the coefficients appearing in the Entanglement Hamiltonian, rather than in the original Hamiltonian, see (3.9) below.

having numerous applications. For reviews the reader could consult [13, 14].

The reasons and the circumstances for the existence of commuting operators in time and band limiting problems are still not fully understood. This has motivated in part the seminal work of Duistermaat and Grünbaum on bispectral problems [15]. With their three-term recurrence relation and their differential/difference equation, the hypergeometric polynomials (which are organized in a hierarchical way in the so-called Askey scheme [16, 17]) are prominent examples of bispectral problems. Over the years, with his collaborators and students, Grünbaum has discovered and developed many realizations of limiting problems with commuting operators. In [18] for example, working in the framework of the classical orthogonal polynomials (Jacobi, Laguerre, Hermite), he has found an analog of the results obtained by Slepian et al. with the Fourier transform. This has been extended to more general orthogonal polynomials in [19, 20]. The questions regarding the origin of the commuting operator were recently revisited in [21]; the concept of algebraic Heun operator[2] attached to bispectral problems was introduced and it was shown that, generically, commuting operators of time and band limiting problems belong to that class of so-called Heun operators thus rediscovering and extending beyond the finite-dimensional case, a result of Perline [25]. It is this simple construction that we here wish to apply to the search of tridiagonal matrices that commute with the hopping matrix for finite free-Fermion chains that are associated to orthogonal polynomials of the Askey scheme.

The relevance of the time and band limiting theory to the study of the entanglement properties of free-Fermion chains is now readily seen. Restricting to a subsystem, i.e. to the first $l+1$ sites of the chain, corresponds to limiting time. Filling the Fermi sea (or exciting a consecutive set of 1-particle energy eigenvalues) is tantamount to band limiting. The set-ups are clearly parallel. The correlation matrix C is the operator that we wish to diagonalize; and its analysis would much benefit from knowing a tridiagonal matrix T that commutes with it, or equivalently with the hopping matrix. We shall point out in what follows that the formula of Perline [25] which specializes the corresponding algebraic Heun operator, readily provides this commuting Jacobi matrix when the chain is associated to orthogonal polynomials of the Askey scheme and the subsystem corresponds to the first $l+1$ sites of the chain and the filling is done with consecutive "momenta". The key point will be to recognize and exploit the presence in these situations of the second operator of the bispectral pair. In a recent study [12] focused on finite free-Fermionic chains with uniform couplings, Eisler and Peschel have obtained the tridiagonal matrix that commutes with the hopping matrix. They have found that it coincides with the results obtained by Grünbaum in [26] and observed that the expression for the commuting T corresponds to what is obtained from conformal field theory [27]. In the following we shall indicate how this tridiagonal commuting matrix is straightforwardly obtained by applying the algebraic Heun construction to a truncation of the Chebychev polynomials of the second kind. We note that there is currently interest also in the study of inhomogeneous chains from the entanglement viewpoint (see for instance [28, 29]). The method highlighted in this paper also lends itself to certain chains of that type, and again easily provides a tridiagonal matrix that commutes with the hopping matrix for the entanglement Hamiltonian. This is done by connecting with hypergeometric orthogonal

[2]The reason for the name is that, when applied [22] to the bispectral operators of the Jacobi polynomials, the construction precisely yields the Heun equation with four regular Fuchsian singularities [23], [24].

polynomials, and will be illustrated for two inhomogeneous free-Fermionic chains respectively associated to the Krawtchouk and the dual Hahn polynomials.

The remainder of the paper is organized as follows. In Section 2, we shall introduce the Hamiltonians of the finite free-Fermionic chains that will be considered. How their eigenstates are obtained from the one-excitation dynamics will be reviewed and the required diagonalization using orthogonal polynomials will be explained. The ground state in which entanglement will be studied, shall be given in Section 3 where the connections between the 1-particle correlation matrix, the entanglement Hamiltonian and the reduced density matrix will be reviewed. With an eye to considering chains with couplings given by the recurrence coefficients of various families of discrete orthogonal polynomials, we shall recall in Section 4 properties that will be used. The construction from the algebraic Heun operator of the operator that commutes with the hopping matrix of the entanglement Hamiltonian will be described in Section 5, and will be seen to exploit the bispectrality of the underlying polynomials. Section 6 will be dedicated to the finite free-Fermion spin chain with uniform couplings and to recovering from the algebraic Heun operator approach applied to truncated Chebychev polynomials, the commuting tridiagonal matrix obtained in [12, 26]. Section 7 will present two inhomogeneous free-Fermionic chains respectively associated to the Krawtchouk and dual Hahn polynomials together with the tridiagonal matrices commuting with the corresponding hopping matrices. Finally, Section 8 will offer concluding remarks.

2 Free-Fermion chains and their diagonalization

We consider the following open quadratic free-Fermion inhomogeneous Hamiltonian

$$\widehat{\mathcal{H}} = \sum_{n=0}^{N-1} J_n (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) - \sum_{n=0}^{N} B_n c_n^\dagger c_n = \sum_{m,n=0}^{N} c_m^\dagger \widehat{H}_{mn} c_n \ , \tag{2.1}$$

where J_n and B_n are real parameters, and $\{c_m^\dagger \, , c_n\} = \delta_{m,n}$. For the sake of simplicity of the following computations, we enumerate the sites of the lattice from 0 to N. Let us remark that the Hamiltonian (2.1) can be obtained by a Jordan–Wigner transformation from the following XX model

$$\widehat{\mathcal{H}} = -\frac{1}{2} \sum_{n=0}^{N-1} J_n (\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y) - \frac{1}{2} \sum_{n=0}^{N} B_n \sigma_n^z \ , \tag{2.2}$$

with $c_n^\dagger = \sigma_0^z \dots \sigma_{n-1}^z \sigma_n^+$ and $c_n = \sigma_0^z \dots \sigma_{n-1}^z \sigma_n^-$.

In order to diagonalize $\widehat{\mathcal{H}}$, it is convenient to first diagonalize the $(N+1) \times (N+1)$ matrix $\widehat{H} = |\widehat{H}_{mn}|_{0 \leq m,n \leq N}$. In the canonical orthonormal basis $\{|0\rangle, |1\rangle, \dots, |N\rangle\}$ of $\mathbb{C}^{N+1}$, called the position basis, $\widehat{H}$ acts as follows

$$\widehat{H}|n\rangle = J_{n-1}|n-1\rangle - B_n|n\rangle + J_n|n+1\rangle \, , \qquad 0 \leq n \leq N \, , \tag{2.3}$$

with the convention $J_N = J_{-1} = 0$. It takes the tridiagonal form

$$\widehat{H} = \begin{pmatrix} -B_0 & J_0 & & & & \\ J_0 & -B_1 & J_1 & & & \\ & J_1 & -B_2 & J_2 & & \\ & & \ddots & \ddots & \ddots & \\ & & & J_{N-2} & -B_{N-1} & J_{N-1} \\ & & & & J_{N-1} & -B_N \end{pmatrix} . \tag{2.4}$$

The spectral problem for $\widehat{H}$ reads

$$\widehat{H}|\omega_k\rangle = \omega_k|\omega_k\rangle \ , \tag{2.5}$$

where

$$|\omega_k\rangle = \sum_{n=0}^{N} \phi_n(\omega_k)|n\rangle \ . \tag{2.6}$$

We choose to order the $N+1$ eigenvalues $\omega_0, \omega_1, \dots \omega_N$ such that $\omega_k < \omega_{k+1}$. We also choose $|\omega_0\rangle, |\omega_1\rangle, \dots |\omega_N\rangle$ such that they form an orthonormal basis of $\mathbb{C}^{N+1}$, called the momentum basis. The eigenfunctions $\phi_n(\omega_k)$ are real, since the matrix $\widehat{H}$ is real and its eigenvalues are non-degenerate (see e.g. Lemma 3.1 in [30], we suppose that $J_n \neq 0$). Therefore, the eigenfunctions satisfy the orthonormality conditions

$$\sum_{n=0}^{N} \phi_n(\omega_k)\phi_n(\omega_p) = \delta_{kp} \, . \tag{2.7}$$

From relation (2.3), we deduce that $\phi_n(\omega_k)$ must satisfy the following recurrence relation

$$\omega_k \phi_n(\omega_k) = J_n \phi_{n+1}(\omega_k) - B_n \phi_n(\omega_k) + J_{n-1}\phi_{n-1}(\omega_k) \, , \qquad 0 \leq n \leq N \, . \tag{2.8}$$

Having diagonalized $\widehat{H}$, we see that the Hamiltonian $\widehat{\mathcal{H}}$ (2.1) can be rewritten as

$$\widehat{\mathcal{H}} = \sum_{k=0}^{N} \omega_k \tilde{c}_k^\dagger \tilde{c}_k \, , \tag{2.9}$$

where the annihilation operators $\tilde{c}_k$ are defined by

$$\tilde{c}_k = \sum_{n=0}^{N} \phi_n(\omega_k)\, c_n \, , \qquad c_n = \sum_{k=0}^{N} \phi_n(\omega_k)\, \tilde{c}_k \, , \tag{2.10}$$

and the corresponding relations for the creation operators $\tilde{c}_k^\dagger$ are given by Hermitian conjugation of (2.10). These operators obey the anticommutation relations

$$\{\tilde{c}_k^\dagger \, , \tilde{c}_p\} = \delta_{k,p} \, , \qquad \{\tilde{c}_k^\dagger \, , \tilde{c}_p^\dagger\} = \{\tilde{c}_k \, , \tilde{c}_p\} = 0 \, . \tag{2.11}$$

The eigenvectors of $\widehat{\mathcal{H}}$ are therefore given by

$$|\Psi\rangle\rangle = \tilde{c}^\dagger_{k_1} \dots \tilde{c}^\dagger_{k_r} |0\rangle\rangle \,, \tag{2.12}$$

where $k_1, \dots, k_r \in \{0, \dots, N\}$ are pairwise distinct, and the vacuum state $|0\rangle\rangle$ is annihilated by all the annihilation operators

$$\tilde{c}_k |0\rangle\rangle = 0 \,, \qquad k = 0 \,, \dots \,, N \,. \tag{2.13}$$

The corresponding energy eigenvalues are simply given by

$$E = \sum_{i=1}^{r} \omega_{k_i} \,. \tag{2.14}$$

3 The entanglement Hamiltonian

For the sake of concreteness, we shall consider entanglement in the ground state, which is described below. We shall further review how the reduced density matrix for the first $l+1$ sites of the chain is determined by the 1-particle correlation matrix, and its relation to the entanglement Hamiltonian. The parallel with the time and band limiting problem will also be drawn.

3.1 Defining the ground state or band limiting

The fact that the ground state is constructed by filling the Fermi sea leads to a "chopping" in frequency. Indeed, the ground state $|\Psi_0\rangle\rangle$ of the Hamiltonian (2.1) is given by

$$|\Psi_0\rangle\rangle = \tilde{c}^\dagger_0 \dots \tilde{c}^\dagger_K |0\rangle\rangle \,, \tag{3.1}$$

where $K \in \{0, 1, \dots, N\}$ is the greatest integer below the Fermi momentum, such that

$$\omega_K < 0 \,, \qquad \omega_{K+1} > 0 \,. \tag{3.2}$$

Let us remark that K can be modified by adding a constant term in the external magnetic field B_n.

The correlation matrix $\widehat{C}$ in the ground state is an $(N+1) \times (N+1)$ matrix with the following entries

$$\widehat{C}_{mn} = \langle\langle \Psi_0 | c^\dagger_m c_n | \Psi_0 \rangle\rangle \,. \tag{3.3}$$

Expressing everything in terms of annihilation and creation operators using (2.10) and (2.12), and then using the anticommutation relations (2.11) and the property (2.13) of the vacuum state, we obtain

$$\widehat{C}_{mn} = \sum_{k=0}^{K} \phi_m(\omega_k) \phi_n(\omega_k) \,, \qquad 0 \leq n, m \leq N \,. \tag{3.4}$$

It is then easy to see that

$$\widehat{C} = \sum_{k=0}^{K} |\omega_k\rangle\langle\omega_k| \,, \tag{3.5}$$

namely, that $\widehat{C}$ is the projector onto the subspace of $\mathbb{C}^{N+1}$ spanned by the vectors $|\omega_k\rangle$ with $k = 0, ..., K$ running over the labels of the excitations in the ground state.

3.2 Space limiting and entanglement

In order to examine entanglement, we must first define a bipartition of our free-Fermionic chain. This is the space limiting. As subsystem we shall take the first $\ell+1$ consecutive sites, and shall find how it is intertwined with the rest of the chain in the ground state $|\Psi_0\rangle\!\rangle$. To that end, we need the reduced density matrix

$$\rho_1 = \mathrm{tr}_2 \, |\Psi_0\rangle\!\rangle\langle\!\langle\Psi_0| \,, \tag{3.6}$$

where part 2, the complement of part 1, is comprised of the sites $\{\ell+1, \ell+2, ..., N\}$.

It has been observed that this reduced density matrix is determined by the spatially "chopped" correlation matrix C , which is the following $(\ell+1) \times (\ell+1)$ submatrix of $\widehat{C}$:

$$C = |\widehat{C}_{mn}|_{0 \le m,n \le \ell} \,. \tag{3.7}$$

The argument which we take from [7] (see also [8]) goes as follows. Because the ground state of the Hamiltonian $\widehat{\mathcal{H}}$ is a Slater determinant, all correlations can be expressed in terms of the one-particle functions, i.e. in terms of the matrix elements of $\widehat{C}$. When all the sites belong to the subsystem, since

$$C_{mn} = \mathrm{tr}(\rho_1 \, c_m^\dagger c_n) \,, \qquad m \,, n \in \{0, 1, \ldots, \ell\}, \tag{3.8}$$

the factorization property will hold according to Wick's theorem if ρ_1 is of the form (1.1) with the entanglement Hamiltonian $\mathcal{H}$ given by

$$\mathcal{H} = \sum_{m,n \in \{0,...,\ell\}} h_{mn} \, c_m^\dagger c_n \,. \tag{3.9}$$

The hopping matrix $h = |h_{mn}|_{0 \le m,n \le \ell}$ is defined so that (3.8) holds, and one finds through diagonalization that

$$h = \log[(1 - C)/C] \,. \tag{3.10}$$

We thus see that ρ_1, and hence the entanglement Hamiltonian $\mathcal{H}$, are obtained from the $(l+1) \times (l+1)$ matrix C.

To calculate the entanglement entropies one therefore has to compute the eigenvalues of C. As explained in [10], this is not easy to do numerically because the eigenvalues of that matrix are exponentially close to 0 and 1. This motivates the search for a tridiagonal matrix T such that

$$[T, C] = 0 \,. \tag{3.11}$$

The parallel between the study of entanglement properties of finite free-Fermion chains and finite-dimensional analogs of time and band limiting problems indicates that this can be achieved. Our aim here is to show that methods developed in the later context can advantageouly be used in the former framework.

Introducing the projectors

$$\pi_1 = \sum_{n=0}^{\ell} |n\rangle\langle n| \quad \text{and} \quad \pi_2 = \sum_{k=0}^{K} |\omega_k\rangle\langle\omega_k| = \widehat{C}\,, \tag{3.12}$$

the chopped correlation matrix can be written as (see for instance [31, 32])

$$C = \pi_1\pi_2\pi_1\ . \tag{3.13}$$

This makes the limiting explicit. We shall hence find a T satisfying (3.11) by looking for a tridiagonal matrix commuting with both projectors:

$$[T, \pi_1] = [T, \pi_2] = 0\,. \tag{3.14}$$

We may observe that the matrix D defined by $D = \pi_2\pi_1\pi_2$ would describe a dual entanglement situation where the vacuum state (2.13) would be filled with excitations labelled by the set $\{0, \ldots, \ell\}$, and the subsystem would consist of the sites $\{0, \ldots, K\}$. Since C and D have the same non-zero eigenvalues, the entanglement entropies will be the same in these two instances. Such dualities have been studied in [33]. We remark that the T commuting with C will also satisfy $[T, D] = 0$ because of (3.14) (see also [11]).

4 Bispectral properties of discrete orthogonal polynomials of the Askey scheme

A family of discrete orthogonal polynomials $\{R_n(\lambda(x))\}$ with $n, x = 0, 1, \ldots, N$, is a sequence of polynomials of degree n in the variable $\lambda(x)$, that are orthogonal with respect to some discrete measure

$$\sum_{x=0}^{N} W(x)\, R_m(\lambda(x))\, R_n(\lambda(x)) = U_n\delta_{mn}\,, \qquad W(x) > 0\,, \quad U_n > 0\,. \tag{4.1}$$

We assume the normalization $R_0(\lambda(x)) = 1$. We consider such polynomials that satisfy a recurrence relation of the form

$$\lambda(x)R_n(\lambda(x)) = A_nR_{n+1}(\lambda(x)) - (A_n + C_n)\, R_n(\lambda(x)) + C_nR_{n-1}(\lambda(x))\,, \quad 0 \le n \le N\,, \tag{4.2}$$

with $C_0 = A_N = 0$; as well as a difference relation of the form

$$f(n)R_n(\lambda(x)) = \overline{A}(x)R_n(\lambda(x+1)) - \left[\overline{A}(x) + \overline{C}(x)\right] R_n(\lambda(x)) + \overline{C}(x)R_n(\lambda(x-1))\,, \quad 0 \le x \le N\,, \tag{4.3}$$

with $\overline{C}(0) = \overline{A}(N) = 0$. A useful reference for such polynomials is [16, 17], which provides standard examples of bispectral problems where one has functions $\psi(x, n)$ that are eigenfunctions with eigenvalues depending on x of an operator L acting on the variable n, and are eigenfunctions as well with eigenvalues depending conversely on n of an operator Z acting on the variable x. This is the central framework that we shall deal with.

Our basic strategy is to engineer the parameters J_n and B_n in the Hamiltonian (2.1) in such a way that the recurrence relation (2.8) for the eigenfunctions $\phi_n(\omega_k)$ can be mapped to the recurrence relation (4.2) for some discrete orthogonal polynomials $R_n(\lambda(x))$. We then exploit the corresponding difference relation (4.3) to construct the sought-after operator T satisfying (3.11), as explained in Sec. 5 below.

In practice, we typically start from the recurrence relation for a given set of discrete orthogonal polynomials from [16, 17], and use it to determine the parameters J_n and B_n. To this end, we set

$$R_n(\lambda(x)) = \frac{\alpha_n}{\sqrt{W_k}}\,\phi_n(\omega_k)\,, \tag{4.4}$$

where α_n are still to be determined. While $R_n(\lambda(x))$ is a polynomial, $\phi_n(\omega_k)$ is generally *not* a polynomial, as it contains a transcendental factor that is proportional to $\sqrt{W_k}$. We observe that the recurrence relations (2.8) and (4.2) can be mapped into each other by means of the identifications

$$J_{n-1} = \frac{\alpha_n}{\alpha_{n-1}} A_{n-1} = \frac{\alpha_{n-1}}{\alpha_n} C_n\,, \qquad k = x\,, \qquad \omega_k = \lambda(x)\,, \qquad W_k = W(x)\,. \tag{4.5}$$

It follows that

$$\alpha_n = \alpha_{n-1}\,\varepsilon \sqrt{\frac{C_n}{A_{n-1}}}\,, \tag{4.6}$$

where $\varepsilon = \pm 1$. Solving for the α's, we obtain

$$\alpha_n = \alpha_0\,\varepsilon^n \prod_{k=1}^{n} \sqrt{\frac{C_k}{A_{k-1}}}\,. \tag{4.7}$$

In particular, we arrive at the important result that the parameters defining the Hamiltonian (2.1) are given by

$$J_n = \varepsilon \sqrt{A_n C_{n+1}}\,, \qquad B_n = A_n + C_n\,, \tag{4.8}$$

where A_n and C_n are the known coefficients in the recurrence relation (4.2) for a given family of discrete orthogonal polynomials.

The difference relation (4.3) for $R_n(\lambda(x))$ implies that the eigenfunctions $\phi_n(\omega_k)$ obey the corresponding equation

$$\lambda_n \phi_n(\omega_k) = \overline{J}_k \phi_n(\omega_{k+1}) - \overline{B}_k \phi_n(\omega_k) + \overline{J}_{k-1} \phi_n(\omega_{k-1})\,, \qquad 0 \le k \le N\,, \tag{4.9}$$

with $\overline{J}_{-1} = \overline{J}_N = 0$, where the coefficients are given by[3]

$$\overline{J}_k = \overline{A}(k)\sqrt{\frac{W_k}{W_{k+1}}} = \overline{C}(k+1)\sqrt{\frac{W_{k+1}}{W_k}}\,, \qquad \overline{B}_k = \overline{A}(k) + \overline{C}(k)\,, \qquad \lambda_n = f(n)\,. \tag{4.10}$$

5 Algebraic Heun operator and commuting tridiagonal matrices

The fact that the eigenfunctions $\phi_n(\omega_k) = \langle n|\omega_k\rangle$ obey the difference relation (4.9) can now be exploited to define an operator $\widehat{X}$ in the basis $\{|n\rangle\}$ by

$$\widehat{X}|n\rangle = \lambda_n|n\rangle\,, \tag{5.1}$$

which consequently acts as follows in the $\{|\omega_k\rangle\}$ basis

$$\widehat{X}|\omega_k\rangle = \overline{J}_{k-1}|\omega_{k-1}\rangle - \overline{B}_k|\omega_k\rangle + \overline{J}_k|\omega_{k+1}\rangle\ . \tag{5.2}$$

The operators $\widehat{H}$ and $\widehat{X}$ thus form a Leonard pair [30], meaning roughly that for these two operators there exist two bases such that in one, $\{|\omega_k\rangle\}$, $\widehat{H}$ is diagonal and $\widehat{X}$ is tridiagonal and in the other, $\{|n\rangle\}$, conversely $\widehat{H}$ is tridiagonal and $\widehat{X}$ is diagonal.

We may now introduce the algebraic Heun operator defined in [21] as the most general bilinear expression in the two bispectral operators $\widehat{H}$ and $\widehat{X}$:

$$\widehat{T} = \{\widehat{X}, \widehat{H}\} + \tau[\widehat{X}, \widehat{H}] + \mu\widehat{X} + \nu\widehat{H}\,, \tag{5.3}$$

where as usual $\{\widehat{X}, \widehat{H}\} = \widehat{X}\widehat{H} + \widehat{H}\widehat{X}$. At this point the parameters τ, μ, ν are free. (Note that allowing for redefinition by an irrelevant overall factor, the coefficient of $\{\widehat{X}, \widehat{H}\}$ has been set to 1.) It is immediate to see that $\widehat{T}$ is tridiagonal in both the position basis

$$\begin{aligned}\widehat{T}|n\rangle \;=\;& J_{n-1}(\lambda_{n-1}(1+\tau) + \lambda_n(1-\tau) + \nu)|n-1\rangle + (\mu\lambda_n - 2B_n\lambda_n - \nu B_n)|n\rangle \\ &+ J_n(\lambda_n(1-\tau) + \lambda_{n+1}(1+\tau) + \nu)|n+1\rangle\ ,\end{aligned} \tag{5.4}$$

and the momentum basis

$$\begin{aligned}\widehat{T}|\omega_k\rangle \;=\;& \overline{J}_{k-1}(\omega_{k-1}(1-\tau) + \omega_k(1+\tau) + \mu)|\omega_{k-1}\rangle + (\nu\omega_k - 2\overline{B}_k\omega_k - \mu\overline{B}_k)|\omega_k\rangle \\ &+ \overline{J}_k(\omega_k(1+\tau) + \omega_{k+1}(1-\tau) + \mu)|\omega_{k+1}\rangle\ .\end{aligned} \tag{5.5}$$

As a matter of fact, it has been shown in [34] that $\widehat{T}$ is the most general operator which is tridiagonal in both bases in finite-dimensional situations.

[3] The consistency condition

$$\frac{\overline{A}(k)}{\overline{C}(k+1)} = \frac{W_{k+1}}{W_k}$$

is a consequence of the fact that the difference operator is symmetrizable.

Let $\widehat{T}_{mn} = \langle m|\widehat{T}|n\rangle$, and define the "chopped" matrix T by

$$T = |\widehat{T}_{mn}|_{0\leq m,n\leq \ell}\,. \tag{5.6}$$

Following the results of [25, 21], we know that T and C will commute

$$[T, C] = 0 \tag{5.7}$$

if the parameters in $\widehat{T}$ (5.3) are given by

$$\tau = 0\ , \quad \mu = -(\omega_K + \omega_{K+1}) \quad \text{and} \qquad \nu = -(\lambda_\ell + \lambda_{\ell+1})\ . \tag{5.8}$$

Indeed, with the particular value of ν given by (5.8), we see that the matrix $\widehat{T}$ leaves the subspace $\{|n\rangle, n = 0, 1, \ldots, \ell\}$ invariant. Therefore T commutes with π_1. Similarly, with the particular value of μ given by (5.8), $\widehat{T}$ leaves the subspace $\{|\omega_k\rangle, k = 0, 1, \ldots, K\}$ invariant. Therefore T commutes with π_2. Finally, in view of (3.13), it is easy to get the result (5.7).

The main result of this section is the tridiagonal matrix T (5.6) i.e.

$$T = \begin{pmatrix} d_0 & t_0 & & & & \\ t_0 & d_1 & t_1 & & & \\ & t_1 & d_2 & t_2 & & \\ & & \ddots & \ddots & \ddots & \\ & & & t_{\ell-2} & d_{\ell-1} & t_{\ell-1} \\ & & & & t_{\ell-1} & d_\ell \end{pmatrix}, \tag{5.9}$$

which commutes with the correlation matrix (5.7) and whose nonzero matrix elements are given by (see (5.4))

$$\begin{aligned} t_n &= J_n(\lambda_n + \lambda_{n+1} - \lambda_\ell - \lambda_{\ell+1})\,, \\ d_n &= -B_n(2\lambda_n - \lambda_\ell - \lambda_{\ell+1}) - \lambda_n(\omega_K + \omega_{K+1})\,. \end{aligned} \tag{5.10}$$

A key ingredient obviously is the operator $\widehat{X}$ defined in (5.1). In the following sections, we apply this construction to both homogeneous and inhomogeneous free-Fermionic chains.

If $t_n \neq 0$ (which is the case in the examples below), T is non-degenerate (see e.g. Lemma 3.1 in [30]) and the commuting matrices T and C have a unique set of common eigenvectors. Since T is tridiagonal, its eigenvectors can be readily computed numerically. By acting with C on these eigenvectors, the eigenvalues of C can be easily obtained. The eigenvalues of the entanglement Hamiltonian $\mathcal{H}$, and therefore the entanglement entropy of the model, can then also be easily obtained.

6 The homogeneous chain

Let us construct the tridiagonal matrix T (5.9) for the homogeneous chain, for which

$$J_0 = \ldots = J_{N-1} = -\frac{1}{2}\,, \qquad B_n = 0\,. \tag{6.1}$$

We make use of a certain discretization of the (continuous) Chebyshev polynomials of the second kind, which are defined by (see e.g. [35, 36])

$$R_n(x) = \frac{\sin(\theta(n+1))}{\sin(\theta)}\,, \qquad x = \cos(\theta)\,, \qquad n = 0, 1, \dots\,, \tag{6.2}$$

which are polynomials in x of degree n. Note that x is not restricted here to integer values. These polynomials satisfy the recurrence relation (c.f. (4.2))

$$2xR_n(x) = R_{n+1}(x) + R_{n-1}(x)\,, \qquad n = 0, 1, \dots\,. \tag{6.3}$$

Comparing the recurrence relations (2.8) with $0 \leq n \leq N-1$ and (6.3), and recalling the parameter values (6.1), we see that $\phi_n(\omega_k) \propto R_n(x)$. Moreover, the recurrence relation (2.8) with $n = N$ leads to the constraint

$$2\cos(\theta)\sin((N+1)\theta) = \sin(N\theta)\,, \tag{6.4}$$

which has solutions

$$\theta = \theta_k = \frac{\pi(k+1)}{N+2} \tag{6.5}$$

for any integer k. Imposing the normalization (2.7), we conclude that the eigenfunctions are given by

$$\phi_n(\omega_k) = \sqrt{\frac{2}{N+2}}\sin(\theta_k)R_n(x_k) = \sqrt{\frac{2}{N+2}}\sin\left[\frac{\pi(k+1)(n+1)}{N+2}\right]\,, \tag{6.6}$$

where

$$\omega_k = -x_k = -\cos(\theta_k)\,, \qquad k = 0, 1, \dots, N\,. \tag{6.7}$$

Starting from the recurrence relation for $\phi_n(\omega_k)$, we can relabel $n \leftrightarrow k$ and use the property $\phi_n(\omega_k) = \phi_k(\omega_n)$ of the eigenfunctions (6.6) to obtain the difference relation

$$\omega_n\phi_n(\omega_k) = -\frac{1}{2}\phi_n(\omega_{k+1}) - \frac{1}{2}\phi_n(\omega_{k-1})\,, \tag{6.8}$$

c.f. (4.9). We can therefore define $\widehat{X}$ as in (5.1), with

$$\lambda_n = \omega_n = -\cos(\theta_n)\,. \tag{6.9}$$

The matrix T is therefore given by (5.9), with

$$\begin{aligned} t_n &= \frac{1}{2}\left[\cos(\theta_n) + \cos(\theta_{n+1}) - \cos(\theta_\ell) - \cos(\theta_{\ell+1})\right]\,, \\ d_n &= -\cos(\theta_n)\left[\cos(\theta_K) + \cos(\theta_{K+1})\right]\,. \end{aligned} \tag{6.10}$$

This result agrees (up to overall and additive constants, accounting for differences in conventions) with the recent result for the same model in [12] (see also [27]). Our new observation is that these results follow from the application of the algebraic Heun construction to truncated Chebychev polynomials of the second kind.

7 Inhomogeneous chains

We now turn to some examples of inhomogeneous chains. We consider models corresponding to Krawtchouk and dual Hahn polynomials in Secs. 7.1 and 7.2, respectively. Let us mention that the commuting matrices associated to these polynomials were first obtained by Perlstadt [19, 20] and recovered algebraically by Perline [25].

7.1 Krawtchouk

The Krawtchouk polynomials, which in general depend on one parameter (p), are defined by [16, 17]

$$R_n(\lambda(x)) = {}_2F_1\left(\begin{matrix}-n, & -x \\ & -N\end{matrix}; \frac{1}{p}\right), \qquad n = 0, 1, \ldots, N, \tag{7.1}$$

where

$$\lambda(x) = -x\,. \tag{7.2}$$

The orthogonality relation is given by (4.1) with [4]

$$W(x) = \binom{N}{x} p^x (1-p)^{N-x}, \qquad U_n = \left(\frac{1-p}{p}\right)^n \Big/ \binom{N}{n}, \tag{7.3}$$

for $0 < p < 1$. The recurrence relation is given by (4.2) with

$$A_n = p(N-n)\,, \qquad C_n = n(1-p)\,, \tag{7.4}$$

while the difference relation is given by (4.3) with

$$\overline{A}(x) = p(N-x)\,, \qquad \overline{C}(x) = x(1-p)\,, \qquad f(n) = -n\,. \tag{7.5}$$

Note that the Krawtchouk polynomials (7.1) are self-dual: they are invariant under the interchange $n \leftrightarrow x$. Hence, the coefficients (7.4) and (7.5) are related by $A \leftrightarrow \overline{A}$ and $C \leftrightarrow \overline{C}$ under this interchange.

The parameters in the corresponding Hamiltonian are given by (4.8) [5]

$$J_n = \sqrt{(N-n)(n+1)p(1-p)}\,, \qquad B_n = -\left[Np + n(1-2p)\right], \tag{7.6}$$

[4] The Pochhammer (or shifted factorial) symbol $(a)_k$ is defined by

$$(a)_0 = 1\,, \qquad (a)_k = a(a+1)(a+2)\cdots(a+k-1)\,, \quad k = 1, 2, \ldots\,.$$

We note the identity

$$\frac{(-N)_n(-1)^n}{n!} = \binom{N}{n}.$$

[5] We choose $\varepsilon = 1$, and we introduce in B_n an extra factor -1 in order to ensure $\omega_k < \omega_{k+1}$.

which corresponds to an inhomogeneous chain. For simplicity, we henceforth consider the special case $p = \frac{1}{2}$, for which the chain is mirror symmetric and admits end-to-end perfect state transfer [37, 38, 39, 40]. The α's are then given by (4.7)

$$\alpha_n = \alpha_0 / \sqrt{\binom{N}{n}} = 1 / \sqrt{\binom{N}{n}}\,, \tag{7.7}$$

where $\alpha_0 = 1$ has been chosen to ensure the normalization in (2.7). The eigenfunctions $\phi_n(\omega_k)$ are given by (4.4)

$$\phi_n(\omega_k) = (-1)^n 2^{-\frac{N}{2}} \sqrt{\binom{N}{n}\binom{N}{k}}\, R_n(\lambda(k))\,, \tag{7.8}$$

where

$$\omega_k = -\lambda(k) = k\,. \tag{7.9}$$

The difference relation is given by (4.9), with

$$\overline{J}_k = -\frac{1}{2}\sqrt{(N-k)(k+1)}\,, \qquad \overline{B}_k = -\frac{N}{2}\,, \qquad \lambda_n = n\,. \tag{7.10}$$

The matrix T is therefore of the form (5.9), with

$$\begin{aligned} t_n &= (n-\ell)\sqrt{(N-n)(n+1)}\,, \\ d_n &= \frac{N}{2}(2n-2\ell-1) - n(2K+1)\,. \end{aligned} \tag{7.11}$$

7.2 Dual Hahn

The dual Hahn polynomials, which in general depend on two parameters $(\gamma\,, \delta)$, are defined by [16, 17]

$$R_n(\lambda(x)) = {}_3F_2\left(\begin{matrix} -n, & -x, & x+\gamma+\delta+1 \\ \gamma+1, & -N & \end{matrix}; 1\right)\,, \qquad n = 0, 1, \ldots, N\,, \tag{7.12}$$

where

$$\lambda(x) = x(x+\gamma+\delta+1)\,. \tag{7.13}$$

They obey the orthogonality relation (4.1) with

$$W(x) = \frac{(2x+\gamma+\delta+1)(\gamma+1)_x N!}{(x+\gamma+\delta+1)_{N+1}(\delta+1)_x}\binom{N}{x}\,, \qquad U_n = \left[\binom{\gamma+n}{n}\binom{\delta+N-n}{N-n}\right]^{-1}\,, \tag{7.14}$$

for $\gamma\,, \delta > -1$ or $\gamma\,, \delta < -N$. These polynomials satisfy the recurrence relation (4.2) with

$$A_n = (n+\gamma+1)(n-N)\,, \qquad C_n = n(n-\delta-N-1)\,, \tag{7.15}$$

and the difference relation (4.3) with $f(n) = -n$ and

$$\overline{A}(x) = \frac{(x+\gamma+1)(x+\gamma+\delta+1)(N-x)}{(2x+\gamma+\delta+1)(2x+\gamma+\delta+2)}\,, \qquad \overline{C}(x) = \frac{x(x+\gamma+\delta+N+1)(x+\delta)}{(2x+\gamma+\delta)(2x+\gamma+\delta+1)}\,. \tag{7.16}$$

The parameters in the corresponding Hamiltonian read (choosing $\varepsilon = -1$) by (4.8)

$$J_n = -\sqrt{(n+1)(n+\gamma+1)(N-n)(N+\delta-n)}\,, \qquad B_n = -N-(N-n)(2n+\gamma)-n\delta\,, \tag{7.17}$$

which also corresponds to an inhomogeneous chain. For simplicity, we henceforth consider the special case $\delta = \gamma > 0$. The α's of (4.7) are then

$$\alpha_n = \alpha_0 \sqrt{\frac{n!\binom{N+\gamma}{n}}{\binom{N}{n}(\gamma+1)_n}} = \sqrt{\frac{N!n!\binom{N+\gamma}{n}}{\binom{N}{n}(\gamma+1)_N(\gamma+1)_n}}\,, \tag{7.18}$$

where α_0 has been chosen to ensure the normalization in (2.7) for the eigenfunctions $\phi_n(\omega_k)$, which obey the recursion relation (2.8), and which are given by (4.4)

$$\phi_n(\omega_k) = \left[\frac{\binom{N}{n}\binom{N}{k}(2k+2\gamma+1)(\gamma+1)_N(\gamma+1)_n}{n!\binom{N+\gamma}{n}(k+2\gamma+1)_{N+1}}\right]^{1/2} R_n(\lambda(k))\,, \tag{7.19}$$

where

$$\omega_k = \lambda(k) = k(k+2\gamma+1)\,. \tag{7.20}$$

These eigenfunctions obey the difference relation (4.9), with

$$\overline{J}_k = \frac{1}{2}\sqrt{\frac{(N-k)(k+1)(k+2\gamma+1)(N+k+2\gamma+2)}{(2k+2\gamma+1)(2k+2\gamma+3)}}\,, \qquad \overline{B}_k = \frac{N}{2}\,, \qquad \lambda_n = -n\,. \tag{7.21}$$

The matrix T is therefore of the form (5.9), with

$$\begin{aligned} t_n &= -2(\ell-n)\sqrt{(n+1)(n+\gamma+1)(N-n)(N+\gamma-n)}\,, \\ d_n &= (2\ell-2n+1)\left[N(\gamma+1)+2Nn-2n^2\right]+2n\left[\gamma+1+K(K+2\gamma+2)\right]\,. \end{aligned} \tag{7.22}$$

8 Conclusions

For any free-Fermion chain associated with a discrete orthogonal polynomial, we have constructed a tridiagonal matrix T that commutes with the "chopped" correlation matrix C, and hence, with the hopping matrix for the entanglement Hamiltonian. This matrix T is nothing but a specialization of the algebraic Heun operator. The provenance of this construction is the remarkable fact that the wavefunctions (orthogonal polynomials) obey both recurrence and difference relations with three terms. We expect that this result will facilitate the computation of the finite-size entanglement entropy for such models.

We "chopped" here in frequency by keeping only the momentum modes in the interval $[0\,,K]$, see e.g. (3.5). It would be interesting to know whether such a matrix T can still be constructed if one chops in other ways, such as in an arbitrary interval $[K_1\,,K_2]$, or in more than one disjoint intervals, etc.

Free-Fermion chains are simple examples of quantum integrable models. It would be instructive to explore whether similar constructions are possible for interacting quantum integrable models. An attractive candidate would be the XXZ spin chain with $\Delta = \pm\frac{1}{2}$, see e.g. [41].

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