

The Fisher-Hartwig Formula and Entanglement Entropy

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Abstract Toeplitz matrices have applications to different problems of statistical mechanics. Recently it was used for calculation of entanglement entropy in spin chains. In the paper we review these recent developments. We use the Fisher-Hartwig formula, as well as the recent results concerning the asymptotics of the block Toeplitz determinants, to calculate entanglement entropy of large block of spins in the ground state of XY spin chain.

Keywords Toeplitz determinant · Fisher-Hartwig formula · Entanglement · Spin chain

1 Introduction

We study von Neumann entropy and Rényi entropy of spin chains by means of the Fisher-Hartwig formula. The concept of entanglement was introduced Schrödinger in 1935 in the course of developing the famous ‘cat paradox’, see [53–56]. Recently it became important as a resource for quantum control, which is central for quantum device building, including quantum computers (it is a primary resource for information processing). Entropy of a subsystem as a measure of entanglement was introduced in [13]. We study spin chains with unique ground state. Von Neumann entropy (and Rényi entropy) of the whole ground state is zero, but it is positive for a subsystem [block of spins]. In order to define entanglement entropy one has to introduce reduced density matrix. The reduced density matrix was first introduced by P.A.M. Dirac in 1930, see [24].

We calculate the entropy of a block of L continuous spins in the ground state of a Hamiltonian. We can think that the ground state is a bipartite system $|GS\rangle = |A\&B\rangle$, where we

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call the block by subsystem A and the rest of the ground state by subsystem B . The density matrix of the ground state is $\rho_{AB} = |GS\rangle\langle GS|$, and the density matrix of the block of L neighboring spins [subsystem A] is $\rho_A = \text{Tr}_B(\rho_{AB})$, where we trace out all degrees of freedom outside the block. The von Neumann entropy of the block is

$$S(\rho_A) = -\text{Tr}_A(\rho_A \ln \rho_A), \tag{1}$$

which measures how much the block is entangled with the rest of the ground state. On the other hand, the Rényi entropy $S(\rho_A, \alpha)$ is defined as

$$S(\rho_A, \alpha) = \frac{1}{1-\alpha} \ln \text{Tr}_A(\rho_A^\alpha), \quad \text{and} \quad \alpha > 0, \tag{2}$$

here α is a parameter. Rényi entropy [52] is important in information theory. The Rényi entropy turns into von Neumann entropy at $\alpha \rightarrow 1$. Knowledge of the Rényi entropy at arbitrary α permits evaluation of spectrum of the density matrix. Our main example is XY spin chain.

The Toeplitz matrix $T_L[\Phi]$ is said to be expressed in terms of the generating function $\Phi(\theta)$ (which is called symbol in mathematical literature):

$$T_L[\Phi] = (\Phi_{i-j}), \quad i, j = 1, \dots, L-1 \tag{3}$$

where

$$\Phi_k = \frac{1}{2\pi} \int_0^{2\pi} \Phi(\theta) e^{-ik\theta} d\theta \tag{4}$$

is the k -th Fourier coefficient of generating function $\Phi(\theta)$. The generating function $\Phi(\theta)$ can be type of $N \times N$ matrix and $T_L[\Phi]$ is a $NL \times NL$ matrix for such case. One of the central objects in the study of the Toeplitz matrix $T_L[\Phi]$ is its determinant, which we will denote as $D_L[\Phi]$,

$$D_L[\Phi] := \det T_L[\Phi]. \tag{5}$$

Starting with Onsager’s celebrated solution of the two-dimensional Ising model in the 1940’s, Toeplitz determinants have played an increasingly central role in modern mathematical physics. We refer the reader to the book [50], and to survey [49] as for comprehensive sources of the classical results and the history concerning the use of the Toeplitz determinants in statistical mechanics.

Another important areas of applications of the Toeplitz determinants are random matrices and combinatorics. We refer the readers to the works [5, 29, 60] for the basic results and for the historic reviews.

Given a generating function $\Phi(\theta)$, a principal question is the evaluation of the large L behavior of the Toeplitz determinant $D_L[\Phi]$. The pioneering works on the asymptotic analysis of Toeplitz determinants were done by Szegő (regular symbol) and by Fisher and Hartwig (singular symbol). These results have been used in the study of spin correlation in two-dimensional Ising model in the classical works of Wu and McCoy, see for example [50] and since then by many other researchers and for a various generating functions.

The main focus of the majority of works in the area has been, so far, the study of spin correlations. The key objects of the analysis have been the relevant correlation functions of the local operators. In this paper, we discuss yet another, more recent application of the asymptotic analysis of Toeplitz determinants in the theory of quantum spin models. Instead

of the local operators, these applications are concerned with the important nonlocal objects appearing in spin chains in connection to their suggested use in quantum informatics [43, 45]. Indeed, we shall survey some of the recent results concerning the *quantum entanglement*. We will consider the two applications—the entanglement in the XX model and in the XY model. The first one is related to a singular scalar generating function, while the second one deals with a regular but (2×2) matrix generating function.

We begin with the brief review of the history and some of the most recent results concerning the asymptotic analysis of Toeplitz determinants.

The *plan* of the paper is:

In the second section we discuss the asymptotical expression of the determinant of a large Toeplitz matrix. The section is divided into subsections. Section 2.2 is devoted to block Toeplitz determinants.

Third section is devoted to XY spin chain. In Sect. 3.1 we remind derivation of determinant representation of entropy of a block of spins in the ground state. Isotropic case, i.e. the XX model, is considered in Sect. 3.2. For anisotropic case we have to use the block Toeplitz matrices.

In Sect. 4 we derive asymptotic expression of entropy of large block of spins in isotropic case: the leading logarithmic term and sub-leading corrections.

In Sect. 5 we derive asymptotic expression of von Neuman entropy of large block of spins in anisotropic case. In the case of XY spin chain the entropy has a limit. We calculate the limit.

In Sect. 6 we calculate limiting expression for Renyi entropy of large block of spins in XY spin chain.

In Sect. 7 we derive the spectrum of the limiting density matrix from Renyi entropy. We prove that the spectrum is exact geometric sequence, see (117) and (124). We also calculate the degeneracy of individual eigenvalues, see (126).

The content of Sects. 4–7 is based on the works [28, 31, 32, 37].

In Sect. 8 we formulate open problems.

2 Szegő and Fisher-Hartwig Asymptotics

Throughout the paper we will follow the usual, in the theory and applications of the Toeplitz determinants, convention to denote the argument of the functions on the unit circle either as θ or as z , $z = e^{i\theta}$, i.e. we will always assume the notational identity,

$$f(z) \equiv f(\theta), \quad z = e^{i\theta}, \quad \theta \in [0, 2\pi).$$

We first consider the case of scalar generating function, i.e. $N = 1$. We shall also use for this case the low case symbol ϕ instead of Φ .

2.1 Szegő and Fisher-Hartwig Asymptotics in the Case of Scalar Symbols

In this subsection we review the basic mathematical facts concerning the asymptotics of Toeplitz determinants $D_L[\phi]$ with scalar generation functions $\phi(z)$.

The large L asymptotic behavior of $D_L[\phi]$ depends significantly on the analytical properties of the generating function $\phi(\theta)$. In the case of the smooth enough functions $\phi(\theta)$, the behavior is exponential and its leading and the pre-exponential terms are given by the following classical result of Szegő, known as the *strong Szegő limit theorem*.

Theorem 1 *Suppose that the generation function $\phi(\theta)$ satisfies the conditions,*

1. $\phi(\theta) \neq 0$, for all $\theta \in [0, 2\pi)$.
2. $\text{index } \phi(\theta) \equiv \arg \phi(2\pi) - \arg \phi(0) = 0$.
3. $\sum_{k=-\infty}^{\infty} |V_k| + \sum_{k=-\infty}^{\infty} |k||V_k|^2 < \infty$, where V_k are the Fourier coefficients of the function,

$$V(\theta) := \ln \phi(\theta), \tag{6}$$

that is,

$$V(z) = \sum_{k=-\infty}^{\infty} V_k z^k, \quad V_k = \frac{1}{2\pi} \int_0^{2\pi} V(\theta) e^{-ki\theta} d\theta. \tag{7}$$

Then,

$$D_L[\phi] \sim E_{Sz}[\phi] \exp(LV_0), \quad L \rightarrow \infty, \tag{8}$$

where the pre-exponential factor, $E_{Sz}[\phi]$, is given by the equation,¹

$$E_{Sz}[\phi] = \exp\left(\sum_{k=1}^{\infty} k V_k V_{-k}\right). \tag{9}$$

Conditions (1) and (2) on the symbol $\phi(\theta)$ ensure that the function $V(z)$ is a well defined function on the unit circle. Condition (3) is a smoothness condition.² It is certainly satisfied by the differentiable functions and is not satisfied by the functions having root and jump singularities. In the context of Toeplitz matrices, this type of singularities is usually called the *Fisher-Hartwig singularities*. The general form of the symbol $\phi(z)$ which has m , $m = 0, 1, 2, \dots$ fixed Fisher-Hartwig singularities is given by the equation,³

$$\phi(z) = e^{V(z)} z^{\sum_{j=0}^m \beta_j} \prod_{j=0}^m |z - z_j|^{2\alpha_j} g_{z_j, \beta_j}(z) z_j^{-\beta_j}, \quad z = e^{i\theta}, \theta \in [0, 2\pi), \tag{10}$$

where

$$z_j = e^{i\theta_j}, \quad j = 0, \dots, m, \quad 0 = \theta_0 < \theta_1 < \dots < \theta_m < 2\pi, \tag{11}$$

$$g_{z_j, \beta_j}(z) \equiv g_{\beta_j}(z) = \begin{cases} e^{i\pi\beta_j}, & 0 \leq \arg z < \theta_j, \\ e^{-i\pi\beta_j}, & \theta_j \leq \arg z < 2\pi, \end{cases} \tag{12}$$

¹It is this equation which is responsible for the term “strong Szegő theorem”. Szegő’s first result, i.e. *Szegő limit theorem* produced the asymptotics of the determinant $D_L[\phi]$ up to an undetermined multiplicative constant.

²In [59], Szegő proved this theorem under a somewhat stronger smoothness assumption on the symbol; namely, he assumed that the symbol is positive, and that the symbol and its derivative are Lipschitz functions. It took a substantial period of time and the efforts of several very skillful analysts to reduce the smoothness conditions to the conditions (1)–(2) above. It also worth noticing that these conditions are already precise, i.e., if they do not satisfy, the asymptotics (8) may not hold.

³In writing the Fisher-Hartwig symbol in form (10) we follow the recent paper [20]. Equation (10) is slightly different from the one accepted in most of the literature devoted to the Fisher-Hartwig generating functions. The “translation” back to the standard form is easy. The main deviation from the standard form is that in (10) the product $z^{\sum_{j=0}^m \beta_j}$ is factored out which allow to better appreciate the non-triviality of the shifting some of the parameters β_j by integers.

$$\Re\alpha_j > -1/2, \beta_j \in \mathbb{C}, \quad j = 0, \dots, m, \tag{13}$$

and $V(z)$ is a sufficiently smooth function on the unit circle so that the first factor of the right hand side of (10) represents the ‘‘Szegő part’’ of the symbol. The condition on α_j insures integrability. As it has already been mentioned before, a single Fisher-Hartwig singularity at z_j consists of a root-type singularity

$$|z - z_j|^{2\alpha_j} = \left| 2 \sin \frac{\theta - \theta_j}{2} \right|^{2\alpha_j} \tag{14}$$

and a jump $g_{\beta_j}(z)$. A point $z_j, j = 1, \dots, m$ is included in (11) if and only if either $\alpha_j \neq 0$ or $\beta_j \neq 0$ (or both); in contrast, we always fix $z_0 = 1$ even if $\alpha_0 = \beta_0 = 0$ (note that $g_{\beta_0}(z) = e^{-i\pi\beta_0}$). Observe that for each $j = 1, \dots, m, z^{\beta_j} g_{\beta_j}(z)$ is continuous at $z = 1$, and so for each j each ‘‘beta’’ singularity produces a jump only at the point z_j .

In 1968, M. Fisher and R. Hartwig [26] suggested a formula for the leading term of the asymptotic behavior for the Toeplitz determinant generated by the symbol (10).⁴ The principal insight of Fisher and Hartwig was the observation that the singularities of the symbol yield the appearance of the power-like factors in the asymptotics. Indeed, in the case of all $\beta_j = 0$, the Fisher-Hartwig formula reads as follows.

$$D_L[\phi] \sim E_{\text{FH}}^0[\phi] L^{\sum_{j=0}^m \alpha_j^2} \exp(LV_0), \quad L \rightarrow \infty. \tag{15}$$

The pre-exponential constant factor, $E_{\text{FH}}^0[\phi]$, is more elaborated than its Szegő counterpart $E_{\text{Sz}}[\phi]$ from the Szegő equation (8). The description of $E_{\text{FH}}^0[\phi]$ involves a rather ‘‘exotic’’ special function—the Barnes’ G -function $G(x)$ which is defined by the equations (see e.g. [62]),

$$G(1+x) = (2\pi)^{x/2} e^{-(x+1)x/2 - \gamma_E x^2/2} \prod_{n=1}^{\infty} \{(1+x/n)^n e^{-x+x^2/(2n)}\}, \tag{16}$$

where γ_E is Euler constant and its numerical value is 0.5772156649... The G -function can be thought of as a ‘‘discrete antiderivative’’ of the Γ -function. The exact expression for $E_{\text{FH}}^0[\phi]$ is given by the equation (cf. (9)),

$$\begin{aligned} E_{\text{FH}}^0[\phi] = & \exp\left(\sum_{k=1}^{\infty} k V_k V_{-k}\right) \prod_{j=0}^m e^{\alpha_j (V_0 - V(z_j))} \\ & \times \prod_{0 \leq j < k \leq m} |z_j - z_k|^{-2\alpha_j \alpha_k} \prod_{j=0}^m \frac{G^2(1 + \alpha_j)}{G(1 + 2\alpha_j)}. \end{aligned} \tag{17}$$

The double product over $j < k$ is set to 1 if $m = 0$, so that in the absence of singularities, we are back to the strong Szegő limit theorem.

The Fisher-Hartwig formula (15) was proven in 1973 by H. Widom [63].

The presence of jumps, under the assumption $|\Re\beta_j - \Re\beta_k| < 1$, does not change the structure much of the large L behavior of the Toeplitz determinant $D_L[\phi]$. Indeed, it is still

⁴Some important partial results concerning the asymptotics of the Toeplitz determinants with singular symbols were also obtained by A. Lenard [44] and used by Fisher and Hartwig as a strong evidence in favor of their formula.

the combination of the exponential and the power terms with the exponential term being determined, as before, by only the Szegő part of the symbol while the power factor is determined by both the α and the β parameters of the Fisher-Hartwig part of the symbol. The Fisher-Hartwig formula for the general case of symbol (10) reads (cf. (15)),

$$D_L[\phi] \sim E_{\text{FH}}[\phi] L^{\sum_{j=0}^m (\alpha_j^2 - \beta_j^2)} \exp(LV_0), \quad L \rightarrow \infty. \tag{18}$$

The pre-exponential constant factor, $E_{\text{FH}}[\phi]$, is now even more complex than in the case of all $\beta_j = 0$. In addition to the Barnes’ G -function, it now involves the canonical Wiener-Hopf factorization of the Szegő part, $e^{V(z)}$, of the symbol $\phi(z)$,

$$e^{V(z)} = b_+(z)e^{V_0}b_-(z), \quad b_+(z) = e^{\sum_{k=1}^{\infty} V_k z^k}, \quad b_-(z) = e^{\sum_{k=-\infty}^{-1} V_k z^k}. \tag{19}$$

Note that $b_+(z)$ and $b_-(z)$ are analytic inside and outside of the unit circle $|z| = 1$, respectively, and they satisfy the normalization conditions $b_+(0) = b_-(\infty) = 1$. The exact expression for $E_{\text{FH}}[\phi]$ is given by the equation (cf. (9) and (17)),

$$\begin{aligned} E_{\text{FH}}[\phi] &= \exp\left(\sum_{k=1}^{\infty} k V_k V_{-k}\right) \prod_{j=0}^m b_+(z_j)^{-\alpha_j + \beta_j} b_-(z_j)^{-\alpha_j - \beta_j} \\ &\times \prod_{0 \leq j < k \leq m} |z_j - z_k|^{2(\beta_j \beta_k - \alpha_j \alpha_k)} \left(\frac{z_k}{z_j e^{i\pi}}\right)^{\alpha_j \beta_k - \alpha_k \beta_j} \\ &\times \prod_{j=0}^m \frac{G(1 + \alpha_j + \beta_j)G(1 + \alpha_j - \beta_j)}{G(1 + 2\alpha_j)} (1 + o(1)). \end{aligned} \tag{20}$$

The proof of the general Fisher-Hartwig formula (18) is due to E. Basor [8] for $\Re\beta_j = 0$, E. Basor [9] for $\alpha_j = 0$, $|\Re\beta_j| < 1/2$, A. Böttcher and B. Silbermann [16] for $|\Re\alpha_j| < 1/2$, $|\Re\beta_j| < 1/2$, T. Ehrhardt [25] for $|\Re\beta_j - \Re\beta_k| < 1$. The precise statement concerning the large L behavior of the Toeplitz determinant $D_L[\phi]$ with the Fisher-Hartwig generating function (10) is given by the following theorem.

Theorem 2 (T. Ehrhardt [25]) *Let $\phi(z)$ be defined in (10), $V(z)$ be C^∞ on the unit circle, $\Re\alpha_j > -1/2$, $|\Re\beta_j - \Re\beta_k| < 1$, and $\alpha_j \pm \beta_j \neq -1, -2, \dots$ for $j, k = 0, 1, \dots, m$. Then, as $L \rightarrow \infty$, the asymptotic behavior of the Toeplitz determinant $D_L[\phi]$ is given by the formulae (18)–(20).*

A. Böttcher and B. Silbermann [16] in 1985 and E. Basor and C. Tracy [11] in 1991 constructed examples with $\Re\beta_j$ not lying in a single interval of length less than 1 and such that the large L asymptotics is very different from the one given by (18). These examples have showed that for the asymptotics (18) to take place, the condition

$$|\Re\beta_j - \Re\beta_k| < 1, \quad \forall j, k = 0, 1, \dots, m, \tag{21}$$

is precise. In the case of arbitrary complex β_j , E. Basor and C. Tracy conjectured in [11] a very elegant structure of the large L asymptotics of the determinant $D_L[\phi]$. They based their arguments on the formal analysis of the behavior of the both sides of estimate (18) with respect to the shifts of the β -parameters by integers. A detail description of the Basor-Tracy conjecture can be found in the original paper [11] as well as in the recent work [20]

were this conjecture was actually proven with the help of the new technique—the *Riemann-Hilbert method*.

We refer the reader to monograph [17] and survey [25] for more on the mathematics of the Toeplitz determinants with the Fisher-Hartwig symbols.

For the Riemann-Hilbert approach in the theory of the Toeplitz determinants, we refer the reader to the papers [20] and [19] where the method was introduced (following the similar approach for the Hankel determinants [27] and the theory of integrable Fredholm determinants [33, 34]) and to the works [41, 42, 47, 48], where the method was further developed. The crucial role in the implementation of the Riemann-Hilbert approach to the Toeplitz determinants is played by the Deift-Zhou nonlinear steepest descent method of the asymptotic analysis of the oscillatory matrix Riemann-Hilbert problems [22] and by its orthogonal polynomial version [21].

2.2 Block Toeplitz Determinants

A general asymptotic representation of the determinant of a block Toeplitz matrix, which generalizes the classical strong Szegő theorem to the block matrix case, was obtained by Widom in [64–66] (see also more recent work [15] and references therein).

Theorem 3 (H. Widom [66]) *Let $\Phi(z)$ be a $N \times N$ matrix function defined on the unit circle and satisfying the conditions,*

1. $\det \Phi(\theta) \neq 0$, for all $\theta \in [0, 2\pi)$.
2. $\text{index } \det \Phi(\theta) \equiv \arg \det \Phi(2\pi) - \arg \det \Phi(0) = 0$.
3. $\sum_{k=-\infty}^{\infty} |\Phi_k| + \sum_{k=-\infty}^{\infty} |k| |\Phi_k|^2 < \infty$,

where Φ_k are the Fourier coefficients of $\Phi(\theta)$, and $|F|$ denote a matrix norm of the matrix F . Then, the asymptotic behavior of the block Toeplitz determinant generated by the symbol $\Phi(z)$ is given by the formulae,

$$D_L[\Phi] \sim E_W[\Phi] \exp\left(\frac{L}{2\pi} \int_0^{2\pi} \ln \det \Phi(\theta) d\theta\right), \quad L \rightarrow \infty, \tag{22}$$

$$E_W[\Phi] = \det(T_\infty[\Phi]T_\infty[\Phi^{-1}]), \tag{23}$$

where $T_\infty[\Phi]$ is a semi-infinite Toeplitz matrix,

$$T_\infty[\Phi] = (\Phi_{i-j}), \quad i, j = 1, 2, \dots \tag{24}$$

From the application point of view, there is an important difference between this result and the Szegő formula (8) for the case of scalar symbols. Indeed, the determinant in the right hand side of (23) is the Fredholm determinant of an infinite matrix, and already for 2×2 matrix symbols the question of effective evaluation of Widom’s pre-factor $E_W[\Phi]$ is a highly nontrivial one, even for a relatively simple matrix functions Φ . Indeed, up until very recently the only general class of matrix functions Φ for which such effective evaluation is possible has been the class of functions with at least one-side truncated Fourier series. This class was singled out by Widom himself in [64, 65], and this Widom’s result has been used in the recent paper [10] of E. Basor and T. Ehrhardt devoted to the dimer model.

Another class of matrix generating functions which admits an explicit evaluation of Widom’s constant are the algebraic symbols. This fact was demonstrated in the works [31,

32, 36] for important cases of the block Toeplitz determinants appearing in the analysis of the entanglement entropy in quantum spin chains. For this class of symbols, Widom’s pre-factor admits an explicit evaluation in terms of Jacobi and Riemann theta functions. To give a flavor of these results, we will now present a detail description of the asymptotics of the block Toeplitz determinant related to the XY spin model obtained in [31, 32]. We shall also use these formulae later in Sect. 4.

The Toeplitz determinant in question is generated by the 2×2 matrix symbol,

$$\Phi(z) = \begin{pmatrix} i\lambda & \phi(z) \\ -\phi^{-1}(z) & i\lambda \end{pmatrix} \tag{25}$$

and

$$\phi(z) = \sqrt{\frac{(z - z_1)(z - z_2)}{(1 - z_1z)(1 - z_2z)}}, \tag{26}$$

where $z_1 \neq z_2$ are complex nonzero numbers not lying on the unit circle. Following the needs of the XY model, we shall assume that the both points are from the right half plane though the result we present below can be easily generalized to the arbitrary position of the points z_1 and z_2 outside of the unit circle. We will also distinguish three possible locations of the points z_1 and z_2 on complex plane.

Case 1a: Both z_1 and z_2 are real, they lie outside of the unit circle, and we assume that $z_1 > z_2 > 1$.

Case 1b: Both z_1 and z_2 are complex, $z_1 = z_2^*$, and we assume that $\Re z_1 > 1$ and $\Im z_1 > 0$.

Case 2: Both z_1 and z_2 are real, they lie at the different sides of the unit circle, and we assume that $z_1 > z_2^{-1} > 1$.

The reason why the Cases 1a and 1b are considered as sub-cases of a single case is that in the both these cases all the root singularities of the function $\phi(z)$ defined in (26) are inside of the unite circle while all its zeros are outside. In Case 2, the zeros and the singularities are evenly distributed between the inside and the outside of the unit circle. This difference in the position of the roots and singularities of $\phi(z)$ has an impact to the derivations of the asymptotics and, as we see below, is reflected in the form of the final answer. We shall also see that in the context of the XY model, Case 1 and Case 2 correspond to the small ($h < 2$) and large ($h > 2$) magnetic field, respectively.

The complex parameter λ plays role of a spectral parameter for the Toeplitz matrix generated by the symbol,

$$\Phi_0(z) \equiv -\Phi(z)|_{\lambda=0} = \begin{pmatrix} 0 & -\phi(z) \\ \phi^{-1}(z) & 0 \end{pmatrix}. \tag{27}$$

Hence the Toeplitz determinant $D_L[\Phi]$ we are dealing with is in fact a Toeplitz *characteristic* determinant,

$$D_L[\Phi] \equiv D_L(\lambda) = \det(i\lambda I_{2L} - T_L[\Phi_0]). \tag{28}$$

Given the branch points z_j of the symbol $\Phi(z)$, we introduce now the elliptic curve,

$$w^2(z) = (z - z_1)(z - z_2)(z - z_2^{-1})(z - z_1^{-1}). \tag{29}$$

Let us also re-label the branch points of this curve by the letters $\lambda_A, \lambda_B, \lambda_C,$ and $\lambda_D,$ according to the following rule. Case 1a: $\lambda_A = z_1^{-1}, \lambda_B = z_2^{-1}, \lambda_C = z_2, \lambda_D = z_1$; Case 1b:

$\lambda_A = z_1^{-1}, \lambda_B = z_2^{-1}, \lambda_C = z_1, \lambda_D = z_2$; Case 2: $\lambda_A = z_1^{-1}, \lambda_B = z_2, \lambda_C = z_2^{-1}, \lambda_D = z_1$. Observe that λ_A and λ_B are always inside the unite circle while λ_C and λ_D are always outside. This new relabeling of the branch points allows to introduce the module parameter of elliptic curve (29) in the universal way,

$$\tau = \frac{2}{c} \int_{\lambda_B}^{\lambda_C} \frac{dz}{w(z)}, \quad c = 2 \int_{\lambda_A}^{\lambda_B} \frac{dz}{w(z)}. \tag{30}$$

Theorem 4 ([31, 32]) *Let*

$$\theta_3(s) = \sum_{n=-\infty}^{\infty} e^{\pi i \tau n^2 + 2\pi i s n}, \tag{31}$$

where τ is taken from (30), be the third Jacobi theta-function associated with the curve (29). Then, the large L asymptotic behavior of the determinant $D_L(\lambda)$ is given by the equations,

$$D_L(\lambda) \sim \frac{\theta_3(\beta(\lambda) + \frac{\sigma\tau}{2})\theta_3(\beta(\lambda) - \frac{\sigma\tau}{2})}{\theta_3^2(\frac{\sigma\tau}{2})} (1 - \lambda^2)^L, \quad L \rightarrow \infty \tag{32}$$

where

$$\beta(\lambda) = \frac{1}{2\pi i} \ln \frac{\lambda + 1}{\lambda - 1}, \tag{33}$$

and $\sigma = 1$ in Case 1 and $\sigma = 0$ in Case 2.

Remark The theta-functions involved in the asymptotic formula (32) has zeros at the points

$$\pm\lambda_m, \quad \lambda_m = \tanh\left(m + \frac{1 - \sigma}{2}\right)\pi\tau_0, \quad m \geq 0, \tag{34}$$

where,

$$\tau_0 = -i\tau = -i \frac{\int_{\lambda_B}^{\lambda_C} \frac{dz}{w(z)}}{\int_{\lambda_A}^{\lambda_B} \frac{dz}{w(z)}} > 0.$$

The asymptotics (32) is uniform outside of the arbitrary fixed neighborhoods of the points $\lambda = \pm 1$ and $\lambda = \pm\lambda_m$.

Observe that in the case under consideration, $\det \Phi(z) \equiv 1 - \lambda^2$. Therefore, the last factor in (32) is exactly the exponential term of the general Widom-Szegö formula (22) written for symbol (25). The rest of (32) gives then the corresponding Widom’s constant, i.e.

$$E_W[\Phi] = \frac{\theta_3(\beta(\lambda) + \frac{\sigma\tau}{2})\theta_3(\beta(\lambda) - \frac{\sigma\tau}{2})}{\theta_3^2(\frac{\sigma\tau}{2})}. \tag{35}$$

Similar formulae for the case of the more general quantum spin chains were obtained in [36]. The relevant generating function has the same matrix structure (25) with the scalar function $\phi(z)$ defined by the equation,

$$\phi(z) := \sqrt{\frac{p(z)}{z^{2n} p(1/z)}} \tag{36}$$

and $p(z)$ is a polynomial of degree $2n$. The analog of the formulae (32)–(35) in the case $n > 1$ involves, instead of elliptic, the hyperelliptic integrals and, instead of the Jacobi theta-function, the $2n - 1$ dimensional Riemann theta-function.

The methods that lead to these results, involves the theory of integrable Fredholm operators [19, 30, 33, 34] and the use of the algebrageometric techniques of the soliton theory (see e.g. [12]).

3 XY Model and Block Entropy

The Hamiltonian of XY model can be written as

$$H = - \sum_{n=-\infty}^{\infty} (1 + \gamma)\sigma_n^x \sigma_{n+1}^x + (1 - \gamma)\sigma_n^y \sigma_{n+1}^y + h\sigma_n^z. \tag{37}$$

Here $\sigma_n^x, \sigma_n^y, \sigma_n^z$ are Pauli matrices and h is a magnetic field; Without loss generality, the anisotropy parameter γ can be taken as $0 \leq \gamma < 1$; Case with $\gamma = 0$ is usually called XX model. The model was solved in [1–3, 6, 7, 46] and it owns a unique ground state $|GS\rangle$. The Toeplitz determinants were used for evaluation of some correlation functions [7, 57, 58]; Integrable Fredholm operators were used for calculation of other correlations [23, 35, 38]. When the system is in the ground state, the entropy for this whole system is zero but the entropy of a sub-system can be positive. We calculate the entropy of a sub-system (a block of L neighboring spins) which can measure the entanglement between this sub-system and the rest part [37]. We treat the whole chain as a binary system $|GS\rangle = |A\&B\rangle$, where we denote the block of L neighboring spins by sub-system A and the rest part by sub-system B . The density matrix of the ground state can be denoted by $\rho_{AB} = |GS\rangle\langle GS|$. The density matrix of sub-system A is $\rho_A = \text{Tr}_B(\rho_{AB})$. Von Neumann entropy $S(\rho_A)$ of the sub-system A can be represented as following:

$$S(\rho_A) = - \text{Tr}_A(\rho_A \ln \rho_A). \tag{38}$$

This entropy also defines the dimension of the Hilbert space of states of the block of L spins.

3.1 Derivation

Following Ref. [46], let us introduce two Majorana operators

$$c_{2l-1} = \left(\prod_{n=1}^{l-1} \sigma_n^z \right) \sigma_l^x \quad \text{and} \quad c_{2l} = \left(\prod_{n=1}^{l-1} \sigma_n^z \right) \sigma_l^y, \tag{39}$$

on each site of the spin chain. Operators c_n are hermitian and obey the anti-commutation relations $\{c_m, c_n\} = 2\delta_{mn}$. In terms of operators c_n , Hamiltonian H_{XX} can be rewritten as

$$H_{XX}(h) = i \sum_{n=1}^N (c_{2n}c_{2n+1} - c_{2n-1}c_{2n+2} + hc_{2n-1}c_{2n}). \tag{40}$$

Here different boundary effects can be ignored because we are only interested in cases with $N \rightarrow \infty$. This Hamiltonian can be subsequently diagonalized by linearly transforming the operators c_n . It has been obtained [6, 46] (also see [43, 45, 61]) that

$$\langle GS|c_m|GS\rangle = 0, \quad \langle GS|c_m c_n|GS\rangle = \delta_{mn} + i(\mathbf{B}_N)_{mn}. \tag{41}$$

Here matrix \mathbf{B}_N can be written in a block form as

$$\mathbf{B}_N = \begin{pmatrix} \Pi_0 & \Pi_{-1} & \dots & \Pi_{1-N} \\ \Pi_1 & \Pi_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ \Pi_{N-1} & \dots & \dots & \Pi_0 \end{pmatrix} \quad \text{and} \quad \Pi_l = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-i l \theta} \Phi_0(\theta), \quad (42)$$

where both Π_l and $\Phi_0(\theta)$ (for $N \rightarrow \infty$) are 2×2 matrix,

$$\Phi_0(\theta) = \begin{pmatrix} 0 & \phi(\theta) \\ -\phi^{-1}(\theta) & 0 \end{pmatrix} \quad \text{and} \quad \phi(\theta) = \frac{\cos \theta - i\gamma \sin \theta - h/2}{|\cos \theta - i\gamma \sin \theta - h/2|}. \quad (43)$$

Other correlations such as $\langle GS|c_m \dots c_n|GS \rangle$ are obtainable by Wick theorem. The Hilbert space of sub-system A can be spanned by $\prod_{i=1}^L \{\sigma_i^-\}^{p_i} |0\rangle_F$, where σ_i^\pm is Pauli matrix, p_i takes value 0 or 1, and vector $|0\rangle_F$ denotes the ferromagnetic state with all spins up. It's possible to construct a set of fermionic operators b_i and b_i^+ by defining

$$d_m = \sum_{n=1}^{2L} v_{mn} c_n, \quad m = 1, \dots, 2L; \quad b_l = (d_{2l} + i d_{2l+1})/2, \quad l = 1, \dots, L \quad (44)$$

with $v_{mn} \equiv (\mathbf{V})_{mn}$. Here the matrix \mathbf{V} is an orthogonal matrix. It's easy to verify that d_m is hermitian operator and

$$b_l^+ = (d_{2l} - i d_{2l+1})/2, \quad \{b_i, b_j\} = 0, \quad \{b_i^+, b_j^+\} = 0, \quad \{b_i^+, b_j\} = \delta_{i,j}. \quad (45)$$

In terms of fermionic operators b_i and b_i^+ , the Hilbert space can also be spanned by $\prod_{i=1}^L \{b_i^+\}^{p_i} |0\rangle_{vac}$. Here p_i takes value 0 or 1, $2L$ fermionic operators b_i, b_i^+ and vacuum state $|0\rangle_{vac}$ can be constructed by requiring

$$b_l |0\rangle_{vac} = 0, \quad l = 1, \dots, L. \quad (46)$$

We shall choose a specific orthogonal matrix \mathbf{V} later.

Let $\{\psi_I\}$ be a set of orthogonal basis for Hilbert space of any physical system. Then the most general form for density matrix of this physical system can be written as

$$\rho = \sum_{I,J} c(I, J) |\psi_I\rangle \langle \psi_J|. \quad (47)$$

Here $c(I, J)$ are complex coefficients. We can introduce a set of operators $P(I, J)$ by $P(I, J) \propto |\psi_I\rangle \langle \psi_J|$ and $\tilde{P}(I, J)$ satisfying

$$\tilde{P}(I, J) P(J, K) = \delta_{I,K} |\psi_I\rangle \langle \psi_I|, \quad P(I, J) \tilde{P}(J, K) = \delta_{I,K} |\psi_I\rangle \langle \psi_I|. \quad (48)$$

There is no summation over a repeated index in these formula. We shall use an explicit summation symbol through the whole paper. Then we can write the density matrix as

$$\rho = \sum_{I,J} \tilde{c}(I, J) P(I, J), \quad \tilde{c}(I, J) = \text{Tr}(\rho \tilde{P}(J, I)). \quad (49)$$

Now let us consider the quantum spin chain defined in (37). For the sub-system A, the complete set of operators $P(I, J)$ can be generated by $\prod_{i=1}^L O_i$. Here we take operator O_i to be

any one of the four operators $\{b_i^+, b_i, b_i^+ b_i, b_i b_i^+\}$ (Remember that b_i and b_i^+ are fermionic operators defined in (44)). It's easy to find that $\tilde{P}(J, I) = (\prod_{i=1}^L O_i)^\dagger$ if $P(I, J) = \prod_{i=1}^L O_i$. Here \dagger means hermitian conjugation. Therefore, the reduced density matrix for sub-system A can be represented as

$$\rho_A = \sum \text{Tr}_{AB} \left(\rho_{AB} \left(\prod_{i=1}^L O_i \right)^\dagger \right) \prod_{i=1}^L O_i. \tag{50}$$

Here the summation is over all possible different terms $\prod_{i=1}^L O_i$. For the whole system to be in pure state $|GS\rangle$, the density matrix ρ_{AB} is represented by $|GS\rangle\langle GS|$. Then we have the expression for ρ_A as following

$$\rho_A = \sum \langle GS | \left(\prod_{i=1}^L O_i \right)^\dagger | GS \rangle \prod_{i=1}^L O_i. \tag{51}$$

This is the expression of density matrix with the coefficients related to multi-point correlation functions. These correlation functions are well studied in the physics literature [14]. Now let us choose matrix \mathbf{V} in (44) so that the set of fermionic basis $\{b_i^+\}$ and $\{b_i\}$ satisfy an equation

$$\langle GS | b_i b_j | GS \rangle = 0, \quad \langle GS | b_i^+ b_j | GS \rangle = \delta_{i,j} \langle GS | b_i^+ b_i | GS \rangle. \tag{52}$$

Then the reduced density matrix ρ_A represented as sum of products in (51) can be represented as a product of sums

$$\rho_A = \prod_{i=1}^L (\langle GS | b_i^+ b_i | GS \rangle b_i^+ b_i + \langle GS | b_i b_i^+ | GS \rangle b_i b_i^+). \tag{53}$$

Here we used the equations $\langle GS | b_i | GS \rangle = 0 = \langle GS | b_i^+ | GS \rangle$ and Wick theorem. This fermionic basis was suggested in Refs. [43, 45, 61].

Now let us find a matrix \mathbf{V} in (44), which will block-diagonalize the correlation functions of Majorana operators c_n . From (44) and (42), we have the following expression for correlation function of d_n operators:

$$\begin{aligned} \langle GS | d_m d_n | GS \rangle &= \sum_{i=1}^{2L} \sum_{j=1}^{2L} v_{mi} \langle GS | c_i c_j | GS \rangle v_{jn}, \\ \langle GS | c_m c_n | GS \rangle &= \delta_{mn} + i(\mathbf{B}_L)_{mn}, \\ \langle GS | d_m d_n | GS \rangle &= \delta_{mn} + i(\tilde{\mathbf{B}}_L)_{mn}. \end{aligned} \tag{54}$$

The last equation is the definition of a matrix $\tilde{\mathbf{B}}_L$. Matrix \mathbf{B}_L is the sub-matrix of \mathbf{B}_N defined in (42) with $m, n = 1, 2, \dots, L$. We also require $\tilde{\mathbf{B}}_L$ to be the form [43, 45, 61]

$$\tilde{\mathbf{B}}_L = \mathbf{V} \mathbf{B}_L \mathbf{V}^T = \bigoplus_{m=1}^L v_m \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \Omega \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{55}$$

Here the matrix Ω is a diagonal matrix with elements v_m (all v_m are real numbers). Therefore, choosing matrix \mathbf{V} satisfying (55) in (44), we obtain $2L$ operators $\{b_l\}$ and $\{b_l^+\}$ with

following expectation values

$$\begin{aligned} \langle GS|b_m|GS\rangle &= 0, & \langle GS|b_m b_n|GS\rangle &= 0, \\ \langle GS|b_m^\dagger b_n|GS\rangle &= \delta_{mn} \frac{1 + v_m}{2}. \end{aligned} \tag{56}$$

Using the simple expression for reduced density matrix ρ_A in (53), we obtain

$$\rho_A = \prod_{i=1}^L \left(\frac{1 + v_i}{2} b_i^\dagger b_i + \frac{1 - v_i}{2} b_i b_i^\dagger \right). \tag{57}$$

This form immediately gives us all the eigenvalues $\lambda_{x_1 x_2 \dots x_L}$ of reduced density matrix ρ_A ,

$$\lambda_{x_1 x_2 \dots x_L} = \prod_{i=1}^L \frac{1 + (-1)^{x_i} v_i}{2}, \quad x_i = 0, 1, \forall i. \tag{58}$$

Note that in total we have 2^L eigenvalues. Hence, the entropy of ρ_A from (38) becomes

$$S(\rho_A) = \sum_{m=1}^L e(1, v_m) \tag{59}$$

with

$$e(x, v) = -\frac{x + v}{2} \ln\left(\frac{x + v}{2}\right) - \frac{x - v}{2} \ln\left(\frac{x - v}{2}\right). \tag{60}$$

3.2 XX Model

Notice further that for XX model, i.e. $\gamma = 0$ case, matrix \mathbf{B}_L can have a direct product form

$$\mathbf{B}_L = \mathbf{G}_L \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \text{with } \mathbf{G}_L = \begin{pmatrix} \phi_0 & \phi_{-1} & \dots & \phi_{1-L} \\ \phi_1 & \phi_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ \phi_{L-1} & \dots & \dots & \phi_0 \end{pmatrix}, \tag{61}$$

where ϕ_l is defined as

$$\phi_l = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-il\theta} \phi(\theta), \quad \phi(\theta) = \begin{cases} 1, & -k_F < \theta < k_F, \\ -1, & k_F < \theta < (2\pi - k_F) \end{cases} \tag{62}$$

and $k_F = \arccos(|h|/2)$. From (55) and (61), we conclude that all v_m are just the eigenvalues of real symmetric matrix \mathbf{G}_L .

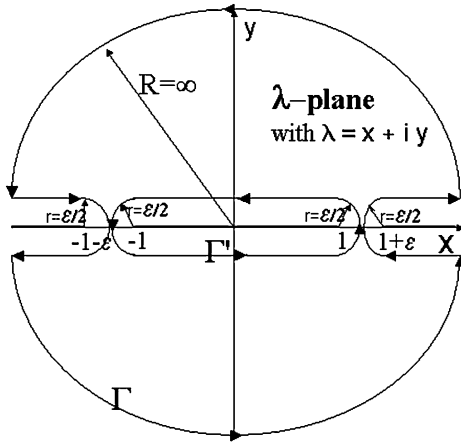
However, to obtain all eigenvalues v_m directly from matrix \mathbf{G}_L is a non-trivial task. Let us introduce

$$D_L(\lambda) = \det(\tilde{\mathbf{G}}_L(\lambda) \equiv \lambda I_L - \mathbf{G}_L). \tag{63}$$

Here $\tilde{\mathbf{G}}_L$ is a Toeplitz matrix and I_L is the identity matrix of dimension L. Obviously we also have

$$D_L(\lambda) = \prod_{m=1}^L (\lambda - v_m). \tag{64}$$

Fig. 1 Contours Γ' (smaller one) and Γ (larger one). Bold lines $(-\infty, -1 - \epsilon)$ and $(1 + \epsilon, \infty)$ are the cuts of integrand $e(1 + \epsilon, \lambda)$. Zeros of $D_L(\lambda)$ (see (64)) are located on bold line $(-1, 1)$. The arrow is the direction of the route of integral we take and r and R are the radius of circles



From the Cauchy residue theorem and analytical property of $e(x, v)$, then $S(\rho_A)$ can be rewritten as

$$S(\rho_A) = \lim_{\epsilon \rightarrow 0^+} \frac{1}{2\pi i} \oint_{\Gamma'} d\lambda e(1 + \epsilon, \lambda) \frac{d}{d\lambda} \ln D_L(\lambda). \tag{65}$$

Here the contour Γ' in Fig. 1 encircles all zeros of $D_L(\lambda)$ and function $e(1 + \epsilon, \lambda)$ is analytic within the contour. Just like the Toeplitz matrix \mathbf{G}_L is generated by function $\phi(\theta)$ in (61) and (62), the Toeplitz matrix $\tilde{\mathbf{G}}_L(\lambda)$ is generated by function $\tilde{\phi}(\theta)$ defined by

$$\tilde{\phi}(\theta) = \begin{cases} \lambda - 1, & -k_F < \theta < k_F, \\ \lambda + 1, & k_F < \theta < (2\pi - k_F). \end{cases} \tag{66}$$

Notice that $\tilde{\phi}(\theta)$ is a piecewise constant function of θ on the unit circle, with jumps at $\theta = \pm k_F$. Hence, if one can obtain the determinant of this Toeplitz matrix analytically, one will be able to get a closed analytical result for $S(\rho_A)$ which is our new result. Now, the calculation of $S(\rho_A)$ reduces to the calculation of the determinant of the Toeplitz matrix $\tilde{\mathbf{G}}_L(\lambda)$.

3.3 XY Model

Similarly let us introduce:

$$\tilde{\mathbf{B}}_L(\lambda) = i\lambda I_L - \mathbf{B}_L, \quad D_L(\lambda) = \det \tilde{\mathbf{B}}_L(\lambda). \tag{67}$$

Here I_L is the identity matrix of dimension $2L$. By definition, we have

$$D_L(\lambda) = (-1)^L \prod_{m=1}^L (\lambda^2 - v_m^2). \tag{68}$$

Using again the Cauchy residue theorem we obtain that, similar to (65),

$$S(\rho_A) = \lim_{\epsilon \rightarrow 0^+} \frac{1}{4\pi i} \oint_{\Gamma'} d\lambda e(1 + \epsilon, \lambda) \frac{d}{d\lambda} \ln D_L(\lambda). \tag{69}$$

Here the contour Γ' in Fig. 1 encircles all zeros of $D_L(\lambda)$.

z-plane with $z = x + i y$

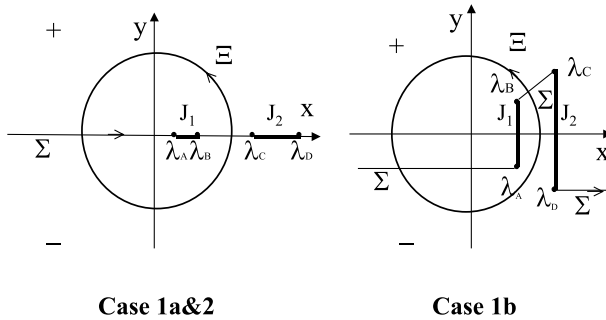


Fig. 2 Polygonal line Σ (direction as labeled) separates the complex z plane into the two parts: the part Ω_+ which lies to the left of Σ , and the part Ω_- which lies to the right of Σ . Curve Ξ is the unit circle in anti-clockwise direction. Cuts J_1, J_2 for functions $\phi(z), w(z)$ are labeled by *bold* on line Σ . Definition of the end points of the cuts λ_{\dots} depends on the case: Case 1a: $\lambda_A = \lambda_1$ and $\lambda_B = \lambda_2^{-1}, \lambda_C = \lambda_2$ and $\lambda_D = \lambda_1^{-1}$. Case 1b: $\lambda_A = \lambda_1$ and $\lambda_B = \lambda_2^{-1}, \lambda_C = \lambda_1^{-1}$ and $\lambda_D = \lambda_2$. Case 2: $\lambda_A = \lambda_1$ and $\lambda_B = \lambda_2, \lambda_C = \lambda_2^{-1}$ and $\lambda_D = \lambda_1^{-1}$

We also realized that $\tilde{\mathbf{B}}_L(\lambda)$ is the block Toeplitz matrix with the generator $\Phi(z)$, i.e.

$$\tilde{\mathbf{B}}_L(\lambda) = \begin{pmatrix} \tilde{\Pi}_0 & \tilde{\Pi}_{-1} & \dots & \tilde{\Pi}_{1-L} \\ \tilde{\Pi}_1 & \tilde{\Pi}_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ \tilde{\Pi}_{L-1} & \dots & \dots & \tilde{\Pi}_0 \end{pmatrix} \tag{70}$$

with

$$\tilde{\Pi}_l = \frac{1}{2\pi i} \oint_{\Xi} dz z^{-l-1} \Phi(z), \quad \Phi(z) = \begin{pmatrix} i\lambda & \phi(z) \\ -\phi^{-1}(z) & i\lambda \end{pmatrix} \tag{71}$$

and

$$\phi(z) = \left(\frac{\lambda_1^* (1 - \lambda_1 z)(1 - \lambda_2 z^{-1})}{\lambda_1 (1 - \lambda_1^* z^{-1})(1 - \lambda_2^* z)} \right)^{1/2}. \tag{72}$$

We fix the branch by requiring that $\phi(\infty) > 0$. We use $*$ to denote complex conjugation and Ξ the unit circle shown in Fig. 2. λ_1 and λ_2 are defined differently for different values of γ and h . There are following three different cases:

In Case 1a ($2\sqrt{1 - \gamma^2} < h < 2$) and Case 2 ($h > 2$), both λ_1 and λ_2 are real

$$\lambda_1 = \frac{h - \sqrt{h^2 - 4(1 - \gamma^2)}}{2(1 + \gamma)}, \quad \lambda_2 = \frac{1 + \gamma}{1 - \gamma} \lambda_1. \tag{73}$$

In Case 1b ($h^2 < 4(1 - \gamma^2)$), both λ_1 and λ_2 are complex

$$\lambda_1 = \frac{h - i\sqrt{4(1 - \gamma^2) - h^2}}{2(1 + \gamma)}, \quad \lambda_2 = 1/\lambda_1^*. \tag{74}$$

Note that in the Case 1 the poles of function $\phi(z)$ (see (72)) coincide with the points λ_A and λ_B , while in the Case 2 they coincide with the points λ_A and λ_C .

4 Block Entropy of XX Model and the Fisher-Hartwig Formula

From (65), one needs the calculation of the Toeplitz determinant $D_L(\lambda)$ with a singular generating function

$$\tilde{\phi}(\theta) = \begin{cases} \lambda - 1, & -k_F < \theta < k_F, \\ \lambda + 1, & k_F < \theta < (2\pi - k_F). \end{cases} \tag{75}$$

It is easy to check that this function admits the canonical Fisher-Hartwig factorization given by (10) with

$$\begin{aligned} m &= 2, & \alpha_j &= 0 \quad \forall j, \\ \beta_0 &= 0, & \beta_2 = -\beta_1 &\equiv \beta(\lambda) = \frac{1}{2\pi i} \ln \frac{\lambda + 1}{\lambda - 1}, \end{aligned} \tag{76}$$

and

$$e^{V(z)} \equiv e^{V_0} = (\lambda + 1) \left(\frac{\lambda + 1}{\lambda - 1} \right)^{-k_F/\pi}. \tag{77}$$

The branch of the logarithm is fixed by the condition,

$$-\pi \leq \arg\left(\frac{\lambda + 1}{\lambda - 1}\right) < \pi., \tag{78}$$

For $\lambda \notin [-1, 1]$, the left inequality is also strict, and hence $|\Re(\beta_1(\lambda))| < \frac{1}{2}$ and $|\Re(\beta_2(\lambda))| < \frac{1}{2}$. Therefore, Theorem 2 is applicable (indeed, even its earlier weaker version proven by É. Basor [9] would suffice) and we see that the determinant $D_L(\lambda)$ of $\lambda L - \mathbf{G}_L$ can be asymptotically represented as

$$\begin{aligned} D_L(\lambda) &= \left(2 - 2 \cos(2k_F)\right)^{-\beta^2(\lambda)} \left\{ G(1 + \beta(\lambda)) G(1 - \beta(\lambda)) \right\}^2 \\ &\times \left\{ (\lambda + 1) \left((\lambda + 1)/(\lambda - 1) \right)^{-k_F/\pi} \right\}^L L^{-2\beta^2(\lambda)}. \end{aligned} \tag{79}$$

Here G is, as before, the Barnes G -function and

$$G(1 + \beta(\lambda)) G(1 - \beta(\lambda)) = e^{-(1+\gamma_E)\beta^2(\lambda)} \prod_{n=1}^{\infty} \left\{ \left(1 - \frac{\beta^2(\lambda)}{n^2}\right)^n e^{\beta^2(\lambda)/n^2} \right\}. \tag{80}$$

Let us substitute the asymptotic form (79) into (65) and after some simplification [37], we have that

$$S(\rho_A) = \frac{1}{3} \ln L + \frac{1}{6} \ln \left(1 - \left(\frac{h}{2}\right)^2\right) + \frac{\ln 2}{3} + \Upsilon_1, \quad L \rightarrow \infty \tag{81}$$

with

$$\Upsilon_1 = - \int_0^{\infty} dt \left\{ \frac{e^{-t}}{3t} + \frac{1}{t \sinh^2(t/2)} - \frac{\cosh(t/2)}{2 \sinh^3(t/2)} \right\} \tag{82}$$

for XX model. The leading term of asymptotic of the entropy $\frac{1}{3} \ln L$ in (81) was first obtained based on numerical calculation and a simple conformal argument in Refs. [43, 45, 61] in the context of entanglement. We also want to mention that a complete conformal derivation for this entropy was found in Ref. [40]. One can numerically evaluate Υ_1 to very high accuracy to be $0.4950179\dots$. For zero magnetic field ($h = 0$) case, the constant term $\Upsilon_1 + \ln 2/3$ for $S(\rho_A)$ is close to but different from $(\pi/3) \ln 2$, which can be found by taking numerical accuracy to be more than five digits.

5 Block Entropy of XY Model and the Block Toeplitz Determinants

For the block entropy of XY model, by virtue of (69), our objective becomes the asymptotic calculation of the determinant of the block Toeplitz matrix $D_L(\lambda)$ or, rather, its λ -derivative $\frac{d}{d\lambda} \ln D_L(\lambda)$.

Let us denote,

$$z_1 := \lambda_1^{-1}, \quad \text{and} \quad z_2 := \lambda_2. \tag{83}$$

It is easy to check that the generating function introduced in (71)–(72) coincides with the one introduced in (25)–(26) together with the case-separations and the $\lambda_A - \lambda_D$ labeling of the branch points. Hence one can use Theorem 4 and substitute the asymptotic form (32) into (69). Deforming the original contour of integration to the contour Γ as indicated in Fig. 1 we arrive at the following expression for the entropy [31, 32]:

$$S(\rho_A) = \frac{1}{2} \int_1^\infty \ln \left(\frac{\theta_3(\beta(\lambda) + \frac{\sigma\tau}{2})\theta_3(\beta(\lambda) - \frac{\sigma\tau}{2})}{\theta_3^2(\frac{\sigma\tau}{2})} \right) d\lambda, \tag{84}$$

which can also be written in the form,

$$S(\rho_A) = \frac{\pi}{2} \int_0^\infty \ln \left(\frac{\theta_3(ix + \frac{\sigma\tau}{2})\theta_3(ix - \frac{\sigma\tau}{2})}{\theta_3^2(\frac{\sigma\tau}{2})} \right) \frac{dx}{\sinh^2(\pi x)}. \tag{85}$$

This is a limiting expression as $L \rightarrow \infty$. In [32] it is also proven that the corrections in (84) are of order of $O(\lambda_c^{-L}/\sqrt{L})$.

The entropy has singularities at *phase transitions*. When $\tau \rightarrow 0$ we can use Landen transform (see [62]) to get the following estimate of the theta-function for small τ and pure imaginary s :

$$\ln \frac{\theta_3(s \pm \frac{\sigma\tau}{2})}{\theta_3(\frac{\sigma\tau}{2})} = \frac{\pi}{i\tau} s^2 \mp \pi i \sigma s + O\left(\frac{e^{-i\pi/\tau}}{\tau^2} s^2\right), \quad \text{as } \tau \rightarrow 0.$$

Now the leading term in the expression for the entropy (84) can be replaced by

$$S(\rho_A) = \frac{i\pi}{6\tau} + O\left(\frac{e^{-i\pi/\tau}}{\tau^2}\right) \quad \text{for } \tau \rightarrow 0. \tag{86}$$

Let us consider two physical situations corresponding to small τ depending on the case defined on the page 2:

1. *Critical magnetic field:* $\gamma \neq 0$ and $h \rightarrow 2$.

This is included in our Case 1a and Case 2, when $h > 2\sqrt{1 - \gamma^2}$. As $h \rightarrow 2$ the end points of the cuts $\lambda_B \rightarrow \lambda_C$, so τ given by (30) simplifies and we obtain from (86) that the entropy is:

$$S(\rho_A) = -\frac{1}{6} \ln |2 - h| + \frac{1}{3} \ln 4\gamma, \quad \text{for } h \rightarrow 2 \text{ and } \gamma \neq 0 \tag{87}$$

correction is $O(|2 - h| \ln^2 |2 - h|)$. This limit agrees with predictions of conformal approach [18, 40]. The first term in the right hand side of (87) can be represented as $(1/6) \ln \xi$, this confirms a conjecture of [18]. The correlation length ξ was evaluated in [6].

2. *An approach to the XX model:* $\gamma \rightarrow 0$ and $h < 2$: It is included in Case 1b, when $0 < h < 2\sqrt{1 - \gamma^2}$. Now $\lambda_B \rightarrow \lambda_C$ and $\lambda_A \rightarrow \lambda_D$, we can calculate τ explicitly. The entropy becomes:

$$S^0(\rho_A) = -\frac{1}{3} \ln \gamma + \frac{1}{6} \ln(4 - h^2) + \frac{1}{3} \ln 2, \quad \text{for } \gamma \rightarrow 0 \text{ and } h < 2 \tag{88}$$

correction is $O(\gamma \ln^2 \gamma)$. This agrees with [37] (see also (81)).

As it has already been indicated, the theta-functions involved in the asymptotic formula (32) has zeros at the points $\pm\lambda_m$ which are defined in (34). Theorem 4 shows, in particular, that in the large L limit, the points $\pm\lambda_m$ are double zeros of the $D_L(\lambda)$. More precisely, we see that in the large L limit the eigenvalues v_{2m} and v_{2m+1} from (59) merge to λ_m :

$$v_{2m}, v_{2m+1} \rightarrow \lambda_m, \tag{89}$$

which in turn implies (cf. (59)) the following equivalent description of the limiting entropy $S(\rho_A)$ [31].

The limiting entropy, $S(\rho_A)$, of the subsystem can be identified with the infinite convergent series,

$$S(\rho_A) = \sum_{m=-\infty}^{\infty} e(1, \lambda_m) = \sum_{m=-\infty}^{\infty} (1 + \lambda_m) \ln \frac{2}{1 + \lambda_m}. \tag{90}$$

Indeed, (90) follows from the substitution of (32) into (69) and integrating over the *original* contour Γ' of Fig. 1.

It is also worth mentioning that relation (89) also indicates the degeneracy of the spectrum of the matrix \mathbf{B}_L and an appearance of an *extra symmetry* in the large L limit.

Remark These numbers λ_m satisfy an estimate:

$$|\lambda_{m+1} - \lambda_m| \leq 4\pi \tau_0 \quad \text{with} \quad \tau_0 = -i\tau.$$

This means that $(\lambda_{m+1} - \lambda_m) \rightarrow 0$ as $\tau \rightarrow 0$ for every m . This is useful for understanding of large L limit of the XX case corresponding to $\gamma \rightarrow 0$, as considered in [37]. The estimate explains why in the XX case the singularities of the logarithmic derivative of the Toeplitz determinant $d \ln D_L(\lambda)/d\lambda$ form a cut along the interval $[-1, 1]$, while in the XY case it has a discrete set of poles at points $\pm\lambda_m$ of (34).

The higher genus analog of formula (84) for the class of quantum spin chains introduced by J. Keating and F. Mezzadri in [39] has been obtained in [36].

Remark It was shown by Peschel in [51] (who also suggested an alternative heuristic derivation of (90) based on the work [18]), the series (90) can be summed up to an elementary function of the complete elliptic integrals corresponding to the modular parameter τ —see (109) and (110) below. It is an open problem whether an analogous representation of the integral equation (84) exists for higher genus. The key issue here is the extreme complexity of the identification of the zero divisor of the theta-functions in the dimension greater than 1.

6 Renyi Entropy and the Spectrum of Reduced Density Matrix of XY Model

The Renyi entropy of $S_\alpha(\rho_A)$ of the block of spins is defined by the expression

$$S_\alpha(\rho_A) = \frac{1}{1 - \alpha} \ln \text{Tr}(\rho_A^\alpha), \quad \alpha \neq 1 \text{ and } \alpha > 0. \tag{91}$$

Here the power α is a parameter. The Renyi entropy is intimately related to the spectrum of the reduced density matrix ρ_A . Indeed, let λ_n , ($0 < \lambda_n < 1$) and a_n denote the eigenvalues and their multiplicities of the operator ρ_A . The spectrum is completely determined by its momentum function, i.e. by the ζ -function of ρ_A ,

$$\zeta_{\rho_A}(\alpha) = \sum_{n=0}^{\infty} a_n \lambda_n^\alpha. \tag{92}$$

The obvious equation takes place,

$$\zeta_{\rho_A}(\alpha) = e^{(1-\alpha)S_R(\rho_A, \alpha)}. \tag{93}$$

The key point is that we can evaluate $S_\alpha(\rho_A)$, and hence $\zeta_{\rho_A}(\alpha)$, explicitly.

As it is shown in [37], the Renyi entropy $S_\alpha(\rho_A)$ of a block of L neighboring spins, before the large L limit is taken, can be represented by the finite sum,

$$S_R(\rho_A, \alpha) = \frac{1}{1 - \alpha} \sum_{k=1}^L \ln \left[\left(\frac{1 + \nu_k}{2} \right)^\alpha + \left(\frac{1 - \nu_k}{2} \right)^\alpha \right], \tag{94}$$

where the numbers

$$\pm i \nu_k, \quad k = 1, \dots, L$$

are the eigenvalues of the same block Toeplitz matrix (68) as we worked with in Sect. 3.4. In virtue of (89), the Renyi entropy in the large L limit can be identified with the convergent series,

$$S_R(\rho_A, \alpha) = \frac{1}{1 - \alpha} \sum_{m=-\infty}^{\infty} \ln \left[\left(\frac{1 + \lambda_m}{2} \right)^\alpha + \left(\frac{1 - \lambda_m}{2} \right)^\alpha \right], \tag{95}$$

with

$$\lambda_m = \tanh \left(m + \frac{1 - \sigma}{2} \right) \pi \tau_0. \tag{96}$$

The summation of the series can be done following the same approach as in [51] in the case of the von Neuman entropy. The result is (for details see [28]) the following,

$$S_R(\rho_A, \alpha) = \frac{\alpha}{1-\alpha} \left(\frac{\pi \tau_0}{12} + \frac{1}{6} \ln \frac{kk'}{4} \right) + \frac{1}{1-\alpha} \ln \prod_{n=0}^{\infty} (1 + q_\alpha^{2n+1})^2, \tag{97}$$

$$q_\alpha = e^{-\alpha\pi\tau_0}, \tag{98}$$

for the case $h > 2$, and

$$S_R(\rho_A, \alpha) = \frac{\alpha}{1-\alpha} \left(-\frac{\pi \tau_0}{6} + \frac{1}{6} \ln \frac{k'}{4k^2} \right) + \frac{1}{1-\alpha} \ln \prod_{n=1}^{\infty} (1 + q_\alpha^{2n})^2 + \frac{1}{1-\alpha} \ln 2, \tag{99}$$

$$q_\alpha = e^{-\alpha\pi\tau_0},$$

for the case $h < 2$. In these equations, $\tau_0 \equiv -i\tau$ is the module parameter defined in (30), and $k \equiv k(q_1)$, $k' \equiv k'(q_1)$ are the standard elliptic modular functions, see e.g. [62]. The quantities k and k' are simply related to the basic physical parameters γ and h . Indeed, one has that

$$k \equiv \begin{cases} \sqrt{(h/2)^2 + \gamma^2 - 1}/\gamma, & \text{Case 1a: } 4(1 - \gamma^2) < h^2 < 4; \\ \sqrt{(1 - h^2/4 - \gamma^2)/(1 - h^2/4)}, & \text{Case 1b: } h^2 < 4(1 - \gamma^2); \\ \gamma/\sqrt{(h/2)^2 + \gamma^2 - 1}, & \text{Case 2: } h > 2. \end{cases} \tag{100}$$

$$k' = \sqrt{1 - k^2}.$$

By standard techniques of the theory of elliptic functions, (30) can be transformed into the following representation for the module τ_0 as a function of k .

$$\tau_0 \equiv \frac{I(k')}{I(k)}, \quad k' = \sqrt{1 - k^2}, \tag{101}$$

$I(k)$ is the complete elliptic integral of the first kind,

$$I(k) = \int_0^1 \frac{dx}{\sqrt{(1-x^2)(1-k^2x^2)}}. \tag{102}$$

The q -products in (97) and (99) can be expressed in terms of the *elliptic lambda function* or λ -*modular function*. The λ -function plays a central role in the theory of modular functions and modular forms, and it is defined by the equation (see e.g. [62]),

$$\lambda(\tau) = \frac{\theta_2^4(0|\tau)}{\theta_3^4(0|\tau)} \equiv k^2(e^{i\pi\tau}), \quad \Im\tau > 0, \tag{103}$$

where $\theta_j(s|\tau)$, $j = 3, 4$ are Jacobi theta-functions; the function $\theta_3(s|\tau)$ has already been defined in (31), while the function $\theta_4(s|\tau)$ is defined by the equation,

$$\theta(s|\tau) = \sum_{n=-\infty}^{\infty} (-1)^n e^{\pi i \tau n^2 + 2\pi i s n}. \tag{104}$$

The λ -function is analytic function of τ , $\Im\tau > 0$, and it satisfies the following symmetry relations with respect to the actions of the generators of the modular group,

$$\lambda(\tau + 1) = \frac{\lambda(\tau)}{\lambda(\tau) - 1}, \tag{105}$$

$$\lambda\left(-\frac{1}{\tau}\right) = 1 - \lambda(\tau). \tag{106}$$

In terms of the λ -modular function, the formulae for Renyi read as follows [28].

$$\begin{aligned} S_R(\rho_A, \alpha) &= \frac{1}{6} \frac{\alpha}{1 - \alpha} \ln(kk') - \frac{1}{12} \frac{1}{1 - \alpha} \ln(\lambda(\alpha i \tau_0)(1 - \lambda(\alpha i \tau_0))) \\ &\quad + \frac{1}{3} \ln 2, \end{aligned} \tag{107}$$

for $h > 2$ and

$$\begin{aligned} S_R(\rho_A, \alpha) &= \frac{1}{6} \frac{\alpha}{1 - \alpha} \ln\left(\frac{k'}{k^2}\right) + \frac{1}{12} \frac{1}{1 - \alpha} \ln \frac{\lambda^2(\alpha i \tau_0)}{1 - \lambda(\alpha i \tau_0)} \\ &\quad + \frac{1}{3} \ln 2, \end{aligned} \tag{108}$$

for $h < 2$.

Equations (107) and (108) allow to apply to the study of the Renyi entropy the apparatus of the theory of modular functions.

Remark Using (107) and (108) one can evaluate the asymptotics of the Renyi entropy as $\alpha \rightarrow 1$. This would lead to the following formulae for the Neumann entropy,

$$S(\rho_A) = \frac{1}{6} \left[\ln\left(\frac{k^2}{16k'}\right) + \left(1 - \frac{k^2}{2}\right) \frac{4I(k)I(k')}{\pi} \right] + \ln 2, \tag{109}$$

in Case 1, and

$$S(\rho_A) = \frac{1}{12} \left[\ln\left(\frac{16}{(k^2 k'^2)}\right) + (k^2 - k'^2) \frac{4I(k)I(k')}{\pi} \right], \tag{110}$$

in Case 2. For the Cases 1a and 2 these formulae were first obtained by Peschel in [51] by a direct summation of series (90).

7 Spectrum of the Limiting Density Matrix

Following our calculations with L.A. Takhtajan and F. Franchini we will show now how to extract from (97) and (99) the information about the spectrum of the density matrix ρ_A .

Consider first the case $h > 2$. Combining (97) and (93), we arrive at the following representation for the ζ -function $\zeta_{\rho_A}(\alpha)$,

$$\zeta_{\rho_A}(\alpha) = e^{\alpha(\frac{\pi\tau_0}{12} + \frac{1}{6} \ln \frac{kk'}{4})} \prod_{n=0}^{\infty} (1 + q_{\alpha}^{2n+1})^2. \tag{111}$$

At the same time, using the classical arguments of the theory of partitions (see e.g. [4], Chap. 11, (11.1.4)) we have that

$$\prod_{n=0}^{\infty} (1 + q^{2n+1}) = \sum_{n=1}^{\infty} p_{\mathcal{O}}^{(1)}(n)q^n, \tag{112}$$

where $p_{\mathcal{O}}^{(1)}(0) = 1$ and $p_{\mathcal{O}}^{(1)}(n)$, for $n > 1$, denote the number of partitions of n into distinct positive odd integers, i.e.

$$\# \{ (m_1, \dots, m_k) : m_j = 2r_j + 1, m_1 > m_2 > \dots > m_k, n = m_1 + m_2 + \dots + m_k \}.$$

Hence (111) becomes,

$$\zeta_{\rho_A}(\alpha) = e^{\alpha(\frac{\pi\tau_0}{12} + \frac{1}{6} \ln \frac{kk'}{4})} \sum_{n=0}^{\infty} a_n q_{\alpha}^n, \tag{113}$$

where,

$$a_0 = 1, \quad a_n = \sum_{l=0}^n p_{\mathcal{O}}^{(1)}(l) p_{\mathcal{O}}^{(1)}(n - l). \tag{114}$$

Finally, observing that

$$q_{\alpha}^n = (e^{-\pi\tau_0 n})^{\alpha}, \tag{115}$$

we conclude that

$$\zeta_{\rho_A}(\alpha) = \sum_{n=0}^{\infty} a_n \lambda_n^{\alpha}, \quad \lambda_n = e^{-\pi\tau_0 n + \frac{\pi\tau_0}{12} + \frac{1}{6} \ln \frac{kk'}{4}}. \tag{116}$$

Comparing the last equation with (92) we arrive at the following theorem.

Theorem 5 *Let the magnetic field $h > 2$. Then, the eigenvalues of the reduced density matrix ρ_A are given by the equation,*

$$\lambda_n = e^{-\pi\tau_0 n + \frac{\pi\tau_0}{12} + \frac{1}{6} \ln \frac{kk'}{4}}, \quad n = 0, 1, 2, \dots, \tag{117}$$

and the corresponding multiplicities a_n are determined by the relation (114).

The case $h < 2$ is treated in a very similar way. Instead of (111) we have now the formula,

$$\zeta_{\rho_A}(\alpha) = 2e^{\alpha(-\frac{\pi\tau_0}{6} + \frac{1}{6} \ln \frac{k'}{4k^2})} \prod_{n=0}^{\infty} (1 + q_{\alpha}^{2n})^2, \tag{118}$$

where q_α as in (98). The analog of the Taylor expansion (112) is the equation,

$$\prod_{n=0}^{\infty} (1 + q^{2n}) = \sum_{n=1}^{\infty} p_{\mathcal{N}}^{(1)}(n) q^{2n}, \tag{119}$$

where $p_{\mathcal{N}}^{(1)}(0) = 1$ and $p_{\mathcal{N}}^{(1)}(n)$, for $n > 1$, denote the number of partitions of n into distinct positive integers, i.e.

$$\#\{(m_1, \dots, m_k) : m_1 > m_2 > \dots > m_k \geq 0, n = m_1 + m_2 + \dots + m_k\}.$$

Hence (118) becomes,

$$\zeta_{\rho_A}(\alpha) = 2e^{\alpha(-\frac{\pi\tau_0}{6} + \frac{1}{6} \ln \frac{k'}{4k^2})} \sum_{n=0}^{\infty} b_n q_\alpha^{2n}, \tag{120}$$

where,

$$b_0 = 1, \quad b_n = \sum_{l=0}^n p_{\mathcal{N}}^{(1)}(l) p_{\mathcal{N}}^{(1)}(n-l). \tag{121}$$

Finally, observing that

$$q_\alpha^{2n} = (e^{-2\pi\tau_0 n})^\alpha, \tag{122}$$

we conclude that

$$\zeta_{\rho_A}(\alpha) = 2 \sum_{n=0}^{\infty} b_n \lambda_n^\alpha, \quad \lambda_n = e^{-2\pi\tau_0 n - \frac{\pi\tau_0}{6} + \frac{1}{6} \ln \frac{k'}{4k^2}}. \tag{123}$$

Comparing the last equation again with (92) we arrive at the analog of Theorem 5 for the case $h < 2$.

Theorem 6 *Let the magnetic field $h < 2$. Then, the eigenvalues of the reduced density matrix ρ_A are given by the equation,*

$$\lambda_n = e^{-2\pi\tau_0 n - \frac{\pi\tau_0}{6} + \frac{1}{6} \ln \frac{k'}{4k^2}}, \quad n = 0, 1, 2, \dots, \tag{124}$$

and the corresponding multiplicities equal $2b_n$ where the integers b_n are determined by the relation (121).

Let

$$f(x) := \sum_{n=0}^{\infty} a_n x^n, \tag{125}$$

be the generating function for the coefficients a_n . Then, (107) and (93) in conjunction with the symmetry property (106) allow to analyze the asymptotic behavior of the function $f(x)$ generating function as $x \rightarrow 1$. In its turn, this fact yields the evaluation of the large n asymptotics of the multiplicities a_n .

Theorem 7 Let a_n be the multiplicities of the eigenvalues of the reduced density matrix for $h > 2$. Then their large n behavior is given by the relation,

$$a_n \sim 2^{-3/2} 3^{-1/4} n^{-3/4} e^{\pi \sqrt{\frac{n}{3}}}, \quad n \rightarrow \infty. \quad (126)$$

We will publish detailed derivation together with L.A. Takhtajan and F. Franchini.

8 Summary and Open Problems

We want to emphasize that the method described here also works for evaluation of correlation functions. For example space, time and temperature dependent correlation function of quantum spins was evaluated in [35]. The book [14] explains how to apply this method for calculation of correlation functions in Bose gas with delta interaction.

On the other hand there are still *open problems*. For example let us consider the XXZ model. The Hamiltonian can be written in terms of Pauli matrices σ_n :

$$H_{XXZ} = - \sum_{n=-\infty}^{\infty} \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta \sigma_n^z \sigma_{n+1}^z. \quad (127)$$

At $\Delta < -1$ the model has a gap and the ground state is anti-ferromagnetic. Challenging problem is to calculate the von Neumann entropy and Rényi entropy of large block of spins on the infinite lattice. It will be interesting to find the dependence of limiting entropy on Δ .

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