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The Onsager Solution and the Bethe Ansatz

By

T. C. Dorlas

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Preface

The two-dimensional Ising model without external field was solved by Onsager in 1944[1]. This was a very important result, because it showed that mathematically, the phase transition comes about in the thermodynamic limit. Moreover, his solution showed that the phase transition is second-order and that the specific heat diverges logarithmically at the critical point.

Since then many different derivations of his solution have been published. First the Onsager solution was simplified by Kauffman[2]. We mention a few other approaches. A combinatorial solution based on an expansion was developed by Kac and Ward[3]. Another ingenious solution was proposed by Feynman[4]. The assumptions made in this proposal were proved by Sherman[5]. Another approach, related to quantum field theory as it relies on the Jordan-Wigner transformation, is due to Schultz, Mattis and Lieb[6]. This solution also clearly demonstrates that the 2-dimensional Ising model can be considered a free fermion field theory. However, there is a twist, in the form of a phase transition. It was shown[7] that this has a topological origin

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by reformulating the model on an infinite lattice in terms of a C*-algebra. The simplest approach is probably via the introduction of Grassmann variables: see Samuel[8] and Ytzykson[9] and the particularly simple approach of Plechko[10]. Although Onsager already proposed a formula for the spontaneous magnetization, a derivation was only published by Yang[11]. Finally, let me mention the solution by Baxter[12] which uses his star-triangle transformation and the related Yang-Baxter equation, which he also used to solve several other models, notably the 8-vertex model and the XYZ Heisenberg chain[13].

Here we consider still another approach, which relies on the original Bethe Ansatz, which was introduced by Bethe[14] in his celebrated paper of 1931. In this work Bethe succeeded in computing the eigenvalues of the homogeneous quantum Heisenberg model in one dimension (XXX model) using an Ansatz for the eigenfunctions. The Bethe Ansatz has led to a veritable revolution in mathematics. A large number of different models, both classical and quan-

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tum, is now known that can be solved using this method or the extension introduced by Baxter and developed further by the St. Petersburg school of Faddeev et al.[15]. It is now often referred to as the *algebraic Bethe Ansatz*. The first application of the Bethe Ansatz to a model other than the Heisenberg model is due to Lieb[16], who computed the residual entropy of square ice. He then extended this to the more general 6-vertex model[17]. Another application is the solution of the non-linear Schrödinger model, or one-dimensional Bose gas with δ-interaction[18]. Their solution for the eigenvalues was extended to a calculation of the thermodynamics by Yang and Yang[19]. This was made rigorous by Dorlas, Lewis and Pulé[20]. The Yang-Yang derivation was generalized to the Heisenberg model by Takahashi[21] and also to other models, and is now know as the *thermodynamic Bethe Ansatz*.

Fortunately, we shall see that for the 2-dimensional Ising model, the Bethe Ansatz solutions are quite simple and explicit. In these notes, we start by considering the 1-dimensional Ising model. We give in fact 3 different solutions: the standard solution using the diagonalization of the transfer matrix, the combinatorial solution given by Ising himself, and another, quite simple approach, which might be new and is also based on the transfer matrix, but

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without diagonalization. Next we consider the Ising model on 2, 3 and 4 linked chains respectively. This should set the scene for the general solution. Adding extra chains introduces new complications at each of these stages and prepares the way for the general solution using Bethe Ansatz diagonalization of a submatrix.

T. C. Dorlas, April 2022.

1 The Ising chain

The Ising chain is a model of spin variables $s_i = \pm 1$ $(i = 1, \ldots, N)$ arranged on a line with nearest-neighbour interaction. Assuming periodic boundary conditions, the interaction Hamiltonian is given by

$$H_N(\{s_i\}_{i=1}^N) = -J \sum_{i=1}^N s_i s_{i+1} - H \sum_{i=1}^N s_i, \tag{1.1}$$

where we set $s_{N+1} = s_1$. The coupling constant J will be assumed to be positive (ferromagnetic). H is an external magnetic field. The corresponding **partition function** is defined by

$$Z_N(\beta) = \sum_{s_1,\ldots,s_N=\pm 1} e^{-\beta H_N(\{s_i\}_{i=1}^N)}, \tag{1.2}$$

where $\beta > 0$ is the inverse temperature (setting $k_B = 1$). The thermodynamics of the model in the **thermodynamic limit** is then given by the free energy density[22]

$$f(\beta, J, H) = -\frac{1}{\beta} \lim_{N\to\infty} \frac{1}{N} \ln Z_N(\beta). \tag{1.3}$$

In the following we give 3 different ways of computing Z_N and the corresponding free energy density for this simple model.

1.1 Transfer matrix solution

This solution is given in many textbooks[23]. We write the partition function as a trace of the N-th power of the so-called **transfer matrix**. Consider two neighbouring spins s_i and s_{i+1}. Dividing the magnetic field equally over the two spins, the corresponding factor in the partition function equals $e^{\beta(J+H)}$

[22] See for example T. C. Dorlas, *Statistical Mechanics, Fundamentals and Model Solutions* (2nd Ed.), Taylor and Francis, 2021.

[23] See for example K. Huang, *Statistical Mechanics.* J. Wiley and Sons, 1963. Section 16.5, or R. J. Baxter, *loc. cit.* Chapter 2, or T. C. Dorlas, *loc. cit.* Chapter 28.

is $s_i = s_{i+1} = +1$, $e^{-\beta J}$ if $s_i s_{i+1} = -1$, and $e^{\beta(J-H)}$ if $s_i = s_{i+1} = -1$. Introducing the transfer matrix

$$T = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix},$$

we can then express Z_N as follows:

$$Z_N = \sum_{s_1,\ldots,s_N=\pm 1} T_{s_1,s_2} T_{s_2,s_3} \cdots T_{s_{N-1},s_N} T_{s_N,s_1} = \mathrm{Tr}\,(T^N). \tag{1.4}$$

If $\lambda_\pm$ are the eigenvalues of the matrix T, then it follows that

$$Z_N = \lambda_+^N + \lambda_-^N, \tag{1.5}$$

and hence

$$f(\beta, J, H) = -\frac{1}{\beta} \ln \lambda_+, \tag{1.6}$$

assuming that $\lambda_+ > \lambda_-$. It is easy to determine $\lambda_\pm$:

$$\lambda_\pm = e^{\beta J} \cosh \beta H \pm \sqrt{e^{2\beta J} \sinh^2 \beta H + e^{-2\beta J}}. \tag{1.7}$$

Thus,

$$\begin{aligned} f(\beta, J, H) &= -\frac{1}{\beta} \ln \left\{ e^{\beta J} \cosh \beta H \pm \sqrt{e^{2\beta J} \sinh^2 \beta H + e^{-2\beta J}} \right\} \\ &= -J - \frac{1}{\beta} \ln \cosh(\beta H) - \frac{1}{\beta} \ln \left(1 + \sqrt{u^2 + (1-u^2) e^{-4\beta J}} \right), \end{aligned} \tag{1.8}$$

where we put

$$u = \tanh(\beta H). \tag{1.9}$$

1.2 Ising's combinatorial solution

We now present Ising's combinatorial derivation of the formula for Z_N. Consider a configuration with N_+ $+$-spins and $N_- = N - N_+$ $-$-spins, e.g.

$$+ + - - + - - - - + + + - + + - --$$

Assume that the first spin is $+$. The minus spins are divided over a number of separate intervals p. The number of possibilities for choosing these intervals (4 in the above case) is $\binom{N_+}{p}$. Given the intervals we can divide the $-$-spins over them in $\binom{N_- -1}{p-1}$ ways (provided $N_- \geq 1$). (To divide the $-$ spins, we put division marks in $p-1$ positions among the $N_- - 1$ possible places.) The corresponding energy (Hamiltonian) is then $-J(N-4p) - H(N_+ - N_-)$.

The resulting expression for Z_N is

$$\begin{aligned} Z_N &= e^{\beta(J+H)N} + e^{\beta(J-H)N} \\ &\quad + \sum_{N_+=1}^{N-1} \sum_{p=1}^{N_+ \wedge N_-} \left[\binom{N_+}{p} \binom{N_- - 1}{p-1} e^{\beta J(N-4p)+\beta H(N_+ - N_-)} \right. \\ &\qquad \left. + \binom{N_-}{p} \binom{N_+ - 1}{p-1} e^{\beta J(N-4p)+\beta H(N_+ - N_-)} \right]. \end{aligned} \tag{1.10}$$

(The first two terms correspond to all spins being $+$ or all $-$; the last term corresponds to the case where the first spin is $-$.) To evaluate these sums, we consider the generating function $\sum_{N=0}^{\infty} Z_N x^N$. Using the formula

$$\sum_{N=p}^{\infty} \binom{N}{p} x^N = \frac{x^p}{(1-x)^{p+1}}, \tag{1.11}$$

we have

$$\begin{aligned}
\sum_{N=0}^{\infty} Z_N x^N &= \frac{1}{1-xe^{\beta(J+H)}} + \frac{1}{1-xe^{\beta(J-H)}} \\
&\quad + \sum_{p=1}^{\infty} e^{-4\beta J p} \sum_{N_+=p}^{\infty} \sum_{N_-=p}^{\infty} x^{N_+ + N_-} e^{\beta(J+H)N_+} e^{\beta(J-H)N_-} \\
&\qquad \times \left[\binom{N_+}{p} \binom{N_- - 1}{p-1} + \binom{N_-}{p} \binom{N_+ - 1}{p-1} \right] \\
&= \frac{1}{1-xe^{\beta(J+H)}} + \frac{1}{1-xe^{\beta(J-H)}} \\
&\qquad + \sum_{p=1}^{\infty} e^{-4\beta J p} \left\{ \frac{x^p e^{\beta(J+H)p}}{(1-xe^{\beta(J+H)})^{p+1}} \frac{x^p e^{\beta(J-H)p}}{(1-xe^{\beta(J-H)})^{p}} \right. \\
&\qquad\qquad \left. + \frac{x^p e^{\beta(J+H)p}}{(1-xe^{\beta(J+H)})^{p}} \frac{x^p e^{\beta(J-H)p}}{(1-xe^{\beta(J-H)})^{p+1}} \right\} \\
&= \left\{ \frac{1}{1-xe^{\beta(J+H)}} + \frac{1}{1-xe^{\beta(J-H)}} \right\} \\
&\qquad \times \sum_{p=0}^{\infty} \left\{ \frac{x^2 e^{-2\beta J}}{(1-xe^{\beta(J+H)})(1-xe^{\beta(J-H)})} \right\}^p \\
&= 2\,\frac{1 - xe^{\beta J}\cosh\beta H}{1 - 2xe^{\beta J}\cosh\beta H + 2x^2 \sinh 2\beta J}. \qquad (1.12)
\end{aligned}$$

Then, using the formula

$$\sum_{N=0}^{\infty} \left[(a+\sqrt{b}\,)^N + (a-\sqrt{b}\,)^N \right] x^N = 2\frac{1-ax}{(1-ax)^2 - bx^2} \qquad (1.13)$$

it follows that

$$Z_N = \lambda_+^N + \lambda_-^N, \qquad (1.14)$$

where $\lambda_\pm$ are given by equation (1.7).

Note that the combinatorial expression (1.10) also gives rise to a variational expression for the free energy:

$$
\begin{aligned}
f(\beta) &= -\frac{1}{\beta} \sup_{x\in[0,1]} \sup_{0\le u\le x\wedge(1-x)} \big\{\beta(J-H)+2\beta Hx-4\beta Ju \\
&\qquad -2u\ln\frac{u}{x}-(x-u)\ln\frac{x-u}{x} \\
&\qquad -u\ln\frac{u}{1-x}-(1-x-u)\ln\frac{1-x-u}{1-x}\big\} \\
&= -J+H-\frac{1}{\beta}\sup_{x\in[\frac{1}{2},1]} \sup_{u\in[0,1-x]} \big\{2\beta Hx-4\beta J\,u-2\,u\ln u \\
&\qquad -(x-u)\ln(x-u)-(1-x-u)\ln(1-x-u) \\
&\qquad +x\ln x+(1-x)\ln(1-x)\big\}.
\end{aligned} \tag{1.15}
$$

Maximising over x yields

$$
\frac{(1-x)(x-u)}{x(1-x-u)} = e^{2\beta H}, \tag{1.16}
$$

and maximising over u yields

$$
(x-u)(1-x-u) = u^2 e^{4\beta J}. \tag{1.17}
$$

Solving for u from (1.16) and substituting in (1.17) yields

$$
\frac{e^{2\beta H}}{(e^{2\beta H}-1)^2}\frac{(2x-1)^2}{x(1-x)} = e^{4\beta J} \tag{1.18}
$$

and hence

$$
x = \frac{1}{2}\left\{1+\frac{\sinh\beta H}{\sqrt{\sinh^2\beta H+e^{-4\beta J}}}\right\}. \tag{1.19}
$$

Inserting into the expression for u gives

$$
u = \frac{1}{2}\frac{e^{-4\beta J}}{\left(\cosh\beta H+\sqrt{\sinh^2\beta H+e^{-4\beta J}}\right)\sqrt{\sinh^2\beta H+e^{-4\beta J}}}. \tag{1.20}
$$

Inserting these expressions into (1.15) finally leads to

$$
\begin{aligned}
f(\beta) &= -J + H - \frac{1}{\beta}\left\{2\beta H - \frac{1}{\beta}\ln\frac{x-u}{x}\right\} \\
&= -J - H - \frac{1}{\beta}\ln\left\{1 - \frac{e^{-4\beta J}}{\sinh\beta H + \sqrt{\sinh^2\beta H + e^{-4\beta J}}}\right. \\
&\qquad\qquad \left.\times\frac{1}{\cosh\beta H + \sqrt{\sinh^2\beta H + e^{-4\beta J}}}\right\} \\
&= -J - H - \frac{1}{\beta}\ln\left\{1 - \frac{\sqrt{\sinh^2\beta H + e^{-4\beta J}} - \sinh\beta H}{\sqrt{\sinh^2\beta H + e^{-4\beta J}} + \cosh\beta H}\right\} \\
&= -J - H - \ln\frac{e^{\beta H}}{\cosh\beta H + \sqrt{\sinh^2\beta H + e^{-4\beta J}}} \\
&= -J - \frac{1}{\beta}\ln\left(\cosh\beta H + \sqrt{\sinh^2\beta H + e^{-4\beta J}}\right). \qquad (1.21)
\end{aligned}
$$

1.3 Algebraic solution

We can derive the expression (1.5), where $\lambda_\pm$ is given by (1.7), algebraically as follows. First we write

$$Z_N = e^{\beta J N}(\cosh\beta H)^N \,\mathrm{Tr}\,(A\,B)^N, \qquad (1.22)$$

where $A = \mathbf{1} + \lambda\sigma^x$ with $\lambda = e^{-2\beta J}$, and $B = \mathbf{1} + u\sigma^z$. To see this, note that instead of (1.4) we can also write separately the interaction term and the magnetic field term thus

$$e^{\beta J s_i s_{i+1}} e^{\beta H s_{i+1}}.$$

Then

$$e^{\beta J s_i s_{i+1}} = e^{\beta J}(\delta_{s_i,s_{i+1}} + \lambda\delta_{s_i,-s_{i+1}}) = e^{\beta J}(\mathbf{1} + \lambda\sigma^x)_{s_i,s_{i+1}},$$

where $\lambda = e^{-2\beta J}$, and

$$e^{\beta H s_{i+1}} = \cosh(\beta H)(1 + u s_{i+1}) = \cosh(\beta H)(\mathbf{1} + u\sigma^z)_{s_{i+1},s_{i+1}}.$$

We put

$$\tilde{Z}_N = \mathrm{Tr}\,(A\,B)^N = \mathrm{Tr}\,((\mathbf{1} + \lambda\sigma^x)(\mathbf{1} + u\sigma^z))^N, \qquad (1.23)$$

so that

$$Z_N = e^{\beta JN} \cosh^N(\beta H) \tilde{Z}_N. \tag{1.24}$$

In deriving an expression for $\tilde{Z}_N$, we now simply use the anti-commutation relations

$$\sigma^x \sigma^z + \sigma^z \sigma^x = 0;\ (\sigma^x)^2 = (\sigma^z)^2 = \mathbf{1}. \tag{1.25}$$

We expand the product $(A\,B)^N$ choosing in each of the factors $A\,B$ of the product the term $\mathbf{1}$ or at least one σ operator. There must be an even number of factors σ^x because otherwise the diagonal is zero, and there must also be an even number of factors σ^z because otherwise the trace is zero. Therefore let $2k$ be the number of factors where we choose at least one σ operator. From those factors we next choose among those the factors containing a σ^x at positions $i_1, \ldots, i_{2p}$ out of the total $2k$. This yields

$$\begin{aligned}
\mathrm{Tr}\,(A\,B)^N &= \sum_{k=0}^{[N/2]} \binom{N}{2k} \sum_{p=0}^{k} \sum_{1 \le i_1 < \cdots < i_{2p} \le 2k} \lambda^{2p} u^{2k-2p} \\
&\quad \times \mathrm{Tr}\,\left((\sigma^z)^{i_1-1}\sigma^x(\mathbf{1}+u\sigma^z)(\sigma^z)^{i_2-i_1-1}\cdots(\sigma^z)^{2k-i_{2p}}\right).
\end{aligned} \tag{1.26}$$

If each second factor $\mathbf{1} + u\sigma^z$ is permuted with the previous factor σ^x it becomes $\mathbf{1} - u\sigma^z$. This can then be combined with the previous factor $\mathbf{1} + u\sigma^z$ to give $(1 - u^2)\mathbf{1}$, which, in all, results in a factor $(1 - u^2)^p$ in front of the trace. The remaining traces are all equal ± 2. We finally notice that, if we keep the position of the even-numbered σ^x factors fixed, and move the odd-numbered ones across the σ^z, the sign of the trace alternates. It follows that the sum over the position of the odd-numbered factors σ^x cancels unless all i_{2j} $(j = 1, \ldots, p)$ are even, and in that case, the sum equals 2. There are thus $\binom{k}{p}$ possible choices for the even-numbered factors, and the result is

$$\begin{aligned}
\tilde{Z}_N &= 2 \sum_{k=0}^{[N/2]} \binom{N}{2k} \sum_{p=0}^{k} \binom{k}{p} \lambda^{2p} (1-u^2)^p u^{2k-2p} \\
&= 2 \sum_{k=0}^{[N/2]} \binom{N}{2k} (u^2 + (1-u^2)\lambda^2)^k.
\end{aligned} \tag{1.27}$$

Finally, we have the expansion

$$(1+\sqrt{x})^N + (1-\sqrt{x})^N = 2\sum_{k=0}^{[N/2]} \binom{N}{2k} x^k, \tag{1.28}$$

so that

$$\tilde{Z}_N = (1+\sqrt{u^2+\lambda^2(1-u^2)})^N + (1-\sqrt{u^2+\lambda^2(1-u^2)})^N. \tag{1.29}$$

Alternatively, in the thermodynamic limit, we have the variational expression

$$\lim_{N\to\infty} \frac{1}{N} \ln \tilde{Z}_N = \sup_{x\in[0,1]} \big\{ x \ln (u^2 + (1-u^2)\lambda^2) - I(2x) \big\} \tag{1.30}$$

where $I(x) = x\,\ln x + (1-x)\ln(1-x)$. The supremum is attained at

$$x = \frac{1}{2} \frac{\sqrt{u^2+(1-u^2)e^{-4\beta J}}}{1+\sqrt{u^2+(1-u^2)e^{-4\beta J}}}$$

and equals

$$\lim_{N\to\infty} \frac{1}{N} \ln \tilde{Z}_N = \ln (1+\sqrt{u^2+(1-u^2)e^{-4\beta J}}\,). \tag{1.31}$$

2 The Ising model on linked chains

In the case of M linked chains, the Hamiltonian reads

$$H_{N,M}(\{s_{i,j}\}_{i=1;j=1}^{N,M}) = -J_1 \sum_{i=1}^{N}\sum_{j=1}^{M} s_{i,j}s_{i+1,j} - J_2 \sum_{i=1}^{N}\sum_{j=1}^{M} s_{i,j}s_{i,j+1}, \qquad (2.1)$$

where we set $s_{N+1,j} = s_{1,j}$ and $s_{i,M+1} = s_{i,1}$ for periodic boundary conditions. The coupling constants J_1, J_2 will be assumed to be positive (ferromagnetic). Note that we consider only the case where the external magnetic field equals zero. The corresponding **partition function** is defined by

$$Z_{N,M}(\beta) = \sum_{\{s_{i,j}\};\, s_{i,j}=\pm 1} e^{-\beta H_{N,M}(\{s_{i,j}\})}. \qquad (2.2)$$

The free energy density is given by

$$f(\beta, J, H) = -\frac{1}{\beta} \lim_{N,M\to\infty} \frac{1}{NM} \ln Z_{N,M}(\beta). \qquad (2.3)$$

Again, we can write a transfer matrix expression for $Z_{N,M}$ analogous to (1.22):

$$Z_{N,M}(\beta) = e^{\beta J_1 NM} \cosh(\beta J_2)^{NM} \tilde{Z}_{N,M}(\beta), \text{ with } \tilde{Z}_{N,M} = \mathrm{Tr}\,(A\,B)^N, \qquad (2.4)$$

where

$$\begin{aligned} A &= \prod_{j=1}^{M} (\mathbf{1} + \lambda \sigma_j^x) \text{ and} \\ B &= \prod_{j=1}^{M} (\mathbf{1} + u \sigma_j^z \otimes \sigma_{j+1}^z). \end{aligned} \qquad (2.5)$$

Here $\sigma_j^x = \mathbf{1} \otimes \cdots \otimes \sigma^x \otimes \cdots \otimes \mathbf{1}$, with σ^x at the j-th position, and similarly, σ_j^z. Moreover, $\lambda = e^{-2\beta J_1}$ and $u = \tanh(\beta J_2)$.

2.1 Two chains

In the case of two linked chains ($M = 2$), note that we have double the interaction $2J_2$ between two vertically connected spins due to the periodic boundary conditions. This may be unnatural but it is more consistent with the case of $M > 2$. We consider the eigenspaces of $\sigma^x \otimes \sigma^x$.

On the eigenspace $\mathcal{H}_+$ of $\sigma^x \otimes \sigma^x$ with eigenvalue $+1$ consider the basis

$$\frac{1}{\sqrt{2}}(|++\rangle \pm |--\rangle), \tag{2.6}$$

where $|\pm\rangle$ denote the eigenstates of σ^x (NOT σ^z). Since $\sigma^z \otimes \sigma^z$ maps $|++\rangle$ to $|--\rangle$ and vice versa, it acts like σ^z on this space. Moreover, $\sigma^x \otimes \mathbf{1}$ and $\mathbf{1} \otimes \sigma^x$ both act like σ^x on this space. On the $+$ eigenspace we therefore have the effective trace expression

$$\begin{aligned} &\mathrm{Tr}\,\left[(\mathbf{1}+\lambda\sigma^x)^2(\mathbf{1}+u\sigma^z)^2\right]^N = \\ &= \;(1+\lambda^2)^N(1+u^2)^N\,\mathrm{Tr}\,\left[(\mathbf{1}+\frac{2\lambda}{1+\lambda^2}\sigma^x)(\mathbf{1}+\frac{2u}{1+u^2}\sigma^z)\right]^N. \end{aligned} \tag{2.7}$$

This trace expression is similar to the expression for the partition function of the 1-dimensional Ising model with field.

Replacing λ by $\frac{2\lambda}{1+\lambda^2}$ and u by $\frac{2u}{1+u^2}$ in (1.29), we get immediately,

$$\begin{aligned} &\mathrm{Tr}\,\left[(\mathbf{1}+\lambda\sigma^x)^2(\mathbf{1}+u\sigma^z)^2\right]^N \\ &= \sum_\pm (1+\lambda^2)^N(1+u^2)^N \\ &\qquad\times\left\{1 \pm \sqrt{\frac{4u^2}{(1+u^2)^2}+\frac{4\lambda^2}{(1+\lambda^2)^2}\left(1-\frac{4u^2}{(1+u^2)^2}\right)}\right\}^N \\ &= \sum_\pm \left((1+\lambda^2)(1+u^2) \pm \sqrt{4u^2(1+\lambda^2)^2+4\lambda^2((1+u^2)^2-4u^2)}\right)^N \\ &= \sum_\pm \left((1+\lambda^2)(1+u^2) \pm 2\sqrt{u^2(1+\lambda^4)+\lambda^2(1+u^4)}\right)^N. \end{aligned} \tag{2.8}$$

The $-$ eigenspace $\mathcal{H}_-$ of $\sigma^x \otimes \sigma^x$ is spanned by

$$\frac{1}{\sqrt{2}}(|+-\rangle \pm |-+\rangle), \tag{2.9}$$

where $|\pm\rangle$ again denote the eigenstates of σ^x. Then $\sigma^z \otimes \sigma^z$ acts like σ^z, whereas $A(|+-\rangle \pm |-+\rangle) = (1-\lambda^2)(|+-\rangle \pm |-+\rangle)$, i.e. A acts like

$(1-\lambda^2)\mathbf{1}$. The two operators therefore commute and we get the contribution

$$(1-\lambda^2)^N[(1-u)^{2N}+(1+u)^{2N}]. \tag{2.10}$$

In total we therefore have

$$\begin{aligned}\tilde{Z}_{N,2} &= [(1+u)^{2N}+(1-u)^{2N}](1-\lambda^2)^N \\ &\quad + \left[(1+\lambda^2)(1+u^2)+2\sqrt{\lambda^2(1+u^4)+u^2(1+\lambda^4)}\right]^N \\ &\quad + \left[(1+\lambda^2)(1+u^2)-2\sqrt{\lambda^2(1+u^4)+u^2(1+\lambda^4)}\right]^N . \end{aligned} \tag{2.11}$$

It is easily seen that the second term is largest, so that

$$\lim_{N\to\infty}\frac{1}{N}\ln\tilde{Z}_{N,2}=\ln\lambda_{\max}$$

where

$$\lambda_{\max}=(1+\lambda^2)(1+u^2)+2\sqrt{\lambda^2(1+u^4)+u^2(1+\lambda^4)}.$$

Remark. Note that the operator $A\,B$ is nonnegative in the sense that $A\,B\,\vec{v}\geq 0$ if $\vec{v}\geq 0$, and $A\,B$ is also irreducible because all matrix elements are positive. It follows from the **Perron-Frobenius theorem** (See Appendix A) that the eigenvector corresponding to the maximal eigenvalue is positive (up to a multiplicative factor). However, on the basis corresponding the eigenvectors of A (more precisely, the σ_j^x) one has to distinguish the space $\mathcal{H}_+$ and the space $\mathcal{H}_-$. On these individual spaces, $A\,B$ is again positive, so the maximal eigenvalue corresponds to the positive vector in $\mathcal{H}_+$ or that in $\mathcal{H}_-$.

Note that the interaction between the chains effectively acts like an external magnetic field. We might then speculate that the case of more chains can also be decomposed in terms of effective fields.

2.2 The Ising model on a three-stranded chain

We write again

$$\tilde{Z}_{N,3}=\mathrm{Tr}\,(AB)^N, \tag{2.12}$$

where in this case

$$A = (\mathbf{1} + \lambda\sigma^x) \otimes (\mathbf{1} + \lambda\sigma^x) \otimes (\mathbf{1} + \lambda\sigma^x), \tag{2.13}$$

and

$$B = (\mathbf{1} + u\sigma^z \otimes \sigma^z \otimes \mathbf{1})(\mathbf{1} + u\sigma^z \otimes \mathbf{1} \otimes \sigma^z)(\mathbf{1} + u\mathbf{1} \otimes \sigma^z \otimes \sigma^z). \tag{2.14}$$

The latter can be written in the form

$$B = (1 + u^3)\mathbf{1} + (u + u^2)(\sigma_1^z\sigma_2^z + \sigma_2^z\sigma_3^z + \sigma_3^z\sigma_1^z). \tag{2.15}$$

Analogous to the two-chain case, we can reason as follows: On the eigenspace of $\sigma^x \otimes \sigma^x \otimes \sigma^x$ with eigenvalue $+1$ there are two invariant subspaces: that spanned by $|+++\rangle$ and $\frac{1}{\sqrt{3}}(|+--\rangle + |-+-\rangle + |--+\rangle)$, and that consisting of the vectors $a_1|+--\rangle + a_2|-+-\rangle + a_3|--+\rangle$ with $a_1 + a_2 + a_3 = 0$. On the latter, the operator

$$B = (1 + u)\left[(1 - u + u^2)\mathbf{1} + u(\sigma_1^z\sigma_2^z + \sigma_2^z\sigma_3^z + \sigma_3^z\sigma_1^z)\right] \tag{2.16}$$

reduces to

$$B_{+,odd} = (1 + u)[(1 - u + u^2)\mathbf{1} - u\mathbf{1}] = (1 + u)(1 - u)^2\,\mathbf{1}. \tag{2.17}$$

Since moreover, A is also diagonal with eigenvalue $(1 - \lambda)^2(1 + \lambda)$ on this subspace, we obtain the contribution $2(1 - \lambda)^2(1 + \lambda)(1 + u)(1 - u)^2$.

On the first subspace, the operator B reduces to

$$B_{+,even} = (1 + u)[(1 - u + u^2)\mathbf{1} + u(\mathbf{1} - \sigma^z) + \sqrt{3}u\sigma^x], \tag{2.18}$$

and A reduces to

$$A_{+,even} = (1 + \lambda)[(1 + \lambda^2)\mathbf{1} + 2\lambda\sigma^z]. \tag{2.19}$$

On this subspace we therefore have to compute

$$\mathrm{Tr}\left[\Big(((1 + u^2)\mathbf{1} - u\sigma^z + \sqrt{3}u\sigma^x)((1 + \lambda^2)\mathbf{1} + 2\lambda\sigma^z)\Big)^N\right]. \tag{2.20}$$

This is similar to the one-dimensional chain. We prove for future reference:

Lemma 2.1 *Define, for any* $\theta \in [0, 2\pi]$,

$$B(\theta) = (1+u^2)\mathbf{1} + 2u\cos(\theta)\,\sigma^z + 2u\sin(\theta)\sigma^x, \tag{2.21}$$

and let

$$A = (1+\lambda^2)\mathbf{1} + 2\lambda\sigma^z. \tag{2.22}$$

Then

$$\mathrm{Tr}\,(A\,B(\theta))^N = (\zeta_+(\theta))^N + (\zeta_-(\theta))^N \tag{2.23}$$

where

$$\zeta_\pm(\theta) = (1+\lambda^2)(1+u^2) + 4u\lambda\cos(\theta) \pm \sqrt{\Delta(\theta)}, \tag{2.24}$$

and

$$\Delta(\theta) = [(1+\lambda^2)(1+u^2) + 4\cos(\theta)u\lambda]^2 - (1-u^2)^2(1-\lambda^2)^2. \tag{2.25}$$

Proof. In expanding the product, we first choose the sites where there is either no σ-operator or two factors σ^z. These factors commute with the others and yield factors $(1+\lambda^2)(1+u^2) + 4\lambda u\cos(\theta)$. The remaining sites must either have a factor σ^x or a single σ^z. Each must occur an even number of times. The result is

$$\begin{aligned}
&\mathrm{Tr}\,(A\,B(\theta))^N = \\
&= \sum_{k=0}^{[N/2]} \binom{N}{2k} [(1+\lambda^2)(1+u^2) + 4\lambda u\cos(\theta)]^{N-2k} \\
&\quad \times \sum_{p=0}^{k} \sum_{1\le i_1<\cdots<i_{2p}\le 2k} [(2\lambda(1+u^2) + 2u\cos(\theta)(1+\lambda^2)]^{2k-2p}(2u\sin(\theta))^{2p} \\
&\quad \times \mathrm{Tr}\,\left[(\sigma^z)^{i_1-1}\sigma^x((1+\lambda^2)\mathbf{1} + 2\lambda\sigma^z)(\sigma^z)^{i_2-i_1-1}\dots(\sigma^z)^{2k-i_{2p}}\right].
\end{aligned} \tag{2.26}$$

The factors $(1+\lambda^2)\mathbf{1}+2\lambda\sigma^z$ combine as in the one-chain case to give a factor $(1-\lambda^2)^{2p}$. As before the remaining traces yield the condition that each i_r must be even and the result is:

$$\begin{aligned}
\mathrm{Tr}\,(A\,B(\theta))^N &= 2\sum_{k=0}^{[N/2]} \binom{N}{2k} [(1+\lambda^2)(1+u^2) + 4\lambda u\cos(\theta)]^{N-2k} \\
&\quad \times \sum_{p=0}^{k} \binom{k}{p} [(2\lambda(1+u^2) + 2u\cos(\theta)(1+\lambda^2)]^{2k-2p} \\
&\quad \times (2u\sin(\theta))^{2p}(1-\lambda^2)^{2p}.
\end{aligned} \tag{2.27}$$

The sum over p can be evaluated to give

$$\begin{aligned} &\left\{[(2\lambda(1+u^2)+2u\cos(\theta)(1+\lambda^2)]^2+(2u\sin(\theta))^2(1-\lambda^2)^2\right\}^k \\ &= \left\{[(1+\lambda^2)(1+u^2)+4u\lambda\cos\theta]^2-(1-u^2)^2(1-\lambda^2)^2\right\}^k \\ &= \Delta(\theta)^k. \end{aligned} \tag{2.28}$$

Inserting this, the sum over k can be evaluated using the expansion (1.28) and yields the formula (2.23). ∎

Taking $\theta = 2\pi/3$ we obtain the contribution

$$(1+\lambda)^N(1+u)^N \sum_{\pm} \left[(1+\lambda^2)(1+u^2)-2u\lambda \pm \sqrt{\Delta_-}\right]^N, \tag{2.29}$$

where

$$\Delta_- = [(1+\lambda^2)(1+u^2)-2u\lambda]^2-(1-u^2)^2(1-\lambda^2)^2. \tag{2.30}$$

On the eigenspace of $\sigma^x \otimes \sigma^x \otimes \sigma^x$ with eigenvalue -1 there are similarly two invariant subspaces: that spanned by $|---\rangle$ and $\frac{1}{\sqrt{3}}(|++-\rangle+|+-+\rangle+|-++\rangle)$, and that consisting of the vectors $a_1|++-\rangle+a_2|+-+\rangle+a_3|-++\rangle$ with $a_1+a_2+a_3=0$. On the latter, the operator

$$B = (1+u)\left[(1-u+u^2)\mathbf{1}+u(\sigma_1^z\sigma_2^z+\sigma_2^z\sigma_3^z+\sigma_3^z\sigma_1^z)\right] \tag{2.31}$$

again reduces to

$$B_{-,odd} = (1+u)[(1-u+u^2)\mathbf{1}-u\mathbf{1}] = (1+u)(1-u)^2\,\mathbf{1}. \tag{2.32}$$

Moreover, A is diagonal on this space with degenerate eigenvalue $(1+\lambda)^2(1-\lambda)$. On this subspace, we therefore obtain the contribution $2(1+\lambda)^2(1-\lambda)(1+u)(1-u)^2$.

On the other subspace, the operator B reduces to

$$B_{-,even} = (1+u)[(1-u+u^2)\mathbf{1}+u(\mathbf{1}+\sigma^z)+\sqrt{3}u\sigma^x], \tag{2.33}$$

and A reduces to

$$A_{-,even} = (1-\lambda)[(1+\lambda^2)\mathbf{1}+2\lambda\sigma^z]. \tag{2.34}$$

On this subspace we therefore have to compute $(1+u)^N(1-\lambda)^N\times$

$$\mathrm{Tr}\left[\Big(((1+u^2)\mathbf{1}+u\sigma^z+\sqrt{3}u\sigma^x)((1+\lambda^2)\mathbf{1}+2\lambda\sigma^z)\Big)^N\right]. \qquad (2.35)$$

Using the lemma above with $\theta=\pi/3$ we get the contribution

$$(1-\lambda)^N(1+u)^N\sum_{\pm}\left[(1+\lambda^2)(1+u^2)+2u\lambda\pm\sqrt{\Delta_+}\right]^N, \qquad (2.36)$$

where

$$\Delta_+=[(1+\lambda^2)(1+u^2)+2u\lambda]^2-(1-u^2)^2(1-\lambda^2)^2. \qquad (2.37)$$

The complete result is thus

$$\begin{aligned}\tilde{Z}_{N,3} &= 2(1-u^2)^N(1-\lambda^2)^N(1-u)^N[(1+\lambda)^N+(1-\lambda)^N]\\ &\quad +(1+u)^N(1+\lambda)^N(\zeta_{1,+}^N+\zeta_{1,-}^N)\\ &\quad +(1+u)^N(1-\lambda)^N(\zeta_{2,+}^N+\zeta_{2,-}^N),\end{aligned} \qquad (2.38)$$

where

$$\zeta_{1,\pm}=(1+u^2)(1+\lambda^2)-2u\lambda\pm\sqrt{\Delta_-} \qquad (2.39)$$

and

$$\zeta_{2,\pm}=(1+u^2)(1+\lambda^2)+2u\lambda\pm\sqrt{\Delta_+}. \qquad (2.40)$$

In the thermodynamic limit we get

$$\begin{aligned}\lim_{N\to\infty}\frac{1}{N}\ln\tilde{Z}_{N,3} &= \ln(1+u)(1+\lambda)+\ln\Big[(1+\lambda^2)(1+u^2)-2\lambda u\\ &\quad +2\sqrt{(\lambda^2+u^2+\lambda u)(1+\lambda^2u^2+\lambda u)}\Big].\end{aligned} \qquad (2.41)$$

2.3 The Ising model on a four-stranded chain

The B-operator now reads

$$B=(\mathbf{1}+u\sigma_1^z\sigma_2^z)(\mathbf{1}+u\sigma_2^z\sigma_3^z)(\mathbf{1}+u\sigma_3^z\sigma_4^z)(\mathbf{1}+u\sigma_4^z\sigma_1^z). \qquad (2.42)$$

We consider again the eigenspaces of $\sigma^x\otimes\sigma^x\otimes\sigma^x\otimes\sigma^x$. The eigenspace with eigenvalue $+1$ now splits into a 4-dimensional space spanned by $|++++\rangle$,

$\frac{1}{2}(|++--\rangle+|-++-\rangle+|--++\rangle+|+--+\rangle)$, $\frac{1}{\sqrt{2}}(|+-+-\rangle+|-+-+\rangle)$ and $|----\rangle$, a 3-dimensional space of vectors $a_1|++--\rangle+a_2|-++-\rangle+a_3|--++\rangle+a_4|+--+\rangle$ with $a_1+a_2+a_3+a_4=0$ and a one-dimensional space spanned by $\frac{1}{\sqrt{2}}(|+-+-\rangle-|-+-+\rangle)$. On the latter the operator B reduces to $(1-u^2)^2\mathbf{1}$ and A has eigenvalue $(1-\lambda^2)^2$ so that the contribution is $(1-u^2)^2(1-\lambda^2)^2$. On the second space B also reduces to $(1-u^2)^2\mathbf{1}$ and A also has eigenvalue $(1-\lambda^2)^2$ so the contribution is $3(1-u^2)^2(1-\lambda^2)^2$.

Finally consider the first subspace. On this space B has the matrix representation

$$B = \begin{pmatrix} 1+u^4 & 2u(1+u^2) & 2\sqrt{2}u^2 & 2u^2 \\ 2u(1+u^2) & 1+u^4+6u^2 & 2\sqrt{2}u(1+u^2) & 2u(1+u^2) \\ 2\sqrt{2}u^2 & 2\sqrt{2}u(1+u^2) & 1+u^4+2u^2 & 2\sqrt{2}u^2 \\ 2u^2 & 2u(1+u^2) & 2\sqrt{2}u^2 & 1+u^4 \end{pmatrix}. \tag{2.43}$$

We change basis by multiplying left and right by the unitary matrix

$$U = U^* = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2.44}$$

The resulting matrix is

$$U\,B\,U = \begin{pmatrix} 1+u^4 & \sqrt{2}u(1+\sqrt{2}u+u^2) & \sqrt{2}u(1-\sqrt{2}u+u^2) & 2u^2 \\ \sqrt{2}u(1+\sqrt{2}u+u^2) & 1+\sqrt{2}u+4u^2+\sqrt{2}u^3+u^4 & 2u^2 & \sqrt{2}u(1+\sqrt{2}u+u^2) \\ \sqrt{2}u(1-\sqrt{2}u+u^2) & 2u^2 & 1-\sqrt{2}u+4u^2-\sqrt{2}u^3+u^4 & \sqrt{2}u(1-\sqrt{2}u+u^2) \\ 2u^2 & \sqrt{2}u(1+\sqrt{2}u+u^2) & \sqrt{2}u(1-\sqrt{2}u+u^2) & 1+u^4 \end{pmatrix} \tag{2.45}$$

This can be written as

$$\begin{aligned} U\,B\,U &= \begin{pmatrix} 1+\sqrt{2}u+u^2 & \sqrt{2}u \\ \sqrt{2}u & 1-\sqrt{2}u+u^2 \end{pmatrix} \\ &\qquad \otimes \begin{pmatrix} 1-\sqrt{2}u+u^2 & \sqrt{2}u \\ \sqrt{2}u & 1+\sqrt{2}u+u^2 \end{pmatrix} \\ &= \big((1+u^2)\mathbf{1}+\sqrt{2}\sigma^z+\sqrt{2}\sigma^x\big)\otimes\big((1+u^2)\mathbf{1}-\sqrt{2}\sigma^z+\sqrt{2}\sigma^x\big). \end{aligned} \tag{2.46}$$

Notice that the matrix of A is unaffected by the transformation U and can be written as

$$A = \big((1+\lambda^2)\mathbf{1}+2\lambda\sigma^z\big)\otimes\big((1+\lambda^2)\mathbf{1}+2\lambda\sigma^z\big). \tag{2.47}$$

We can thus apply the lemma to both factors and obtain the contribution

$$\begin{aligned} \mathrm{Tr}\,(A\,B_{+,even})^N &= \left(\sum_{\pm}\left[(1+\lambda^2)(1+u^2)+2\sqrt{2}u\lambda\pm\sqrt{\Delta(\frac{\pi}{4})}\right]^N\right) \\ &\qquad \times\left(\sum_{\pm}\left[(1+\lambda^2)(1+u^2)-2\sqrt{2}u\lambda\pm\sqrt{\Delta(\frac{3\pi}{4})}\right]^N\right), \end{aligned} \tag{2.48}$$

where

$$\Delta(\frac{\pi}{4}) = [(1+\lambda^2)(1+u^2)+2\sqrt{2}u\lambda]^2-(1-u^2)^2(1-\lambda^2)^2 \tag{2.49}$$

and

$$\Delta(\frac{3\pi}{4}) = [(1+\lambda^2)(1+u^2)-2\sqrt{2}u\lambda]^2-(1-u^2)^2(1-\lambda^2)^2. \tag{2.50}$$

The representation (2.46) can in fact be derived more simply as follows. We have obtained B as

$$\begin{aligned} \cosh(\beta J_2)^4 B &= \exp[\beta J_2 B_0], \text{ where} \\ B_0 &= \sigma_1^z\sigma_2^z+\sigma_2^z\sigma_3^z+\sigma_3^z\sigma_4^z+\sigma_4^z\sigma_1^z. \end{aligned} \tag{2.51}$$

On the 4-dimensional subspace B_0 acts as follows.

$$B_0 = \begin{pmatrix} 0 & 2 & 0 & 0 \\ 2 & 0 & 2\sqrt{2} & 2 \\ 0 & 2\sqrt{2} & 0 & 0 \\ 0 & 2 & 0 & 0 \end{pmatrix}.$$

To bring this into the form $B_1 \otimes \mathbf{1} + \mathbf{1} \otimes B_2$ where $B_i = \begin{pmatrix} a_i & b_i \\ b_i & c_i \end{pmatrix}$, using an orthogonal matrix of the form affecting only the states with total spin 0, we write

$$B_1 \otimes \mathbf{1} + \mathbf{1} \otimes B_2 = \begin{pmatrix} a_1 + a_2 & b_2 & b_1 & 0 \\ b_2 & a_1 + c_2 & 0 & b_1 \\ b_1 & 0 & c_1 + a_2 & b_2 \\ 0 & b_1 & b_2 & c_1 + c_2 \end{pmatrix}.$$

It follows that we must diagonalize the centre matrix, i.e. $\begin{pmatrix} 0 & 2\sqrt{2} \\ 2\sqrt{2} & 0 \end{pmatrix}$, which leads to the unitary matrix U above. We obtain

$$UB_0U = \begin{pmatrix} 0 & \sqrt{2} & \sqrt{2} & 0 \\ \sqrt{2} & 2\sqrt{2} & 0 & \sqrt{2} \\ \sqrt{2} & 0 & -2\sqrt{2} & \sqrt{2} \\ 0 & \sqrt{2} & \sqrt{2} & 0 \end{pmatrix}$$

and hence

$$B_1 = \begin{pmatrix} \sqrt{2} & \sqrt{2} \\ \sqrt{2} & -\sqrt{2} \end{pmatrix} = \sqrt{2}(\sigma^x + \sigma^z)$$

and

$$B_2 = \begin{pmatrix} -\sqrt{2} & \sqrt{2} \\ \sqrt{2} & \sqrt{2} \end{pmatrix} = \sqrt{2}(\sigma^x - \sigma^z).$$

Now, $\sigma^x \pm \sigma^z = \sqrt{2} U_\pm \sigma^z U_\pm$ for some orthogonal matrices $U_\pm$, so

$$\begin{aligned} \exp(\beta J_2 \sqrt{2}(\sigma^x \pm \sigma^z)) &= U_\pm(\cosh(2\beta J_2) + \sinh(2\beta J_2)\sigma^z)U_\pm \\ &= \cosh(2\beta J_2)\mathbf{1} + \frac{1}{\sqrt{2}}(\sigma^x \pm \sigma^z)\sinh(2\beta J_2) \\ &= \cosh^2(\beta J_2)[(1 + \tanh^2(\beta J_2))\mathbf{1} + \sqrt{2}\tanh(\beta J_2)(\sigma^x \pm \sigma^z)]. \end{aligned} \tag{2.52}$$

This implies (2.46).

Next consider the eigenspace with eigenvalue -1. This space decomposes into two two-dimensional spaces and four one-dimensional spaces. The first two-dimensional space is spanned by the vectors

$$\frac{1}{2}(|+++-\rangle + |++-+\rangle + |+-++\rangle + |-+++\rangle)$$

and

$$\frac{1}{2}(|+---\rangle + |-+--\rangle + |--+-\rangle + |---+\rangle);$$

the second is spanned by the vectors

$$\frac{1}{2}(|+++-\rangle - |++-+\rangle + |+-++\rangle - |-+++\rangle)$$

and

$$\frac{1}{2}(|+---\rangle - |-+--\rangle + |--+-\rangle - |---+\rangle).$$

The one-dimensional spaces are spanned by the vectors

$$\frac{1}{2}(|+++-\rangle - |+-++\rangle \pm (|++-+\rangle - |-+++\rangle))$$

and

$$\frac{1}{2}(|+---\rangle - |--+-\rangle \pm (|-+--\rangle - |---+\rangle))$$

respectively.

On the first space the operator B reduces to

$$\begin{aligned} B_{\mathrm{red},1} &= (1+u^4)\mathbf{1} + 2u(1+u^2)(\mathbf{1}+\sigma^x) + 2u^2(\mathbf{1}+2\sigma^x) \\ &= (1+u)^2\left[(1+u^2)\mathbf{1} + 2u\sigma^x\right]. \end{aligned} \tag{2.53}$$

The operator A on the other hand reduces to

$$A_{\mathrm{red},1} = (1-\lambda^2)[(1+\lambda^2)\mathbf{1} + 2\lambda\sigma^z]. \tag{2.54}$$

We can thus apply the lemma with $\theta = \pi/2$ to obtain the contribution

$$(1+u)^{2N}(1-\lambda^2)^N \sum_{\pm} \left[(1+\lambda^2)(1+u^2) \pm \sqrt{\Delta(\pi/2)}\right]^N, \tag{2.55}$$

where

$$\Delta(\pi/2) = [(1+\lambda^2)(1+u^2)]^2 - (1-\lambda^2)^2 1 - u^2)^2 = 4u^2(1+\lambda^4) + 4\lambda^2(1+u^4). \tag{2.56}$$

Similarly, on the second space, B reduces to

$$\begin{aligned} B_{\mathrm{red},2} &= (1+u^4)\mathbf{1} - 2u(1+u^2)(\mathbf{1} - \sigma^x) + 2u^2(\mathbf{1} - 2\sigma^x) \\ &= (1-u)^2\left[(1+u^2)\mathbf{1} + 2u\sigma^x\right]. \end{aligned} \tag{2.57}$$

and A reduces to

$$A_{\mathrm{red},2} = (1-\lambda^2)[(1+\lambda^2)\mathbf{1} + 2\lambda\sigma^z] \tag{2.58}$$

as before. The resulting contribution is

$$(1-u)^{2N}(1-\lambda^2)^N \sum_{\pm}\left[(1+\lambda^2)(1+u^2) \pm \sqrt{\Delta(\pi/2)}\right]^N. \tag{2.59}$$

On the one-dimensional spaces, B reduces to $(1-u^2)^2\mathbf{1}$. On the first two spaces, $A = (1+\lambda)^3(1-\lambda)$, on the other two, $A = (1+\lambda)(1-\lambda)^3$. We thus obtain the contributions

$$2(1-u^2)^{2N}(1-\lambda^2)^N\,[(1+\lambda)^{2N} + (1-\lambda)^{2N}]. \tag{2.60}$$

In total, we obtain the following expression for $\tilde{Z}_{N,4}$.

$$\begin{aligned} \tilde{Z}_{N,4} &= 4\rho^{2N} + 2\rho^N\gamma_{N,-} + \gamma_{N,+}(\zeta_{2,+}^N + \zeta_{2,-}^N) \\ &\quad +(\zeta_{1,+}^N + \zeta_{1,-}^N)(\zeta_{3,+}^N + \zeta_{3,-}^N), \end{aligned} \tag{2.61}$$

where

$$\rho = (1-u^2)(1-\lambda^2), \tag{2.62}$$

and

$$\begin{aligned} \gamma_{N,+} &= (1-\lambda^2)^N[(1+u)^{2N} + (1-u)^{2N}] \\ \gamma_{N,-} &= (1-u^2)^N[(1+\lambda)^{2N} + (1-\lambda)^{2N}], \end{aligned} \tag{2.63}$$

and

$$\zeta_{j,\pm} = \zeta_\pm(j\pi/4) = (1+u^2)(1+\lambda^2) - 4u\lambda\cos\frac{j\pi}{4} \pm \sqrt{\Delta(j\pi/4)}. \tag{2.64}$$

In the thermodynamic limit,

$$\lim_{N\to\infty}\ln\tilde{Z}_{N,4} = \ln\zeta_{1,+} + \ln\zeta_{3,+}. \tag{2.65}$$

3 The 2-dimensional Ising model

The general case with M chains is of course equivalent to the 2-dimensional Ising model. To generalize the above approach, we want to transform B into a tensor product of 2-dimensional matrices. Equivalently, since $\cosh(\beta J_2)^M B = \exp(\beta J_2 B_0)$, we need to find a transformation such that B_0 has the form

$$B_0 = \sum_{i=1}^{[M/2]} B_i, \text{ where } B_i = \mathbf{1} \otimes \cdots \otimes \begin{pmatrix} a_i & b_i \\ b_i & -a_i \end{pmatrix} \otimes \cdots \otimes \mathbf{1}.$$

(Here the matrix $\begin{pmatrix} a_i & b_i \\ b_i & -a_i \end{pmatrix}$ is at the i-th position.)

Note that $A = \bigotimes_{i=1}^M (\mathbf{1} + \lambda \sigma_i^x) = \frac{1}{\cosh(\gamma)^M} e^{\gamma \oplus_{i=1}^M \sigma_i^x}$ if $\lambda = \tanh(\gamma)$. Therefore we can subdivide the Hilbert space $\mathcal{H} = \mathbb{C}^{2^M}$ into subspaces $\mathcal{H}_n$ where $\oplus_{i=1}^M \sigma_i^x$ has eigenvalue $M - 2n$ with $n \leq M/2$, i.e. in the representation in which σ^x is diagonal, the number of minuses equals n. On the subspace $\mathcal{H}_n$, A has the eigenvalue $(1+\lambda)^{M-n}(1-\lambda)^n$. We can therefore diagonalize the restriction $\tilde{B}_0$ of B_0 to each $\mathcal{H}_n$ as we did in the case $M = 4$ above. This does not affect the matrix A. Note also that B_0 only connects $\mathcal{H}_n$ with $\mathcal{H}_{n-2}$ and $\mathcal{H}_{n+2}$. We shall see below that the connections are in fact more restricted.

In order to diagonalize $\tilde{B}_0$ on $\mathcal{H}_n$ we need a more general approach. Consider first again the case of 2 negative signs ($n = 2$). We restrict ourselves to the translation-invariant states. For the case of 8 linked chains for example, $\mathcal{H}_{n,\mathrm{sym}}$ is spanned by

$$\begin{aligned}
\psi_{+,1} &= \frac{1}{\sqrt{8}} \sum_{k=0}^{7} \tau^k |+ + + + + + - -\rangle, \\
\psi_{+,2} &= \frac{1}{\sqrt{8}} \sum_{k=0}^{7} \tau^k |+ + + + + - + -\rangle, \\
\psi_{+,3} &= \frac{1}{\sqrt{8}} \sum_{k=0}^{7} \tau^k |+ + + + - + + -\rangle \text{ and} \\
\psi_{+,4} &= \frac{1}{2} \sum_{k=0}^{3} \tau^k |+ + + - + + + -\rangle, \qquad (3.1)
\end{aligned}$$

where τ is the (periodized) translation operator. (For example, $\tau|++++++--\rangle = |-++++++-\rangle$.) The matrix $\tilde{B}$ acts as follows: $\tilde{B}\psi_{+,1} = 2\psi_{+2}$; $\tilde{B}\psi_{+,2} = 2\psi_{+,1} + 2\psi_{+,3}$; $\tilde{B}\psi_{+,3} = 2\psi_{+,2} + 2\sqrt{2}\psi_{+,4}$; $\tilde{B}\psi_{+,4} = 2\sqrt{2}\psi_{+,3}$, i.e. the matrix is

$$\tilde{B} = 2\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{2} \\ 0 & 0 & \sqrt{2} & 0 \end{pmatrix}.$$

The factor $\sqrt{2}$ is obviously due to the normalization of $\psi_{+,4}$. Replacing $\psi_{+,4}$ by $\psi'_{+,4} = \sqrt{2}\psi_{+,4}$ the matrix becomes

$$\tilde{B}' = 2\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 2 & 0 \end{pmatrix}.$$

We can rewrite the eigenvalue equation as

$$2\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_3 \\ v_2 \\ v_1 \end{pmatrix} = \lambda\begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_3 \\ v_2 \\ v_1 \end{pmatrix}.$$

The latter matrix can be diagonalized by Fourier transformation, but with a zero boundary condition, i.e. setting $v_k = \omega^k - \omega^{-k}$ ($k = 1, \ldots, 7$). Then

$$2\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \end{pmatrix} = 2(\omega + \omega^{-1})\begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \\ v_5 \\ v_6 \\ v_7 \end{pmatrix}$$

provided $\omega^{16} = 1$. But $v_5 = v_3$, i.e. $\omega^5 - \omega^{-5} = \omega^3 - \omega^{-3}$, if $\omega^4 + \omega^2 + 1 + \omega^{-2} + \omega^{-4} = \omega^2 + 1 + \omega^{-2}$, so $\omega^4 + \omega^{-4} = 0$, i.e. $\omega^8 = -1$. In that case also $\omega^6 - \omega^{-6} = \omega^2 - \omega^{-2}$ and $\omega^7 - \omega^{-7} = \omega - \omega^{-1}$. Taking the renormalization of $\psi_{+,4}$ into account, the eigenvectors of $\tilde{B}$ are given by $(\omega - \omega^{-1}, \omega^2 - \omega^{-2}, \omega^3 - \omega^{-3}, \frac{1}{\sqrt{2}}(\omega^4 - \omega^{-4}))^T$, where $\omega = e^{(2j-1)\pi/8}$, where $j = 1, 2, 3, 4$. (Note that replacing ω by $\overline{\omega}$ one obtains the same eigenvector but with opposite sign.) Normalizing the vectors and multiplying by i, we obtain the following unitary matrix.

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} \sin\frac{\pi}{8} & \sin\frac{3\pi}{8} & \sin\frac{3\pi}{8} & \sin\frac{\pi}{8} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \sin\frac{3\pi}{8} & -\sin\frac{\pi}{8} & -\sin\frac{\pi}{8} & \sin\frac{3\pi}{8} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}. \tag{3.2}$$

This easily generalizes to arbitrary M.

3.1 Bethe Ansatz approach

In the case of higher numbers of minus signs $n > 2$, there are more boundary conditions, corresponding to the case where several minuses are adjacent. This can be solved using the Bethe Ansatz.

Note that the introduction of a factor $\sqrt{2}$ in $\psi_{+,4}$ above just corresponds to the different normalization of $\psi_{+,4}$, which has only 4 terms rather than the 8 terms of the other basis vectors. This suggests that we need to introduce the Fourier transform for the original basis vectors, but with equal coefficients for translates. Moreover, the boundary conditions generalize to the case of higher numbers of minus signs. To deal with this , let $\varphi(x_1, \dots, x_n)$ denote the basis vector with minus signs at the positions $x_1, \dots, x_n$, where $1 \le x_1 < \cdots < x_n \le M$. We write the eigenvectors as

$$\psi = \sum_{1 \le x_1 < \cdots < x_n \le M} f(x_1, \dots, x_n)\, \varphi(x_1, \dots, x_n). \tag{3.3}$$

In the case $n = 2$ we then put

$$f(x_1, x_2) = A\omega_1^{x_1}\omega_2^{x_2} + B\omega_1^{x_2}\omega_2^{x_1}, \tag{3.4}$$

where ω_1, ω_2 and the ratio of the coefficients A and B have to be determined. We first write the general expression for $\tilde{B}_n$ on the n-particle space:

$$\begin{aligned}\tilde{B}_n f(x_1, \ldots, x_n) &= \sum_{i=1}^{n} (1 - \delta_{x_i - x_{i-1},1})\, f(x_1, \ldots, x_i - 1, \ldots, x_n) \\ &\quad + \sum_{i=1}^{n} (1 - \delta_{x_{i+1} - x_i,1})\, f(x_1, \ldots, x_i + 1, \ldots, x_n) \\ &\quad + \delta_{x_1,1}(1 - \delta_{x_n,M})\, f(x_2, \ldots, x_n, M) \\ &\quad + \delta_{x_n,M}(1 - \delta_{x_1,1})\, f(1, x_1, \ldots, x_{n-1}), \end{aligned} \tag{3.5}$$

where we set $x_0 = 0$ and $x_{n+1} = M + 1$.

3.1.1 The case $n = 2$

Let us apply this to the Bethe Ansatz expression (3.4). Assuming first $1 < x_1 < x_2 - 1 < M - 1$, we see easily that

$$\tilde{B}_2 f(x_1, x_2) = \lambda\, f(x_1, x_2), \text{ where } \lambda = \omega_1 + \omega_1^{-1} + \omega_2 + \omega_2^{-1}.$$

We then have to consider the boundary conditions. First assume $x_2 = x_1 + 1 < M$ and $x_1 > 1$. Then

$$\begin{aligned}\tilde{B}_2 f(x_1, x_1 + 1) &= A\omega_1^{x_1-1}\omega_2^{x_1+1} + B\omega_2^{x_1-1}\omega_1^{x_1+1} \\ &\quad + A\omega_1^{x_1}\omega_2^{x_1+2} + B\omega_2^{x_1}\omega_1^{x_1+2}.\end{aligned}$$

For this to equal $\lambda\, f(x_1, x_1 + 1)$ we need the missing terms to add to 0, i.e.

$$(\omega_1 + \omega_2^{-1})A\omega_1^{x_1}\omega_2^{x_1+1} + (\omega_1^{-1} + \omega_2)B\omega_1^{x_1+1}\omega_2^{x_1} = 0,$$

i.e. $(\omega_1\omega_2 + 1)(A + B) = 0$. Thus $\omega_1\omega_2 = -1$ and $\lambda = 0$ or $A + B = 0$.

Next consider the case that $1 < x_1 < M - 1$ and $x_2 = M$. In that case

$$\begin{aligned}\tilde{B}_2 f(x_1, M) &= A\omega_1^{x_1}\omega_2^{M}(\omega_1 + \omega_1^{-1}) + B\omega_2^{x_1}\omega_1^{M}(\omega_2 + \omega_2^{-1}) \\ &\quad + A\omega_1^{x_1}\omega_2^{M-1} + A\omega_1\omega_2^{x_1} + B\omega_2^{x_1}\omega_1^{M-1} + B\omega_2\omega_1^{x_1}.\end{aligned}$$

This equals $\lambda\, f(x_1, M)$ provided

$$A\omega_1\omega_2^{x_1} + B\omega_2\omega_1^{x_1} = A\omega_1^{x_1}\omega_2^{M+1} + B\omega_2^{x_1}\omega_1^{M+1}.$$

If $A+B=0$ this leads to

$$\omega_1\omega_2^{x_1}-\omega_2\omega_1^{x_1}=\omega_1^{x_1}\omega_2^{M+1}-\omega_2^{x_1}\omega_1^{M+1},$$

so

$$\left(\frac{\omega_1}{\omega_2}\right)^{x_1-1}=\frac{1+\omega_1^M}{1+\omega_2^M}\text{ or }\omega_2^M=-1.$$

Since $\omega_1\neq\omega_2$ and x_1 is arbitrary, we conclude that $\omega_1^M=\omega_2^M=-1$.

If $\omega_1\omega_2=-1$ and $\lambda=0$ then we have

$$f(x_1,x_2)=A\omega_1^{x_1-x_2}(-1)^{x_2}+B\omega_1^{x_2-x_1}(-1)^{x_1},$$

and the boundary condition becomes

$$A((-1)^{x_1}\omega_1^{1-x_1}+(-1)^M\omega_1^{x_1-M-1})=B(\omega_1^{x_1-1}+(-1)^{x_1}\omega_1^{M+1-x_1})$$

or

$$(A-B\omega_1^M)(-1)^{x_1}\omega_1^{1-x_1}+(A(-1)^M\omega_1^{-M}-B)\omega_1^{x_1-1}=0.$$

Again, since x_1 is arbitrary, we need $A=B\omega_1^M=(-1)^MB\omega_1^M$, and in particular M must be even.

Similarly, if $x_1=1$ and $2<x_2<M$, we have the condition

$$A\omega_1^{x_2}\omega_2^M+B\omega_2^{x_2}\omega_1^M=A\omega_2^{x_2}+B\omega_1^{x_2}.$$

If $A+B=0$ this again implies $\omega_1^M=\omega_2^M=-1$. If $\omega_1\omega_2=-1$, we obtain

$$(A(-1)^M\omega_1^{-M}-B)\omega_1^{x_2}=(A-B\omega_1^M)(-1)^{x_2}\omega_1^{-x_2}$$

and hence $A=(-1)^M\omega_1^MB=\omega_1^MB$ as above.

Finally, the case $x_1=1$ and $x_2=M$ we have $(1+\omega_1\omega_2)\omega^M=(1+\omega_1\omega_2)\omega_1^M$ and hence $\omega_1^M=\omega_2^M$ or $\omega_1\omega_2=-1$, i.e. it does not lead to any new conditions.

In the first case we therefore obtain the eigenfunctions

$$\sum_{1\leq x_1<x_2\leq M}f(x_1,x_2)\,\varphi(x_1,x_2),$$

where

$$f(x_1,x_2) = \omega_1^{x_1}\omega_2^{x_2} - \omega_2^{x_1}\omega_1^{x_2}, \tag{3.6}$$

and where $\omega_1 \neq \omega_2$ are M-th roots of -1. There are obviously exactly $\frac{1}{2}M(M-1)$ such pairs of roots. We compute the scalar products of functions f and g of this form:

$$\begin{aligned}
\langle f\,|\,g\rangle &= \sum_{1\le x_1<x_2\le M} (\overline{\omega}_1^{x_1}\overline{\omega}_2^{x_2} - \overline{\omega}_2^{x_1}\overline{\omega}_1^{x_2})((\omega_1')^{x_1}(\omega_2')^{x_2} - (\omega_2')^{x_1}(\omega_1')^{x_2}) \\
&= \frac{1}{2}\sum_{x_1,x_2=1}^{M} (\overline{\omega}_1^{x_1}\overline{\omega}_2^{x_2} - \overline{\omega}_2^{x_1}\overline{\omega}_1^{x_2})((\omega_1')^{x_1}(\omega_2')^{x_2} - (\omega_2')^{x_1}(\omega_1')^{x_2}) \\
&= \sum_{x_1,x_2=1}^{M} (\overline{\omega}_1^{x_1}\overline{\omega}_2^{x_2}(\omega_1')^{x_1}(\omega_2')^{x_2} - \overline{\omega}_2^{x_1}\overline{\omega}_1^{x_2}(\omega_1')^{x_1}(\omega_2')^{x_2}) \\
&= M^2(\delta_{\overline{\omega_1}\omega_1',1}\delta_{\overline{\omega_2}\omega_2',1} - \delta_{\overline{\omega_2}\omega_1',1}\delta_{\overline{\omega_1}\omega_2',1}) \\
&= M^2(\delta_{\omega_1,\omega_1'}\delta_{\omega_2,\omega_2'} - \delta_{\omega_2,\omega_1'}\delta_{\omega_1,\omega_2'}).
\end{aligned}$$

Assuming a given ordering of the M-th roots of -1, the eigenfunctions are therefore orthogonal and should be normalized with a factor $1/M$. These eigenfunctions then form an orthonormal basis for a $\frac{1}{2}M(M-1)$-dimensional space, and since the space spanned by $\varphi(x_1,x_2)$ with $1 \le x_1 < x_2 \le M$ is also $\frac{1}{2}M(M-1)$-dimensional, these functions already span this space. The other eigenfunctions obtained in case $\omega_1\omega_2 = -1$ must therefore be linear combinations of the functions (3.6). To see this explicitly, note that the former are of the form

$$f(x_1,x_2) = (-1)^{x_2}\lambda^{M+x_1-x_2} + (-1)^{x_1}\lambda^{x_2-x_1},$$

where M is even and $\lambda \neq 0$ is arbitrary. This only depends on $x_2 - x_1$ and the sign of $(-1)^{x_2}$. Moreover, if $x_2 - x_1 > M/2$ then $x_1 < M/2$ and $x_2 > M/2$, so we can set $x_2' = x_1 + M/2$ and $x_1' = x_2 - M/2$. Then

$$f(x_1',x_2') = (-1)^{x_1+M/2}\lambda^{x_2-x_1} + (-1)^{x_2-M/2}\lambda^{M+x_1-x_2} = (-1)^{M/2}f(x_1,x_2).$$

It follows that there are $M/2$ independent values, i.e. these functions span an $M/2$-dimensional space. A basis for this space is obtained by taking $\lambda = e^{(2j-1)\pi i/M}$ with $j = 1,\ldots,M/2$. Then $\lambda^M = -1$ and we can write

$$f(x_1,x_2) = (-1)^{x_2}\lambda^{x_1-x_2} - (-1)^{x_1}\lambda^{x_2-x_1},$$

where we have also multiplied by a minus sign. This is exactly of the form (3.6) with $\omega_1 = \lambda$ and $\omega_2 = -\lambda^{-1}$. (Note that this also proves that these functions are orthogonal and hence indeed form a basis for the $M/2$-dimensional space.)

To summarize, the functions

$$f(x_1, x_2) = \frac{1}{M}(\omega_1^{x_1}\omega_2^{x_2} - \omega_2^{x_1}\omega_1^{x_2}) \tag{3.7}$$

form an orthonormal basis for $\mathcal{H}_2$. Moreover, the translation-invariant eigenfunctions are given by those where $\omega_2 = \overline{\omega_1}$. Indeed,

$$f(x_1+1, x_2+1) = \omega_1^{x_1+1}\omega_2^{x_2+1} - \omega_2^{x_1+1}\omega_1^{x_2+1} = \omega_1\omega_2 f(x_1, x_2),$$

so we need $\omega_1\omega_2 = 1$.

3.1.2 Higher numbers of minuses

For larger numbers of minuses we put

$$f(x_1, \dots, x_n) = \sum_{P \in \mathcal{S}_n} A(P) \prod_{j=1}^{n} \omega_{P(j)}^{x_j}. \tag{3.8}$$

If $x_{j+1} > x_j - 1$ for all $j = 0, \dots, n$, then we get

$$\tilde{B}_n f(x_1, \dots, x_n) = \lambda\, f(x_1, \dots, x_n); \qquad \lambda = \sum_{j=1}^{n}(\omega_j + \omega_j^{-1}).$$

If $x_{j+1} = x_j$ for some j then the missing terms must vanish:

$$\sum_{P \in \mathcal{S}_n} A(P) \prod_{i=1}^{n} \omega_{P(i)}^{x_i}(\omega_{P(j)} + \omega_{P(j+1)}^{-1}) = 0.$$

Combining P with $P(j) = p$, $P(j+1) = q$ and P' with $P'(j) = q$, $P'(j+1) = p$, we have the condition

$$A(P)(\omega_p + \omega_q^{-1})\omega_p^{x_j}\omega_q^{x_j+1} + A(P')(\omega_q + \omega_p^{-1})\omega_q^{x_j}\omega_p^{x_j+1} = 0,$$

which holds if either $\omega_p\omega_q = -1$, or $A(P) + A(P') = 0$. Moreover, if $x_n = M$, we have

$$\begin{aligned}
&\tilde{B}_n f(x_1, \dots, x_{n-1}, M) \\
&\quad = \sum_{P\in\mathcal{S}_n} A(P) \left\{ \prod_{j=1}^{n-1} \omega_{P(j)}^{x_j} \left(\sum_{k=1}^{n-1} (\omega_{P(k)} + \omega_{P(k)}^{-1}) \omega_{P(n)}^{-1} \right) \omega_{P(n)}^{M} \right. \\
&\quad \left. \sum_{P\in\mathcal{S}_n} A(P) \left(\prod_{j=1}^{n-1} \omega_{P(j)}^{x_j} \omega_{P(n)}^{M-1} + \omega_{P(1)} \prod_{j=1}^{n-1} \omega_{P(j+1)}^{x_j} \right) \right\}.
\end{aligned}$$

We therefore have the condition

$$\sum_{P\in\mathcal{S}_n} A(P) \prod_{j=1}^{n-1} \omega_{P(j+1)}^{x_j} \omega_{P(1)} = \sum_{P\in\mathcal{S}_n} A(P) \prod_{j=1}^{n-1} \omega_{P(j)}^{x_j} \omega_{P(n)}^{M+1}.$$

For $P = (p_1, \dots, p_n)$ and $P' = (p_n, p_1, \dots, p_{n-1})$ we get $A(P') \prod_{j=1}^{n-1} \omega_{p_j}^{x_j} \omega_{p_n} = A(P) \prod_{j=1}^{n-1} \omega_{p_j}^{x_j} \omega_{p_n}^{M+1}$. Therefore $\omega_{p_n}^M = (-1)^{n-1}$. The eigenfunctions therefore are given by

$$f(x_1, \dots, x_n) = \sum_{P\in\mathcal{S}_n} (-1)^{|P|} \prod_{j=1}^{n} \omega_{P(j)}^{x_j}, \tag{3.9}$$

where the ω_i ($i = 1, \dots, n$) are distinct M-th roots of $(-1)^{n-1}$. For translation-invariant states we have in addition that $\prod_{i=1}^n \omega_i = 1$.

Example 3.1: $M = 8$; $n = 4$. For $n = 4$, the ω_j are 8-th roots of -1. These are $e^{\pm\pi i/8}, e^{\pm 3\pi i/8}, e^{\pm 5\pi i/8}$ and $e^{\pm 7\pi i/8}$. Denote $\omega_j = e^{(2j-1)\pi i/8}$ ($j = 1, 3, 5, 7$). The possible quadruples satisfying the condition $\prod \omega_i = 1$ are

$$\begin{array}{ll}
(\omega_1, \omega_2, \omega_3, \omega_4), & (\omega_1, \omega_2, \overline{\omega_2}, \overline{\omega_1}) \\
(\omega_1, \omega_3, \overline{\omega_3}, \overline{\omega_1}), & (\omega_1, \omega_4, \overline{\omega_3}, \overline{\omega_2}) \\
(\omega_1, \omega_4, \overline{\omega_4}, \overline{\omega_1}), & (\omega_2, \omega_3, \overline{\omega_4}, \overline{\omega_1}) \\
(\omega_2, \omega_3, \overline{\omega_3}, \overline{\omega_2}), & (\omega_2, \omega_4, \overline{\omega_4}, \overline{\omega_2}) \\
(\omega_3, \omega_4, \overline{\omega_4}, \overline{\omega_3}), & (\overline{\omega_4}, \overline{\omega_3}, \overline{\omega_2}, \overline{\omega_1}).
\end{array}$$

There are exactly 10 states, corresponding to the 10-dimensional space considered previously. There are 4 states with non-zero eigenvalues: $(\omega_1, \omega_2, \overline{\omega_2}, \overline{\omega_1})$,

$(\omega_1, \omega_3, \overline{\omega_3}, \overline{\omega_1})$, $(\omega_2, \omega_4, \overline{\omega_4}, \overline{\omega_2})$ and $(\omega_3, \omega_4, \overline{\omega_4}, \overline{\omega_3})$ with eigenvalues

$$\begin{aligned} 2(\omega_1 + \overline{\omega_1}) + 2(\omega_2 + \overline{\omega_2}) &= \lambda_1 + \lambda_2, \\ 2(\omega_1 + \overline{\omega_1}) + 2(\omega_3 + \overline{\omega_3}) &= \lambda_1 - \lambda_2, \\ 2(\omega_2 + \overline{\omega_2}) + 2(\omega_4 + \overline{\omega_4}) &= -\lambda_1 + \lambda_2, \\ 2(\omega_3 + \overline{\omega_3}) + 2(\omega_4 + \overline{\omega_4}) &= -\lambda_1 - \lambda_2. \end{aligned}$$

(Here $\lambda_1 = 4\cos\frac{\pi}{8}$ and $\lambda_2 = 4\cos\frac{3\pi}{8}$.)

We compute the scalar products:

$$\begin{aligned} \langle f \,|\, g \rangle &= \sum_{1 \le x_1 < \cdots < x_n \le M} \sum_{P,Q \in \mathcal{S}_n} (-1)^{|P|+|Q|} \prod_{j=1}^{n} (\overline{\omega_{P(j)}})^{x_j} (\omega'_{Q(j)})^{x_j} \\ &= \frac{1}{n!} \sum_{x_1,\ldots,x_n=1}^{M} \sum_{P,Q \in \mathcal{S}_n} (-1)^{|P|+|Q|} \prod_{j=1}^{n} (\overline{\omega_{P(j)}})^{x_j} (\omega'_{Q(j)})^{x_j} \\ &= \frac{1}{n!} M^n \sum_{P,Q \in \mathcal{S}_n} (-1)^{|P|+|Q|} \prod_{j=1}^{n} \delta_{\overline{\omega_{P(j)}}\omega'_{Q(j)},1} \\ &= M^n \sum_{P \in \mathcal{S}_n} (-1)^{|P|} \prod_{j=1}^{n} \delta_{\omega_{P(j)},\omega'_j}. \end{aligned}$$

Therefore two Bethe Ansatz eigenstates are orthogonal unless upon reordering the ω_j are the same as the ω'_j. Assuming a given ordering of the M-th roots of ± 1, the eigenstates have to be normalized with a factor $1/M^{n/2}$. The normalized eigenfunctions are thus

$$f(x_1, \ldots, x_n) = \frac{1}{M^{n/2}} \sum_{P \in \mathcal{S}_n} (-1)^{|P|} \prod_{j=1}^{n} \omega_{P(j)}^{x_j}, \tag{3.10}$$

where the ω_i $(i = 1, \ldots, n)$ are distinct M-th roots of $(-1)^{n-1}$.

Next, we need to compute the matrix elements of B_0 connecting $\mathcal{H}_n$ and $\mathcal{H}_{n-2}$. The corresponding matrix $C_n = P_{n-2} B_0\big|_{\mathcal{H}_n}$ is given by

$$\begin{aligned} (Cf_n)(x_1, \ldots, x_{n-2}) &= \sum_{j=0}^{n-2} \sum_{x=x_j+1}^{x_{j+1}-2} f_n(x_1, \ldots, x_j, x, x+1, x_{j+1}, \ldots, x_{n-2}) \\ &\quad + f_n(1, x_1, \ldots, x_{n-2}, M)\,(1 - \delta_{x_1,1})(1 - \delta_{x_{n-2},M}), \end{aligned} \tag{3.11}$$

where $x_0 = 0$ and $x_{n-1} = M+1$. We therefore have to compute $\langle f_{n-2} \,|\, C f_n \rangle$, where f_n is given by (3.10) and

$$f_{n-2}(x_1, \ldots, x_{n-2}) = \frac{1}{M^{(n-2)/2}} \sum_{Q \in \mathcal{S}_{n-2}} (-1)^{|Q|} \prod_{i=1}^{n-2} (\omega'_{Q(i)})^{x_i}.$$

We have

$$\begin{aligned}
\langle f_{n-2} \,|\, C f_n \rangle &= \frac{1}{M^{(n-2)/2}} \sum_{1 \le x_1 < \cdots < x_{n-2} \le M} \sum_{Q \in \mathcal{S}_{n-2}} (-1)^{|Q|} \\
&\qquad \times \prod_{i=1}^{n-2} (\overline{\omega'_{Q(i)}})^{x_i} (C f_n)(x_1, \ldots, x_{n-2}) \\
&= \frac{1}{M^{n-1}} \sum_{1 \le x_1 < \cdots < x_{n-2} \le M} \sum_{Q \in \mathcal{S}_{n-2}} (-1)^{|Q|} \prod_{i=1}^{n-2} (\overline{\omega'_{Q(i)}})^{x_i} \sum_{P \in \mathcal{S}_n} (-1)^{|P|} \\
&\qquad \times \left\{ \sum_{j=0}^{n-2} \sum_{x=x_j+1}^{x_{j+1}-2} \prod_{i=1}^{j} \omega_{P(i)}^{x_i} \omega_{P(j+1)}^{x} \omega_{P(j+2)}^{x+1} \prod_{i=j+1}^{n-2} \omega_{P(i+2)}^{x_i} \right. \\
&\qquad\qquad \left. + (1 - \delta_{x_1,1})(1 - \delta_{x_{n-2},M}) \omega_{P(1)} \prod_{i=1}^{n-2} \omega_{P(i+1)}^{x_i} \omega_{P(n)}^{M} \right\} \\
&= \frac{1}{M^{n-1}} \frac{1}{(n-2)!} \sum_{x_1, \ldots, x_{n-2}=1}^{M} \sum_{x=1}^{M} \sum_{Q \in \mathcal{S}_{n-2}} (-1)^{|Q|} \sum_{P \in \mathcal{S}_n} (-1)^{|P|} \\
&\qquad \times \prod_{i=1}^{n-2} \left\{ \left(\overline{\omega'_{Q(i)}}\right)^{x_i} \omega_{P(i)}^{x_i} \right\} \omega_{P(n-1)}^{x} \omega_{P(n)}^{x+1} \\
&= \frac{1}{M^{n-1}} \frac{1}{(n-2)!} \sum_{Q \in \mathcal{S}_{n-2}} (-1)^{|Q|} \sum_{P \in \mathcal{S}_n} (-1)^{|P|} \\
&\qquad \times M^{n-2} \prod_{i=1}^{n-2} \delta_{\omega'_{Q(i)}, \omega_{P(i)}} \sum_{x=1}^{M} \omega_{P(n-1)}^{x} \omega_{P(n)}^{x+1} \\
&= \sum_{P \in \mathcal{S}_n} (-1)^{|P|} \prod_{i=1}^{n-2} \delta_{\omega'_i, \omega_{P(i)}} \delta_{\omega_{P(n-1)} \omega_{P(n)}, 1} \omega_{P(n)}.
\end{aligned}$$

The third equality is obtained as follows. We can interchange the x_j at the cost of a factor $1/(n-2)!$. The terms where two $x_i = x_j$ for some $i \neq j$ vanish because of the factor $(-1)^{|Q|}$, and similarly the terms where $x = x_j$ or $x+1 = x_j$ because of the factor $(-1)^{|P|}$. In the terms with

$j = 0, \ldots, n-2$ it is obvious that we can move the factors $\omega^{x}_{P(j+1)}\omega^{x+1}_{P(j+2)}$ to $\omega^{x}_{P(n-1)}\omega^{x+1}_{P(n)}$ since it involves an even number of transpositions. In the last term we distinguish the cases where n is even and odd. If n is even, we can interchange $\omega_{P(1)}$ and $\prod_{i=1}^{n-2} \omega^{x_i}_{P(i+1)}$ to get $\prod_{i=1}^{n-2} \omega^{x_i}_{P(i)}\omega_{P(n-1)}$. Then using the fact that $\omega_j^M = -1$, we have $\omega_{P(n-1)}\omega^M_{P(n)} = -\omega_{P(n-1)} = -\omega^M_{P(n)}\omega^{M+1}_{P(n-1)}$ and interchanging $P(n-1)$ and $P(n)$ the minus sign cancels. If n is odd, then $\omega_j^M = 1$ and we have $-\omega_{P(n-1)}\omega^M_{P(n)} = -\omega_{P(n-1)} = -\omega^M_{P(n)}\omega^{M+1}_{P(n-1)}$ after which we again interchange $P(n-1)$ and $P(n)$.

This means that the scalar product $\langle f_{n-2} \,|\, C f_n\rangle$ equals zero unless among the ω_j ($j = 1, \ldots, n$) defining f_n there are $n-2$ which are equal to the ω'_i defining f_{n-2}, and the remaining two are complex conjugates. In that case, the corresponding matrix element equals $\omega - \overline{\omega}$, where ω and $\overline{\omega}$ are the remaining two ω_j.

Example 3.2: $M = 8$**.** The only translation-invariant eigenstates with $n = 4$ for which $\langle f_2 \,|\, C f_4\rangle \neq 0$ are those given by two pairs of complex conjugate roots of -1, i.e.

$$f(x_1, \ldots, x_4) = \frac{1}{M^2} \sum_{P \in \mathcal{S}_4} (-1)^{|P|} \omega_1^{x_{P(1)}} \overline{\omega_1}^{x_{P(2)}} \omega_2^{x_{P(3)}} \overline{\omega_2}^{x_{P(4)}},$$

where

$$\begin{aligned}(\omega_1, \omega_2) \;\; &= \;\; (e^{\pi i/8}, e^{3\pi i/8}), (e^{\pi i/8}, e^{5\pi i/8}), (e^{\pi i/8}, e^{7\pi i/8}), \\ &\qquad (e^{3\pi i/8}, e^{5\pi i/8}), (e^{3\pi i/8}, e^{7\pi i/8}), (e^{5\pi i/8}, e^{7\pi i/8}).\end{aligned}$$

We can label the Bethe Ansatz eigenfunction (3.10) by the M-th roots of ± 1 defining it, i.e. by $(\omega_{j_1}, \ldots, \omega_{j_n})$, where

$$\omega_j = e^{(2j-1)\pi i/M}, \qquad j = 1, \ldots, M, \tag{3.12}$$

for n even, and

$$\omega_j = e^{2j\pi i/M}, \qquad j = 0, \ldots, M-1, \tag{3.13}$$

for n odd, and where we assume $1 \le j_1 < \cdots < j_n \le M$.

3.2 The maximal eigenvalue and contribution to $\tilde{Z}$.

Note that the eigenvalues of A are all positive and that B restricted to the subspaces $\mathcal{H}_\pm$ is a strictly positive matrix on the basis $\{\varphi(x_1, \ldots, x_n) : 0 \le n \le M; 1 \le x_1 < \cdots < x_n \le M\}$ of eigenvectors of A, where $\mathcal{H}_\pm$ are the subspaces of $\mathbb{C}^{2^M}$ given by the eigenvalue ± 1 of $\sigma^x \otimes \cdots \otimes \sigma^x$, that is, with with even, respectively odd, numbers of minuses. Note that a matrix $\exp(B_0)$ is (strictly) positive if B_0 is nonnegative and irreducible. Now, the general expression (3.5) for $\tilde{B}_0$ shows that any two basis vectors $\varphi(x_1, \ldots, x_n)$ and $\varphi(x'_1, \ldots, x'_n)$ such that $x'_i = x_i$ except for $i = j$, and $x'_j = x_j \pm 1$ are connected by a positive matrix element in $\tilde{B}_0$, so by repeated application, any two vectors $\varphi(x_1, \ldots, x_n)$ and $\varphi(x'_1, \ldots, x'_n)$ are connected by positive matrix elements of $\tilde{B}_0^m$ for some m. Moreover, looking at the expression for $C_n = P_{n-2}B_0\big|_{\mathcal{H}_n}$ given by (3.11), we see that vectors $\varphi(x_1, \ldots, x_n)$ and $\varphi(x'_1, \ldots, x'_{n-2})$ are connected by positive matrix elements provided that *either* $x_j + 1 = x_{j+1}$ for some $j = 1, \ldots, M-1$ and $x_1 = x'_1, \ldots, x_{j-1} = x'_{j-1}$, $x_{j+2} = x'_j, \ldots, x_n = x'_{n-2}$, *or* $x_1 = 1$ and $x_n = M$ and $x_2 = x'_1, \ldots, x_{n-1} = x'_{n-2}$. Again, by iterating, we find that all basis vectors of $\mathcal{H}_n$ are connected by positive matrix elements of powers of B_0 to vectors of $\mathcal{H}_{n-2}$.

It follows from the Perron-Frobenius theorem (see Appendix A), that the eigenvector with maximum eigenvalue of AB must be either a vector with positive components on the eigenbasis of A in $\mathcal{H}_+$, or a vector with positive components in $\mathcal{H}_-$ (both up to a multiplicative factor). Since A and B are both translation-invariant, it follows that these eigenvectors must belong to the subspaces of translation-invariant vectors. We now consider separately the cases $\mathcal{H}_+$ and $\mathcal{H}_-$.

3.2.1 The case of even n.

The space $\mathcal{H}_+$ corresponds to the case of even n, namely

$$\mathcal{H}_+ = \bigoplus_{k=0}^{[M/2]} \mathcal{H}_{2k}. \tag{3.14}$$

Note that the maximal eigenvector ψ must have positive components in each $\mathcal{H}_{2k}$. We consider first the case that M is also even.

The case that M is even.
Then $\mathcal{H}_M$ is 1-dimensional, and the Bethe Ansatz vector f_M is defined by the sequence $\omega_1, \ldots, \omega_M$, where ω_j is given by (3.12) for the case n even. Note that $\omega_{M+1-j} = \overline{\omega_j}$. Now, by the fact that $\langle f_{n-2} \,|B_0\, f_n\rangle = 0$ unless f_{n-2} is defined by a sequence $\omega_{j'_1}, \ldots, \omega_{j'_{n-2}}$ obtained from the sequence $\omega_{j_1}, \ldots, \omega_{j_n}$ defining f_n by omitting a conjugate pair, it follows that the projection $P_{2k}\psi$ of ψ onto $\mathcal{H}_{2k}$ must be spanned by Bethe Ansatz vectors f_{2k} defined by sequences $\omega_{j_1}, \ldots, \omega_{j_{2k}}$ such that $\omega_{j_{2k+1-p}} = \overline{\omega_{j_p}}$, i.e. $j_{2k+1-p} = M + 1 - j_p$ for $p = 1, \ldots, k$. (see Example 3.1.)

On this basis, B_0 has the matrix elements

$$
\begin{aligned}
\langle f'_{2k} \,|\, B_0\, f_{2k}\rangle &= \begin{cases} \sum_{p=1}^n (\omega_{j_p} + \omega_{j_p}^{-1}) & \text{if } \omega'_{j_p} = \omega_{j_p} \text{ for all } p = 1, \ldots, k; \\ 0 & \text{otherwise;} \end{cases} \\
\langle f'_{2k-2} \,|\, B_0\, f_{2k}\rangle &= \begin{cases} \omega_j - \omega_j^{-1} & \text{if } \{\omega_{j_p}\}_{p=1}^k = \{\omega'_{j_q}\}_{q=1}^{k-1} \cup \{\omega_j\} \\ 0 & \text{otherwise.} \end{cases} \\
\langle f'_{2k} \,|\, B_0\, f_{2k-2}\rangle &= \overline{\langle f_{2k-2} \,|\, B_0\, f'_{2k}\rangle}, \\
\langle f'_{2l} \,|\, B_0\, f_{2k}\rangle &= 0 \text{ if } |k - l| > 1.
\end{aligned} \tag{3.15}
$$

In particular, $\langle f_0 \,|\, B_0 f_0\rangle = 0$ and also $\langle f_M \,|\, B_0\, f_M\rangle = 0$ since

$$\sum_{j=1}^M \omega_j = 0. \tag{3.16}$$

At this stage it is convenient to multiply the basis vectors f_{2k} by $(-i)^k$. This does not change the diagonal elements of B, but the off-diagonal elements are multiplied by $-i$.

Moreover, we now label the vectors f_n defined by $(\omega_{j_1}, \ldots, \omega_{j_n})$ such that $j_{n+1-p} = j_p$, $(p = 1, \ldots, n)$ by a sequence $(s_1, \ldots, s_{M/2})$ where s_j is an Ising spin such that $s_j = +1$ if $\omega_j \in \{\omega_{j_1}, \ldots, \omega_{j_n}\}$ and $s_j = -1$ if

$\omega_j \notin \{\omega_{j_1}, \ldots, \omega_{j_n}\}$. We write this vector as $|\{s_j\}_{j=1}^{M/2}\rangle$. Thus,

$$|s_1, \ldots, s_{M/2}\rangle = (-i)^{n/2} f_{n;\omega_{j_1},\ldots,\omega_{j_n}}, \text{ where}$$
$$j_{n+1-p} = j_p \text{ and } s_j = \begin{cases} +1 & \text{if } j \in \{j_1, \ldots, j_{n/2}\}; \\ -1 & \text{if } j \in \{j_1, \ldots, j_{n/2}\}. \end{cases} \tag{3.17}$$

On this basis, B_0 has the matrix elements

$$\langle s'_1, \ldots, s'_{M/2} \,|\, B_0 \,| s_1, \ldots, s_{M/2}\rangle = \begin{cases} 4\sum_{j=1}^{M/2} \delta_{s_j,1} \cos\frac{(2j-1)\pi}{M} \\ \qquad \text{if } s'_j = s_j \text{ for all } j = 1, \ldots, M/2; \\ 2\sin\frac{(2j-1)\pi}{M} \\ \qquad \text{if } s'_j s_j = -1 \text{ and } s'_i = s_i \text{ for } i \neq j; \\ 0 \quad \text{otherwise.} \end{cases} \tag{3.18}$$

This is just the matrix

$$\overline{B_0} = \sum_{j=1}^{M/2} (\mathbf{1} \otimes \cdots \otimes B_j \otimes \cdots \otimes \mathbf{1}), \tag{3.19}$$

where the factor B_j appears in the j-th position and equals

$$\begin{aligned} B_j &= 2 \begin{pmatrix} \cos\frac{(2j-1)\pi}{M} & \sin\frac{(2j-1)\pi}{M} \\ \sin\frac{(2j-1)\pi}{M} & -\cos\frac{(2j-1)\pi}{M} \end{pmatrix} \\ &= 2\cos\theta_{2j-1}\,\sigma^z + 2\sin\theta_{2j-1}\,\sigma^x, \end{aligned} \tag{3.20}$$

where

$$\theta_r = \frac{r\pi}{M}. \tag{3.21}$$

To see this, note that

$$\begin{aligned} &\langle s_1, \ldots, s_{M/2} \,|\, \overline{B_0} \,| s_1, \ldots, s_{M/2}\rangle \\ &= \sum_{j=1}^{M/2} 2(\delta_{s_j,1} \cos\theta_{2j-1} - \delta_{s_j,-1} \cos\theta_{M+1-2j} \\ &= 4\sum_{j=1}^{M/2} \delta_{s_j,1} \cos\theta_{2j-1}. \end{aligned} \tag{3.22}$$

Indeed, note that, by (3.16),

$$\sum_{j=1}^{M/2} \cos \frac{(2j-1)\pi}{M} = 0. \tag{3.23}$$

Example 3.3. Consider the case $M = 6$. Then (3.19) reads

$$\overline{B}_0 = \begin{pmatrix} 0 & 1 & 2 & 0 & 1 & 0 & 0 & 0 \\ 1 & 2\sqrt{3} & 0 & 2 & 0 & 1 & 0 & 0 \\ 2 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 2 & 1 & 2\sqrt{3} & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & -2\sqrt{3} & 1 & 2 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 2 \\ 0 & 0 & 1 & 0 & 2 & 0 & -2\sqrt{3} & 1 \\ 0 & 0 & 0 & 1 & 0 & 2 & 1 & 0 \end{pmatrix}.$$

Indeed,

$$B_1 = \begin{pmatrix} \sqrt{3} & 1 \\ 1 & -\sqrt{3} \end{pmatrix}, \quad B_1 = \begin{pmatrix} 0 & 2 \\ 2 & 0 \end{pmatrix}, \quad B_1 = \begin{pmatrix} -\sqrt{3} & 1 \\ 1 & \sqrt{3} \end{pmatrix}.$$

The entries are in the order $+++$, $++-$, $+-+$, $+--$, $-++$, $-+-$, $--+$, $---$. Thus, on the diagonal, the entries are

$$0, \; -4\cos\frac{5\pi}{6}, \; -4\cos\frac{\pi}{2}, \; 4\cos\frac{\pi}{6}, \; -4\cos\frac{\pi}{6}, \; 4\cos\frac{\pi}{2}, \; 4\cos\frac{5\pi}{6}, 0.$$

Exponentiating, we find that the matrix of B given by $\cosh^M(\beta J_2)B = e^{\beta J_2 B_0}$ on the Bethe basis is

$$\overline{B} = \frac{1}{\cosh^M(\beta J_2)} \bigotimes_{j=1}^{M/2} e^{\beta J_2 B_j}, \tag{3.24}$$

where

$$\frac{e^{\beta J_2 B_j}}{\cosh^2(\beta J_2)} = (1+u^2)\mathbf{1} + 2u\cos\theta_{2j-1}\,\sigma^z + 2u\sin\theta_{2j-1}\,\sigma^x, \tag{3.25}$$

where θ_r is given by (3.21).

On this same basis, the matrix A is diagonal with diagonal elements $(1-\lambda)^n(1+\lambda)^{M-n}$. Thus,

$$\overline{A} = \bigotimes_{j=1}^{M/2} A_j, \text{ where}$$
$$A_j = \begin{pmatrix} (1-\lambda)^2 & 0 \\ 0 & (1+\lambda)^2 \end{pmatrix} = (1+\lambda^2)\mathbf{1} - 2\lambda\sigma^z. \tag{3.26}$$

Applying Lemma 2.1 we obtain the following contribution to $\tilde{Z}_{N,M}$:

$$\tilde{Z}_{\max,+} = \prod_{j=1}^{M/2} (\zeta_{2j-1,+}^N + \zeta_{2j-1,-}^N), \tag{3.27}$$

where

$$\begin{cases} \zeta_{r,\pm} = (1+\lambda^2)(1+u^2) - 4u\lambda\cos\frac{r\pi}{M} \pm \sqrt{\Delta_r}, \quad \text{where} \\ \Delta_r = \left[(1+\lambda^2)(1+u^2) - 4u\lambda\cos\frac{r\pi}{M}\right]^2 - (1-\lambda^2)^2(1-u^2)^2. \end{cases} \tag{3.28}$$

The case that M is odd.
In this case, $\mathcal{H}_{M-1}$ is M-dimensional, but the translation-invariant Bethe Ansatz vector f_{M-1} is unique, and defined by the sequence

$$\omega_1, \ldots, \omega_{(M-1)/2}, \omega_{(M+3)/2}, \ldots, \omega_M.$$

(Note that $\omega_{(M+1)/2} = -1$ is excluded. Thus, $j_{M-1} = M$. Also, $\omega_{M+1-j} = \overline{\omega_j}$ for $j = 1, \ldots, \frac{M-1}{2}$.) The matrix elements of B_0 on the Bethe Ansatz vectors f_{2k} defined by $(\omega_{j_1}, \ldots, \omega_{j_{2k}})$ such that $\omega_{j_{2k+1-p}} = \overline{\omega_{j_p}}$, i.e. $j_{2k+1-p} = M+1-j_p$, are again given by (3.15). However, there is no symmetry, since in this case

$$\langle f_{M-1} \,|\, B_0\, f_{M-1} \rangle = 2\sum_{j=1}^{(M-1)/2} (\omega_j + \overline{\omega_j}) = 2\sum_{j=1}^{M} \omega_j - 2\omega_{(M+1)/2} = 2.$$

We introduce again spin variables $s_1, \ldots, s_{(M-1)/2}$ such that $s_j = +1$ if $j \in$

$\{j_1, \ldots, j_k\}$ and $s_j = -1$ otherwise. The matrix B_0 on this basis becomes

$$\langle s'_1, \ldots, s'_{(M-1)/2} \,|\, B_0 \,|s_1, \ldots, s_{(M-1)/2}\rangle$$
$$= \begin{cases} 4\sum_{j=1}^{(M-1)/2} \delta_{s_j,1} \cos\frac{(2j-1)\pi}{M} \\ \qquad \text{if } s'_j = s_j \text{ for all } j = 1, \ldots, (M-1)/2; \\ 2\sin\frac{(2j-1)\pi}{M} \\ \qquad \text{if } s'_j s_j = -1 \text{ and } s'_i = s_i \text{ for } i \neq j; \\ 0 \qquad \text{otherwise.} \end{cases} \tag{3.29}$$

Using the identity (3.16) we can now write

$$\sum_{j=1}^{(M-1)/2} \delta_{s_j,1} \cos\frac{(2j-1)\pi}{M} = \frac{1}{2} - \sum_{j=1}^{(M-1)/2} \delta_{s_j,-1} \cos\frac{(2j-1)\pi}{M}.$$

It follows similarly to (3.22) that

$$B_0 = \mathbf{1}_{2^{(M-1)/2}} + \sum_{j=1}^{(M-1)/2} (\mathbf{1}_2 \otimes \cdots \otimes B_j \otimes \cdots \otimes \mathbf{1}_2), \tag{3.30}$$

where B_j is given by (3.20).

Example 3.4. Consider the case $M = 5$. Then B_0 is a 4×4 matrix: f_0 and f_4 are unique, and there are two Bethe Ansatz vectors f_2 defined by (ω_1, ω_5) and (ω_2, ω_4) respectively. Thus,

$$B_0 = \begin{pmatrix} 0 & 2\sin\frac{\pi}{5} & 2\sin\frac{3\pi}{5} & 0 \\ 2\sin\frac{\pi}{5} & 4\cos\frac{\pi}{5} & 0 & 2\sin\frac{3\pi}{5} \\ 2\sin\frac{3\pi}{5} & 0 & 4\cos\frac{3\pi}{5} & 2\sin\frac{\pi}{5} \\ 0 & 2\sin\frac{3\pi}{5} & 2\sin\frac{\pi}{5} & 2 \end{pmatrix}.$$

Using the fact that $2(\cos\frac{\pi}{5} + \cos\frac{3\pi}{5}) = 1$, this can be written as

$$B_0 = \mathbf{1} + \begin{pmatrix} -1 & 2\sin\frac{\pi}{5} & 2\sin\frac{3\pi}{5} & 0 \\ 2\sin\frac{\pi}{5} & 2(\cos\frac{\pi}{5} - \cos\frac{3\pi}{5}) & 0 & 2\sin\frac{3\pi}{5} \\ 2\sin\frac{3\pi}{5} & 0 & 2(\cos\frac{3\pi}{5} - \cos\frac{\pi}{5}) & 2\sin\frac{\pi}{5} \\ 0 & 2\sin\frac{3\pi}{5} & 2\sin\frac{\pi}{5} & 1 \end{pmatrix},$$

and using this identity once more, we have $B_0 = \mathbf{1}_4 + B_1 \otimes \mathbf{1}_2 + \mathbf{1}_2 \otimes B_2$, where

$$\begin{aligned} B_1 &= 2\sin\frac{3\pi}{5}\sigma^x - 2\cos\frac{3\pi}{5}\sigma^z \text{ and} \\ B_2 &= 2\sin\frac{\pi}{5}\sigma^x - 2\cos\frac{\pi}{5}\sigma^z. \end{aligned}$$

Noting that

$$\frac{e^{\beta J_2}}{\cosh(\beta J_2)} = 1 + u,$$

we find that the matrix of B on the Bethe basis is given by

$$\begin{aligned} \overline{B} &= \frac{e^{\beta J_2}}{\cosh^M(\beta J_2)} \bigotimes_{j=1}^{(M-1)/2} e^{\beta J_2 B_j} \\ &= (1+u) \bigotimes_{j=1}^{(M-1)/2} [(1+u^2)\mathbf{1} + 2u\cos\theta_{2j-1}\sigma^z + 2u\sin\theta_{2j-1}\sigma^x] \end{aligned} \tag{3.31}$$

On this same basis, the matrix A is diagonal with diagonal elements $(1-\lambda)^n(1+\lambda)^{M-n}$. Thus,

$$\begin{aligned} \overline{A} &= (1+\lambda) \bigotimes_{j=1}^{(M-1)/2} A_j, \text{ where} \\ A_j &= \begin{pmatrix} (1-\lambda)^2 & 0 \\ 0 & (1+\lambda)^2 \end{pmatrix} = (1+\lambda^2)\mathbf{1} - 2\lambda\sigma^z. \end{aligned} \tag{3.32}$$

Applying Lemma 2.1 we obtain the following contribution to $\tilde{Z}_{N,M}$:

$$\tilde{Z}_{\max,+} = (1+u)^N(1+\lambda)^N \prod_{j=1}^{(M-1)/2} (\zeta_{2j-1,+}^N + \zeta_{2j-1,-}^N), \tag{3.33}$$

where

$$\begin{cases} \zeta_{r,\pm} = (1+\lambda^2)(1+u^2) - 4u\lambda\cos\frac{r\pi}{M} \pm \sqrt{\Delta_r}, \quad \text{where} \\ \Delta_r = \left[(1+\lambda^2)(1+u^2) - 4u\lambda\cos\frac{r\pi}{M}\right]^2 - (1-\lambda^2)^2(1-u^2)^2. \end{cases} \tag{3.34}$$

3.2.2 The case of odd n.

Similarly to the even case, the maximal eigenvector $\psi \in \mathcal{H}_-$ must be a vector in the space spanned by the Bethe Ansatz vectors f_n with $n = 2k-1$, such that each f_n is defined by a sequence $\omega_{j_0}, \ldots, \omega_{j_{n-1}}$ where apart from ω_{j_0} all other ω_j occur together with their complex conjugates. Again we distinguish the cases M even and odd.

In case that M is even, then

$$\mathcal{H}_- = \oplus_{k=1}^{M/2} \mathcal{H}_{2k-1}.$$

The highest space $\mathcal{H}_{M-1}$ is M-dimensional but the translation-invariant subspace is 1-dimensional and spanned by the vector f_{M-1} defined by

$$(1, \omega_1, \ldots, \omega_{M/2-1}, \omega_{M/2+1}, \ldots, \omega_{M-1}),$$

where

$$\omega_j = e^{2\pi j i/M} \qquad (j = 0, 1, \ldots, M-1) \tag{3.35}$$

are the M-th roots of 1 (see (3.13)). Indeed, the only missing root of unity must be real-valued, and since $\prod_{p=1}^{M} \omega_j = 1$, the missing root must be -1. Similarly, $f_1 \in \mathcal{H}_1$ is also unique and given by $f_1(x_1) = 1/\sqrt{M}$. We have $\langle f_1 \,|\, B_0\, f_1\rangle = \langle f_{M-1} \,|\, B_0\, f_{M-1}\rangle = 2$. In general, f_{2k-1} is defined by $(1, \omega_{j_1}, \ldots, \omega_{j_{2k-2}})$ such that $\omega_{j_{2k-1-p}} = \overline{\omega_{j_p}}$ for $p = 1, \ldots, (n-1)/2 = k-1$. Introducing again a sequence of spin variables $s_1, \ldots, s_{M/2-1}$ such that $s_j = +1$ if $j \in \{j_1, \ldots, j_{k-1}\}$ and $s_j = -1$ otherwise, we have

$$\begin{aligned} &\langle s'_1, \ldots, s'_{M/2-1} \,|\, B_0 \,|s_1, \ldots, s_{M/2-1}\rangle \\ &= \begin{cases} 2 + 4\sum_{j=1}^{M/2-1} \delta_{s_j,1} \cos\frac{2j\pi}{M} \\ \qquad \text{if } s'_j = s_j \text{ for all } j = 1, \ldots, M/2-1; \\ 2\sin\frac{2j\pi}{M} \\ \qquad \text{if } s'_j s_j = -1 \text{ and } s'_i = s_i \text{ for } i \neq j; \\ 0 \qquad \text{otherwise.} \end{cases} \end{aligned} \tag{3.36}$$

Note that in this case, we have

$$\sum_{j=1}^{M/2-1} \cos\frac{2\pi j}{M} = 0. \tag{3.37}$$

Therefore,

$$4\sum_{j=1}^{M/2-1}\delta_{s_j,1}\cos\frac{2j\pi}{M}=2\sum_{j=1}^{M/2-1}s_j\cos\frac{2j\pi}{M}.$$

This implies that $\overline{B_0}$ can be written as

$$\overline{B_0}=2\mathbf{1}_{2^{M/2-1}}+\sum_{j=1}^{M/2-1}(\mathbf{1}_2\otimes\cdots\otimes B_j\otimes\cdots\otimes\mathbf{1}_2), \tag{3.38}$$

where there are $M/2-1$ factors. Moreover, the eigenvalues of A are $(1-\lambda)^{2k-1}(1+\lambda)^{M+1-2k}=(1-\lambda^2)(1-\lambda)^{2(k-1)}(1+\lambda)^{2(M/2-k)}$, so that A can be written as

$$A=(1-\lambda^2)\otimes_{j=1}^{M/2-1}((1+\lambda^2)\mathbf{1}_2-2\lambda\sigma^z). \tag{3.39}$$

Applying Lemma 2.1, we get the contribution

$$\tilde{Z}_{\max,-}=(1+u)^{2N}(1-\lambda^2)^N\prod_{j=1}^{M/2-1}(\zeta_{2j,+}^N+\zeta_{2j,-}^N), \tag{3.40}$$

where

$$\begin{cases}\zeta_{r,\pm}=(1+\lambda^2)(1+u^2)-4u\lambda\cos\frac{r\pi}{M}\pm\sqrt{\Delta_r}, \quad \text{where}\\ \Delta_r=\left[(1+\lambda^2)(1+u^2)-4u\lambda\cos\frac{r\pi}{M}\right]^2-(1-\lambda^2)^2(1-u^2)^2.\end{cases} \tag{3.41}$$

If M is odd, then

$$\mathcal{H}_-=\oplus_{k=1}^{(M+1)/2}\mathcal{H}_{2k-1}.$$

The highest space $\mathcal{H}_M$ is 1-dimensional and is given by f_M defined by the sequence of all roots $(1,\omega_1,\ldots,\omega_{M-1})$. The corresponding diagonal element of B_0 is zero. The space $\mathcal{H}_1$ has one translation-invariant element, $\langle f_1\,|\,B_0\,f_1\rangle=2$. For other $n=2k-1$, f_n is defined by a sequence $(1,\omega_{j_1},\ldots,\omega_{j_{2k-2}})$ with $\omega_{j_{2k-1-p}}=\overline{\omega_{j_p}}$. Introducing spin variables $s_1,\ldots,s_{(M-1)/2}$, the matrix elements of B_0 are

$$\langle s'_1, \dots, s'_{(M-1)/2} \,|\, B_0 \,|s_1, \dots, s_{(M-1)/2}\rangle$$
$$= \begin{cases} 2 + 4\sum_{j=1}^{(M-1)/2} \delta_{s_j,1} \cos \frac{2j\pi}{M} \\ \qquad\qquad \text{if } s'_j = s_j \text{ for all } j = 1, \dots, (M-1)/2; \\ 2\sin\frac{2j\pi}{M} \\ \qquad\qquad \text{if } s'_j s_j = -1 \text{ and } s'_i = s_i \text{ for } i \neq j; \\ 0 \qquad \text{otherwise.} \end{cases} \tag{3.42}$$

In this case,

$$\frac{1}{2} + \sum_{j=1}^{(M-1)/2} \cos\frac{2\pi j}{M} = 0. \tag{3.43}$$

Therefore we can write

$$2 + 4\sum_{j=1}^{(M-1)/2} \delta_{s_j,1} \cos\frac{2j\pi}{M} = 1 + 2\sum_{j=1}^{(M-1)/2} s_j \cos\frac{2j\pi}{M}.$$

We conclude that

$$\overline{B_0} = \mathbf{1}_{2^{(M-1)/2}} + \sum_{j=1}^{(M-1)/2} (\mathbf{1}_2 \otimes \cdots \otimes B_j \otimes \cdots \otimes \mathbf{1}_2). \tag{3.44}$$

Also, the eigenvalues of A are $(1-\lambda)^{2k-1}(1+\lambda)^{M+1-2k} = (1-\lambda)(1-\lambda)^{2k-2}(1+\lambda)^{M-1-(2k-2)}$, so we have

$$A = (1-\lambda) \otimes_{j=1}^{(M-1)/2} ((1+\lambda^2)\mathbf{1}_2 - 2\lambda\sigma^z). \tag{3.45}$$

The resulting contribution is

$$\tilde{Z}_{\max,-} = (1+u)^N(1+\lambda)^N \prod_{j=1}^{(M-1)/2} (\zeta_{2j,+}^N + \zeta_{2j,-}^N). \tag{3.46}$$

Remark. In the same way one can of course obtain all contributions to $\tilde{Z}$ since all Bethe Ansatz eigenstates are given. We give the general result in Appendix B.

3.3 The thermodynamic limit.

The thermodynamic limit is given by

$$\begin{aligned}
\lim_{N,M\to\infty} \frac{1}{NM} \ln \tilde{Z}_{N,M} &= \lim_{M\to\infty} \frac{1}{M} \max\{\sum_{j=1}^{[M/2]} \ln \zeta_{2j-1,+}, \sum_{j=1}^{[M/2]} \ln \zeta_{2j,+}\} \\
&= \frac{1}{2\pi} \int_0^\pi d\theta \, \ln \zeta(\lambda, u; \theta), \qquad (3.47)
\end{aligned}$$

where

$$\begin{aligned}
\zeta(\lambda, u; \theta) &= (1+\lambda^2)(1+u^2) - 4u\lambda \cos\theta \\
&\quad + \sqrt{[(1+\lambda^2)(1+u^2) - 4u\lambda\cos\theta]^2 - (1-\lambda^2)^2(1-u^2)^2}. \qquad (3.48)
\end{aligned}$$

We want to rewrite this in terms of the original variables. Let $K_1 = \beta J_1$ and $K_2 = \beta J_2$. Note that $\frac{1}{NM} \ln Z_{N,M}(K_1, K_2) = K_1 + \ln\cosh(K_2) + \frac{1}{NM} \ln \tilde{Z}_{N,M}$. Moreover,

$$e^{2K_1}(1+\lambda^2) = 2\cosh(2K_1) \text{ and } \cosh^2(K_2)(1+u^2) = \cosh(2K_2),$$

and $e^{2K_1}\lambda = 1$ and $\cosh^2(K_2)u = \frac{1}{2}\sinh(2K_2)$, and finally,

$$e^{2K_1}(1-\lambda^2) = 2\sinh(2K_1) \text{ and } \cosh^2(K_2)(1-u^2) = 1.$$

Therefore, we have for the free energy density,

$$-\beta f(\beta, J_1, J_2) = \frac{1}{2\pi} \int_0^\pi d\theta \, \ln z(\beta J_1, \beta J_2; \theta), \qquad (3.49)$$

where

$$\begin{aligned}
z(K_1, K_2; \theta) &= 2[\cosh(2K_1)\cosh(2K_2) - \sinh(2K_2)\cos(\theta)] \\
&\quad + 2\sqrt{[\cosh(2K_1)\cosh(2K_2) - \sinh(2K_2)\cos(\theta)]^2 - \sinh^2(2K_1)}. \qquad (3.50)
\end{aligned}$$

This can be expressed more elegantly in terms of a double integral. First note that the inverse hyperbolic cosine function is given by

$$\cosh^{-1}(x) = \ln[x + \sqrt{x^2 - 1}].$$

We can thus express $\ln z(K_1, K_2; \theta)$ in terms of this function:

$$\begin{aligned}
&\ln z(K_1, K_2; \theta) \\
&= \ln \sinh(2K_1) \\
&\quad + \ln \left\{ 2[\coth(2K_1)\cosh(2K_2) - \frac{\sinh(2K_2)}{\sinh(2K_1)}\cos(\theta)] \right. \\
&\quad \left. + 2\sqrt{\left[\coth(2K_1)\cosh(2K_2) - \frac{\sinh(2K_2)}{\sinh(2K_1)}\cos(\theta)\right]^2 - 1} \right\} \\
&= \ln 2\sinh(2K_1) \\
&\quad + \cosh^{-1}\left(\coth(2K_1)\cosh(2K_2) - \frac{\sinh(2K_2)}{\sinh(2K_1)}\cos(\theta)\right).
\end{aligned} \tag{3.51}$$

We next use the following remarkable identity:

$$|z| = \frac{1}{\pi}\int_0^\pi dt\ \ln[2\cosh(z) - 2\cos(t)]. \tag{3.52}$$

This can be proved as follows. Differentiating, we have,

$$\frac{d}{dz}\frac{1}{\pi}\int_0^\pi dt\ \ln[2\cosh(z) - 2\cos(t)] = \frac{1}{\pi}\int_0^\pi dt\, \frac{\sinh(z)}{\cosh(z) - \cos(t)}.$$

This integral can be evaluated using the substitution $\tan\frac{1}{2}t = x$, which yields

$$\begin{aligned}
\frac{1}{\pi}\int_0^\pi dt\, \frac{\sinh(z)}{\cosh(z) - \cos(t)} &= \frac{2}{\pi}\int_0^\infty \frac{\sinh(z)\,dx}{\cosh(z) - 1 + (\cosh(z)+1)x^2} \\
&= \frac{2}{\pi}\frac{\sinh(z)}{\sqrt{\cosh^2(z) - 1}}\int_0^\infty \frac{dy}{1+y^2} = \mathrm{sgn}(z),
\end{aligned}$$

where $y = \sqrt{\frac{\cosh(z)+1}{\cosh(z)-1}}x$. To fix the constant, note that, as $|z| \to \infty$,

$$\begin{aligned}
\frac{1}{\pi}\int_0^\pi dt\ \ln[2\cosh(z) - 2\cos(t)] &= \ln 2\cosh(z) + \frac{1}{\pi}\int_0^\pi dt\ \ln\left(1 - \frac{\cos(t)}{\cosh(z)}\right) \\
&\sim \ln(2\cosh(z)) - \frac{1}{\pi}\int_0^\pi dt\, \frac{\cos(t)}{\cosh(z)} \\
&\sim |z| + O(e^{-2z}).
\end{aligned}$$

Setting $z = \cosh^{-1}(u)$, we have

$$\cosh^{-1}(u) = \frac{1}{\pi}\int_0^\pi dt\ \ln[2u - 2\cos(t)],$$

and therefore

$$\ln z(K_1, K_2; \theta) = \ln 2\sinh(2K_1) \\ + \frac{1}{\pi}\int_0^\pi dt\ \ln\left(2\coth(2K_1)\cosh(2K_2) - 2\frac{\sinh(2K_2)}{\sinh(2K_1)}\cos(\theta) - 2\cos(t)\right).$$

Inserting this into the formula (3.49) we obtain the well-known expression

$$\begin{aligned} -\beta f(\beta, J_1, J_2) &= \ln 2 + \frac{1}{2\pi^2}\int_0^\pi d\theta_1 \int_0^\pi d\theta_2 \ln\left[\cosh(2\beta J_1)\cosh(2\beta J_2)\right. \\ &\qquad \left. - \sinh(2\beta J_1)\cos(\theta_1) - \sinh(2\beta J_2)\cos(\theta_2)\right]. \end{aligned} \tag{3.53}$$

This result is analyzed in[24] in the case $J_1 = J_2$. There it was shown that there is a second-order phase transition at the critical temperature T_c given by $\sinh(2\beta_c J) = 1$, with $\beta_c = 1/(k_B T_c$. In the inhomogeneous case, we see that there can be a singularity when the argument of the logarithm becomes zero. Now $\cosh(2\beta J_1)\cosh(2\beta J_2) \geq \sinh(2\beta J_1) + \sinh(2\beta J_2)$. Indeed, writing $a = 2\beta J_1$ and $b = 2\beta J_2$, we have

$$\begin{aligned} &\cosh^2(a)\cosh^2(b) - (\sinh(a) + \sinh(b))^2 \\ &= \sinh^2(a)\sinh^2(b) - 2\sinh(a)\sinh(b) + 1 \\ &= (\sinh(a)\sinh(b) - 1)^2 \geq 0. \end{aligned}$$

This also shows that the singularity must occur for $\theta_1 = \theta_2 = 0$ and for $\sinh(2\beta J_1)\sinh(2\beta J_2) = 1$.

[24] T. C. Dorlas, *loc. sit.*, Chapter 28.

A The Perron-Frobenius Theorem

A vector $\vec{v} \in \mathbb{R}^n$ is called **nonnegative** if $v_i \geq 0$ for all $i = 1, \ldots, n$. A matrix $B \in \mathcal{M}_n(\mathbb{R})$ is said to be **nonnegative** if its entries $B_{ij} \geq 0$. B is called **positive** if $B_{ij} > 0$ for all $i, j = 1, \ldots, n$.

Lemma A.1 *A matrix $B \in \mathcal{M}_n(\mathbb{R})$ is nonnegative if and only if $B\vec{v} \geq 0$ whenever $\vec{v} \geq 0$. Moreover, B is positive if and only if $B\vec{v} > 0$ whenever $\vec{v} \geq 0$ and $\vec{v} \neq 0$.*

Proof. The 'if' part of these statements follows because we can take $\vec{v}$ to be a standard basis vector. It is also clear that if B is nonnegative then $B\vec{v} \geq 0$ once $\vec{v} \geq 0$. Now suppose that B is positive. Suppose that $v_i \geq 0$ for all $i = 1, \ldots, n$ and $v_j > 0$. Then

$$(B\vec{v})_i = \sum_{k=1}^{n} B_{ik} v_k \geq B_{ij} v_j > 0$$

since $B_{ij} > 0$. ∎

A matrix $B \in \mathcal{M}_n(\mathbb{R})$ is said to be **reducible** if there exists a partition of $\{1, \ldots, n\}$ into non-empty subsets I and J such that $B_{ij} = 0$ for all $i \in I$ and $j \in J$. Otherwise B is said to be **irreducible**. Note that B is irreducible if and only if for all $i, j \in \{1, \ldots, n\}$, there is a sequence $j_0 = i, \ldots, j_k = j$ such that $B_{j_{p-1}, j_p} \neq 0$ for $p = 1, \ldots, k$. In particular, a symmetric matrix B is irreducible if the graph on the vertices $1, \ldots, n$ formed by connecting i and j if $B_{ij} \neq 0$ is connected.

Lemma A.2 *If $B \in \mathcal{M}_n(\mathbb{R})$ is an irreducible nonnegative matrix then $(\mathbf{1} + B)^{n-1}$ is positive.*

Proof. Fix $\vec{v} \geq 0$ with $v_k > 0$. Clearly, $((\mathbf{1} + B)^m \vec{v})_j \geq 0$ for all $m \geq 0$ and $j = 1, \ldots, n$. For $m \geq 0$, let J_m be the set of indices j such that $((\mathbf{1} + B)^m \vec{v})_j > 0$. Then $|J_0| > 0$ since $k \in J_0$. Moreover, since B is nonnegative, $((\mathbf{1} + B)\vec{u})_i \geq u_i$ for all vectors $\vec{u}$, and therefore $J_m \subset J_{m+1}$ and hence $|J_{m+1}| \geq |J_m|$. Now suppose $J_m \neq \{1, \ldots, n\}$. We want to show that in that case, $|J_{m+1}| > |J_m|$. Suppose $J_{m+1} = J_m$. Let $I = J_m^c$. Because B is irreducible, there exist $j \in J_m$, and $i \in I$ such that $B_{ij} > 0$. But then

$$((\mathbf{1} + B)^{m+1}\vec{v})_i \geq B_{ij}((\mathbf{1} + B)^m\vec{v})_j > 0,$$

so that $i \in J_{m+1}$, contradicting $J_{m+1} = J_m$. We conclude that $|J_m| \geq \min\{m+1, n\}$ and hence $|J_{n-1}| = n$. ∎

Remark. Note that $e^B \geq \frac{1}{m!}(\mathbf{1} + B)^m$, so that e^B is also positive once B is nonnegative and irreducible.

Lemma A.3 *Let $B \in \mathcal{M}_n(\mathbb{R})$ be an irreducible nonnegative matrix. Then a nonnegative eigenvector $\vec{v}$ of B is in fact positive, and, moreover, the corresponding eigenvalue is positive.*

Proof. If $\vec{v}$ is a nonnegative eigenvector with eigenvalue λ then $\lambda \geq 0$. In addition, $\vec{v}$ is also an eigenvector of $(\mathbf{1} + B)^{n-1}$ with eigenvalue $(1 + \lambda)^{n-1}$, and therefore

$$\vec{v} = \frac{1}{(1 + \lambda)^{n-1}}(\mathbf{1} + B)^{n-1}\vec{v}.$$

By the previous lemma, $(\mathbf{1} + B)^{n-1}$ is positive, and since $\vec{v} \neq 0$, it follows that $\vec{v}$ is positive. Since B is irreducible, we conclude that also $B\vec{v}$ is positive, which implies that $\lambda > 0$. ∎

The Perron-Frobenius Theorem reads as follows.

Theorem A.1 (Perron-Frobenius) *Let $B \in \mathcal{M}_n(\mathbb{R})$ be an irreducible nonnegative $n \times n$ matrix. Then the spectral radius $\rho(B)$ is an eigenvalue of B, and there is a corresponding positive eigenvector $\vec{v}$ such that $B\vec{v} = \rho(B)\vec{v}$. Moreover, $\rho(B) > 0$.*

Proof. [25] It is convenient to use the 1-norm on $\mathbb{R}^n$ defined by

$$||\vec{v}||_1 = \sum_{i=1}^{n} |v_i|.$$

[25] See: D. Serre: *Matrices. Theory and Applications.* Second Ed. Graduate Texts in Mathematics 216. Springer, 2010.

For $r \geq 0$, define the set $C_r \subset \mathbb{R}^n$ by

$$C_r = \{\vec{x} \in \mathbb{R}^n : \vec{x} \geq 0, \, ||\vec{x}||_1 = 1, \, B\vec{x} \geq r\vec{x}\}.$$

Then C_r is a convex compact set. Moreover, $C_{\rho(B)} \neq \emptyset$. Indeed, if $\vec{v}$ is an eigenvector with eigenvalue λ and $||\vec{v}||_1 = 1$ then $B\,|\vec{v}| = |B\vec{v}| = |\lambda\vec{v}| = |\lambda|\,|\vec{v}|$, i.e. $|\vec{v}|$ is a nonnegative eigenvector with eigenvalue $|\lambda|$. There is an eigenvalue λ with $|\lambda| = \rho(B)$ and therefore $\rho(B)$ is also an eigenvalue with nonnegative eigenvector. Conversely, if $C_r \neq \emptyset$ then for $\vec{x} \in C_r$,

$$r = r||\vec{x}||_1 = ||r\vec{x}||_1 \leq ||B\vec{x}||_1 \leq ||B||_1||\vec{x}||_1 = ||B||_1.$$

Therefore, $C_r = \emptyset$ for $r > ||B||_1$. If $R = \sup\{r \geq 0 : C_r \neq \emptyset\}$, then $R \in [\rho(B), ||B||_1]$. Obviously, $C_{r'} \subset C_r$ for $r' > r$. Therefore, if $r < R$ then $C_r \neq \emptyset$. More precisely, $C_R = \bigcap_{r<R} C_r$, because if $(r_p)_{p\in\mathbb{N}}$ is an increasing sequence converging to R and $\vec{x}_p \in C_{r_p}$ then there is a converging subsequence $\vec{x}'_p$, the limit of which lies in C_R. This also shows that $C_R \neq \emptyset$. Let $\vec{v} \in C_R$. We claim that $\vec{v}$ is an eigenvector with eigenvalue R. Indeed, suppose the contrary. Set $\vec{u} = (\mathbf{1} + B)^{n-1}\vec{v}$. Since B is irreducible and $\vec{v}$ is nonnegative and nonzero, it follows that $\vec{u}$ is positive. Since B commutes with $\mathbf{1} + B$, we have $(B - R)\vec{u} = (\mathbf{1} + B)^{n-1}(B\vec{v} - R\vec{v}) > 0$. Define $r' = \min_{j=1}^n (B\vec{u})_j/u_j$. Then $r' > R$ and $C_{r'} \neq \emptyset$ since $B\vec{u} \geq r'\vec{u}$. This contradicts the definition of R. Therefore R is an eigenvalue with eigenvector $\vec{v}$ and since $B\vec{v} \geq \rho(B)\vec{v}$, we conclude that $R = \rho(B)$. Positivity of $\vec{v}$ and $\rho(B)$ now follow from Lemma A.3. ∎

Remark. One can prove that $\rho(B)$ is in fact a non-degenerate eigenvalue of B.

B Complete Solution

B.1 The case M odd.

Consider first the case that M is odd. In that case we have the following expression for $\tilde{Z}_{N,M}$:

$$\begin{aligned}\tilde{Z}_{N,M} &= \sum_{k=0}^{(M-1)/2} (2\rho^N)^{\frac{M-1}{2}-k} \sum_{1\leq j_1<\cdots<j_k\leq\frac{M-1}{2}} \\ &\times \left\{ \zeta_{M,\pm}^{N/2} \prod_{r=1}^{k} (\zeta_{2j_r-1,+}^N + \zeta_{2j_r-1,-}^N) + \zeta_{2M,\pm}^{N/2} \prod_{r=1}^{k} (\zeta_{2j_r,+}^N + \zeta_{2j_r,-}^N) \right\},\end{aligned} \tag{B.1}$$

where the index $\pm$ is $+$ if $\frac{M-1}{2} - k$ is even and $-$ if $\frac{M-1}{2} - k$ is odd. Here

$$\rho = (1-\lambda^2)(1-u^2), \tag{B.2}$$

and $\zeta_{r,\pm}$ are given by

$$\zeta_{r,\pm} = (1+\lambda^2)(1+u^2) - 4u\lambda\cos\frac{r\pi}{M} \pm \sqrt{\Delta_r}, \text{ where} \tag{B.3}$$

$$\Delta_r = ((1+\lambda^2)(1+u^2) - 4u\lambda\cos\frac{r\pi}{M})^2 - \rho^2. \tag{B.4}$$

In particular,

$$\zeta_{M,\pm} = (1\pm\lambda)^2(1\pm u)^2 \text{ and } \zeta_{2M,\pm} = (1\pm u)^2(1\mp\lambda)^2. \tag{B.5}$$

B.2 Example: $M = 5$.

For $M = 5$ we get:

$$\begin{aligned}\tilde{Z}_{N,5} &= (1+u)^N(1+\lambda)^N(\zeta_{1,+}^N + \zeta_{1,-}^N)(\zeta_{3,+}^N + \zeta_{3,-}^N) \\ &+(1+u)^N(1-\lambda)^N(\zeta_{2,+}^N + \zeta_{2,-}^N)(\zeta_{4,+}^N + \zeta_{4,-}^N) \\ &+2(1-u^2)^N(1-\lambda^2)^N(1-u)^N(1-\lambda)^N(\zeta_{1,+}^N + \zeta_{1,-}^N + \zeta_{3,+}^N + \zeta_{3,-}^N) \\ &+2(1-u^2)^N(1-\lambda^2)^N(1-u)^N(1+\lambda)^N(\zeta_{2,+}^N + \zeta_{2,-}^N + \zeta_{4,+}^N + \zeta_{4,-}^N) \\ &+4(1-u^2)^{2N}(1-\lambda^2)^{2N}(1+u)^N[(1+\lambda)^N + (1-\lambda)^N].\end{aligned} \tag{B.6}$$

Here

$$\begin{aligned}\zeta_{r,\pm} &= (1+\lambda^2)(1+u^2) - 4u\lambda\cos\frac{r\pi}{5} \\ &\qquad \pm\sqrt{\left[(1+\lambda^2)(1+u^2) - 4u\lambda\cos\frac{r\pi}{5}\right]^2 - (1-\lambda^2)^2(1-u^2)^2}.\end{aligned} \tag{B.7}$$

B.3 The case M even.

In this case we have

$$\begin{aligned}\tilde{Z}_{N,M} &= \sum_{\substack{k=0 \\ M/2-k \text{ even}}}^{M/2} (2\rho^N)^{\frac{M}{2}-k} \sum_{1\le j_1<\cdots<j_k\le\frac{M}{2}} \prod_{r=1}^{k} (\zeta^N_{2j_r-1,+} + \zeta^N_{2j_r-1,-}) + \\ &\quad + \sum_{k=0}^{\frac{1}{2}M-1} (2\rho^N)^{\frac{M}{2}-k-1} \gamma_\pm \sum_{1\le j_1<\cdots<j_k\le\frac{1}{2}M-1} \prod_{r=1}^{k} (\zeta^N_{2j_r,+} + \zeta^N_{2j_r,-}),\end{aligned} \tag{B.8}$$

where the sign $\pm$ is $+$ if $\frac{M}{2}-k-1$ is even and $-$ if $\frac{M}{2}-k-1$ is odd. Here $\gamma_\pm$ are defined by

$$\gamma_+ = \zeta^{N/2}_{M,+}\zeta^{N/2}_{2M,+} + \zeta^{N/2}_{M,-}\zeta^{N/2}_{2M,-} = (1-\lambda^2)^N[(1+u)^{2N} + (1-u)^{2N}] \tag{B.9}$$

and

$$\gamma_- = \zeta^{N/2}_{M,+}\zeta^{N/2}_{2M,-} + \zeta^{N/2}_{M,-}\zeta^{N/2}_{2M,+} = (1-u^2)^N[(1+\lambda)^{2N} + (1-\lambda)^{2N}]. \tag{B.10}$$

B.4 Example: $M = 6$.

For $M = 6$ we get

$$\begin{aligned}
\tilde{Z}_{N,6} &= 4(1-\lambda^2)^{2N}(1-u^2)^{2N}(\zeta_{1,+}^N+\zeta_{1,-}^N+\zeta_{3,+}^N+\zeta_{3,-}^N+\zeta_{5,+}^N+\zeta_{5,-}^N) \\
&+(\zeta_{1,+}^N+\zeta_{1,-}^N)(\zeta_{3,+}^N+\zeta_{3,-}^N)(\zeta_{5,+}^N+\zeta_{5,-}^N) \\
&+4(1-\lambda^2)^{3N}(1-u^2)^{2N}((1+u)^{2N}+(1-u)^{2N}) \\
&+2(1-\lambda^2)^{N}(1-u^2)^{2N}((1+\lambda)^{2N}+(1-\lambda)^{2N})\big\{\zeta_{2,+}^N+\zeta_{2,-}^N+\zeta_{4,+}^N+\zeta_{4,-}^N\big\} \\
&+(1-\lambda^2)^{N}((1+u)^{2N}+(1-u)^{2N})(\zeta_{2,+}^N+\zeta_{2,-}^N)(\zeta_{4,+}^N+\zeta_{4,-}^N).
\end{aligned} \tag{B.11}$$

B.5 Example: $M = 8$.

For $M = 8$ we have

$$\begin{aligned}
\tilde{Z}_{N,8} &= 16(1-\lambda^2)^{4N}(1-u^2)^{4N} \\
&+4(1-\lambda^2)^{2N}(1-u^2)^{2N}\big\{(\zeta_{1,+}^N+\zeta_{1,-}^N)(\zeta_{3,+}^N+\zeta_{3,-}^N) \\
&+(\zeta_{1,+}^N+\zeta_{1,-}^N)(\zeta_{5,+}^N+\zeta_{5,-}^N)+(\zeta_{1,+}^N+\zeta_{1,-}^N)(\zeta_{7,+}^N+\zeta_{7,-}^N) \\
&+(\zeta_{3,+}^N+\zeta_{3,-}^N)(\zeta_{5,+}^N+\zeta_{5,-}^N)+(\zeta_{3,+}^N+\zeta_{3,-}^N)(\zeta_{7,+}^N+\zeta_{7,-}^N) \\
&+(\zeta_{5,+}^N+\zeta_{5,-}^N)(\zeta_{7,+}^N+\zeta_{7,-}^N)\big\} \\
&+(\zeta_{1,+}^N+\zeta_{1,-}^N)(\zeta_{3,+}^N+\zeta_{3,-}^N)(\zeta_{5,+}^N+\zeta_{5,-}^N)(\zeta_{7,+}^N+\zeta_{7,-}^N) \\
&+8(1-\lambda^2)^{4N}(1-u^2)^{3N}((1+u)^{2N}+(1-u)^{2N}) \\
&+4(1-\lambda^2)^{2N}(1-u^2)^{3N}((1-\lambda)^{2N}+(1-\lambda)^{2N})\big\{\zeta_{2,+}^N+\zeta_{2,-}^N \\
&+\zeta_{4,+}^N+\zeta_{4,-}^N+\zeta_{6,+}^N+\zeta_{6,-}^N\big\} \\
&+2(1-\lambda^2)^{2N}(1-u^2)^{N}((1+u)^{2N}+(1-u)^{2N}) \\
&\times\big\{(\zeta_{2,+}^N+\zeta_{2,-}^N)(\zeta_{4,+}^N+\zeta_{4,-}^N) \\
&+(\zeta_{2,+}^N+\zeta_{2,-}^N)(\zeta_{6,+}^N+\zeta_{6,-}^N)+(\zeta_{4,+}^N+\zeta_{4,-}^N)(\zeta_{6,+}^N+\zeta_{6,-}^N)\big\} \\
&+(1-u^2)^{N}((1-\lambda)^{2N}+(1-\lambda)^{2N}) \\
&\times(\zeta_{2,+}^N+\zeta_{2,-}^N)(\zeta_{4,+}^N+\zeta_{4,-}^N)(\zeta_{6,+}^N+\zeta_{6,-}^N).
\end{aligned} \tag{B.12}$$