Journal of Statistical Physics, Vol. 116, Nos. 1/4, August 2004 (© 2004)

Quantum Spin Chain, Toeplitz Determinants and the Fisher–Hartwig Conjecture

B.-Q. Jin[1] and V. E. Korepin[1]

Received April 15, 2003; accepted December 3, 2003

We consider the one-dimensional quantum spin chain, which is called the XX model (XX0 model or isotropic XY model) in a transverse magnetic field. We are mainly interested in the entropy of a block of L neighboring spins at zero temperature and of an infinite system. We represent the entropy in terms of a Toeplitz determinant and calculate the asymptotic analytically. We derive the first two terms of the asymptotic decomposition. Interestingly, these two terms of decomposition clearly show a length scale related to the field h.

KEY WORDS: Quantum spin chain; XX0 model; entropy; Toeplitz determinant; quantum entanglement.

1. INTRODUCTION

The derivation of macroscopic thermodynamics from microscopic dynamics is not *a priori* and one should examine it critically when possible. As is well known, the entropy is the main object in thermodynamics and statistical physics. The exact calculation of the entropy in some simple yet nontrival systems is interesting. Not only is it interesting for physics, it may also be interesting for information theory.[1–3]

The physical system we consider is the XX model in a transverse magnetic field and the entropy in which we are interested is that of a block of L neighboring spins at zero temperature and of an infinite system. The Hamiltonian for this model can be written as

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

[1] C. N. Yang Institute for Theoretical Physics, State University of New York at Stony Brook, Stony Brook, New York 11794-3840; e-mail: korepin@insti.physics.sunysb.edu

0022-4715/04/0800-0079/0

Here σ_n^x, σ_n^y, and σ_n^z are Pauli matrices, which describe spin operators on the nth lattice site, h is the magnetic field and N is the number of total lattice sites of the spin chain (we take $N \to \infty$ in this paper). This model has been solved by E. Lieb, T. Schultz, and D. Mattis in the zero-magnetic field case[4] and by E. Barouch and B. M. McCoy in the presence of a constant magnetic field.[5] Some exact calculations of time-dependent properties also exist; for examples, see ref. 6 by E. Barouch, B. M. McCoy, and M. Dresden and ref. 7 by D. B. Abraham, E. Barouch, G. Gallavotti, and A. Martin-Löf. The ground state and excitation spectrum are well known. The ground state is ferromagnetic for $|h| > 2$, while it is critical for $|h| < 2$. Let us denote the first L neighboring spins as sub-system A and the rest as sub-system B. Meanwhile the whole system is in ground state $|GS\rangle$. Then von Neumann entropy $(S(\rho_A))$ and Rényi entropy $(S_\alpha(\rho_A))$[2] for subsystem A are defined as follows:

$$S(\rho_A) = -\mathrm{Tr}(\rho_A \ln \rho_A), \tag{2}$$

$$S_\alpha(\rho_A) = \frac{1}{1-\alpha} \ln \mathrm{Tr}(\rho_A^\alpha), \qquad \alpha \neq 1 \quad \text{and} \quad \alpha > 0. \tag{3}$$

Von Neumann entropy is a well known object and Rényi entropy may also be important for both information theory and statistical physics.[8] When $\alpha \to 1$, the related Rényi entropy becomes von Neumann entropy. Here ρ_A is the reduced density matrix of subsystem A, i.e., $\rho_A = \mathrm{Tr}_B(\rho_{AB})$ and the density matrix of the whole system is $\rho_{AB} = |GS\rangle\langle GS|$ for zero temperature. Since the calculations for von Neumann entropy and Rényi entropy are very similar, we give a detailed calculation for the von Neumann entropy only. The explicit result for Rényi entropy will be given without derivation.

Before we give the full derivation in the following sections, we first summarize our results here. It is very interesting that one can introduce a scaling variable $\mathscr{L} = 2\mathrm{L}/\mathrm{L}_h$ with $\mathrm{L}_h = (1-(\frac{h}{2})^2)^{-\frac{1}{2}}$ for $|h| < 2$ and L_h infinite for $|h| \geqslant 2$. Then, both the von Neumann entropy and Rényi entropy of block spins have a very simple expression in the case of large $\mathscr{L}$ and small $\mathscr{L}$ as follows:

$$S_\alpha(\rho_A) \approx \begin{cases} \begin{cases} \frac{1}{1-\alpha} \ln\left((\frac{\mathscr{L}}{2\pi})^\alpha + (1-\frac{\mathscr{L}}{2\pi})^\alpha \right) & (\alpha \neq 1) \\ \frac{\mathscr{L}}{\pi} \ln \frac{\pi}{\mathscr{L}} & (\alpha = 1) \end{cases} & \text{if} \quad 0 < \mathscr{L} < 1 \\ \frac{1+\alpha^{-1}}{6} \ln \mathscr{L} + \Upsilon_1^{\{\alpha\}} & \text{if} \quad \mathscr{L} \gg 1. \end{cases} \tag{4}$$

Here $\Upsilon_1^{\{\alpha\}}$ is the constant defined in Eq. (64). When $\alpha = 1$, the Rényi entropy $S_\alpha(\rho_A)$ becomes the von Neumann entropy, the coefficient for $\log \mathscr{L}$ in the large $\mathscr{L}$ expression becomes $\frac{1}{3}$ and $\Upsilon_1^{\{\alpha\}}$ becomes

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

Following ref. 4, let us introduce the two Majorana operators

$$c_{2l-1}=\left(\prod_{n=1}^{l-1}\sigma_n^z\right)\sigma_l^x \qquad \text{and} \qquad c_{2l}=\left(\prod_{n=1}^{l-1}\sigma_n^z\right)\sigma_l^y \tag{5}$$

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, the Hamiltonian H_{XX} can be rewritten as

$$H_{\text{XX}}(h)=i\sum_{n=1}^{N}(c_{2n}c_{2n+1}-c_{2n-1}c_{2n+2}+hc_{2n-1}c_{2n}). \tag{6}$$

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[4, 5] (also see refs. 10 and 11) that

$$\langle GS|\, c_m\, |GS\rangle=0, \qquad \langle GS|\, c_m c_n\, |GS\rangle=\delta_{mn}+i(\mathbf{B}_N)_{mn}. \tag{7}$$

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

$$\mathbf{B}_N=\begin{pmatrix} \Pi_0 & \Pi_{-1} & \cdots & \Pi_{1-N} \\ \Pi_1 & \Pi_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ \Pi_{N-1} & \cdots & \cdots & \Pi_0 \end{pmatrix} \quad \text{and} \quad \Pi_l=\frac{1}{2\pi}\int_0^{2\pi} d\theta\, e^{-il\theta}\mathcal{G}(\theta), \tag{8}$$

where both Π_l and $\mathcal{G}(\theta)$ (for $N\to\infty$) are 2×2 matrices,

$$\mathcal{G}(\theta)=\begin{pmatrix} 0 & g(\theta) \\ -g(\theta) & 0 \end{pmatrix}, \qquad g(\theta)=\begin{cases} 1, & -k_F<\theta<k_F, \\ -1, & k_F<\theta<(2\pi-k_F) \end{cases} \tag{9}$$

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

$$d_m=\sum_{n=1}^{2L} v_{mn}c_n, \quad m=1,\ldots,2\mathrm{L}; \qquad b_l=(d_{2l}+id_{2l+1})/2, \quad l=1,\ldots,\mathrm{L}, \tag{10}$$

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

$$b_l^+ = (d_{2l} - i d_{2l+1})/2, \quad \{b_i, b_j\} = 0, \quad \{b_i^+, b_j^+\} = 0, \quad \{b_i^+, b_j\} = \delta_{i,j}. \tag{11}$$

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

$$b_l\, |0\rangle_{\mathrm{vac}} = 0, \qquad l = 1, \ldots, \mathrm{L}. \tag{12}$$

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

2. DENSITY MATRIX OF SUBSYSTEM A

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

$$\rho = \sum_{I,J} c(I,J)\, |\psi_I\rangle\langle\psi_J|. \tag{13}$$

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

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

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

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

Now let us consider the quantum spin chain defined in Eq. (1). For the subsystem 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 the fermionic operators defined in Eq. (10).) It is easy to find that $\tilde{P}(J,I) = (\prod_{i=1}^{\mathrm{L}} O_i)^\dagger$ if

$P(I, J) = \prod_{i=1}^{L} O_i$. Here $\dagger$ means hermitian conjugation. Therefore, the reduced density matrix for subsystem A can be represented as

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

Here the summation is over all possible different terms $\prod_{i=1}^{L} O_i$. For the whole system to be in the 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 follows:

$$\rho_A = \sum \langle GS|\left(\prod_{i=1}^{L} O_i\right)^{\dagger}|GS\rangle \prod_{i=1}^{L} O_i. \tag{17}$$

This is the expression of the density matrix with coefficients related to multi-point correlation functions. These correlation functions are well studied in the physics literature.[9] Now let us choose matrix $\mathbf{V}$ in Eq. (10) so that the set of fermionic bases $\{b_i^+\}$ and $\{b_i\}$ satisfy the equations

$$\langle GS|\, b_i b_j\, |GS\rangle = 0, \qquad \langle GS|\, b_i^+ b_j\, |GS\rangle = \delta_{i,j}\langle GS|\, b_i^+ b_i\, |GS\rangle. \tag{18}$$

Then the reduced density matrix ρ_A represented as the sum of products in Eq. (17) can be represented as a product of sums:

$$\rho_A = \prod_{i=1}^{L} (\langle GS|\, b_i^+ b_i\, |GS\rangle\, b_i^+ b_i + \langle GS|\, b_i b_i^+\, |GS\rangle\, b_i b_i^+). \tag{19}$$

Here we used the equations $\langle GS|\, b_i\, |GS\rangle = 0 = \langle GS|\, b_i^+\, |GS\rangle$ and the Wick theorem. This fermionic basis was suggested by G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev in refs. 10 and 11. A similar result for the density matrix of a subsystem in terms of the free spinless fermion model was obtained by C. A. Cheong and C. L. Henley in ref. 12.

3. CLOSED FORM FOR THE ENTROPY

Now let us find a matrix $\mathbf{V}$ in Eq. (10), which will block-diagonalize correlation functions of the Majorana operators c_n. From Eqs. (8) and (10), we have the following expression for the correlation function of d_n operators:

$$\begin{aligned}
\langle GS|\, d_m d_n\, |GS\rangle &= \sum_{i=1}^{2L}\sum_{j=1}^{2L} v_{mi}\langle GS|\, c_i c_j\, |GS\rangle\, v_{jn},\\
\langle GS|\, c_m c_n\, |GS\rangle &= \delta_{mn} + \mathrm{i}(\mathbf{B}_{\mathrm{L}})_{mn},\\
\langle GS|\, d_m d_n\, |GS\rangle &= \delta_{mn} + \mathrm{i}(\tilde{\mathbf{B}}_{\mathrm{L}})_{mn}.
\end{aligned} \tag{20}$$

The last equation is the definition of matrix $\tilde{\mathbf{B}}_\mathrm{L}$. Matrix $\mathbf{B}_\mathrm{L}$ is the submatrix of $\mathbf{B}_\mathrm{N}$ defined in Eq. (8) with $m, n = 1, 2, \ldots, \mathrm{L}$. We also require $\tilde{\mathbf{B}}_\mathrm{L}$ to be of the form[10, 11]

$$\tilde{\mathbf{B}}_\mathrm{L} = V\mathbf{B}_\mathrm{L}V^T = \bigoplus_{m=1}^{\mathrm{L}} v_m \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \mathbf{\Omega} \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{21}$$

Here the matrix $\mathbf{\Omega}$ is a diagonal matrix with elements v_m (all v_m are real numbers). Therefore, choosing matrix $\mathbf{V}$ satisfying Eq. (21) in Eq. (10), we obtain 2L operators $\{b_l\}$ and $\{b_l^+\}$ with the following expectation values:

$$\langle GS|\, b_m \,|GS\rangle = 0, \quad \langle GS|\, b_m b_n \,|GS\rangle = 0, \quad \langle GS|\, b_m^+ b_n \,|GS\rangle = \delta_{mn}\frac{1+v_m}{2}. \tag{22}$$

Using the simple expression for the reduced density matrix ρ_A in Eq. (19), we obtain

$$\rho_A = \prod_{i=1}^{\mathrm{L}} \left(\frac{1+v_i}{2} b_i^+ b_i + \frac{1-v_i}{2} b_i b_i^+ \right). \tag{23}$$

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

$$\lambda_{x_1 x_2 \cdots x_\mathrm{L}} = \prod_{i=1}^{\mathrm{L}} \frac{1+(-1)^{x_i} v_i}{2}, \qquad x_i = 0, 1 \quad \forall i. \tag{24}$$

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

$$S(\rho_A) = \sum_{m=1}^{\mathrm{L}} e(1, v_m) \tag{25}$$

with

$$e(x, v) = -\frac{x+v}{2} \ln\left(\frac{x+v}{2}\right) - \frac{x-v}{2} \ln\left(\frac{x-v}{2}\right). \tag{26}$$

We shall use this result further to obtain the analytical asymptotic. Function $e(1, v)$ in Eq. (25) is equal to the Shannon entropy function $H(\frac{1+v}{2})$. However, in the following calculation [Eq. (31)], we will need the more general function $e(x, v)$ instead of $H(v)$. Note further that the matrix $\mathbf{B}_{\mathrm{L}}$ can have a direct product form, i.e.,

$$\mathbf{B}_{\mathrm{L}} = \mathbf{G}_{\mathrm{L}} \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \text{with} \quad \mathbf{G}_{\mathrm{L}} = \begin{pmatrix} g_0 & g_{-1} & \cdots & g_{1-L} \\ g_1 & g_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ g_{L-1} & \cdots & \cdots & g_0 \end{pmatrix}, \tag{27}$$

where g_l is defined as

$$g_l = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta \, e^{-il\theta} g(\theta) \qquad \text{and} \qquad g(\theta) = \begin{cases} 1, & -k_F < \theta < k_F, \\ -1, & k_F < \theta < (2\pi - k_F) \end{cases} \tag{28}$$

and $k_F = \arccos(|h|/2)$. From Eqs. (21) and (27), we conclude that all v_m are just the eigenvalues of the real symmetric matrix $\mathbf{G}_{\mathrm{L}}$.

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

$$D_{\mathrm{L}}(\lambda) = \det(\tilde{\mathbf{G}}_{\mathrm{L}}(\lambda) \equiv \lambda I_{\mathrm{L}} - \mathbf{G}_{\mathrm{L}}). \tag{29}$$

Here $\tilde{\mathbf{G}}_{\mathrm{L}}$ is a Toeplitz matrix (see ref. 17) and I_{L} is the identity matrix of dimension L. Obviously we also have

$$D_{\mathrm{L}}(\lambda) = \prod_{m=1}^{\mathrm{L}} (\lambda - v_m). \tag{30}$$

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

$$S(\rho_A) = \lim_{\epsilon \to 0^+} \lim_{\delta \to 0^+} \frac{1}{2\pi \mathrm{i}} \oint_{c(\epsilon, \delta)} e(1+\epsilon, \lambda) \, \mathrm{d} \ln D_{\mathrm{L}}(\lambda). \tag{31}$$

Here the contour $c(\epsilon, \delta)$ in Fig. 1 encircles all zeros of $D_{\mathrm{L}}(\lambda)$, but the function $e(1+\epsilon, \lambda)$ is analytic within the contour. Just as the Toeplitz matrix $\mathbf{G}_{\mathrm{L}}$ is generated by the function $g(\theta)$ in Eqs. (27) and (28) [see next section], the Toeplitz matrix $\tilde{\mathbf{G}}_{\mathrm{L}}(\lambda)$ is generated by the function $\tilde{g}(\theta)$ defined by

$$\tilde{g}(\theta) = \begin{cases} \lambda - 1, & -k_F < \theta < k_F, \\ \lambda + 1, & k_F < \theta < (2\pi - k_F). \end{cases} \tag{32}$$

Note 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

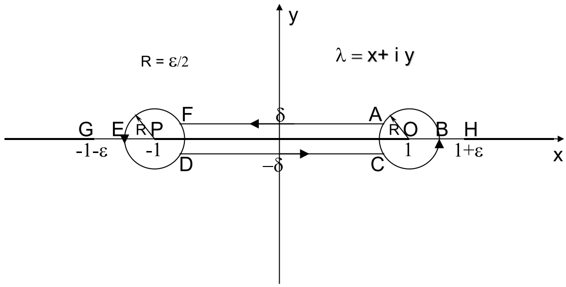

Fig. 1. The contour $c(\epsilon, \delta)$. Bold lines $(-\infty, -1-\epsilon)$ and $(1+\epsilon, \infty)$ are the cuts of integrand $e(1+\epsilon, \lambda)$. Zeros of $D_{\mathrm{L}}(\lambda)$ [Eq. (30)] are located on bold line $(-1, 1)$ and this line becomes the cut of $\mathrm{d}\log D_{\mathrm{L}}(\lambda)$ for $L \to \infty$ [Eq. (47)]. The arrow is the direction of the route of the integral we take and R is the radius of the circle.

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 $\tilde{\mathbf{G}}_{\mathrm{L}}(\lambda)$. Before we calculate the determinant of the Toeplitz matrix $\tilde{\mathbf{G}}_{\mathrm{L}}(\lambda)$, we also want to point out two special cases which allow us to obtain an explicit form for these eigenvalues v_m and hence the entropy $S(\rho_A)$. These are cases with a small lattice size of the subsystem A and magnetic h close to the critical values ± 2. Let us take $\tilde{k}_F = k_F$ for $k_F < \frac{\pi}{2}$ or $\tilde{k}_F = \pi - k_F$ for $k_F > \frac{\pi}{2}$. For the case $\tilde{k}_F L \ll 1$, the Toeplitz matrix $\mathbf{G}_{\mathrm{L}}$ can be well approximated by a matrix with diagonal elements $(2\tilde{k}_F/\pi - 1)$ and all other matrix elements equal to $2\tilde{k}_F/\pi$. Hence, we can obtain all eigenvalues for the Toeplitz matrix $\mathbf{G}_{\mathrm{L}}$ as $\{2\mathrm{L}\tilde{k}_F/\pi - 1, -1, -1, \ldots, -1\}$ and $S(\rho_A)$ becomes

$$S(\rho_A) \approx \frac{2\mathrm{L}\tilde{k}_F}{\pi} \ln \frac{\pi}{2\mathrm{L}\tilde{k}_F}, \qquad 0 < \tilde{k}_F \mathrm{L} \ll 1. \tag{33}$$

The expression above can also be re-expressed in terms of h as

$$S(\rho_A) \approx \frac{2\mathrm{L}(1-h^2/4)^{\frac{1}{2}}}{\pi} \ln \frac{\pi}{2\mathrm{L}(1-h^2/4)^{\frac{1}{2}}}, \qquad 0 < (1-h^2/4)^{\frac{1}{2}}\,\mathrm{L} \ll 1. \tag{34}$$

4. THE TOEPLITZ MATRIX AND THE FISHER–HARTWIG CONJECTURE

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

$$T_{\mathrm{L}}[\phi] = (\phi_{i-j}), \qquad i, j = 1, \ldots, \mathrm{L}-1 \tag{35}$$

where

$$\phi_l = \frac{1}{2\pi} \int_0^{2\pi} \phi(\theta)\, e^{-il\theta}\, \mathrm{d}\theta \tag{36}$$

is the lth Fourier coefficient of the generating function $\phi(\theta)$. The determinant of $T_L[\phi]$ is denoted by D_{L}. The study of the asymptotic behavior of the determinant of the Toeplitz matrix with a singular generating function was initiated by T. T. Wu[13] in his calculation of spin correlation in the two-dimensional Ising model. Later his result was incorporated into a more general conjecture, i.e., the famous Fisher–Hartwig conjecture.[14–17]

Fisher–Hartwig Conjecture. Suppose the generating function of the Toeplitz matrix $\phi(\theta)$ is singular in the following form:

$$\phi(\theta) = \psi(\theta) \prod_{r=1}^{R} t_{\beta_r,\theta_r}(\theta)\, u_{\alpha_r,\theta_r}(\theta), \tag{37}$$

where

$$t_{\beta_r,\theta_r}(\theta) = \exp[-i\beta_r(\pi-\theta+\theta_r)], \qquad \theta_r < \theta < 2\pi+\theta_r \tag{38}$$

$$u_{\alpha_r,\theta_r}(\theta) = (2-2\cos(\theta-\theta_r))^{\alpha_r}, \qquad \Re\alpha_r > -\tfrac{1}{2} \tag{39}$$

and ψ: $\mathbf{T}\to\mathbf{C}$ is a smooth non-vanishing function with zero winding number. Then as $n\to\infty$, the determinant of $T_{\mathrm{L}}[\phi]$ can be expressed as follows

$$D_{\mathrm{L}} = (\mathscr{F}[\psi])^{\mathrm{L}} \left(\prod_{i=1}^{R} \mathrm{L}^{\alpha_i^2-\beta_i^2}\right) \mathscr{E}[\psi, \{\alpha_i\}, \{\beta_i\}, \{\theta_i\}], \qquad \mathrm{L}\to\infty. \tag{40}$$

Here $\mathscr{F}[\psi] = \exp(\frac{1}{2\pi}\int_0^{2\pi} \ln\psi(\theta)\, \mathrm{d}\theta)$. Further assuming that there exists the Weiner–Hopf factorization

$$\psi(\theta) = \mathscr{F}[\psi]\, \psi_+(\exp(\mathrm{i}\theta))\, \psi_-(\exp(-\mathrm{i}\theta)), \tag{41}$$

the constant $\mathscr{E}[\psi, \{\alpha_{\mathrm{i}}\}, \{\beta_{\mathrm{i}}\}, \{\theta_{\mathrm{i}}\}]$ in Eq. (40) can be written as

$$\begin{aligned}\mathscr{E}[\psi, \{\alpha_i\}, \{\beta_i\}, \{\theta_i\}] &= \mathscr{E}[\psi] \\ &\times \prod_{i=1}^{R} G(1+\alpha_i+\beta_i)\, G(1+\alpha_i-\beta_i)/G(1+2\alpha_i) \\ &\times \prod_{i=1}^{R} (\psi_-(\exp(\mathrm{i}\theta_i)))^{-\alpha_i-\beta_i}\, (\psi_+(\exp(-\mathrm{i}\theta_i)))^{-\alpha_i+\beta_i} \\ &\times \prod_{1\leqslant i\neq j\leqslant R} (1-\exp(\mathrm{i}(\theta_i-\theta_j)))^{-(\alpha_i+\beta_i)(\alpha_j-\beta_j)},\end{aligned} \tag{42}$$

where G is the Barnes G-function, $\mathscr{E}[\psi]=\exp(\sum_{k=1}^{\infty} k s_k s_{-k})$, and s_k is the kth Fourier coefficient of $\ln \psi(\theta)$. The Barnes G-function is defined as

$$G(1+z)=(2\pi)^{z/2}\, e^{-(z+1)\,z/2-\gamma_E z^2/2} \prod_{n=1}^{\infty} \{(1+z/n)^n\, e^{-z+z^2/(2n)}\}, \tag{43}$$

where γ_E is the Euler constant and its numerical value is $0.5772156649\cdots$. This conjecture has not been proven for the general case. However, there are various special cases for which the conjecture was proven.

For our case, the generating function $\tilde{g}(\theta)$ has two jumps at $\theta=\pm k_F$ and it has the following canonical factorization:

$$\tilde{g}(\theta)=\psi(\theta)\, t_{\beta_1(\lambda),\,k_F}(\theta)\, t_{\beta_2(\lambda),\,-k_F}(\theta) \tag{44}$$

with

$$\psi(\theta)=(\lambda+1)\left(\frac{\lambda+1}{\lambda-1}\right)^{-k_F/\pi}, \qquad \beta(\lambda)=-\beta_1(\lambda)=\beta_2(\lambda)=\frac{1}{2\pi \mathrm{i}}\ln\frac{\lambda+1}{\lambda-1}. \tag{45}$$

The function t was defined in Eq. (38). We fix the branch of the logarithm in the following way:

$$-\pi \leqslant \arg\left(\frac{\lambda+1}{\lambda-1}\right) < \pi. \tag{46}$$

For $\lambda \notin [-1, 1]$, we know that $|\Re(\beta_1(\lambda))|<\frac{1}{2}$ and $|\Re(\beta_2(\lambda))|<\frac{1}{2}$ and the Fisher–Hartwig conjecture was proven by E. L. Basor for this case.[15] Therefore, we will call it a theorem instead of a conjecture for our application. Hence following the theorem in Eq. (40), the determinant $D_{\mathrm{L}}(\lambda)$ of $\lambda I_{\mathrm{L}}-\mathbf{G}_{\mathrm{L}}$ can be asymptotically represented as

$$\begin{aligned} D_{\mathrm{L}}(\lambda) &= (2-2\cos(2k_F))^{-\beta^2(\lambda)}\, \{G(1+\beta(\lambda))\, G(1-\beta(\lambda))\}^2 \\ &\quad \times \{(\lambda+1)((\lambda+1)/(\lambda-1))^{-k_F/\pi}\}^{\mathrm{L}}\, \mathrm{L}^{-2\beta^2(\lambda)}. \end{aligned} \tag{47}$$

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

$$G(1+\beta(\lambda))\, G(1-\beta(\lambda)) = e^{-(1+\gamma_E)\,\beta^2(\lambda)} \prod_{n=1}^{\infty}\left\{\left(1-\frac{\beta^2(\lambda)}{n^2}\right)^n e^{\beta^2(\lambda)/n^2}\right\}. \tag{48}$$

5. ASYMPTOTIC FORM OF THE ENTROPY

Now let us come back to the calculation of the entropy $S(\rho_A)$. For later convenience, let us define

$$\Upsilon(\lambda) = \sum_{n=1}^{\infty} \frac{n^{-1}\beta^2(\lambda)}{n^2 - \beta^2(\lambda)}. \tag{49}$$

Taking the logarithmic derivative of $D_{\mathrm{L}}(\lambda)$ [Eq. (47)], we obtain

$$\frac{\mathrm{d}\ln D_{\mathrm{L}}(\lambda)}{\mathrm{d}\lambda} = \left(\frac{1-k_F/\pi}{1+\lambda} - \frac{k_F/\pi}{1-\lambda}\right)\mathrm{L}$$
$$-\frac{4}{\mathrm{i}\pi}\frac{\beta(\lambda)}{(1+\lambda)(1-\lambda)}(\ln \mathrm{L} + \ln(2\,|\sin k_F|) + (1+\gamma_E) + \Upsilon(\lambda)). \tag{50}$$

Let us substitute the asymptotic form above for $\mathrm{d}\ln D_{\mathrm{L}}(\lambda)/\mathrm{d}\lambda$ into Eq. (31) for the entropy $S(\rho_A)$:

$$S(\rho_A) = S_1(\rho_A) + S_2(\rho_A) \tag{51}$$

with

$$S_1(\rho_A) = \lim_{\epsilon \to 0^+} \lim_{\delta \to 0^+} \frac{1}{2\pi \mathrm{i}} \oint_{c(\epsilon,\delta)} e(1+\epsilon,\lambda)\left(\frac{1-k_F/\pi}{1+\lambda} - \frac{k_F/\pi}{1-\lambda}\right)\mathrm{L},$$
$$S_2(\rho_A) = \lim_{\epsilon \to 0^+} \lim_{\delta \to 0^+} \frac{2}{\pi^2} \oint_{c(\epsilon,\delta)} \mathrm{d}\lambda\, \frac{e(1+\epsilon,\lambda)\,\beta(\lambda)}{(1+\lambda)(1-\lambda)}$$
$$\times (\ln \mathrm{L} + \ln(2\,|\sin k_F|) + (1+\gamma_E) + \Upsilon(\lambda)), \tag{52}$$

where the contour is taken as shown in Fig. 1. The first integral in Eq. (52) can be carried out by using the residue theorem and the definition of the function $e(x, v)$ in Eq. (26). We found that the linear term in L for the entropy $S(\rho_A)$ vanishes. The second integral can be calculated as follows: First, we note that

$$\oint_{c(\epsilon,\delta)} \mathrm{d}\lambda(\cdots) = \left(\int_{\overrightarrow{\mathrm{AF}}} + \int_{\overrightarrow{\mathrm{FED}}} + \int_{\overrightarrow{\mathrm{DC}}} + \int_{\overrightarrow{\mathrm{CBA}}}\right)\mathrm{d}\lambda\,(\cdots). \tag{53}$$

Second, we can show that the contribution of the integral from the circular arcs $\overrightarrow{\mathrm{FED}}$ and $\overrightarrow{\mathrm{CAB}}$ vanishes. Therefore, the entropy [Eq. (52)] can be written as

$$S(\rho_A) = \lim_{\epsilon\to 0^+} \frac{2}{\pi^2}\left(\int_{1+\mathrm{i}0^+}^{-1+\mathrm{i}0^+} + \int_{-1+\mathrm{i}0^-}^{1+\mathrm{i}0^-}\right) \mathrm{d}\lambda \; \frac{e(1+\epsilon,\lambda)\,\beta(\lambda)}{(1+\lambda)(1-\lambda)}$$
$$\times\, (\ln L + \ln(2\,|\sin k_F|) + (1+\gamma_E) + \Upsilon(\lambda)). \tag{54}$$

For further simplification, we shall use the fact that

$$\beta(x+\mathrm{i}0^{\pm}) = \frac{1}{2\mathrm{i}\pi}\left(\ln\frac{1+x}{1-x} \mp \mathrm{i}(\pi-0^+)\right) = -\mathrm{i}W(x) \mp \left(\frac{1}{2} - 0^+\right) \tag{55}$$

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

$$W(x) = \frac{1}{2\pi}\ln\frac{1+x}{1-x}. \tag{56}$$

We can now write the entropy $S(\rho_A)$ as

$$S(\rho_A) = \frac{2}{\pi^2}\int_{-1}^{1} \mathrm{d}x\, \frac{e(1,x)}{1-x^2}\,(\ln \mathrm{L} + \ln(2\,|\sin k_F|) + (1+\gamma_E))$$
$$+ \sum_{n=1}^{\infty} \frac{2n^{-1}}{\pi^2}\int_{-1}^{1} \mathrm{d}x\, \frac{e(1,x)}{1-x^2}\left(\frac{(\frac{1}{2}+\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}+\mathrm{i}W(x))^2} + \frac{(\frac{1}{2}-\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}-\mathrm{i}W(x))^2}\right), \tag{57}$$

where $e(1,x)$ is defined in Eq. (26). This expression for $S(\rho_A)$ contains two integrals. The first integral can be expressed exactly as

$$\frac{2}{\pi^2}\int_{-1}^{1}\mathrm{d}x\left(-\frac{1+x}{2}\ln\frac{1+x}{2} - \frac{1-x}{2}\ln\frac{1-x}{2}\right)\frac{1}{1-x^2} = \frac{1}{3}. \tag{58}$$

The second integral in Eq. (57) can be written as

$$\Upsilon_0 = \sum_{n=1}^{\infty}\frac{n^{-1}}{\pi^2}\int_{-1}^{1}\mathrm{d}x\left(-\frac{1}{1-x}\ln\frac{1+x}{2} - \frac{1}{1+x}\ln\frac{1-x}{2}\right)$$
$$\times\left(\frac{(\frac{1}{2}+\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}+\mathrm{i}W(x))^2} + \frac{(\frac{1}{2}-\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}-\mathrm{i}W(x))^2}\right), \tag{59}$$

which can be further simplified.[18] Finally we have that

$$S(\rho_A) = \frac{1}{3}\ln \mathrm{L} + \frac{1}{6}\ln\left(1-\left(\frac{h}{2}\right)^2\right) + \frac{\ln 2}{3} + \Upsilon_1, \qquad \mathrm{L}\to\infty, \tag{60}$$

with

$$\Upsilon_1 = -\int_0^\infty \mathrm{d}t \left\{\frac{e^{-t}}{3t} + \frac{1}{t\sinh^2(t/2)} - \frac{\cosh(t/2)}{2\sinh^3(t/2)}\right\} \tag{61}$$

for the XX model. The leading term of the asymptotic of the entropy $\frac{1}{3}\ln \mathrm{L}$ in Eq. (60) was first obtained based on numerical calculation and a simple conformal argument in refs. 10 and 11 in the context of entanglement. We also want to mention that a complete conformal derivation for this entropy was found in ref. 19. One can numerically evaluate Υ_1 to a very high accuracy to be $0.4950179\cdots$. For the 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 the numerical accuracy to be more than five digits.

6. SUMMARY

In this paper, we study the entropy of a block of L neighboring spins in the XX model with the presence of a transverse magnetic field. We obtain Eqs. (34) and (60) for the von Neumann entropy of a block of L neighboring spins in XX with small L and large L respectively. It is interesting to note that there is a natural length scale $\mathrm{L}_h = 1/(1-(\frac{h}{2})^2)^{\frac{1}{2}}$ for $|h|<2$ and $\mathrm{L}_h=\infty$ for $|h|\geqslant 2$ to incorporate the magnetic field effects. When $|h|$ increases from less than 2 to larger than 2, the system evolves from the critical phase into the ferromagnetic phase and the length scale L_h increases. L_h shows the singular behavior at the phase-transition point. Let us introduce the scaling variable $\mathscr{L} = 2\mathrm{L}/\mathrm{L}_h$, i.e.,

$$\mathscr{L} \equiv 2\mathrm{L}\left(1-\left(\frac{h}{2}\right)^2\right)^{\frac{1}{2}}$$

for $|h|<2$. Then we can express the von Neumann entropy of L neighboring spins in the following simple form:

$$S(\rho_A) = \begin{cases} \frac{\mathscr{L}}{\pi}\ln\frac{\pi}{\mathscr{L}} & \text{if} \quad 0<\mathscr{L}<1 \\ \frac{1}{3}\ln\mathscr{L} + \Upsilon_1 & \text{if} \quad \mathscr{L}\gg 1 \end{cases} \tag{62}$$

with

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

For a small lattice and a magnetic field close to ± 2, we obtain the result directly. To obtain the result for large L asymptotically, we first expressed the entropy in terms of the determinant of a Toeplitz matrix. Then we used a special case of the Fisher–Hartwig conjecture;[14] this special case was proven in ref. 15.

From similar calculations, we also obtain the Rényi entropy in Eq. (3) to be

$$S_\alpha(\rho_A) = \begin{cases} \frac{1}{1-\alpha} \ln\left(\left(\frac{\mathscr{L}}{2\pi}\right)^\alpha + \left(1-\frac{\mathscr{L}}{2\pi}\right)^\alpha\right) & \text{if} \quad 0 < \mathscr{L} < 1 \\ \frac{1+\alpha^{-1}}{6} \ln \mathscr{L} + \Upsilon_1^{\{\alpha\}} & \text{if} \quad \mathscr{L} \gg 1. \end{cases} \tag{63}$$

Here

$$\Upsilon_1^{\{\alpha\}} = -\frac{1}{\pi^2}\int_{-1}^{1} \mathrm{d}x \, \frac{s_\alpha(x)}{1-x^2}\left(\psi\left(\frac{1}{2} - \mathrm{i}W(x)\right) + \psi\left(\frac{1}{2} + \mathrm{i}W(x)\right)\right), \tag{64}$$

$$s_\alpha(x) = \frac{1}{1-\alpha} \ln\left(\left(\frac{1+x}{2}\right)^\alpha + \left(\frac{1-x}{2}\right)^\alpha\right), \qquad \alpha \neq 1, \tag{65}$$

$$\psi(x) \equiv \frac{\mathrm{d}}{\mathrm{d}x} \ln \Gamma(x) = -\gamma_E + \sum_{n=0}^{\infty}\left(\frac{1}{n+1} - \frac{1}{n+x}\right), \tag{66}$$

$$W(x) = \frac{1}{2\pi} \ln \frac{1+x}{1-x} \tag{67}$$

with γ_E the Euler constant and $\Gamma(x)$ the well known Gamma function.

APPENDIX: SIMPLIFICATION OF FORMULA

In this Appendix, we show more details for simplification of Υ_0 (59) in detail. In order to simplify Υ_0, we will use the function $\psi(x)$, which is defined as

$$\psi(x) \equiv \frac{\mathrm{d}}{\mathrm{d}x} \ln \Gamma(x) = -\gamma_E + \sum_{n=0}^{\infty} \frac{1}{n+1} - \sum_{n=0}^{\infty} \frac{1}{n+x} \tag{68}$$

with γ_E the Euler constant and $\Gamma(x)$ the well known Gamma function, and the property

$$\psi(x+1) = \psi(x) + \frac{1}{x}. \tag{69}$$

Introducing $z\ (\bar{z}) \equiv \frac{1}{2} + (-)\ \mathrm{i}W(x)$ and using Eqs. (68) and (69), we obtain

$$\sum_{n=1}^{\infty} n^{-1} \left(\frac{(\frac{1}{2}+\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}+\mathrm{i}W(x))^2} + \frac{(\frac{1}{2}-\mathrm{i}W(x))^3}{n^2-(\frac{1}{2}-\mathrm{i}W(x))^2} \right)$$
$$= \psi(1) - 1 - \frac{1}{2}\psi\left(\frac{1}{2} - \mathrm{i}W(x)\right) - \frac{1}{2}\psi\left(\frac{1}{2} + \mathrm{i}W(x)\right) \tag{70}$$

by using Eq. (69) and the definition of z and $\bar{z}$. Hence, we obtain

$$\begin{aligned} \Upsilon_0 &= \frac{1}{\pi^2}\int_{-1}^{1} \mathrm{d}x \left(-\frac{1}{1-x} \ln \frac{1+x}{2} - \frac{1}{1+x} \ln \frac{1-x}{2} \right) \\ &\quad \times \left[\psi(1) - 1 - \frac{1}{2}\psi\left(\frac{1}{2} - \mathrm{i}W(x)\right) - \frac{1}{2}\psi\left(\frac{1}{2} + \mathrm{i}W(x)\right) \right] \\ &= \Upsilon_1 - \frac{1+\gamma_E}{3} \end{aligned} \tag{71}$$

with Υ_1 defined as

$$\begin{aligned} \Upsilon_1 = -\frac{1}{2\pi^2}\int_{-1}^{1} \mathrm{d}x \left(-\frac{1}{1-x} \ln \frac{1+x}{2} - \frac{1}{1+x} \ln \frac{1-x}{2} \right) \\ \times \left[\psi\left(\frac{1}{2} - \mathrm{i}W(x)\right) + \psi\left(\frac{1}{2} + \mathrm{i}W(x)\right) \right]. \end{aligned} \tag{72}$$

We now perform a change of variable using $w = \frac{1}{2\pi} \ln \frac{1+x}{1-x}$:

$$\begin{aligned} \Upsilon_1 = \frac{-2}{\pi}\int_{0}^{\infty} \mathrm{d}w (\ln[2\cosh(\pi w)] - \pi w \tanh(\pi w)) \\ \times \left[\psi\left(\frac{1}{2} - \mathrm{i}w\right) + \psi\left(\frac{1}{2} + \mathrm{i}w\right) \right]. \end{aligned} \tag{73}$$

We note that

$$\ln[2\cosh(\pi w)] - \pi w \tanh(\pi w) = \left(1 - \frac{\mathrm{d}}{\mathrm{d}\alpha}\right) \ln(1 + e^{-2\pi w \alpha}) \bigg|_{\alpha=1}. \tag{74}$$

and that

$$\Upsilon_1 = \frac{-2\mathrm{i}}{\pi}\int_0^\infty \mathrm{d}w(\ln[2\cosh(\pi w)] - \pi w \tanh(\pi w)) \cdot \frac{\mathrm{d}}{\mathrm{d}w}\ln\frac{\Gamma(\frac{1}{2}-\mathrm{i}w)}{\Gamma(\frac{1}{2}+\mathrm{i}w)}. \tag{75}$$

Use the following expression for the logarithm of the Gamma function:

$$\ln\Gamma(z) = \int_0^\infty \left[z-1-\frac{1-e^{-(z-1)t}}{1-e^{-t}}\right]\frac{e^{-t}}{t}\,\mathrm{d}t \tag{76}$$

which is particularly convenient because we need only the imaginary part of it:

$$\ln\frac{\Gamma(\frac{1}{2}-\mathrm{i}w)}{\Gamma(\frac{1}{2}+\mathrm{i}w)} = -\mathrm{i}\int_0^\infty \left[2we^{-t} - \frac{\sin(wt)}{\sinh(t/2)}\right]\frac{\mathrm{d}t}{t}. \tag{77}$$

After some elementary but tedious calculations, we finally obtain

$$\Upsilon_1 = -\int_0^\infty \mathrm{d}t\left\{\frac{e^{-t}}{3t} + \frac{1}{t\sinh^2(t/2)} - \frac{\cosh(t/2)}{2\sinh^3(t/2)}\right\}. \tag{78}$$

ACKNOWLEDGMENTS

We would like to thank Prof. B. M. McCoy, Prof. A. Abanov, and Mr. F. Franchini for useful discussions. This work was supported by the National Science Foundation (USA) under Grants DMR-0302758 and PHY-9988566.

REFERENCES

1. C. H. Bennett, H. J. Bernstein, S. Popescu, and B. Schumacher, *Phys. Rev. A* **53**:2046 (1996).
2. A. Rényi, *Probability Theory* (North-Holland, Amsterdam, 1970).
3. S. Abe and A. K. Rajagopal, *Phys. Rev. A* **60**:3461 (1999).
4. E. Lieb, T. Schultz, and D. Mattis, *Ann. Phys.* **16**:407 (1961).
5. E. Barouch and B. M. McCoy, *Phys. Rev. A* **3**:786 (1971)
6. E. Barouch, B. M. McCoy, and M. Dresden, *Phys. Rev. A* **2**:1075 (1970)
7. D. B. Abraham, E. Barouch, G. Gallavotti, and A. Martin-Löf, *Phys. Rev. Lett.* **25**:1449 (1970); *Studies in Appl. Math.* **50**:121 (1971); *ibid.* **51**:211 (1972).
8. C. Tsallis, *J. Stat. Phys.* **52**:479 (1988).
9. N. M. Bogoliubov, A. G. Izergin, and V. E. Korepin, *Quantum Inverse Scattering Method and Correlation Functions* (Cambridge University Press, Cambridge, 1993).
10. G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, *Phys. Rev. Lett.* **90**:227902 (2003).
11. J. I. Latorre, E. Rico, and G. Vidal, arXiv: quant-ph/0304098.

12. C. A. Cheong and C. L. Henley, arXiv: cond-mat/0206196.
13. T. T. Wu, *Phys. Rev.* **149**:380 (1966).
14. M. E. Fisher and R. E. Hartwig, *Adv. Chem. Phys.* **15**:333 (1968).
15. E. L. Basor, *Indiana Math. J.* **28**:975 (1979).
16. E. L. Basor and C. A. Tracy, *Physica A* **177**:167 (1991).
17. A. Böttcher and B. Silbermann, *Analysis of Toeplitz Operators* (Springer-Verlag, Berlin, 1990).
18. F. Franchini, private communication.
19. V. E. Korepin, *Phys. Rev. Lett.* **92**:096402 (2004).