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Entanglement in the XY spin chain

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Abstract
We consider the entanglement in the ground state of the XY model of an infinite chain. Following Bennett, Bernstein, Popescu and Schumacher, we use the entropy of a sub-system as a measure of entanglement. Vidal, Latorre, Rico and Kitaev have conjectured that the von Neumann entropy of a large block of neighbouring spins approaches a constant as the size of the block increases. We evaluate this limiting entropy as a function of anisotropy and transverse magnetic field. We use the methods based on the integrable Fredholm operators and the Riemann–Hilbert approach. It is shown how the entropy becomes singular at the phase transition points.

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1. Introduction

There is an essential interest in quantifying entanglement in various quantum systems [1–22]. Entanglement is a fundamental measure of 'quantumness' of a system: how many quantum effects we can observe and use. It is the primary resource in quantum computation and quantum information processing [23, 24]. Stable and large scale entanglement is necessary for the scalability of quantum computation [12, 13]. For an experimental demonstration one can look, for example, in [25].

The XY model in a transverse magnetic field was studied from the point of view of quantum information in [2, 3, 26, 27]. It was conjectured [2] that in the ground state of non-critical XY and other gapped models the entropy of a block of L neighbouring spins approaches a constant as $L \to \infty$. The conjecture has been proven for the AKLT-VBS models [19].

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In this paper, we evaluate the entropy of a block of L neighbouring spins in the ground state of the XY model in the limit $L \to \infty$ analytically. Our approach uses the Riemann–Hilbert method of the theory of integrable Fredholm operators. The final answer is given in terms of the elliptic functions and is presented in equation (74).

2. The XY model and the entropy of a sub-system

The Hamiltonian of the XY model can be written as

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

Here, $0 < \gamma < 1$ is the anisotropy parameter; σ_n^x, σ_n^y and σ_n^z are the Pauli matrices and h is the magnetic field. The model was solved in [28–31]. The methods of Toeplitz determinants, as well as the techniques based on integrable Fredholm operators, were used for the evaluation of some correlation functions, see [30, 32] and also [33–36].

The model has the unique ground state $|\mathrm{GS}\rangle$. In the ground state $|\mathrm{GS}\rangle$, the entropy for the whole system vanishes but the entropy of a sub-system can be positive. We shall calculate the entropy of a sub-system (a block of L neighbouring spins) which can measure the entanglement between this sub-system and the rest of the chain [1]. We treat the whole chain as a binary system $|\mathrm{GS}\rangle = |\mathrm{A\&B}\rangle$. We denote this block of L neighbouring spins by sub-system A and the rest of the chain by sub-system B. The density matrix of the ground state can be denoted by $\rho_{\mathrm{AB}} = |\mathrm{GS}\rangle\langle\mathrm{GS}|$. The density matrix of sub-system A is $\rho_A = \mathrm{Tr}_B(\rho_{\mathrm{AB}})$. The von Neumann entropy $S(\rho_A)$ of sub-system A can be represented as follows:

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

This entropy also defines the dimension of the Hilbert space of states of sub-system A.

A set of Majorana operators were used in [2] with self-correlations described 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,

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

and

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

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

$$V\mathbf{B}_L V^T = \oplus_{m=1}^{L} \nu_m \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{4}$$

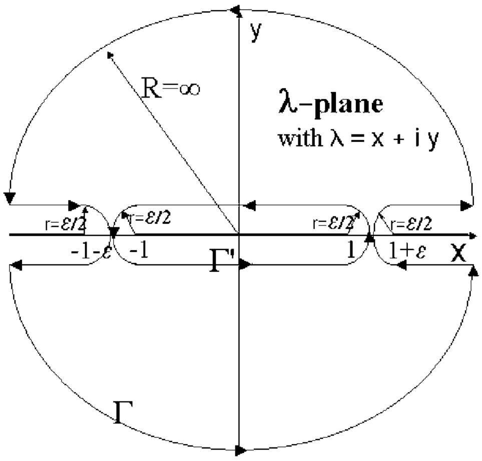

Figure 1. Contours Γ' (smaller one) and Γ (larger one). Bold lines $(-\infty, -1-\epsilon)$ and $(1+\epsilon, \infty)$ are the cuts of the integrand $e(1+\epsilon, \lambda)$. Zeros of $D_L(\lambda)$ (equation (9)) are located on the bold line $(-1, 1)$. The arrows indicate the directions of integrations, and r and R are the radius of the circles.

The real numbers $-1 < \nu_m < 1$ play an important role. We shall call them eigenvalues. The entropy of a block of L neighbouring spins was represented in [2] as

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

with

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

In order to calculate the asymptotic form of the entropy it is not convenient to use formule (4) and (5) directly. Following the idea we have already used in [6], let us introduce

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

and

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

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

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

With the help of the Cauchy residue theorem, we rewrite formula (5) in the following form:

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

Here the contour Γ' is depicted in figure 1; it encircles all zeros of $D_L(\lambda)$. We also note that $\widetilde{\mathbf{B}}_L(\lambda)$ is the block Toeplitz matrix,

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

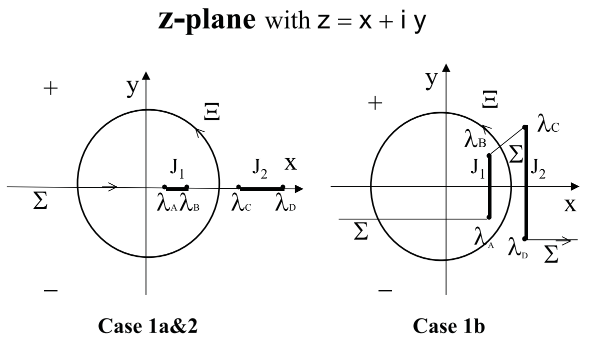

Figure 2. The polygonal line Σ (oriented as it is indicated) separates the complex z plane into two parts: the part Ω_+ which lies to the left of Σ and the part Ω_- which lies to the right of Σ. Curve Ξ is the unit circle in the anti-clockwise direction. Cuts J_1, J_2 for the functions $\phi(z)$, $w(z)$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

with

$$\widetilde{\Pi}_l = \frac{1}{2\pi \mathrm{i}} \oint_{\Xi} \mathrm{d}z\, z^{-l-1} \Phi(z), \tag{11}$$

where the matrix generator $\Phi(z)$ is defined by the equations

$$\Phi(z) = \begin{pmatrix} \mathrm{i}\lambda & \phi(z) \\ -\phi^{-1}(z) & \mathrm{i}\lambda \end{pmatrix} \tag{12}$$

and

$$\phi(z) = \left(\frac{\lambda_1^*}{\lambda_1} \frac{(1-\lambda_1 z)(1-\lambda_2 z^{-1})}{(1-\lambda_1^* z^{-1})(1-\lambda_2^* z)} \right)^{1/2}. \tag{13}$$

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

Case 1(a) $\left(2\sqrt{1-\gamma^2} < h < 2\right)$ and *Case* 2 $(h > 2)$. Both λ_1 and λ_2 are real and given by the formulae

$$\lambda_1 = \frac{h - \sqrt{h^2 - 4(1-\gamma^2)}}{2(1+\gamma)}, \qquad \lambda_2 = \frac{1+\gamma}{1-\gamma}\lambda_1. \tag{14}$$

Case 1(b) $(h^2 < 4(1-\gamma^2))$. Both λ_1 and λ_2 are complex and given by the equations

$$\lambda_1 = \frac{h - \mathrm{i}\sqrt{4(1-\gamma^2) - h^2}}{2(1+\gamma)}, \qquad \lambda_2 = 1/\lambda_1^*. \tag{15}$$

Note that in Case 1 the poles of the function $\phi(z)$ (equation 13) coincide with the points λ_A and λ_B, while in Case 2 they coincide with the points λ_A and λ_C.

3. Integrable Fredholm operators and the Riemann–Hilbert problem

By virtue of equation (10), our objective becomes the asymptotic evaluation of the determinant of block Toeplitz matrix $D_L(\lambda)$ or, rather, its λ-derivative $\frac{\mathrm{d}}{\mathrm{d}\lambda} \ln D_L(\lambda)$. 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 [37] (see also more recent work [38] and references therein). The important difference with the scalar case is the non-commutativity of the associated Weiner–Hopf factorization. This creates serious technical difficulties. In our work, we circumvent this obstacle by using an alternative approach to Toeplitz determinants suggested by Deift in [39]. It is based on the Riemann–Hilbert technique of the theory of 'integrable Fredholm operators', which was developed in [40, 41] and [43] for evaluation of the correlation functions of quantum completely integrable (exactly solvable) models. It turns out that, using the block matrix version of [40] suggested in [45], 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 asymptotics of the entropy $S(\rho_A)$. The final result is formulated in terms of the elliptic functions and is given in equation (74). In what follows we shall outline our calculations providing the necessary facts concerning integrable Fredholm operators. More details, including the evaluation of error terms, will be presented in a separate publication.

(It should also be mentioned that the Riemann–Hilbert apparatus of [40], which is used in this paper, is in turn built upon the ideas of [42] and that some of the important elements of modern theory of integrable Fredholm operators were already implicitly present in the earlier work [44].)

Let K be an integral operator acting in $L_2(\Xi, \mathbb{C}^m)$, i.e.,

$$(K\,X)(z) = \oint_{\Xi} K(z, z')\,X(z')\,\mathrm{d}z' \qquad \text{for} \quad X \in L_2.$$

According to [40, 45], the operator K is called an *integrable Fredholm operator* (on the unite circle) if its kernel $K(z, z')$ can be represented in the form

$$K(z, z') = \frac{f^T(z)h(z')}{z - z'}, \tag{16}$$

with some $p \times m$ matrix functions $f(z)$ and $h(z)$. These functions are supposed to satisfy the nonsingularity condition,

$$f^T(z)h(z) \equiv 0.$$

In what follows we will be dealing with the class of 2×2 matrix integrable Fredholm operators. Indeed, the integer parameters m and p will be 2 and 4, respectively.

Let $f_j(z)$ and $h_j(z)$, $j = 1, 2$, be the 2×2 matrix functions defined by the equations

$$f_1(z) = z^L I_2, \qquad f_2(z) = I_2 \tag{17}$$

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

where I_2 denote the 2×2 identity matrix and the 2×2 matrix function $\Phi(z)$ is defined in equation (12). We specify the operator K by putting in equation (16)

$$f(z) = \begin{pmatrix} f_1(z) \\ f_2(z) \end{pmatrix} \qquad \text{and} \qquad h(z) = \begin{pmatrix} h_1(z) \\ h_2(z) \end{pmatrix}. \tag{19}$$

Then, essentially repeating the arguments of [39], we come to the relation

$$D_L(\lambda) = \det(I - K) \tag{20}$$

which represents $D_L(\lambda)$ as a Fredholm determinant of an integrable operator.

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

$$\frac{d}{d\lambda}K(z,z')=-\mathrm{i}K(z,z')(I_2-\Phi(z'))^{-1},$$

can be rewritten as

$$\frac{d}{d\lambda}\ln D_L(\lambda)=\mathrm{i}\oint_{\Xi}\mathrm{tr}\,[R(z,z)(I_2-\Phi(z))^{-1}]\,dz. \tag{21}$$

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 of the theory of integrable Fredholm operators is that the resolvent operator R also belongs to the integrable class. Indeed, its kernel is given by the formula (see, e.g., [45])

$$R(z,z')=\frac{F^T(z)H(z')}{z-z'}, \tag{22}$$

where

$$F^T=(I-K)^{-1}f^T, \qquad \text{and} \qquad H=h(I-K)^{-1},$$

and in the first relation the operator $(I-K)^{-1}$ is understood as acting to the right, while in the second relation it acts to the left. In its turn, equation (22) leads to the equation

$$R(z,z)=\frac{dF^T(z)}{dz}H(z). \tag{23}$$

Another key result of the integrable operator theory is the possibility to write for the (4×2 in our case) matrix functions $F(z)$ and $H(z)$ the alternative representations (see, e.g., again [45])

$$F(z)=Y_+(z)f(z), \qquad z\in\Xi, \tag{24}$$

$$H(z)=\left(Y_+^T\right)^{-1}(z)h(z), \qquad z\in\Xi, \tag{25}$$

where the (4×4 in our case) matrix function $Y_+(z)$ can be found from the (unique) solution of the following *Riemann–Hilbert problem*:

(i) $Y(z)$ is analytic for $z\notin\Xi$.

(ii) $Y(\infty)=I_4$, where I_4 denotes the 4×4 identity matrix.

(iii) $Y_-(z)=Y_+(z)J(z)$ 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 equation

$$J(z)=I_4+2\pi\mathrm{i}f(z)h^T(z). \tag{26}$$

In our case, general equation (26) reads as follows:

$$J(z)=\begin{pmatrix}2I_2-\Phi^T(z) & -z^L(I_2-\Phi^T(z))\\ z^{-L}(I_2-\Phi^T(z)) & \Phi^T(z)\end{pmatrix}. \tag{27}$$

y

Equations (21)–(25) reduce the original question of the large L evaluation of the Toeplitz determinant D_L to the asymptotic analysis of the solution $Y(z)$ of the Riemann–Hilbert problems (1)–(3).

4. Asymptotic solution of the Riemann–Hilbert problem

Our observation is that once again we can generalize the arguments of [39] to the case of matrix generator $\Phi(z)$ and proceed with the asymptotic solution of the Riemann–Hilbert problems (1)–(3) as follows.

We note that the matrix $J(z)$ admits the following algebraic factorization (cf [39]):

$$J(z) = J_1(z)J_0(z)J_2(z), \tag{28}$$

where

$$J_1(z) = \begin{pmatrix} I_2 & z^L(I_2 - (\Phi^T)^{-1}(z)) \\ 0_2 & I_2 \end{pmatrix}, \tag{29}$$

$$J_2(z) = \begin{pmatrix} I_2 & 0_2 \\ -z^{-L}(I_2 - (\Phi^T)^{-1}(z)) & I_2 \end{pmatrix}, \tag{30}$$

and

$$J_0(z) = \begin{pmatrix} (\Phi^T)^{-1}(z) & 0_2 \\ 0_2 & \Phi^T(z) \end{pmatrix}. \tag{31}$$

Choose now a small ϵ and define the matrix function $X(z)$ according to the equations

$$X(z) = Y(z) \qquad \text{if} \quad |z| > 1+\epsilon, \qquad \text{or} \qquad |z| < 1-\epsilon, \tag{32}$$

$$X(z) = Y(z)J_1(z) \qquad \text{if} \quad 1-\epsilon < |z| < 1, \tag{33}$$

$$X(z) = Y(z)J_2^{-1}(z) \qquad \text{if} \quad 1 < |z| < 1+\epsilon. \tag{34}$$

The new function has a jump across the unit circle Ξ with the jump matrix $J_0(z)$ and two more jumps across the circles,

$$\Xi_1 : |z| = 1-\epsilon, \qquad \text{jump matrix } J_1(z)$$

and

$$\Xi_2 : |z| = 1+\epsilon, \qquad \text{jump matrix } J_2(z).$$

In other words, the original Rimeann–Hilbert problems (1)–(3) are equivalent to the problem

(1) $X(z)$ is analytic outside of the contour $\Gamma \equiv \Xi \cup \Xi_1 \cup \Xi_2$.
(2) $X(\infty) = I_4$, where I_4 denotes the 4×4 identity matrix.
(3) The jumps of the function $X(z)$ across the contour Γ are given by the equations
- $X_-(z) = X_+(z)J_1(z), \qquad z \in \Xi_1$
- $X_-(z) = X_+(z)J_2(z), \qquad z \in \Xi_2$
- $X_-(z) = X_+(z)J_0(z), \qquad z \in \Xi$

where the jump matrices $J_1(z)$, $J_2(z)$ and $J_0(z)$ are defined in equations (29)–(31), respectively, and each circle is oriented counterclockwise.

Observe that the jump matrices on Ξ_1 and Ξ_2 are exponentially close to the identity matrix as $L \to \infty$. This means the following asymptotic relation for $X(z)$:

$$X(z) \sim X^0(z), \tag{35}$$

where $X^0(z)$ solves the Riemann–Hilbert problem which is the same as the Y problem but with the jump matrix $J_0(z)$ instead of $J(z)$.

To conclude our formal asymptotic analysis it remains to note that the function $X^0(z)$ can be found explicitly in terms of the 2×2 matrix-valued functions $U_\pm(z)$ and $V_\pm(z)$ solving the following Weiner–Hopf factorization problem:

(i) $\Phi(z) = U_+(z)U_-(z) = V_-(z)V_+(z), \qquad z \in \Xi$
(ii) $U_-(z)$ ($U_+(z)$) and $V_-(z)$ ($V_+(z)$) are analytic outside (inside) the unit circle Ξ.
(iii) $U_-(\infty) = V_-(\infty) = I$.

Indeed, we have that

$$X^0(z) = \begin{pmatrix} U_+^T(z) & 0_2 \\ 0_2 & \left(V_+^T\right)^{-1}(z) \end{pmatrix}, \qquad \text{if} \quad |z| < 1, \tag{36}$$

and

$$X^0(z) = \begin{pmatrix} (U_-^T)^{-1}(z) & 0_2 \\ 0_2 & V_-^T(z) \end{pmatrix}, \qquad \text{if} \quad |z| > 1. \tag{37}$$

Combining these equations with equations (33) and (34), we arrive to the following asymptotic solution of the problems (1)–(3) ($L \to \infty$):

$$Y_+(z) = \begin{pmatrix} U_+^T(z) & -z^L U_+^T(z)\, M(z) \\ 0_2 & \left(V_+^T\right)^{-1}(z) \end{pmatrix} \tag{38}$$

and

$$(Y_+)^{-1}(z) = \begin{pmatrix} \left(U_+^T\right)^{-1}(z) & z^L M(z)\, V_+^T(z) \\ 0_2 & V_+^T(z) \end{pmatrix}. \tag{39}$$

Here, $z \in \Xi$ and

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

We can use equations (38) and (39) in equations (21)–(25) and obtain the following asymptotic formula:

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} \ln D_L(\lambda) = -\frac{2\lambda}{1-\lambda^2} L + \frac{1}{2\pi} \int_\Xi \mathrm{tr}[\Psi(z)]\, \mathrm{d}z \qquad (L \to \infty), \tag{40}$$

$$\Psi(z) = \left[U_+'(z)U_+^{-1}(z) + V_+^{-1}(z)V_+'(z)\right] \Phi^{-1}(z). \tag{41}$$

Here, $'$ means a derivative in the z variable. In our analysis, this formula plays the role of the strong Szegö theorem (and it would be of interest to understand its meaning in the context of the general result of Widom [37]). In the following section, we give an explicit Weiner–Hopf factorization of $\Phi(z)$.

5. Weiner–Hopf factorization of matrix operator $\Phi(z)$

By explicit calculation, one can find that

$$(1-\lambda^2)\sigma_3 \Phi^{-1}(z)\sigma_3 = \Phi(z), \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{42}$$

Hence,

$$V_-(z) = \sigma_3 U_-^{-1}(z)\sigma_3 \tag{43}$$

$$V_+(z) = \sigma_3 U_+^{-1}(z)\sigma_3(1-\lambda^2), \qquad \lambda \neq \pm 1, \tag{44}$$

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 problems (i)–(iii) exists;

moreover, the functions $U_\pm(z)$ can be expressed in terms of the Jacobi theta functions. Indeed, the auxiliary Riemann–Hilbert problems (i)–(iii) can easily be 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 [46]). Before we give detailed expressions, let us first define some basic objects:

$$w(z) = \sqrt{(z-\lambda_1)(z-\lambda_2)\left(z-\lambda_2^{-1}\right)\left(z-\lambda_1^{-1}\right)}, \tag{45}$$

$$\beta(\lambda) = \frac{1}{2\pi \mathrm{i}} \ln \frac{\lambda+1}{\lambda-1}, \tag{46}$$

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

$$\tau = \frac{2}{c}\int_{\lambda_B}^{\lambda_C} \frac{\mathrm{d}z}{w(z)}, \qquad c = 2\int_{\lambda_A}^{\lambda_B} \frac{\mathrm{d}z}{w(z)}, \tag{47}$$

$$\delta = \frac{2}{c}\left(-\pi\mathrm{i} - \int_{\lambda_A}^{\lambda_B} \frac{z\,\mathrm{d}z}{w(z)}\right), \qquad \omega(z) = \frac{1}{c}\int_{\lambda_A}^{z} \frac{\mathrm{d}z}{w(z)}, \tag{48}$$

$$\Delta(z) = \frac{1}{2}\int_{\lambda_A}^{z} \frac{z+\delta}{w(z)}\,\mathrm{d}z, \qquad \kappa = \int_{\lambda_A}^{\infty} \mathrm{d}\omega(z), \tag{49}$$

The points $\lambda_A, \lambda_B, \lambda_C, \lambda_D$, the cuts J_1, J_2 and the curves Σ and Ξ are shown in figure 2. We shall also need

$$\Delta_0 = \lim_{z\to\infty}\left[\Delta(z) - \tfrac{1}{2}\ln(z-\lambda_1)\right]. \tag{50}$$

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 (50) are taken along the line Σ to the left from λ_A; also in (50), $\arg(z-\lambda_1) = \pi$. 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 noting that $\mathrm{i}\tau < 0$.

Having defined the parameter τ, we introduce the Jacobi theta function

$$\theta_3(s) \equiv \theta_3(s;\tau) = \sum_{n=-\infty}^{\infty} \exp(\pi\mathrm{i}\tau n^2 + 2\pi\mathrm{i}sn). \tag{51}$$

We recall the following properties of this theta function (see, e.g., [47]):

$$\theta_3(-s) = \theta_3(s), \qquad \theta_3(s+1) = \theta_3(s) \tag{52}$$

$$\theta_3(s+\tau) = \exp(-\pi\mathrm{i}\tau - 2\pi\mathrm{i}s)\theta_3(s) \tag{53}$$

$$\theta_3\left(n + m\tau + \frac{1}{2} + \frac{\tau}{2}\right) = 0, \qquad n, m \in \mathbb{Z}. \tag{54}$$

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

$$\Theta_{11}(z) = (z-\lambda_1)^{-\frac{1}{2}} e^{\Delta(z)} \frac{\theta_3\left(\omega(z) + \beta(\lambda) - \kappa + \frac{\sigma\tau}{2}\right)}{\theta_3\left(\omega(z) + \frac{\sigma\tau}{2}\right)}$$

$$\Theta_{12}(z) = -(z-\lambda_1)^{-\frac{1}{2}} e^{-\Delta(z)} \frac{\theta_3\left(\omega(z) - \beta(\lambda) + \kappa - \frac{\sigma\tau}{2}\right)}{\theta_3\left(\omega(z) - \frac{\sigma\tau}{2}\right)}$$

$$\Theta_{21}(z) = -(z-\lambda_1)^{-\frac{1}{2}} e^{-\Delta(z)} \frac{\theta_3\left(\omega(z)+\beta(\lambda)+\kappa-\frac{\sigma\tau}{2}\right)}{\theta_3\left(\omega(z)-\frac{\sigma\tau}{2}\right)}$$

$$\Theta_{22}(z) = (z-\lambda_1)^{-\frac{1}{2}} e^{\Delta(z)} \frac{\theta_3\left(\omega(z)-\beta(\lambda)-\kappa+\frac{\sigma\tau}{2}\right)}{\theta_3\left(\omega(z)+\frac{\sigma\tau}{2}\right)}, \tag{55}$$

where $\sigma = 1$ in Case 1 and $\sigma = 0$ in Case 2, and $\beta(\lambda)$, $\omega(z)$ and κ are defined in equations (45)–(50). 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 $\mathbb{C}\backslash\Sigma$. However, analysing the jumps of the integrals $\omega(z)$ and $\Delta(z)$ over the line Σ and taking into account the properties (52) and (53) of the theta function, one can see that $\Theta(z)$ is actually extended to the analytic function defined on $\mathbb{C}\backslash\{J_1 \cup J_2\}$. Moreover, it satisfies the jump relations

$$\Theta_+(z) = \Theta_-(z)\sigma_1, \qquad z \in J_1 \tag{56}$$

$$\Theta_+(z) = \Theta_-(z)\Lambda\sigma_1\Lambda^{-1}, \qquad z \in J_2. \tag{57}$$

$$\Lambda = \mathrm{i}\begin{pmatrix} \lambda+1 & 0 \\ 0 & \lambda-1 \end{pmatrix}, \qquad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{58}$$

Also note

$$\Theta_{11}(\infty) = \mathrm{e}^{\Delta_0} \frac{\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)}{\theta_3\left(\kappa+\frac{\sigma\tau}{2}\right)} \tag{59}$$

$$\Theta_{22}(\infty) = \mathrm{e}^{\Delta_0} \frac{\theta_3\left(\beta(\lambda)-\frac{\sigma\tau}{2}\right)}{\theta_3\left(\kappa+\frac{\sigma\tau}{2}\right)} \tag{60}$$

$$\Theta_{12}(\infty) = \Theta_{21}(\infty) = 0, \tag{61}$$

and

$$\det\Theta(z) \equiv \phi(z)\det\Theta(\infty)\sqrt{\frac{\lambda_2}{\lambda_1}}. \tag{62}$$

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

$$Q(z) = \begin{pmatrix} \phi(z) & -\phi(z) \\ \mathrm{i} & \mathrm{i} \end{pmatrix}. \tag{63}$$

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

$$\Phi(z) = Q(z)\Lambda Q^{-1}(z) \tag{64}$$

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

$$Q_+(z) = Q_-(z)\sigma_1, \qquad z \in J_1 \cup J_2. \tag{65}$$

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

$$A = Q(\infty)\Lambda^{-1}\Theta^{-1}(\infty). \tag{66}$$

Then,

$$U_-(z) = A\Theta(z)\Lambda Q^{-1}(z), \qquad |z| \geqslant 1 \tag{67}$$

$$U_+(z) = Q(z)\Theta^{-1}(z)A^{-1}, \qquad |z| \leqslant 1. \tag{68}$$

Indeed, by virtue of equation (64), 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 cancelled out in the products (67), (68). The excluded values of λ for which the above construction fails are $\lambda = \pm 1$ and, in view of equation (62), the zeros of $\theta_3\left(\beta(\lambda) + \frac{\sigma\tau}{2}\right)$, i.e. (see (54)),

$$\pm\,\lambda_m, \qquad \lambda_m = \tanh\left(m + \frac{1-\sigma}{2}\right)\pi\tau_0, \qquad m \geqslant 0, \tag{69}$$

where

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

The explicit formulae (67), (68) allow us to transform our basic equation (40) into the form

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln D_L(\lambda) + \frac{2\lambda}{1-\lambda^2}L = \frac{\mathrm{i}}{\pi(1-\lambda^2)}\int_\Xi \mathrm{tr}\left[\Theta^{-1}(z)\frac{\mathrm{d}}{\mathrm{d}z}\Theta(z)\sigma_3\right]\mathrm{d}z. \tag{70}$$

Here $\lambda \neq \pm 1,\ \pm\lambda_m$. Using the same arguments as for equation (62), one can see that

$$\mathrm{tr}\left[\Theta^{-1}(z)\frac{\mathrm{d}}{\mathrm{d}z}\Theta(z)\sigma_3\right] = \frac{1}{cw(z)}\frac{\mathrm{d}}{\mathrm{d}\beta}\ln\left[\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)\theta_3\left(\beta(\lambda)-\frac{\sigma\tau}{2}\right)\right]. \tag{71}$$

This relation allows further simplification of equation (40). Indeed, we have

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln D_L(\lambda) + \frac{2\lambda}{1-\lambda^2}L = \frac{\mathrm{d}}{\mathrm{d}\lambda}\ln\left[\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)\theta_3\left(\beta(\lambda)-\frac{\sigma\tau}{2}\right)\right]. \tag{72}$$

Here $\lambda \neq \pm 1,\ \pm\lambda_m$. Taking into account the fact that as $\lambda \to \infty$, $D_L(\lambda) \to (-1)^L\lambda^{2L}$, we obtain from equation (72) 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 the fixed but arbitrary neighbourhoods of the points ± 1 and $\pm\lambda_m$, $m \geqslant 0$. It is worth noting that the asymptotic representation for the Toeplitz determinant above shows that, in the large L limit, the points λ_m (69) 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.

6. Asymptotic expression for the entropy $S(\rho_A)$

Substituting equation (72) into equation (10), we obtain the formula

$$S(\rho_A) = -L\lim_{\epsilon\to 0^+}\frac{1}{4\pi\mathrm{i}}\oint_{\Gamma'}\mathrm{d}\lambda\, e(1+\epsilon,\lambda)\frac{2\lambda}{1-\lambda^2} + \lim_{\epsilon\to 0^+}\frac{1}{4\pi\mathrm{i}}\oint_{\Gamma'}\mathrm{d}\lambda\, e(1+\epsilon,\lambda)$$
$$\times\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln\left[\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)\theta_3\left(\beta(\lambda)-\frac{\sigma\tau}{2}\right)\right]. \tag{73}$$

The first integral in the rhs of this equation can easily be evaluated by residues at $\lambda = \pm 1$,

$$\frac{1}{4\pi \mathrm{i}} \oint_{\Gamma'} \mathrm{d}\lambda\, e(1+\epsilon, \lambda) \frac{2\lambda}{1-\lambda^2} = \frac{\epsilon+2}{2} \ln\left(1+\frac{\epsilon}{2}\right) - \frac{\epsilon}{2}\ln\frac{\epsilon}{2},$$

and we see that its limit as $\epsilon \to 0^+$ is zero. In order to simplify the second term in the rhs of equation (73) we observe that

- the logarithmic derivative $\frac{\mathrm{d}}{\mathrm{d}\lambda} \ln\left[\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)\theta_3\left(\beta(\lambda)-\frac{\sigma\tau}{2}\right)\right]$ is an odd, single-valued (indeed meromorphic) function in the λ-plane which, in addition, decays as λ^{-3} when $\lambda \to \infty$,
- the boundary values of the function $e(1+\epsilon, \lambda)$ on the cuts $[1+\epsilon, +\infty)$ and $(-\infty, -1-\epsilon]$ satisfy the relations

  $$e_+(1+\epsilon, \lambda) - e_-(1+\epsilon, \lambda) = \pi \mathrm{i}(1+\epsilon-\lambda),$$

  and

  $$e_+(1+\epsilon, \lambda) - e_-(1+\epsilon, \lambda) = -\pi \mathrm{i}(1+\epsilon+\lambda),$$

  respectively.

Therefore, by deforming the original contour of integration to the contour Γ as indicated in figure 1, we conclude that

$$\begin{aligned}
&\frac{1}{4\pi \mathrm{i}} \oint_{\Gamma'} \mathrm{d}\lambda\, e(1+\epsilon, \lambda) \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln\left[\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)\theta_3\left(\beta(\lambda)-\frac{\sigma\tau}{2}\right)\right] \\
&\quad = \frac{1}{2}\int_{1+\epsilon}^{\infty} \mathrm{d}\lambda\, (1+\epsilon-\lambda) \frac{\mathrm{d}}{\mathrm{d}\lambda} \ln\left[\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)\theta_3\left(\beta(\lambda)-\frac{\sigma\tau}{2}\right)\right] \\
&\quad = \frac{1}{2}\int_{1+\epsilon}^{\infty} \ln\left(\frac{\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)\theta_3\left(\beta(\lambda)-\frac{\sigma\tau}{2}\right)}{\theta_3^2\left(\frac{\sigma\tau}{2}\right)}\right)\mathrm{d}\lambda,
\end{aligned}$$

where the last equation is obtained by performing the integration by parts. One can now note that equation (53) implies the general estimate

$$\ln\theta_3(\mathrm{i}s) = \frac{\pi}{\tau_0}s^2\left(1+O\left(\frac{1}{s}\right)\right), \qquad s \to \pm\infty.$$

This allows us to take the limit $\epsilon \to 0^+$ in the last integral and arrive at the following final expression for the *entropy*:

$$S(\rho_A) = \frac{1}{2}\int_1^{\infty} \ln\left(\frac{\theta_3\left(\beta(\lambda)+\frac{\sigma\tau}{2}\right)\theta_3\left(\beta(\lambda)-\frac{\sigma\tau}{2}\right)}{\theta_3^2\left(\frac{\sigma\tau}{2}\right)}\right)\mathrm{d}\lambda. \tag{74}$$

We can change the variable of integration in equation (74) and represent our final answer in the form

$$S(\rho_A) = \frac{\pi}{2}\int_0^{\infty} \ln\left(\frac{\theta_3\left(\mathrm{i}x+\frac{\sigma\tau}{2}\right)\theta_3\left(\mathrm{i}x-\frac{\sigma\tau}{2}\right)}{\theta_3^2\left(\frac{\sigma\tau}{2}\right)}\right)\frac{\mathrm{d}x}{\sinh^2(\pi x)}, \tag{75}$$

which involves the standard functions only. This representation of the entropy $S(\rho_A)$ is convenient for the analysis of the critical cases which we discuss in the next section.

We recall that $\sigma = 0$ for Case 2 and $\sigma = 1$ in Case 1. The entropy $S(\rho_A)$ depends on the basic physical quantities γ and h through the elliptic modulus τ. Indeed, the parameter τ is the ratio (see equation (47)) of the elliptic integrals corresponding to the branch points $\lambda_A, \lambda_B, \lambda_C$ and λ_D, which in turn are given directly in terms of γ and h via equations (14), (15).

Remark. After substituting equation (72) into equation (10), we can in fact integrate over the original contour Γ' of figure 1. This will give us an alternative representation for the entropy $S(\rho_A)$ in terms of an infinite series:

$$S(\rho_A) = 2\sum_{m=0}^{\infty} H(\lambda_m) = \sum_{m=-\infty}^{\infty} (1+\lambda_m)\ln\frac{2}{1+\lambda_m}. \tag{76}$$

Here, the numbers λ_m are defined in equation (69).

The above formulae are the limiting expressions as $L \to \infty$. We can prove that the corrections in equations (74)–(76) are of the order of $O\big(\lambda_C^{-L}\big/\sqrt{L}\big)$. These asymptotic expressions constitute a theorem, whose complete proof we shall publish elsewhere.

It would be interesting to generalize our approach to a new class of quantum spin chains introduced recently by Keating and Mezzadri, while studying matrix models [26].

7. Some limiting cases

The entropy has singularities at the *phase transitions*. When $\tau \to 0$ we can use the Landen transform (see [47]) to get the following estimate of the theta function for the small τ and the pure imaginary s:

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

Now the leading term in equation (75) for the entropy can be replaced by

$$S(\rho_A) = \frac{\mathrm{i}\pi}{6\tau} + O\left(\frac{\mathrm{e}^{-\mathrm{i}\pi/\tau}}{\tau^2}\right) \qquad \text{for} \quad \tau \to 0. \tag{77}$$

Let us consider the following two physical situations corresponding to the small τ and arising the cases introduced in section 2:

(i) *Critical magnetic field* ($\gamma \neq 0$ and $h \to 2$). This is included in our Case 1(a) and Case 2, when $h > 2\sqrt{1-\gamma^2}$. The Ising model belongs to this class. As $h \to 2$ the end points of the cuts $\lambda_B \to \lambda_C$, so τ given by equation (47) is simplified and we obtain from equation (77) that the entropy is

$$S(\rho_A) = -\tfrac{1}{6}\ln|2-h| + \tfrac{1}{3}\ln 4\gamma, \qquad \text{for} \quad h \to 2 \quad \text{and} \quad \gamma \neq 0. \tag{78}$$

The correction is $O(|2-h|\ln^2|2-h|)$. This limit agrees with the predictions of the conformal approach [8, 9]. The first term in the right-hand side of (78) can be represented as $(1/6)\ln\xi$, this confirms the conjecture of [9]. The correlation length ξ was evaluated in [29].

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

$$S(\rho_A) = -\tfrac{1}{3}\ln\gamma + \tfrac{1}{6}\ln(4-h^2) + \tfrac{1}{3}\ln 2, \qquad \text{for} \quad \gamma \to 0 \quad \text{and} \quad h < 2. \tag{79}$$

The correction is $O(\gamma\ln^2\gamma)$. This agrees with [6].

It is interesting to compare this critical behaviour to the one of the Lipkin–Meshkov–Glick model. The latter is similar to the XY model but each pair of the spins interacts with an equal force, and one can say that it is a model on a complete graph. The critical behaviour in the Lipkin–Meshkov–Glick model was described in [22], it is similar to the XY model, but the actual critical exponents are different.

Remark. From equation (69) it follows that the numbers λ_m satisfy the estimate

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

This means that $(\lambda_{m+1} - \lambda_m) \to 0$ as $\tau \to 0$ for every m. This estimate explains why in the XX case considered in [6] the singularities of the logarithmic derivative of the Toeplitz determinant $\mathrm{d}\ln D_L(\lambda)/\mathrm{d}\lambda$ form at the large L limit a cut along the interval $[-1, 1]$, while in the XY case the singular set remains a discrete set of poles (at the points $\pm\lambda_m$).

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Appendix

After our paper appeared in quant-ph, Peschel [48] simplified our expression for the entropy in Cases 1(a) and 2. He used the approach of [9]. He showed that in these cases our formula (76) is equivalent to formula (4.33) of [9]. Moreover, Peschel was able to sum it up into the following expressions for the entropy:

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

in Case 1(a) and

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

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

$$k = \begin{cases} \sqrt{(h/2)^2 + \gamma^2 - 1}/\gamma, & \text{Case 1(a)} \\ \gamma/\sqrt{(h/2)^2 + \gamma^2 - 1}, & \text{Case 2.} \end{cases} \tag{A.3}$$

In our work, we have shown, in particular, that equation (76) is valid in Case 1(b) as well. Therefore, for Case 1(b) we can apply the summation procedure of [48] and obtain the same formula equation A.1 but with $k = \sqrt{(1 - h^2/4 - \gamma^2)/(1 - h^2/4)}$.

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