Entanglement in XY Spin Chain

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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.

There is an essential interest in quantifying entanglement in various quantum systems. Entanglement in spin chains, strongly correlated electrons and interacting bosons was recently published [2–13, 17–19, 28, 39]. Entanglement is a fundamental measure of 'quantumness' of the system: how much quantum effects we can observe and use. It is the primary resource in quantum computation and quantum information processing [14, 15]. Stable, large scale entanglement is necessary for scalability of quantum computation [18, 19]. For experimental demonstration one can look, for example in [5, 16]. The XY model in a transverse magnetic was studied from the point for view of quantum information in [2, 3], [29], [44]. It was conjectured in [2] that in XY and other gapped models the entropy of a block of L neighboring spins approaches a constant as $L \to \infty$ (see comment [45]). In this paper we evaluated the entropy of a block of L neighboring spins in the ground state of XY model in the limit $L \to \infty$ analytically, see (60). Hamiltonian of XY model can be written as

$$H_{XY} = -\sum_{n=-\infty}^{\infty} (1+\gamma)\sigma_n^x\sigma_{n+1}^x + (1-\gamma)\sigma_n^y\sigma_{n+1}^y + h\sigma_n^z \quad (1)$$

Here γ is anisotropy parameter $(0 < \gamma < 1)$; σ_n^x, σ_n^y σ_n^z are Pauli matrices and h is a magnetic field. The model was solved in [30], [31], [32], [42]. Toeplitz determinants were used for evaluation of some correlation functions, see [38] and [37]. Integrable Fredholm operators were used for calculation of other correlations, see [33–36].

The ground state of the model $|GS\rangle$ is unique. So the entropy of the whole infinite ground state is zero, but it can be positive for a subsystem [a part of the ground state]. We shall calculate the entropy of a block of L neighboring spins. We can think that the ground state is a binary system $|GS\rangle = |A\&B\rangle$. We can call the block of L neighboring spins by sub-system A and the rest of the ground state by sub-system B. The density matrix of the ground state is $|GS\rangle\langle GS|$. We shall denote it by $\rho_{AB} = |GS\rangle\langle GS|$. The density matrix of the L neighboring spins [subsystem A] is $\rho_A = Tr_B(\rho_{AB})$. Von Neumann entropy $S(\rho_A)$ of the subsystem A can be represented as following:

$$S(\rho_A) = -Tr_A(\rho_A \ln \rho_A), \quad (2)$$

This entropy defines the dimension of the Hilbert space of states of the block of L spins. Majorana operators were used in [2] to describe the entropy (2) by the following matrix:

$$\mathbf{B}_L = \begin{pmatrix} \Pi_0 & \Pi_{-1} & \dots & \Pi_{1-L} \\ \Pi_1 & \Pi_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ \Pi_{L-1} & \dots & \dots & \Pi_0 \end{pmatrix}$$

Here

$$\Pi_l = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta\, e^{-\mathrm{i}l\theta}\mathcal{G}(\theta), \quad \mathcal{G}(\theta) = \begin{pmatrix} 0 & g(\theta) \\ -g^{-1}(\theta) & 0 \end{pmatrix}$$

$$\text{and} \qquad g(\theta) = \frac{\cos\theta - \mathrm{i}\gamma\sin\theta - h/2}{|\cos\theta - \mathrm{i}\gamma\sin\theta - h/2|} \quad . \quad (3)$$

One can use an orthogonal matrix V to transform $\mathbf{B}_L$ to a canonical form:

$$V\mathbf{B}_L V^T = \oplus_{m=1}^{L}\nu_m \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad (4)$$

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 [2] as

$$S(\rho_A) \;=\; \sum_{m=1}^{L} H(\nu_m) \quad (5)$$

with

$$H(\nu) = -\frac{1+\nu}{2}\ln\frac{1+\nu}{2} - \frac{1-\nu}{2}\ln\frac{1-\nu}{2}. \quad (6)$$

In order to calculate the asymptotic form of the entropy let us introduce:

$$\widetilde{\mathbf{B}}_L(\lambda) = \mathrm{i}\lambda I_L - \mathbf{B}_L, \quad D_L(\lambda) = \det\widetilde{\mathbf{B}}_L(\lambda) \quad (7)$$

and

$$e(x,\nu) = -\frac{x+\nu}{2}\ln\frac{x+\nu}{2} - \frac{x-\nu}{2}\ln\frac{x-\nu}{2}. \qquad (8)$$

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

$$D_L(\lambda) = (-1)^L \prod_{m=1}^{L} (\lambda^2 - \nu_m^2). \qquad (9)$$

In [28] we used Cauchy residue theorem to rewrite formula (5) in the following form:

$$S(\rho_A) = \lim_{\epsilon\to 0^+} \frac{1}{4\pi \mathrm{i}} \oint_{\Gamma'} \mathrm{d}\lambda\, e(1+\epsilon,\lambda) \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln D_L(\lambda)\ . \qquad (10)$$

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

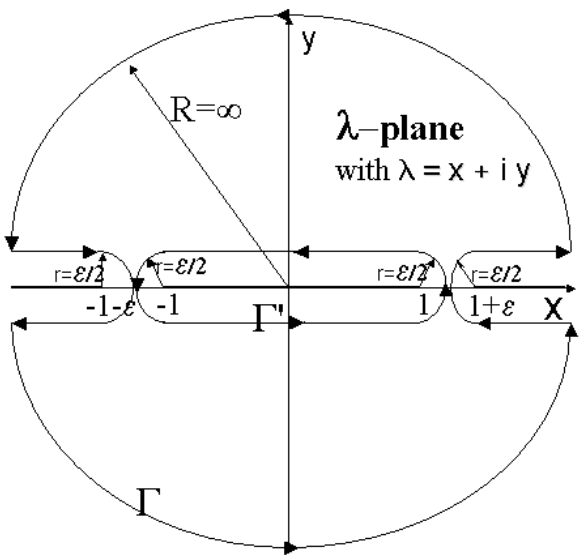

FIG. 1: *Contours Γ' (smaller one) and Γ (larger one). Bold lines $(-\infty,-1-\epsilon)$ and $(1+\epsilon,\infty)$ are the cuts of integrand $e(1+\epsilon,\lambda)$. Zeros of $D_L(\lambda)$ (Eq. 9) are located on bold line $(-1,1)$. The arrow is the direction of the route of integral we take and* r *and* R *are the radius of circles.* ¶

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

$$\widetilde{\mathbf{B}}_L(\lambda) = \begin{pmatrix} \widetilde{\Pi}_0 & \widetilde{\Pi}_{-1} & \dots & \widetilde{\Pi}_{1-L} \\ \widetilde{\Pi}_1 & \widetilde{\Pi}_0 & & \vdots \\ \vdots & & \ddots & \vdots \\ \widetilde{\Pi}_{L-1} & \dots & \dots & \widetilde{\Pi}_0 \end{pmatrix} \quad \text{with}$$

$$\widetilde{\Pi}_l = \frac{1}{2\pi \mathrm{i}} \oint_{\Xi} \mathrm{d}z\, z^{-l} \Phi(z), \quad \Phi(z) = \begin{pmatrix} \mathrm{i}\lambda & \phi(z) \\ -\phi^{-1}(z) & \mathrm{i}\lambda \end{pmatrix} \qquad (11)$$

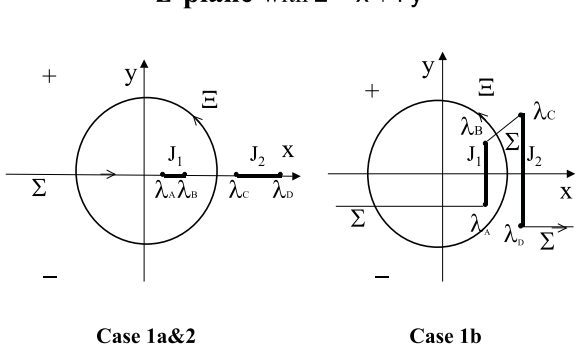

FIG. 2: *Polygonal line Σ (direction as labeled) separates the complex z plane into the two parts: the part Ω_+ which lies to the left of Σ, and the part Ω_- which lies to the right of Σ. Curve Ξ is the unit circle in anti-clockwise direction. Cuts J_1, J_2 for functions $\phi(z), w(z)$ are labeled by bold on line Σ.* **Case** 1*a: $h<2$ and $h^2 > 4(1-\gamma^2)$ then $\lambda_A = \lambda_1$ and $\lambda_B = \lambda_2^{-1}$, $\lambda_C = \lambda_2$ and $\lambda_D = \lambda_1^{-1}$.* **Case** 1*b: $h^2 < 4(1-\gamma^2)$, then $\lambda_A = \lambda_1$ and $\lambda_B = \lambda_2^{-1}$, $\lambda_C = \lambda_1^{-1}$ and $\lambda_D = \lambda_2$.* **Case** 2*: $h>2$ and $h^2 > 4(1-\gamma^2)$ then $\lambda_A = \lambda_1$ and $\lambda_B = \lambda_2$, $\lambda_C = \lambda_2^{-1}$ and $\lambda_D = \lambda_1^{-1}$.* ¶

$$\text{and} \quad \phi(z) = \left(\frac{\lambda_1^*}{\lambda_1} \frac{(1-\lambda_1 z)(1-\lambda_2 z^{-1})}{(1-\lambda_1^* z^{-1})(1-\lambda_2^* z)} \right)^{1/2} \qquad (12)$$

We use $*$ to denote complex conjugation and Ξ is the unite circle shown in Fig. 2. The points λ_1, λ_2 are different depending on the **Case** defined in end of caption to Fig. 2.
In two cases 1a and 2:

$$\lambda_1 = \frac{h - \sqrt{h^2 - 4(1-\gamma^2)}}{2(1+\gamma)}, \quad \lambda_2 = \frac{1+\gamma}{1-\gamma}\lambda_1. \qquad (13)$$

These λ are real because $h^2 > 4(1-\gamma^2)$ for both cases.
In case 1b:

$$\lambda_1 = \frac{h - \mathrm{i}\sqrt{4(1-\gamma^2) - h^2}}{2(1+\gamma)}, \quad \lambda_2 = 1/\lambda_1^*. \qquad (14)$$

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 λ_A and λ_B, while in the Case 2 they coincide with the points λ_A and λ_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 λ -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 [40] (see also more recent work [41] 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 [20]. It is based on the Riemann-Hilbert technique of the theory of "integrable integral operators", which was developed in [21], [43] for evaluation of correlation functions of quantum completely integrable [exactly solvable] models (see also comment [46]). It turns out that, using the block matrix version of [21] suggested in [25], 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. (61) 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 2×2 matrix functions. We introduce the class of **integrable operators** K defined on $L_2(\Xi, \mathbb{C}^2)$ by the following equations (cf. [25]),

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

where

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

$$h(z) = \begin{pmatrix} h_1(z) \\ h_2(z) \end{pmatrix}. \quad (16)$$

Let I_2 denote the 2×2 identity matrix. Put

$$f_1(z) = z^L I_2, \quad f_2(z) = I_2 \quad (17)$$

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

Then, essentially repeating the arguments of [20], we have the following relation

$$D_L(\lambda) = \det(I - K), \quad (19)$$

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,

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

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

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

In the formulae above, "Tr" means the trace taking in the space $L_2(\Xi, \mathbb{C}^2)$, while "tr" is the 2×2 matrix trace. An important general fact is that the resolvent kernel satisfies the equation (see e.g. [25]),

$$R(z,z) = \frac{dF^T(z)}{dz}H(z). \quad (21)$$

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

$$F(z) = Y_+(z)f(z), \quad z \in \Xi, \quad (22)$$

$$H(z) = (Y_+^T)^{-1}(z)h(z), \quad z \in \Xi, \quad (23)$$

where the 4×4 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 4×4 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 Ξ (Note: "+" means from inside of the unit circle). The 4×4 jump matrix $J(z)$ is defined by the equations,

$$J(z) = I_4 + 2\pi i f(z)h^T(z)$$

$$= \begin{pmatrix} 2I_2 - \Phi^T(z) & -z^L(I_2 - \Phi^T(z)) \\ z^{-L}(I_2 - \Phi^T(z)) & \Phi^T(z) \end{pmatrix}. \quad (24)$$

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 [20] to the case of matrix generator $\Phi(z)$ and arrive to the following asymptotic solution of the problem (1-3) ($L \to \infty$):

$$Y_+(z) = \begin{pmatrix} U_+^T(z) & -z^L U_+^T(z)\,M(z) \\ 0_2 & (V_+^T)^{-1}(z) \end{pmatrix} \quad (25)$$

and

$$(Y_+)^{-1}(z) = \begin{pmatrix} (U_+^T)^{-1}(z) & z^L M(z)\,V_+^T(z) \\ 0_2 & V_+^T(z) \end{pmatrix}. \quad (26)$$

Here

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

and $U_\pm(z)$ and $V_\pm(z)$ are 2×2 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 Ξ.

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

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

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

$$\Psi(z) = \left[U'_+(z)U_+^{-1}(z) + V_+^{-1}(z)V'_+(z)\right] \Phi^{-1}(z), \quad (28)$$

as $L \to \infty$ (see also comment [47]). 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,

$$V_-(z) = \sigma_3 U_-^{-1}(z)\sigma_3 \quad (30)$$

$$V_+(z) = \sigma_3 U_+^{-1}(z)\sigma_3(1-\lambda^2), \quad \lambda \neq \pm 1, \quad (31)$$

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

Our last principal observation is that, for all λ 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 [26]). 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

$$\tau = \frac{2}{c} \int_{\lambda_B}^{\lambda_C} \frac{\mathrm{d}z}{w(z)}, \quad c = 2\int_{\lambda_A}^{\lambda_B} \frac{\mathrm{d}z}{w(z)}, \quad (34)$$

$$\delta = \frac{2}{c}\left(-\pi i - \int_{\lambda_A}^{\lambda_B} \frac{z\mathrm{d}z}{w(z)}\right), \quad \omega(z) = \frac{1}{c}\int_{\lambda_A}^{z} \frac{\mathrm{d}z}{w(z)}, \quad (35)$$

$$\Delta(z) = \frac{1}{2}\int_{\lambda_A}^{z} \frac{z+\delta}{w(z)}\mathrm{d}z, \quad \kappa = \int_{\lambda_A}^{\infty} \mathrm{d}\omega(z), \quad (36)$$

Points $\lambda_A, \lambda_B, \lambda_C, \lambda_D$ and cuts J_1, J_2 and curves Σ and Ξ 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 δ are taken along the left side of the cut J_1. The contour of integration for τ is the segment $[\lambda_B, \lambda_C]$. The contours of integration for κ and in (37) are taken along the line Σ to the left from λ_A; also in (37), $\arg(z-\lambda_1) = \pi$. 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 Ω_+ (Ω_-) for z belonging to Ω_+ (Ω_-). It also worth noticing that $i\tau < 0$.

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

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

We remind the following properties of this theta-function (see e.g. [27]):

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

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

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

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

$$\begin{aligned}
\Theta_{11}(z) &= (z-\lambda_1)^{-\frac{1}{2}} e^{\Delta(z)} \\
&\quad \times \frac{\theta_3\left(\omega(z) + \beta(\lambda) - \kappa + \frac{\sigma\tau}{2}\right)}{\theta_3\left(\omega(z) + \frac{\sigma\tau}{2}\right)} \\
\Theta_{12}(z) &= -(z-\lambda_1)^{-\frac{1}{2}} e^{-\Delta(z)} \\
&\quad \times \frac{\theta_3\left(\omega(z) - \beta(\lambda) + \kappa - \frac{\sigma\tau}{2}\right)}{\theta_3\left(\omega(z) - \frac{\sigma\tau}{2}\right)} \\
\Theta_{21}(z) &= -(z-\lambda_1)^{-\frac{1}{2}} e^{-\Delta(z)} \\
&\quad \times \frac{\theta_3\left(\omega(z) + \beta(\lambda) + \kappa - \frac{\sigma\tau}{2}\right)}{\theta_3\left(\omega(z) - \frac{\sigma\tau}{2}\right)} \\
\Theta_{22}(z) &= (z-\lambda_1)^{-\frac{1}{2}} e^{\Delta(z)} \\
&\quad \times \frac{\theta_3\left(\omega(z) - \beta(\lambda) - \kappa + \frac{\sigma\tau}{2}\right)}{\theta_3\left(\omega(z) + \frac{\sigma\tau}{2}\right)}, \quad (42)
\end{aligned}$$

where $\sigma = 1$ in Case 1 and $\sigma = 0$ in Case 2, and $\beta(\lambda)$, $\omega(z)$ and κ are defined in Eqs. (32-37). The branch of $(z-\lambda_1)^{-\frac{1}{2}}$ is defined on the z-plane cut along the part of the line Σ 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 Σ 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

$$\Theta_+(z)=\Theta_-(z)\sigma_1 \qquad z\in J_1 \tag{43}$$

$$\Theta_+(z)=\Theta_-(z)\Lambda\sigma_1\Lambda^{-1} \quad z\in J_2. \tag{44}$$

$$\Lambda=i\begin{pmatrix}\lambda+1 & 0\\ 0 & \lambda-1\end{pmatrix}, \quad \sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \tag{45}$$

Also note:

$$\Theta_{11}(\infty) \;=\; e^{\Delta_0}\frac{\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)}{\theta_3\left(\kappa+\frac{\sigma\tau}{2}\right)} \tag{46}$$

$$\Theta_{22}(\infty) \;=\; e^{\Delta_0}\frac{\theta_3\left(\beta(\lambda)-\frac{\sigma\tau}{2}\right)}{\theta_3\left(\kappa+\frac{\sigma\tau}{2}\right)} \tag{47}$$

$$\Theta_{12}(\infty) \;=\; \Theta_{21}(\infty)=0\;, \tag{48}$$

and

$$\det\Theta(z)\equiv\phi(z)\det\Theta(\infty)\sqrt{\frac{\lambda_2}{\lambda_1}}. \tag{49}$$

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

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

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

$$\Phi(z)=Q(z)\Lambda Q^{-1}(z) \tag{51}$$

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

$$Q_+(z)=Q_-(z)\sigma_1, \quad z\in J_1\cup J_2. \tag{52}$$

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

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

Then,

$$U_-(z)=A\Theta(z)\Lambda Q^{-1}(z), \quad |z|\geq 1 \tag{54}$$

$$U_+(z)=Q(z)\Theta^{-1}(z)A^{-1}, \quad |z|\leq 1. \tag{55}$$

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 $\lambda_{1,2},\lambda_{1,2}^{-1}$. 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 λ for which the above construction fails are $\lambda=\pm1$ and, in view of Eq. (49), the zeros of $\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)$, i.e. (see (41)),

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

where,

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

Using explicit formulae (54)-(55) one can transform our basic Eq. (27) into the form

$$\frac{d}{d\lambda}\ln D_L(\lambda)+\frac{2\lambda}{1-\lambda^2}L= \\ =\;\frac{i}{\pi(1-\lambda^2)}\int_\Xi \mathrm{tr}\left[\Theta^{-1}(z)\frac{d}{dz}\Theta(z)\sigma_3\right]dz, \tag{57}$$

here $\lambda\neq\pm1,\ \pm\lambda_m$. Using the same arguments as for Eq. (49), one can see that

$$\mathrm{tr}\left[\Theta^{-1}(z)\frac{d}{dz}\Theta(z)\sigma_3\right]= \\ =\frac{1}{cw(z)}\frac{d}{d\beta}\ln\left[\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)\theta_3\left(\beta(\lambda)-\frac{\sigma\tau}{2}\right)\right]. \tag{58}$$

This relation allows further simplification of Eq. (27). Indeed, we have,

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

here $\lambda\neq\pm1,\ \pm\lambda_m$. Taking into account the fact that as $\lambda\to\infty$, $D_L(\lambda)\to(-1)^L\lambda^{2L}$, we obtain from Eq. (59) the following asymptotic representation for the *Toeplitz determinant* $D_L(\lambda)$:

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

here λ lies outside of fixed but arbitrary neighborhoods of the points ±1 and $\pm\lambda_m$, $m\geq0$.

It is worth noticing that the asymptotic representation for the Toeplitz determinant above shows that the points λ_m (56) are double zeros of the $D_L(\lambda)$. This suggests that in the large L limit the eigenvalues ν_{2m} and ν_{2m+1} from (5), (4) merge: $\nu_{2m},\nu_{2m+1}\to\lambda_m$. In turn it indicates the degeneracy of the spectrum of the matrix $\mathbf{B}_L$ 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 Γ as indicated in Fig. 1 we arrive at the following expression for the **entropy**:

$$S(\rho_A)= \tag{60}$$

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

We remind that $\sigma = 0$ for Case 2 and $\sigma = 1$ in Case 1. We can change variables and represent the final answer in the form:

$$S(\rho_A) = \tag{61}$$

$$= \frac{\pi}{2}\int_0^\infty \ln\left(\frac{\theta_3\left(\mathrm{i}x+\frac{\sigma\tau}{2}\right)\theta_3\left(\mathrm{i}x-\frac{\sigma\tau}{2}\right)}{\theta_3^2\left(\frac{\sigma\tau}{2}\right)}\right)\frac{dx}{\sinh^2(\pi x)}$$

This is a limiting expression as $L\to\infty$. Indeed, it can be shown that the corrections in Eq. (60) and Eq. (61) are of order of $O\left(\lambda_C^{-L}/\sqrt{L}\right)$.

Note: $S(\rho_A)$ implicitly depends on γ and h introduced in (1) by means of τ defined in Eq. (34), this τ is a ratio of periods for the theta function $\theta_3(z)$. The γ and h define λ_A, λ_B, λ_C and λ_D by means of Eqs. (13,14) and Fig. 2. Eq. (34) and Eqs. (60) or (61) define $S(\rho_A)$ ¶.

Note also, that, by integrating over the original contour Γ', one can also suggest an alternative representation for $S(\rho_A)$ in terms of the infinite series (cf. Eq. (5)):

$$S(\rho_A) = 2\sum_{m=0}^{\infty} H(\lambda_m) = \sum_{m=-\infty}^{\infty}(1+\lambda_m)\ln\frac{2}{1+\lambda_m}, \tag{62}$$

here the numbers λ_m are defined in Eq. (56).

Now let us discuss some interesting limiting cases which correspond $\tau\to 0$. The *Landen transform* (see [27]) yields the following estimate of the theta-function for small τ and pure imaginary s

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

The leading term in the expression for the entropy (60) in these cases can be replaced by

$$S(\rho_A) = \frac{\mathrm{i}\pi}{6\tau} + O\left(\frac{e^{-i\pi/\tau}}{\tau^2}\right) \quad \text{for } \tau\to 0. \tag{63}$$

There are two physical situations corresponding to small τ:

1. *Critical magnetic field*: $\gamma\neq 0$ and $h\to 2$. It is included in Case 1a i.e. $h^2-4(1-\gamma^2)>0$. Evaluating the h-asymptotic of τ, we obtain from Eq. (63) that

$$S(\rho_A) = -\tfrac{1}{6}\ln|2-h| + \tfrac{1}{3}\ln 4\gamma, \qquad h\to 2 \qquad \gamma\neq 0 \tag{64}$$

   Correction is $O(|2-h|\ln^2|2-h|)$.

2. *An approach to XX model*: $\gamma\to 0$ and $h<2$: It is included in Case 1b i.e. $h^2-4(1-\gamma^2)<0$:

$$S^0(\rho_A) = -\tfrac{1}{3}\ln\gamma + \tfrac{1}{6}\ln(4-h^2) + \tfrac{1}{3}\ln 2, \qquad \gamma\to 0 \qquad h<2 \tag{65}$$

   Correction is $O(\gamma\ln^2\gamma)$.

Remark. The zeros λ_m satisfy an estimate:

$$|\lambda_{m+1}-\lambda_m| \le 4\pi\tau_0,$$

and hence, $\lambda_{m+1}-\lambda_m\to 0$ as $\tau\to 0$ for every m. This is useful for understanding of large L limit of the XX case corresponding to $\gamma\to 0$ and considered in [28]. The estimate explains why in the XX case the singularities of the logarithmic derivative of the Toeplitz determinant form a cut along the interval $[-1,1]$, while in the XY case we have a discrete set of poles (at points $\pm\lambda_m$).

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 [29].

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[45] For AKLT-VBS models this was proved in [39]

[46] In its turn, the approach of [21] is based on the ideas of [22]. 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 [23]. Some of the important elements of modern theory of integrable operators were already implicitly present in the earlier work [24].

[47] 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 [40].