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Long-Range Inverse Two-Spin Correlations in One-Dimensional Potts Lattices

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The inverse two-spin correlation function of a one-dimensional three-state Potts lattice with constant nearest-neighbor interactions in a uniform external field is derived exactly. It is shown that the external field induces long-range correlations. The inverse two-spin correlation function decays in a monotonic exponential fashion for a ferromagnetic lattice, while it decays in an oscillatory exponential fashion for an antiferromagnetic lattice. With no external field the inverse two-spin correlation function has a finite range equal to that of the interactions.

KEY WORDS: Inverse two-spin correlation function; one-dimensional; Potts model; Ising model; lattice model.

1. INTRODUCTION

The central point in the Ornstein–Zernike[1] theory of the pair correlation function $\nu(r)$ is the observation that near the critical point of a fluid $\nu(r)$ develops a very long tail, that is, its Fourier transform at zero wave vector is infinite at the critical point. As usual when infinities are present in a theory, one shifts attention to a less singular function that can be handled conveniently. The direct correlation function $c(r)$ (or, equivalently, the inverse pair correlation function) introduced by Ornstein and Zernike is in this sense a more convenient function because it is shorter ranged than $\nu(r)$. In particular, the Fourier transform of $c(r)$ at zero wave vector is finite at the critical point. It was supposed further by Ornstein and Zernike that $c(r)$ is so short-ranged as to have a finite second moment at the critical point. These assumptions lead to a qualitatively very good description of

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the long tail of $\nu(r)$ in three dimensions, but completely fail in a one- or two-dimensional space.[2]

Since the pioneering work of Ornstein and Zernike in 1914, $c(r)$ has been proved to be one of the most important functions in equilibrium statistical mechanics. It plays a central role in the density functional theory of both uniform and nonuniform classical systems of which any application requires some prescription for $c(r)$.

In the case of spin systems, the role of $\nu(r)$ is played by the two-spin correlation function $\nu(n)$,[2] which has properties quite similar to $\nu(r)$. The inverse of $\nu(n)$, which we denote henceforth by $k(n)$, has been widely studied in model systems.[2] One-dimensional lattice systems have been considered in detail because all calculations can usually be done without approximation. Percus[3] showed that $k(n)$ has the range of the interactions for an Ising chain with constant nearest-neighbor interactions in an arbitrary external field. Recently, it was proved[4,6] that this result also holds for nonconstant nearest-neighbor interactions. That $k(n)$ is also of the interaction range for next-nearest-neighbor interactions was proved by Robert[5] in the absence of external field. Borzi *et al.*[6] showed numerically that for a next-nearest-neighbor Ising model in a uniform external field $k(n)$ has an oscillating tail and that further interactions induce long-range correlations.

In this paper we present an exact calculation of $k(n)$ for a three-state Potts lattice with constant nearest-neighbor interactions in a uniform external field. We show that, in contrast to the case of the Ising model, the uniform external field induces long-range inverse two-spin correlations for ferromagnetic as well as for antiferromagnetic lattices. With no external field, $k(n)$ has exactly the range of the interactions.

2. AN EXACTLY SOLVABLE MODEL

Our model is a one-dimensional lattice of N three-state Potts variables s_i $(i = 1, 2,..., N)$ with constant nearest-neighbor interactions in a uniform external field. The Hamiltonian for a configuration $\{s_i\}$ of these variables is

$$H_N\{s_i\} = -\sum_{i=1}^{N} \left\{ J\delta(s_i, s_{i+1}) + \sum_{\alpha=0,\pm1} B_\alpha \delta(s_i, \alpha) \right\} \tag{1}$$

where each Potts variable s_i may take the values $\alpha = 0, \pm 1$ and a periodic boundary condition $s_{N+1} = s_1$ has been assumed. Here, J is the nearest-neighbor potential, $J > 0$ for ferromagnetic interaction and $J < 0$ for antiferromagnetic interaction, and the Kronecker delta in the potential energy of interaction ensures that any two like values are equally favored on neighboring sites, while any two unlike values are equally unfavored. The external field couples to a Potts variable s_i via $B_\alpha \delta(s_i, \alpha)$, B_α being the strength of the external field on the α state. This dependence favors the α state with large B_α strength. We take henceforth $B_\alpha = \alpha B$.

The equilibrium statistical mechanics of our model is fully contained in the partition function

$$Z_N(K, h_\alpha) = \sum_{\{s_i\}} \exp(-\beta H_N\{s_i\})$$

$$= \sum_{\{s_i\}} \exp\left\{ \sum_{i=1}^{N} \left[K\delta(s_i, s_{i+1}) + \sum_{\alpha=0,\pm1} h_\alpha \delta(s_i, \alpha) \right] \right\} \tag{2}$$

where the sum is over all the lattice configurations and we have defined the dimensionless constants $K = \beta J$ and $h_\alpha = \beta B_\alpha$, with $\beta = 1/k_B T$, k_B Boltzmann's constant, and T the absolute temperature. The partition function $Z_N(K, h_\alpha)$ can be exactly computed using standard transfer matrix techniques, with the result

$$Z_N(K, h_\alpha) = \mathrm{tr}\{P^N\} = \sum_{\alpha=0,\pm1} \lambda_\alpha^N \tag{3}$$

where tr denotes the trace operator, P is the 3×3 symmetric positive-semi-definite matrix

$$P_{ij} = \exp\left\{ K\delta(i, j) + \sum_{\alpha=0,\pm1} h_\alpha [\delta(i, \alpha) + \delta(j, \alpha)]/2 \right\} \tag{4}$$

with $i, j = 0, \pm 1$ and λ_α its real eigenvalues. Solving the characteristic equation of P, we get the following cubic equation:

$$\lambda^3 - \lambda^2 \Gamma_2 y + \lambda \Gamma_1 (y^2 - 1) - \Gamma_0 (y - 1)^2 (y + 2) = 0 \tag{5}$$

with

$$y = \exp(K) \tag{6a}$$

$$\Gamma_2 = \sum_{\alpha=0,\pm1} \exp(h_\alpha) \tag{6b}$$

$$\Gamma_1 = \tfrac{1}{2} \sum\sum_{\alpha,\alpha'=0,\pm1} \exp(h_\alpha + h_{\alpha'}) \qquad (\alpha \neq \alpha') \tag{6c}$$

$$\Gamma_0 = \exp\left(\sum_{\alpha=0,\pm1} h_\alpha \right) \tag{6d}$$

[2] For dichotomic spins $k(n)$ can be shown to be equivalent, to within a numerical factor, to the direct correlation function, say $c(n)$, but this equivalence is not valid for higher dimensional spins.

Equation (5) has three positive and unequal roots for $K>0$ (ferromagnetic lattice) and one positive root and two unequal negative roots for $K<0$ (antiferromagnetic lattice). One important exception to this rule should be mentioned. When $h_\alpha=0$ for all α, i.e., when the three states are equivalent, two of these roots become equal. This special case will be discussed below. The analytical expression for the eigenvalues λ_α can be written in the following trigonometric form[7]:

$$\lambda_1 = A\cos(\phi/3)+A' \quad (7a)$$

$$\lambda_0 = A\cos[(\phi+2\pi)/3]+A' \quad (7b)$$

$$\lambda_{-1} = A\cos[(\phi+4\pi)/3]+A' \quad (7c)$$

with

$$A=\tfrac{2}{3}[\Gamma_2^2 y^2+3\Gamma_1(1-y^2)]^{1/2}>0 \quad (8a)$$

$$A'=\Gamma_2 y/3>0 \quad (8b)$$

$$\cos\phi=[2\Gamma_2^3 y^3-9\Gamma_1\Gamma_2 y(y^2-1)+27\Gamma_0(y-1)^2(y+2)] \times\{2[\Gamma_2^2 y^2-3\Gamma_1(y^2-1)]^{3/2}\}^{-1} \quad (8c)$$

Equations (6)–(8) accomplish the desired goal of evaluating analytically $Z_N(K, h_\alpha)$ in terms of the dimensionless constants K and h_α. From these exact results it is an easy matter to derive any equilibrium distribution function by usual transfer matrix methods.

3. TWO-SPIN CORRELATION FUNCTION

Let us restrict ourselves to the two-spin correlation function defined as

$$v(n)=\lim_{N\to\infty} v_N(n) \quad (9)$$

with

$$v_N(n)=\langle \Delta s_i\, \Delta s_{i+n}\rangle \quad (10)$$

where

$$\Delta s_i = s_i-\langle s_i\rangle \quad (11)$$

and

$$\langle f\{s_i\}\rangle = Z_N^{-1}(K,h_\alpha)\sum_{\{s_i\}} f\{s_i\}\exp(-\beta H_N\{s_i\}) \quad (12)$$

i.e., $\langle f\{s_i\}\rangle$ denotes the statistical average of any well-behaved function of the Potts variables $f\{s_i\}$ over a canonical distribution function with Hamiltonian $H_N\{s_i\}$. We proceed to evaluate $v_N(n)$, noting that

$$\langle \delta(s_i,\gamma)\rangle = Z_N^{-1}(K,h_\alpha)\,\mathrm{tr}\{(P')^N U^+ M_\gamma U\} \quad (13a)$$

$$\langle \delta(s_i,\gamma)\,\delta(s_{i+n},\sigma)\rangle = Z_N^{-1}(K,h_\alpha)\,\mathrm{tr}\{(P')^{N-n} U^+ M_\gamma U (P')^n U^+ M_\sigma U\} \quad (13b)$$

where U is the unitary matrix (U^+ being its adjoint) that transforms P to a diagonal matrix $P'=U^+PU$ with matrix element $P'_{ij}=\lambda_i\delta(i,j)$ and

$$(M_\gamma)_{ij}=\delta(i,j)\,\delta(j,\gamma) \quad (14)$$

It is straightforward to calculate the traces in (13), the final expressions being considerably simplified at the thermodynamic limit $N\to\infty$. Using the identities

$$s_i=\delta(s_i,1)-\delta(s_i,-1) \quad (15a)$$

$$s_is_j=\delta(s_i,1)\,\delta(s_j,1)+\delta(s_i,-1)\,\delta(s_j,-1) - [\delta(s_i,1)\,\delta(s_j,-1)+\delta(s_i,-1)\,\delta(s_j,1)] \quad (15b)$$

the statistical averages $\langle s_i\rangle$ and $\langle s_is_{i+n}\rangle$ can be expressed as a superposition of terms in the form (13a) and (13b). Let λ_1 be the largest eigenvalue of P. After some algebra one finds

$$v(n)=A_0(\lambda_0/\lambda_1)^{|n|}+A_{-1}(\lambda_{-1}/\lambda_1)^{|n|} \quad (16)$$

where A_0 and A_{-1}, expressed in terms of the matrix elements U_{ij}, are given by

$$A_0=(U_{11}U_{10}-U_{-11}U_{-10})^2 \quad (17a)$$

$$A_{-1}=(U_{11}U_{1-1}-U_{-11}U_{-1-1})^2 \quad (17b)$$

For a ferromagnetic lattice ($\lambda_0>0$ and $\lambda_{-1}>0$) the two-spin correlation function decays as a superposition of two monotonic decreasing exponentials, while for an antiferromagnetic lattice ($\lambda_0<0$ and $\lambda_{-1}<0$) the two-spin correlation function decreases as a superposition of two oscillatory exponentials. As quoted before, with no external field, $\lambda_0^*=\lambda_{-1}^*$ and the two-spin correlation function is $[\lambda_i^*=\lambda_i(h_\alpha=0),\ A_i^*=A_i(h_\alpha=0)]$

$$v(n)=(A_0^*+A_{-1}^*)(\lambda_0^*/\lambda_1^*)^{|n|} \quad (18)$$

decreasing as a simple monotonic ($K>0$) or oscillatory ($K<0$) exponential. Equations (16) and (18) are the main results in this paper, though the effect of the external field will become more transparent in terms of the inverse two-spin correlation function.

4. THE INVERSE TWO-SPIN CORRELATION FUNCTION

Let us rewrite equation (16) as

$$v(n) = (\pm 1)^n \left[A_0 \exp(-|n|/\xi_0) + A_{-1} \exp(-|n|/\xi_{-1})\right] \tag{19}$$

with $+1$ (-1) corresponding to the ferromagnetic (antiferromagnetic) lattice and

$$1/\xi_0 = \ln|\lambda_1/\lambda_0| \tag{20a}$$

$$1/\xi_{-1} = \ln|\lambda_1/\lambda_{-1}| \tag{20b}$$

Defining the discrete Fourier transform of $v(n)$ as

$$\hat{v}(q) = \sum_{n=-\infty}^{\infty} v(n) \exp(-iqn) \tag{21}$$

we find that a simple calculation leads to

$$\hat{v}(q) = (\eta_1 \mp \eta_2 \cos q)/(\eta_3 \mp \eta_4 \cos q + \cos^2 q) \tag{22}$$

where the upper (lower) sign corresponds to a ferromagnetic (antiferromagnetic) lattice and we have defined

$$\eta_1 = A_0 \sinh(1/\xi_0)\cosh(1/\xi_{-1}) + A_{-1}\sinh(1/\xi_{-1})\cosh(1/\xi_0) \tag{23a}$$

$$\eta_2 = A_0 \sinh(1/\xi_0) + A_{-1}\sinh(1/\xi_{-1}) \tag{23b}$$

$$\eta_3 = \cosh(1/\xi_0)\cosh(1/\xi_{-1}) \tag{23c}$$

$$\eta_4 = \cosh(1/\xi_0) + \cosh(1/\xi_{-1}) \tag{23d}$$

The Fourier transform of the inverse two-spin correlation function $k(n)$ is then simply obtained as

$$\hat{k}(q) = \hat{v}^{-1}(q) \tag{24}$$

with an inverse Fourier transform $k(n)$ given by

$$k(n) = (1/2\pi)\int_0^{2\pi} dq\, \hat{k}(q)\exp(iqn) = (1/2\pi)\int_0^{2\pi} dq\, \frac{\eta_3 \mp \eta_4 \cos q + \cos^2 q}{\eta_1 \mp \eta_2 \cos q}\exp(iqn) \tag{25}$$

The integral (25) can be evaluated as follows. Let $z = \exp(iq)$ and write the integral (25) in terms of this complex variable to get

$$k(n) = \mp(1/4\pi i \eta_2)\int_\Gamma dz\, z^{n-2}\,\frac{z^4 \mp 2\eta_4 z^3 + 2(1+2\eta_3)z^2 \mp 2\eta_4 z + 1}{(z-z_1)(z-z_2)} \tag{26}$$

where the contour of integration Γ consists of the circumference $|z|=1$ and

$$z_1 = \pm\{\eta_1/\eta_2 + [(\eta_1/\eta_2)^2 - 1]^{1/2}\} \tag{27a}$$

$$z_2 = \pm\{\eta_1/\eta_2 - [(\eta_1/\eta_2)^2 - 1]^{1/2}\} \tag{27b}$$

the upper (lower) sign in (26) and (27) corresponding to $K>0 (K<0)$. The integrand of (26) has two simple poles at z_1 and z_2 for all n, a pole of second order at $z=0$ for $n=0$, and a simple pole at $z=0$ for $n=1$. Using the method of residues and taking into account that z_1 lies outside the integration contour $|z|=1$ (notice that $\eta_1>\eta_2$), we find

$$k(n) = \frac{(\eta_4 - \eta_1/\eta_2)\,\delta(n,0)}{\eta_2} \mp \frac{\delta(n,1)}{2\eta_2} + (\pm 1)^n \frac{\{\eta_1/\eta_2 - [(\eta_1/\eta_2)^2 - 1]^{1/2}\}^n\,[(\eta_1/\eta_2)^2 - \eta_4\eta_1/\eta_2 + \eta_3]}{(\eta_1^2 - \eta_2^2)^{1/2}} \tag{28}$$

the upper (lower) sign corresponding to $K>0$ $(K<0)$. The right-hand side of (28) is a sum of two short-range δ terms [the contributions of the residues at $z=0$ in (26)] and a long-range exponential term [the contribution of the residue at $z=z_2$ in (26)].

It can be easily seen from (23) that

$$(\eta_1/\eta_2)^2 - \eta_4\eta_1/\eta_2 + \eta_3 = -A_0 A_{-1}\sinh(1/\xi_0)\sinh(1/\xi_{-1})[\cosh(1/\xi_0) - \cosh(1/\xi_{-1})]^2 \tag{29}$$

is nonzero because $\xi_0 \neq \xi_{-1}$, $A_0 \neq 0$, and $A_{-1} \neq 0$. Therefore $k(n)$ is long-ranged.

Remark that a necessary condition for $k(n)$ to be long-ranged is $\eta_2 \neq 0$. Indeed, coming back to (25) and writing its right-hand side in terms of the complex variable $z = \exp(iq)$, it can be readily seen that $\eta_2 = 0$ implies that there is not other pole than $z = 0$ inside the integration contour $|z| = 1$. In the present model $\eta_1 > \eta_2 > 0$ and therefore in (22) the numerator is a first-degree polynomial in $\cos q$ with nonvanishing coefficients. Another necessary condition in order for $k(n)$ to have a long range is that in (22) the numerator cannot be a multiple of the denominator because this would turn $\hat{k}(q)$ into the form $a + b\cos q$ with no other pole than the origin inside the integration contout $|z| = 1$. This last condition implies $(\eta_1/\eta_2)^2 - \eta_4\eta_1/\eta_2 + \eta_3 \neq 0$, which we have proved to be a direct implication of the no-simple-exponential form of the two-spin correlation function.

We thus get the following results. For a ferromagnetic lattice, $k(0) > 0$ and $k(n) < 0\ (n > 1)$, $k(n)$ having a monotonic exponential decay as $|n| \to \infty$ (see Fig. 1). For an antiferromagnetic lattice, $k(0) > 0$, $k(1) > 0$, and $\operatorname{sgn} k(n) = (-1)^{n+1}$ (for all $n > 1$), $k(n)$ having an oscillatory exponential decay as $|n| \to \infty$ (see Fig. 2). This behavior resembles that reported by Borzi *et al.*[6] in their study of the next-nearest-neighbor Ising chain in a uniform external field. The oscillating tail appeared there because they considered a negative next-nearest-neighbor interaction constant, while they found $k(1) < 0$ because they took a positive nearest-neighbor interaction constant.

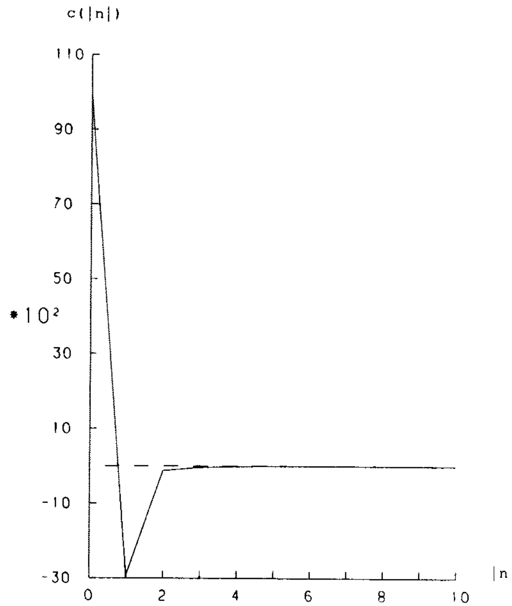

Fig. 1. The inverse two-spin correlation function $k(n)$ of a ferromagnetic lattice ($b = 0.8$, $K = 5.0$) versus n.

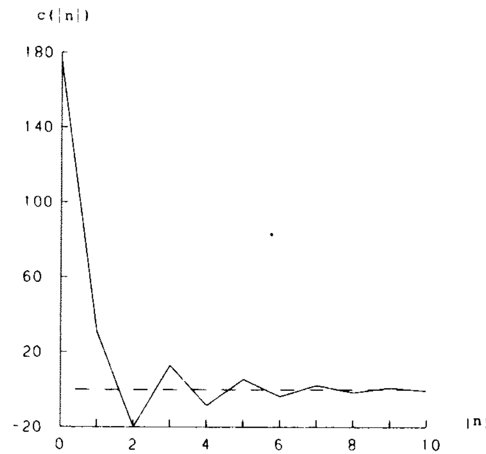

Fig. 2. The inverse two-spin correlation function $k(n)$ of an antiferromagnetic lattice ($b = 5.0$, $K = -10.0$) versus n

Let us consider now the three-state Potts lattice with no external field. The novelty here is that $v(n)$ decreases as a simple exponential [see (18)]. Since in this case $\xi_0 = \xi_{-1}$, the right-hand side of (29) vanishes identically and only the δ terms in (28) contribute to $k(n)$, the η_i constants appearing therein having to be replaced by $\eta_i^* = \eta_i(b_\alpha = 0)$. Consequently, $k(n)$ has the range of the interactions.

5. CONCLUSIONS

We have derived an exact calculation of the inverse two-spin correlation function $k(n)$ of the one-dimensional three-state Potts lattice with constant nearest-neighbor interactions in a uniform external field. We have shown that the external field induces long-range correlations. The method we have used starts with the exact calculation of the two-spin correlation function $v(n)$ by usual transfer matrix techniques. This functions decays as a superposition of two exponentials, this number being a unit less than the number of independent roots of the characteristic equation. With no external field, two of the three roots are equal and, consequently, $v(n)$ decays as a simple exponential. Notice that for an Ising lattice with nearest-neighbor interactions there are two independent roots (with external field as well as with no external field) and therefore $\upsilon(n)$ always decays as a simple exponential.

The inverse two-spin correlation function $k(n)$ has been derived from $\upsilon(n)$ by using discrete Fourier transforms. We have shown that the external field induces a long tail in $k(n)$, its mathematical origin being a direct consequence of the no-simple-exponential behavior of $\upsilon(n)$. With no external field, $k(n)$ has exactly the range of the interactions. However, it should be kept in mind that the inverse two-spin correlation function of a next-nearest-neighbor Ising lattice with no external field has the range of the interactions[5] in spite of the fact that $\upsilon(n)$ is a sum of two exponentials[8] as it is in the present model. It can be shown that for that model η_2 [see (23b)] vanishes identically and the integrand in Eq. (26) has no other pole than $z=0$ inside the integration contour Γ.

We finally remark that our findings do not contradict the result of Percus,[9] who extended previous investigations to a one-dimensional Ising chain of D-dimensional spins with nearest-neighbor interactions. He found that in all cases the direct correlation function $c(n)$ has nearest-neighbor support. As pointed out in footnote 2, $c(n)$ and $k(n)$ are not equivalent for nondichotomic spins.

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REFERENCES

1. L. S. Ornstein and F. Zernike, *Proc. Acad. Sci. Amsterdam* **17**:793 (1914).
2. M. E. Fisher, *J. Math. Phys.* **5**:944 (1964).
3. J. K. Percus, *J. Stat. Phys.* **16**:299 (1977).
4. C. F. Tejero, *J. Stat. Phys.* **48**:531 (1987).
5. M. Robert, *Phys. Rev. A* **29**:2854 (1984); *Phys. Rev. A* **33**:2825 (1986).
6. C. Borzi, G. Ord, and J. K. Percus, *J. Stat. Phys.* **46**:51 (1987).
7. CRC, *Standard Mathematical Tables* (Chemical Rubber Publishing Company, Cleveland, Ohio, 1962).
8. J. Stephenson, *Can. J. Phys.* **48**:1724 (1970).
9. J. K. Percus, *J. Math. Phys.* **23**:1162 (1982).

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