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R. Benzi and G. Martinelli: CORRECTIONS TO SCALING LAWS IN THE SELF-AVOIDING WALK.

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ABSTRACT.

A reconsideration of data obtained from high temperature expansion shows the validity of the scaling law $\alpha = 2 - D\nu$ for the three dimensional self-avoiding walk. Corrections to the scaling law are computed in the two and three dimensional cases. The results are in agreement with those obtained in quantum field theory.

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It is well known that the statistical mechanics of diluite solutions of synthetic polymers has many properties analogous to those of the Ising and related models of ferromagnetism and it is possible to model the representation of a polymer molecule as a self-avoiding walk on a regular crystal lattice[1, 2]. These models, like the Ising one, show a second order phase transition and it is possible to define exponents α and ν to describe the asymptotic behaviour of the total number of self-avoiding polygons U_n and of the root-mean square end to end length R_n in a n-step self-avoiding walk (x)

$$R_n \sim R_o \; n^{\nu} \tag{1}$$

$$U_n \sim U_o \; n^{\alpha - 2} \tag{2}$$

Table I[3-6] shows values of α and ν computed in two and three dimensions for different crystal lattices [Hereafter PS stands for plane square (P = 2), T for triangular (D = 2), BCC for the body-centered cubic (D = 3), FCC for face-centered cubic and D is the dimension].

Lattice	α	ν	D
PS	1/2	3/4	2
T	1/2	3/4	2
BEC	1/4	3/5	3
FCC	1/4	3/5	3

Table I - Review of numerical results for the critical exponents α and ν after Mc Kenzie [1].

(x) In the case of the Ising model α and ν refer respectively to the specific heat and to the correlation length.

By analogy with the Ising model one can show that α and ν must satisfy the scaling relation

$$D\nu = 2 - \alpha \tag{3}$$

We see from Table I that in D = 3 there is a disagreement between the computed value of α and ν and scling law (3). Also for the three dimensional Ising model there is such a disagreement between the computed value of critical exponents and the scaling law (3). However in the case of the Ising model it has been shown recently[7] that this scaling law is valid and that the disagreement can be explained in terms of corrections to scaling law for the specific heat which were not previously taken into account. Let us clarify this point. In the case of the Ising model the critical exponent α for the specific heat C is extracted from the high temperature expansions assuming a scaling law of the kind

$$C(T) \cong (T - T_c)^{-\alpha}\left[1 + O(T - T_c)\right] \tag{4}$$

where T_c is the critical temperature. On the other hand renormalization group theory implies a scaling law of the kind:

$$C(T) \cong (T - T_c)^{-\alpha}\left[1 + O(T - T_c)^{\omega\nu} + O(T - T_c)\right] \tag{5}$$

where $\omega\nu \simeq 1/2$.

If we use standard extrapolation techniques starting from scaling law (4) we get a numerical value of α in disagreement with the theory. To get out of the impasse we have to test scaling law (3) directly without computing in an independent way α and ν as shown in ref. (7). How to do this will be shortly reviewed later.

The same considerations can be made in the case of the self avoiding walk. Indeed it has been suggested [8] that the self avoiding walk is equivalent to a $\lambda(\sum_{i=1}^{N} \Phi_i \Phi^i)^2$ quantum field theory (QFT) in the case N = 0 and so the same arguments lead to scaling laws in QFT can be applied.

Let us now review the method which allows a direct test of scaling law (3). We define the quantity Q in the following way:

$$Q = \frac{\partial^2 K}{\partial V^2} \quad \frac{R^{3+D/2}}{(\partial R/\partial V)^3} \tag{6}$$

where $K = \sum_{n \geq 3} U_n V^n$ and $R = \frac{I - V}{V} \sum_{n \geq 1} R_n V^n$.

Things are so defined that phase transition occurs for $V \to 1$ and $\partial K/\partial V$ and R are the analogous of the specific heat and the square of the correlation length in the Ising model. Indeed for $R_n \sim R_o n^{\nu}$ we have $R \sim (1 - V)^{\nu}$. The term $(1 - V)/V$ arises from the definitions of R. If $G(p^2, V)$ is the Fourier transform of the two point correlation function then $R = \frac{1}{G} \frac{dG}{dp^2}\Big|_{p^2 = 0}$. In our case this is equivalent to:

$$R = \sum_1 R_n V^n / \sum_1^{\infty} V^n \tag{7}$$

Renormalization group theory tells us [7] that if scaling law (3) is valid Q has the following behaviour near the phase transition:

$$Q(V) \simeq Q(o) + A(1 - V)^{\omega\nu} + B(1 - V) + O(1 - V)^2 \tag{8}$$

That is Q(V) has a regular behaviour. On the other hand if scaling law (3) is not valid we get:

$$Q(V) \simeq Q(o)\,(1 - V)^{-(\alpha - 2 + D\nu)} \tag{9}$$

We see that the computed values of α and ν in D = 3 predict for Q(V) a singular behaviour. Thus we get the following result: to test directly the scaling law (3) we have to compute the behaviour of Q near the phase transition (V = 1); if Q has a singular behaviour then the scaling law (3) is not valid; if Q has a regular behaviour then the scaling law (3) is valid.

From numerical value of U_n and R_n it is possible to get Q in the

following form:

$$Q = \frac{\Sigma A_n V^n}{\Sigma B_n V^n} \tag{10}$$

If Δ is the exponent of the leading term of Q then by standard arguments [9]

$$\Delta = \lim_{n\to\infty} \Delta_n \tag{11}$$

where

$$\Delta_n = n\left[1 - \frac{A_n}{A_{n-1}} \frac{B_{n-1}}{B_n}\right] \tag{12}$$

(Let us recall that if Δ is positive then scaling law (3) is valid if Δ is negative then scaling law (3) is not valid). We have computed Δ_n for the PS, T, BCC and FCC lattices making use of numerical values of U_n and R_n [12-15].

In Table II values of the Δ_n are shown. We see that there is no violation of scaling (3) either in D = 2, as we expected, or in D = 3. Moreover it is possible from Table II to get rough estimate of $\omega\nu$ that is:

$$\begin{aligned} &0.35 \div 0.45 \qquad D = 2 \\ &0.50 \div 0.55 \qquad D = 3 \end{aligned} \tag{13}$$

It is possible to compute $\omega\nu$ in quantum-field-theory by means of other techniques and the known results are [10, 11]:

$$\begin{aligned} &\omega\nu \cong 0.43 \qquad D = 2 \\ &\omega\nu \cong 0.50 \qquad D = 3 \end{aligned} \tag{14}$$

in agreement with those we have found. Let us make another remark:

n	T x D=2	PS x D=2	BCC x D=3	FCC x D=3
1	.2088312	.2860045	.2603074	.2675639
2	.3401360	.1305051	.2623109	.3629629
3	.3965895	.3282076	.3911846	.4240633
4	.4284606	.2819463	.4034326	.4654090
5	.4446146	.3475668	.4594001	.4939484
6	.4532706	.3208612	.4219353	.5137090
7	.4568743	.3507615	.4486909	.5271892
8	.4573438	.3307286	.4605056	x
9	.4555342	.3447290	.5014306	x
10	.4517880	.3269321	x	x
11	.4466750	.3329861	x	x
12	x	.3162668	x	x
13	x	x	x	x
14	x	x	x	x
15	x	x	x	x
16	x	x	x	x

Table II - Computed values of Δ_n for various crystal lattices in 2 and 3 dimensions.

in the case of the Ising model $\lim_{n\to\infty} \Delta_n = 0$ and then it was not possible to estimate (7). It was suggested that, due to non-universal nature of the coefficient A and B in eq. (7), when $A \ll B$ one can estimate only the coefficient of the regular correction, $O(T - T_c)$, to the scaling law. This suggestion seem to be confirmed by the analysis we have done in the case of the self avoiding walk where one can reasonably argue that $A \simeq B$.

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REFERENCES.

(1) - For a review on the subject see: D. S. Mc Kenzie, Polimers and scaling, Phys. Reports C27, 35 (1976).
(2) - D. S. Mc Kenzie and C. Domb, Proc. Phys. Soc. 92 632 (1967).
(3) - M. G. Watts, J. Phys. A7 489 (1974).
(4) - M. F. Sykes, A. J. Guttman, M. G. Watts and P. D. Roberts, J. Phys. A5 653 (1972).
(5) - J. L. Martin, N. F. Sykes and F. T. Hioe, J. Chem. Phys. 46 3478 (1967).
(6) - J. L. Martin and M. G. Watts, J. Phys. A4 456 (1971).
(7) - R. Benzi and G. Martinelli, Validity of the scaling law for specific heat in three dimensional Ising model, Frascati Preprint, LNF-77/54 (1977).
(8) - P.G. De Gennes, Phys. Letters 38A, 339 (1972).
(9) - D. Jasnow and M. Wortis, Phys. Rev. 176, 739 (1968).
(10)- G. Parisi, Lectures given at the 1973 Cargese Summer School. Edited by Brezin and J. M. Charap (Gordon and Breach, to be published).
(11)- Le Guillon and J. C. Zinn-Justin Phys. Rev. Letters 39, 95 (1977).
(12)- C. Domb, J. Chem. Phys. 38, 2957 (1963).
(13)- J. L. Martin and M. G. Watts, J. Phys. A4, 456 (1971).
(14)- C. Domb and F. T. Hioe, J. Chem. Phys. 51 1915 (1969).
(15)- See also references quoted in ref. (1).

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