Entanglement in XY Spin Chain

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(Dated: April 1, 2022)

We consider the ground state of the XY model on an infinite chain at zero temperature. Following Bennett, Bernstein, Popescu, and Schumacher we use entropy of a sub-system as a measure of entanglement. Vidal, Latorre, Rico and Kitaev conjectured that von Neumann entropy of a large block of neighboring spins approaches a constant as the size of the block increases. We evaluated this limiting entropy as a function of anisotropy and transverse magnetic field. We used the methods based on integrable Fredholm operators and Riemann-Hilbert problem. The entropy is singular at phase transitions.

There is an essential interest in quantifying entanglement in various quantum systems. In this paper we evaluated the entropy of a block of neighboring spins. We can think that the ground state is the ground state. We shall calculate the entropy of a block of L spins approaching a constant as the size of the block increases. We evaluated this entropy by the following:

\[ S(\rho_A) = -Tr_A(\rho_A \ln \rho_A), \] (2)

This entropy defines the dimension of the Hilbert space of states of the block of L spins. Majorana operators were used in [3] to describe the entropy [4] by the following matrix:

\[ B_L = \begin{pmatrix} \Pi_0 & \Pi_1 & \cdots & \Pi_{L-1} \\ \Pi_1 & \Pi_0 & & \\ & & \ddots & \\ \Pi_{L-1} & \cdots & & \Pi_0 \end{pmatrix} \]

Here

\[ \Pi_\ell = \frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-i\theta} G(\theta), \quad G(\theta) = \begin{pmatrix} 0 & g(\theta) \\ -g^{-1}(\theta) & 0 \end{pmatrix} \] (3)

and

\[ g(\theta) = \frac{\cos \theta - i\gamma \sin \theta - h/2}{\cos \theta - i\gamma \sin \theta - h/2}. \]

One can use an orthogonal matrix V to transform B_L to a canonical form:

\[ V B_L V^T = \oplus_{m=1}^L \nu_m \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \] (4)

The real numbers \(-1 < \nu_m < 1\) play an important role. We shall call them eigenvalues. The entropy of a block of L neighboring spins was represented in [3] as

\[ S(\rho_A) = \sum_{m=1}^L H(\nu_m) \] (5)

with

\[ H(\nu) = -\frac{1+\nu}{2} \ln \frac{1+\nu}{2} - \frac{1-\nu}{2} \ln \frac{1-\nu}{2}. \] (6)
In order to calculate the asymptotic form of the entropy let us introduce:

\[ \mathbf{B}_L(\lambda) = i\lambda \mathbf{I}_L - \mathbf{B}_L, \quad D_L(\lambda) = \det \mathbf{B}_L(\lambda) \]  

and

\[ e(x, \nu) = -\frac{x + \nu}{2} \ln \frac{x + \nu}{2} - \frac{x - \nu}{2} \ln \frac{x - \nu}{2}. \]  

Here \( I_L \) is the identity matrix of dimension \( 2L \). By definition, we have \( H(\nu) = e(1, \nu) \) and

\[ D_L(\lambda) = (-1)^L \prod_{m=1}^{L} (\lambda^2 - \nu_m^2). \]  

In [33] we used Cauchy residue theorem to rewrite formula (2) in the following form:

\[ S(\rho_A) = \lim_{\epsilon \to 0^+} \frac{1}{4\pi i} \int_{\Gamma} d\lambda \epsilon(1 + \epsilon, \lambda) \frac{d}{d\lambda} \ln D_L(\lambda). \]  

Here the contour \( \Gamma' \) in Fig. 1 encircles all zeros of \( D_L(\lambda) \). We also realized that \( \mathbf{B}_L(\lambda) \) is a block Toeplitz matrix

\[ \mathbf{B}_L(\lambda) = \begin{pmatrix} \tilde{B}_1 & \tilde{B}_2 & \cdots & \tilde{B}_L \\ \tilde{B}_2 & \tilde{B}_1 & \cdots & \tilde{B}_{L-1} \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{B}_L & \cdots & \cdots & \tilde{B}_1 \end{pmatrix} \]  

with the generator \( \Phi(z) \), i.e.

\[ \Pi_l = \frac{1}{2\pi i} \oint_{\Gamma} dz \ z^{-l-1} \Phi(z), \quad \Phi(z) = \begin{pmatrix} i \lambda \\ -\phi^{-1}(z) \ i \lambda \end{pmatrix} \]  

and \( \phi(z) = \frac{\lambda^*_1 (1 - \lambda_1 z)(1 - \lambda_2 z^{-1})}{\lambda^*_1 (1 - \lambda_1^* z^{-1})(1 - \lambda_2^* z)} \) \( \rightarrow \frac{1}{\sqrt{2}} \) (12)

\[ \Phi(z) = \begin{pmatrix} \lambda^*_1 (1 - \lambda_1 z)(1 - \lambda_2 z^{-1}) \ \
\lambda^*_1 (1 - \lambda_1^* z^{-1})(1 - \lambda_2^* z) \end{pmatrix} \]  

\[ \rightarrow \frac{1}{\sqrt{2}} \] (12)

\[ \text{z-plane with } z = x + iy \]

\[ \begin{array}{c|c|c}
\text{Case 1a&2} & \text{Case 1b} \\
\hline
\end{array} \]

We fix the branch by requiring that \( \phi(\infty) > 0 \). We use * to denote complex conjugation and \( \Xi \) is the unite circle.

Definition of the end points of the cuts \( \lambda_{\pm} \) depends on the case:

1. Case 1a: \( \lambda_A = \lambda_1 \) and \( \lambda_B = \lambda_2^* \), \( \lambda_C = \lambda_2 \) and \( \lambda_D = \lambda_1^* \).
2. Case 1b: \( \lambda_A = \lambda_1 \) and \( \lambda_B = \lambda_2 \), \( \lambda_C = \lambda_2^* \) and \( \lambda_D = \lambda_1^* \).
3. Case 2: \( h > 2 \).

In two cases 1a and 2:

\[ \lambda_1 = \frac{h - \sqrt{h^2 - 4(1 - \gamma^2)}}{2(1 + \gamma)} \quad \lambda_2 = \frac{1 + \gamma}{1 - \gamma} \lambda_1. \]  

These \( \lambda \) are real because \( h^2 > 4(1 - \gamma^2) \) for both cases.

In case 1b:

\[ \lambda_1 = \frac{h - i\sqrt{4(1 - \gamma^2) - \gamma^2}}{2(1 + \gamma)} \quad \lambda_2 = 1/\lambda_1^*. \]  

In this case \( h^2 < 4(1 - \gamma^2) \).

(Note that in the Case 1 the poles of the function \( \phi(z) \) coincide with the points \( \lambda_A \) and \( \lambda_B \), while in the Case 2 they coincide with the points \( \lambda_A \) and \( \lambda_C \).)
By virtue of Eq. (10), our objective becomes the asymptotic calculation of the determinant of block Toeplitz matrix \( D_L(\lambda) \) or, rather, its \( \lambda \) -derivative \( \frac{d}{d\lambda} \ln D_L(\lambda) \). A general asymptotic representation of the determinant of a block Toeplitz matrix, which generalizes the classical strong Szegö theorem to the block matrix case, was obtained by Widom in [17] (see also more recent work [18] and references therein). The important difference with the scalar case is the non-commutativity of the associated Weiner-Hopf factorization. This creates serious technical problems. In our work we circumvent this obstacle by using an alternative approach to Toeplitz determinants suggested by Deift in [23]. It is based on the Riemann-Hilbert technique of the theory of “integrable integral operators”, which was developed in [20, 29] for evaluation of correlation functions of quantum completely integrable [exactly solvable] models (see also comment [33]). It turns out that, using the block matrix version of [20] suggested in [30], one can generalize Deift’s scheme to the block Toeplitz matrices. In addition, we were able to find the explicit Weiner-Hopf factorization of the generator \( \Phi(z) \) which eventually made it possible to perform an explicit evaluation of the asymptotic of the entropy \( S(\rho_A) \). The final result is given in terms of elliptic functions and is presented in Eq. (65) below. In what follows we shall outline our calculation providing the necessary facts concerning integrable Fredholm operators. More details, including the evaluation of error terms, will be presented in a separate publication.

Let \( f_j(z) \) and \( h_j(z), \ j = 1, 2, \) be \( 2 \times 2 \) matrix functions. We introduce the class of **integrable operators** \( \Sigma \) defined on \( L_2(\Xi, \mathbb{C}^2) \) by the following equations (cf. [30]),

\[
(KX)(z) = \oint_{\Xi} K(z, z')X(z')dz' \quad \text{for} \quad X \in L_2, \tag{15}
\]

where

\[
K(z, z') = \frac{f^T(z)h(z')}{z - z'}, \quad f(z) = \begin{pmatrix} f_1(z) \\ f_2(z) \end{pmatrix},
\]

\[
h(z) = \begin{pmatrix} h_1(z) \\ h_2(z) \end{pmatrix}. \tag{16}
\]

Let \( I_2 \) denote the \( 2 \times 2 \) identity matrix. Put

\[
f_1(z) = z^L I_2, \quad f_2(z) = I_2 \tag{17}
\]

\[
h_1(z) = z^{-L} I_2 - \Phi(z), \quad h_2(z) = -\frac{I_2 - \Phi(z)}{2\pi i}. \tag{18}
\]

Then, essentially repeating the arguments of [23], we have the following relation

\[
D_L(\lambda) = \det(I - K), \tag{19}
\]

So we represented \( D_L(\lambda) \) as a Fredholm determinant of the integral operator \( K \). Define the resolvent operator \( R \) by

\[
(I - K)(I + R) = I.
\]

Here \( I \) is the identity operator in \( L_2(\Xi, \mathbb{C}^2) \). Then we have the general equation,

\[
\frac{d}{d\lambda} \ln D_L(\lambda) = -\text{Tr} \left[ (I - K)^{-1} \frac{d}{d\lambda} K \right],
\]

which, taking into account that in our case

\[
\frac{d}{d\lambda} K(z, z') = -iK(z, z')(I_2 - \Phi(z'))^{-1},
\]

can be rewritten as

\[
\frac{d}{d\lambda} \ln D_L(\lambda) = i \oint_{\Xi} \text{tr} \left[ R(z, z)(I_2 - \Phi(z'))^{-1} \right] dz. \tag{20}
\]

In the formulae above, “Tr” means the trace taking in the space \( L_2(\Xi, \mathbb{C}^2) \), while “tr” is the \( 2 \times 2 \) matrix trace. An important general fact is that the resolvent kernel satisfies the equation (see e.g. [30]),

\[
R(z, z) = \frac{dF^T(z)}{dz}H(z). \tag{21}
\]

In this equation, the \( 4 \times 2 \) matrix functions \( F(z) \) and \( H(z) \) are determined by the relations,

\[
F(z) = Y_+(z)f(z), \quad z \in \Xi, \tag{22}
\]

\[
H(z) = (Y_T)^{-1}(z)h(z), \quad z \in \Xi, \tag{23}
\]

where the \( 4 \times 4 \) matrix function \( Y_+(z) \) can be found from the (unique) solution of the following Riemann-Hilbert problem:

1. \( Y(z) \) is analytic for \( z \notin \Xi \).

2. \( Y(\infty) = I_4 \), where \( I_4 \) denotes the \( 4 \times 4 \) identity matrix.

3. \( Y^-(z) = Y_+(z)J(z) \) for \( z \in \Xi \) where \( Y_+(z) \) \( (Y^-(z)) \) denotes the left (right) boundary value of \( Y(z) \) on unit circle \( \Xi \) (Note: “+” means from inside of the unit circle). The \( 4 \times 4 \) jump matrix \( J(z) \) is defined by the equations,

\[
J(z) = I_4 + 2\pi i f(z)h^T(z) = \begin{pmatrix} 2I_2 - \Phi T(z) & -z^L(I_2 - \Phi T(z)) \\ z^{-L}(I_2 - \Phi T(z)) & \Phi T(z) \end{pmatrix}. \tag{24}
\]
Eqs. (20) and (21) reduce the original question to the asymptotic analysis of the solution \( Y(z) \) of the Riemann-Hilbert problem (1-3). Our observation is that once again we can generalize the arguments of [23] to the case of matrix generator \( \Phi(z) \) and arrive to the following asymptotic solution of the problem (1-3) \( (L \to \infty) \):

\[
Y_+(z) = \begin{pmatrix} U_T^+(z) & -zL^+ U_T^+(z) M(z) \\ 0_2 & (V_T^+)^{-1}(z) \end{pmatrix}
\]  

and

\[
(Y_+)^{-1}(z) = \begin{pmatrix} (U_T^+)^{-1}(z) & zLM(z) V_T^+(z) \\ 0_2 & V_T^+(z) \end{pmatrix}.
\]

Here

\[ M(z) = I_2 - (\Phi^T)^{-1}(z) \]

and \( U_+(z) \) and \( V_+(z) \) are \( 2 \times 2 \) matrices solving the Weiner-Hopf factorization problem:

(i)  \( \Phi(z) = U_+(z)U_-(z) = V_-(z)V_+(z), \quad z \in \Xi \)

(ii) \( U_-(z) \) and \( V_-(z) \) (\( U_+(z) \) and \( V_+(z) \)) are analytic outside (inside) the unit circle \( \Xi \).

(iii) \( U_-(\infty) = V_-(\infty) = I \).

We can use Eqs. (25) and (26) in Eqs. (20) - (23) and obtain the following asymptotic formula:

\[
\frac{d}{d\lambda} \ln D_L(\lambda) = -\frac{2\lambda}{1 - \lambda^2} L + \frac{1}{2\pi} \int_{\Xi} \text{tr} [\Phi(z)] \, dz, \quad (27)
\]

\[
\Phi(z) = \left[ U_+(z) \overline{U_-(z)} + V_-(z) \overline{V_+(z)} \right] \Phi^{-1}(z), \quad (28)
\]

as \( L \to \infty \) (see also comment [56]). Here ’ means a derivative in \( z \) variable.

By explicit calculation, one can find that

\[
(1 - \lambda^2) \sigma_3 \Phi^{-1}(z) \sigma_3 = \Phi(z), \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (29)
\]

Hence,

\[
V_-(z) = \sigma_3 U_-(z) \sigma_3, \quad (30)
\]

\[
V_+(z) = \sigma_3 U_+(z) \sigma_3 (1 - \lambda^2), \quad \lambda \neq \pm 1, \quad (31)
\]

and one only needs the explicit expressions for \( U_\pm(z) \).

Our last principal observation is that, for all \( \lambda \) outside of a certain discrete subset of the interval \([-1, 1]\), the solution to the auxiliary Riemann-Hilbert problem (i-iii) exists; moreover, the functions \( U_\pm(z) \) can be expressed in terms of the Jacobi theta-functions. Indeed, the auxiliary Riemann-Hilbert problem (i-iii) can be easily reduced to a type of the “finite-gap” Riemann-Hilbert problems which have already appeared in the analysis of the integrable statistical mechanics models (see [31]).

Before we give detail expressions, let us first define some basic objects:

\[
w(z) = \sqrt{(z - \lambda_1)(z - \lambda_2)(z - \lambda_2^{-1})(z - \lambda_1^{-1})}, \quad (32)
\]

\[
\beta(\lambda) = \frac{1}{2\pi i} \ln \frac{\lambda + 1}{\lambda - 1}, \quad (33)
\]

where \( w(z) \) is analytic on the domain \( \mathbb{C} \setminus \{ J_1 \cup J_2 \} \) shown in Fig. 2 and fixed by the condition: \( w(z) \to z^2 \) as \( z \to \infty \). Next we define

\[
\tau = \frac{2}{c} \int_{\lambda \in J} dz, \quad c = 2 \int_{\lambda \in J} \frac{dz}{w(z)} \cdot (34)
\]

\[
\delta = \frac{2}{c} \left( -\pi i - \int_{\lambda \in J} dz \frac{\omega(z)}{w(z)} \right), \quad (35)
\]

\[
\Delta(z) = \frac{1}{2} \int_{\lambda \in J} \frac{dz + \delta}{w(z)}, \quad (36)
\]

Points \( \lambda_A, \lambda_B, \lambda_C, \lambda_D \) and cuts \( J_1, J_2 \) and curves \( \Sigma \) and \( \Xi \) are shown in Fig. 2. We shall also need:

\[
\Delta_0 = \lim_{z \to \infty} \left( \Delta(z) - \frac{1}{2} \ln(z - \lambda_1) \right). \quad (37)
\]

Here, the contours of integration for \( c \) and \( \delta \) are taken along the left side of the cut \( J_1 \). The contour of integration for \( \tau \) is the segment \([\lambda_B, \lambda_C]\). The contours of integration for \( \kappa \) and in \([32]\) are taken along the line \( \Sigma \) to the left from \( \lambda_A \); also in \([31]\), \( \arg(z - \lambda_1) = \pi \). The contours of integration in the integrals \( \Delta(z) \) and \( \omega(z) \) are taking according to the rule: The contour lies entirely in the domain \( \Omega_+ (\Omega_-) \) for \( z \) belonging to \( \Omega_+ (\Omega_-) \). It also worth noticing that \( i\tau < 0 \).

Now we are ready to introduce the Jacobi theta-function,

\[
\theta_3(s) = \sum_{n=-\infty}^{\infty} e^{\pi i r^2 + 2\pi i n s}. \quad (38)
\]

We remind the following properties of this theta-function (see e.g. [32]):

\[
\theta_3(-s) = \theta_3(s), \quad \theta_3(s + 1) = \theta_3(s) \quad (39)
\]

\[
\theta_3(s + \tau) = e^{-\pi i r - 2\pi i s} \theta_3(s) \quad (40)
\]

\[
\theta_3 \left( n + m \tau + \frac{1}{2} + \frac{\tau}{2} \right) = 0, \quad n, m \in \mathbb{Z} \quad (41)
\]

We also introduce the \( 2 \times 2 \) matrix valued function \( \Theta(z) \) with the entries,

\[
\Theta_{11}(z) = (z - \lambda_1)^{-\frac{1}{2}} e^{\Delta(z)} \times \frac{\theta_3 \left( \omega(z) + \beta(\lambda) - \kappa + \frac{\tau}{2} \right)}{\theta_3 \left( \omega(z) + \frac{\tau}{2} \right)}. \quad (42)
\]
\[ \Theta_{12}(z) = -(z - \lambda_1)^{-\frac{1}{2}} e^{-\Delta(z)} \times \frac{\theta_3(\omega(z) - \beta(\lambda) + \kappa - \frac{\sigma \tau}{2})}{\theta_3(\omega(z) - \frac{\sigma \tau}{2})} \]
\[ \Theta_{21}(z) = -(z - \lambda_1)^{-\frac{1}{2}} e^{-\Delta(z)} \times \frac{\theta_3(\omega(z) + \beta(\lambda) + \kappa - \frac{\sigma \tau}{2})}{\theta_3(\omega(z) - \frac{\sigma \tau}{2})} \]
\[ \Theta_{22}(z) = (z - \lambda_1)^{-\frac{1}{2}} e^{\Delta(z)} \times \frac{\theta_3(\omega(z) - \beta(\lambda) - \kappa + \frac{\sigma \tau}{2})}{\theta_3(\omega(z) + \frac{\sigma \tau}{2})} \] (42)

where \( \sigma = 1 \) in Case 1 and \( \sigma = 0 \) in Case 2, and \( \beta(\lambda), \omega(z) \) and \( \kappa \) are defined in Eqs. (32-34). The branch of \( (z - \lambda_1)^{-\frac{1}{2}} \) is defined on the \( \omega \)-plane cut along the part of the line \( \Sigma \) which is to the right of \( \lambda_1 \equiv \lambda_A \), and it is fixed by the condition \( \arg(z - \lambda_1) = \pi \), if \( z - \lambda_1 < 0 \).

The matrix function \( \Theta(z) \) is defined on \( \mathbb{C} \setminus \Sigma \). However, analyzing the jumps of the integrals \( \omega(z) \) and \( \Delta(z) \) over the line \( \Sigma \) and taking into account the properties (39) and (40) of the theta function, one can see that \( \Theta(z) \) is actually extended to the analytic function defined on \( \mathbb{C} \setminus \{J_1 \cup J_2\} \). Moreover, it satisfies the jump relations

\[ \Theta_+(z) = \Theta_-(z) \sigma_1, \quad z \in J_1 \] (43)
\[ \Theta_+(z) = \Theta_-(z) \Lambda \sigma_1 \Lambda^{-1}, \quad z \in J_2 \] (44)
\[ \Lambda = i \begin{pmatrix} \lambda + 1 & 0 \\ 0 & \lambda - 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \] (45)

Also note:

\[ \Theta_{11}(\infty) = e^{\Delta} \frac{\theta_3(\beta(\lambda) + \frac{\sigma \tau}{2})}{\theta_3(\kappa + \frac{\sigma \tau}{2})} \] (46)
\[ \Theta_{22}(\infty) = e^{\Delta} \frac{\theta_3(\beta(\lambda) - \frac{\sigma \tau}{2})}{\theta_3(\kappa + \frac{\sigma \tau}{2})} \] (47)
\[ \Theta_{12}(\infty) = \Theta_{21}(\infty) = 0 \] (48)

and

\[ \det \Theta(z) \equiv \phi(z) \det \Theta(\infty) \sqrt{\frac{\lambda_2}{\lambda_1}} \] (49)

The latter equation follows from the comparison of the jumps and singularities of its sides. Finally, we introduce the matrix

\[ Q(z) = \begin{pmatrix} \phi(z) & -\phi(z) \\ i & i \end{pmatrix} \] (50)

Note that \( Q(z) \) diagonalizes original jump matrix \( \Phi(z) \):

\[ \Phi(z) = Q(z) \Lambda Q^{-1}(z) \] (51)

and \( Q(z) \) is analytic on \( \mathbb{C} \setminus \{J_1 \cup J_2\} \) and

\[ Q_+(z) = Q_-(z) \sigma_1, \quad z \in J_1 \cup J_2 \] (52)

We are now ready to present the solution \( U_\pm(z) \) of the Riemann-Hilbert problem (i-iii). Put

\[ A = Q(\infty) \Lambda^{-1} \Theta^{-1}(\infty). \] (53)

Then,

\[ U_-(z) = A \Theta(z) A Q^{-1}(z), \] \[ |z| \geq 1 \] (54)
\[ U_+(z) = Q(z) \Theta^{-1}(z) A^{-1}, \] \[ |z| \leq 1. \] (55)

Indeed, by virtue of Eq. (51), we only need to be sure that \( U_-(z) \) and \( U_+(z) \) are analytic for \( |z| > 1 \) and \( |z| < 1 \) respectively. From the jump properties of \( \Theta(z) \) and \( Q(z) \) it follows that \( U_\pm \) have no jumps across \( J_{1,2} \), and hence they might have only possible isolated singularities at \( \lambda_{1,2}, \lambda_{1,\pm} \). The analyticity at these points can be shown by observing that the singularities, which the functions \( \Theta(z) \) and \( Q(z) \) do have at the end points of the segments \( J_{1,2} \), are canceled out in the products (54)-(55).

The excluded values of \( \lambda \) for which the above construction fails are \( \lambda = \pm 1 \) and, in view of Eq. (49), the zeros of \( \theta_3(\beta(\lambda) + \frac{\sigma \tau}{2}) \), i.e. (see (11)),

\[ \pm \lambda_m, \quad \lambda_m = \tanh \left( m + \frac{1 - \sigma}{2} \right) \pi \tau_0, \quad m \geq 0 \] (56)

where,

\[ \tau_0 = -i \tau = -i \frac{\int_{\lambda_B}^{\lambda_C} \frac{dz}{\theta_3(\omega(z))}}{\int_{\lambda_A}^{\lambda_B} \frac{dz}{\theta_3(\omega(z))}} > 0. \]

Using explicit formulae (41-45) one can transform our basic Eq. (24) into the form

\[ \frac{d}{d\lambda} \ln D_L(\lambda) + \frac{2\lambda}{1 - \lambda^2} L = \frac{i}{\pi(1 - \lambda^2)} \int_\infty^{\gamma \lambda} \left[ \Theta^{-1}(z) \frac{dz}{dz} \Theta(z) \sigma_3 \right] dz, \] (57)

here \( \lambda \neq \pm 1, \pm \lambda_m \). Using the same arguments as for Eq. (49), one can see that

\[ \text{tr} \left[ \Theta^{-1}(z) \frac{dz}{dz} \Theta(z) \sigma_3 \right] = \frac{1}{c w(z)} \frac{d}{d\beta} \left[ \theta_3(\beta(\lambda) + \frac{\sigma \tau}{2}) \theta_3(\beta(\lambda) - \frac{\sigma \tau}{2}) \right]. \] (58)

This relation allows further simplification of Eq. (24). Indeed, we have,

\[ \frac{d}{d\lambda} \ln D_L(\lambda) + \frac{2\lambda}{1 - \lambda^2} L = \frac{d}{d\lambda} \ln \left[ \theta_3(\beta(\lambda) + \frac{\sigma \tau}{2}) \theta_3(\beta(\lambda) - \frac{\sigma \tau}{2}) \right], \] (59)

here \( \lambda \neq \pm 1, \pm \lambda_m \). Taking into account the fact that as \( \lambda \rightarrow \infty, D_L(\lambda) \rightarrow (-1)^k \Lambda^{2k} \), we obtain from Eq. (59)
the following asymptotic representation for the Toeplitz determinant $D_L(\lambda)$:

$$D_L(\lambda) = \frac{(-1)^L}{\theta_3^2(\ell_2)} \left( \lambda^2 - 1 \right) L \theta_3 \left( \beta(\lambda + \frac{\sigma \tau}{2}) \theta_3 \left( \beta(\lambda - \frac{\sigma \tau}{2}) \right) \right)$$

here $\lambda$ lies outside of fixed but arbitrary neighborhoods of the points $\pm 1$ and $\pm \lambda_m, m \geq 0$.

It is worth noticing that the asymptotic representation for the Toeplitz determinant above shows that, in the large $L$ limit, the eigenvalues $\nu_{2m}$ and $\nu_{2m+1}$ from $[0, \pi]$ merge: $\nu_{2m}, \nu_{2m+1} \to \lambda_m$. In turn it indicates the degeneracy of the spectrum of the matrix $B_L$ and an appearance of an extra symmetry in the large $L$ limit.

Substituting Eq. (59) into the original equation Eq. (10), and deforming the original contour of integration to the contour $\Gamma$ as indicated in Fig. 1 we arrive at the following expression for the entropy:

$$S(\rho_A) = \frac{1}{2} \int_1^{\infty} \ln \left( \frac{\theta_3 (\beta(\lambda + \frac{\sigma \tau}{2}) \theta_3 (\beta(\lambda - \frac{\sigma \tau}{2}))}{\theta_3^2 (\ell_2)} \right) d\lambda$$

This is a limiting expression as $L \to \infty$. We can prove that the corrections in Eq. (60) are of order of $O \left( \lambda_m^{-L}/\sqrt{L} \right)$. The asymptotic expression (60) is a theorem, we shall publish a complete proof later.

The entropy has singularities at phase transitions. When $\tau \to 0$ we can use Landen transform (see (52)) to get the following estimate of the theta-function for small $\tau$ and pure imaginary $s$:

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

Now the leading term in the expression for the entropy (60) can be replaced by

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

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

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

   This is included in our Case 1a and Case 2, when $h > 2\sqrt{1 - \gamma^2}$. As $h \to 2$ the end points of the cuts $\lambda_B \to \lambda_C$, so $\tau$ given by Eq. (64) simplifies and we obtain from Eq. (65) that the entropy is:

   $$S(\rho_A) = -\frac{1}{6} \ln |2 - h| + \frac{1}{3} \ln 4 \gamma, \quad h \to 2 \quad \gamma \neq 0$$  \hspace{1cm} (62)

   This means that $(\lambda_{m+1} - \lambda_m) \to 0$ as $\tau \to 0$ for every $m$. This is useful for understanding of large $L$ limit of the XX case corresponding to $\gamma \to 0$, as considered in (33). 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 Eq. (65).

   It would be interesting to generalize our approach to the a new class of quantum spin chains introduced recently by J. Keating and F. Mezzadri, while study matrix models (33).

**SUMMARY**

Our main result is the theorem that the expression for the limit (as $L \to \infty$) of the entropy of a block of $L$
neighboring spins on the infinite lattice is given by formula (4.33). We are preparing a larger file with all the details of the proof. We can change variables and represent it in the form:

$$S(\rho_A) =$$

$$= \frac{\pi}{2} \int_0^\infty \ln \left( \frac{\theta_3 \left( \frac{ix}{2} \right) \theta_3 \left( \frac{-ix}{2} \right)}{\theta_3 \left( \frac{ix}{2} \right)} \right) \frac{dx}{\sinh^2(\pi x)}$$

We remind that $\sigma = 0$ for Case 2 and $\sigma = 1$ in Case 1, see page 2. $S(\rho_A)$ implicitly depends on $\gamma$ and $h$ introduced in [1] by means of $\tau$ defined in Eq. (4.33), this $\tau$ is a ratio of periods for the theta function $\theta_3(z)$, see [83]. The $\gamma$ and $h$ define $\lambda_A, \lambda_B, \lambda_C$ and $\lambda_D$ by means of Eqs. (13), (14), Fig. 2, and its caption. Finally Eq. (4.33) and Eqs. (60) or (65) define $S(\rho_A)$.

**APPENDIX**

After our paper appeared in quant-ph, I.Peschel [51] simplified our expression for the entropy in the Cases 1a and 2. He used the approach of [83]. He showed that in these cases our formula (4.33) is equivalent to formula (4.33) of [1]. Moreover, I. Peschel was able to sum it up into the following expressions for the entropy.

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

in Case 1a, and

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

in Case 2.

Here, $I(k)$ denotes the complete elliptic integral of the first kind, $k' = \sqrt{1 - k^2}$, and

$$k = \begin{cases} \sqrt{(h/2)^2 + \gamma^2 - 1} / \gamma, & \text{Case 1a} \\ \gamma / \sqrt{(h/2)^2 + \gamma^2 - 1}, & \text{Case 2} \end{cases}$$

(67)

In our work, we have shown, in particular, that equation (60) is valid in Case 1b as well. Therefore, we can apply the summation procedure of [51] and obtain that in Case 1b

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

with $k' = \sqrt{1 - k^2}$, and

$$k = \sqrt{\frac{1 - (h/2)^2 - \gamma^2}{1 - (h/2)^2}}$$

(68)

**Acknowledgments.** We thank B. McCoy, P. Deift, P. Calabrese and I. Peschel for useful discussions. This work was supported by NSF Grants DMR-0302758, DMS-0099812 and DMS-0410109. The first co-author thanks B. Conrey, F. Mezzardi, P. Sarnak, and N. Snaith - the organizers of the 2004 program at the Isaac Newton Institute for Mathematical Sciences on Random Matrices, where part of this work was done, for an extremely stimulating research environment and hospitality during his visit.

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[54] For AKLT-VBS models this was proved in [45]

[55] In its turn, the approach of [26] is based on the ideas of [27]. Several principal aspects of the integrable operator theory, especially the ones concerning with the integrable differential systems appearing in random matrix theory, have been developed in [28]. Some of the important elements of modern theory of integrable operators were already implicitly present in the earlier work [29].

[56] This formula plays in our analysis the role of the strong Szegö theorem. We think it would be of interest to understand its meaning in context of the general result of Widom [17].