HIGH-TEMPERATURE EXPANSION OF SURFACE CRITICAL EXPONENTS FOR THE CLASSICAL n-VECTOR MODEL

Kaoru OHNO and Yutaka OKABE [1]
Department of Physics, Tohoku University, Sendai 980, Japan

Received 15 November 1982
Revised manuscript received 5 January 1983

The surface critical exponents of the classical n-vector model are investigated in the high-temperature series expansion. The first nine coefficients of the layer susceptibility for the semi-infinite simple cubic lattice are presented. The n-dependence of surface exponents is compared with the results of other theories.

The critical phenomena of spin systems with a free surface have been the subject of recent studies [1–8]. The assumption that there exists only one correlation length as a length scale leads to several scaling relations among surface and bulk critical exponents [1,2]. Such naive scaling laws assert that only one surface exponent is independent. Although Bray and Moore [3] proposed an additional relation in which all the surface exponents for the ordinary transition [1,3] can be expressed in terms of bulk exponents, the renormalization-group studies have revealed that this is not true at $O(\epsilon^2)$ [4,5]. Subsequently, the $1/n$ expansion up to $O(1/n)$ by the present authors [6] which is based on Bray and Moore's exact calculation for $n = \infty$ [3], also has shown this violation at $d = 3$ and another dimensionality.

In discussing critical exponents, the conventional high-temperature series expansion serves to give a plausible value of the exponents. However, the series expansion has been applied so far to the study of surface critical exponents only for $n = 0$ [7] and $n = 1$ [1,8]. A systematic investigation of the surface exponents as a function of n is highly desirable for the purpose of (i) testing the various scaling relations, (ii) making a comparison with the results of the ϵ and $1/n$ expansions, and also (iii) providing the standards to be compared with experiments [9].

We consider the classical n-vector model [10] for the semi-infinite simple cubic lattice. Our hamiltonian is

$$H = -J \sum_{\langle i,j \rangle} \sum_{\alpha=1}^{n} S_i^\alpha S_j^\alpha \,, \tag{1}$$

where the lattice summation is over pairs of nearest-neighbor sites. We fix the length of spins as $\sqrt{n}$. Stanley [10] studied the bulk properties of this model using the high-temperature series expansion. We follow the approach by Stanley and apply it to the calculation of surface critical exponents. Since the exchange parameter on the surface is taken to have the same value as in the bulk, this model is expected to describe the ordinary transition. With the knowledge of the spin correlation function $G(r; r')$, we can evaluate the layer susceptibility χ_1 and the local susceptibility $\chi_{1,1}$ through the relations

$$\chi_1 = \sum_{z' \geqslant 1, \boldsymbol{\rho}} G(\boldsymbol{\rho}, 1; \boldsymbol{\rho}', z') \tag{2}$$

and

$$\chi_{1,1} = \sum_{\boldsymbol{\rho}'} G(\boldsymbol{\rho}, 1; \boldsymbol{\rho}', 1) \,, \tag{3}$$

respectively. Hereafter, we deal only with χ_1 as in ref. [8], because a reliable estimate of a small and negative exponent is difficult to form from the series, and $\gamma_{1,1}$ is expected to be such.

[1] Present address: Department of Physics, University of Waterloo, Waterloo, Canada N2L 3G1.

 0 031-9163/83/0000–0000/$ 03.00

The coefficients of the correlation-function series were derived with the help of diagrams up to ninth order by Stanley [10]. In order to get the layer susceptibility χ_1, eq. (2), we should count the number of configurations which satisfy the condition for the sum. The layer susceptibility coefficients a_k, defined by

$$\chi_1 = 1 + \sum_{k=1}^{\infty} a_k (J/k_B T)^k \,, \tag{4}$$

are tabulated as a function of n up to ninth order in the appendix. As was pointed out by Stanley [10], the series becomes smoother if we expand in the variable

$$y = (\partial/n\partial\mathcal{J}) \log[\mathcal{J}^{1-n/2} I_{n/2-1}(n\mathcal{J})] \,, \tag{5}$$

where I_ν is the modified Bessel function and $\mathcal{J} = J/k_B T$. The new coefficients A_k are defined by

$$\chi_1 = 1 + \sum_{k=1}^{\infty} A_k y^k \,. \tag{6}$$

For the direct relations between a_k and A_k, we refer to Stanley [10]. It should be noted that we get the same coefficients A_k as in ref. [8] if we put $n = 1$.

Now that we have obtained the layer susceptibility coefficients, we analyze the critical exponent γ_1. We employ the standard ratio method. In order to reduce the oscillatory behavior in the series, we consider the ratio of alternate coefficients A_k/A_{k-2}. The exponent γ_1 can be obtained from the asymptotic behavior of the ratios [1,8]

$$A_k/A_{k-2} \simeq y_c^{-2}\{1 + 2(\gamma_1 - 1)/[k(k-1)]^{1/2}\} \,, \tag{7}$$

where y_c is the value of y at the critical point.

In this letter, we only show the result. Our estimates of γ_1 are

$$\begin{aligned} \gamma_1 &= 0.79 \pm 0.05 \,, \quad n = 1 \,, \\ &= 0.83 \pm 0.05 \,, \quad n = 2 \,, \\ &= 0.91 \pm 0.05 \,, \quad n = 3 \,. \end{aligned} \tag{8}$$

In deriving these values, we have used the series estimates for y_c made in ref. [11]. The γ_1 estimate for $n = 1$ by Whittington et al. [8] was 0.78 ± 0.02. As a check, we have also treated γ_1 for $n = \infty$, which is known exactly as 3/2 for $d = 3$ [3]. Our series estimate is 1.45 ± 0.05.

We plot the surface critical exponent $\eta_\parallel$ in fig. 1

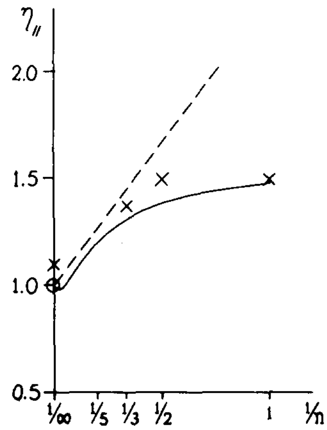

Fig. 1. The surface critical exponent $\eta_\parallel$ at $d = 3$. The crosses are plots of the present result obtained from γ_1 via scaling relations. The circle denotes the exact value for $n = \infty$ [3]. The solid and dashed lines represent the results of the ϵ [4,5] and $1/n$ [6] expansion, respectively.

via the relations [1,2] $\gamma_1 = \nu(2 - \eta_\perp)$ and $\eta = 2\eta_\perp - \eta_\parallel$. The result of the ϵ expansion [4,5] (ϵ is set to be 1)

$$\eta_\parallel = 2 - \frac{n+2}{n+8}\epsilon - \frac{(n+2)(17n+76)}{2(n+8)^2}\epsilon^2 \tag{9}$$

and that of the $1/n$ expansion [6]

$$\eta_\parallel = 1 + 4/3n \tag{10}$$

are also shown in fig. 1 for the sake of comparison. If we regard the series data as reliable ones, the $O(1/n)$ result of the $1/n$ expansion is satisfactory, especially for large n, while the result of the ϵ expansion represents the overall behavior well.

Finally, we make a remark on the additional scaling law due to Bray and Moore [3]. According to their argument, γ_1 could be expressed as

$$\gamma_1 = \nu + (\gamma - 1)/2 \,. \tag{11}$$

If we use the recent data for bulk exponents [12], we get

$$\begin{aligned} \nu + (\gamma - 1)/2 &= 0.7501 \,, \quad n = 1 \,, \\ &= 0.8273 \,, \quad n = 2 \,, \\ &= 0.8987 \,, \quad n = 3 \,. \end{aligned} \tag{12}$$

Comparing (12) with (8), we may say that there is no appreciable deviation from γ_1 for $n = 1$–3 at $d = 3$. It is within the extent of the error of the estimates. A clear deviation has been reported only in the case of $n = 0$ at $d = 2$ [7].

We have thus obtained the first nine coefficients of the layer susceptibility for general n and estimated the surface critical exponent γ_1.

The authors thank Professor A. Morita for helpful discussions. One of the authors (Y.O.) thanks the Sakkokai foundation for financial aid.

Appendix. The first nine coefficients of the layer susceptibility χ_1 for the semi-infinite simple cubic lattice. Refer to ref. [10] for the definitions of Q_j and T_j, which are functions of n.

$$a_1 = 5\,, \quad a_2 = 21\,, \quad a_3 = 93 + 5Q_1\,,$$

$$a_4 = 409 + 42Q_1\,, \quad a_5 = 1853 + 327Q_1 + 5Q_2\,,$$

$$a_6 = 8333 + 1960Q_1 + 42Q_2 + 16T_1 + 21T_2\,,$$

$$a_7 = 37965 + 11869Q_1 + 359Q_2 + 5Q_3 + 112T_1 + 423T_2 + 16T_3\,,$$

$$a_8 = 172265 + 65262Q_1 + 2176Q_2 + 42Q_3 + 1028T_1 + 3750T_2 + 108T_3 + 32T_5 + 32T_6 + 42T_7\,,$$

$$a_9 = 787557 + 359343Q_1 + 13785Q_2 + 391Q_3 + 5Q_4 + 6536T_1 + 32702T_2 + 1064T_3 + 40T_4 + 224T_5 + 336T_6 + 942T_7 + 237T_{10} + 80T_{11}\,.$$

References

[1] K. Binder and P.C. Hohenberg, Phys. Rev. B6 (1972) 3461; B9 (1974) 2194.
[2] M.N. Barber, Phys. Rev. B8 (1973) 407.
[3] A.J. Bray and M.A. Moore, Phys. Rev. Lett. 38 (1977) 735, 1046; J. Phys. A10 (1977) 1927.
[4] J.S. Reeve and A.J. Guttmann, Phys. Rev. Lett. 45 (1980) 1581; J. Phys. A14 (1981) 3357.
[5] H.W. Diehl and S. Dietrich, Phys. Lett. 80A (1980) 408; Z. Phys. B42 (1981) 65.
[6] K. Ohno and Y. Okabe, Phys. Lett. 95A (1983) 41.
[7] M.N. Barber, A.J. Guttmann, K.M. Middlemiss, G.M. Torrie and S.G. Whittington, J. Phys. A11 (1978) 1833.
[8] S.G. Whittington, G.M. Torrie and A.J. Guttmann, J. Phys. A12 (1979) 2449.
[9] S. Alvarado, M. Campagna and H. Hopster, Phys. Rev. Lett. 48 (1982) 51.
[10] E. Stanley, Phys. Rev. Lett. 20 (1968) 589; in: Phase transitions and critical phenomena, Vol. 3, eds. C. Domb and M.S. Green (Academic Press, New York, 1974).
[11] M.F. Sykes, D.S. Gaunt, P.D. Roberts and J.A. Wyles, J. Phys. A5 (1972) 640;
P.G. Bowers and G.S. Joyce, Phys. Rev. Lett. 19 (1967) 630;
P.J. Wood and G.S. Rushbrooke, Phys. Rev. Lett. 17 (1966) 307.
[12] J.C. Le Guillou and J. Zinn-Justin, Phys. Rev. Lett. 39 (1977) 95.