Entanglement, Toeplitz Determinants and Fisher-Hartwig Conjecture

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Abstract

We consider one-dimensional quantum spin chain, which is called XX model (XX0 model or isotropic XY model) in a transverse magnetic field. We are interested in the case of zero temperature and infinite volume. We study the entanglement of a block L of neighboring spins with the rest of the system. We represent the entanglement in terms of a Toeplitz determinant and calculate the asymptotic analytically . We derive first two terms of asymptotic decomposition.

1 Introduction

The entangled states are regarded as a valuable resource for processing information in novel ways [1, 2]. The entropy of entanglement is one possible way to quantify this valuable resource [3]. We consider following physical system. This system can be separated into two interacting sub-systems A and B and the whole system is in a pure state $|GS\rangle$. For this case, the entropy of entanglement E (Later we shall call it entanglement) between two sub-systems A and B can be measured as the von Neumann entropy of either sub-system A or B, i.e.,

$$E(\mathrm{A}) = E(\mathrm{B}) = -tr(\rho_A \log_2 \rho_A) = -tr(\rho_B \log_2 \rho_B). \tag{1}$$

Here ρ_A (ρ_B) is the reduced density matrix of sub-system A (B), i.e., $\rho_A = Tr_B(\rho_{AB})$ ($\rho_B = Tr_A(\rho_{AB})$). The density matrix of the whole system is $\rho_{AB} = |GS\rangle\langle GS|$ (since the system is in state $|GS\rangle$).

More specifically, let us take the physical system to be XX model in a transverse magnetic field. The Hamiltonian for this model can be written as

$$H_{\mathrm{XX}}(h) = -\sum_{n=1}^{N}(\sigma_n^x\sigma_{n+1}^x + \sigma_n^y\sigma_{n+1}^y + h\sigma_n^z), \quad -2 < h < 2. \tag{2}$$

Here σ_n^x, σ_n^y, σ_n^z are Pauli matrix, which describe spin operators on n-th lattice site, h is the magnetic field and N is the number of total lattice sites of spin chain (or called length of the lattice). This model has been solved by E. Lieb, T. Schultz and D. Mattis in zero-magnetic field case [6] and by E. Barouch and B.M. McCoy in the presence of a constant magnetic field [7]. The ground state and excitation spectrum are well-known. Following Ref. [6], let us introduce two Majorana operators

$$c_{2l-1} = (\prod_{n=1}^{l-1}\sigma_n^z)\sigma_l^x \quad \text{and} \quad c_{2l} = (\prod_{n=1}^{l-1}\sigma_n^z)\sigma_l^y, \tag{3}$$

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

$$H_{\mathrm{XX}}(h) = i\sum_{n=1}^{N}(c_{2n}c_{2n+1} - c_{2n-1}c_{2n+2} + hc_{2n-1}c_{2n}). \tag{4}$$

Here different boundary effects can be ignored because we are only interested in cases with $N \to \infty$. This Hamiltonian can be subsequently diagonalized by linearly transforming the operators c_n. It has been obtained [6, 7] (also see [5]) that

$$\langle GS|c_m|GS\rangle = 0, \quad \langle GS|c_m c_n|GS\rangle = \delta_{mn} + i(\mathbf{B}_N)_{mn}. \tag{5}$$

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

$$\mathbf{B}_N = \begin{pmatrix} \Pi_0 & \Pi_{-1} & \dots & \Pi_{1-N} \\ \Pi_1 & \Pi_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ \Pi_{N-1} & \dots & \dots & \Pi_0 \end{pmatrix}, \tag{6}$$

where block Π_l (for $N \to \infty$) is a 2×2 matrix given by

$$\Pi_l = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\theta \, e^{-\mathrm{i}l\theta} \mathcal{G}(\theta), \tag{7}$$

$$\mathcal{G}(\theta) = \begin{pmatrix} 0 & g(\theta) \\ -g(\theta) & 0 \end{pmatrix} \quad \text{and} \quad g(\theta) = \begin{cases} 1, & -k_F < \theta < k_F, \\ -1, & k_F < \theta < (2\pi - k_F) \end{cases} \tag{8}$$

and $k_F = \arccos(h/2)$. Other correlations such as $\langle GS|c_m \cdots c_n|GS\rangle$ are obtainable by Wick theorem. In terms of spin operators, the Hilbert space of the physical states for first-L sequential lattice sites can be spanned by $\prod_{i=1}^{\mathrm{L}} \{\sigma_i^-\}^{p_i}|0\rangle_F$, where $\sigma_i^{\pm}$ is Pauli matrix, p_i takes value 0 or 1, and vector $|0\rangle_F$ denotes the ferromagnetic state with all spins up. Besides, we are also able to construct a set of fermionic operators b_i and b_i^+ by defining

$$d_m = \sum_{n=1}^{2\mathrm{L}} v_{mn} c_n, \quad m = 1, \cdots, 2\mathrm{L}; \quad b_l = (d_{2l} + i d_{2l+1})/2, \quad l = 1, \cdots, \mathrm{L} \tag{9}$$

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

$$b_l^+ = (d_{2l} - i d_{2l+1})/2, \quad \{b_i, b_j\} = 0, \quad \{b_i^+, b_j^+\} = 0, \quad \{b_i^+, b_j\} = \delta_{i,j}. \tag{10}$$

In terms of fermionic operators b_i and b_i^+, the Hilbert space can also be spanned by $\prod_{i=1}^{\mathrm{L}} \{b_i^+\}^{p_i}|0\rangle_{vac}$. 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

$$b_l|0\rangle_{vac} = 0, \quad l = 1, \cdots, \mathrm{L}. \tag{11}$$

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

2 Density Matrix of Subsystem

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

$$\rho = \sum_{I,J} c(I,J)|\psi_I\rangle\langle\psi_J|. \tag{12}$$

Here $c(I,J)$ are complex coefficients. We can introduce a set of operators $P(I,J)$ by

$$P(I,J) \propto |\psi_I\rangle\langle\psi_J| \tag{13}$$

and $\widetilde{P}(I,J)$ satisfying

$$\widetilde{P}(I,J)P(J,K) = \delta_{I,K}|\psi_I\rangle\langle\psi_I|, \quad P(I,J)\widetilde{P}(J,K) = \delta_{I,K}|\psi_I\rangle\langle\psi_I|. \tag{14}$$

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

$$\rho = \sum_{I,J} \tilde{c}(I,J)P(I,J), \quad \tilde{c}(I,J) = Tr(\rho\widetilde{P}(J,I)). \tag{15}$$

Now let us consider quantum spin chain defined in Eq. 2. Define the sub-system A as spins on first-L sequential lattice sites of chain. The complete set of operators $P(I,J)$ can be generated by $\prod_{i=1}^{\mathrm{L}} O_i$. Here operator O_i can be any one of the following four operators $\{\sigma_i^+, \sigma_i^-, \sigma_i^+\sigma_i^-, \sigma_i^-\sigma_i^+\}$, where $\sigma^{\pm} = \frac{1}{2}(\sigma^x \pm \mathrm{i}\sigma^y)$. Equivalently operators $P(I,J)$ can also be generated by $\prod_{i=1}^{\mathrm{L}} O_i$ where O_i can be any one of the four operators $\{b_i^+, b_i, b_i^+b_i, b_ib_i^+\}$ (Remember that b_i and b_i^+ are fermionic operators). It's easy to find that $\widetilde{P}(J,I) = (\prod_{i=1}^{\mathrm{L}} O_i)^\dagger$ if $P(I,J) = \prod_{i=1}^{\mathrm{L}} O_i$. Here $\dagger$ means hermitian conjugation. Therefore, in both descriptions, the reduced density matrix for sub-system A can be represented as

$$\rho_A = \sum Tr_A\left(\rho_A(\prod_{i=1}^{\mathrm{L}} O_i)^\dagger\right)\prod_{i=1}^{\mathrm{L}} O_i. \tag{16}$$

Here the summation is over all possible different terms $\prod_{i=1}^{\mathrm{L}} O_i$. One immediately find that

$$\begin{aligned}\rho_A &= \sum Tr_A\left(Tr_B(\rho_{AB})(\prod_{i=1}^{\mathrm{L}} O_i)^\dagger\right)\prod_{i=1}^{\mathrm{L}} O_i &(17)\\ &= \sum Tr_{AB}\left(\rho_{AB}(\prod_{i=1}^{\mathrm{L}} O_i)^\dagger\right)\prod_{i=1}^{\mathrm{L}} O_i\ . &(18)\end{aligned}$$

For the whole system to be in pure state $|GS\rangle$ (the ground state), the density matrix ρ_{AB} can be represented by $|GS\rangle\langle GS|$. Then we have the expression for ρ_A as following

$$\rho_A = \sum \langle GS|(\prod_{i=1}^{\mathrm{L}} O_i)^\dagger |GS\rangle \prod_{i=1}^{\mathrm{L}} O_i \ . \tag{19}$$

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 [4]. Now let us choose matrix $\mathbf{V}$ in Eq. 9 so that the set of fermionic basis $\{b_i^+\}$ and $\{b_i\}$ satisfy an equation

$$\langle GS|b_i b_j|GS\rangle = 0, \quad \langle GS|b_i^+ b_j|GS\rangle = \delta_{i,j}\langle GS|b_i^+ b_i|GS\rangle. \tag{20}$$

Then the reduced density matrix ρ_A represented as sum of products in Eq. 19 can be represented as a product of sums

$$\rho_A = \prod_{i=1}^{\mathrm{L}} (\langle\langle GS|b_i^+ b_i|GS\rangle b_i^+ b_i + \langle GS|b_i b_i^+|GS\rangle b_i b_i^+). \tag{21}$$

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 by G. Vidal, J.I. Latorre, E. Rico and A. Kitaev in Ref. [5].

3 Closed Form for The Entanglement

Following Ref. [5], let us find a matrix $\mathbf{V}$ in Eq. 9, which will block-diagonalize correlation functions of Majorana operators c_n. From Eqs. 9 and 6, we have the following expression for correlation function of d_n operators:

$$\begin{aligned}
\langle GS|d_m d_n|GS\rangle &= \sum_{i=1}^{2\mathrm{L}}\sum_{j=1}^{2\mathrm{L}} v_{mi}\langle GS|c_i c_j|GS\rangle v_{jn} \ , \\
\langle GS|c_m c_n|GS\rangle &= \delta_{mn} + \mathrm{i}(\mathbf{B}_{\mathrm{L}})_{mn}, \\
\langle GS|d_m d_n|GS\rangle &= \delta_{mn} + \mathrm{i}(\widetilde{\mathbf{B}}_{\mathrm{L}})_{mn}.
\end{aligned} \tag{22}$$

The last equation is the definition of a matrix $\tilde{\mathbf{B}}_{\mathrm{L}}$. Matrix $\mathbf{B}_{\mathrm{L}}$ can be represented in a block form as

$$\mathbf{B}_{\mathrm{L}} = \begin{pmatrix} \Pi_0 & \Pi_{-1} & \dots & \Pi_{1-\mathrm{L}} \\ \Pi_1 & \Pi_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ \Pi_{\mathrm{L}-1} & \dots & \dots & \Pi_0 \end{pmatrix}. \tag{23}$$

Here block Π_l is a 2×2 matrix and can be expressed as a Fourier transform of 2×2 matrix $\mathcal{G}(\theta)$, i.e.

$$\Pi_l = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\theta \, e^{-\mathrm{i}l\theta} \mathcal{G}(\theta), \tag{24}$$

$$\mathcal{G}(\theta) = \begin{pmatrix} 0 & g(\theta) \\ -g(\theta) & 0 \end{pmatrix} \quad \text{and} \quad g(\theta) \;=\; \begin{cases} 1, & -k_F < \theta < k_F, \\ -1, & k_F < \theta < (2\pi - k_F) \end{cases} \tag{25}$$

and $k_F = \arccos(h/2)$. We also require $\tilde{\mathbf{B}}_{\mathrm{L}}$ to be block-diagonal [5]

$$\tilde{\mathbf{B}}_{\mathrm{L}} = V \mathbf{B}_{\mathrm{L}} V^T = \oplus_{m=1}^{\mathrm{L}} \nu_m \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \mathbf{\Omega} \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{26}$$

Here matrix $\mathbf{\Omega}$ is a diagonal matrix with elements ν_m (all ν_m are real numbers). Therefore, choosing matrix $\mathbf{V}$ satisfying Eq. 26 in Eq. 9, we obtain 2L operators $\{b_l\}$ and $\{b_l^+\}$ with following expectation values

$$\langle GS|b_m|GS\rangle = 0 \, , \langle GS|b_m b_n|GS\rangle = 0 \, , \langle GS|b_m^+ b_n|GS\rangle = \delta_{mn} \frac{1+\nu_m}{2}. \tag{27}$$

Using the simple expression for reduced density matrix ρ_A in Eq. 21, we obtain

$$\rho_A = \prod_{i=1}^{\mathrm{L}} \left(\frac{1+\nu_i}{2} b_i^+ b_i + \frac{1-\nu_i}{2} b_i b_i^+ \right). \tag{28}$$

This form immediately gives us all the eigenvalues $\lambda_{x_1 x_2 \cdots x_{\mathrm{L}}}$ of reduced density matrix ρ_A,

$$\lambda_{x_1 x_2 \cdots x_{\mathrm{L}}} = \prod_{i=1}^{\mathrm{L}} \frac{1+(-1)^{x_i}\nu_i}{2}, \quad x_i = 0, 1 \;\; \forall i. \tag{29}$$

Note that in total we have 2^{L} eigenvalues. Hence, the entanglement (von Neumann entropy of ρ_A) from Eq. 1 becomes

$$E_A = \sum_{m=1}^{\mathrm{L}} e(1, \nu_m) \tag{30}$$

with

$$e(x,\nu) = -\frac{x+\nu}{2}\log_2(\frac{x+\nu}{2}) - \frac{x-\nu}{2}\log_2(\frac{x-\nu}{2}). \tag{31}$$

More generally, we also can consider Rényi entropy $S_\alpha(\rho)$, which is defined as

$$S_\alpha(\rho) = \frac{1}{1-\alpha}\log Tr(\rho^\alpha), \qquad \alpha \neq 1 \tag{32}$$

and becomes von Neumann entropy when $\alpha \to 1$. Then Rényi entropy becomes

$$S_\alpha = \sum_{m=1}^{\mathrm{L}} s_\alpha(1,\nu_m) \tag{33}$$

with

$$s_\alpha(x,\nu) = \frac{1}{1-\alpha}\log\left((\frac{x+\nu}{2})^\alpha + (\frac{x-\nu}{2})^\alpha\right). \tag{34}$$

Since all calculations for von Neumann entropy and Rényi entropy are similiar, we will show the detail of calculation for von Neumann entropy only and give the result for Rényi entropy directly. This form of entanglement E_A is the main result of paper [5] and we shall use this result further to obtain analytical asymptotic of the entanglement. Function $e(1,\nu)$ in Eq. 30 is equal to the Shannon entropy function $H_2(\frac{1+\nu}{2})$, which is used in Ref. [5]. However, in the following calculation (Eq. 39), we will need the more general function $e(x,\nu)$ instead of $H_2(\nu)$. Let us further notice that matrix $\mathbf{B}_\mathrm{L}$ can have a direct product form, i.e.

$$\mathbf{B}_\mathrm{L} = \mathbf{G}_\mathrm{L} \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{35}$$

with

$$\mathbf{G}_\mathrm{L} = \begin{pmatrix} g_0 & g_{-1} & \cdots & g_{1-L} \\ g_1 & g_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ g_{L-1} & \cdots & \cdots & g_0 \end{pmatrix}, \tag{36}$$

where g_l is defined as

$$g_l = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta\, e^{-\mathrm{i}l\theta} g(\theta) \;\; \text{and} \;\; g(\theta) = \begin{cases} 1, & -k_F < \theta < k_F, \\ -1, & k_F < \theta < (2\pi - k_F) \end{cases} \tag{37}$$

and $k_F = \arccos(h/2)$. From Eqs. 26 and 35, we know that all ν_m are just the eigenvalues of real symmetric matrix $\mathbf{G}_{\mathrm{L}}$.

However, to obtain all eigenvalues ν_m directly from matrix $\mathbf{G}_{\mathrm{L}}$ is a non-trivial task. Let us introduce function $D_{\mathrm{L}}(\lambda)$ as

$$D_{\mathrm{L}}(\lambda) = \prod_{m=1}^{\mathrm{L}} (\lambda - \nu_m) \tag{38}$$

to circumvent this difficulty. From the Cauchy residue theorem and analytical property of $e(x, \nu)$, the entanglement can be rewritten as

$$E_A = \lim_{\epsilon \to 0^+} \lim_{\delta \to 0^+} \frac{1}{2\pi \mathrm{i}} \oint_{c(\epsilon,\delta)} e(1+\epsilon, \lambda) \mathrm{d} \ln D_{\mathrm{L}}(\lambda) \ . \tag{39}$$

Here the contour $c(\epsilon, \delta)$ in Fig 1 encircles all zeros of $D_{\mathrm{L}}(\lambda)$, but Both functions $e(1+\epsilon, \lambda)$ and $s_\alpha(1+\epsilon, \lambda)$ are analytic within the contour. It's easy to find that

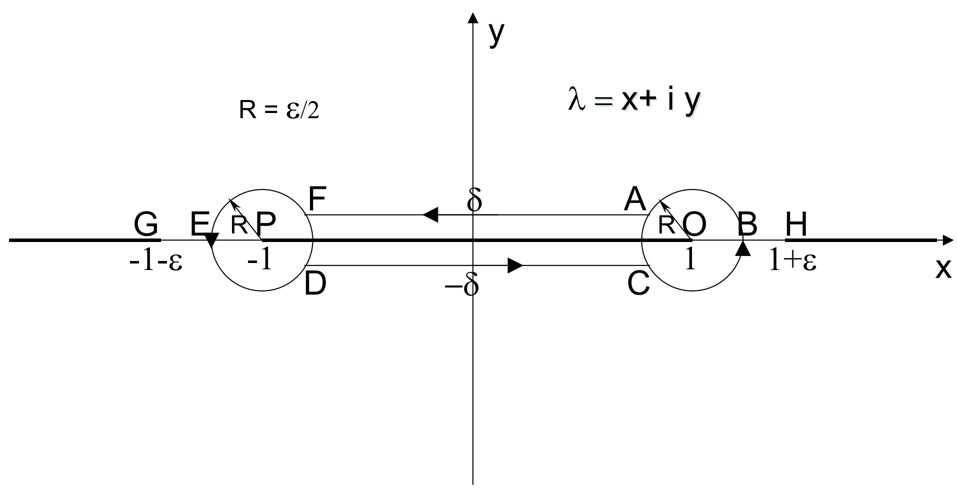

Figure 1: The contour $c(\epsilon, \delta)$. Bold lines $(-\infty, -1-\epsilon)$ and $(1+\epsilon, \infty)$ are the cuts of integrand $e(1+\epsilon, \lambda)$. Zeros of $D_{\mathrm{L}}(\lambda)$ (Eq. 38) are located on bold line $(-1, 1)$ and this line becomes the cut of $\mathrm{d} \log D_{\mathrm{L}}(\lambda)$ for $L \to \infty$ (Eq. 56). The arrow is the direction of the route of integral we take and R is the radius of circles.

$$D_{\mathrm{L}}(\lambda) = \det(\widetilde{\mathbf{G}}_{\mathrm{L}} \equiv \lambda I_{\mathrm{L}} - \mathbf{G}_{\mathrm{L}}) \ . \tag{40}$$

Here $\widetilde{\mathbf{G}}_{\mathrm{L}}$ is a Toeplitz matrix (see [12]) and I_{L} is the identity matrix of dimension L. Just like Toeplitz matrix $\mathbf{G}_{\mathrm{L}}$ is generated by function $g(\theta)$ in Eqs. 36 and 37, Toeplitz matrix $\widetilde{\mathbf{G}}_{\mathrm{L}}$ is generated by function $\tilde{g}(\theta)$, which is defined by

$$\tilde{g}(\theta) = \begin{cases} \lambda - 1, & -k_F < \theta < k_F, \\ \lambda + 1, & k_F < \theta < (2\pi - k_F). \end{cases} \tag{41}$$

Notice that $\tilde{g}(\theta)$ 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 the entanglement which is our new result. Now, the calculation of the entanglement reduces to the calculation of the determinant of Toeplitz matrix $\widetilde{\mathbf{G}}_{\mathrm{L}}$. Before we calculate the determinant of Toeplitz matrix $\widetilde{\mathbf{G}}_{\mathrm{L}}$, we also want to point out two special cases which allow us to obtain an explicit form for these eigenvalues ν_m and hence the entanglement. These are cases with small lattice size of subsystem A and magnetic h close to critical values ± 2, more accurately to be said, cases with $k_F \mathrm{L} << 1$ or $(\pi - k_F)\mathrm{L} << 1$. For the case of $k_F \mathrm{L} << 1$, Toeplitz matrix $\mathbf{G}_{\mathrm{L}}$ can be well approximated by a matrix with diagonal elements $(2k_F/\pi - 1)$ and all other matrix elements equal to $2k_F/\pi$. Hence, if $k_F \mathrm{L} << 1$, we can obtain all eigenvalues for Toeplitz matrix $\mathbf{G}_{\mathrm{L}}$ as $\{2\mathrm{L}k_F/\pi - 1, -1, -1, \cdots, -1\}$ and the approximate entanglement becomes

$$E_A = \frac{2\mathrm{L}k_F}{\pi} \log_2 \frac{\pi}{2\mathrm{L}k_F}, \quad 0 < k_F \mathrm{L} << 1. \tag{42}$$

Similarly, we obtain the entanglement for the case of $(\pi - k_F)\mathrm{L} << 1$ as

$$E_A = \frac{2\mathrm{L}(\pi - k_F)}{\pi} \log_2 \frac{\pi}{2\mathrm{L}(\pi - k_F)}, \quad 0 < (\pi - k_F)\mathrm{L} << 1. \tag{43}$$

Both Eqs. 42 and 43 can be re-expressed in terms of h as

$$E_A = \frac{2\mathrm{L}(1 - h^2/4)^{\frac{1}{2}}}{\pi} \log_2 \frac{\pi}{2\mathrm{L}(1 - h^2/4)^{\frac{1}{2}}}, \quad 0 < (1 - h^2/4)^{\frac{1}{2}}\mathrm{L} << 1. \tag{44}$$

4 Determinant of The Toeplitz Matrix

The Toeplitz matrix $T_{\mathrm{L}}[\phi]$ is said to be generated by function $\phi(\theta)$ if

$$T_{\mathrm{L}}[\phi] = (\phi_{i-j}), \quad i, j = 1, \cdots, \mathrm{L} - 1 \tag{45}$$

where

$$\phi_l = \frac{1}{2\pi} \int_0^{2\pi} \phi(\theta) e^{-\mathrm{i}l\theta} \mathrm{d}\theta \tag{46}$$

is the l-th Fourier coefficient of generating function $\phi(\theta)$. The determinant of $T_{\mathrm{L}}[\phi]$ is denoted by D_{L}. The asymptotic behavior of the determinant of Toeplitz matrix with singular generating function was initiated by T.T. Wu [8] in his study of spin correlation in two-dimensional Ising model and later incorporated into a more general conjecture, i.e., the famous Fisher-Hartwig conjecture [9, 10, 11, 12]. For our application, we will not need the general case of Fisher-Hartwig conjecture. Instead, we only need the singular generating function $\phi(\theta)$ with discontinuities only. This case was first considered in [8] . This function allows a canonical factorization:

$$\phi(\theta) = \psi(\theta) \prod_{i=1}^{R} t_{(\beta_i,\theta_i)}(\theta). \tag{47}$$

Here

$$t_{(\beta_i,\theta_i)}(\theta) = \exp\Big(-\mathrm{i}\beta_i(\pi - \theta + \theta_i)\Big) \tag{48}$$

is defined on the interval $\theta_i < \theta < (2\pi + \theta_i)$. In this way, we factorizes the function $\phi(\theta)$ into a product of a smooth function $\psi(\theta)$ (with winding number zero) and jump-only functions $t_{(\beta_i,\theta_i)}(\theta)$. We also assume that there exists Weiner-Hopf factorization

$$\psi(\theta) = \mathcal{F}[\psi]\psi_+\Big(\exp(\mathrm{i}\theta)\Big)\psi_-\Big(\exp(-\mathrm{i}\theta)\Big). \tag{49}$$

Here ψ_+ is analytical inside the unit circle, ψ_- is analytical outside the unit circle (with $\psi_+(0) = \psi_-(\infty) = 1$), and normalization factor $\mathcal{F}[\psi] = \exp\Big(\frac{1}{2\pi}\int_0^{2\pi} \ln\psi(\theta)\mathrm{d}\theta\Big)$. It was proved by E.L. Basor in Ref. [10] that if $|\Re(\beta_i)| < \frac{1}{2}$, then the determinant D_{L} of related Toeplitz matrix has the following asymptotic expression

$$D_{\mathrm{L}} = (\mathcal{F}[\psi])^{\mathrm{L}} \left(\prod_{i=1}^{R} \mathrm{L}^{-\beta_i^2}\right) \mathcal{E}[\psi, \{\beta_i\}, \{\theta_i\}], \quad \mathrm{L} \to \infty. \tag{50}$$

Here $\mathcal{E}[\psi, \{\beta_i\}, \{\theta_i\}]$ is a constant defined as

$$\begin{aligned} \mathcal{E}[\psi, \{\beta_i\}, \{\theta_i\}] &= \mathcal{E}[\psi] \prod_{i=1}^{R} G(1+\beta_i)G(1-\beta_i) \\ &\times \prod_{i=1}^{R} \Big(\psi_-\Big(\exp(\mathrm{i}\theta_i)\Big)\Big)^{-\beta_i} \Big(\psi_+\Big(\exp(-\mathrm{i}\theta_i)\Big)\Big)^{\beta_i} \\ &\times \prod_{1\le i\ne j\le R} \Big(1 - \exp\Big(\mathrm{i}(\theta_i - \theta_j)\Big)\Big)^{\beta_i\beta_j}. \end{aligned} \tag{51}$$

Let us explain notations: G is the Barnes G-function, $\mathcal{E}[\psi] = \exp(\sum_{k=1}^{\infty} k s_k s_{-k})$, and s_k is the k-th Fourier coefficient of $\ln \psi(\theta)$. The Barnes G-function is defined as

$$G(1+z) = (2\pi)^{z/2} e^{-(z+1)z/2-\gamma_E z^2/2} \prod_{n=1}^{\infty} \{(1+z/n)^n e^{-z+z^2/(2n)}\}, \tag{52}$$

where γ_E is Euler constant and its numerical value is $0.5772156649\cdots$. In our case, we have $|\Re(\beta_i)| < \frac{1}{2}$ (see Eqs. 53, 54 and 55) and hence the Fisher-Hartwig conjecture is **PROVEN** by E.L. Basor for our case [10]. Therefore, we will call it the theorem instead of conjecture, which is suitable name for more general cases.

5 Asymptotic Form of The Entanglement

Now, let us come back to the calculation of Toeplitz matrix with generating function $\tilde{g}(\theta)$ defined in Eq. 41, which corresponds to XX quantum spin chain. This generating function $\tilde{g}(\theta)$ has two jumps at $\theta = \pm k_F$ and it has the following canonical factorization

$$\tilde{g}(\theta) = \psi(\theta) t_{(\beta_1(\lambda), k_F)}(\theta) t_{(\beta_2(\lambda), -k_F)}(\theta) \tag{53}$$

with

$$\psi(\theta) = (\lambda+1)\left(\frac{\lambda+1}{\lambda-1}\right)^{-k_F/\pi}, \quad \beta(\lambda) = -\beta_1(\lambda) = \beta_2(\lambda) = \frac{1}{2\pi \mathrm{i}} \ln \frac{\lambda+1}{\lambda-1}. \tag{54}$$

The function t was defined in Eq. 48. We fix the branch of the logarithm in the following way

$$-\pi \le \arg\left(\frac{\lambda+1}{\lambda-1}\right) < \pi. \tag{55}$$

For $\lambda \notin [-1, 1]$, we know that $|\Re(\beta_1(\lambda))| < \frac{1}{2}$ and $|\Re(\beta_2(\lambda))| < \frac{1}{2}$ and Fisher-Hartwig conjecture was proved. From the factorization, we also have $\psi_+(\theta) = \psi_-(\theta) = 1$. Hence following the theorem in Eq. 50, the determinant $D_{\mathrm{L}}(\lambda)$ of $\lambda I_{\mathrm{L}} - \mathbf{G}_{\mathrm{L}}$ can be asymptotically represented as

$$\begin{aligned} D_{\mathrm{L}}(\lambda) &= \Big(2 - 2\cos(2k_F)\Big)^{-\beta^2(\lambda)} \Big\{G\Big(1+\beta(\lambda)\Big) G\Big(1-\beta(\lambda)\Big)\Big\}^2 \\ &\quad \Big\{(\lambda+1)\Big((\lambda+1)/(\lambda-1)\Big)^{-k_F/\pi}\Big\}^{\mathrm{L}} \mathrm{L}^{-2\beta^2(\lambda)}. \end{aligned} \tag{56}$$

Here L is the length of sub-system A and G is the Barnes G-function and

$$G(1+\beta(\lambda))G(1-\beta(\lambda)) = e^{-(1+\gamma_E)\beta^2(\lambda)} \prod_{n=1}^{\infty} \left\{ \left(1 - \frac{\beta^2(\lambda)}{n^2}\right)^n e^{\beta^2(\lambda)/n^2} \right\}. \tag{57}$$

For later convenience, let us define

$$\Upsilon(\lambda) = \sum_{n=1}^{\infty} \frac{n^{-1}\beta^2(\lambda)}{n^2 - \beta^2(\lambda)}. \tag{58}$$

Taking logrithmic derivative of $D_{\mathrm{L}}(\lambda)$, we obtain

$$\begin{aligned} \frac{\mathrm{d}\ln D_{\mathrm{L}}(\lambda)}{\mathrm{d}\lambda} &= \left(\frac{1-k_F/\pi}{1+\lambda} - \frac{k_F/\pi}{1-\lambda}\right)\mathrm{L} \\ &- \frac{4}{\mathrm{i}\pi}\frac{\beta(\lambda)}{(1+\lambda)(1-\lambda)}\Big(\ln \mathrm{L} + \ln(2|\cos k_F|) + (1+\gamma_E) + \Upsilon(\lambda)\Big). \end{aligned} \tag{59}$$

Eq. 39 represents the entanglement in terms of the log-determinant

$$E_A = \lim_{\epsilon\to 0^+}\lim_{\delta\to 0^+} \frac{1}{2\pi\mathrm{i}} \oint_{c(\epsilon,\delta)} e(1+\epsilon,\lambda) \frac{\mathrm{d}\ln D_{\mathrm{L}}(\lambda)}{\mathrm{d}\lambda}\mathrm{d}\lambda \tag{60}$$

with contour shown in Fig 1. Let us substitute the asymptotic form Eq. 59 for $\mathrm{d}\ln D_{\mathrm{L}}(\lambda)/\mathrm{d}\lambda$ into the expression above:

$$\begin{aligned} E_A = \lim_{\epsilon\to 0^+}\lim_{\delta\to 0^+} \frac{1}{2\pi\mathrm{i}} \oint_{c(\epsilon,\delta)} e(1+\epsilon,\lambda) \left(\frac{1-k_F/\pi}{1+\lambda} - \frac{k_F/\pi}{1-\lambda}\right)\mathrm{L} + \\ \lim_{\epsilon\to 0^+}\lim_{\delta\to 0^+} \frac{2}{\pi^2} \oint_{c(\epsilon,\delta)} \mathrm{d}\lambda \frac{e(1+\epsilon,\lambda)\beta(\lambda)}{(1+\lambda)(1-\lambda)}\Big(\ln \mathrm{L} + \ln(2|\cos k_F|) + (1+\gamma_E) + \Upsilon(\lambda)\Big), \end{aligned} \tag{61}$$

where the contour is taken as shown in Fig. 1. The first integral which is linear in L term in Eq. 61 vanishes:

$$\begin{aligned} &\lim_{\epsilon\to 0^+}\lim_{\delta\to 0^+} \frac{1}{2\pi\mathrm{i}} \oint_{c(\epsilon,\delta)} e(1+\epsilon,\lambda) \left(\frac{1-k_F/\pi}{1+\lambda} - \frac{k_F/\pi}{1-\lambda}\right)\mathrm{L} \\ = &\lim_{\epsilon\to 0^+} \Big(e(1+\epsilon,-1)(1-k_F/\pi) + e(1+\epsilon,1)k_F/\pi\Big)\mathrm{L} \\ = &\ 0. \end{aligned} \tag{62}$$

Here, we applied the residue theorem by knowing the analyticity of $e(1+\epsilon,\lambda)$ in λ within the contour $c(\epsilon,\delta)$. We also used the fact that $\lim_{\epsilon\to 0^+} e(1+\epsilon,\pm 1) = 0$ (Definition of function $e(x,\nu)$ in Eq. 31). Hence, there is no linear in L term in the expression for entanglement E_A. The second integral can be calculated as follows: First, we notice that

$$\oint_{c(\epsilon,\delta)} \mathrm{d}\lambda\ (\cdots) = \left(\int_{\overrightarrow{\mathrm{AF}}} + \int_{\overrightarrow{\mathrm{FED}}} + \int_{\overrightarrow{\mathrm{DC}}} + \int_{\overrightarrow{\mathrm{CBA}}}\right) \mathrm{d}\lambda\ (\cdots) \tag{63}$$

Second, we can show that the contribution of the circular arc $\overrightarrow{\mathrm{FED}}$ vanishes

$$\lim_{\epsilon\to 0^+}\lim_{\delta\to 0^+}\int_{\overrightarrow{\mathrm{FED}}}\mathrm{d}\lambda\frac{e(1+\epsilon,\lambda)\beta(\lambda)}{(1+\lambda)(1-\lambda)}\Big(\ln\mathrm{L}+\ln(2|\cos k_F|)+(1+\gamma_E)+\Upsilon(\lambda)\Big)=0. \quad (64)$$

Third, we show that the contribution of the circular arc $\overrightarrow{\mathrm{CBA}}$ vanishes

$$\lim_{\epsilon\to 0^+}\lim_{\delta\to 0^+}\int_{\overrightarrow{\mathrm{CBA}}}\mathrm{d}\lambda\frac{e(1+\epsilon,\lambda)\beta(\lambda)}{(1+\lambda)(1-\lambda)}\Big(\ln\mathrm{L}+\ln(2|\cos k_F|)+(1+\gamma_E)+\Upsilon(\lambda)\Big)=0. \quad (65)$$

Let us explain how we obtained these results:

For points λ on the circular arc FED, we rewrote λ as

$$\lambda=-1-\frac{\epsilon}{2}e^{\mathrm{i}\phi}. \quad (66)$$

So, we can show that

$$\begin{aligned}&\frac{1}{1+\lambda}\sim\frac{1}{\epsilon},\quad\frac{1}{1-\lambda}\sim 1,\quad\beta(\lambda)\sim\ln\epsilon,\\ &e(1+\epsilon,\lambda)\sim\epsilon\ln\epsilon\quad\text{and}\quad\Upsilon(\lambda)\sim 1\end{aligned} \quad (67)$$

for $\lambda=-1-\frac{\epsilon}{2}e^{\mathrm{i}\phi}$ and ϵ small enough. Hence,

$$\int_{\overrightarrow{\mathrm{FED}}}\mathrm{d}\lambda\frac{e(1+\epsilon,\lambda)\beta(\lambda)}{(1+\lambda)(1-\lambda)}\Big(\ln\mathrm{L}+\ln(2|\cos k_F|)+(1+\gamma_E)+\Upsilon(\lambda)\Big)\sim\epsilon\ln^2\epsilon, \quad (68)$$

which leads to Eq. 64. Similarly we can obtain Eq. 65. Therefore, the entanglement (Eq. 61) can be written as

$$\begin{aligned}E_A &= \lim_{\epsilon\to 0^+}\frac{2}{\pi^2}\Big(\int_{1+\mathrm{i}0^+}^{-1+\mathrm{i}0^+}+\int_{-1+\mathrm{i}0^-}^{1+\mathrm{i}0^-}\Big)\mathrm{d}\lambda\frac{e(1+\epsilon,\lambda)\beta(\lambda)}{(1+\lambda)(1-\lambda)}\\ &\times\Big(\ln L+\ln(2|\cos k_F|)+(1+\gamma_E)+\Upsilon(\lambda)\Big).\end{aligned} \quad (69)$$

For further simplification, we shall use the fact that

$$\beta(x+\mathrm{i}0^\pm)=\frac{1}{2\mathrm{i}\pi}\left(\ln\frac{1+x}{1-x}\mp\mathrm{i}(\pi-0^+)\right)=-\mathrm{i}W(x)\mp(\frac{1}{2}-0^+) \quad (70)$$

for $x\in(-1,1)$ and

$$W(x)=\frac{1}{2\pi}\ln\frac{1+x}{1-x}. \quad (71)$$

We can now write the entanglement E_A as

$$\begin{aligned}E_A &= \frac{2}{\pi^2}\int_{-1}^{1}\mathrm{d}x\,\frac{e(1,x)}{1-x^2}\Big(\ln\mathrm{L}+\ln(2|\cos k_F|)+(1+\gamma_E)\Big)\\ &+\sum_{n=1}^{\infty}\frac{2n^{-1}}{\pi^2}\int_{-1}^{1}\mathrm{d}x\,\frac{e(1,x)}{1-x^2}\left(\frac{(\frac{1}{2}+\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}+\mathrm{i}W(x))^2}+\frac{(\frac{1}{2}-\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}-\mathrm{i}W(x))^2}\right),\end{aligned} \quad (72)$$

where $e(1,x)$ is defined in Eq. 31.

This expression for E_A contains two integrals. The first integral can be done exactly as

$$\begin{aligned}
& \frac{2}{\pi^2}\int_{-1}^{1} \mathrm{d}x\,(-\frac{1+x}{2}\log_2\frac{1+x}{2} - \frac{1-x}{2}\log_2\frac{1-x}{2})\frac{1}{1-x^2} \\
= & \frac{1}{\pi^2}\int_{-1}^{1} \mathrm{d}x\,(-\frac{1}{1-x}\ln\frac{1+x}{2} - \frac{1}{1+x}\ln\frac{1-x}{2})\frac{1}{\ln 2} \\
= & \frac{1}{3\ln 2}.
\end{aligned} \tag{73}$$

The second integral in Eq. 72 becomes

$$\begin{aligned}
& \sum_{n=1}^{\infty}\frac{2n^{-1}}{\pi^2}\int_{-1}^{1} \mathrm{d}x\,(-\frac{1+x}{2}\log_2\frac{1+x}{2} - \frac{1-x}{2}\log_2\frac{1-x}{2}) \\
& \quad \times\frac{1}{1-x^2}\left(\frac{(\frac{1}{2}+\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}+\mathrm{i}W(x))^2} + \frac{(\frac{1}{2}-\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}-\mathrm{i}W(x))^2}\right) \\
= & \sum_{n=1}^{\infty}\frac{2n^{-1}}{\pi^2\ln 2}\int_{-1}^{1} \mathrm{d}x\,(-\frac{1}{1-x}\ln\frac{1+x}{2} - \frac{1}{1+x}\ln\frac{1-x}{2}) \\
& \quad \times\left(\frac{(\frac{1}{2}+\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}+\mathrm{i}W(x))^2} + \frac{(\frac{1}{2}-\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}-\mathrm{i}W(x))^2}\right),
\end{aligned} \tag{74}$$

which is hard to treat analytically and is very close to $-1/(30\ln 2)$ numerically. Hence, we find that

$$E_A = \frac{1}{3}\log_2 \mathrm{L} + \frac{1}{6}\log_2\left(1-(\frac{h}{2})^2\right) + \frac{1}{3} + \frac{1+\gamma_E}{3\ln 2} + \Upsilon_0, \quad \mathrm{L}\to\infty \tag{75}$$

for XX model. The constant Υ_0 can be obtained as

$$\begin{aligned}
\Upsilon_0 = & \sum_{n=1}^{\infty}\frac{2n^{-1}}{\pi^2\ln 2}\int_{-1}^{1} \mathrm{d}x\,(-\frac{1}{1-x}\ln\frac{1+x}{2} - \frac{1}{1+x}\ln\frac{1-x}{2}) \\
& \quad \times\left(\frac{(\frac{1}{2}+\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}+\mathrm{i}W(x))^2} + \frac{(\frac{1}{2}-\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}-\mathrm{i}W(x))^2}\right) \\
\simeq & -\frac{1}{30\ln 2}.
\end{aligned} \tag{76}$$

The series here is convergent and we think that $\Upsilon_0 = -1/(30\ln 2)$.

6 Summary

In this paper, we study asymptotic behavior of entanglement of XX model in the transverse magnetic field. We first expressed the entanglement in terms of a determinant of a Toeplitz matrix. Then we used Fisher-Hartwig conjecture [9] (the special case, which we need, was first considered in [8] and proved in [10]) to obtain its asymptotic behavior. We proved that

$$E_A = \frac{1}{3}\log_2 \mathrm{L} + \frac{1}{6}\log_2\left(1-(\frac{h}{2})^2\right) + \frac{1}{3} + \frac{1+\gamma_E}{3\ln 2} + \Upsilon_0, \quad \mathrm{L}\to\infty. \tag{77}$$

$$\Upsilon_0 = \sum_{n=1}^{\infty}\frac{2n^{-1}}{\pi^2\ln 2}\int_{-1}^{1}\mathrm{d}x\,(-\frac{1}{1-x}\ln\frac{1+x}{2} - \frac{1}{1+x}\ln\frac{1-x}{2}) \times\left(\frac{(\frac{1}{2}+\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}+\mathrm{i}W(x))^2} + \frac{(\frac{1}{2}-\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}-\mathrm{i}W(x))^2}\right), \tag{78}$$

$$W(x) = \frac{1}{2\pi}\ln\frac{1+x}{1-x}, \quad \gamma_E \text{ is Euler constant.} \tag{79}$$

The leading term of asymptotic of the entanglement $\frac{1}{3}\log_2 \mathrm{L}$ coincides what has been published in Ref. [5] . The next leading term of asymptotic,

$$\frac{1}{6}\log_2\left(1-(\frac{h}{2})^2\right) + \frac{1}{3} + \frac{1+\gamma_E}{3\ln 2} + \Upsilon_0, \tag{80}$$

is our new result. It is a constant (in the sense of no L dependence) showing explicit dependence on magnetic field h and we conjecture the constant just as simple as

$$\frac{1}{6}\log_2\left(1-(\frac{h}{2})^2\right) + \frac{1}{3} + \frac{\gamma_E}{3\ln 2} + \frac{3}{10\ln 2}. \tag{81}$$

Besides asymptotic case (with very large lattice size of subsystem A), we also obtain the analytical expression Eq. 44 for the entanglement for the case with small lattice size of subsystem A and the transverse magnetic field h close to critical values ± 2.

Similiar to Eq. 72, Rényi entropy can be written as

$$S_\alpha = \frac{2}{\pi^2}\int_{-1}^{1}\mathrm{d}x\,\frac{s_\alpha(1,x)}{1-x^2}\big(\ln \mathrm{L} + \ln(2|\cos k_F|) + (1+\gamma_E)\big) + \sum_{n=1}^{\infty}\frac{2n^{-1}}{\pi^2}\int_{-1}^{1}\mathrm{d}x\,\frac{s_\alpha(1,x)}{1-x^2}\left(\frac{(\frac{1}{2}+\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}+\mathrm{i}W(x))^2} + \frac{(\frac{1}{2}-\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}-\mathrm{i}W(x))^2}\right) \tag{82}$$

with

$$s_\alpha(x,\nu) = \frac{1}{1-\alpha}\log\left((\frac{x+\nu}{2})^\alpha + (\frac{x-\nu}{2})^\alpha\right). \tag{83}$$

The lead term of Rényi entropy in this critical model is linear with $\ln \mathrm{L}$ and we have its coefficient $C_R(\alpha)$ as

$$C_R(\alpha) = \frac{2}{\pi^2(1-\alpha)}\int_{-1}^{1}\mathrm{d}x\,\frac{1}{1-x^2}\log\left((\frac{1+x}{2})^\alpha + (\frac{1-x}{2})^\alpha\right). \tag{84}$$

Note:

- When $\alpha \to 1$, i.e. $\alpha = 1+\delta$ and $\delta \to 0$, Rényi entropy becomes von Neumann entropy and we can show $\lim_{\alpha\to 1} C_R(\alpha) = \frac{1}{3}$ as following:

$$\begin{aligned}
\lim_{\delta\to 0} C_R(\alpha) &= \lim_{\delta\to 0} \frac{-2}{\pi^2\delta} \int_{-1}^{1} \mathrm{d}x \, \frac{1}{1-x^2} \log\left((\frac{1+x}{2})^{1+\delta} + (\frac{1-x}{2})^{1+\delta} \right) && (85)\\
&= \frac{2}{\pi^2} \int_{-1}^{1} \mathrm{d}x \, \frac{-1}{(1-x^2)} (\frac{1+x}{2} \log \frac{1+x}{2} + \frac{1-x}{2} \log \frac{1-x}{2}) && (86)\\
&= \frac{1}{3} && (87)
\end{aligned}$$

- We also can show the related results rigorously for XY model. At the critical point, the leading term is the half of the corresponding term for XX model. This is related to the number of jumps in generating function for correlation function.

Acknowlegment

We would like to thank Prof. B.M. McCoy for useful discussions. This work was supported by National Science Foundation (USA) under Grant No. DMR-0073058 and PHY-9988566.

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