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FISHER HARTWIG DETERMINANTS, CONFORMAL FIELD THEORY AND UNIVERSALITY IN GENERALISED XX MODELS

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ABSTRACT. We discuss certain quadratic models of spinless fermions on a 1D lattice, and their corresponding spin chains. These were studied by Keating and Mezzadri in the context of their relation to the Haar measures of the classical compact groups. We show how these models correspond to translation invariant models on an infinite or semi-infinite chain, which in the simplest case reduce to the familiar XX model. We give physical context to mathematical results for the entanglement entropy, and calculate the spin-spin correlation functions using the Fisher-Hartwig conjecture. These calculations rigorously demonstrate universality in classes of these models. We show that these are in agreement with field theoretical and renormalization group arguments that we provide.

1. INTRODUCTION

Universality is a central concept in statistical physics, and in many contexts modern understanding is based on renormalization group (RG) arguments. Physical systems exhibit universal behaviour when they share an effective theory. This effective theory is reached by systematically removing irrelevant degrees of freedom, usually in the context of a flow of parameters in the space of Hamiltonians of quantum field theories. In this area rigorous arguments are scarce. In this paper, for a class of 1D spin systems which can be related to certain free fermion models, we present rigorously derived physical properties. We see that they correspond exactly to those expected from the analysis of the effective theory. In particular, the systems we are interested in are critical – the effective description is generically scale invariant and in fact has conformal symmetry, so can be described by a conformal field theory (CFT). We give the CFT description of our class of models, which takes the form of a direct sum of non-interacting massless fermions.

Ground states of 1D critical models are characterised by algebraic decay of correlations and recently much interest has been shown in their entanglement structure. In [2, 3] it is seen that the von Neumann entanglement entropy of a subsystem of linear size N diverges logarithmically as

$$S(N) = |A| \frac{c}{6} \log_2 N + O(1). \quad (1)$$

Here $|A|$ is the size of the boundary of the subsystem, and c is the central charge of the corresponding CFT. A similar formula for the XX model was observed numerically in [4] and then, including the extension to the Rényi entropies, was proved in [5] using the Fisher-Hartwig conjecture. This was then substantially generalised in [6, 7] to wider classes of models susceptible to random matrix theory techniques. We review these results and see that (1), including the correction up to $o(1)$, as well as the expected spin correlations are verified exactly in these models.

Our main results are the following:

- We give a physical interpretation of the large class of mathematical models studied in [6].
- This allows us to understand the universal entanglement entropy scaling found rigorously in that paper, and to predict the universal leading asymptotic scaling of equal time spin-spin correlation functions, as well as the oscillatory prefactors.
- Where calculation is possible, we show that this prediction is indeed correct and find the coefficients of the leading terms using proven cases of the generalized Fisher-Hartwig conjecture. This corrects part of a similar calculation in [8].

The paper is organised as follows: in Section 2 we introduce the lattice model that is the framework for our rigorous calculations. We then give a generic diagonal form of the Hamiltonian for the cases we will consider and analyse this diagonal form using standard quantum field theoretic methods. We aim to keep the discussion self contained so review some details. We postulate the effective theory, and its dependence on microscopic parameters, and show that this is consistent using RG arguments. From this conformally invariant effective theory we can read off the central charge and give an argument, via bosonization, for the expected leading order behaviour of the correlation functions.

We then review the Fisher-Hartwig conjecture, proved in [9], which is essential for the rigorous analysis that follows. First in Section 5 we study the translation invariant (TI) chain, reviewing previous results in context and deriving the corrected correlators. Then in Section 6 we introduce two further classes of lattice model which permit some further analysis and explain their physical relevance as well as the connection to the work of Keating and Mezzadri [6, 7].

We note that the bulk universality classes of our models, parameterised by a finite number of Fermi momenta and velocities, are identified in [10] from the perspective of quantum integrable systems. The connection between integrals over classical compact groups and boundary conditions is also demonstrated in [11]. We also remark that an analysis of fermionic dispersion relations with four Fermi points was made in [12] and the entropy scaling with the number of these points was observed numerically in [13]. Similar conclusions about the utility of identifying the discontinuities of the Fisher-Hartwig symbol with Fermi points are reached in [14]. Finally, there is a complementary approach to identifying scaling dimensions and the central charge of the low energy

theory via finite size scaling [15, 16, 10] – we will not pursue this, but note that it would also be accessible from the exact solution of our models.

2. THE QUADRATIC FERMION MODEL – DEFINITIONS

We will consider the following model for free fermions on a lattice:

$$H = \sum_{j,k=0}^{M-1} b_j^\dagger A_{jk} b_k - 2h \sum_{j=0}^{M-1} b_j^\dagger b_j; \quad \text{tr} A = 0 \quad (2)$$

which is equivalent, under Jordan-Wigner transformation, to the spin model

$$H = -\frac{1}{2} \sum_{0 \leq j < k \leq M-1} A_{jk} (\sigma_j^x \sigma_k^x + \sigma_j^y \sigma_k^y) \left(\prod_{l=j+1}^{k-1} \sigma_l^z \right) - h \sum_{j=0}^{M-1} \sigma_j^z. \quad (3)$$

The b_i are the usual complex fermionic operators, and the σ^i are the Pauli matrices. To fix conventions, the Jordan-Wigner transformation is given by:

$$\begin{aligned} b_i^\dagger &= \frac{1}{2} (\sigma_i^x + i\sigma_i^y) \left(\prod_{l=1}^{i-1} \sigma_l^z \right); \\ b_i &= \frac{1}{2} (\sigma_i^x - i\sigma_i^y) \left(\prod_{l=1}^{i-1} \sigma_l^z \right); \\ b_i^\dagger b_i &= \frac{1 + \sigma_i^z}{2}. \end{aligned} \quad (4)$$

The matrix A is Hermitian and traceless, and without loss of generality we take it to contain only real parameters. We take periodic boundary conditions (PBCs) for the fermions¹, i.e. $b_M = b_0$. As with any quadratic fermion model, we can diagonalise by the methods of Lieb, Schulz and Mattis [17] – although we will see that after specialising to our cases of interest that a Fourier transform suffices. We will eventually take the thermodynamic limit $M \rightarrow \infty$. This system has a $U(1)$ symmetry. For the spin model this corresponds to rotations in the XY plane: the action on the spin operators is conjugation by $R(\alpha) = \prod_j \exp(i\frac{\alpha}{2}\sigma_z)$. For the fermions this is a uniform phase shift $b_j \rightarrow \exp(i\alpha)b_j$. In order to express the entanglement entropy and the correlation functions of the model in a way amenable to random matrix theory techniques we restrict the form of the matrices A – the precise forms are given in Table 1. Essentially we restrict to either TI chains, or to half chains where the TI bulk is broken by a boundary. In all cases we obtain, in the thermodynamic limit, a Hamiltonian of the form:

$$H = \int_{-\pi}^{\pi} dq \Lambda(q) \psi^\dagger(q) \psi(q) \quad (5)$$

where $\psi(q)$ is a fermionic annihilation operator – the Fourier transform of the lattice fermion annihilation operator ψ_j – and the energy is zero at the Fermi surface. As the system is non-interacting we have an exact single particle ‘Fermi sea’ picture for our

¹We note that this is inequivalent to periodic boundary conditions for the spins, but not drastically. Differences are of order $1/M$ as explained in [17], so in the thermodynamic limit we are calculating properties of the periodic spin chain.

eigenstates, however $\Lambda(q)$ may be very general: we can construct any continuous periodic function that is symmetric in q . (More precisely, an arbitrarily good approximation at the cost of longer distance interactions.)

An important distinction should be made between two regions in parameter space – the gapped region where $|\Lambda(q)|$ is strictly greater than zero and we have a ground state empty of particles, and a gapless region where $\Lambda(q)$ has zeroes. The gapless region is critical (it is at a quantum phase transition for an anisotropic variant of the model (2) – a generalised XY model – defined in [6]) and is characterised by algebraic decay of correlation functions, as well as logarithmic scaling of entanglement entropy. We will focus our discussion on this gapless region.

3. PHYSICAL PICTURE

We will continue schematically, working with the quadratic Hamiltonian (5). The strategy is to isolate the low energy form of the Hamiltonian by linearisation and to see that this is consistent. More detailed accounts are given in, for example, [18]; although much of the literature focuses on the nearest neighbour XX model: $A_{jk} = \delta_1(j-k) + \delta_{-1}(j-k) + U\delta_0(j-k)$, where $\Lambda(q) = \cos(q) + U$. The aim of this section is to see how the rigorous results for the entropy and the correlation functions given later can be argued from a physical perspective. In particular, for the ground state of the system, we are interested in computing the leading asymptotic dependence of spin-spin correlation functions such as $\langle \sigma^x(N)\sigma^x(0) \rangle$ as $N \rightarrow \infty$, as well as identifying the central charge which controls the asymptotics of the entanglement entropy through (1).

3.1. Linearisation and irrelevance of local nonlinear corrections: We have an oscillatory dispersion which we may linearise about its zeroes (the 1D Fermi surface) to get:

$$\begin{aligned} H &\simeq \sum_{i=1}^{2R} v_i \int_{-\delta_i}^{\delta_i} dq_i q_i \psi_i^\dagger(q_i) \psi_i(q_i) \\ &= \sum_{i=1}^R |v_i| \int_{-\delta_i}^{\delta_i} dq_i q_i (\psi_{i+}^\dagger(q_i) \psi_{i+}(q_i) - \psi_{i-}^\dagger(q_i) \psi_{i-}(q_i)) \end{aligned} \quad (6)$$

$$\begin{aligned} S(\Delta) &= \sum_{i=1}^R \int_{-\infty}^{\infty} d\omega \int_{-\delta_i}^{\delta_i} dq_i (-i\omega + |v_i|q_i) \times \\ &\quad (\psi_{i+}^\dagger(\omega, q_i) \psi_{i+}(\omega, q_i) - \psi_{i-}^\dagger(\omega, q_i) \psi_{i-}(\omega, q_i)) \end{aligned} \quad (7)$$

where q_i is a coordinate around the i th point of the Fermi surface, which we will label θ_i , and $v_i = \frac{\partial}{\partial q} \Lambda(q)|_{\theta_i}$ is the local Fermi velocity. R is the number of zeroes between $(0, \pi)$. For the RG analysis, we consider the action $S(\Delta)$, where ω is the Matsubara frequency, and where we put a uniform cutoff in the energy, Δ , which locally restricts the momenta to an interval of width $2\delta_i = 2\Delta/|v_i|$. The action with unbounded ω would appear in path integral calculations of zero temperature correlation functions. As $\Lambda(q)$ is symmetric, we have pairs of points with equal and opposite velocity as illustrated in Figure 1; we label these ψ_{i+}, ψ_{i-} for right and left movers respectively. The approximate ('low-energy') equality is because we are losing all details of the band curvature, and

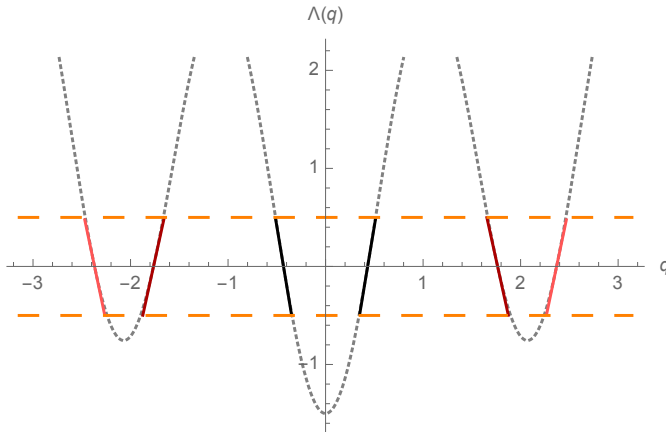


FIGURE 1. Example of a linearised dispersion with energy cutoff.

also, if we allow high energy excitation of the fields, we are overcounting degrees of freedom.

We note that it is possible that the linearisation fails – this happens at points where both Λ and a finite number of its derivatives vanish. We address this in detail in Appendix A, but for now we will limit our discussion to the generic case $\Lambda'(\theta_i) \neq 0$.

Corrections to the linearised Hamiltonian to account for the approximation do not affect the low energy physics in which we are interested. Following the discussion in [19, 20], we first note that the action (7) is a fixed point under the following RG transformation: we reduce the cutoff to δ_i/s , for some $s > 1$ to reach a new action $S'(\Delta/s)$; then we rescale $(q, \omega, \psi_{i\pm}) \rightarrow (sq, s\omega, s^{-3/2}\psi_{i\pm})$ to restore the cutoff $S'(\Delta)$. For the linearised action we indeed have $S' = S$. The idea now is to see that our original action, before linearisation but with an energy cutoff, is in the basin of attraction of this fixed point. To do this we consider diagonal perturbations of the form:

$$\delta S = \sum_{i,\pm} \int_{-\infty}^{\infty} d\omega \int_{-\delta_i}^{\delta_i} dq_i \psi_{i\pm}^\dagger(\omega, q_i) \mu(\omega, q_i) \psi_{i\pm}(\omega, q_i). \quad (8)$$

Expanding $\mu(\omega, q) = \sum_{j,k=0}^{\infty} \mu_{jk} (i\omega)^j q^k$, we see that μ_{jk} scales as s^{1-j-k} . Hence as we reduce our cutoff, when $j+k \geq 1$ all such perturbations are irrelevant, the coefficient goes to zero. We are left with μ_{01} and μ_{10} which do not change under such a rescaling – they are called marginal – and their precise value is important. They correspond to the value of the Fermi velocity, which we fixed from our full Hamiltonian, and we see that this value does not change under the rescaling so does characterise different fixed points. Hence we have a different fixed point for each set of Fermi velocities, and we remark that this difference will manifest itself in the correlation functions. Finally the operator μ_{00} is transformed to $s\mu_{00}$, so grows as we reduce our cutoff – it is relevant and can change which effective theory we need. This is a change in chemical potential, so naturally affects which effective theory we're looking at – by moving the local² zero of energy we can remove the degree of freedom entirely by going past a local minimum or maximum,

²We are looking at each mode separately so can artificially rescale the chemical potential in each one.

or less drastically it will change the local Fermi velocity. As we have expanded around the true zeroes of our dispersion, we do not need need to consider perturbations of this type.

The conclusion to take from this discussion is that the only important information from the full nonlinear Hamiltonian is the number of crossings, the Fermi momentum, θ_i , at each crossing and the Fermi velocity at each crossing. All of the curvature is irrelevant as we look at low energies. We need the $\{\theta_i\}$ to ensure the correct charge density and relative phases between the different Fermi points. We then have universality classes of Hamiltonians which share these parameters.

We remark that we should work always with some cutoff so as not to allow overcounting of modes at high energy q values, and we need not include couplings between the different modes as our full Hamiltonian is diagonal in q . We have neglected quadratic perturbations of the type $\psi^\dagger\psi^\dagger, \psi\psi$ which break the U(1) fermion number symmetry. Allowing such terms corresponds to considering anisotropic spin chains or superconducting fermionic chains – these have a gap in the spectrum. Rigorous techniques are used in [21, 22] to calculate the leading order entanglement entropy for these systems, which is a constant. Finally we note that the analysis of interacting perturbations leads, as one would expect, to a much broader class of models with different physics to that described here – however the rigorous techniques used below do not apply directly to such models so we will not discuss them further.

3.2. The central charge and entanglement entropy. Based on the above discussion, we fix the effective Hamiltonian as (6). To facilitate the CFT method, we note that:

$$H_{CFT} = \sum_{i=1}^R |v_i| \int_{-\infty}^{\infty} dq q (\psi_{i+}^\dagger(q)\psi_{i+}(q) - \psi_{i-}^\dagger(q)\psi_{i-}(q)) \quad (9)$$

is clearly in the same low energy universality class (we have just extended the high energy cutoff) and should have the same long distance physical properties. The advantage is that now we have a real space continuum conformal field theory, corresponding to the continuum limit³ of our chain, and can use textbook methods. We maintain a fixed density of fermions in our ground state.

We should pay attention to the boundary conditions of the chain that led to (5), and carry them over to (9). We note that we have a direct sum of $2R$ chiral fermions, each with a central charge of $1/2$ [23]. In total the model has $c = R$. Hence on the basis of [2] we expect, for a system with PBCs, the entanglement entropy of any block of length N to scale as:

$$S(N) = \frac{R}{3} \log_2 N + \kappa_\Lambda + o(1). \quad (10)$$

For a system with a boundary, irrespective of the boundary condition, we expect:

$$S(N) = \frac{R}{6} \log_2 2N + \frac{1}{2}\kappa_\Lambda + (\log_2(g)) + o(1), \quad (11)$$

³Roughly, after defining a lattice spacing a , let $\psi(x) = \lim_{a \rightarrow 0} \frac{1}{\sqrt{a}} b_{x/a}$. In our microscopic models factors of a are suppressed throughout. Care should be taken in the presence of a boundary, as the lattice may need to be shifted before this identification.

where we consider blocks of length N starting at the boundary. (This choice of block is motivated by the random matrix theory calculations below - we note that [24] discusses blocks away from the boundary in that language.)

To interpret these formulae, first we see that the constant κ_Λ is not universal, but agrees for systems with different boundary conditions sharing a (proportional) bulk dispersion relation $\Lambda(q)$. Going between (10) and (11) there is a factor of two separating the ‘bulk terms’ originating in the fact that our block from site 1 to site N has gone from having two bulk-facing edges to one (this is the $|\mathcal{A}|$ in (1)). The scaling by $2N$ inside the logarithm is a result of a method of images argument given in [2] - broadly: studying N sites with a boundary can be mapped into $2N + 1$ sites without a boundary, we will see this in more detail below. We include the bracketed $\log_2(g)$ for completeness. This is the boundary entropy introduced in [25], where it is also shown that for free fermions $g = 1$ - hence this term will be zero for our systems.

3.3. Spin correlation functions. We can use the effective theory (9) to find the asymptotics of the spin-spin correlation functions by bosonization methods [18, 26, 27, 28, 29, 30]. The aim of this section is to motivate an expected leading asymptotic term, rather than make an explicit first principles derivation. This method was originally applied to the XX model case in [31].

We defer to the literature for detailed definitions and discussion, for our purposes we need the bosonization formula⁴ [29]:

$$\psi_i(x) \simeq \exp i\Phi_i(x) \left(A_{i+} \exp i(\vartheta_i(x) + \theta_i x) + A_{i-} \exp -i(\vartheta_i(x) + \theta_i x) \right); \quad (12)$$

where Φ_i , ϑ_i are canonical free, massless, bosonic fields which bosonize each of the R complex fermions ψ_i . For each fermion, θ_i is the Fermi momentum and the A_i are constants. Again, we have a ‘low energy’ equality, i.e. this is the dominant part of the operator when calculating long distance correlation functions. Physically $\exp(i\Phi_i)$ creates a unit charge excitation, while $\pm(\theta_i + \partial_x \vartheta_i)/\pi$ is the relevant charge density $\partial Q_i/\partial x$ - the expression above is thus analogous to the Jordan-Wigner transformation (4) for these continuum fields. For convenience we will also define the left and right moving boson fields:

$$\varphi_{i\pm} = \Phi_i \pm \vartheta_i. \quad (13)$$

Now we argue on general grounds that the spin operator must take the form:

$$\sigma^+(x) = (-1)^{bx} \sum_{\tilde{\beta}} C_{\tilde{\beta}} \exp i \left(\sum_{j=1}^R \tilde{\beta}_j (\varphi_{j+}(x) + Q_j(x)) + \tilde{\beta}_{2R+1-j} (\varphi_{j-}(x) - Q_j(x)) \right) \quad (14)$$

where we consider all strings $\tilde{\beta}_j = \pm 1/2$ such that $\sum_j \tilde{\beta}_j = 1$. This equality is exact in the CFT and thus valid for long distance correlation functions in our lattice model. $Q_j(x)$ is the cumulative charge to the left of x for the j th fermion and $C_{\tilde{\beta}}$ are constants.

⁴All expressions are subject to appropriate normal ordering. We suppress the Klein factors which fix the correct mutual anticommutation relations between the fermionic operators as they do not play a role in our calculations.

The Néel order factor $(-1)^{bx}$ for b either 0 or 1 is included for consistency with the lattice spin operator and the Jordan-Wigner transformation⁵.

First, we expect by analogy with the single complex fermion XX model case [18] that we will deal with vertex operators – exponentials of our left and right moving bosonic fields. Vertex operators give local expressions for certain non-local operators in the fermionic degrees of freedom, and the continuum limit of the spin operator must be among these. Such operators take the form $V_{\alpha,\gamma} := \exp i \sum_i (\alpha_i \varphi_{i+} + \gamma_i \varphi_{i-})$. In order for $V_{\alpha,\gamma}$ to be well defined, we must have that $\alpha_i - \gamma_i \in \mathbb{Z}$ and $\alpha_i + \gamma_i \in \mathbb{Z}$. The correlation functions of such operators are easily derived, giving:

$$\langle V_{\alpha,\gamma}(x) V_{\alpha',\gamma'}(0) \rangle = \frac{\delta_{\alpha+\alpha',0} \delta_{\gamma+\gamma',0}}{x^{\frac{1}{2} \sum (\alpha_i^2 + \gamma_i^2)}}. \quad (15)$$

Clearly, then, the dominant vertex operators in the large x limit have either $\alpha_i = \gamma_i = 0$ or $\alpha_i, \gamma_i = \pm 1/2$. The lattice spin operator satisfies nontrivial commutation relations which must carry over to the continuum in each fermion sector, hence we can exclude the first case. This gives us that, to leading order, all $\tilde{\beta}_j = \pm 1/2$ in the spin operator above. The condition $\sum_j \tilde{\beta}_j = 1$ is due to the constraint that the spin operator creates a single particle, or equivalently that it transforms under the U(1) rotation symmetry in the same way as a single fermion. The condition enforces this by noting that for $\psi_i \rightarrow \exp(i\alpha)\psi_i$, we have $\Phi_i \rightarrow \Phi_i + \alpha$ and $\vartheta_i \rightarrow \vartheta_i$. Finally, every appearance of ϑ_i is through integrating the charge density and so should be accompanied by $Q_i(x)$ – the form of (14) ensures this. The bosonization method cannot give the coefficients so we assume that they are nonzero.

Then, using (14) and (15), we can give the expected form of the asymptotics for our lattice spin-spin correlators as:

$$\langle \sigma^+(N) \sigma^-(0) \rangle \sim (-1)^{bN} N^{-R/2} \sum_{\tilde{\beta}} |C_{\tilde{\beta}}|^2 \exp i \left(\sum_{j=1}^R (\tilde{\beta}_j - \tilde{\beta}_{2R+1-j}) Q_j(N) \right) \quad (16)$$

$$\sim (-1)^{bN} N^{-R/2} \sum_{\tilde{\beta}} |C_{\tilde{\beta}}|^2 \exp i N \left(\sum_{j=1}^R (\tilde{\beta}_j - \tilde{\beta}_{2R+1-j}) \theta_j \right). \quad (17)$$

This gives us $\Re \langle \sigma^+(N) \sigma^-(0) \rangle / 2 = \langle \sigma^x(N) \sigma^x(0) \rangle = \langle \sigma^y(N) \sigma^y(0) \rangle$ by the isotropy of the Hamiltonian (and that there can be no spontaneous breaking of this continuous rotation symmetry in the ground state by the result of [32]). We note that for every allowed string $\{\beta_j\}$ in the sum there is a corresponding string $\{\beta'_j\}$ with the opposite angle in the exponential – if we assume $|C_{\beta}| = |C_{\beta'}|$ then the right hand side of (17) is real. This property is verified in the exact calculation below. Finally we note that physically this operator is a sum of operators, each of which create and annihilate charges (always with an overall +1) and create particle-hole excitations. When R is odd we have some non-oscillating terms which contain only the charged Φ_i fields.

⁵In any particular lattice model this term is removable by a redefinition of the on-site spin basis. Starting from a fixed basis it should in principle be derived from treating boundary conditions and branch cuts in the field theory carefully, however we will not pursue this here.

For completeness, we have from (4) that σ_z on the lattice is, up to a constant shift, the fermion number operator. Hence the analogous continuum operator is $\sigma^z(x) \sim \sum_i \partial_x \vartheta_i$ from which we quickly see that $\langle \sigma^z(x) \sigma^z(0) \rangle \sim x^{-2}$.

We implicitly assumed above that we were working with periodic spatial boundary conditions. We expect the same asymptotic correlations in the presence of a boundary, via a method of images argument as in [23]. Note that in the presence of a boundary we must have a conformally invariant boundary condition, for example $\psi(x) = 0$ or $\psi(x) = \infty$, which respectively correspond to the ‘ordinary’ and ‘extraordinary’ transitions discussed later.

4. ASYMPTOTICS FOR DETERMINANTS OF TOEPLITZ MATRICES

We use this section to recall some results on the generalised Fisher Hartwig conjecture for asymptotics of certain Toeplitz matrices, and related Toeplitz+Hankel matrices. Theorem 1 below is essential to our analysis of the lattice model. It is this form of the theorem that allows us to correct⁶ the derivation of the $\sigma^{x,y}$ correlators in [8].

We note first that a Toeplitz matrix has the form $M_{jk} = M_{j-k}$ and a Hankel matrix has the form $M_{jk} = M_{j+k}$. We will make use of these results in the following section to compute both the entanglement entropy and the correlators. Originally conjectured by Basor and Tracy [33], Dieft, Its and Kravsovsky [9] proved the Fisher Hartwig conjecture for the situations we will now describe. We note that these determinants are often equivalent to integrals over random matrix distributions, as discussed in [6, 11].

We wish to compute the determinants of matrices with Toeplitz structure, with entries given by the Fourier coefficients of a function $f(z)$ called the symbol (or generating function);

$$D_N(f(z)) = \det(f_{j-k})_{j,k=0}^{N-1}, \quad f_j = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) e^{-ij\theta} d\theta. \quad (18)$$

We will be interested only in symbols whose m singularities are jump discontinuities, thus $f(z)$ can be written in the following form on the unit circle:

$$f(z) = e^{V(z)} z^{\sum_{j=1}^m \beta_j} \prod_{j=1}^m g_{z_j, \beta_j}(z) z_j^{-\beta_j} \quad z = e^{i\theta}, \quad \theta \in [0, 2\pi), \quad (19)$$

where $z_j = e^{i\theta_j}$, $\beta_j \in \mathbb{C}$ for $j = 1, \dots, m$, $0 = \theta_1 < \dots < \theta_m < 2\pi$,

$$g_{z_r, \beta_r}(z) = \begin{cases} e^{i\pi\beta_r}, & 0 \leq \arg z < \theta_r, \\ e^{-i\pi\beta_r}, & \theta_r \leq \arg z < 2\pi, \end{cases} \quad (20)$$

and the function $V(e^{i\theta})$ satisfies some smoothness conditions, explained in [9].

In general there can be multiple ways of writing this decomposition, each giving different representations of $f(z)$. We will use the nomenclature of [9] and define these other representations relative to an initial one in the following way. Start with one such

⁶In that paper the representation of the symbol did not satisfy the relevant hypotheses, leading to a divergent term in the coefficient.

representation, in terms of a set $\{\beta_j\}$, and then modify the right hand side of (19) by $\tilde{\beta}_j = \beta_j + n_j$, subject to the constraint

$$\sum_{j=1}^m n_j = 0. \quad (21)$$

This is called a *Fisher-Hartwig representation* $f(z; n_1, \dots, n_m)$, relative to the initial $f(z; 0, \dots, 0)$. Importantly we note that our initial symbol is given by:

$$f(z) = \prod_{j=1}^m z_j^{n_j} f(z; n_1, \dots, n_m). \quad (22)$$

To find the leading term of the asymptotics of the determinant we need the subset of these representations which minimise $\sum_{j=1}^m \tilde{\beta}_j^2$. For symbols that are even and with image $\{+\exp(i\phi), -\exp(i\phi)\}$, for some $\phi \in \mathbb{R}$, (featuring prominently below) we find that these minimal representations have $\tilde{\beta}_j = \pm \frac{1}{2}$ and $n_j \in \{1, -1, 0\}$.

We now quote the following theorem, after simplifications which occur in our cases of interest. In particular, our symbols will always have $V(z) = \text{constant}$, so the only Fourier coefficient is V_0 .

Theorem 1 (Deift, Its, Krasovsky 2011). *As the matrix dimension, N , goes to infinity:*

$$\det(f_{j-k})_{j,k=0}^{N-1} = \sum_{\text{Reps: } \{n_j\}} \left(\prod_{j=1}^m z_j^{n_j} \right)^N \mathcal{R}(f(z; \{n_j\}))(1 + o(1)). \quad (23)$$

Where:

$$\begin{aligned} \mathcal{R}(f(z; \{n_j\})) &= N^{-\sum_{j=1}^m \tilde{\beta}_j^2} \exp(NV_0) \prod_{1 \leq j < k \leq m} |z_j - z_k|^{2\tilde{\beta}_j \tilde{\beta}_k} \prod_{j=1}^m G(1 + \tilde{\beta}_j) G(1 - \tilde{\beta}_j) \\ \tilde{\beta}_j &= \beta_j + n_j. \end{aligned}$$

We emphasise that V_0 is unaltered when passing between representations. $G(z)$ is the Barnes G-function [34, §5.17]. For imaginary V_0 , the dominant behaviour of this determinant is an algebraic decay. We also note that, using the methods of [9], one can write Hankel determinants and Toeplitz+Hankel determinants in terms of purely Toeplitz determinants which can then be put into the full version of the above theorem – we return to this point below.

5. THE TRANSLATION INVARIANT CHAIN

We will specialise (2) to three models which encompass all the models labelled by the classical compact groups introduced in [6] - the first of which is the translation invariant case or $U(N)$ model. The translation symmetry of the chain corresponds to the translation symmetry of the Haar measure on $U(N)$, and we will see later that the entanglement entropy and correlation functions are given by Toeplitz determinants which can be written as integrals over $U(N)$.

In the Hamiltonian (2) we separate for clarity of interpretation the kinetic term with hopping matrix A from the term proportional to h which acts as a chemical potential

for the fermions, or as an external field for the spins. Below, though, we will summarise the whole Hamiltonian by $\bar{A} = A - 2h\mathbb{I}$. Let: $\bar{A}_{jk} = a(j-k)$ where a is an even function on $\mathbb{Z}/M\mathbb{Z}$. Let M be odd, even M is very similar with formulae given in [6]. Defining

$$\delta_i(j) = \begin{cases} 1 & i = j \pmod{M} \\ 0 & i \neq j \pmod{M} \end{cases} \quad (24)$$

we have:

$$a(j) = \alpha_0 \delta_0(j) + \sum_{i=1}^{(M-1)/2} \alpha_i (\delta_i(j) + \delta_{-i}(j)). \quad (25)$$

We can diagonalise the Hamiltonian by Fourier transform to get:

$$H = \sum_q \Lambda_q b_q^\dagger b_q; \quad \text{for} \quad \Lambda_q = \alpha_0 + 2 \sum_{j=1}^{(M-1)/2} \alpha_j \cos(jq). \quad (26)$$

Now taking the limit $M \rightarrow \infty$ we get $\Lambda(q) = \alpha_0 + 2 \sum_{j=1}^{\infty} \alpha_j \cos(jq)$ where α_j decays sufficiently fast that this series converges. This decay is physically natural as α_j is a coupling of sites j lattice spacings apart and so implies that our Hamiltonian is local in both the fermion and spin operators. In this limit we have also, after redefining particle/hole excitations relative to the Fermi level:

$$\psi^\dagger(q) := \begin{cases} b_q^\dagger, & \Lambda(q) > 0 \\ b_q, & \Lambda(q) < 0, \end{cases} \quad (27)$$

the Hamiltonian:

$$H = \int_{-\pi}^{\pi} dq |\Lambda(q)| \psi^\dagger(q) \psi(q). \quad (28)$$

We see from the results of [6, 8] that for all models discussed in this paper, the asymptotics of both the entanglement entropy and certain spin-spin correlation functions may be related to determinants of Toeplitz matrices. These matrices are generated by the symbol:

$$f(\theta) = \frac{\Lambda(\theta)}{|\Lambda(\theta)|} = \text{sign}(\Lambda(\theta)). \quad (29)$$

This is an even function with jump discontinuities taking values ± 1 . $\Lambda(\theta)$ is the $M \rightarrow \infty$ limit of the dispersion relation. We remind the reader that R is the number of zeroes of Λ in $(0, \pi)$ and θ_i are the points where $\Lambda(\theta_i) = 0$ (and the first nonzero derivative of Λ is odd). The number of jump discontinuities of our symbol is given by $m = 2R$. We shift the Brillouin zone to $[0, 2\pi)$ in order to get the correct branches in Theorem 1. We note that the fermionic correlators, and hence the σ_z two point functions, are simply related to the Fourier coefficients themselves.

5.1. Entanglement entropy. We begin by stating the results from the entanglement computation in [6]. Thanks to the connection between the reduced density matrix and ground state correlation functions for one dimensional free fermions noted in [35, 4], we can relate the entanglement entropy of such a system to the ‘correlation matrix’ - the eigenvalues of which are simply related to the fermionic correlations *within* the

subsystem. More precisely, the entanglement entropy of a subchain of length N can be shown to be given by the contour integral:

$$S(N) = \lim_{\epsilon \rightarrow 0^+} \lim_{\delta \rightarrow 0^+} \frac{1}{2\pi i} \oint_{c(\epsilon, \delta)} e(1 + \epsilon, \lambda) \frac{d \ln D_N[f](\lambda)}{d\lambda} d\lambda. \quad (30)$$

This is a result of the residue theorem, as this integral sums the bipartite entanglement function:

$$e(x, \nu) = -\frac{x + \nu}{2} \log_2 \left(\frac{x + \nu}{2} \right) - \frac{x - \nu}{2} \log_2 \left(\frac{x - \nu}{2} \right) \quad (31)$$

at each of the eigenvalues of the correlation matrix - which are themselves zeroes of the characteristic polynomial:

$$D_N[f](\lambda) = \det(\lambda \mathbb{I} - \mathcal{M}_N[f]). \quad (32)$$

Physics constrains the eigenvalues to lie in $[-1, 1]$, hence we take $c(\epsilon, \delta)$ to be any curve enclosing the interval $[-1, 1]$ and approaching it as $\epsilon, \delta \rightarrow 0$. \mathcal{M}_N is the Toeplitz matrix generated by (29). Now, $D_N[f](\lambda)$ is a Toeplitz determinant and has leading asymptotics given by the relevant extended form of Theorem 1 given in [6].

By analysing the derivatives of $\ln D_N[f](\lambda)$, and then doing the resulting contour integrals, Keating and Mezzadri showed the following:

$$S(N) = \frac{R}{3} \log N + \frac{R}{3} (K / \ln 2 - 6I_3) + o(1). \quad (33)$$

Where:

$$K = 1 + \gamma_E + \frac{1}{R} \left(\sum_{r=1}^R \ln |1 - e^{i2\theta_r}| - 2 \sum_{1 \leq r < s \leq R} (-1)^{(r+s)} \ln \left| \frac{1 - e^{i(\theta_r - \theta_s)}}{1 - e^{i(\theta_r + \theta_s)}} \right| \right), \quad (34)$$

$\gamma_E \simeq 0.58$ is the Euler-Mascheroni constant, and $I_3 \simeq 0.022$ is a definite integral evaluated in [5]. We can see that (33) exactly verifies the CFT prediction (10). We note in (34) the dependence of the constant on fine details of the dispersion relation - i.e. the values of $\{\theta_i\}$.

5.2. Correlation functions. We will now compute the ground state σ^x and σ^y correlators using the Fisher-Hartwig conjecture. We also review the correct calculation given in [8] for the the σ^z -string correlator. We note that the correlators for the XX model were evaluated using the Fisher-Hartwig conjecture in [30] - our results agree when specialised to this case.

The general method in this section is given in [17]. To summarise: we can rewrite, say, a two point spin-spin correlation function by the Jordan-Wigner transform as a fermionic $O(N)$ -point function. As we have a quadratic theory in the fermions, we can use Wick's theorem to expand this as a determinant of a matrix of fermionic correlators. We know these fermionic correlators and so may then use the Fisher-Hartwig conjecture and related techniques to find the asymptotics of the spin-spin correlation functions. Note that all three correlators below may be shifted to anywhere on the chain by translation invariance.

5.2.1. $\left\langle \prod_{i=0}^{N-1} \sigma_i^z \right\rangle$. The expectation value of the σ^z -string operator in the ground state is given by:

$$\left\langle \prod_{i=0}^{N-1} \sigma_i^z \right\rangle = \det \mathcal{M}_N, \quad (35)$$

where the matrix \mathcal{M}_N is generated by (29). We use this for illustration as it is the simplest Fisher-Hartwig type correlator to calculate. The field theory prediction will be as in (14), except as σ_z does not transform under the U(1) symmetry we must have that the operator corresponds to no overall charge creation – i.e. $\sum \tilde{\beta}_j = 0$. This does not affect the leading order scaling which is $N^{-R/2}$.

As \mathcal{M}_N is Toeplitz we can directly apply Theorem 1. We find that there are many representations for the symbol (29) of this matrix, but since it is of the form described in Section 4, those that are minimal will have $\tilde{\beta}_j = \pm \frac{1}{2}$ and $n_j \in \{1, -1, 0\}$ along with constraint (21). In order for $V(z)$ to satisfy the smoothness requirements we additionally require that $\sum_{r=1}^{2R} \beta_r = 0$, then the symbol can be written in the form given by (19) with

$$V(z) = V_0 = i \left(\sum_{r=1}^R \theta_r (\beta_r - \beta_{2R+1-r}) + 2\pi \sum_{r=R+1}^{2R} \beta_r \right) + (i\pi) \quad (36)$$

where we have used the evenness of the symbol. The final term $i\pi$ fixes the correct overall sign of the symbol at zero, so is included here if and only if the symbol is negative at zero.

There are $\binom{2R}{R}$ different combinations $\tilde{\beta}_j = \pm 1/2$ which satisfy the constraints, thus there are $\binom{2R}{R}$ different representations with minimal weight. The labels $\beta, \tilde{\beta}$ and n are fixed by an arbitrary initial representation $\{\beta_j\}$, but the final answer is independent of this choice.

Theorem 1 then gives us the following leading asymptotic behaviour in the limit $N \rightarrow \infty$:

$$\begin{aligned} \left\langle \prod_{i=0}^{N-1} \sigma_i^z \right\rangle &\sim N^{-\frac{R}{2}} (-1)^{RN} \left(G\left(\frac{3}{2}\right) G\left(\frac{1}{2}\right) \right)^{2R} \\ &\sum_{\text{Reps: } \{\tilde{\beta}_j\}} \exp iN \sum_{r=1}^R \theta_r (\tilde{\beta}_r - \tilde{\beta}_{2R+1-r}) \prod_{1 \leq j < k \leq 2R} |\exp(i\theta_j) - \exp(i\theta_k)|^{2\tilde{\beta}_j \tilde{\beta}_k}. \end{aligned} \quad (37)$$

Here we did not include the extra $i\pi$, i.e. we assume the symbol is positive at zero – this term would give an additional coefficient $(-1)^N$ if included. This is in exact agreement with the field theory calculation, and gives us the coefficients.

5.3. $\langle \sigma_0^x \sigma_N^x \rangle$ and $\langle \sigma_0^y \sigma_N^y \rangle$. The ground state two-point functions have the form:

$$\langle \sigma_0^x \sigma_N^x \rangle = \det (\mathcal{M}_{j,k+1})_{j,k=0}^{N-1} = \det (\mathcal{M}_{j,k}^x)_{j,k=0}^{N-1} \quad (38)$$

$$\langle \sigma_0^y \sigma_N^y \rangle = \det (\mathcal{M}_{j+1,k})_{j,k=0}^{N-1} = \det (\mathcal{M}_{j,k}^y)_{j,k=0}^{N-1}, \quad (39)$$

where the matrices \mathcal{M}^x , \mathcal{M}^y have symbol

$$f^x(\theta) = e^{i\theta} \frac{\Lambda(\theta)}{|\Lambda(\theta)|}, \quad f^y(\theta) = e^{-i\theta} \frac{\Lambda(\theta)}{|\Lambda(\theta)|}. \quad (40)$$

The matrices $\mathcal{M}^{x,y}$ are Toeplitz and we can use Theorem 1. This results in the same analysis as for the previous correlator and we obtain asymptotics of the same form as the right hand side of (37). The only difference is that the condition on the set of $\{\beta_j\}$ is

$$\sum_{r=1}^{2R} \beta_r = \pm 1 \quad (41)$$

where the sum is $+1$ for the σ^x correlator and -1 for σ^y . We find the $\{\tilde{\beta}_j\}$ subject to the same constraint (21). One must also check whether to include the additional $i\pi$ in V_0 – here it corresponds to a positive symbol at zero. This gives $\binom{2R}{R+1}$ different Fisher Hartwig representations to sum over. The condition (41) on the $\{\beta_j\}$ is what we need to correct the calculation in [8].

We remark that the form of the right hand side of (37) combined with the conditions (41) gives us that the σ_x and σ_y correlators are equal – as we expect from rotation invariance. We see agreement with the field theory calculation for both of these correlators.

5.4. Example: $\langle \sigma_i^x \sigma_{i+N}^x \rangle$ and $\langle \sigma_i^y \sigma_{i+N}^y \rangle$ for $R = 2$. We consider any dispersion which has two zeroes of $\Lambda(\theta)$ in $(0, \pi)$, with $\Lambda(0) > 0$. This could be, for example, a model with positive nearest neighbour hopping on the even and odd sublattices. We find $V(z)$ takes the form

$$V(z) = i(\theta_1(\beta_1 - \beta_4) + \theta_2(\beta_2 - \beta_3)) + 2\pi i(\beta_3 + \beta_4) + i\pi, \quad (42)$$

and we have the following four representations which satisfy the constraints: $f(z; 0, 0, 0, 0)$, $f(z; 0, 0, -1, +1)$, $f(z; -1, 0, 0, +1)$ and $f(z; 0, -1, 0, +1)$; where $\tilde{\beta}_i = (1/2, 1/2, 1/2, -1/2)$, $(1/2, 1/2, -1/2, 1/2)$, $(-1/2, 1/2, 1/2, 1/2)$ and $(1/2, -1/2, 1/2, 1/2)$ respectively.

Summing over the contribution of these representations as in (37) gives the following result:

$$\begin{aligned} \langle \sigma_i^x \sigma_{i+N}^x \rangle &\sim (-1)^N N^{-1} \left(G\left(\frac{3}{2}\right) G\left(\frac{1}{2}\right) \right)^4 \\ &\times \left(\sqrt{\frac{\sin \theta_2}{\sin \theta_1}} 2 \cos(N\theta_1) + \sqrt{\frac{\sin \theta_1}{\sin \theta_2}} 2 \cos(N\theta_2) \right). \end{aligned} \quad (43)$$

The σ_y calculation is similar: we have the same formula for V , but the signs of n and $\tilde{\beta}$ in the representations are reversed. Doing the sum we get identical asymptotics to (43) as expected.

6. MODELS RELATED TO THE OTHER CLASSICAL COMPACT GROUPS

We now give two further models that give physical context to the results of [6, 7]. In the spirit of the Altland-Zirnbauer ten-fold way [36] we see a connection between classical compact groups and discrete symmetries.

6.1. Semi-infinite chain – ordinary transition. We work directly in the thermodynamic limit, however specialisation to the finite chain is similar and described in, for example, [24] where random matrix techniques are used to study the Rényi entanglement entropies in the XX model on open chains. The following is close to the method of images from differential equation theory and also to the same method in CFT with a boundary as explained in [23, Chapter 11].

Consider the Hamiltonian for fermionic operators $\{B_j\}_{j \in \mathbb{Z}_+}$ on the semi-infinite chain:

$$H' = \sum_{j=1}^{\infty} B_{j+1}^\dagger B_j + h.c. , \quad (44)$$

where h.c. stands for the hermitian conjugate. This is the nearest neighbour fermionic chain with open boundary conditions (OBCs). We will use this model as an example to illustrate the main ideas of the calculations given in detail in Appendix B. To diagonalise this model we introduce the ‘mirrored’ operators $B_{-j} := -B_j$. Then⁷:

$$H' = \frac{1}{2} \sum_{j=-\infty}^{\infty} B_{j+1}^\dagger B_j + h.c. = 2 \int_{-\pi}^{\pi} dq \cos(q) B^\dagger(q) B(q) . \quad (45)$$

where the Fourier transformed operators $B(q) \propto \sum_{j=-\infty}^{\infty} \exp(iqj) B_j$ or, in terms of the original, unmirrored variables, $B(q) \propto \sum_{j=1}^{\infty} \sin(qj) B_j$.

To make contact with the models and methods of [6, 8] and the canonical Hamiltonian (2), suppose we start with fermions $\{b_j\}_{j \in \mathbb{Z}}$ on the whole chain. We can use these to simulate the above half chain by introducing the parity odd combination: $B_j := (b_j - b_{-j})/\sqrt{2}$. Inserting this into the Hamiltonian (44) we get:

$$\begin{aligned} H' &= \frac{1}{2} \sum_{j=1}^{\infty} (b_{j+1}^\dagger - b_{-(j+1)}^\dagger)(b_j - b_{-j}) + h.c. \\ &= \frac{1}{2} \sum_{j=-\infty}^{\infty} b_{j+1}^\dagger b_j - \frac{1}{2} \sum_{j=-\infty}^{\infty} b_{j+1}^\dagger b_{-j} + h.c. . \end{aligned} \quad (46)$$

In the b_j degrees of freedom we now have a non-local Hamiltonian, with hopping between sites i and j if $|i - j| = 1$ or if $|i + j| = 1$. As a final step we shift the chain by one lattice site to align with the model (2) which starts at $j = 0$ (with a b_0 not identically 0) and so send $j \rightarrow j - 1$. Hence we see (44) is a particular case of (2) with $A_{jk} = \delta_1(|j - k|) - \delta_1(|j + k + 2|)$. This is in turn a particular case of the model labelled $\text{Sp}(2N)$ in [6], with hopping matrix given in Table 1. Note that combining the steps above we also have the spectrum and eigenfunctions of this particular model.

We now assert, with details left to Appendix B, that all of the nonlocal models in [6] that are related to the groups $\text{Sp}(2N)$, $\text{O}^-(2N + 2)$, $\text{O}^+(2N + 1)$ are more naturally viewed as local models on the half chain, after mirroring with the parity transformation

⁷We also include $B_0 = -B_0 = 0$. The factor of two in front of the dispersion is due to the density of modes and is explained in Appendix B.

Physical model	Classical compact group	Structure of matrices $\bar{A}_{j,k}$	Matrix entries $(\mathcal{M}_N)_{j,k}$
TI, PBC	$U(N)$	$a(j-k)$	$f_{j-k}, j, k \geq 0$
TI, Edge, $P = 1$	$O^+(2N)$	$a(j-k) + a(j+k)$	f_0 if $j = k = 0$ $\sqrt{2}f_l$ if either $j = 0, k = l$ or $j = l, k = 0$
TI, Edge, $P = -1$	$Sp(2N),$ $O^-(2N+2)$	$a(j-k) - a(j+k+2)$	$f_{j-k} + f_{j+k}, j, k > 0$ $f_{j-k} - f_{j+k+2}, j, k \geq 0$
TI, Edge, $P = \mp 1$	$O^\pm(2N+1)$	$a(j-k) \mp a(j+k+1)$	$f_{j-k} \mp f_{j+k+1}, j, k \geq 0$

TABLE 1. Entries of matrices $\bar{\mathbf{A}} = \mathbf{A} - 2h\mathbf{I}$ in terms of the function $a(j)$. The f_k s are the Fourier coefficients of the symbol $f(\theta)$ of \mathcal{M}_N . P corresponds to the parity of the operators $B_j \propto b_j \pm b_{-j}$, which in turn indicate the nature of the boundary transition.

$B_j = -B_{-j}$. These models are defined by the hopping strengths $a(j-k)$ in:

$$H' = \sum_{j,k=1}^{\infty} a(j-k) B_k^\dagger B_j + h.c. + H_{edge}, \quad (47)$$

where $H_{edge} = -\sum_{j,k=1}^{\infty} a(j+k) B_j^\dagger B_k$. H_{edge} is localised near the boundary (due to the decay of α_j) and is needed so that the transformation to the full chain yields a translation invariant Hamiltonian. Note that this gives an overall weakening of hopping amplitude near the boundary. Such models have $\langle B_0^\dagger B_0 \rangle = 0$ by definition, and correspond to the ‘ordinary’ transition for our critical system, as described in [37, 23]. Ideas from boundary CFT then suggest that the long distance correlation functions will be identical to those of the infinite chain with a hopping matrix $A_{jk} = a(j-k)$.

6.2. Semi-infinite chain – extraordinary transition. It is then natural to consider the alternative parity transformation $B_{-j} := B_j$ and $H_{edge} = +\sum_{j,k=1}^{\infty} a(j+k) B_j^\dagger B_k$. The analysis goes through mostly as before, with details in Appendix B. The dispersion relation is identical to that of the models in 6.1.

Importantly we no longer have $B_0 = 0$. In fact for finite chain size $\langle B_0^\dagger B_0 \rangle \sim N_e/M$, the filling fraction (which will be finite in the thermodynamic limit). We have enhanced hopping amplitudes near the boundary, giving a finite order parameter there at the transition (again see [37, 23]). Thus we are now in models representing the ‘extraordinary’ transition of a system with a bulk corresponding to some $U(N)$ model. As a final remark we note that the nonzero expectation value here will manifest itself as the conformally invariant $\psi(0) = \infty$ boundary condition in the continuum limit, due to scaling by inverse powers of the lattice constant in the definition of $\psi(x)$.

6.3. Summary of models: In Table 1 we summarise all of the models related to classical compact groups. First we identify the physical model with a TI bulk, which can be easily transferred to a predictive CFT description. Then we give the corresponding

compact group model of [6], which is fully specified by the \bar{A} matrix in the Hamiltonian (2) and allows rigorous analysis via random matrix theory methods. We denote the different connected components of the orthogonal group by $O^+(2N)$, $O^+(2N+1)$, $O^-(2N+1)$ and $O^-(2N+2)$ with plus and minus corresponding to positive and negative determinant respectively. The column $(\mathcal{M}_N)_{j,k}$ gives us the immediate generalisation of the TI calculations above to these models – we simply need to replace all of the Toeplitz matrices generated by (29) by the relevant Toeplitz+Hankel matrix generated by the same symbol according to this column.

6.4. Entanglement entropy and σ^z string correlator. For the entanglement entropy Keating and Mezzadri derive, using a different proven case of the Fisher-Hartwig conjecture from [11], that:

$$S(N) = \frac{R}{6} \log 2N + \frac{R}{6} (K/\ln 2 - 6I_3) + o(1). \quad (48)$$

We see agreement with the CFT prediction (11), in particular we note that the boundary entropy is confirmed to be zero for these models.

For the correlators, we still have (35) – but now the matrix \mathcal{M}_N has a Toeplitz+Hankel structure as dictated by Table 1. The method to find asymptotics of such matrices is outlined in [9] – they are transformed first to Hankel matrices and then to Toeplitz matrices multiplied by certain orthogonal polynomials. Using the results of the paper, the asymptotics of the Toeplitz part is controlled by Theorem 1, and the asymptotics of the orthogonal polynomials are derived by the Riemann-Hilbert method, a discussion of which is beyond the scope of this paper.

A general theorem for Toeplitz+Hankel matrices with symbols containing jump discontinuities is not given in [9] – however combining [9, Theorem 1.25 and Remark 1.22], we have the following:

$$\left\langle \prod_{i=0}^{N-1} \sigma_i^z \right\rangle \sim N^{-\sum \beta_j^2} (A \exp(iF(N)) + o(1)) = N^{-\frac{R}{2}} (A \exp(iF(N)) + o(1)). \quad (49)$$

A is an unknown constant, and F is an unknown real function. Both could in principle, however, be determined rigorously according to the arguments of [9]. In particular, the additional Riemann-Hilbert analysis required due to our symbol violating the hypotheses of [9, Theorem 1.25] only affects the coefficient, and not the leading order algebraic decay. We also note in the derivation of [9, Theorem 1.25], and in the theorem itself, the determinant scales as $(2N)^{-R/2}$ – this is another clear connection with the method of images and conformal field theoretic calculations where we would expect to make such a replacement. This reasoning applies to all the models with boundary that we consider, and in each case we get the bulk scaling as we would expect from the field theory.

We note that for systems with these Toeplitz+Hankel structures we lack translation invariance, so this result is restricted to the σ^z -string on the first N sites.

For the σ^x and σ^y correlators, we see in Table 1 that we have a particular Toeplitz+Hankel matrix to deal with. However, to use the methods of [9] we need to shift the indices on the matrices as above by multiplying the symbol by an exponential. This means that the symbol is no longer even in θ so we can no longer use the results of [9] for Toeplitz+Hankel matrices.

7. CONCLUSIONS AND DISCUSSION

In this paper we reconciled a rigorous mathematical approach to calculating properties of spin chains with the intuition gained from more heuristic physical arguments. To do this we worked within a framework of mathematically tractable models introduced in [6]. We motivated an effective CFT description of each of these models which gave predictions consistent with the rigorous calculations. This was particularly informative after noting that some of the models in [6] represent systems with a boundary. We then gave the results of rigorous calculations in [6] for the entanglement entropy, and [8] for the translation invariant correlation functions. We fixed an error in [8] and gave a partial extension to the expectation of the σ_z string operator for systems with a boundary. All of these agreed with the field theory expectation. We could not directly extend this method in the presence of a boundary to the more physically relevant spin-spin correlation functions, but we note the formal similarity between the Jordan-Wigner transformed σ_x and σ_y operators to the σ_z string. It is interesting to compare the partial result (17) with the full lattice results. Given a more thorough field theoretic calculation perhaps the entire Fisher-Hartwig result could be recovered – for example we might expect the combinations of sine functions in (43) to come from the theory of form factors in integrable quantum field theories [38, 39]. The universal appearance of the combination $(G(1/2)G(3/2))^2$ for each complex fermionic field suggests this is simply a normalisation of the field operators relative to the normalisation chosen on the lattice. We also remark that the oscillating prefactor $(-1)^N$ which we included in (14) in an ad-hoc manner is found to be present⁸ if and only if there is a difference (± 1) in the number of fermion types with positive v_i and those with negative v_i in $(0, \pi)$. If we imagine a ‘Dirac cone’ where we extend the linearised dispersion to an intersection at $\theta = 0$ in each fermionic sector, the sign of v_i corresponds to a vacuum filled with either particles or holes. This picture could be a way of fixing the correct continuum spin operator, although we could not see how to apply it directly in our heuristics.

To summarise the universality results, we see that for our critical systems in both the effective theory and the Fisher-Hartwig calculation, the most important feature affecting the physics is the number of zeroes of the dispersion relation. Interestingly, both calculations are sensitive to the values of the zeroes, or Fermi momenta, of the dispersion, but the gradient at these zeroes, or the Fermi velocities, are invisible to the Fisher-Hartwig analysis. They do, however, feature prominently in the physics – in particular the spacetime mixing conformal symmetries must act on coordinates $(x, v_{\text{F}}t)$. For this reason, attempting to extend this analysis to dynamic correlators would be an interesting question. We note that from the boundary CFT perspective, for correlation functions between sites at the boundary (but displaced in time) we would expect different scaling exponents to the bulk correlators. There is also an interesting question about the enhanced symmetry for systems where the Fermi velocity is the same at two or more crossings. This system has a new symmetry at the effective theory level – we can now mix these different fermion sectors – however the lattice results imply that the physics does not change in this case.

⁸After fixing a lattice Jordan-Wigner convention that corresponds to anti-ferromagnetic order.

To address universality more precisely, we have rigorously demonstrated different classifications depending on the macroscopic quantity of interest as follows:

- Classification I: The divergence of the entanglement entropy of a block for translation invariant periodic systems of free fermions which preserve fermion number (and related spin chains) is universal for systems with the same number of zeroes of their dispersion.
- Classification Ia: The divergence of the entanglement entropy at the boundary for free fermion systems with a boundary which preserve fermion number and which have a translation invariant bulk (and related spin chains) is universal for systems with the same number of zeroes of their dispersion.
- Classification II, IIa: The subclass of such systems sharing entanglement entropy up to $O(1)$ is given by systems with equal Fermi momenta $\{\theta_i\}$.
- The leading asymptotics of the equal time spin-spin correlation functions for the spin chains in Class I have universal scaling and are universal for Class II.

We now make some general remarks on the mathematical methods and further applicability. The Fisher-Hartwig conjecture as proved in [9] relies on a matrix with Toeplitz structure or some special Toeplitz+Hankel structures. In the approach above, these structures correspond to bulk translation invariance. If we restrict to free fermion models (and related spin chains), the class of microscopic systems we have studied effectively saturates those with bulk translation invariance. In particular, the finite chain must be either a ring or have two open ends and our analysis covers both in the thermodynamic limit. We would thus need some other rigorous arguments to extend the microscopic universality classes to systems without translation invariance, but which we would expect to have the same universal behaviour based on an effective description. Another open problem would be moving the analysis away from the edge in the case of the open chain – this would require Toeplitz+Hankel results beyond those given in [9]. The rigorous analysis above also relied heavily on the fact that our system had a description as a quadratic fermionic Hamiltonian. This allowed us to write the entanglement entropy in terms of eigenvalues of the correlation matrix, and also allowed us to use Wick's theorem to compute correlation functions. Hence we cannot expect to use Fisher-Hartwig type asymptotics directly in interacting systems.

We note the link between matrix Riemann-Hilbert problems, via the results of [9], and rigorously providing asymptotics for systems with a CFT description. This may be unsurprising when we consider the strong links to the theory of differential equations from both sides. Other interesting results would follow from solving related Riemann-Hilbert problems. For example it should also be possible to use the ideas contained in [40] to understand finite size effects for our lattice model – i.e. studying long distance correlation functions before taking the limit $M \rightarrow \infty$. In [41] and [42] uniform asymptotics are obtained for two merging Fisher-Hartwig singularities and a single emerging singularity respectively, giving information about the phase transition between different asymptotic behaviours. The phase transitions in our model, due to the form of the symbol, correspond to two singularities emerging at the same time – hence these results are not directly applicable. It would thus be another interesting open question to study the case of the simultaneous emergence of two Fisher-Hartwig singularities via the Riemann-Hilbert method.

Finally we remark that we have far from utilised all of the symbols amenable to Fisher-Hartwig analysis. It would be interesting to see if any other spin chain models could be connected to symbols with different Fisher-Hartwig singularity structures, or indeed if in general there is a corresponding physical model for each symbol. We would expect a connection to Bethe ansatz solvable models through the methods contained in [38].

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APPENDIX A. TREATMENT OF POINTS WHERE LINEARISATION FAILS

We need to consider what happens at an exceptional point θ_i where $\Lambda(\theta_i) = 0$ and $\Lambda'(\theta_i) = 0$. At such points we *may* get different critical behaviour. For example in the XX model in a magnetic field, $|\Lambda(q)| = |\cos(q) + h|$. The model is gapped for $|h| > 1$, has two crossings and is linearisable when $|h| < 1$, but when $h = 1$ it has a low energy parabolic dispersion (about $q = \pi$) and the effective theory is that of a non-relativistic massless fermion, which is not a CFT.

We note that the rigorous argument based on the Fisher-Hartwig conjecture is only sensitive to the following question: does the sign of the dispersion change at the crossing? If it does - i.e. if the first non-zero derivative is odd - then we get identical Fisher-Hartwig behaviour to a linear crossing at the same point. This can be understood physically in the following way: an infinitesimal perturbation $\Lambda \rightarrow \Lambda \pm \epsilon$ will now have a linear crossing in the neighbourhood of θ_i . There is thus stability here - infinitesimally either side of our exceptional parameters we have a system with n linear crossings - hence we should expect by continuity that such an effective description still applies at such exceptional points.

In the case that the first non-zero derivative is even, we have an instability of the type described above for the XX model. An infinitesimal shift changes the number of crossings, and hence this exceptional point is at a phase transition between different critical theories. Due to the nature of this singularity, the symbol cannot be written in the general Fisher-Hartwig form [9] at this point, so that form of analysis fails. Hence we do not seek to describe these transition points in the same terms, and exclude such exceptional $\Lambda(q)$ from our discussion. We note that this automatically excludes any zeroes at $q = 0$ and $q = \pi$ by symmetry.

APPENDIX B. METHOD OF IMAGES FOR THE CHAIN WITH BOUNDARY AND RELATION TO CLASSICAL COMPACT GROUPS

B.1. $\text{Sp}(2N)$. Consider the model on the half chain:

$$H = \sum_{j,k=1}^{\infty} a(j-k) B_j^\dagger B_k - \sum_{j,k=1}^{\infty} a(j+k) B_j^\dagger B_k, \quad (50)$$

where $a(j) = a(-j)$ and decays for large j . We will show that:

- this model is solvable by the method of images,
- this can be written as an $\text{Sp}(2N)$ model in the language of [6].

To do the first, let us define $B_{-j} := -B_j$. Then, as in 6.1, we can write:

$$\begin{aligned} H &= \frac{1}{2} \left(\sum_{j,k=1}^{\infty} a(j-k) B_j^\dagger B_k + \sum_{j,k=1}^{\infty} a(j-k) B_{-j}^\dagger B_{-k} \right) - \sum_{j,k=1}^{\infty} a(j+k) B_j^\dagger B_k \\ &= \frac{1}{2} \sum_{j,k=-\infty}^{\infty} a(j-k) B_j^\dagger B_k. \end{aligned} \quad (51)$$

This is now a TI model which can be solved by Fourier transform.

Now to relate this to $\text{Sp}(2N)$, we define $B_j = \frac{b_j - b_{-j}}{\sqrt{2}}$. Then:

$$\begin{aligned} H &= \frac{1}{2} \left(\sum_{j,k=1}^{\infty} a(j-k)(b_j^\dagger - b_{-j}^\dagger)(b_k - b_{-k}) - \sum_{j,k=1}^{\infty} a(j+k)(b_j^\dagger - b_{-j}^\dagger)(b_k - b_{-k}) \right) \\ &= \frac{1}{2} \sum_{j,k=-\infty}^{\infty} (a(j-k) - a(j+k)) b_j^\dagger b_k \end{aligned} \quad (52)$$

As in section 6.1, we need to shift the lattice by one site to see that this is our model (2) with $\bar{A}_{jk} = a(j-k) - a(j+k+2)$. Hence we see that the half-line model (50) is the $\text{Sp}(2N)$ model of [6] in full generality. Note that (52) may be transformed to (51) due to the equivalence $B_j = -B_{-j}$ which carries over to the Fourier transformed operators $B_q = -B_{-q}$. This means any eigenstate $B_q^\dagger |0\rangle$ will have an eigenvalue of $2\Lambda(q)$ where $\Lambda(q)$ is the dispersion one would get by naively applying the diagonalisation in (26) to (51). Equivalently one can write the Hamiltonian purely in terms of the independent k modes, evenly spaced in $(-\pi, \pi]$, and send $\Lambda(q) \rightarrow 2\Lambda(q)$ in the process. This doubled dispersion is seen directly in the diagonalisation carried out in [6] where the same modes are written twice as densely in the interval $[0, \pi)$. We prefer $(-\pi, \pi]$ as it gives the same density of states as the translation invariant model when counting the gapless degrees of freedom. We remark that the initial model (50) is the natural physical interpretation of all three models in this section, as it is the only one which is local in the thermodynamic limit.

B.2. $\text{O}^-(2N+2)$ and $\text{O}^+(2N+1)$. The structure of the \bar{A} matrix for the group $\text{O}^-(2N+2)$ is identical to that for $\text{Sp}(2N)$ so all of the above applies in exactly the same way. The fermion chain related to $\text{O}^+(2N+1)$ is structurally very similar, but naturally lives on the half integer sites, i.e. we should shift the labels by $j \rightarrow j' = j + 1/2$ and then repeat the above calculation for

$$H = \sum_{j,k=0}^{\infty} a(j-k) B_{j+1/2}^\dagger B_{k+1/2} - \sum_{j,k=0}^{\infty} a(j+k) B_{j+1/2}^\dagger B_{k+1/2}. \quad (53)$$

Alternatively, the $\text{O}^+(2N+1)$ chain can be embedded in the $\text{Sp}(2N)$ chain by shifting the chain by half a lattice space and then relabelling sites by integers $j' \rightarrow 2j'$. Both are consistent with the diagonalisation given in [6]. As we can embed the chain corresponding to each of these groups in the $\text{Sp}(2N)$ chain, we do not extend the class of models by including them.

B.3. $\text{O}^+(2N)$ and $\text{O}^-(2N+1)$. One can repeat the above manipulations for the following Hamiltonian on the half chain (starting at zero):

$$H = \sum_{j,k=0}^{\infty} a(j-k) B_j^\dagger B_k + \sum_{j,k=1}^{\infty} a(j+k) B_j^\dagger B_k. \quad (54)$$

We put $B_{-j} := B_j$ to reach a translation invariant model, and $B_j = \frac{1}{\sqrt{2}}(b_j + b_{-j})$ to reach the $\text{O}^+(2N)$ model of [6]. The only novelty is that the site at zero now has $B_0 \neq 0$, and we must include $B_{-0} = B_0$. This is seen in the $\text{O}^+(2N)$ model where the

operator $b_0 = \sqrt{2}B_0$ has a heavier weight in calculations (see Table 1). We also note that this subtlety is seen at the level of the dispersion as well: we should not send the TI $\Lambda(0) \rightarrow 2\Lambda(0)$ for the $\{B_k\}$ model (54), but it does appear doubled in the $\{b_k\}$ $O^+(2N)$ model.

We may also send $j \rightarrow j + 1/2$ and consider the model:

$$H = \sum_{j,k=0}^{\infty} a(j-k)B_{j+1/2}^\dagger B_{k+1/2} + \sum_{j,k=0}^{\infty} a(j+k)B_{j+1/2}^\dagger B_{k+1/2}. \quad (55)$$

Again we obtain a TI model after reflection and, with $B_j = \frac{1}{\sqrt{2}}(b_j + b_{-j})$, we reach the $O^-(2N+1)$ model. As there is no site reflected into itself, we do not get any special weights. These are again in agreement with the diagonalisation in [6].

We note that the connected subgroups of the orthogonal groups containing the negative of the identity matrix, $-\mathbb{I}$, correspond to systems at the extraordinary transition, and those not containing $-\mathbb{I}$ to systems at the ordinary transition. Finally we remark that by the addition of a second auxiliary site between the reflected site $-M$ and the boundary site M , the method of images can be used for a finite system with two boundaries. Care should be taken with the quantised momentum for the finite system, but the manipulations are otherwise identical. This method is used in [24] to study the XX model on a finite chain.