Sum Rule Identities and the Duality Relation for the Potts *n*-Point Boundary Correlation Function

F. Y. Wu and H. Y. Huang

Department of Physics, Northeastern University, Boston, Massachusetts 02115 (Received 20 June 1997)

It is shown that certain sum rule identities exist which relate correlation functions for n Potts spins on the boundary of a planar lattice for $n \ge 4$. Explicit expressions of the identities are obtained for n = 4. It is also shown that the identities provide the missing link needed for a complete determination of the duality relation for the *n*-point boundary correlation function. The n = 4 duality relation is obtained explicitly. More generally we deduce the number of sum rule identities as well as a cyclic inversion relation for any *n*, and conjecture on the general form of the duality relation. [S0031-9007(97)04886-2]

PACS numbers: 05.50.+q, 75.10.Hk

The Potts model [1], which is a generalization of the two-component Ising model to q components for arbitrary q, has been the subject matter of intense interest in many fields ranging from condensed matter to highenergy physics. For reviews on the Potts model and its relevance, see, for example, [2,3]. However, exact results on the Potts model have proven to be extremely elusive. Rigorous results known to this date are limited, and include essentially only a closed-form evaluation of its free energy for q = 2, the Ising model [4], and critical properties for the square, triangular, and honeycomb lattices [5,6]. Much less is known about its correlation functions.

In this Letter we report on new sum rule identities for the Potts *n*-point boundary correlation function. Specifically, we show that, as a consequence of being a manycomponent system, the correlation functions of Potts spins on the boundary of a planar lattice must necessarily satisfy certain identities when $n \ge 4$. We further show that these identities lead to the complete determination of a correlation duality relation which, in its simplest form, relates the correlation length and the domain wall free energy and has proven to be useful in determining the equilibrium crystal shape of the Ising model [7]. Our results are very general and hold for any planar lattice or graph with arbitrary (nonuniform) edge interactions.

Consider the *q*-state Potts model on a planar lattice \mathcal{L} with open boundary conditions, or more generally any planar graph, of *N* sites and *E* edges. Let i, j, \ldots, m, ℓ be *n* sites on the boundary ordered as shown in Fig. 1, and let σ_i denote the state of the spin at site *i*. Two spins of \mathcal{L} at sites *i'* and *j'* interact with an interaction $K_{ij}\delta(\sigma_{i'}, \sigma_{j'})$, where $\sigma'_i, \sigma'_j = 1, 2, \ldots, q$. Define the *n*-point correlation function [8]

$$P_n(\sigma, \sigma', \dots, \sigma^{(n-1)}) = \langle \delta(\sigma_i, \sigma) \delta(\sigma_j, \sigma') \\ \dots \delta(\sigma_\ell, \sigma^{(n-1)}) \rangle$$
(1)

as the probability that the *n* spins are in respective *definite* spin states $\sigma, \sigma', \ldots, \sigma^{(n)}$. In particular, the correlation function

$$\Gamma_n = q^n P_n(\sigma, \sigma, \dots, \sigma) - 1 \tag{2}$$

vanishes identically if the n spins are completely uncorrelated.

It is convenient to write $P_{ij\dots\ell} = P_n(i, j, \dots, \ell) = Z_{ij\dots\ell}/Z$, where $i, j, \dots, \ell = 1, 2, \dots, q$, Z is the partition function, and $Z_{ij\dots\ell}$ the partial partition function, namely, the sum of Boltzmann factors with the boundary spin states fixed at i, j, \dots, ℓ . Then we have the following theorem.

Theorem: (i) The boundary correlation functions P_n , $n \ge 4$, are related by certain sum rule identities. Particularly, for n = 4, the identity is

$$P_{1212} = P_{1213} + P_{2131} - P_{1234}.$$
 (3)

(ii) The number of correlation identities for a given n is $a_n = b_n - c_n$, where b_n and c_n are generated, respectively, from

$$\exp(e^{t} - 1) = \sum_{n=0}^{\infty} b_{n} t^{n} / n!, \qquad (4)$$

$$(1 - \sqrt{1 - 4t})/2t = \sum_{n=0}^{\infty} c_n t^n.$$
 (5)

Proof: The identity (3) is equivalent to $Z_{1212} = Z_{1213} + Z_{2131} - Z_{1234}$, which we represent graphically in Fig. 2. Consider the high-temperature expansion of $Z_{ijk\ell}$ in the form [9] of

$$Z_{ijk\ell} = \sum_{G} q^{n(G)} \prod_{i',j' \in G} (e^{K_{i'j'}} - 1).$$
 (6)



FIG. 1. A planar lattice \mathcal{L} and *n* sites i, j, \ldots, m, ℓ on the boundary.

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FIG. 2. Graphical representation of the sum rule identity (3).

Here, as a consequence of the fact that the four boundary sites are fixed in definite spin states, the summation is taken over all graphs $G \subseteq \mathcal{L}$ in which there are n(G) clusters excluding those connected to the four boundary sites.

Apply the expansion (6) to the four Z's. It is clear that, as a consequence of sites being on the boundary and \mathcal{L} being planar, we have $Z_{1212} = T_1 + T_2 + T_3$, where T_1 is the sum of graphs where sites *i* and *k* belong to the same cluster, T_2 those graphs where sites j and ℓ belong to the same cluster, and T_3 graphs i, j, k, ℓ all belong to different clusters. It is also clear that we have $Z_{1213} = T_1 + T_3$, $Z_{2131} = T_2 + T_3$, and $Z_{1234} = T_3$. The identity (3) now follows as a sum rule condition. The identity (3) can also be deduced from an application of the principle of inclusion-exclusion [10]: Z_{1212} is equal to the sum of Z_{1213} and Z_{2131} minus the overcounted terms, Z_{1234} . Clearly, the existence of (3) is a consequence of the planar connectivity topology and the fact that the sites are on the boundary. One can proceed in a similar fashion to derive sum rules for $n \ge 5$, and thus we have established (i). We remark that the sum rules manifest themselves only for $q \ge 4$.

To enumerate a_n , the number of correlation identities for a given *n*, it is instructive to consider the case n = 4. First, by enumeration we find that there are 15 distinct $Z_{ijk\ell}$. For each $Z_{ijk\ell}$ we connect sites in the same state by drawing connecting lines exterior to \mathcal{L} , resulting in a "connectivity" of the four points. A well-nested connectivity, or planar Z for brevity, is one in which the connecting lines do not intersect [11]. For n = 4, the 14 Z's shown in Fig. 3 are planar. Only Z_{1212} , which is not shown, is nonplanar.

More generally for a given *n*-point correlation function $Z_{ij\dots m\ell}$, or Z for brevity, one connects sites in the same state to arrive at an *n*-point connectivity. Let there be altogether b_n distinct connectivities of which c_n are planar. To each Z which is nonplanar, we follow the procedure described above, namely, expanding graphically in a high-temperature series. By applying the aforementioned principle of inclusion-exclusion we eventually arrive at a



FIG. 3. The 14 planar connectivities for n = 4 corresponding to (a) Z_{1234} ; (b) Z_{1111} ; (c) Z_{1112} , occurring four times; (d) Z_{1123} , four times; (e) Z_{1213} , two times; and (f) Z_{1122} , two times.

sum rule expressing the particular correlation function in question in terms of planar ones. This gives rise to an identity for this particular Z. Furthermore, since each Z has a unique graphical expansion, all identities are distinct. It follows that the number of sum rule identities, a_n , is equal to the number of Z's which are nonplanar, namely, $b_n - c_n$.

The number c_n has been evaluated in a consideration of the transfer matrix formulation of the Potts model [12], and is found to be generated by (5). To enumerate b_n we note that it is precisely the number of ways that *n* objects can be partitioned into indistinguishable parts. Let there be m_{ν} parts of ν objects each subject to $\sum_{m_{\nu=1}}^{\infty} \nu m_{\nu} = n$. Then we have $b_n =$ $\sum_{m_{\nu=0}}^{\infty} \prod_{\nu=1}^{\infty} n! / (\nu!)^{m_{\nu}} m_{\nu}!$. This leads to the generating function (4). Particularly, we find $a_4 = 15 - 14 = 1$, $a_5 = 52 - 42 = 10$, $a_6 = 203 - 132 = 71$. Q.E.D.

Duality relation for P_n .—It has been known for some time that the two-point boundary correlation function of an Ising model is related to its counterpart in the dual space. The usual derivation of this relation involves embedding expansions of the correlation functions on the lattice followed by an explicit term-by-term identification [13,14]. In a recent paper one of us [8] introduced a new approach to this problem which invokes only a repeated use of an elementary duality consideration [15]. The new approach, which is very general, also permits the extension of the duality analysis to the Potts model for n = 2, 3 [8]. However, an extension of the analysis of [8] to $n \ge 4$ ran into an apparent snag of inadequacy of conditions [16]. Here we show that the correlation identities derived above provide the missing link, and with the help of these identities we determine the duality relation for any n.

The consideration of [8] is based on the fundamental duality relation [15]

$$Z = qCZ^* \tag{7}$$

relating the partition function Z of any planar lattice, or graph, to the partition function Z^* on the dual. Here, $C = q^{-N^*} \prod_{\text{edges}} (e^{K_{ij}} - 1)$, with N^* being the number of sites of the dual and the product taken over all edges. The interaction K_{ij}^* dual to K_{ij} is given by $(e^{K_{ij}} - 1)(e^{K_{ij}^*} - 1) = q$.

Starting from \mathcal{L} we consider a lattice \mathcal{L}^* formed by introducing *n* spins $\alpha, \beta, \gamma, \ldots, \delta$ to the boundary of the dual of \mathcal{L} (cf. Fig. 1), each interacting with neighboring dual spins within \mathcal{L} . (Note that \mathcal{L}^* has $N^* + n - 1$ sites and is not the dual of \mathcal{L} .) Let $Z^*_{\alpha\beta\gamma\cdots\delta}$ be the partial dual partition function of \mathcal{L}^* with the *n* boundary spins fixed in the respective definite states. Our goal is to obtain a duality relation in the form of a linear transformation relating the $Z_{ij\cdots m\ell}$ to $Z^*_{\alpha\beta\gamma\cdots\delta}$.

Regard the b_n planar connectivities as auxiliary lattices, and apply the fundamental duality relation to each one of them [16]. Applying the duality on \mathcal{L} itself, for example, we obtain (7) which can be written as an equation relating linear combinations of the Z and Z^* [8]. Applying the duality to the planar connectivity \mathcal{L}_n in which all *n* points are connected to a common point with interactions *K* as in \mathcal{L}_4 shown in Fig. 3(b), we obtain

$$Z_{aux(n)} = Cq^{-(n-2)}(u-1)^n Z^*_{aux(n)}, \qquad (8)$$

where $u = e^{K}$, and $Z_{aux(n)}$ and $Z_{aux(n)}^{*}$ are, respectively, the partition functions of \mathcal{L}_{n} and its dual. Now, both

$$Z_{1111} = Cq^{-2} [Z_{1111}^* + q_1 (Z_{2111}^* + Z_{1211}^* + Z_{1121}^* + Z_{1112}^*) + q_1 (Z_{1122}^* + Z_{1221}^*) + q_1 q_2 (Z_{1123}^* + Z_{2113}^* + Z_{2311}^* + Z_{1231}^*) + q_1 (Z_{1212}^* + q_2 Z_{1213}^* + q_2 Z_{2131}^* + q_2 q_3 Z_{1234}^*)] = \{1 + q_1 (1, 1, 1, 1) + q_1 (1, 1) + q_1 q_2 (1, 1, 1, 1) + q_1 (1, q_2, q_2, q_2 q_3)\},$$
(9)

where $q_m = q - m$, m = 1, 2, ..., and in the last line we have introduced a short-handed notation. An immediate consequence of (9) is the result

$$\Gamma_{4} = q_{1}(p_{2111} + p_{1211} + p_{1121} + p_{1112} + p_{1212} + p_{1212} + p_{1122} + p_{1221}) + q_{1}q_{2}(p_{1123} + p_{2113} + p_{2311} + p_{1231} + p_{1213} + p_{2131}) + q_{1}q_{2}q_{3}p_{1234},$$
(10)

where we have introduced (7), $Z^* = q Z_{1111}^*$, as well as $p_{\alpha\beta\gamma\delta} = Z_{\alpha\beta\gamma\delta}^*/Z_{1111}^*$. For general *n* the consideration of \mathcal{L}_n leads to

sides of (8) are polynomials of degree *n* in *u*. Since (8) holds for arbitrary *u*, the coefficients of all powers of *u* must be equal. However, it suffices to equate only the coefficients of the highest power of *u*. On the left-hand side we have $Z_{aux(n)} = q(u + q - 1)^n Z_{11\dots 1}^n + \text{terms of}$ the order of $O(u^{n-1})$. On the right-hand side we have $(u - 1)^n Z_{aux(n)}^* = q(u + q - 1)^n Z_{11\dots 1}^* + \text{other terms}$. This leads immediately to an expression for $Z_{11\dots 1}$. For n = 4, for example, we obtain

$$\Gamma_n = q_1 \sum p_{211\cdots 1} + q_1 q_2 \sum p_{231\cdots 1} + \cdots + q_1 q_2 \cdots q_{n-1} p_{123\cdots n} .$$
(11)

Applying (7) to all c_n auxiliary lattices of planar connectivities in this fashion and equating the coefficients of the highest power of u in each case, we obtain c_n equations for the b_n unknown Z's. Combining the c_n equations with the $b_n - c_n$ sum rule identities, we have precisely b_n equations, and the duality relation can now be determined.

In the case of n = 4, the solution of the 15 equations leads to, in addition to (9),

$$Z_{2111} = \{1 + (-1, -1, q_1, q_1) + (q_1, -1) + q_2(q_1, -1, -1, -1) - (1, q_2, q_2, q_2q_3)\},$$

$$Z_{1122} = \{1 + (-1, q_1, -1, q_1) - (1, 1) - q_2(1, 1, 1, 1) + (q_1, q_1q_2, -q_2, -q_2q_3)\},$$

$$Z_{1123} = \{1 - (1, -q_1, 1, 1) - (1, 1) + (2, 2, -q_2, -q_2) + (-1, -q_2, 2, 2q_3)\},$$

$$Z_{1212} = \{1 - (1, 1, 1, 1) + q_1(1, 1) - q_2(1, 1, 1, 1) + Q(-1, q_1q_2, q_1q_2, q_2q_3r)\},$$

$$Z_{1213} = \{1 - (1, 1, 1, 1) + (-1, q_1) + (2, -q_2, 2, -q_2) + Q(q_1, s, s, q_3t)\},$$

$$Z_{1234} = \{1 - (1, 1, 1, 1) - (1, 1) + 2(1, 1, 1, 1) + Q[r, t, t, q_3(2 - 5q)]\},$$
(12)

where $Q = 1/(q^2 - 3q + 1)$, r = 2q - 1, $s = q^2 - 4q + 2$, $t = q^2 - 5q + 2$. Expressions for other $Z_{ijk\ell}$ are given by cyclic permutations.

The solutions (9) and (12) can be written in the form of a partition expansion

$$P_{4}(\sigma_{1}, \sigma_{2}, \sigma_{3}, \sigma_{4}) = A_{1234} + A_{1123}\delta_{12} + A_{2113}\delta_{23} + A_{2311}\delta_{34} + A_{1231}\delta_{14} + A_{1213}\delta_{13} + A_{2131}\delta_{24} + A_{1122}\delta_{12}\delta_{34} + A_{1221}\delta_{14}\delta_{23} + A_{1212}\delta_{13}\delta_{24} + A_{2111}\delta_{234} + A_{1211}\delta_{134} + A_{1121}\delta_{124} + A_{1112}\delta_{123} + A_{1111}\delta_{1234},$$

$$(13)$$

where $\delta_{12} = \delta(\sigma_1, \sigma_2)$, $\delta_{123} = \delta_{12}\delta_{23}$, etc. We find

$$\begin{split} A_{1234} &= q^{-4} [1 - (p_{2111} + p_{1211} + p_{1121} + p_{1112} + p_{1122} + p_{1221} + p_{1212}) \\ &\quad + 2(p_{1123} + p_{1231} + p_{2113} + p_{2311} + p_{1213} + p_{2131}) - 6p_{1234}], \\ A_{1123} &= q^{-3}(p_{1211} - p_{1231} - p_{2311} - p_{1213} + 2p_{1234}), \\ A_{2113} &= q^{-3}(p_{1121} - p_{1123} - p_{1231} - p_{2131} + 2p_{1234}), \\ A_{2311} &= q^{-3}(p_{1112} - p_{2113} - p_{1123} - p_{1213} + 2p_{1234}), \\ A_{1231} &= q^{-3}(p_{2111} - p_{2311} - p_{2113} - p_{2131} + 2p_{1234}), \end{split}$$

$$\begin{aligned} A_{1213} &= q^{-3}(p_{1221} - p_{1231} - p_{2113} + p_{1234}), \\ A_{2131} &= q^{-3}(p_{1122} - p_{1123} - p_{2311} + p_{1234}), \\ A_{1122} &= q^{-2}(p_{1213} - p_{1234}), \qquad A_{1221} &= q^{-2}(p_{2131} - p_{1234}) \\ A_{1212} &= 0, \qquad A_{2111} &= q^{-2}(p_{1123} - p_{1234}) \\ A_{1211} &= q^{-2}(p_{2113} - p_{1234}), \qquad A_{1121} &= q^{-2}(p_{2311} - p_{1234}) \\ A_{1112} &= q^{-2}(p_{1231} - p_{1234}), \qquad A_{1111} &= q^{-1}p_{1234}, \end{aligned}$$

where we have used the fact that Z^* satisfies the same sum rules as the Z, including $Z_{1212}^* = Z_{1213}^* + Z_{2131}^* - Z_{1234}^*$.

For general n we write in analogous to (13) the partition expansions

$$P_{n}(\sigma_{1}, \sigma_{2}, \dots, \sigma_{n}) = A_{12\dots n} + A_{1123\dots (n-1)}\delta_{12} + \dots + A_{11\dots 1}\delta_{12\dots n}, \quad (15)$$

$$P_{\alpha\beta\cdots\delta} = Z_{\alpha\beta\cdots\delta}/Z_{11\cdots1}$$

$$= B_{12\cdots n} + B_{1123\cdots(n-1)}\delta_{\alpha\beta}$$

$$+ \cdots + B_{11\cdots 1}\delta_{\alpha\beta\cdots\delta}.$$
(16)

Regard the diagram in Fig. 1 as representing $A_{ij\cdots\ell}$. Construct for each *A* the associated connectivity as in Fig. 3, and label indices $\alpha, \beta, \ldots, \delta$ such that neighboring indices are the same if there is no line in between. Then we are led to the following *conjecture:*

$$A_{ij\cdots\ell} = q^{-d(ij\cdots\ell)} B_{\alpha\beta\cdots\delta} \quad \text{if the connectivity is planar,} = 0, \quad \text{otherwise,} \quad (17)$$

where $d(ij \cdots \ell)$ is the number of distinct indices in $\{i, j, \ldots, \ell\}$. The conjecture is readily verified for n = 2, 3, 4. In practice, for any given *n*, one can solve from (16) for $B_{\alpha\beta\cdots\delta}$ by applying the principle of inclusion-exclusion.

A cyclic inversion relation.—Since $\alpha \beta \gamma \cdots \delta$ are boundary sites of \mathcal{L}^* , the transformation relating Z^* to Z, an inversion process, is given precisely by the same transformation relating Z to Z^* . Now \mathcal{L}^* has $N^* + n - 1$ sites and its dual has N - n + 1 sites. Also \mathcal{L} and \mathcal{L}^* have the same number of edges. Therefore we have

$$Z_{ijk\cdots m\ell} = \left(\frac{\Pi(e^{\kappa_{ij}} - 1)}{q^{N^* + (n-2)}}\right) \times \sum_{\{\alpha\beta\gamma\cdots\delta\}} \mathbf{T}_n(ij\cdots m\ell \mid \alpha\beta\gamma\cdots\delta) Z^*_{\alpha\beta\gamma\cdots\delta},$$
(18)

$$Z^*_{\alpha\beta\gamma\cdots\delta} = \left(\frac{\Pi(e^{K^*_{ij}} - 1)}{q^{N-n+1+(n-2)}}\right)$$
$$\times \sum_{\{ij\cdots m\ell\}} \mathbf{T}_n(\alpha\beta\gamma\cdots\delta \mid \ell ij\cdots m) Z_{\ell ij\cdots m},$$
(19)

where \mathbf{T}_n is a $b_n \times b_n$ matrix, and the summations are over the set of b_n distinct partitions of the *n* indices. Substituting (19) into (18) and making use of the Euler relation $E = N + N^* - 2$, we are led to the identity, which we refer to as a cyclic inversion relation,

$$\mathbf{\Gamma}_n^2(ijk\cdots\ell\mid i'j'k'\cdots\ell') = q^{n-1}\delta_{ij'}\delta_{jk'}\cdots\delta_{\ell i'}.$$
 (20)

Further discussions including properties of \mathbf{T}_n and the extension to the Ashkin-Teller model will be given elsewhere [17].

We are grateful to J. L. Jacobsen for discussions and a comment [16] which has led to this investigation. This work is supported in part by National Science Foundation Grant No. DMR-9614170.

Note added.—The conjecture (17) has since been established rigorously [18].

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