

Representations of $O(N)$ Spin Models by Self-Avoiding Random Walks

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Abstract: We establish that correlation functions of classical lattice spin models can be represented by series expansions in terms of self-avoiding random walks. Using this, we get new upper bounds of critical temperatures of the $O(N)$ symmetric classical Heisenberg models.

1. Introduction

Based on the idea of Symanzik [20], the authors of [5, 4, 9] formulated the random walk representations of classical lattice spin systems and used them to derive various correlation inequalities and bounds for the critical inverse temperatures β_c . We tried to combine the idea of renormalization group with the random walk representations, and succeeded in the first step of transformations of block spin type. Namely we could renormalize the contribution of the smallest loops (self-crossing points) in the expansion as the changes of the single spin distributions and obtain an improvement of β_c for the $O(N)$ Heisenberg model [10, 11], in which the method of blockwise diagonalization of matrices is used to remove smallest loops from the random walk.

The purpose of this paper is to show that all loops can be removed from the random walk representations. In other words, we give a self-avoiding random walk representation of correlation functions of classical lattice spin systems, by which we obtain a new lower bound of β_c of the $O(N)$ Heisenberg model. It is better than the bound in [11] and is the most accurate among the theoretical values so far obtained. See the table. For example, we recover $\beta_c = \infty$ for every N on the one dimensional lattice, and we expect that this provides us with new methods to solve the long standing conjecture of non-existence of

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the phase transition in the two dimensional Heisenberg models [19]. A brief review of this paper is in [12] with some extended numerical analysis toward the problem.

In Sect. 2, the correlation function of two spins of the $O(N)$ spin model is represented in terms of a sum over self-avoiding walks that connect the two spin locations. Each term consists of the contour integration of determinants which depend on the walk. Section 3 is devoted to preparations of some mathematical devices about the contour integration which generalize the splitting arguments of [5, 10]. Applying to each term the block diagonalization method used in [10, 11] successively along the walk and then using an inequality of Sect. 3, we obtain bounds of the terms in Sect. 4. As a summary, we get in Sect. 5 the lower bound of β_c of the $O(N)$ spin model as a function of N and the connective constant. We also discuss the two limiting cases $N \rightarrow 0$ and $N \rightarrow \infty$.

2. Spin Models and Self-Avoiding Walks

Let Λ be a ν dimensional lattice, i.e., a finite subset of \mathbf{Z}^ν . We consider $O(N)$ symmetric classical Heisenberg model (N -vector model) on Λ with free boundary condition. Its partition function is given by

$$Z = \int_{\mathbf{R}^{N|\Lambda|}} \exp \left(\sum_{j,k \in \Lambda} J_{jk} \mathbf{S}_j \cdot \mathbf{S}_k / 2 \right) \prod_{j \in \Lambda} \frac{\delta(\mathbf{S}_j^2 - 1) d\mathbf{S}_j}{(2\pi)^{N/2}}, \tag{2.1}$$

where

$$J_{jk} = \begin{cases} \beta & \text{if } |j - k| = 1 \\ 0 & \text{otherwise} \end{cases} \tag{2.2}$$

for $j, k \in \Lambda$ and for the inverse temperature $\beta > 0$. We adopt the convention $|j| = \sum_{\mu=1}^\nu |j_\mu|$ for the norm of $j \in \Lambda$ in this paper.

Let Γ_λ be the contour given by the map

$$t \rightarrow \begin{cases} t\lambda e^{-i\pi/8} & (-\infty < t \leq -1) \\ \lambda e^{i(5t-4)\pi/8} & (-1 \leq t \leq 1) \\ t\lambda e^{i\pi/8} & (1 \leq t < \infty) \end{cases} \tag{2.3}$$

for $\lambda > 0$. Then we get the representations:

Lemma 1.

$$\begin{aligned} Z &= \int_{\Gamma_\lambda^{|\Lambda|}} \det^{-N/2}(2iA - J) \prod_{j \in \Lambda} \frac{e^{ia_j} da_j}{2\pi}, \tag{2.4} \\ &= \int_{\mathbf{R}^{N|\Lambda|}} S_i^{(1)} S_m^{(1)} \exp((\mathbf{S}, J\mathbf{S})/2) \prod_{j \in \Lambda} \frac{\delta(\mathbf{S}_j^2 - 1) d\mathbf{S}_j}{(2\pi)^{N/2}} \\ &= \int_{\Gamma_\lambda^{|\Lambda|}} (2iA - J)_{lm}^{-1} \det^{-N/2}(2iA - J) \prod_{j \in \Lambda} \frac{e^{ia_j} da_j}{2\pi}. \tag{2.5} \end{aligned}$$

Here, $l, m \in \Lambda$, $\mathbf{S}_j = (S_j^{(1)}, \dots, S_j^{(N)}) \in \mathbf{R}^N$ and A denotes the diagonal matrix given by $A_{jk} = a_j \delta_{jk}$ ($j, k \in \Lambda$).

Proof. After approximating $\delta(S^2 - 1)$ by the gaussian function, we perform the Fourier transformations by the formula

$$(2\pi\epsilon^2)^{-1/2} \exp(- (S^2 - 1)^2/2\epsilon^2) = \int_{-i\lambda + \mathbf{R}} \exp\left(-ia(S^2 - 1) - \frac{\epsilon^2 a^2}{2}\right) \frac{da}{2\pi}. \quad (2.6)$$

Then the lemma follows from Fubini's theorem and the integration with respect to S_l 's, followed by the replacement of the contour $-i\lambda + \mathbf{R}$ by Γ_λ . \square

Note that the representation of Lemma 1 is valid for all $\lambda > 0$. We set λ large in the following sections. Now, we develop self-avoiding random walk representations for $\langle S_l^{(\alpha)} S_m^{(\alpha)} \rangle$. We regard the matrices A and J as the operators acting on the linear space \mathbf{C}^Λ of all the \mathbf{C} -valued mappings defined on Λ . The set of mappings

$$e_k : \Lambda \ni j \mapsto \delta_{jk} \in \mathbf{C} \quad (k \in \Lambda) \quad (2.7)$$

forms a basis of the space. Let (\cdot, \cdot) be the bilinear form on \mathbf{C}^Λ defined by

$$\left(\sum_{j \in \Lambda} z_j e_j, \sum_{k \in \Lambda} w_k e_k\right) = \sum_{j \in \Lambda} z_j w_j. \quad (2.8)$$

Then $\{e_k\}_{k \in \Lambda}$ is the orthonormal basis with respect to (\cdot, \cdot) defined in the obvious way. The operators A and J are defined by

$$(e_j, A e_k) = A_{jk} = a_k \delta_{jk}, \quad (2.9)$$

$$(e_j, J e_k) = J_{jk} = \beta \delta_{|j-k|, 1}. \quad (2.10)$$

Let ω be a self-avoiding walk starting from l and ending at m . That is, let ω be a set of ordered pairs

$$\{(\omega(n-1), \omega(n)) \in \Lambda^2 \mid n = 1, \dots, \|\omega\|\} \quad (2.11)$$

satisfying

$$\begin{aligned} \omega(0) &= l, \quad \omega(\|\omega\|) = m, \\ |\omega(n-1) - \omega(n)| &= 1 \quad (n = 1, \dots, \|\omega\|), \\ \omega(n) &\neq \omega(n') \quad (n \neq n'), \end{aligned}$$

where $\|\omega\| \in \mathbf{N}$ is called the number of steps of the walk ω . Let Q_ω be the orthonormal projection to the subspace spanned by $\{e_{\omega(0)}, \dots, e_{\omega(\|\omega\|)}\}$:

$$Q_\omega \left(\sum_{j \in \Lambda} z_j e_j\right) = \sum_{n=0}^{\|\omega\|} z_{\omega(n)} e_{\omega(n)}. \quad (2.12)$$

We set $P_\omega = I_d - Q_\omega$. Now we have the following representation of the correlation function of the $O(N)$ Heisenberg model in terms of the self-avoiding random walk.

Theorem 1.

$$\langle S_l^{(1)} S_m^{(1)} \rangle = \sum_{\omega: l \rightarrow m} \beta^{|\omega|} Z(\omega) / Z. \tag{2.13}$$

Here, the summation is taken over all self-avoiding nearest neighbor walks ω on Λ starting from l and ending at m . The weight $Z(\omega)$ is given by

$$Z(\omega) = \int_{\Gamma_\lambda^{|\Lambda|}} \det(P_\omega(2iA - J)P_\omega) \det^{-(N+2)/2}(2iA - J) \left(\prod_{j \in \Lambda} \frac{e^{ia_j} da_j}{2\pi} \right), \tag{2.14}$$

where $\det(P_\omega(2iA - J)P_\omega)$ is the determinant of $P_\omega(2iA - J)P_\omega$ as the operator acting on the space $P_\omega \mathbb{C}^\Lambda$, i.e., the corresponding minor determinant of $2iA - J$.

Remark 1. We frequently deal with operators of type $\tilde{T} = PTP$ in the sequel as well as in the theorem, where T is an operator on \mathbb{C}^Λ and P is an orthonormal projection like P_ω or Q_ω . By $\det \tilde{T}$, we always mean the determinant of \tilde{T} which is regarded as the operator acting on PC^Λ as in the theorem. The operator which acts as the inverse of \tilde{T} on PC^Λ and 0 on $(I_d - P)\mathbb{C}^\Lambda$ is denoted by \tilde{T}^{-1} , i.e., \tilde{T}^{-1} satisfies

$$\tilde{T}^{-1}\tilde{T} = \tilde{T}\tilde{T}^{-1} = P, \quad (I_d - P)\tilde{T}^{-1} = \tilde{T}^{-1}(I_d - P) = 0. \tag{2.15}$$

Proof. Let $D(l_1, \dots, l_n; m_1, \dots, m_n)$ be the minor determinant made by eliminating the l_1, \dots, l_n^{th} rows and m_1, \dots, m_n^{th} columns from the matrix $2iA - J$. In order to define determinants of operators on \mathbb{C}^Λ , we number all $j \in \Lambda$ by $\{1, 2, \dots, |\Lambda|\}$. Let N_j be the number of j . If $l = m$, we have $(2iA - J)_{ll}^{-1} = D(l; l) / \det(2iA - J)$ in (2.5), which corresponds to the self-avoiding walk of zero step from l to l . For $l \neq m$, applying the Laplace expansion along the l^{th} column to $D(l; m)$, we have

$$\begin{aligned} (2iA - J)_{lm}^{-1} &= \epsilon_l \epsilon_m D(l; m) / \det(2iA - J) \\ &= \sum_{k_1} \epsilon_l \epsilon_m \epsilon_{k_1} \epsilon_{k_1 l} \epsilon_l \epsilon_{lm} (-\beta) D(k_1, l; l, m) / \det(2iA - J), \end{aligned}$$

where $\epsilon_l = (-1)^{N_l - 1}$ and $\epsilon_{kl} = 1$ if $N_k < N_l$, -1 if $N_k > N_l$. The summation is taken over all $k_1 \in \Lambda - \{l\}$ satisfying $|k_1 - l| = 1$, because of (2.2). When the term corresponding to $k_1 = m$ is allowed, it equals $\beta D(m, l; l, m)$. Except for the term $k_1 = m$, we apply the Laplace expansion along the k_1^{th} column to $D(k_1, l; l, m)$:

$$D(k_1, l; l, m) = \sum_{k_2} \epsilon_{k_2} \epsilon_{k_2 k_1} \epsilon_{k_2 l} \epsilon_{k_1} \epsilon_{k_1 l} \epsilon_{k_1 m} (-\beta) D(k_2, k_1, l; k_1, l, m), \tag{2.16}$$

where all $k_2 \in \Lambda - \{l, k_1\}$ satisfying $|k_2 - k_1| = 1$ are to be summed. We repeat the procedure until no non-zero terms remain except for the terms of type $\beta^{n+1} D(m, k_n, \dots, k_1, l; k_n, \dots, k_1, l, m)$, which corresponds to the self-avoiding nearest neighbor walk $l \rightarrow k_1 \rightarrow \dots \rightarrow k_n \rightarrow m$. Note that each of these terms has the sign plus. Since the lattice Λ is finite, the procedure terminates after finite iterations. Thus we get the formula. \square

Remark 2. In order to get the representations of the correlation functions in terms of the self-avoiding random walk, we used only the Fourier transformations of single spin distributions and the Laplace expansions of determinants. Then the n -point functions of various lattice spin systems with various boundary conditions have similar representations. However, we may not apply the method to get a similar formula for lattice gauge systems.

3. Integration on $\Gamma_\lambda^{|\Lambda|}$

In this section, we prepare some properties of the integration with respect to the complex variables $\{a_j\}_{j \in \Lambda}$ on $\Gamma_\lambda^{|\Lambda|}$. We give them for a certain class of functions specified below for later convenience.

Let $\delta > 0$ be an arbitrary but fixed constant. For a function f and a matrix valued function T defined on the polydisc

$$D_\delta^{|\Lambda|} = \left\{ z = \{z_j\}_{j \in \Lambda} \in \mathbb{C}^\Lambda \mid |z_j| \leq \delta (\forall j \in \Lambda) \right\},$$

we introduce norms

$$\|f\|_\delta = \sup_{z \in D_\delta^{|\Lambda|}} |f(z)|, \quad \|T\|_\delta = \sup_j \sum_k \|T_{jk}\|_\delta.$$

We define a class of analytic functions on $D_\delta^{|\Lambda|}$ by

$$\mathcal{F}_\delta = \left\{ f(z) = \sum_{\alpha \in \bar{\mathbf{N}}^\Lambda} c_\alpha z^\alpha \mid c_\alpha \geq 0 (\forall \alpha \in \bar{\mathbf{N}}^\Lambda), \|f\|_\delta = \sum_{\alpha \in \bar{\mathbf{N}}^\Lambda} c_\alpha \delta^{|\alpha|} < \infty \right\}.$$

Here, $\bar{\mathbf{N}} = \{0, 1, 2, \dots\}$ and $|\alpha| = \sum_{j \in \Lambda} \alpha_j, z^\alpha = \prod_{j \in \Lambda} z_j^{\alpha_j}$ for the multi-index $\alpha = \{\alpha_j\}_{j \in \Lambda} \in \bar{\mathbf{N}}^\Lambda$. We will need another class of analytic functions defined by

$$\mathcal{E}^s = \left\{ h(z) = C z^{(s)+\alpha} \exp\left(\sum_{j \in \Lambda} c_j z_j\right) \mid C > 0, \alpha \in \bar{\mathbf{N}}^\Lambda, c_j \geq 0 (\forall j \in \Lambda) \right\}$$

for an arbitrary but fixed $s > 0$. Here, $z^{(s)+\alpha} = \prod_{j \in \Lambda} z_j^{s+\alpha_j}$. Then the following proposition holds:

Proposition 1. (i) \mathcal{F}_δ contains all polynomials with positive coefficients.

(ii) $f, g \in \mathcal{F}_\delta \implies e^f, f + g, fg \in \mathcal{F}_\delta$.

Proof. Substituting $f \in \mathcal{F}_\delta$ into the Maclaurin expansion of e^z , we find $e^f \in \mathcal{F}_\delta$. The other properties are obvious. \square

Let us introduce an integration of functions of the form fh ($f \in \mathcal{F}_\delta, h \in \mathcal{E}^s$). We put

$$\llbracket fh \rrbracket = \int_{\Gamma_\lambda^{|\Lambda|}} f\left(\frac{1}{2ia}\right) h\left(\frac{1}{2ia}\right) \prod_{j \in \Lambda} \frac{e^{ia_j} da_j}{2\pi} \tag{3.1}$$

for $f \in \mathcal{F}_\delta$ and $\lambda \in (1/2\delta, \infty)$. Since f and h are bounded and $e^{ia} da$ is a finite (complex valued) measure on Γ_λ , the integral is well-defined. Note also that the expectation value $\llbracket fh \rrbracket$ does not depend on the choice of $\lambda > 1/2\delta$ because of Cauchy's integral theorem.

Proposition 2. For $\alpha \in \bar{\mathbf{N}}^\Lambda, f, g \in \mathcal{F}_\delta$ and $h \in \mathcal{E}^s$, the following relations hold:

(i) $\llbracket z^{(s)+\alpha} \rrbracket = \prod_{j \in \Lambda} 2^{-(s+\alpha_j)} \Gamma(s + \alpha_j)^{-1},$

(ii) $\llbracket fh \rrbracket \geq 0, \llbracket fh \rrbracket = 0 \iff f = 0,$

(iii) $\llbracket fgh \rrbracket \llbracket h \rrbracket \leq \llbracket fh \rrbracket \llbracket gh \rrbracket. \tag{3.2}$

Proof. To prove the first relation, it is enough to show

$$\int_{\Gamma_\lambda} \frac{e^{ia}}{(2ia)^u} \frac{da}{2\pi} = \frac{1}{2^u \Gamma(u)} \tag{3.3}$$

for any $u > 0$;

$$\begin{aligned} \text{l.h.s. of (3.3)} &= \lim_{\epsilon \downarrow 0} \int_{\mathbf{R}-i\lambda} \frac{da}{2\pi(2ia)^u} \exp \left[ia - \frac{\epsilon^2 a^2}{2} \right] \\ &= \lim_{\epsilon \downarrow 0} \int_{\mathbf{R}-i\lambda} \frac{da}{2\pi} \frac{1}{\Gamma(u)} \int_0^\infty \exp \left[ia(1-2t) - \frac{\epsilon^2 a^2}{2} \right] t^{u-1} dt \\ &= \lim_{\epsilon \downarrow 0} \frac{1}{\Gamma(u)} \int_0^\infty \frac{t^{u-1}}{\sqrt{2\pi\epsilon^2}} \exp \left[-\frac{(2t-1)^2}{2\epsilon^2} \right] dt \\ &= \frac{1}{2^u \Gamma(u)}. \end{aligned}$$

The case that f is a monomial in (ii) is an obvious consequence of (i). The dominated convergence theorem leads to the general case because $f \in \mathcal{F}_\delta$ has non-negative coefficients.

For the third relation, it is enough to show

$$\mathcal{I}_{s+2}(c)\mathcal{I}_s(c) \leq \mathcal{I}_{s+1}(c)^2, \tag{3.4}$$

where

$$\mathcal{I}_s(c) \equiv \int_{\Gamma_\lambda} \exp\left(ia + \frac{c}{2ia}\right) \frac{da}{(2ia)^s 2\pi} = \frac{I_{s-1}(\sqrt{2c})}{2(\sqrt{2c})^{s-1}},$$

s and c are non-negative constants and I_s is the s^{th} modified Bessel function. In fact, using (3.4) repeatedly, we get

$$\mathcal{I}_{s+n+m}(c)\mathcal{I}_s(c) \leq \mathcal{I}_{s+m}(c)\mathcal{I}_{s+n}(c) \tag{3.5}$$

for $n, m \in \bar{\mathbf{N}}$. The case where f and g are monomials is the multiplication of those inequalities with appropriate numbers n, m and c . Bilinearity of the inequality in f and g , the dominated convergence theorem and (3.5) establish the general case. For the proof of (3.4), we refer to [15]. (See also [10].) \square

Let us apply this formulation to the $O(N)$ Heisenberg model. We choose λ and δ^{-1} so large that

$$\lambda > 1/2\delta > 3\nu\beta \tag{3.6}$$

holds. The condition is sufficient for the arguments in the proof of Lemma 3 in Sect.4. Let $2iA - J$ be the operator on \mathbf{C}^Λ defined in Sect.2, and Q the orthonormal projection onto the subspace spanned by $\{e_j\}_{j \in \Delta}$ defined similarly as (2.12), where Δ is an arbitrary subset of Λ . Then we have

Proposition 3. *As functions of complex variables $z_j = (2ia_j)^{-1}$ ($j \in \Lambda$),*

$$\det^{-N/2}(2iA) \in \mathcal{E}^{N/2},$$

and the following functions belong to \mathcal{F}_δ :

$$(2iA - J)_{jk}^{-1}, (Q(2iA - J)Q)_{jk}^{-1}, \det^{N/2}(2iA)\det^{-N/2}(2iA - J), \\ \det^{N/2}(Q2iAQ) \det^{-N/2}(Q(2iA - J)Q),$$

where the determinants and the inverses of the operators $Q(2iA - J)Q$ and $Q2iAQ$ are considered as those of the corresponding matrices with the index set Δ . (See Remark 1.)

Proof. As a function of the complex variables $z_j = (2ia_j)^{-1}$,

$$\det^{-N/2}(2iA) = \prod_{j \in \Delta} (2ia_j)^{-N/2} \in \mathcal{E}^{N/2}.$$

From the relations

$$(Q(2iA - J)Q)^{-1} = (2iA)^{-1}Q \sum_{n=0}^{\infty} (J(2iA)^{-1}Q)^n, \\ \det^{N/2}(2iA)\det^{-N/2}(2iA - J) = \exp \left[\frac{N}{2} \sum_{n=1}^{\infty} \frac{1}{n} \text{Tr} \left(J(2iA)^{-1} \right)^n \right],$$

and so on, these quantities are the series of the variables $z_j = (2ia_j)^{-1}$ whose coefficients are all non-negative since the matrices J and Q have only non-negative components. And we get

$$\| (Q(2iA - J)Q)_{jk}^{-1} \|_{\delta} \leq \| (Q(2iA - J)Q)^{-1} \|_{\delta} \\ \leq \delta \sum_{n=0}^{\infty} (2\nu\beta\delta)^n = \delta / (1 - 2\nu\beta\delta), \tag{3.7} \\ \| \det^{N/2}(2iA)\det^{-N/2}(2iA - J) \|_{\delta} \leq 1 / (1 - 2\nu\beta\delta)^{N|\Delta|/2},$$

and so on, where we have used the relations $\|ST\|_{\delta} \leq \|S\|_{\delta}\|T\|_{\delta}$, $\|\text{Tr } T\|_{\delta} \leq |\Delta|\|T\|_{\delta}$ and $\|2iA\|_{\delta} = \delta^{-1}$, $\|Q\|_{\delta} = 1$, $\|J\|_{\delta} = 2\nu\beta$. Thus we have the proposition under condition (3.6). \square

4. Estimates of $Z(\omega)/Z$

In this section, we estimate $Z(\omega)/Z$ using the formulation of the preceding section. The result is summarized in

Theorem 2. For every self-avoiding walk ω on the lattice Λ ,

$$0 < Z(\omega)/Z \leq \frac{1}{N\beta^{|\omega|}} \left(\frac{I_{N/2}(\beta)}{I_{(N-2)/2}(\beta)} \right)^{|\omega|}. \tag{4.1}$$

We prove the theorem in three steps. First, we perform successive block diagonalization of $2iA - J$ along the walk ω . Next, we shift the integral variables $\{a_j\}$ living on ω . And finally, Prop. 2 is applied to get the bound. Let B, C, K and K^T denote the operators

$$B = P_{\omega}(2iA - J)P_{\omega}, \quad C = Q_{\omega}(2iA - J)Q_{\omega}, \quad K = P_{\omega}JQ_{\omega}$$

and the transpose of K , $K^T = Q_{\omega}JP_{\omega}$. Then we have the first block diagonalization.

Lemma 2. *The representations*

$$\begin{aligned} Z(\omega) &= \llbracket \det^{-N/2} B \det^{-(N+2)/2} (C - K^T B^{-1} K) \rrbracket, \\ Z &= \llbracket \det^{-N/2} B \det^{-N/2} (C - K^T B^{-1} K) \rrbracket \end{aligned}$$

hold, where $\det B$ and $\det(C - K^T B^{-1} K)$ denote the determinants of B and $C - K^T B^{-1} K$ in the sense of Remark 1.

Proof. Operating $P_\omega + Q_\omega = I_d$ to $2iA - J$ from both sides and diagonalizing blockwise by the triangular matrices $I_d - K^T B^{-1}$ and $I_d - B^{-1} K$, we obtain

$$\begin{aligned} 2iA - J &= B + C - K - K^T \\ &= (I_d - K^T B^{-1})(B + C - K^T B^{-1} K)(I_d - B^{-1} K), \end{aligned} \tag{4.2}$$

or equivalently

$$\begin{aligned} 2iA - J &= \begin{pmatrix} B & -K \\ -K^T & C \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ -K^T B^{-1} & 1 \end{pmatrix} \begin{pmatrix} B & 0 \\ 0 & C - K^T B^{-1} K \end{pmatrix} \begin{pmatrix} 1 & -B^{-1} K \\ 0 & 1 \end{pmatrix} \end{aligned}$$

on $(P_\omega \mathbf{C}^A) \oplus (Q_\omega \mathbf{C}^A)$ in the block matrix notation used in [10, 11]. For B^{-1} , recall Remark 1 and Prop. 3. Since the determinants of the first and the third factors of (4.2) are 1, we have

$$\det(2iA - J) = \det B \det(C - K^T B^{-1} K). \quad \square$$

Next, we diagonalize $C - K^T B^{-1} K$ blockwise by triangular matrices successively along ω . For $n = 0, 1, \dots, \|\omega\|$, Q_n denotes the orthonormal projection to the one dimensional subspace $\mathbf{C}e_{\omega(n)}$ of \mathbf{C}^A . Let the operator C_n and the function V_n be given inductively by

$$V_n = \left(e_{\omega(n)}, J(B^{-1} + (I_d + B^{-1} J)C_{n+1}^{-1}(I_d + JB^{-1}))J e_{\omega(n)} \right), \tag{4.3}$$

$$C_n^{-1} = C_{n+1}^{-1} + \frac{(I_d + C_{n+1}^{-1} J(I_d + B^{-1} J))Q_n(I_d + (I_d + JB^{-1})JC_{n+1}^{-1})}{2ia_{\omega(n)} - V_n}, \tag{4.4}$$

$$C_{|\omega|+1}^{-1} = 0. \tag{4.5}$$

Then we have the following lemma.

Lemma 3.

$$\det(C - K^T B^{-1} K) = \prod_{n=0}^{|\omega|} (2ia_{\omega(n)} - V_n). \tag{4.6}$$

Proof. Put $R_1 = Q_\omega - Q_0$, which is the orthonormal projection to the subspace spanned by $\{e_{\omega(1)}, \dots, e_{\omega(|\omega|)}\}$. Then we have

$$\begin{aligned} C_0 &\equiv C - K^T B^{-1} K = Q_\omega(2iA - J - JB^{-1} J)Q_\omega \\ &= (2ia_{\omega(0)} - (e_{\omega(0)}, JB^{-1} J e_{\omega(0)}))Q_0 - K_1 - K_1^T + C_1 \\ &= \begin{pmatrix} C_1 & -K_1 \\ -K_1^T & 2ia_{\omega(0)} - (e_{\omega(0)}, JB^{-1} J e_{\omega(0)}) \end{pmatrix}, \end{aligned}$$

where $C_1 = R_1(2iA - J - JB^{-1}J)R_1$, $K_1 = R_1(J + JB^{-1}J)Q_0$ and its transpose $K_1^T = Q_0(J + JB^{-1}J)R_1$. Let us perform the block diagonalization of C_0 by the triangular matrices $I_d - K_1^T C_1^{-1}$ and $I_d - C_1^{-1} K_1$:

$$C_0 = \begin{pmatrix} 1 & 0 \\ -K_1^T C_1^{-1} & 1 \end{pmatrix} \begin{pmatrix} C_1 & 0 \\ 0 & 2ia_{\omega(0)} - V_0 \end{pmatrix} \begin{pmatrix} 1 & -C_1^{-1} K_1 \\ 0 & 1 \end{pmatrix} \\ = (I_d - K_1^T C_1^{-1})(C_1 + Q_0(2ia_{\omega(0)} - V_0))(I_d - C_1^{-1} K_1), \tag{4.7}$$

where $V_0 = (e_{\omega(0)}, J(B^{-1} + (I_d + B^{-1}J)C_1^{-1}(I_d + JB^{-1}))Je_{\omega(0)})$ and C_1^{-1} denotes the inverse of the operator C_1 in the sense of Remark 1. It is given by the expansion $C_1^{-1} = (2iA)^{-1}R_1 \sum_{n=0}^{\infty} ((J + JB^{-1}J)(2iA)^{-1}R_1)^n$. Note that each component of C_1^{-1} belongs to \mathcal{F}_δ . In fact, B^{-1} is in \mathcal{F}_δ componentwise, so the expansion consists of powers of the variables $z_j = (2ia_j)^{-1}$ with non-negative coefficients. Furthermore

$$\|C_1^{-1}\|_\delta \leq \delta \sum_{n=0}^{\infty} \left[\left(2\nu\beta + 2\nu\beta \frac{\delta}{1 - 2\nu\beta\delta} 2\nu\beta \right) \delta \right]^n \\ = \delta(1 - 2\nu\beta\delta)/(1 - 4\nu\beta\delta) < \infty \tag{4.8}$$

holds because of (3.6), where we used the estimate (3.7). We get $V_0 \in \mathcal{F}_\delta$ and $\|V_0\|_\delta \leq 8\nu^2\beta^2\delta/(1 - 4\nu\beta\delta) < \delta^{-1} \leq |2ia_{\omega(0)}|$ under the condition (3.6) similarly. So, $2ia_{\omega(0)} - V_0$ does not vanish on $D_\delta^{|A|}$. Thus we can invert (4.7), and obtain

$$C_0^{-1} = (I_d + C_1^{-1} K_1) \left(C_1^{-1} + \frac{Q_0}{2ia_{\omega(0)} - V_0} \right) (I_d + K_1^T C_1^{-1}) \\ = C_1^{-1} + \frac{(I_d + C_1^{-1} J(I_d + B^{-1}J))Q_0(I_d + (I_d + JB^{-1})JC_1^{-1})}{2ia_{\omega(0)} - V_0}.$$

From (4.7), we also have

$$\det C_0 = (2ia_{\omega(0)} - V_0) \det C_1. \tag{4.9}$$

We make a similar procedure with $\omega(1)$ instead of $\omega(0)$, and so on. In general, we put $R_n = R_{n-1} - Q_{n-1}$ ($n = 1, 2, \dots$), which is the orthonormal projection to the subspace spanned by $\{e_{\omega(n)}, \dots, e_{\omega(|\omega|)}\}$. Then we have

$$C_{n-1} \equiv R_{n-1}(2iA - J - JB^{-1}J)R_{n-1} \tag{4.10}$$

$$= (2ia_{\omega(n-1)} - (e_{\omega(n-1)}, JB^{-1}Je_{\omega(n-1)}))Q_{n-1} \\ - K_n - K_n^T + C_n, \tag{4.11}$$

where $C_n = R_n(2iA - J - JB^{-1}J)R_n$, $K_n = R_n(J + JB^{-1}J)Q_{n-1}$ and its transpose $K_n^T = Q_{n-1}(J + JB^{-1}J)R_n$. We again perform the block diagonalization of C_{n-1} by the triangular matrices:

$$C_{n-1} = (I_d - K_n^T C_n^{-1})(C_n + Q_{n-1}(2ia_{\omega(n-1)} - V_{n-1}))(I_d - C_n^{-1} K_n).$$

It follows from (4.10) that $\|C_{n-1}\|_\delta$ and $\|V_{n-1}\|_\delta$ have the same bounds as $\|C_1\|_\delta$ and $\|V_0\|_\delta$ respectively. Hence, $2ia_{\omega(n-1)} - V_{n-1}$ does not vanish. Then we get (4.3), (4.4) and

$$\det C_{n-1} = (2ia_{\omega(n-1)} - V_{n-1}) \det C_n. \tag{4.12}$$

This completes the proof of the lemma. \square

As the second step, let us shift the integration variables living on the walk ω . Let the operators \tilde{C}_n , and the functions \tilde{V}_n be defined inductively by

$$\tilde{V}_n = \left(e_{\omega(n)}, J(B^{-1} + (I_d + B^{-1}J)\tilde{C}_{n+1}^{-1}(I_d + JB^{-1}))Je_{\omega(n)} \right), \tag{4.13}$$

$$\begin{aligned} \tilde{C}_n^{-1} &= \tilde{C}_{n+1}^{-1} \\ &+ \frac{(I_d + \tilde{C}_{n+1}^{-1}J(I_d + B^{-1}J))Q_n(I_d + (I_d + JB^{-1})J\tilde{C}_{n+1}^{-1})}{2ia_{\omega(n)}}, \end{aligned} \tag{4.14}$$

$$\tilde{C}_{|\omega|+1}^{-1} = 0, \tag{4.15}$$

where $n = 0, 1, \dots, \|\omega\|$. Then we have the following lemma.

Lemma 4.

$$Z(\omega)/Z = \frac{\llbracket \det^{-N/2} B \exp \left(\sum_{n=0}^{|\omega|} \tilde{V}_n/2 \right) \prod_{n=0}^{|\omega|} (2ia_{\omega(n)})^{-(N+2)/2} \rrbracket}{\llbracket \det^{-N/2} B \exp \left(\sum_{n=0}^{|\omega|} \tilde{V}_n/2 \right) \prod_{n=0}^{|\omega|} (2ia_{\omega(n)})^{-N/2} \rrbracket}. \tag{4.16}$$

Proof. We obtain the lemma from Lemma 3 by changing the integral variables. From (4.3), (4.4), and (4.5), it is obvious that C_{n+1} and V_n do not depend on the complex variables $\{a_{\omega(0)}, \dots, a_{\omega(n)}\}$. Let us consider the integration with respect to $a_{\omega(0)}$ for fixed $\{a_j\}_{j \in \Lambda - \{\omega(0)\}} \in \Gamma_\lambda^{|\Lambda|-1}$. We shift the integral variable $\tilde{a}_{\omega(0)} = a_{\omega(0)} - V_0/2i$, and then deform the contour of integration with respect to $\tilde{a}_{\omega(0)}$ from $\Gamma_\lambda - V_0/2i$ to Γ_λ . Note that the deformation can be made by avoiding the singularity $\tilde{a}_{\omega(0)} = 0$ as in the proof of the above lemma. It follows from Cauchy’s integral theorem that

$$Z(\omega) = \llbracket \det^{-N/2} B \exp(V_0/2) (2ia_{\omega(0)})^{-(N+2)/2} \prod_{n=1}^{|\omega|} (2ia_{\omega(n)} - V_n)^{-(N+2)/2} \rrbracket, \tag{4.17}$$

where we put the notation $\tilde{a}_{\omega(0)}$ back to $a_{\omega(0)}$. Next, using Fubini’s theorem, we consider the integration with respect to $a_{\omega(1)}$ for fixed $\{a_j\}_{j \in \Lambda - \{\omega(1)\}} \in \Gamma_\lambda^{|\Lambda|-1}$. We perform the shift $a_{\omega(1)} \rightarrow a_{\omega(1)} + V_1/2i$, followed by the deformation of the contour of integration. Note that V_0 is changed by this shift. After performing these operations on variables $\{a_{\omega(0)}, a_{\omega(1)}, \dots, a_{\omega(|\omega|)}\}$, we get the representation for $Z(\omega)$. The same procedure also yields the denominator. \square

To finish the proof of the theorem, we apply the inequality (2) to the expression (4.16). It is seen from (4.13), (4.14), (4.15) that $\tilde{V}_n \in \mathcal{F}_\delta$ and \tilde{V}_n contains the term $\beta^2/2ia_{\omega(n+1)}$. Extracting these terms from $\tilde{V}_0, \dots, \tilde{V}_{|\omega|-1}$, we have the decomposition

$$\det^{-N/2} B \exp \left(\sum_{n=0}^{|\omega|} \tilde{V}_n/2 \right) \prod_{n=0}^{|\omega|} (2ia_{\omega(n)})^{-N/2} = hf,$$

where $f \in \mathcal{F}_\delta$ and

$$h = \exp \left(\sum_{n=1}^{|\omega|} \beta^2/4ia_{\omega(n)} \right) \prod_{j \in \Lambda} (2ia_j)^{-N/2} \in \mathcal{E}^{N/2},$$

thanks to Prop. 3. Using (2) for the above f, h and

$$g = \prod_{n=0}^{|\omega|} (2ia_{\omega(n)})^{-1} \in \mathcal{F}_\delta,$$

we get

$$\begin{aligned} Z(\omega)/Z &= \frac{\llbracket h f g \rrbracket}{\llbracket h f \rrbracket} \leq \frac{\llbracket h g \rrbracket}{\llbracket h \rrbracket} \\ &= \frac{1}{N} \left(\frac{I_{(N+2)/2}(\beta^2/2)}{I_{N/2}(\beta^2/2)} \right)^{|\omega|} = \frac{1}{N\beta^{|\omega|}} \left(\frac{I_{N/2}(\beta)}{I_{(N-2)/2}(\beta)} \right)^{|\omega|}. \quad \square \end{aligned}$$

Remark 3. The shifts of those integration variables may be interpreted as a renormalization of the single spin distributions. The integrand e^{ia_j} , which comes from the Fourier transformation of $\delta(S_j^2 - 1)$ is replaced by $\exp(ia_j + \beta^2/4ia_j)$, which absorbs the complicated effects of the interaction.

Remark 4. A slightly stronger bound holds in Theorem 2. In fact, we note that \tilde{V}_n contains the terms

$$\sum_{\substack{m \in \{n+1, \dots, \|\omega\|\} \\ |\omega(m) - \omega(n)| = 1}} \frac{\beta^2}{2ia_{\omega(m)}}.$$

Extracting these terms from $\tilde{V}_0, \dots, \tilde{V}_{|\omega|-1}$, we can get the following bound as in the last step of the above proof:

$$Z(\omega)/Z \leq \frac{1}{N} \prod_{m=1}^{|\omega|} \frac{1}{\beta\sqrt{\tau(m, \omega)}} \frac{I_{N/2}(\beta\sqrt{\tau(m, \omega)})}{I_{(N-2)/2}(\beta\sqrt{\tau(m, \omega)})}, \tag{4.18}$$

where $\tau(m, \omega) = \#\left\{ n \in \{0, 1, \dots, m-1\} \mid |\omega(m) - \omega(n)| = 1 \right\}$, i.e., the number of times the self-avoiding walk ω visits the nearest neighbor points of $\omega(m)$ before the m^{th} step.

5. Lower Bounds of β_c

In this section, we discuss lower bounds of the inverse critical temperatures of the $O(N)$ symmetric Heisenberg models. From Theorem 1 and 2, we get

$$0 < \langle S_l^{(1)} S_m^{(1)} \rangle \leq \sum_{\omega: l \rightarrow m} \frac{1}{N} \left(\frac{I_{N/2}(\beta)}{I_{(N-2)/2}(\beta)} \right)^{|\omega|}. \tag{5.1}$$

Here the summation is taken over all self-avoiding walks starting from l and ending at m on Λ . This is a bound of the correlation function of the $O(N)$ spin model by the generating function of self-avoiding walks that connect the two spin locations with activity $I_{N/2}(\beta)/I_{(N-2)/2}(\beta)$. It is a generalization of the case $N = 1$ [6] to all N . If all the self-avoiding walks in Z^ν connecting l and m are taken into account in the summation in (5.1), the bound is uniform in Λ . Then the above inequality also holds for the thermodynamic limit taken under the free boundary condition. Let μ_ν be the connective

constant in the ν -dimensional lattice defined by $\log \mu_\nu = \lim_{l \rightarrow \infty} l^{-1} \log s_l'$, where s_l' is the total number of self-avoiding nearest neighbor walks in \mathbb{Z}^ν of length l starting from the origin (see e.g. [17]). Then the correlation function decays exponentially when the activity $I_{N/2}(\beta)/I_{(N-2)/2}(\beta)$ is smaller than the inverse of the connective constant μ_ν^{-1} . Since the critical inverse temperature β_c is defined as the maximum number of those β below which the correlation function exhibits exponential decay, we have:

Corollary 1. *For the ν -dimensional $O(N)$ symmetric Heisenberg model,*

$$\beta_c \geq \inf \{ \beta > 0 \mid \mu_\nu I_{N/2}(\beta)/I_{(N-2)/2}(\beta) \geq 1 \}. \tag{5.2}$$

Let us apply the corollary to one-dimensional cases. The connective constant μ_1 is 1. The inequality $I_{N/2}(\beta) < I_{(N-2)/2}(\beta)$ holds for every $\beta > 0$ and $N \in \mathbb{N}$. So we recover the fact $\beta_c = \infty$.

For the cases $\nu \geq 2$, the precise values of the connective constants have not been known, yet. But it is rigorously known that $\mu_2 \leq 2.69576, \mu_3 \leq 4.756, \mu_4 \leq 6.832$ [1], and it is expected that $\mu_2 = 2.638, \mu_3 = 4.683, \mu_4 = 6.775$ [18]. The numerical values using Corollary 1 and the above upper bounds and expected values of μ_ν are listed in Table 1, and they are in good agreement with experimental results except for two dimensional cases.

The following properties of the modified Bessel functions can be obtained readily ((5) is proved in the appendix):

(i) $I_s(x)/I_{s-1}(x) \leq x/2s, \quad (s > 0, x > 0), \tag{5.3}$

(ii) $I_s(x)/I_{s-1}(x) \leq \frac{x}{s-1+\sqrt{s^2+x^2}}. \quad (s \geq 1/2, x > 0). \tag{5.4}$

Summarizing these arguments, we have the following bounds.

Corollary 2.

$$\begin{aligned} \text{(i)} \quad & \beta_c \geq N/\mu_\nu, && \text{for all } N, \\ \text{(ii)} \quad & \beta_c \geq \mu_\nu N/(\mu_\nu^2 - 1) + O(1), && N \rightarrow \infty, \\ \text{(iii)} \quad & \beta_c = \infty && \text{for } \nu = 1. \end{aligned}$$

Finally, we mention the two limiting cases $N \rightarrow 0$ and $N \rightarrow \infty$, briefly. For these limits, we vary N and β while $\bar{\beta} = \beta/N$ fixed, and investigate $N \langle S_i^{(1)} S_m^{(1)} \rangle$. This is equivalent to examine $\langle S_i^{(1)} S_m^{(1)} \rangle$ under the normalization $\delta(\mathbb{S}^2 - N)$ instead of $\delta(\mathbb{S}^2 - 1)$ and $\bar{\beta}$ instead of β in (2.1), (2.2) and (2.5). From (5.1) and (5), we have

$$N \langle S_i^{(1)} S_m^{(1)} \rangle \leq \sum_{\omega: l \rightarrow m} \left(\frac{I_{N/2}(N\bar{\beta})}{I_{(N-2)/2}(N\bar{\beta})} \right)^{|\omega|} \leq \sum_{\omega: l \rightarrow m} \bar{\beta}^{|\omega|}.$$

It is known that in the limit $N \rightarrow 0$ the left-hand side converges to the right-hand side in these inequalities[17]. Hence, our bound is sharp in this limit. The self-avoiding random walk representation in this paper may be considered as a generalization of the relation between the $O(N)$ spin model with $N = 0, 1$ and the self-avoiding walks. For the $N \rightarrow \infty$ case, it follows from (5.1) and (5) that

$$\limsup_{N \rightarrow \infty} N \langle S_l^{(1)} S_m^{(1)} \rangle \leq \sum_{\omega: l \rightarrow m} \left(\frac{2\bar{\beta}}{1 + \sqrt{1 + 4\bar{\beta}^2}} \right)^{|\omega|},$$

where the right-hand side decays exponentially if and only if $\bar{\beta} < \mu_\nu / (\mu_\nu^2 - 1)$. Thus in the present method, we unfortunately could not confirm the well-known result $\bar{\beta} = \infty$ for $\nu = 2$, which was suggested, e.g. by Ma [16] by the $1/N$ expansion. As is seen from our numerical results, accuracy of our results decreases as N increases.

As a conclusion, we could not prove our long standing conjecture $\beta_c(\nu = 2, N \geq 3) = \infty$ [19] in the present framework, even if we used the better bound (4.18). If the conjecture is true after all, we believe that this could be proved by taking more effects of \tilde{V}_n into our considerations, or by simplifying (renormalizing) walks at longer distance scales.

Table 1. Comparison of our results with MC Simulations

ν	N	β_0	β_1	β_2	β_{SAW1}	β_{SAW2}	β_c
1	1	0.7500	1.2705		∞	∞	∞
	2	1.3000	2.4632		∞	∞	∞
	3	1.8753	3.5581		∞	∞	∞
	4	2.4000	4.6141		∞	∞	∞
2	1	0.3000	0.3415	0.3720	0.3895	0.3989	0.4407
	2	0.5714	0.6838	0.7368	0.7996	0.8201	1.06
	3	0.8333	1.0232	1.0921	1.2186	1.2508	
	4	1.0909	1.3606	1.4412	1.6418	1.6862	
3	1	0.1875	0.2018	0.2078	0.2134	0.2168	0.2217
	2	0.3636	0.4038	0.4135	0.4301	0.4372	0.4542
	3	0.5357	0.6053	0.6177	0.6482	0.6589	0.6930
	4	0.7059	0.8063	0.8206	0.8669	0.8813	0.9360
4	1	0.1364	0.1435	0.1453	0.1474	0.1486	0.1503
	2	0.2667	0.2871	0.2901	0.2959	0.2984	
	3	0.3947	0.4305	0.4343	0.4448	0.4487	
	4	0.5271	0.5738	0.5782	0.5940	0.5991	0.6090

$\beta_0, \beta_1, \beta_2$: the lower bounds obtained in [5, 10, 11] respectively.

β_{SAW1} : the lower bounds obtained by Corollary 1 where the upper bounds of connective constants $\mu_2 \leq 2.69576, \mu_3 \leq 4.756$ and $\mu_4 \leq 6.832$ [1] are used.

β_{SAW2} : the lower bounds obtained by Corollary 1 where the expected values of connective constants $\mu_2 = 2.638, \mu_3 = 4.683$ and $\mu_4 = 6.775$ [18] are used.

β_c : data obtained by Monte Carlo simulations except for that of the 2 dimensional Ising model which is exactly soluble. Data are taken from [2, 3, 7, 8, 13, 14, 21].

Appendix

Here, we prove the inequality (5.4). Substituting $I_s(x) = \sum_{n=0}^{\infty} (x/2)^{2n+s} / n! \Gamma(n+s+1)$, we see

$$f(x) \equiv xI_{s-1}(x) - (s - 1 + \sqrt{s^2 + x^2})I_s(x)$$

$$\geq \sum_{n=0}^{\infty} \frac{x(x/2)^{2n+s-1}}{n!\Gamma(n+s)} - \sum_{n=0}^{\infty} \frac{s-1+\frac{b_n}{2}+\frac{s^2+x^2}{2b_n}}{n!\Gamma(n+s+1)} \left(\frac{x}{2}\right)^{2n+s},$$

where we have used

$$\sqrt{s^2+x^2} \leq \frac{b_n}{2} + \frac{s^2+x^2}{2b_n}$$

for $b_n > 0$ in the n -th term. Choosing $b_n = s + 2n + 2$, we get

$$f(x) \geq \sum_{n=0}^{\infty} \frac{s^2(x/2)^{2n+s}}{n!\Gamma(n+s+1)(s+2n)(s+2n+2)} \geq 0. \quad \square$$

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