Random Matrix Theory and Entanglement in Quantum Spin Chains

J.P. Keating, F. Mezzadri

School of Mathematics, University of Bristol, Bristol BS8 1TW, UK. E-mail: j.p.keating@bristol.ac.uk;
f.mezzadri@bristol.ac.uk

Abstract: We compute the entropy of entanglement in the ground states of a general class of quantum spin-chain Hamiltonians — those that are related to quadratic forms of Fermi operators — between the first N spins and the rest of the system in the limit of infinite total chain length. We show that the entropy can be expressed in terms of averages over the classical compact groups and establish an explicit correspondence between the symmetries of a given Hamiltonian and those characterizing the Haar measure of the associated group. These averages are either Toeplitz determinants or determinants of combinations of Toeplitz and Hankel matrices. Recent generalizations of the Fisher-Hartwig conjecture are used to compute the leading order asymptotics of the entropy as $N \to \infty$. This is shown to grow logarithmically with N. The constant of proportionality is determined explicitly, as is the next (constant) term in the asymptotic expansion. The logarithmic growth of the entropy was previously predicted on the basis of numerical computations and conformal-field-theoretic calculations. In these calculations the constant of proportionality was determined in terms of the central charge of the Virasoro algebra. Our results therefore lead to an explicit formula for this charge. We also show that the entropy is related to solutions of ordinary differential equations of Painlevé type. In some cases these solutions can be evaluated to all orders using recurrence relations.

1. Introduction

Random Matrix Theory, as developed by, amongst others, Freeman Dyson, provides the natural framework for calculating statistical properties of quantum fluctuations. It has had a profound impact in many of the traditional application areas of quantum mechanics, including condensed matter physics and nuclear physics. Our purpose here is to establish a new application: to calculating entanglement in quantum spin chains.

The importance of entangled quantum states lies in their ability to exhibit correlations that cannot be accounted for classically. This feature of quantum mechanics has been

known to physicists for almost seven decades — since Einstein, Podolsky and Rosen introduced their famous gedankenexperiment. However, it is only relatively recently that entanglement has come to be viewed as a physical resource for manipulating quantum information. As for any other physical resource, like energy or entropy, it important to be able to quantify entanglement; that is, to assign a measure to it. This aspect of entangled states is still poorly understood, especially when the entanglement is shared between more than two systems. However, when the entanglement of a pure state is shared between two parties, i.e. in a *bipartite system*, Bennett *et al* [1] have shown that it is consistent to define it as the von Neumann entropy of either of the two parts.

We consider here the general class of quantum spin chains arising from quadratic chains of fermionic operators in their ground state. These systems are partitioned into two contiguous subchains. If the ground state is non-degenerate, this subdivision creates a pure bipartite system and we investigate its entanglement of formation.

As is well known, the systems we are studying exhibit quantum phase transitions. These manifest themselves as qualitative changes in the decay of correlations: algebraic in the proximity of a critical point and exponential decay away from it. Entanglement plays a fundamental role in the quantum phase transitions that occur in interacting lattice systems at zero temperature [2–6]. Under these conditions the system is in the ground state, which is also a pure state, and any correlations must be a consequence of the fact the ground state is entangled. It follows immediately that the entanglement changes qualitatively in the proximity of critical points.

Vidal *et al* [3] studied the ground states of the XY and XXZ models, partitioning them into two consecutive subchains; they observed numerically that, when the Hamiltonian undergoes a phase transition, the entanglement of formation of this bipartite system grows logarithmically with the size N of one of the two parts. Jin and Korepin [4] considered the XX model, which corresponds to an XY spin chain with an isotropic interaction, and expressed the von Neumann entropy in terms of a Toeplitz determinant, which they evaluated asymptotically using the Fisher-Hartwig conjecture [7]. Their result coincides with the numerical observations of Vidal *et al* [3], in that they found that the entropy grows like $\frac{1}{3}\log_2 N$. Subsequently Korepin [5] and Calabrese and Cardy [6] showed, using conformal field-theoretic arguments, that the logarithmic divergence of the entanglement in one dimensional systems is a general consequence of the logarithmic growth of the entropy with the size of the system at phase transitions. These arguments determine the constant multiplying the leading order $\log_2 N$ term in the asymptotics to be one-third of the central charge of the associated Virasoro algebra.

Our goal here is to show that if a quantum spin-chain Hamiltonian possesses certain symmetries, the entanglement can be expressed as an average over one of the classical compact groups equipped with Haar measure, i.e. one of the following groups: $U(N)$, $Sp(2N)$ and $O^{\pm}(N)$, where the superscript $\pm$ indicates the connected component of the orthogonal group with determinant ± 1. Indeed, we establish a precise correspondence between the functional form of the appropriate Haar measure and the symmetries of the Hamiltonian. The XX model turns out to be an example of a system with $U(N)$ symmetry. The averages that occur can be expressed either as Toeplitz determinants, in the case of $U(N)$, or as determinants of specific combinations of Toeplitz and Hankel matrices for the other compact groups. Recently, Basor and Ehrhardt [8] and Forrester and Frankel [9] have computed asymptotic formulae for such determinants, and these allow us to write down the leading-order and next-to-leading-order terms in the asymptotics of the entanglement in the limit as the total number of spins tends to infinity and then as $N \to \infty$.

We find that in the proximity of a critical point the entanglement grows logarithmically with N, in agreement with the prediction of Korepin [5] and Calabrese and Cardy [6]. We derive a general formula for the associated constant of proportionality. This is a rational number, the numerator of which is shown to factorize into a universal part, related to symmetries of the quantum Hamiltonian and which can be calculated from the random-matrix averages, and a non-universal (i.e. Hamiltonian-specific) part, which we also evaluate. Comparing with Korepin's result leads to an explicit formula for the central charge, which plays a fundamental role in the conformal-field-theoretic approach. In addition, we obtain the sub-leading (constant) term in the asymptotics.

We also show that the random-matrix averages are related to solutions of certain *Painlevé equations*. In the case of Hamiltonians possessing U(N) symmetry, these solutions, and thus the entropy of the entanglement, can be determined exactly by means of recurrence relations.

The structure of the paper is as follows. In Sect. 2 we review the results of Vidal *et al* [3] and Jin and Korepin [4]. In Sect. 3 we introduce the models that we investigate. Sects. 4, 5, 6 and 7 are devoted to identifying the symmetry classes of Hamiltonians that are associated to each compact group. In Sect. 8 we apply generalizations of the Fisher-Hartwig conjecture to compute the entanglement for each symmetry class. Finally, in Sect. 9 we investigate the connection between the interpretation of the entanglement as an average over a compact group and the theory of Painlevé equations.

2. Bipartite Entanglement in the XY Model

We begin by reviewing the results of Vidal *et al* [3] and Jin and Korepin [4] concerning the entanglement in the ground states of the XY and XX models. These systems are spin-1/2 ferromagnetic chains with an exchange coupling α in a constant transversal magnetic field h. The Hamiltonian $H = h H_\alpha$ with H_α given by

$$H_\alpha = -\frac{\alpha}{2} \sum_{j=0}^{M-1} \left[(1+\gamma)\sigma_j^x \sigma_{j+1}^x + (1-\gamma)\sigma_j^y \sigma_{j+1}^y \right] - \sum_{j=0}^{M-1} \sigma_j^z, \qquad (2.1)$$

where σ^a denotes the Pauli matrices and $a = x, y, z$. It is sometimes convenient to work with the spin operators $S_j^a = \sigma_j^a/2$ instead of the Pauli matrices. The parameter γ lies in the interval $[0, 1]$ and measures the geometric anisotropy of H_α. Throughout this paper we will assume periodic boundary conditions, i.e. $\sigma_M^a = \sigma_0^a$. At zero temperature the system is in the ground state $|\Psi_g\rangle$. In the limit $M \to \infty$ the Hamiltonian (2.1) undergoes a quantum phase transition at $\alpha_c = 1/(2h)$: the spin-spin correlation functions $\langle \Psi_g | S_j^x S_k^x | \Psi_g \rangle$ and $\langle \Psi_g | S_j^y S_k^y | \Psi_g \rangle$ decay algebraically at the critical point and exponentially when $\alpha \neq \alpha_c$.

Let us partition the Hamiltonian (2.1) into two subchains, which we denote by P and Q. The subsystem P is composed of the first N spins, with $1 \ll N \ll M$. The Hilbert space where the Hamiltonian (2.1) acts is the direct product $\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_Q$, where $\mathcal{H}_P$ and $\mathcal{H}_Q$ are generated by the spins in P and Q respectively and are spanned by the vectors

$$\prod_{j=0}^{N-1} (\sigma_j^-)^{r_j} |\Psi_F\rangle \quad \text{and} \quad \prod_{j=N}^{M-1} (\sigma_j^-)^{r_j} |\Psi_F\rangle, \quad r_j = 0, 1, \qquad (2.2)$$

where $\sigma_j^{\pm} = (\sigma_j^x \pm i\sigma_j^y)/2$ and $|\Psi_F\rangle$ denotes the ferromagnetic state with all spins up. Since the ground state is non-degenerate this subdivision creates a pure bipartite system. The measure of entanglement is defined as the von Neumann entropy of either subchain:

$$E_P = E_Q = -\operatorname{Tr}\rho_P \log_2 \rho_P = -\operatorname{Tr}\rho_Q \log_2 \rho_Q, \tag{2.3}$$

where ρ_P and ρ_Q are the reduced density matrices of P and Q, i.e.

$$\rho_P = \operatorname{Tr}_Q \rho_{PQ} \quad \text{and} \quad \rho_Q = \operatorname{Tr}_P \rho_{PQ}. \tag{2.4}$$

The operators ρ_{PQ} form the density matrix of the whole system, $\rho_{PQ} = |\Psi_g\rangle\langle\Psi_g|$.

Let us introduce the Jordan-Wigner transformations at each site of the lattice $\{0, \ldots, M-1\}$:

$$m_{2l+1} = \left(\prod_{j=0}^{l-1}\sigma_j^z\right)\sigma_l^x \quad \text{and} \quad m_{2l} = \left(\prod_{j=0}^{l-1}\sigma_j^z\right)\sigma_l^y. \tag{2.5a}$$

The inverse relations are

$$\sigma_l^z = im_{2l}m_{2l+1},$$

$$\sigma_l^x = \left(\prod_{j=0}^{l-1}im_{2j}m_{2j+1}\right)m_{2l+1},$$

$$\sigma_l^y = \left(\prod_{j=0}^{l-1}im_{2j}m_{2j+1}\right)m_{2l}. \tag{2.5b}$$

These operators are Hermitian and obey the anticommutation relations $\{m_j, m_k\} = 2\delta_{jk}$. We also define

$$b_l = (m_{2l+1} - im_{2l})/2 \quad \text{and} \quad b^\dagger = (m_{2l+1} + im_{2l})/2, \tag{2.6}$$

which obey the anticommutation relations

$$\{b_j, b_k\} = 0 \quad \text{and} \quad \{b_j^\dagger, b_k\} = \delta_{jk} \tag{2.7}$$

and therefore are Fermi operators.

The expectation values of the operators (2.5a) with respect to $|\Psi_g\rangle$ are

$$\langle\Psi_g|m_k|\Psi_g\rangle = 0, \tag{2.8a}$$

$$\langle\Psi_g|m_j m_k|\Psi_g\rangle = \delta_{jk} + i(C_M)_{jk}, \tag{2.8b}$$

where the correlation matrix C_M has the block structure

$$C_M = \begin{pmatrix} C_{11} & C_{12} & \cdots & C_{1M} \\ C_{21} & C_{22} & \cdots & C_{2M} \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ C_{M1} & C_{M2} & \cdots & C_{MM} \end{pmatrix} \tag{2.9a}$$

with

$$C_{jk} = \begin{pmatrix} 0 & g_{j-k} \\ -g_{k-j} & 0 \end{pmatrix}. \tag{2.9b}$$

For large M, the real numbers g_l are the Fourier coefficients

$$g_l = \frac{1}{2\pi} \int_0^{2\pi} \frac{\alpha \cos\theta - 1 + i\alpha\gamma \sin\theta}{\sqrt{(\alpha\cos\theta - 1)^2 + \gamma^2\alpha^2 \sin^2\theta}} \, e^{-il\theta} \, d\theta. \qquad (2.10)$$

Formulae (2.8) were first computed (in a slightly different form) by Lieb *et al* [10] and Barouch and McCoy [11]. The expectation values of products of arbitrary numbers of the operators (2.5a) can be obtained from (2.8) using Wick's theorem. Equation (2.8a) follows from the invariance of H_α under the map $(\sigma_j^x, \sigma_j^y, \sigma_j^z) \mapsto (-\sigma_j^x, -\sigma_j^y, \sigma_j^z)$. In Appendix B we extend (2.8b) to a class of Hamiltonians that generalizes the XY model.

In order to compute the entropy (2.3) we need an expression for the reduced density matrix ρ_P. We therefore restrict our analysis to the first N consecutive spins. The correlation matrix is simply constructed by removing the last $2(M - N)$ rows and columns from the matrix (2.8b); we shall denote this restriction by C_N. If V is an orthogonal matrix, then the operators

$$d_j = \sum_{k=0}^{2N-1} V_{jk} m_k \qquad (2.11)$$

are Hermitian and obey the anti-commutation relations $\{d_j, d_k\} = 2\delta_{jk}$ too. Furthermore, since the Fourier coefficients defined in Eq. (2.10) are real, there exists an appropriate $V \in SO(2N)$ that block-diagonalizes C_N:

$$V C_N V^t = \bigoplus_{j=0}^{N-1} \nu_j \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \qquad (2.12)$$

where the ν_j are real and, for reasons that will become apparent later, lie in the interval $[-1, 1]$. Now, let us define

$$c_j = (d_{2j+1} - id_{2j})/2, \quad j = 0, \ldots, N - 1, \qquad (2.13)$$

which are Fermi operators, i.e.

$$\{c_j, c_k\} = 0 \quad \text{and} \quad \{c_j^\dagger, c_k\} = \delta_{jk} \qquad (2.14)$$

and are linearly related to those ones defined in (2.6). A basis for $\mathcal{H}_P$ is also given by the 2^N vectors

$$\prod_{j=0}^{N-1} (c_j^\dagger)^{r_j} |\Psi_{\text{vac}}\rangle, \quad r_j = 0, 1, \qquad (2.15)$$

where the state $|\Psi_{\text{vac}}\rangle$ is defined by the condition

$$c_j |\Psi_{\text{vac}}\rangle = 0, \quad j = 0, \ldots, N - 1. \qquad (2.16)$$

The expectation values of the c_js are readily obtained from Eq. (2.12):

$$\langle \Psi_g | c_j | \Psi_g \rangle = \langle \Psi_g | c_j c_k | \Psi_g \rangle = 0, \qquad (2.17a)$$

$$\langle \Psi_g | c_j^\dagger c_k | \Psi_g \rangle = \delta_{jk} \frac{1 - \nu_j}{2}. \qquad (2.17b)$$

The reduced density matrix ρ_P can be computed directly from the expectation values (2.17); we describe the details of the derivation in Appendix A. The final expression is

$$\rho_P = \prod_{j=0}^{N-1} \left(\frac{1 - \nu_j}{2} c_j^\dagger c_j + \frac{1 + \nu_j}{2} c_j c_j^\dagger \right). \tag{2.18}$$

In other words, as Eqs. (2.17) already suggest, these fermionic modes are in a product of uncorrelated states, therefore the density matrix is the direct product

$$\rho_P = \bigotimes_{j=0}^{N-1} \rho_j \quad \text{with} \quad \rho_j = \frac{1 - \nu_j}{2} c_j^\dagger c_j + \frac{1 + \nu_j}{2} c_j c_j^\dagger. \tag{2.19}$$

As a consequence, if one of the ν_js lies outside the interval $[-1, 1]$, then either $(1 + \nu_j)/2$ or $(1 - \nu_j)/2$ would be negative and so ρ_j could not be a density matrix. At this point the entropy of the entanglement between the two subsystems can be easily derived from Eq. (2.3):

$$E_P = \sum_{j=0}^{N-1} e(1, \nu_j), \tag{2.20}$$

where

$$e(x, \nu) = -\frac{x + \nu}{2} \log_2 \left(\frac{x + \nu}{2} \right) - \frac{x - \nu}{2} \log_2 \left(\frac{x - \nu}{2} \right). \tag{2.21}$$

Vidal *et al* [3] computed E_P numerically for the XY model and observed that for values of α and γ close to a critical point it grows logarithmically with N, while away from the phase transitions it is either zero or saturates to a constant value. Jin and Korepin [4] computed E_P when $\gamma = 0$, i.e. for the XX model, using the Fisher-Hartwig conjecture, which gives the leading order asymptotics of determinants of Toeplitz matrices whose symbols have zeros or discontinuities. This is also central to our own approach, so we will give a brief account of their method.

When $\gamma = 0$ the numbers (2.10) are the Fourier coefficients of the step function

$$g(\theta) = \begin{cases} 1 & \text{if } -k \leq \theta < k \\ -1 & \text{if } k \leq \theta < 2\pi - k, \end{cases} \tag{2.22}$$

where $k = \arccos(1/\alpha)$. In order to be in a critical regime, the parameter $1/\alpha$ must lie in the interval $(-1, 1)$; for $|\alpha| \leq 1$ the entanglement E_P is trivially zero. In physical terms this means that outside the critical regime the magnetic field is strong enough to align all the spins, therefore entangled states cannot appear. Since $g(\theta)$ is even its Fourier coefficients have the symmetry $g_l = g_{-l}$, therefore the correlation matrix C_N factorizes into the direct product

$$C_N = T_N[g] \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{2.23}$$

where $T_N[g]$ is the matrix

$$(T_N[g])_{jk} = g_{j-k}. \tag{2.24}$$

Matrices of this type are called *Toeplitz matrices* and $g(\theta)$ is called the *symbol* of $T_N[g]$. Toeplitz matrices and their determinants, known as *Toeplitz determinants*, will play an important role in our analysis.

As a consequence of (2.23) the ν_js are simply the eigenvalues of $T_N[g]$. One can then rewrite (2.20) using Cauchy's theorem [4]:

$$E_{\mathrm{P}} = \lim_{\epsilon \to 0^+} \lim_{\delta \to 0^+} \frac{1}{2\pi \mathrm{i}} \oint_{c(\epsilon,\delta)} \mathrm{e}(1+\epsilon, \lambda) \frac{\mathrm{d} \ln D_N[g](\lambda)}{\mathrm{d}\lambda} \, \mathrm{d}\lambda, \qquad (2.25)$$

where $D_N(\lambda)$ is the characteristic polynomial

$$D_N[g](\lambda) = \det (\lambda I - T_N[g]), \qquad (2.26)$$

which is also a Toeplitz determinant with symbol

$$g(\theta; \lambda) = \begin{cases} \lambda - 1 & \text{if } -k \le \theta < k \\ \lambda + 1 & \text{if } k \le \theta < 2\pi - k. \end{cases} \qquad (2.27)$$

The contour of integration $c(\epsilon, \delta)$ depends on the parameters ϵ and δ and includes the interval $[-1, 1]$; as ϵ and δ tend to zero the contour approaches the interval $[-1, 1]$. This technical expedient is necessary in order to guarantee that the branch points of $\mathrm{e}(1+\epsilon, \lambda)$ lie outside the contour of integration and thus that $\mathrm{e}(1+\epsilon, \lambda)$ is analytic inside $c(\epsilon, \delta)$. As already mentioned, the polynomial $D_N(\lambda)$ can be estimated for large N using a formula, which we will discuss in detail in Sect. 8, known as the *Fisher-Hartwig conjecture* [7]. This asymptotic formula can then be inserted in Eq. (2.25) and the integral explicitly evaluated. We will not go into the details of the computation, which can be found in Jin and Korepin's original paper. Their result is that for the XX model,

$$E_{\mathrm{P}} \sim \frac{1}{3} \log_2 N, \quad N \to \infty. \qquad (2.28)$$

This logarithmic divergence is a direct consequence of a general theorem on the spectra of Toeplitz matrices [12], which in our case reduces to the statement that in the limit $N \to \infty$ all except for $O(\ln N)$ of the eigenvalues of $T_N[g]$ migrate toward the points 1 and -1, where, trivially, we have $\mathrm{e}(1, 1) = \mathrm{e}(1, -1) = 0$.

We now make an observation relating to (2.25) that will have important consequences for the way we shall proceed. Toeplitz determinants are equivalent to averages of appropriate functions over the group of unitary matrices $\mathrm{U}(N)$. Let us make this statement more precise. The group $\mathrm{U}(N)$ is compact and therefore has a unique left and right invariant measure known as Haar measure. The invariance of the measure makes it a natural probability density for unitary matrices, because different regions in $\mathrm{U}(N)$ are equally weighted. This is usually referred to as the *Circular Unitary Ensemble* (CUE) of random matrices. After having integrated over the degrees of freedom associated with the eigenvectors, the explicit expression of Haar measure becomes

$$P_{\mathrm{U}(N)}(\theta_1, \dots, \theta_N) = \frac{1}{(2\pi)^N N!} \prod_{1 \le j < k \le N} \left| \mathrm{e}^{\mathrm{i}\theta_j} - \mathrm{e}^{\mathrm{i}\theta_k} \right|^2. \qquad (2.29)$$

Now, let $G(U)$ be a function on $\mathrm{U}(N)$ that depends only on the eigenvalues of U and is such that

$$G(U) = \prod_{j=1}^N g(\theta_j), \qquad (2.30)$$

where $g(\theta)$ is 2π-periodic. An identity due to Heine [13] and — in the form that we use — Szegő [14], pp. 27 and 288, asserts that

$$
\begin{aligned}
\left\langle G(U) \right\rangle_{\mathrm{U}(N)} &= \left\langle \prod_{j=1}^{N} g(\theta_j) \right\rangle_{\mathrm{U}(N)} \\
&= \frac{1}{(2\pi)^N N!} \int_0^{2\pi} \cdots \int_0^{2\pi} \left(\prod_{j=1}^{N} g(\theta_j) \right) \\
&\quad \times \prod_{1 \le j < k \le N} |\,\mathrm{e}^{\mathrm{i}\theta_j} - \mathrm{e}^{\mathrm{i}\theta_k}|^2 \, \mathrm{d}\theta_1 \cdots \mathrm{d}\theta_N \\
&= \det \left(g_{j-k} \right)_{j,k=0,\dots,N-1},
\end{aligned}
\tag{2.31}
$$

where

$$
g_l = \frac{1}{2\pi} \int_0^{2\pi} g(\theta) \, \mathrm{e}^{-\mathrm{i}l\theta} \, \mathrm{d}\theta.
\tag{2.32}
$$

Throughout this paper the brackets $\langle \cdot \rangle$ denote the average with respect to Haar measure (not necessarily just that of $\mathrm{U}(N)$).

For the XX model this remarkable identity allows us to express (2.25) as an average over $\mathrm{U}(N)$. Two questions now arise. First, can (2.25) be generalized to other Hamiltonians? And second, since there are no obvious reasons why $\mathrm{U}(N)$ should be singled out with respect to the other compact groups, are there systems for which the symmetries of the interaction give rise to a von Neumann entropy that can be re-expressed in terms of averages over $\mathrm{Sp}(2N)$ and $\mathrm{O}^{\pm}(N)$?

We note first that when $\gamma \ne 0$ the symbol of the matrix $T_N[g]$ is

$$
g(\theta) = \frac{\alpha \cos\theta - 1 + \mathrm{i}\alpha\gamma \sin\theta}{\sqrt{(\alpha \cos\theta - 1)^2 + \gamma^2 \alpha^2 \sin^2\theta}}.
\tag{2.33}
$$

The numbers ν_j that appear in formula (2.12) are not the eigenvalues of $T_N[g]$, which is not symmetric and as a consequence need not have a real spectrum. Instead they are the eigenvalues of the matrix $S = \left(T_N[g] T_N[g]^t \right)^{1/2}$. As a consequence, the entanglement is not straightforwardly expressible in terms of a Toeplitz determinant and so in terms of an average over $\mathrm{U}(N)$. Even so, it can again be expressed as an integral transform of the characteristic polynomial of S. It is worth remarking that the spin-spin correlation functions can still be expressed in terms of Toeplitz determinants and so related to averages over $\mathrm{U}(N)$.

In the following sections we shall show that for Hamiltonians that can be expressed as quadratic forms of fermionic oscillators, of which the XY model is an example, there exists a one-to-one correspondence between the symmetries of the Hamiltonian and the interpretation of the von Neumann entropy in terms of averages over one of the classical compact groups when $\gamma = 0$. In Sect. 9 we establish a connection between a generalization of formula (2.25) and the theory of Painlevé equations.

3. Quadratic Chains of Fermionic Operators

The most general form of Hamiltonian related to quantum spin chains is

$$H_\alpha = \alpha \left[\sum_{j,k=0}^{M-1} b_j^\dagger A_{jk} b_k + \frac{\gamma}{2} \left(b_j^\dagger B_{jk} b_k^\dagger - b_j B_{jk} b_k \right) \right] - 2 \sum_{j=0}^{M-1} b_j^\dagger b_j, \qquad (3.1)$$

where α and γ are real parameters, $0 \leq \gamma \leq 1$ and the b_js are the Fermi oscillators defined in Eq. (2.6). We take periodic boundary conditions, i.e. $b_M = b_0$. Since H_α is Hermitian, A must be a Hermitian matrix, and because of the anticommutation relation of the Fermi operators, B must be antisymmetric. Without loss of generality, we will consider only matrices A and B with real elements.

Up to an overall constant, the XY model (2.1) maps into the Hamiltonian (3.1)[1] with the matrices A and B given by

$$A = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 1 \\ 1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & 1 & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 & 1 & 0 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & -1 \\ -1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \cdots & -1 & 0 & 1 \\ 1 & 0 & 0 & \cdots & 0 & -1 & 0 \end{pmatrix}. \qquad (3.2)$$

Similarly, Eq. (2.5b) maps the Hamiltonian (3.1) into the spin chain

$$H_\alpha = -\frac{\alpha}{2} \sum_{0 \leq j \leq k \leq M-1} \left[(A_{jk} + \gamma B_{jk}) \sigma_j^x \sigma_k^x \left(\prod_{l=j+1}^{k-1} \sigma_l^z \right) \right.$$
$$\left. + (A_{jk} - \gamma B_{jk}) \sigma_j^y \sigma_k^y \left(\prod_{l=j+1}^{k-1} \sigma_l^z \right) \right] - \sum_{j=0}^{M-1} \sigma_j^z. \qquad (3.3)$$

In other words, the two systems (3.1) and (3.3) are equivalent. One sees that the second sum in (3.1) is the analogue of a uniform magnetic field, the parameter γ introduces a geometric anisotropy in the interaction, and α is an exchange coupling constant.

We will here be concerned with the entanglement between the first N oscillators and the rest of the chain, when the system is in the ground state $|\Psi_g\rangle$ and as the length of chain tends to infinity. In a similar fashion as for the XY model we decompose the Hilbert space into the direct product $\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_Q$, where $\mathcal{H}_P$ is generated by the first N sequential oscillators and $\mathcal{H}_Q$ by the remaining $M - N$. They are spanned by the vectors

$$\prod_{j=0}^{N-1} (b_j^\dagger)^{r_j} |\Psi_{\text{vac}}\rangle \quad \text{and} \quad \prod_{j=N}^{M-N} (b_j^\dagger)^{r_j} |\Psi_{\text{vac}}\rangle, \quad r_j = 0, 1, \qquad (3.4)$$

respectively, where the vacuum state $|\Psi_{\text{vac}}\rangle$ is defined by

$$b_j |\Psi_{\text{vac}}\rangle = 0, \quad j = 0, \ldots, M - 1. \qquad (3.5)$$

---

[1] This is strictly true only for open-end Hamiltonians. If we assume periodic boundary conditions, then the term $b_{M-1}^\dagger b_0$ should be replaced by $\left[\prod_{j=0}^{M-1} \left(2b_j^\dagger b_j - 1 \right) \right] b_{M-1} b_0$. However, because we are interested in the limit $M \to \infty$, the extra factor in front of $b_{M-1} b_0$ can be neglected.

Our goal is to determine the asymptotic behaviour for large N, with $N = o(M)$, of the von Neumann entropy

$$E_{\mathrm{P}} = - \operatorname{Tr} \rho_{\mathrm{P}} \log_2 \rho_{\mathrm{P}}, \tag{3.6}$$

where $\rho_{\mathrm{P}} = \operatorname{Tr}_{\mathrm{Q}} \rho_{\mathrm{PQ}}$ and $\rho_{\mathrm{PQ}} = |\Psi_{\mathrm{g}}\rangle \langle \Psi_{\mathrm{g}}|$.

The first step involves determining the expectation values with respect to $|\Psi_{\mathrm{g}}\rangle$ of products of arbitrary numbers of operators (2.5a). From the invariance of the Hamiltonian (3.1) under the transformation $b_j \mapsto -b_j$, it follows that $\langle \Psi_{\mathrm{g}}| m_l |\Psi_{\mathrm{g}}\rangle = 0$; for the same reason, the expectation value of the product of an odd number of m_js must be zero. The expectation values of the product of an even number of m_js can be computed using Wick's theorem

$$\langle \Psi_{\mathrm{g}}| m_{j_1} m_{j_2} \cdots m_{j_{2n}} |\Psi_{\mathrm{g}}\rangle = \sum_{\text{all pairings}} (-1)^p \prod_{\text{all pairs}} (\text{contraction of the pair}), \tag{3.7}$$

where a contraction of a pair is defined by $\langle \Psi_{\mathrm{g}}| m_{j_l} m_{j_m} |\Psi_{\mathrm{g}}\rangle$ and p is the signature of the permutation, for a given pairing, necessary to bring operators of the same pair next to one another from the original order.

Before continuing our analysis it is worth noting that the spin-spin correlation functions $\langle \Psi_{\mathrm{g}}| S_j^x S_k^x |\Psi_{\mathrm{g}}\rangle$ and $\langle \Psi_{\mathrm{g}}| S_j^y S_k^y |\Psi_{\mathrm{g}}\rangle$ of the XY models are products of the type (3.7). These correlations were first studied by Barouch and McCoy [11], who showed that in general they are Pfaffians, which, when the system reaches thermal equilibrium, reduce to Toeplitz determinants and can be computed using Szegő's theorem and the Fisher-Hartwig conjecture. The different behaviour of these determinants away from and in the proximity of critical points determines how quantum phase transitions appear. Thus, in the same way that we can ask which features of the Hamiltonian (3.1) lead to expressions for the entropy of entanglement in terms of an average over $\mathrm{U}(N)$, so we can enquire which properties of H_α ensure that its physical correlations are expressible as averages over $\mathrm{U}(N)$. In view of the way physical correlations and entanglement affect each other, these two questions are closely related. Similarly, we can pose the same questions for the other classical compact groups $\mathrm{Sp}(2N)$ and $\mathrm{O}^\pm(N)$.

The expectation values $\langle \Psi_{\mathrm{g}}| m_j m_k |\Psi_{\mathrm{g}}\rangle$ can be deduced from the work of Lieb et al [10]; as already mentioned in Sect. 2, we give the details of this computation in Appendix B. They generalize formula (2.8b), in that the Fourier coefficients g_{j-k} and g_{k-j} in the 2×2 block (2.9b) are replaced by the matrix elements $(T_M)_{jk}$ and $(T_M)_{kj}$, where the matrix T_M is defined by

$$(T_M)_{jk} = \sum_{l=0}^{M-1} \psi_{lj} \phi_{lk}, \quad j, k = 0, \ldots, M-1, \tag{3.8}$$

and the vectors ϕ_k and ψ_k are real and orthogonal and obey the eigenvalue equations

$$\alpha^2 (A - (2/\alpha)I - \gamma B)(A - (2/\alpha)I + \gamma B)\phi_k = |\Lambda_k|^2 \phi_k, \tag{3.9a}$$

$$\alpha^2 (A - (2/\alpha)I + \gamma B)(A - (2/\alpha)I - \gamma B)\psi_k = |\Lambda_k|^2 \psi_k. \tag{3.9b}$$

These vectors are related by

$$\alpha (A - (2/\alpha)I + \gamma B)\phi_k = |\Lambda_k| \psi_k, \tag{3.10a}$$

$$\alpha (A - (2/\alpha)I - \gamma B)\psi_k = |\Lambda_k| \phi_k. \tag{3.10b}$$

From Eqs. (3.9) it follows that the $\boldsymbol{\phi}_k$s and $\boldsymbol{\psi}_k$s are eigenvectors of positive symmetric matrices, therefore the corresponding eigenvalues are always real and positive; for later convenience, here and in Appendix B we express them as the square of the absolute value of a complex number.

Now, the derivation of the von Neumann entropy (3.6) is identical to the analogous computation for the XY model described in Sect. 2. The formula for the entropy of the subchain P that one obtains is

$$E_{\mathrm{P}} = \lim_{\epsilon \to 0^+} \lim_{\delta \to 0^+} \frac{1}{2\pi i} \oint_{c(\epsilon,\delta)} e(1 + \epsilon, \lambda) \frac{d \ln D_N(\lambda)}{d\lambda} \, d\lambda, \qquad (3.11)$$

where

$$D_N(\lambda) = \det(I\lambda - S), \qquad (3.12)$$

S is the real symmetric matrix $\left(T_N T_N^t\right)^{1/2}$ and T_N is obtained from the matrix (3.8) by removing the last $M - N$ rows and columns. The path of integration of the integral in (3.11) is the same as that in (2.25). In order for (3.11) to have physical meaning, the eigenvalues of S must all be in the interval $[-1, 1]$. This will have to be verified for the various Hamiltonians of the type (3.1) that we shall consider.

4. U(N) Symmetry

If there is a connection between the entanglement of the ground state or, more generally, between the physical correlations of the ground state and the classical compact groups, it must be reflected somehow in the symmetries of the system of fermionic oscillators (3.1). The most obvious symmetry that the XY model has in common with U(N) is the invariance under translations: for the XY model it manifests itself in the fact that the matrices (3.2) are mapped into themselves if their rows and columns are simultaneously shifted by the same integer q (the periodicity of H_α is of course inherited by the periodicity of the rows and columns of A and B); for U(N) such symmetry is reflected in the invariance of the integral (2.31) if all the θ_js are shifted by the same amount χ. It is worth noting that the integral (2.31) can also be written in the form

$$\left\langle \prod_{j=1}^N g(\theta_j) \right\rangle_{\mathrm{U}(N)} = \int_0^{2\pi} \cdots \int_0^{2\pi} \left(\prod_{j=1}^N g(\theta_j) \right)$$
$$\times \det \left[S_N \left(\theta_j - \theta_k \right) \right]_{j,k=1,\ldots,N} \, d\theta_1 \cdots d\theta_N, \qquad (4.1)$$

where $S_N(z)$ is the kernel of the Haar measure of U(N) and is given by

$$S_N(z) = \frac{1}{2\pi} \frac{\sin(Nz/2)}{\sin(z/2)}. \qquad (4.2)$$

The invariance under translations of the Haar measure is then evident in the kernel (4.2). We shall now determine a general formula for the matrix (3.8) in the limit $M \to \infty$ by assuming that the physical interaction in the Hamiltonian (3.1) is invariant under translations; we shall also deduce under which conditions the characteristic polynomial appearing in the integrand of formula (3.11) can be interpreted as an average over U(N).

In order to simplify the algebra we shall denote $\overline{A} = \alpha A - 2I$ and $\overline{B} = \alpha \gamma B$. If H_α is invariant under translations of the lattice $\{0, 1, \ldots, M - 1\}$, then the elements of

the matrices $\overline{A}$ and $\overline{B}$ must depend only on the difference between the row and column indices, i.e. $\overline{A}$ and $\overline{B}$ must be Toeplitz matrices. In addition, because of the periodic boundary conditions, $\overline{A}$ and $\overline{B}$ must be *cyclic*.

Now, let a and b be two real functions on $\mathbb{Z}/M\mathbb{Z}$, even and odd respectively. The matrix elements of $\overline{A}$ and $\overline{B}$ can be written as

$$\overline{A}_{jk} = a(j-k) \quad \text{and} \quad \overline{B}_{jk} = b(j-k), \quad j, k = 0, \dots, M-1. \tag{4.3}$$

A complete set of orthonormal eigenvectors of cyclic matrices are the complex exponentials:

$$\phi_{kj} = \frac{\exp\left(\frac{2\pi i k j}{M}\right)}{\sqrt{M}}, \quad j, k = 0, \dots, M-1, \tag{4.4}$$

as can be easily verified by direct substitution. Now, the matrices $\overline{A}$ and $\overline{B}$ defined in Eq. (4.3) commute. This becomes straightforward if we notice that $(\overline{AB})_{jk}$ is the convolution of a and b evaluated at $j-k$:

$$\begin{aligned}
(\overline{AB})_{jk} &= \sum_{l=0}^{M-1} a(j-l)b(l-k) = \sum_{l=0}^{M-1} a(l)b(j-k-l) \\
&= \sum_{l=0}^{M-1} a(l-k)b(j-l) = (\overline{BA})_{jk}. \tag{4.5}
\end{aligned}$$

As a consequence, the complex exponentials (4.4) are a complete set of eigenvectors of $\overline{A} + \overline{B}$ too. Therefore, we have

$$\sum_{l=0}^{M-1} [a(p-l) + b(p-l)] \phi_{kl} = \Lambda'_k \phi_{kp} = |\Lambda_k| \psi_{kp}, \tag{4.6}$$

with $\boldsymbol{\psi}_k = \boldsymbol{\phi}_k \Lambda'_k / |\Lambda_k|$. Because both $\boldsymbol{\phi}_k$ and $\boldsymbol{\psi}_k$ are normalized, $\Lambda'_k / |\Lambda_k|$ is a phase factor and we can set $\Lambda'_k = \Lambda_k$. It is important to notice that since we have taken the $\boldsymbol{\phi}_k$s and $\boldsymbol{\psi}_k$s to be common eigenvectors of A and B they are not in general real. The matrix (3.8) should therefore be replaced by

$$\left(\overline{T}_M\right)_{jk} = \sum_{l=0}^{M-1} \overline{\psi}_{lj} \phi_{lk}, \quad j, k = 0, \dots, M-1, \tag{4.7}$$

which a priori need not be real. However, the matrix (4.7) is unitarily equivalent to (3.8); indeed, we shall prove that (4.7) is real too and as consequence there is an orthogonal matrix O such that $O T_M O^t = \overline{T}_M$. Therefore, we shall not distinguish between them.

The eigenvalues of $\overline{A} + \overline{B}$ can be determined simply by inserting the eigenvectors (4.4) into the left-hand-side of Eq. (4.6) and using the parities of the functions $a(j)$ and $b(j)$. We have

$$\Lambda_k = \begin{cases} a(0) + 2\sum_{j=1}^{(M-1)/2} (a(j)\cos kj + ib(j)\sin kj) & \text{if } M \text{ is odd} \\ a(0) + (-1)^l a(M/2) + 2\sum_{j=1}^{M/2-1} (a(j)\cos kj + ib(j)\sin kj) & \text{if } M \text{ is even,} \end{cases} \tag{4.8}$$

where k does not denote an integer anymore but the wave number

$$k = \frac{2\pi l}{M}, \quad l = 0, \ldots, M - 1. \tag{4.9}$$

The matrix (4.7) now becomes

$$(T_M)_{jl} = \frac{1}{2\pi} \sum_{k=0}^{2\pi(1-1/M)} \frac{\overline{\Lambda_k}}{|\Lambda_k|} e^{-ik(j-l)} \Delta k, \tag{4.10}$$

where $\Delta k = 2\pi/M$. From (4.10) it follows that taking the complex conjugate of the right-hand side of (4.10) is equivalent to replacing k by $2\pi - k$ in the sum, therefore T_M is real. If now we focus on the system consisting of the first N oscillators and let $M \to \infty$, we obtain

$$(T_N)_{jk} \xrightarrow[M\to\infty]{} \frac{1}{2\pi} \int_0^{2\pi} \frac{\Lambda(\theta)}{|\Lambda(\theta)|} e^{-i(j-k)\theta} \, d\theta, \tag{4.11}$$

where $\Lambda(\theta)$ is the periodic function

$$\Lambda(\theta) = \sum_{j=-\infty}^{\infty} \Lambda_j \, e^{ij\theta} \tag{4.12}$$

with $\Lambda_j = a(j) - b(j)$ if $j > 0$ and $\Lambda_j = a(j) + b(j)$ if $j < 0$. (We have also implicitly assumed that as $j \to \infty$, $a(j)$ and $b(j)$ tend to zero sufficiently fast for the Fourier series (4.12) to converge.) Thus, $T_N[g]$ is a Toeplitz matrix with symbol $g(\theta) = \Lambda(\theta)/|\Lambda(\theta)|$. It is worth emphasizing that (4.11) has been obtained by assuming only the translation invariance of the Hamiltonian (3.1) and periodic boundary conditions. Finally, if we define

$$\delta_l(j) = \begin{cases} 1 & \text{if } l \equiv j \bmod N \\ 0 & \text{otherwise,} \end{cases} \tag{4.13}$$

then we recover the XY model with the choice

$$a(j) = \alpha \left[\delta_1(j) + \delta_1(-j)\right] - 2\delta_0(j) \quad \text{and} \quad b(j) = -\alpha\gamma \left[\delta_1(j) - \delta_1(-j)\right]. \tag{4.14}$$

At this point a few remarks relating to (4.11) should be made. First, because the interaction is invariant under translations, we can take any set of N consecutive oscillators and the corresponding matrix $T_N[g]$ will still be a Toeplitz matrix. Second, as a consequence of the Jordan-Wigner transformations (2.5b) and Wick's theorem (3.7) the spin-spin correlation functions are Toeplitz determinants, i.e. averages over $U(N)$. Finally, there are important implications for formula (3.11). We mentioned that in order to have physical meaning the eigenvalues of $(T_N[g]T_N[g]^t)^{1/2}$ must lie in the interval $[-1, 1]$. Since the symbol $g(\theta)$ has absolute value one, a theorem on the spectrum of Toeplitz matrices [12] — the same theorem mentioned in Sect. 2 — states that the eigenvalues of $T_N[g]$ are all inside the unit circle and approach the image of g in the limit $N \to \infty$. It follows that all the eigenvalues of $(T_N[g]T_N[g]^t)^{1/2}$ lie in the interval $[-1, 1]$. It remains to establish when (3.11) is an average over $U(N)$. The condition is that $T_N[g]$ should be symmetric, in which case the correlation matrix C_N factorizes into the direct product as in (2.23). A necessary and sufficient condition in order for $T_N[g]$

to be symmetric is that $\Lambda(\theta)$ should be real and even, or equivalently γ should be zero; in other words, the interaction in the Hamiltonian (3.1) must be isotropic. When $\gamma = 0$ the symbol $g(\theta)$ is a piece-wise continuous function that takes the values 1 and -1 and has discontinuities at all points θ_r where the equation

$$\Lambda(\theta_r) = 0 \tag{4.15}$$

is satisfied, with the additional condition that the first non-zero derivative of $\Lambda(\theta)$ at θ_r is odd.

5. $O^+(2N)$ Symmetry

We now address the question of finding a class of symmetries of the Hamiltonian (3.1) which leads to an interpretation of the spin-spin correlation functions and the formula for the entropy of the entanglement (3.11) as averages over $O^+(2N)$, the group of orthogonal matrices of dimension $2N \times 2N$ and determinant 1. We have seen that the expression of the von Neumann entropy in terms of an average over $U(N)$ is a direct consequence of the invariance under translations of the Hamiltonian (3.1) and of its geometrical isotropy. We now proceed in the same way as with $U(N)$ and try to infer how the structure of the kernel of the Haar measure of $O^+(2N)$ is reflected into the invariance properties of H_α.

Eigenvalues of orthogonal and symplectic matrices come in complex conjugate pairs, therefore $O^+(2N)$ has only N independent eigenvalues. When dealing with the classical compact groups, we shall adopt the convention of denoting by $\tilde{N}$ the total number of eigenvalues and by N the number of independent ones. In general we shall denote an arbitrary group by $G_{(\sigma_1, \sigma_2)}(\tilde{N})$. Each of the classical compact groups is identified by specific values of (σ_1, σ_2). This correspondence is described in Appendix C; for $O^+(2N)$, $(\sigma_1, \sigma_2) = (1/2, 1/2)$. Let $F(U)$ be a *class function* on $G_{(\sigma_1, \sigma_2)}(\tilde{N})$, i.e. a symmetric function depending only on the eigenvalues of U. Furthermore, suppose that

$$F(U) = \prod_{j=1}^{\tilde{N}} f(\theta_j), \tag{5.1}$$

where $f(\theta)$ is even and 2π-periodic. The averages discussed in Appendix C can all be written as

$$\begin{aligned}
\left\langle F(U) \right\rangle_{G_{(\sigma_1, \sigma_2)}(\tilde{N})} &= \left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{G_{(\sigma_1, \sigma_2)}(\tilde{N})} \\
&= \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \det\left[f(\theta_j) f(\theta_k) Q_N^{(\sigma_1, \sigma_2)}(\theta_j, \theta_k) \right]_{j,k=1,\dots,N} \\
&\quad \times d\theta_1 \cdots d\theta_N.
\end{aligned} \tag{5.2}$$

The quantity $Q_N^{(\sigma_1, \sigma_2)}(\theta_1, \theta_2)$ is called the *kernel* of the Haar measure and

$$\begin{aligned}
\det&\left[f(\theta_j) f(\theta_k) Q_{(\sigma_1, \sigma_2)}^N(\theta_j, \theta_k) \right]_{j,k=1,\dots,N} \\
&= \left(\prod_{j=1}^{N} f(\theta_j) f(-\theta_j) \right) P_{(\sigma_1, \sigma_2)}^N(\theta_1, \dots, \theta_N),
\end{aligned} \tag{5.3}$$

where $P^N_{(\sigma_1,\sigma_2)}(\theta_1, \ldots, \theta_N)$ is the Haar measure (C.25). The integral (5.2) can always be expressed in terms of the independent eigenvalues; indeed in Appendix C it is shown that it is always proportional to the integral

$$\left\langle \prod_{j=1}^{N} g(\theta) \right\rangle_{G_{(\sigma_1,\sigma_2)}(\tilde{N})} = \int_0^\pi \cdots \int_0^\pi \left(\prod_{j=1}^{N} g(\theta_j) \right) P^N_{(\sigma_1,\sigma_2)} \left(\theta_j, \ldots, \theta_N \right) \, d\theta_1 \cdots d\theta_N$$

$$= \det(\alpha^{(\sigma_1,\sigma_2)}_{jk})_{j,k=0,\ldots,N-1}, \tag{5.4}$$

with a constant of proportionality that depends on the group and on the function $f(\theta)$. In Eq. (5.4) we have set $g(\theta) = f(\theta)f(-\theta)$. Explicit expressions for the matrix elements $\alpha^{(\sigma_1,\sigma_2)}_{jk}$ and the relations between the averages (5.2) and (5.4) for the various compact groups are reported in Table 1, Appendix C. In the rest of the paper we shall concern ourselves only with integrals of the form (5.4).

Let us now go back to $O^+(2N)$. In Appendix C we show that

$$\alpha_{00} = g_0, \tag{5.5a}$$
$$\alpha_{0j} = \alpha_{j0} = \sqrt{2} g_j, \quad j > 0, \tag{5.5b}$$
$$\alpha_{jk} = g_{j-k} + g_{j+k}, \quad j, k > 0, \tag{5.5c}$$

where for simplicity we have dropped the superscript (σ_1, σ_2) and

$$g_l = \frac{1}{2\pi} \int_0^{2\pi} g(\theta) e^{-il\theta} \, d\theta \tag{5.6}$$

is the lth Fourier coefficient of $g(\theta)$. Matrices of the form $\{h_{j+k}\}_{j,k=0,\ldots,N-1}$ are called Hankel matrices, therefore the matrix $\{\alpha_{jk}\}_{j,k=0,\ldots,N-1}$ is always the sum of a Toeplitz and a Hankel matrix.

How can we infer from (5.3) the structure of the matrices $\overline{A}$ and $\overline{B}$ that appear in the Hamiltonian (3.1)? After all, the geometry of H_α is that of a discrete lattice while the kernel of $O^+(2N)$ lives on the circle, its explicit form being

$$Q^N_{O^+(2N)}(\phi, \psi) = S_{2N-1}(\phi - \psi) + S_{2N-1}(\phi + \psi), \quad \phi, \psi \in [0, \pi), \tag{5.7}$$

where $S_N(z)$ is the kernel (4.2). In Appendix C it is shown that the matrix elements α_{jk} can be expressed as integral transforms involving a particular class of orthogonal polynomials, known as Jacobi polynomials. Furthermore, the kernel of Haar measure can be expressed in the form (see, e.g., [14], p. 24)

$$Q^N_{O^+(2N)}(\phi, \psi) = \sum_{j=0}^{N-1} p_j(\cos \phi) p_j(\cos \psi), \tag{5.8}$$

where $p_j(x)$ is the jth Chebyshev polynomial of the first kind:

$$p_0(x) = \frac{1}{\sqrt{\pi}} \quad \text{and} \quad p_j(x) = \sqrt{\frac{2}{\pi}} \cos\left(j \cos^{-1} x \right), \quad j > 0. \tag{5.9}$$

Formula (5.8) leads to the following expression for the matrix elements that appear in the determinant of the left-hand side of (5.3):

$$f(\phi)f(\psi)Q_{\mathrm{O}+(2N)}^{N}(\phi,\psi) = f(\phi)f(\psi)\sum_{j=0}^{N-1} p_j(\cos\phi)p_j(\cos\psi). \qquad (5.10)$$

Then, if we compare the integral transforms (C.35) with the sum (5.10), we note that the expressions are the same, but the role of the continuous and discrete variables is exchanged. In other words, the functional form of the kernel (5.7) is complementary to the intrinsic structure of the matrix $\{\alpha_{jk}\}_{j,k=0,\ldots,N-1}$ as a Toeplitz plus Hankel matrix. It is therefore natural to assume that the matrices A and B defining the quadratic form (3.1) should be the sum of Toeplitz plus Hankel matrices. As for U(N), the periodic boundary conditions will impose on them a further structure which will turn out to be essential to our study. It is worth noting that the analysis presented in Sect. 4 in terms of invariance under translations of the Haar measure of U(N) and of H_α is equivalent to the one discussed here; in the case of U(N) the orthogonal polynomials $p_j(\cos\phi)$ are replaced by the complex exponentials $\mathrm{e}^{ij\phi}/\sqrt{2\pi}$.

The above considerations lead one to consider matrices $\overline{A}$ of the form

$$\overline{A}_{jl} = a(j-l) + a(j+l), \quad j,l = 0,\ldots,M-1. \qquad (5.11)$$

Because of the periodic boundary conditions a must be a function on $\mathbb{Z}/M\mathbb{Z}$, which must also be even in order for $\overline{A}$ to be symmetric. Clearly, a Hankel matrix cannot be antisymmetric, therefore γ must be zero: the Hamiltonian (3.1) must be isotropic. A brief look to Table 1 in Appendix C shows that this is a necessary condition for all the other compact groups too. Since $\overline{A}$ is a real symmetric matrix, its eigenvalues Λ_k are real and therefore

$$\boldsymbol{\psi}_k = \frac{\Lambda_k}{|\Lambda_k|}\boldsymbol{\phi}_k = \operatorname{sign}\Lambda_k\boldsymbol{\phi}_k, \qquad (5.12)$$

where the $\boldsymbol{\phi}_k$s are the eigenvectors of $\overline{A}$.

We now need to diagonalize $\overline{A}$; as for the unitary group, this can be done explicitly. Because

$$\overline{A}_{jl} = \overline{A}_{j\,M-l}, \qquad (5.13)$$

any odd function on $\mathbb{Z}/M\mathbb{Z}$ will be in the kernel of $\overline{A}$. Therefore,

$$\phi_{kj} = \sqrt{\frac{2}{M}}\sin kj, \quad k = \frac{2\pi l}{M}, \quad l = 1,\ldots,[(M-1)/2], \qquad (5.14)$$

are a set of independent eigenvectors with eigenvalue zero whose multiplicity is at least $[(M-1)/2]$, where $[\cdot]$ denotes the integer part.

The eigenvectors with non-zero eigenvalues can be found by exploiting the symmetries of the matrix (5.11). For simplicity, we assume that the non-zero eigenvalues are non-degenerate. An immediate consequence of (5.13) and of the condition $\Lambda_k \neq 0$ is that any eigenvector $c_k(j)$ must be an even function on $\mathbb{Z}/M\mathbb{Z}$; thus, we can always write

$$c_k(j) = \mathrm{e}_k(j) + \mathrm{e}_k(-j), \quad j \in \mathbb{Z}/M\mathbb{Z}. \qquad (5.15)$$

Furthermore, using the periodicity of $a(j)$, it is easy to show that if $c(j)$ is an eigenvector of $\overline{A}$, then $c_k(j + p) + c_k(j - p)$, where p is an arbitrary integer, is also an eigenvector corresponding to the same eigenvalue Λ_k. It follows that

$$c_k(j + p) + c_k(j - p) \propto e_k'(p)c_k(j). \tag{5.16}$$

Since $c_k(j)$ is even, the role of j and p can be interchanged, and since they are both arbitrary, we can choose $e_k'(j) = e_k(j)$. Then it follows from Eqs. (5.15) and (5.16) that

$$e_k(j + p) = e_k(j)e_k(p), \tag{5.17}$$

for an appropriate choice of the constant of proportionality in (5.16). Thus, the $e_k(j)$ are additive-multiplicative functions. Because they are periodic too, it must be that

$$e_k(M) = e_k(1)^M = 1. \tag{5.18}$$

Therefore the $e_k(j)$s are roots of unity:

$$e_k(j) = \frac{e^{ikj}}{\sqrt{M}}, \quad k = \frac{2\pi l}{M}, \quad j, l = 0, \dots M - 1. \tag{5.19}$$

As an immediate consequence of (5.15) the remaining normalized eigenvectors of matrix (5.11) are

$$\begin{cases} \phi_{0j} = \frac{1}{\sqrt{M}}, \quad \phi_{kj} = \sqrt{\frac{2}{M}}\cos kj, \quad 0 < k < \pi & \text{for } M \text{ odd,} \\ \phi_{0j} = \frac{1}{\sqrt{M}}, \quad \phi_{kj} = \sqrt{\frac{2}{M}}\cos kj, \quad 0 < k < \pi, \quad \phi_{\pi j} = \frac{(-1)^j}{\sqrt{M}} & \text{for } M \text{ even,} \end{cases} \tag{5.20}$$

where $k = 2\pi l/M$. The corresponding eigenvalues can be obtained by direct substitution:

$$\Lambda_k = \begin{cases} 2a(0) + 4\sum_{j=1}^{(M-1)/2} a(j)\cos kj & \text{if } M \text{ is odd,} \\ 2\left[a(0) + (-1)^l a(M/2)\right] + 4\sum_{j=1}^{M/2-1} a(j)\cos kj & \text{if } M \text{ is even.} \end{cases} \tag{5.21}$$

In Appendix B we show that there exists a canonical transformation of the Fermi operators b_j that diagonalizes (3.1). Using the same notation as in Appendix B, let us denote by η_k the Fermi operators in term of which H_α is diagonal. The fact that approximately half of the Λ_ks are zero means that the corresponding η_ks do not appear in H_α. In other words, H_α is isomorphic to a system with half the number of degrees of freedom. This is not surprising; it is a reflection of the fact that only half of the eigenvalues of a matrix in $O^+(2N)$ are independent. In the same way as statistical properties of orthogonal and symplectic matrices are computed only in terms of the independent eigenvalues, so the extra degrees of freedom in H_α can be ignored. The matrix (3.8) can therefore be determined from the eigenvectors (5.20).

Following the same steps as for $U(N)$ we fix our attention on the subsystem P composed of the first N consecutive oscillators and let $M \to \infty$. The eigenvalues (5.21) converge to the even function

$$\Lambda(\theta) = \Lambda_0 + 2\sum_{j=1}^{\infty} \Lambda_j \cos \theta j, \tag{5.22}$$

where $\Lambda_j = 2a(j)$. Finally, by substituting the vectors (5.20) into (3.8) and taking the limit $M \to \infty$, we obtain

$$(T_N)_{jl} = \frac{2}{\pi} \sum_{k=0}^{\pi} \frac{\Lambda_k}{|\Lambda_k|} \cos kj \cos kl \Delta k \xrightarrow[M \to \infty]{} \alpha_{jk}, \qquad (5.23)$$

where the α_{jk} are precisely those of Eq. (5.5) with symbol

$$g(\theta) = \frac{\Lambda(\theta)}{|\Lambda(\theta)|}. \qquad (5.24)$$

We can then define an XX model with orthogonal symmetry by choosing

$$a(j) = \alpha \left[\delta_1(j) + \delta_1(-j) \right] - 2\delta_0(j). \qquad (5.25)$$

It is important to notice that in order for $T_N[g]$ to be the sum of a Toeplitz and a Hankel matrix the subchain P must be made of the first N sequential oscillators: we cannot shift the subsystem P because H_α is not translation invariant. This property was to be expected because the kernel (5.7) is not invariant under translations. In other words, the origin of the lattice defining the spin chain is a privileged point, in the same way as the point 1 on the unit circle is a symmetry point for the spectra of orthogonal and symplectic matrices. A consequence of the absence of translational invariance is that the determinant expressing the spin-spin correlations (3.7) is an average over $O^+(2N)$ only if one of the spins is the first in the chain.

It turns out that the structure of the matrix $T_N[g]$ so obtained has important consequences for the formula (3.11). First, since $\Lambda(-\theta) = \Lambda(\theta)$, $T_N[g]$ is symmetric, therefore the correlation matrix C_N factorizes as in (2.23). Thus, the characteristic polynomial

$$D_N[g](\lambda) = \det (\lambda I - T_N[g]) \qquad (5.26)$$

in the integral (3.11) is an average over $O^+(2N)$. We compute this integral in Sect. 8. The symbol $\Lambda(\theta)/|\Lambda(\theta)|$ is the same as the one discussed in Sect. 4 for the case when $\gamma = 0$: it is a piecewise continuous function that takes the values 1 and -1 and whose jumps are located at the points θ_r which are solutions of Eq. (4.15). In Sect. 4 we have seen that the eigenvalues of the corresponding Toeplitz matrix are in the interval $[-1, 1]$; similar arguments lead to the same conclusion for the eigenvalues of a matrix which is the sum of a Toeplitz and a Hankel matrix with the same symbol. Therefore, formula (3.11) gives the entropy of the subchain P and can be expressed in term of an average over $O^+(2N)$.

6. Sp(2*N*) and O⁻(2*N* + 2) Symmetry

The treatment of these two groups turns out to be the same – see (C.49d). The arguments are analogous to those presented for $O^+(2N)$. The elements in $Sp(2N)$ are $2N \times 2N$ unitary matrices U such that

$$U J U^t = J, \quad J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}, \qquad (6.1)$$

where I is the $N \times N$ identity matrix. The number of independent eigenvalues in both $O^-(2N+2)$ and $Sp(2N)$ is N. Without loss of generality, we shall concentrate only on $Sp(2N)$. The kernel of the Haar measure is

$$Q_{Sp(2N)}^N(\phi, \psi) = S_{2N+1}(\phi - \psi) - S_{2N+1}(\phi + \psi), \quad \phi, \psi \in [0, \pi), \qquad (6.2)$$

and the matrix elements appearing in the determinant (5.4) are

$$\alpha_{jk} = g_{j-k} - g_{j+k+2}. \qquad (6.3)$$

As for $O^+(2N)$ the structure of formulae (6.2) and (6.3) is incompatible with $\gamma \neq 0$. The choice of the matrix $\overline{A}$ is

$$\overline{A}_{jk} = a(j - k) - a(j + k + 2), \qquad (6.4)$$

where a is an even function on $\mathbb{Z}/M\mathbb{Z}$. The diagonalization of the matrix (6.4) is analogous to the one of (5.11). Therefore, we just present the results. The eigenvectors that span the kernel of $\overline{A}$ are

$$\phi_{kj} = \sqrt{\frac{2}{M}} \cos k(j + 1), \quad k = \frac{2\pi l}{M}, \quad l = 0, \dots, [M/2], \qquad (6.5a)$$

while those corresponding to $\Lambda_k \neq 0$ are

$$\phi_{kj} = \sqrt{\frac{2}{M}} \sin k(j + 1), \quad k = \frac{2\pi l}{M}, \quad l = 1, \dots, [(M - 1)/2]. \qquad (6.5b)$$

As in the case of $O^+(2N)$ the Hamiltonian (3.1) is isomorphic to a system with half the number of degrees of freedom. The eigenvectors associated to the relevant degrees of freedom are those in (6.5b). Similarly, the eigenvalues can be computed by direct substitution; they turn out to be given by formula (5.21). By fixing the number N of oscillators in the subchain P and letting $M \to \infty$, the matrix T_N converges to

$$(T_N)_{jl} = \frac{2}{\pi} \sum_{k=0}^{\pi} \frac{\Lambda_k}{|\Lambda_k|} \sin k(j + 1) \sin k(l + 1) \Delta k$$

$$\xrightarrow[M\to\infty]{} \frac{1}{2\pi} \int_0^{2\pi} \frac{\Lambda(\theta)}{|\Lambda(\theta)|} \left(e^{-i(j-l)\theta} - e^{-i(j+l+2)\theta} \right) d\theta, \qquad (6.6)$$

which are the integral transforms (C.39); $\Lambda(\theta)$ is the same real and even function as in (5.22), therefore $T_N[g]$ is symmetric. An immediate consequence is that the entropy formula (3.11) can be expressed in terms of an average over $Sp(2N)$.

7. $O^\pm(2N+1)$ Symmetry

The treatments of $O^+(2N+1)$ and of $O^-(2N+1)$ follow a similar pattern, indeed averages over these two groups are intertwined by Eqs. (C.49b) and (C.49c). The kernels of the Haar measures are

$$Q_{O^\pm(2N+1)}^N(\phi, \psi) = S_{2N}(\phi - \psi) \mp S_{2N}(\phi + \psi), \quad \phi, \psi \in [0, \pi), \qquad (7.1)$$

and the matrix elements in the average (5.4) are

$$\alpha_{jk} = g_{j-k} \mp g_{j+k+1}, \tag{7.2}$$

where in Eqs. (7.1) and (7.2) the minus sign refers to $O^+(2N+1)$ and the plus sign to $O^-(2N+1)$. Consequently, the choices of the matrix $\overline{A}$ compatible with (7.1) and (7.2) are

$$\overline{A}_{jk} = a(j-k) \mp a(j+k+1), \tag{7.3}$$

where a is an even function on $\mathbb{Z}/M\mathbb{Z}$. As with the groups treated previously, Eqs. (7.1) and (7.2) are incompatible with $\gamma \neq 0$.

The matrix (7.3) can be diagonalized adopting the same techniques used for the other groups,

$$\phi_{kj} = \sqrt{\frac{2}{M}} \sin\left[k\left(\frac{2j+1}{2}\right)\right], \quad k = \frac{2\pi l}{M}, \quad l = 1, \ldots, [M/2], \tag{7.4a}$$

$$\phi_{kj} = \sqrt{\frac{2}{M}} \cos\left[k\left(\frac{2j+1}{2}\right)\right], \quad k = \frac{2\pi l}{M}, \quad l = 0, \ldots, [(M-1)/2]. \tag{7.4b}$$

These are the eigenvectors of the matrix (7.3) for both choice of signs; however, the functions (7.4b) are in the kernel of $\overline{A}$ when the sign between the two terms in (7.3) is minus, i.e. for $O^+(2N+1)$ symmetry, while their eigenvalues are not zero when the sign is plus, i.e. for $O^-(2N+1)$ symmetry. For the eigenvectors (7.4a) the role is reversed. The eigenvalues are given by formula (5.21) for these groups too. It is now straightforward to determine the matrices T_N for both groups:

$$\begin{aligned}
(T_N)_{jl} &= \frac{2}{\pi} \sum_{k=0}^{\pi} \frac{\Lambda_k}{|\Lambda_k|} \sin\left[k\left(\frac{2j+1}{2}\right)\right] \sin\left[k\left(\frac{2l+1}{2}\right)\right] \Delta k \\
&\xrightarrow[M\to\infty]{} \frac{1}{2\pi} \int_0^{2\pi} \frac{\Lambda(\theta)}{|\Lambda(\theta)|} \left(e^{-i(j-l)\theta} - e^{-i(j+l+1)\theta}\right) d\theta
\end{aligned} \tag{7.5a}$$

for $O^+(2N+1)$ and

$$\begin{aligned}
(T_N)_{jl} &= \frac{2}{\pi} \sum_{k=0}^{\pi} \frac{\Lambda_k}{|\Lambda_k|} \cos\left[k\left(\frac{2j+1}{2}\right)\right] \cos\left[k\left(\frac{2l+1}{2}\right)\right] \Delta k \\
&\xrightarrow[M\to\infty]{} \frac{1}{2\pi} \int_0^{2\pi} \frac{\Lambda(\theta)}{|\Lambda(\theta)|} \left(e^{-i(j-l)\theta} + e^{-i(j+l+1)\theta}\right) d\theta
\end{aligned} \tag{7.5b}$$

for $O^-(2N+1)$. The function $\Lambda(\theta)$ is even and the symbol $g(\theta) = \Lambda(\theta)/|\Lambda(\theta)|$ is the same function analyzed in connection with the other groups. The matrix $T_N[g]$ is real and symmetric and therefore the formula (3.11) for the entropy of the entanglement has an interpretation as average over $O^+(2N+1)$ or over $O^-(2N+1)$.

8. Generalizations of the Fisher-Hartwig Formula and the Computation of Entanglement

The computation of Toeplitz determinants, and in particular of their asymptotics, is important in many branches of Physics. The first and most famous application goes back to 1946 and is due to Osanger, who showed that the diagonal spin-spin correlations in the classical two-dimensional Ising model can be expressed in terms of Toeplitz determinants. It turns out that the behaviour of the leading order term as the dimension of the matrix tends to infinity changes radically when the symbol has discontinuities or zeros. Indeed, phase transitions in quantum and classical lattice systems often appear as changes in the analytic properties of symbols in Toeplitz determinants.

When the symbol $g(\theta)$ is a continuous function on the unit circle and the c_ks are the Fourier coefficients of $\log g(\theta)$, Szegő's theorem [15] states that

$$\ln \det T_N[g] = c_0 N + \sum_{k=1}^{\infty} k c_k c_{-k} + o(1), \quad N \to \infty, \tag{8.1}$$

provided that the series $\sum_{k=-\infty}^{\infty} |c_k|$ and $\sum_{k=-\infty}^{\infty} |k||c_k|^2$ converge. If $g(\theta)$ has zeros or discontinuities, then it can always be reduced to the form

$$g(\theta) = \phi(\theta) \prod_{r=1}^{L} u_{\alpha_r}(\theta - \theta_r) t_{\beta_r}(\theta - \theta_r), \tag{8.2}$$

where ϕ is smooth, has winding number zero and

$$t_\beta(\theta) = \exp[-i\beta(\pi - \theta)], \quad 0 \le \theta < 2\pi, \quad \beta \notin \mathbb{Z} \tag{8.3a}$$

$$u_\alpha(\theta) = (2 - 2\cos\theta)^\alpha, \quad \mathrm{Re}\,\alpha > -\frac{1}{2}. \tag{8.3b}$$

Note that L represents the number of zeros/discontinuities in the interval $[0, 2\pi)$. Fisher and Hartwig [7] conjectured that

$$\ln D_N[g] = c_0 N + \left(\sum_{r=1}^{L} \alpha_r^2 - \beta_r^2\right) \ln N + \ln E + o(1), \quad N \to \infty, \tag{8.4}$$

where now the c_ks are the Fourier coefficients of $\ln \phi(\theta)$. Basor [16] determined the constant E:

$$\begin{aligned}
E = \exp\left(\sum_{k=1}^{\infty} k c_k c_{-k}\right) &\prod_{r=1}^{L} \phi_+\left(e^{i\theta_r}\right)^{-(\alpha_r + \beta_r)} \phi_-\left(e^{-i\theta_r}\right)^{-(\alpha_r - \beta_r)} \\
&\times \prod_{1 \le r \ne s \le L} (1 - \exp[i(\theta_s - \theta_r)])^{-(\alpha_r + \beta_r)(\alpha_s - \beta_s)} \\
&\times \prod_{r=1}^{L} \frac{G(1 + \alpha_r + \beta_r)\,G(1 + \alpha_r - \beta_r)}{G(1 + 2\alpha_r)},
\end{aligned} \tag{8.5}$$

where $G(z)$ is the *Barnes G-function*[2] and

$$\ln \phi_+(t) = \sum_{j=1}^{\infty} c_j t^j, \quad \ln \phi_-(t) = \sum_{j=1}^{\infty} c_{-j} t^{-j}. \tag{8.6}$$

The Fisher-Hartwig conjecture has been proved for $|\operatorname{Re} \alpha_r| < 1/2$ and $|\operatorname{Re} \beta_r| < 1/2$ [17] and for other specific values of α_r, β_r and L. (The reader is referred to [18], pp. 469–474, for a complete discussion.) The most important difference between Eqs. (8.1) and (8.4) is the extra term proportional to $\ln N$ in the Fisher-Hartwig formula.

Formula (8.4) was used by Jin and Korepin [4] to compute the entropy of the entanglement for the XX model, that is for the Hamiltonian (2.1) with $\gamma = 0$. Their computation can be easily generalized to all Hamiltonians of the form (3.1) that are invariant under translations and isotropic, for which, therefore, the formula (3.11) becomes an average over U(N). However, before entering in the details of the computation, we discuss the generalization of formula (8.4) to determinants of combinations of Toeplitz and Hankel matrices, or, more specifically, determinants that can be interpreted as averages over the other classical compact groups.

Basor and Ehrhardt [8] proved a generalization of the Fisher-Hartwig formula to determinants of matrices of the type

$$g_{j-k} + g_{j+k+1}, \quad j, k = 0, \dots, N-1, \tag{8.7}$$

i.e. determinants that are averages over $O^-(2N+1)$. Using Eqs. (C.49b) and (C.49c), their formulae can be applied to averages over $O^+(2N+1)$ by a change of variable in the integral (5.3). In a recent paper Forrester and Frankel [9] extended the results of Basor and Ehrhardt conjecturally to averages over Sp($2N$), $O^+(2N)$ and $O^-(2N+2)$. These formulae provide a very efficient means to compute the integral (3.11) for chains of fermionic oscillators whose symmetries are associated to one of these groups.

From the discussion of the previous sections it has emerged that we are only interested in the symbol $g(\theta) = \Lambda(\theta)/|\Lambda(\theta)|$ when $\Lambda(\theta)$ is real. This symbol takes only two values: 1 and -1. Its discontinuities are located at the points where Eq. (4.15) has solutions. If such an equation has no solutions, then $g(\theta)$ is a constant and $T_N[g] = \pm I$ for all the compact groups. It follows from Eq. (2.20) that $E_P = 0$. In physical terms this means that the Hamiltonian H_α is away from the critical point or, equivalently, the magnetic field is so strong that all the spins are aligned, thus there are no correlations and correspondingly the entanglement must be zero.

The Fisher-Hartwig formula extended to all the compact groups is fairly complicated when expressed for a general symbol of the form (8.2). For simplicity, we shall report only the expression for the case that concerns us directly, i.e. $g(\theta)$ is even and has only discontinuities; for the general case we refer to [8]. Eq. (8.2) becomes

$$g(\theta) = \phi(\theta) \prod_{r=1}^{R} t_{\beta_r}(\theta - \theta_r) t_{-\beta_r}(\theta + \theta_r), \tag{8.8}$$

---

[2] The definition of the Barnes G-function is

$$G(z) = (2\pi)^{z/2} e^{-\left[z(z+1) + \gamma_E z^2\right]/2} \prod_{n=1}^{\infty} \left[\left(1 + \frac{z}{n}\right)^n e^{-z + z^2/(2n)}\right],$$

where γ_E is Euler's constant. It generalizes the Gamma function, in the sense that it obeys $G(z+1) = \Gamma(z)G(z)$.

where now all the discontinuities θ_r lie in the interval $[0, \pi)$ and therefore $L = 2R$; we exclude the case $\theta_r = 0, \pi$ and still require $|\text{Re}\,\beta_r| < 1/2$. We have

$$\ln D_N[g](\lambda)_{(\sigma_1, \sigma_2)} = Nc_0 - \left(\sum_{r=1}^{R} \beta_r^2\right) \ln N$$

$$+ \frac{1}{2}\sum_{k=1}^{\infty} kc_k^2 + \sum_{k=1}^{\infty} c_{2k-1} + \ln F_{(\sigma_1, \sigma_2)}$$

$$+ \ln E + o(1), \quad N \to \infty, \tag{8.9}$$

where

$$F_{(\sigma_1, \sigma_2)} = \prod_{r=1}^{R} (1 + e^{i\theta_r})^{(\sigma_1 - 1/2)\beta_r} (1 + e^{-i\theta_r})^{-(\sigma_1 - 1/2)\beta_r}$$

$$\times (1 + e^{i\theta_r})^{(\sigma_2 + 1/2)\beta_r} (1 + e^{-i\theta_r})^{-(\sigma_2 + 1/2)\beta_r}$$

$$\times \exp\left\{-\sum_{k=1}^{\infty} c_k \left[\sigma_1 - 1/2 + (-1)^k (\sigma_2 + 1/2)\right]\right\}, \tag{8.10a}$$

$$E = \prod_{r=1}^{R} 2^{-\beta_r^2} G(1 + \beta_r) G(1 - \beta_r) |1 - e^{2i\theta_r}|^{-\beta_r^2} \frac{(1 - e^{-i\theta_r})^{\beta_r/2} (1 - e^{i\theta_r})^{-\beta_r/2}}{(1 + e^{-i\theta_r})^{\beta_r/2} (1 + e^{i\theta_r})^{-\beta_r/2}}$$

$$\times \prod_{1 \le r < s \le R} \left|\frac{1 - e^{i(\theta_r - \theta_s)}}{1 - e^{i(\theta_r + \theta_s)}}\right|^{2\beta_r \beta_s} \prod_{r=1}^{R} \phi_+\left(e^{i\theta_r}\right)^{\beta_r} \phi_-\left(e^{i\theta_r}\right)^{-\beta_r}. \tag{8.10b}$$

Note that the main differences between the various groups appear only in the O(1) terms of (8.9): when an even symbol with discontinuities is averaged over a compact group the term linear in N in formulae (8.4) and (8.9) is the same in every case, and the term logarithmic in N has just an extra factor of two in front of it for U(N). This factor is due to the fact that averages over U(N) are computed by integrating over $[0, 2\pi)^N$, while for the other compact groups the domain of integration is $[0, \pi)^N$, therefore, in the latter case the singularities located at $-\theta_r$ do not contribute.

The representation (8.8) of $g(\theta) = \Lambda(\theta)/|\Lambda(\theta)|$ is given by the following choices of $\phi(\theta)$ and β_r:

$$\phi(\lambda) = (\lambda + 1) \left(\frac{\lambda + 1}{\lambda - 1}\right)^{\left(\sum_{r=1}^{R}(-1)^r \theta_r\right)/\pi}, \tag{8.11a}$$

$$\beta_r(\lambda) = (-1)^r \beta(\lambda), \quad \beta(\lambda) = \frac{1}{2\pi i} \ln\left(\frac{\lambda + 1}{\lambda - 1}\right), \tag{8.11b}$$

with $-\pi \le \arg[(\lambda + 1)/(\lambda - 1)] < \pi$. Therefore, we have $|\text{Re}\,\beta_r| < 1/2$ on the contour of integration $c(\epsilon, \delta)$ and we can apply formula (8.9). The leading order asymptotic of the entropy (3.11) is then given by

$$E_P = I_1 N - 2^{w_G} R\, I_2 \ln N + O(1), \quad N \to \infty, \tag{8.12}$$

where R is the number of discontinuities in the interval $[0, \pi)$ and

$$w_G = \begin{cases} 1 & \text{if the average is over U}(N) \\ 0 & \text{if the average is over the other compact groups.} \end{cases} \tag{8.13}$$

I_1 and I_2 are the integrals

$$I_1 = \lim_{\epsilon \to 0^+} \lim_{\delta \to 0^+} \frac{1}{2\pi i} \oint_{c(\epsilon, \delta)} e(1 + \epsilon, \lambda) \frac{\phi'(\lambda)}{\phi(\lambda)} \, d\lambda = 0, \tag{8.14a}$$

$$I_2 = \lim_{\epsilon \to 0^+} \lim_{\delta \to 0^+} \frac{1}{\pi i} \oint_{c(\epsilon, \delta)} e(1 + \epsilon, \lambda) \beta(\lambda) \beta'(\lambda) \, d\lambda = -1/(6 \ln 2). \tag{8.14b}$$

The first integral can be computed straightforwardly using the residue theorem; the second was computed in [4] (in this case the integrand is a multivalued function inside the contour). Finally, we have

$$E_{\mathrm{P}} \sim \frac{2^{w_{\mathrm{G}}} R}{6} \log_2 N, \quad N \to \infty. \tag{8.15}$$

The asymptotic relation (8.15) represents one of our main results. As mentioned in Sect. 2, the logarithmic growth of the entanglement is a general consequence of the fact that in one dimensional systems near quantum phase transitions the entropy is a logarithmic function of the size of the system [5, 6]. These thermodynamic arguments give the value of the coefficient in front of the logarithm to be one-third of the central charge of the associated Virasoro algebra. Our expression therefore leads to an explicit formula for the central charge, which depends in a non-trivial way on the geometry of the Hamiltonian. The factor $2^{w_{\mathrm{G}}}$ is universal, depending only on the symmetries determining the classical compact group to be averaged over. The factor R corresponds to the number of solutions of (4.15).

We now proceed to compute the next-to-leading-order term. This can be determined by integrating with respect to λ the terms independent of N in the Fisher-Hartwig formulae (8.4) and (8.9). We begin with $U(N)$.

Since the symbol is even, using (8.8) and (8.11a), the constant (8.5) becomes

$$E(\lambda) = \prod_{r=1}^{R} |1 - e^{i2\theta_r}|^{-2\beta(\lambda)^2} \prod_{1 \leq r < s \leq R} \left| \frac{1 - e^{i(\theta_r - \theta_s)}}{1 - e^{i(\theta_r + \theta_s)}} \right|^{4(-1)^{(r+s)} \beta(\lambda)^2} \\ \times [G(1 + \beta(\lambda)) G(1 - \beta(\lambda))]^{2R}, \tag{8.16}$$

where only the independent discontinuities, located in the interval $[0, \pi)$, are taken into account. The logarithmic derivative of (8.16) is the sum of two terms. The first one is

$$4\beta(\lambda)\beta'(\lambda) \left(2 \sum_{1 \leq r < s \leq R} (-1)^{(r+s)} \ln \left| \frac{1 - e^{i(\theta_r - \theta_s)}}{1 - e^{i(\theta_r + \theta_s)}} \right| - \sum_{r=1}^{R} \ln|1 - e^{i2\theta_r}| \right). \tag{8.17}$$

The second term is more delicate; we have

$$G(1 + \beta(\lambda)) G(1 - \beta(\lambda)) = e^{-\beta(\lambda)^2(1 + \gamma_{\mathrm{E}})} \prod_{n=1}^{\infty} \left(1 - \frac{\beta(\lambda)^2}{n^2} \right)^n e^{\beta(\lambda)^2/n}, \tag{8.18}$$

where γ_{E} is Euler's constant. The logarithmic derivative of the right-hand side of (8.18) is

$$-2\beta(\lambda)\beta'(\lambda) \left[1 + \gamma_{\mathrm{E}} + \Upsilon(\lambda) \right], \tag{8.19}$$

where

$$\Upsilon(\lambda) = \sum_{n=1}^{\infty} \frac{\beta(\lambda)^2/n}{n^2 - \beta(\lambda)^2}. \tag{8.20}$$

Let us define

$$K = 1 + \gamma_E + \frac{1}{R}\left(\sum_{r=1}^{R}\ln|1 - e^{i2\theta_r}| - 2\sum_{1 \le r < s \le R}(-1)^{(r+s)}\ln\left|\frac{1 - e^{i(\theta_r - \theta_s)}}{1 - e^{i(\theta_r + \theta_s)}}\right|\right) \tag{8.21}$$

and

$$I_3 = \lim_{\epsilon \to 0^+}\lim_{\delta \to 0^+}\frac{1}{\pi i}\oint_{c(\epsilon,\delta)}e(1+\epsilon,\lambda)\beta(\lambda)\beta'(\lambda)\Upsilon(\lambda)\,d\lambda. \tag{8.22}$$

This integral was evaluated in [4] where it was found that $I_3 = 0.0221603\ldots$.

Combining Eqs. (8.16), (8.17) and (8.19), we obtain that the O(1) contribution to the entropy of entanglement is

$$C_{U(N)} = 2RI_2 K - 2RI_3 = \frac{R}{3\ln 2}\left(K - 6I_3\ln 2\right). \tag{8.23}$$

When $R = 1$ this equation reduces to the result of Jin and Korepin for the XX model.

Let us now consider the other compact groups. From Eqs. (8.10) it is clear that the next-to-leading-order term is composed of two parts, one, common to all groups, coming from Eq. (8.10b) and the other, depending on the particular choice of the group, given by (8.10a). By taking the logarithmic derivative of Eq. (8.10b) one immediately realizes that only two integrals contribute to this term: the first one is I_2; the second one is

$$I_4 = \frac{1}{2\pi i}\oint_{c(\epsilon,\delta)}e(1+\epsilon,\lambda)\beta'(\lambda)\,d\lambda. \tag{8.24}$$

This integral can be evaluated using the residue theorem to obtain $I_4 = 0$. Therefore, by proceeding as for U(N) we can determine the contribution to the sub-leading term coming from Eq. (8.10b):

$$C_G = \frac{R}{6\ln 2}\left(K - 6I_3\ln 2 + \ln 2\right). \tag{8.25}$$

This expression differs from that for $C_{U(N)}$ by a factor $1/2$, the origin of which is the same as in the leading order term, and an additional term equal to $R/6$.

We are left to determine the contribution coming from Eq. (8.10a). It is evident that, up to a constant depending only on the θ_rs, by taking the logarithmic derivative of the right-hand-side we are left just with integrals of the type (8.24). Hence, the next-to-leading-order term for the groups Sp($2N$) and O$^\pm$(N) is simply (8.25).

9. Painlevé VI and Gap Probability Generating Functions

The averages we have discussed turn out to be related to solutions of integrable second order ODEs of Painlevé type. There exist six Painlevé equations; any second order differential equation free of moveable essential singularities of the form

$$y'' = R(y', y, t), \tag{9.1}$$

where R is a rational function, can be reduced to one of them.

Let us consider a generating function $g(\theta) = \Lambda(\theta)/|\Lambda(\theta)|$ with only two discontinuities at θ_1 and $-\theta_1$ and set $\phi = 2\theta_1$. We then look at the characteristic polynomial (3.12) when $g(\theta)$ is averaged over U(N), which can be written as the integral

$$
\begin{aligned}
D_N[g](\lambda) &= \frac{(\lambda+1)^N}{(2\pi)^N N!} \int_0^{2\pi} \cdots \int_0^{2\pi} \\
&\quad \times \prod_{j=1}^N \left[1 - \xi \chi_{I_{[\pi-\phi,\pi)}}(\theta_j)\right] \prod_{1 \le j < k \le N} \left| e^{i\theta_j} - e^{i\theta_k} \right|^2 d\theta_1 \cdots d\theta_N \\
&= (\lambda+1)^N E_N^{\mathrm{CUE}}(I_{[\pi-\phi,\pi)}; \xi),
\end{aligned}
\tag{9.2}
$$

where we have set $\xi = 2/(\lambda+1)$. The function $E_N^{\mathrm{CUE}}(I_{[\pi-\phi,\pi)}; \xi)$ is known in random matrix theory as the generating function of the gap probabilities. Here CUE stands for *Circular Unitary Ensemble*, which, as already noted, denotes the probability space given by U(N) equipped with the Haar measure. Differentiating one obtains

$$
E_N^{\mathrm{CUE}}(n; I_{[\pi-\phi,\pi)}) = (-1)^n \left. \frac{d^n E_N^{\mathrm{CUE}}(I_{[\pi-\phi,\pi)}; \xi)}{d\xi^n} \right|_{\xi=1}, \tag{9.3}
$$

where $E_N^{\mathrm{CUE}}(n; I_{[\pi-\phi,\pi)})$ is the probability that the interval $I_{[\pi-\phi,\pi)}$ contains n eigenvalues. Making the substitution

$$
e^{i\theta} = \frac{1 + ix}{1 - ix}, \quad x = \tan\frac{\theta}{2}, \tag{9.4}
$$

Eq. (9.2) becomes

$$
\begin{aligned}
E_N^{\mathrm{CyUE}}(s; \xi) &= \frac{2^{N^2}}{(2\pi)^N N!} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{j=1}^N \frac{\left[1 - \xi \chi_{I_{[s,\infty)}}(x_j)\right]}{\left(1 + x_j^2\right)^N} \\
&\quad \times \prod_{1 \le j < k \le N} |x_j - x_k|^2 \, dx_1 \cdots dx_N,
\end{aligned}
\tag{9.5}
$$

where $s = \cot(\phi/2)$. The integral (9.5) is the gap probability generating function of the Cauchy ensemble (CyUE) for the interval $[s, \infty)$.

If we let the exponent in the denominator in the integrand (9.5) vary, we can define

$$
\begin{aligned}
E_N^{\mathrm{CyUE}}(s; \eta, \xi) &= \frac{2^{N^2}}{(2\pi)^N N!} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{j=1}^N \frac{\left[1 - \xi \chi_{I_{[s,\infty)}}(x_j)\right]}{\left(1 + x_j^2\right)^\eta} \\
&\quad \times \prod_{1 \le j < k \le N} |x_j - x_k|^2 \, dx_1 \cdots dx_N.
\end{aligned}
\tag{9.6}
$$

The connection between the gap probability generating function of $U(N)$ and the theory of Painlevé equations is mediated by the function

$$\sigma(s) = (1 + s^2)\frac{d}{ds}\ln E_N^{CyUE}(s; a + N, \xi), \tag{9.7}$$

which is a solution of the equation

$$(1 + s^2)^2(\sigma'')^2 + 4(1 + s^2)(\sigma')^3 - 8s\sigma(\sigma')^2 + 4\sigma^2(\sigma' - a^2)$$
$$+ 8a^2 s\sigma\sigma' + 4[N(N + 2a) - a^2 s^2](\sigma')^2 = 0. \tag{9.8}$$

The above equation is known in the literature as the σ-form of the Painlevé VI equation.

Solutions of Eq. (9.8), and therefore the determinant (9.2), obey a recurrence relation which allows one to determine an exact formula for them for each value of N. Therefore, at least in principle, it is possible to compute the entropy of the entanglement (3.11) exactly for each N. In terms of of the gap probability generating function, these recurrence relations assume the following form [19]:

$$\frac{E_{N-1}^{CUE} E_{N+1}^{CUE}}{(E_N^{CUE})^2} = 1 - x_N^2 \tag{9.9}$$

with initial conditions

$$E_0^{CUE} = 1 \quad E_1^{CUE} = 1 - \frac{\xi}{2\pi}\phi. \tag{9.10}$$

In turn x_N obeys the recurrence relation

$$2x_N x_{N-1} - 2\cos\frac{\phi}{2} = \frac{1 - x_N^2}{x_N}\left[(N + 1)x_{N+1} - (N - 1)x_{N-1}\right]$$
$$- \frac{1 - x_{N-1}^2}{x_{N-1}^2}\left[N x_N - (N - 2)x_{N-2}\right] \tag{9.11}$$

with initial conditions

$$x_{-1} = 0, \quad x_0 = 1 \quad \text{and} \quad x_1 = -\frac{\xi}{\pi}\frac{\sin\frac{\phi}{2}}{1 - \frac{\xi}{2\pi}\phi}. \tag{9.12}$$

These recurrence relations can be used to compute higher order terms in the asymptotics of E_N^{CUE} as $N \to \infty$, and therefore of the entropy of the entanglement. Substituting the Fisher-Hartwig formula (8.4) into (9.9) gives

$$x_N \sim \frac{\sqrt{2}|\beta(\lambda)|}{N}, \quad N \longrightarrow \infty, \tag{9.13}$$

where $\beta(\lambda)$ was defined in (8.11a). This suggests that x_N has an asymptotic expansion of the form

$$x_N \sim \frac{\sqrt{2}|\beta(\lambda)|}{N} + \frac{c_1(\lambda)}{N^2} + \frac{c_2(\lambda)}{N^3} + \cdots \quad N \to \infty. \tag{9.14}$$

Inserting this expansion into (9.11) it is possible to compute recursively the coefficients $c_j(\lambda)$; for the second order term we obtain

$$c_2(\lambda) = 2^{1/3}|\beta(\lambda)|^3. \tag{9.15}$$

This coefficient determines the contribution to the integral (3.11) given by Eq. (8.23). Higher order terms can be computed in a similar way.

When the average is over the other compact groups, the determinant (3.12) can still be interpreted as a gap probability generating function for the respective group and its logarithm is still a solution of a differential equation related to the Painlevé VI equation. However, although recurrence formulae analogous to (9.9) exist, at each step the values of (σ_1, σ_2) that label the integral (5.4) change and in general do not even identify one of the classical compact groups (see, e.g., [20]).

10. Conclusions

We have investigated the entanglement of formation of the ground state of the general class of quantum spin chains related to quadratic Hamiltonians of fermionic oscillators partitioned into two contiguous subchains. The number of oscillators in the first subsystem is N and we let the total size of the system grow to infinity. We have discovered that for certain Hamiltonians the measure of entanglement, which in these circumstances is given by the von Neumann entropy of the first subchain, can be expressed in term of an average over one of the classical compact groups $U(N)$, $Sp(2N)$ and $O^{\pm}(N)$. Indeed, we show that there exists a one-to-one correspondence between the symmetries of the fermionic chain and the functional form of the Haar measures of the classical compact groups. Using generalizations of the Fisher-Hartwig conjecture it is possible to compute asymptotic formulae for such averages in the limit $N \to \infty$. The entanglement is either zero, away from the critical point, or grows logarithmically with N in the proximity of quantum phase transitions. Generalizations of the Fisher-Hartwig formula allow one to determine the constant in front of the logarithm explicitly, and the next-to-leading-order term in the asymptotics. Furthermore, these averages turn out to be related to solutions of Painlevé equations.

The fact that one can compute the leading order terms in the asymptotics of the entanglement of formation of the ground state of such a significant class of systems suggests that the connection between lattice models and random matrices may be deeper than being simply a calculational device. For example, the diagonal spin-spin correlations of the two-dimensional classical Ising model are Toeplitz determinants with symbols analogous to the one associated to the XY model; it is likely that a similar association between classical compact groups and symmetries of the Hamiltonian exists also for classical lattice models. If it does, random-matrix techniques could then be used to deduce thermodynamic quantities like critical exponents. After all, two-dimensional classical spin chains are mathematically equivalent to one-dimensional quantum spin chains. Furthermore, these type of random matrix averages already appear in the calculation of the ground state density matrices for an impenetrable Bose gas in an interval of finite length [9].

It is likely that these applications of group averages will prompt further studies of the analytical properties of the determinants and spectra of combination of Toeplitz and Hankel matrices, the investigation of which has started only recently.

Appendix A. The Density Matrix of a Subchain

Let $\{|\psi_j\rangle\}$ be a basis of the Hilbert space $\mathcal{H}$ of a system composed of two parts, P and Q, so that $\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_Q$. The density matrix of a statistical ensemble expressed in the basis $\{|\psi_j\rangle\}$ is a positive Hermitian matrix given by

$$\rho_{PQ} = \sum_{jk} c_{jk} |\psi_j\rangle\langle\psi_k|, \tag{A.1}$$

with the condition $\mathrm{Tr}_{PQ}\, \rho_{PQ} = 1$. Let us introduce the operators $S(j,k)$ and $\overline{S}(j,k)$ defined by the relations

$$S(j,k) = |\psi_j\rangle\langle\psi_k|, \tag{A.2a}$$

$$\overline{S}(j,k)S(k,l) = \delta_{jl} |\psi_j\rangle\langle\psi_j| \quad \text{and} \quad S(j,k)\overline{S}(k,l) = \delta_{jl} |\psi_j\rangle\langle\psi_j|. \tag{A.2b}$$

(In this formula repeated indices are not summed over.) Clearly, we have

$$c_{jk} = \mathrm{Tr}_{PQ}\left[\rho_{PQ}\, \overline{S}(k,j)\right]. \tag{A.3}$$

Let us now suppose that the Hamiltonian of our physical system is (3.1) and that the subsystem P is composed of the first N oscillators. Then a set of operators $S(j,k)$ for the subchain P can be generated by products of the type $\prod_{j=1}^{N} G_j$, where G_j can be any of the operators $\{c_j, c_j^\dagger, c_j^\dagger c_j, c_j c_j^\dagger\}$ and the c_js are Fermi operators that span $\mathcal{H}_P$; it is straightforward to check that $\overline{S}(k,j) = \left(\prod G_{j=1}^{N}\right)^\dagger$. We then have

$$\begin{aligned}
\rho_P &= \sum_{\text{All the } S(l,k)} \mathrm{Tr}_P \left[\rho_P \left(\prod_{j=1}^{N} G_j\right)^\dagger \right] \prod_{j=1}^{N} G_j \\
&= \sum_{\text{All the } S(l,k)} \mathrm{Tr}_P \left[\mathrm{Tr}_Q\left(\rho_{PQ}\right) \left(\prod_{j=1}^{N} G_j\right)^\dagger \right] \prod_{j=1}^{N} G_j \\
&= \sum_{\text{All the } S(l,k)} \mathrm{Tr}_{PQ} \left[\rho_{PQ} \left(\prod_{j=1}^{N} G_j\right)^\dagger \right] \prod_{j=1}^{N} G_j.
\end{aligned} \tag{A.4}$$

Since $\rho_{PQ} = |\Psi_g\rangle\langle\Psi_g|$, this expression simply reduces to

$$\rho_P = \sum_{\text{All the } S(l,k)} \langle\Psi_g| \left(\prod_{j=1}^{N} G_j\right)^\dagger |\Psi_g\rangle \prod_{j=1}^{N} G_j. \tag{A.5}$$

The correlation functions in the above sum can be computed using Wick's theorem (3.7). Finally, if the correlations of the c_js are given by (2.8), we immediately obtain formula (2.18).

Appendix B. The Correlation Matrix C_M

The purpose of this appendix is to provide an explicit derivation of the expectation values

$$\langle \Psi_g | m_j m_k | \Psi_g \rangle \tag{B.6}$$

when the dynamics is determined by the Hamiltonian (3.1).

First, we need to diagonalize H_α, which is achieved by finding a linear transformation of the operators b_j of the form

$$\eta_k = \sum_{j=0}^{M-1} \left(g_{kj} b_j + h_{kj} b_j^\dagger \right), \tag{B.7}$$

such that the Hamiltonian (3.1) becomes

$$H_\alpha = \sum_{k=0}^{M-1} |\Lambda_k| \, \eta_k^\dagger \eta_k + C, \tag{B.8}$$

where the coefficients g_{kj} and h_{kj} are real, the η_ks are Fermi operators and C is a constant. We use the notation $|\Lambda_k|$ because it is convenient for the computations carried out in Sect. 4 to allow the coefficients of the number operators $\eta_k^\dagger \eta_k$ to be the absolute values of the complex numbers Λ_k. The quadratic form (3.1) can be transformed into (B.8) by (B.7) if the system of equations

$$[\eta_k, H_\alpha] - |\Lambda_k| \eta_k = 0, \quad k = 0, \ldots, M-1 \tag{B.9}$$

has a solution. Substituting (3.1) and (B.7) into (B.9) we obtain the eigenvalue equations

$$|\Lambda_k| g_{kj} = \sum_{l=0}^{M-1} \left(g_{kl} \overline{A}_{lj} - h_{kl} \overline{B}_{lj} \right), \tag{B.10a}$$

$$|\Lambda_k| h_{kj} = \sum_{l=0}^{M-1} \left(g_{kl} \overline{B}_{lj} - h_{kl} \overline{A}_{lj} \right), \tag{B.10b}$$

where $\overline{A} = \alpha A - 2I$ and $\overline{B} = \alpha \gamma B$. These equations can be simplified by setting

$$\phi_{kj} = g_{kj} + h_{kj}, \tag{B.11a}$$
$$\psi_{kj} = g_{kj} - h_{kj}, \tag{B.11b}$$

in terms of which Eqs. (B.10) become

$$(\overline{A} + \overline{B}) \boldsymbol{\phi}_k = |\Lambda_k| \boldsymbol{\psi}_k, \tag{B.12a}$$
$$(\overline{A} - \overline{B}) \boldsymbol{\psi}_k = |\Lambda_k| \boldsymbol{\phi}_k. \tag{B.12b}$$

Combining these two expressions, we obtain

$$(\overline{A} - \overline{B})(\overline{A} + \overline{B}) \boldsymbol{\phi}_k = |\Lambda_k|^2 \boldsymbol{\phi}_k, \tag{B.13a}$$
$$(\overline{A} + \overline{B})(\overline{A} - \overline{B}) \boldsymbol{\psi}_k = |\Lambda_k|^2 \boldsymbol{\psi}_k. \tag{B.13b}$$

When $\Lambda_k \neq 0$, $\boldsymbol{\phi}_k$ and $|\Lambda_k|$ can be determined by solving the eigenvalue Eq. (B.13a), then $\boldsymbol{\psi}_k$ can be computed using (B.12a). Alternatively, one can solve Eq. (B.13b) and then obtain $\boldsymbol{\phi}_k$ from (B.12b). When $\Lambda_k = 0$, $\boldsymbol{\phi}_k$ and $\boldsymbol{\psi}_k$ differ at most by a sign and can be deduced directly either from (B.12) or from (B.13).

Since $\overline{A}$ and $\overline{B}$ are real, the matrices $(\overline{A} - \overline{B})(\overline{A} + \overline{B})$ and $(\overline{A} + \overline{B})(\overline{A} - \overline{B})$ are symmetric and positive, which guarantees that all of their eigenvalues are positive. Furthermore, the $\boldsymbol{\phi}_k$s and $\boldsymbol{\psi}_k$s can be chosen to be real and orthonormal. As a consequence the coefficients g_{kj} and h_{kj} obey the constraints

$$\sum_{k=0}^{M-1} \left(g_{kj} g_{kl} + h_{kj} h_{kl} \right) = \delta_{jl}, \tag{B.14a}$$

$$\sum_{k=0}^{M-1} \left(g_{kj} h_{kl} + h_{kj} g_{kl} \right) = 0, \tag{B.14b}$$

which are necessary and sufficient conditions for the η_ks to be Fermi operators.

The constant in Eq. (B.8) can be computed by taking the trace of H_α using the two expressions (3.1) and (B.8):

$$\text{Tr } H_\alpha = 2^{M-1} \sum_{k=0}^{M-1} (\alpha A_{kk} - 2) = 2^{M-1} \sum_{k=0}^{M-1} |\Lambda_k| + 2^M C. \tag{B.15}$$

Therefore, we have

$$C = \frac{1}{2} \sum_{k=0}^{M-1} \left(\alpha A_{kk} - 2 - |\Lambda_k| \right). \tag{B.16}$$

We are now in a position to compute the contraction pair (B.6). Substituting (B.11) into (B.7) we have

$$\eta_k = \frac{1}{2} \sum_{j=0}^{M-1} \left(\phi_{kj} m_{2j+1} - i \psi_{kj} m_{2j} \right). \tag{B.17}$$

Since the $\boldsymbol{\phi}_k$s and $\boldsymbol{\psi}_k$s are two sets of real and orthogonal vectors, (B.17) can be inverted to give

$$m_{2j} = i \sum_{k=0}^{M-1} \psi_{kj} \left(\eta_k - \eta_k^\dagger \right), \tag{B.18a}$$

$$m_{2j+1} = \sum_{k=0}^{M-1} \phi_{kj} \left(\eta_k + \eta_k^\dagger \right). \tag{B.18b}$$

Since the vacuum state of the operators η_k coincides with $|\Psi_g\rangle$, the expectation values (B.6) are easily computed from the expressions (B.18). We have

$$\langle \Psi_g | m_{2j} m_{2k} | \Psi_g \rangle = \sum_{l=0}^{M-1} \psi_{lj} \psi_{lk} = \delta_{jk},$$

$$\left\langle \Psi_{\mathrm{g}} \right| m_{2j+1} m_{2k+1} \left| \Psi_{\mathrm{g}} \right\rangle = \sum_{l=0}^{M-1} \phi_{lj} \phi_{lk} = \delta_{jk}, \tag{B.19a}$$

and

$$\left\langle \Psi_{\mathrm{g}} \right| m_{2j} m_{2k+1} \left| \Psi_{\mathrm{g}} \right\rangle = \mathrm{i} \sum_{l=0}^{M-1} \psi_{lj} \phi_{lk},$$

$$\left\langle \Psi_{\mathrm{g}} \right| m_{2j+1} m_{2k} \left| \Psi_{\mathrm{g}} \right\rangle = -\mathrm{i} \sum_{l=0}^{M-1} \psi_{lk} \phi_{lj}. \tag{B.19b}$$

Finally, by introducing the real $M \times M$ matrix

$$(T_M)_{jk} = \sum_{l=0}^{M-1} \psi_{lj} \phi_{lk}, \quad j, k = 0, \dots, M-1 \tag{B.20}$$

and combining the expressions (B.19) we obtain

$$\left\langle \Psi_{\mathrm{g}} \right| m_j m_k \left| \Psi_{\mathrm{g}} \right\rangle = \delta_{jk} + \mathrm{i}(C_M)_{jk}, \tag{B.21}$$

where the matrix C_M has the block structure

$$C_M = \begin{pmatrix} C_{11} & C_{12} & \cdots & C_{1M} \\ C_{21} & C_{22} & \cdots & C_{2M} \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ C_{M1} & C_{M2} & \cdots & C_{MM} \end{pmatrix} \tag{B.22a}$$

with

$$C_{jk} = \begin{pmatrix} 0 & (T_M)_{jk} \\ -(T_M)_{kj} & 0 \end{pmatrix}. \tag{B.22b}$$

We call C_M the correlation matrix. It is worth noting that because of the definition (B.20), the matrix T_M contains all of the physical information relating to the ground state of H_α.

Appendix C. Averages Over the Classical Compact Groups

Let $f(\theta)$ be a 2π-periodic even function and let $\mathrm{G}_{(\sigma_1,\sigma_2)}(\tilde{N})$ be one of the classical compact groups $\mathrm{O}^+(2N)$, $\mathrm{O}^-(2N+2)$, $\mathrm{Sp}(2N)$, $\mathrm{O}^+(2N+1)$ and $\mathrm{O}^-(2N+1)$, where the superscript $\pm$ denotes the connected component of the orthogonal group with positive and negative determinant respectively. The integer $\tilde{N}$ denotes the total number of eigenvalues, while N denotes the number of independent ones. For any $U \in \mathrm{G}_{(\sigma_1,\sigma_2)}(\tilde{N})$, let $F(U)$ be the class function defined by

$$F(U) = \prod_{j=1}^{\tilde{N}} f(\theta_j). \tag{C.23}$$

In this appendix we want to compute averages of the type

$$\left\langle F(U) \right\rangle_{G_{(\sigma_1,\sigma_2)}(\tilde{N})} = \left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{G_{(\sigma_1,\sigma_2)}(\tilde{N})}. \tag{C.24}$$

The Haar measure of $G_{(\sigma_1,\sigma_2)}(\tilde{N})$ expressed in terms of the independent eigenvalues is given by (see, e.g., [21], pp. 218 and 224)

$$P^N_{(\sigma_1,\sigma_2)}(\theta_1, \ldots, \theta_N) = \frac{1}{Z_N^{(\sigma_1,\sigma_2)}} \prod_{l=1}^{N} (1 + \cos\theta_l)^{\sigma_1 + 1/2} (1 - \cos\theta_l)^{\sigma_2 + 1/2}$$
$$\times \prod_{1 \le j < k \le N} (\cos\theta_j - \cos\theta_k)^2, \tag{C.25}$$

where $Z_N^{(\sigma_1,\sigma_2)}$ is a normalization constant whose specific value will not be relevant to what follows. The parameters $(\sigma_1, \sigma_2) = (-1/2, -1/2), (1/2, 1/2), (-1/2, 1/2), (1/2, -1/2)$ refer to $O^+(2N)$, $Sp(2N)$, $O^+(2N + 1)$ and $O^-(2N + 1)$ respectively; we will consider $O^-(2N + 2)$ separately.

Averages of the type (C.24) can be evaluated by making the substitutions

$$x_j = \cos\theta_j, \tag{C.26}$$

which reduces (C.24) to the computation of the integral

$$I_N(\sigma_1, \sigma_2) = \frac{1}{Z_N^{(\sigma_1,\sigma_2)}} \int_{-1}^{1} \cdots \int_{-1}^{1} \left(\prod_{j=1}^{N} g(\cos^{-1} x) \right) \prod_{j=1}^{N} (1 + x_j)^{\sigma_1} (1 - x_j)^{\sigma_2}$$
$$\times \prod_{1 \le j < k \le N} (x_j - x_k)^2 \, dx_1 \cdots dx_N, \tag{C.27}$$

where $g(\theta) = f(\theta)f(-\theta)$. For $\sigma_1, \sigma_2 > -1$ the integral (C.27) can be evaluated using orthogonal polynomial techniques; the details of the computation can be found, for example, in Sects. 2.1 and 2.2 of [14]. Let us introduce the weight

$$w_{(\sigma_1,\sigma_2)}(x) = (1 + x)^{\sigma_1} (1 - x)^{\sigma_2}, \quad -1 < x < 1 \tag{C.28}$$

together with the set of polynomials $\{p_j^{(\sigma_1,\sigma_2)}(x)\}$ orthogonal with respect to $w_{(\sigma_1,\sigma_2)}$, i.e.

$$\int_{-1}^{1} w_{(\sigma_1,\sigma_2)}(x) p_j^{(\sigma_1,\sigma_2)}(x) p_k^{(\sigma_1,\sigma_2)}(x) \, dx = \delta_{jk}. \tag{C.29}$$

We have

$$I_N(\sigma_1, \sigma_2) = \det(\alpha_{jk}^{(\sigma_1,\sigma_2)})_{j,k=0,\ldots,N-1}, \tag{C.30}$$

where

$$\alpha_{jk}^{(\sigma_1,\sigma_2)} = \int_{-1}^{1} g(\cos^{-1} x) w_{(\sigma_1,\sigma_2)}(x) p_j^{(\sigma_1,\sigma_2)}(x) p_k^{(\sigma_1,\sigma_2)}(x) \, dx. \tag{C.31}$$

The orthogonal polynomials $\{p_j^{(\sigma_1,\sigma_2)}(x)\}$ are called *Jacobi polynomials*.

1. $O^+(2N)$. The average to compute is

$$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{O^+(2N)} = \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \left(\prod_{j=1}^{N} f(\theta_j) f(-\theta_j) \right)$$
$$\times P_{(-1/2,-1/2)}^N (\theta_1, \ldots, \theta_N) \, d\theta_1 \cdots d\theta_N. \qquad (C.32)$$

The substitution (C.26) gives

$$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{O^+(2N)} = I_N(-1/2, -1/2) = \det \left(\alpha_{jk} \right)_{j,k=0,\ldots,N-1}. \qquad (C.33)$$

(For simplicity, from now on we shall drop the superscript (σ_1, σ_2) when denoting the orthogonal polynomials, their weight and the matrix elements (C.31).) When the weight is $w(x) = (1-x^2)^{-1/2}$ the Jacobi polynomials are also known as Chebyshev polynomials of the first kind; these are

$$p_0(x) = \frac{1}{\sqrt{\pi}} \quad \text{and} \quad p_j(x) = \sqrt{\frac{2}{\pi}} \cos \left(j \cos^{-1} x \right), \quad j > 0. \qquad (C.34)$$

Substituting $x = \cos \theta$ in Eq. (C.31) we have

$$\alpha_{00} = \frac{1}{2\pi} \int_0^{2\pi} g(\theta) \, d\theta = g_0, \qquad (C.35a)$$

$$\alpha_{0j} = \alpha_{j0} = \frac{\sqrt{2}}{\pi} \int_0^{\pi} g(\theta) \cos(j\,\theta) \, d\theta = \sqrt{2} g_j, \quad j > 0, \qquad (C.35b)$$

$$\alpha_{jk} = \frac{2}{\pi} \int_0^{\pi} g(\theta) \cos(j\,\theta) \cos(k\,\theta) \, d\theta = g_{j-k} + g_{j+k}, \quad j, k > 0, (C.35c)$$

where $g_j = \frac{1}{2\pi} \int_0^{2\pi} g(\theta) e^{-ij\theta} \, d\theta$.

2. $Sp(2N)$. The average to compute is

$$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{Sp(2N)} = \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \left(\prod_{j=1}^{N} f(\theta_j) f(-\theta_j) \right)$$
$$\times P_{(1/2,1/2)}^N (\theta_1, \ldots, \theta_N) \, d\theta_1 \cdots d\theta_N. \qquad (C.36)$$

The substitution (C.26) gives

$$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{Sp(2N)} = I_N(1/2, 1/2) = \det \left(\alpha_{jk} \right)_{j,k=0,\ldots,N-1}. \qquad (C.37)$$

When the weight is $w(x) = (1-x^2)^{1/2}$ the Jacobi polynomials reduce to the Chebyshev polynomials of the second kind:

$$p_j(x) = \sqrt{\frac{2}{\pi}} \frac{\sin \left[(j+1) \cos^{-1} x \right]}{\sin \left(\cos^{-1} x \right)}, \quad j \geq 0. \qquad (C.38)$$

The matrix element (C.31) becomes

$$\alpha_{jk} = \frac{2}{\pi} \int_0^\pi g(\theta) \sin\left[(j+1)\theta\right] \sin\left[(k+1)\theta\right] d\theta$$
$$= g_{j-k} - g_{j+k+2}, \quad j, k = 0, \dots, N-1. \tag{C.39}$$

3. $O^+(2N+1)$. Since the determinant is positive and the dimension is odd, the eigenvalues come in complex conjugate pairs and the extra eigenvalue is 1. This property must be taken into account when computing the average (C.24). We have the formula

$$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{O^+(2N+1)} = f(0) \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \left(\prod_{j=1}^{N} f(\theta_j) f(-\theta_j) \right)$$
$$\times P_{(-1/2,1/2)}^N(\theta_1, \dots, \theta_N) \, d\theta_1 \cdots d\theta_N, \tag{C.40}$$

which can be rearranged to give

$$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{O^+(2N+1)} = f(0) I_N(-1/2, 1/2) = f(0) \det\left(\alpha_{jk}\right)_{j,k=0,\dots,N-1}. \tag{C.41}$$

The Jacobi polynomials with weight $w(x) = \sqrt{(1-x)/(1+x)}$ are

$$p_j(x) = \frac{1}{\sqrt{\pi}} \frac{\sin\left[\left(\frac{2j+1}{2}\right)\cos^{-1}(x)\right]}{\sin\left[\frac{1}{2}\cos^{-1}(x)\right]}, \quad j \geq 0. \tag{C.42}$$

The matrix elements (C.31) become

$$\alpha_{jk} = \frac{2}{\pi} \int_0^\pi g(\theta) \sin\left[\left(\frac{2j+1}{2}\right)\theta\right] \sin\left[\left(\frac{2k+1}{2}\right)\theta\right] d\theta$$
$$= g_{j-k} - g_{j+k+1}, \quad j, k = 0, \dots, N-1. \tag{C.43}$$

4. $O^-(2N+1)$. The treatment in this case is similar to the one for $O^+(2N+1)$, except that now the extra eigenvalue is -1. Therefore, we have

$$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{O^-(2N+1)} = f(\pi) I_N(1/2, -1/2) = f(\pi) \det\left(\alpha_{jk}\right)_{j,k=0,\dots,N-1}. \tag{C.44}$$

The weight is $w(x) = \sqrt{(1+x)/(1-x)}$ and the corresponding Jacobi polynomials are

$$p_j(x) = \frac{1}{\sqrt{\pi}} \frac{\cos\left[\left(\frac{2j+1}{2}\right)\cos^{-1}(x)\right]}{\cos\left[\frac{1}{2}\cos^{-1}(x)\right]}, \quad j \geq 0. \tag{C.45}$$

The matrix elements (C.31) are given by the integral transform

$$\alpha_{jk} = \frac{2}{\pi} \int_0^\pi g(\theta) \cos\left[\left(\frac{2j+1}{2}\right)\theta\right] \cos\left[\left(\frac{2k+1}{2}\right)\theta\right] d\theta$$
$$= g_{j-k} + g_{j+k+1}, \quad j, k = 0, \dots, N-1. \tag{C.46}$$

5. $O^-(2N + 2)$. Since the determinant is negative, one eigenvalue must be -1, and since they come in complex conjugate pairs 1 is also an eigenvalue. The number of independent eigenvalues is therefore only N and not $N + 1$. The Haar measure is given by formula (C.25) with $(\sigma_1, \sigma_2) = (1/2, 1/2)$, the same as $Sp(2N)$. Therefore, we have

$$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{O^-(2N+2)} = f(0)f(\pi) \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} \left(\prod_{j=1}^{N} f(\theta_j)f(-\theta_j) \right)$$
$$\times P_{(1/2,1/2)}^N(\theta_1, \ldots, \theta_N)\, d\theta_1 \cdots d\theta_N, \quad (C.47)$$

which becomes

$$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{O^-(2N+2)} = f(0)f(\pi)I_N(1/2, 1/2)$$
$$= f(0)f(\pi)\det\left(\alpha_{jk}\right)_{j,k=0,\ldots,N-1}, \quad (C.48)$$

where the α_{jk} are given by Eq. (C.39).

Table 1. Summary of the averages over the different compact groups of $F(U) = \prod_{j=1}^{\tilde{N}} f(\theta_j)$. The function f is even and $g(\theta) = f(\theta)f(-\theta)$; f_l and g_l are the corresponding Fourier coefficients; $\tilde{N}$ is the dimension of the matrices and N the number of independent eigenvalues

$G_{(\sigma_1,\sigma_2)}(\tilde{N})$	$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{G_{(\sigma_1,\sigma_2)}(\tilde{N})}$	$\alpha_{jk}^{(\sigma_1,\sigma_2)}$	
$U(N)$	$\det\left(\alpha_{jk}\right)_{j,k=0,\ldots,N-1}$	$f_{j-k}, \quad j,k \geq 0$	
$O^+(2N)$	$\det\left(\alpha_{jk}\right)_{j,k=0,\ldots,N-1}$	g_0	if $j = k = 0$
		$\sqrt{2}g_l$	if either $j = 0, k = l$ or $j = l, k = 0$
		$g_{j-k} + g_{j+k}$	if $j, k > 0$
$Sp(2N)$	$\det\left(\alpha_{jk}\right)_{j,k=0,\ldots,N-1}$	$g_{j-k} - g_{j+k+2}, \quad j,k \geq 0$	
$O^+(2N+1)$	$f(0)\det\left(\alpha_{jk}\right)_{j,k=0,\ldots,N-1}$	$g_{j-k} - g_{j+k+1}, \quad j,k \geq 0$	
$O^-(2N+1)$	$f(\pi)\det\left(\alpha_{jk}\right)_{j,k=0,\ldots,N-1}$	$g_{j-k} + g_{j+k+1}, \quad j,k \geq 0$	
$O^-(2N+2)$	$f(0)f(\pi)\det\left(\alpha_{jk}\right)_{j,k=0,\ldots,N-1}$	$g_{j-k} - g_{j+k+2}, \quad j,k \geq 0$	

There exist useful relations among averages of functions over the classical compact groups. Those that are relevant to this paper are the following:

$$\left\langle \prod_{j=1}^{2N+1} g(\theta_j) \right\rangle_{U(2N+1)} = \left\langle \prod_{j=1}^{2N+2} f(\theta_j) \right\rangle_{O^+(2N+2)} \left\langle \prod_{j=1}^{2N} f(\theta_j) \right\rangle_{Sp(2N)}, \quad (C.49a)$$

$$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{O^+(2N+1)} = \left\langle \prod_{j=1}^{\tilde{N}} f(\pi - \theta_j) \right\rangle_{O^-(2N+1)}, \quad (C.49b)$$

$$\left\langle \prod_{j=1}^{\tilde{N}} f(\theta_j) \right\rangle_{O^-(2N+1)} = \left\langle \prod_{j=1}^{\tilde{N}} f(\pi - \theta_j) \right\rangle_{O^+(2N+1)}, \tag{C.49c}$$

$$\left\langle \prod_{j=1}^{2N} f(\theta_j) \right\rangle_{Sp(2N)} = \frac{1}{f(0)f(\pi)} \left\langle \prod_{j=1}^{2N+2} f(\theta_j) \right\rangle_{O^-(2N+2)}. \tag{C.49d}$$

References

1. Bennett, C.H., Bernstein, H.J., Popescu, S., Schumacher, B.: Concentrating partial entanglement by local operations. Phys. Rev. A **53**, 2046–2052 (1996)
2. Amico, L., Osterloh, A., Plastina, F., Fazio, R., Palma, G.M.: Dynamics of entanglement in one-dimensional spin systems. Phys. Rev. A **69**, 022304 (2004); Aharonov, D.: Quantum to classical phase transitions in noisy quantum computer. Phys. Rev. A **62**, 062311 (2000); Osborne, T.J., Nielsen, M.A.: Entanglement in a simple quantum phase transition. Phys. Rev. A **66**, 032110 (2002); Osterloh, A., Amico, L., Falci, G., Fazio, R.: Scaling of entanglement close to a quantum phase transition. Nature **416**, 608–610 (2002)
3. Vidal, G., Latorre, J.I., Rico, E., Kitaev, A.: Entanglement in quantum critical phenomena. Phys. Rev. Lett. **90**, 227902 (2003)
4. Jin, B.Q., Korepin, V.E.: Entanglement, Toeplitz determinants and Fisher-Hartwig conjecture. J. Stat. Phys. **116**, 79–95 (2004)
5. Korepin, V.E.: Universality of entropy scaling in 1D gap-less models. Phys. Rev. Lett. **92**, 096402 (2004)
6. Calabrese, P., Cardy, J.: Entanglement Entropy and Quantum Field Theory. J. Stat. Mech. Theor. Exp. P06002 (2004)
7. Fisher, M.E., Hartwig, R.E.: Toeplitz determinants, some applications, theorems and conjectures. Adv. Chem. Phys. **15**, 333–353 (1968)
8. Basor, E.L., Ehrhardt, T.: Asymptotic formulas for the determinants of symmetric Toeplitz plus Hankel matrices. In: *Toeplitz matrices and singular integral equations (Pobershau, 2001), Oper. Theory Adv. Appl.* **135**, Basel: Birkhäuser 2002, pp. 61–90
9. Forrester, P.J., Frankel, N.E.: Applications and generalizations of Fisher-Hartwig asymptotics. J. Math. Phys. **45**, 2003–2028 (2004)
10. Lieb, E., Schultz, T., Mattis, D.: Two soluble models of an antiferromagnetic chain. Ann. Phys. **16**, 407–466 (1961)
11. Barouch, E., McCoy, M.: Statistical mechanics of the XY model II. Spin-correlation functions. Phys. Rev. A **3**, 786–804 (1971)
12. Basor, E.L., Morrison, K.E.: The Fisher-Hartwig conjecture and Toeplitz eigenvalues. Lin. Alg. App. **202**, 129–142 (2004)
13. Heine, H.: *Kugelfunktionen*, Berlin, 1878 and 1881. Reprinted by Würzburg: Physica Verlag, 1961
14. Szegő, G.: *Orthogonal Polynomials*. New York: AMS, 1959
15. Szegő, G.: *On certain hermitian forms associated with the Fourier series of a positive function*. Lund: Festkrift Marcel Riesz, 1952, pp. 222–238
16. Basor, E.L.: Asymptotic formulas for Toeplitz determinants. Trans. Amer. Math. Soc. **239**, 33–65 (1978)
17. Böttcher, A., Silbermann, B.: Toeplitz operators and determinants generated by symbols with one Fisher-Hartwig singularity. Math. Nachr. **127**, 95–124 (1986)
18. Böttcher, A., Silbermann, B.: *Analysis of Toeplitz Operators*. Berlin: Springer-Verlag, 1990
19. Forrester, P.J., Witte, N.S.: Discrete Painlevé equations, orthogonal polynomial on the unit circle and N-recurrences for averages over U(N) — P_{VI} τ-functions. http://arxiv.org/abs/math-ph/0308036, 2003
20. Forrester, P.J., Witte, N.S.: Application of the τ-function theory of Painlevé equations to random matrices: P_{VI}, the JUE, CyUE, cJUE and scaled limits. Nagoya Math. J. **174**, 29–114 (2004)
21. Weyl, H.: *The Classical Groups*. Princeton, NJ: Princeton University Press, 1946