J. Phys. A: Math. Gen. 19 (1986) 2599-2609. Printed in Great Britain

Critical behaviour of the loop gas model on the square lattice

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Received 23 August 1985, in final form 21 November 1985

Abstract. The critical behaviour of the two-dimensional self-avoiding loop gas model with multiplicity $m=1$ (singly counted non-intersecting loops) is studied numerically on a square lattice using a recently developed Monte Carlo method. The critical exponents α, β, γ and δ are evaluated in the 'critical window' between the finite-size rounding and the non-critical ('correction-to-scaling') regime using a recently calculated accurate value of T_c. Within error bars, Ising-like critical exponents of the loop gas are obtained.

1. Introduction

Recently [3], a statistical model of non-intersecting loops (loop gas (LG) model) was proposed to study the influence of the excluded-volume repulsion on the critical equilibrium properties of statistical line systems. The LG model is useful in describing various physical systems (such as the defect-line-mediated smectic A–nematic transition [3], the equilibrium polymerisation of sulphur [4] and the roughening phenomenon of solid surfaces [7]). The model is defined by the grand canonical partition function

$$Z = \exp(-\beta F) = \sum_c m^{n_L(c)} \exp(-\beta l(c)) \tag{1}$$

where the sum extends over all configurations c of $n_L(c)$ self-avoiding and mutually self-avoiding (SAW) loops on a given domain L^2 of a two-dimensional square lattice. F is the free energy of the system. The configurational energy is proportional to the total length $l(c)$ of all loops and β is proportional to the inverse temperature

$$\beta = \varepsilon / k_B T \tag{2}$$

where ε is the energy of a single link. The chemical potential of the *loops* is given by

$$\mu = kT \log m \tag{2'}$$

where m is the loop multiplicity. The model describes various physical systems. For example, $m=0$ defines the one-loop (i.e. the dilute-polymer) problem, $m=1$ describes thermally equilibrated polymer rings, as occurring, for example, in the equilibrium polymerisation problem of sulphur [4], $m=2$ describes polar (i.e. oriented) loops, as occurring, for example, in a defect-line-mediated smectic A–nematic phase transition

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of liquid crystals [3], and $m \geq 2$ describes a generalised roughening problem [7]. Moreover, an analogous model is considered in the lattice theory of fermions [9].

In the present paper we show numerically the equivalence of the multiplicity $m = 1$ LG and the Ising model on a square lattice ($d = 2$).

The Ising model on the square lattice is defined, for instance, by its low temperature expansion graphs [5] (and, by the Kramers-Wannier duality [6], its equivalent high temperature expansion graphs). Typically, any component of the Ising partition function expansion graph is defined by a set of bonds connecting the nearest-neighbour lattice sites once at most and ending in a lattice point in pairs or quadruplets. Thus, the bond coordination number at any site is $c = 0, 2$ or 4; no open lines are allowed. In contrast, for the LG model, no bond crossings are allowed: $c \neq 4$. This difference between the LG and the Ising model graphs has three consequences: (i) the Kramers-Wannier duality is destroyed on passing from the Ising to the LG model, (ii) a so-called 'disorder point' appears in the high temperature phase of the LG model, as shown in [8], and (iii) the shift of the critical temperature to higher values is given by $T_c^{\text{Ising}} = 1.135$, $T_c^{\text{LG}} = 1.157$ (in units of ε/k_B). However, from our results, *no modification of the critical behaviour occurs.*

We use a convenient Monte Carlo (MC) computation technique described recently in [1, 9]. A Monte Carlo step can modify a configuration of loops in a plaquette by replacing empty bonds by occupied ones and vice versa, provided that the final configuration satisfies again the SAW property. This means, for instance, creating (or annihilating) an elementary loop of length 4, lengthening (or shortening) a loop by two bonds, or cutting one loop into two loops (or vice versa). The finite-size behaviour of the LG specific heat was analysed in various dimensions and for various multiplicities m [1]. Unfortunately, the extrapolation method does not yield a sufficiently precise value of the critical exponent α and thus, in [1], it could not be decided, for example, whether or not the LG model for $m = 1$ is in the Ising universality class. In fact, for $d = 2$, $m = 1$ a rather large uncertainty of $0 \leq \alpha \leq 0.4$ and correspondingly, from the assumed hyperscaling relation, of $\nu (= 1 - \alpha/2)$, $0.8 \leq \nu \leq 1$, was obtained. In the present paper, we use an accurate value of T_c from a recent numerical study of the corresponding seven-vertex model [2] ($\beta_c = 0.864 \pm 0.001$) obtained with a finite-size transfer matrix method (yielding, in addition, $\nu = 1$ rather accurately [2]). This result was, in fact, the first reliable numerical evidence for an Ising value of the LG exponents α and ν. Using T_c from reference [2], we are able to find a temperature regime within the critical region of the infinite-lattice LG, which is limited, close to T_c, by the finite-size rounding temperature (where diverging thermodynamic quantities round off) on one side, and the end of the critical regime away from T_c (where correction-to-scaling terms become important) on the other side. In this 'critical window' (whose extension increases with increasing system size) the critical exponents near T_c, such as α, β and γ, are calculated from the slope of the linear portion of the corresponding quantity in a doubly logarithmic plot. Furthermore, the exponent δ is determined from the isotherm at the critical temperature T_c (of the *infinite* system). We find Ising-like values for all exponents considered. In addition, as a sharpening of the result $\alpha = 0$ the specific heat is found to diverge logarithmically. Also, the critical amplitudes are determined and, as a result, we conclude that the loop gas model on a square lattice lies, for $m = 1$, in the *Ising universality class.*

Thus, the introduction of the total self-avoidingness of the LG with $m = 1$ ($c = 0, 2, c \neq 4$; i.e. of the non-crossing property of closed lines) in addition to the at most single occupancy of bonds of Ising graphs does not alter the corresponding universality

Table 1. Summary of the results for the critical exponents (E) and critical amplitudes (A) of the investigated thermodynamic variables for the two-dimensional loop gas on a square lattice with $L = 80$ and the Ising model. Except for the order parameter, the *extrapolated* critical quantities of the LG on the infinite lattice lie within the error bars.

	Loop gas	Ising
Specific heat: $T < T_c$	E: $\alpha' = 0$	0
	A: $a' = 0.61 \pm 0.02$	$2/\pi = 0.637$
Specific heat: $T > T_c$	E: $\alpha = 0$	0
	A: $a = 0.59 \pm 0.04$	$2/\pi = 0.637$
Order parameter: $T < T_c$	E: $\beta = 0.115 \pm 0.002$	
	A: $B = 1.17 \pm 0.01$	
Order parameter extrapolated ($L = \infty$)	E: $\beta_\infty = 0.124 \pm 0.002$	$\frac{1}{8} = 0.125$
	A: $B_\infty = 1.17 \pm 0.01$	1.22
Susceptibility: $T < T_c$	E: $\gamma' = 1.77 \pm 0.03$	$\frac{7}{4} = 1.75$
	A: $C_- = 0.024 \pm 0.003$	0.026
Susceptibility: $T > T_c$	E: $\gamma = 1.70 \pm 0.08$	$\frac{7}{4} = 1.75$
	A: $C_+ = 1.3 \pm 0.1$	0.96
Critical isotherm: $T = T_c$	E: $\delta = 15.1 \pm 0.2$	15
	A: $D = 1.06 \pm 0.01$	1.06
Derived exponents		
Correlation length: $T < T_c$	E: $\nu' = 1$	1
Correlation length: $T > T_c$	E: $\nu = 1$	1
Correlation function: $T = T_c$	E: $\eta = 0.25 \pm 0.002$	$\frac{1}{4} = 0.25$

class. From the equivalence of the LG and the Ising model on the honeycomb lattice (where crossing lines ($c = 4$) cannot occur) and our result, further support is given to the general assertion that the critical exponents of lattice models of a given dimensionality are independent of the lattice structure. An analogous result in two dimensions has been reported some time ago [10]. Using exact enumeration data the trail walk problem (in which each lattice *bond* is visited at most once) was shown to be numerically equivalent to the SAW (i.e. dilute polymer) problem. The extension of this equivalence to the corresponding loop problems leads to the $m = 0$ LG case.

In § 2, an analysis of the specific heat near T_c is presented and in § 3 the order parameter is defined for the LG and analysed together with its susceptibility. The critical isotherm is analysed in § 4 and in § 5 concluding remarks as well as a summary of our results for the critical exponents α, β, γ, δ, and amplitudes $A_\pm$, B, $C_\pm$, D are presented in table 1.

2. Specific heat

The specific heat per site

$$c = \frac{\partial E}{\partial T} = \varepsilon \frac{\partial}{\partial T} \langle l^2 \rangle / L^2 \tag{3}$$

is studied near the critical point. From equations (1) and (2), it is related to the energy fluctuations by

$$c k_B T^2 / \varepsilon^2 = \langle (l - \langle l \rangle)^2 \rangle / L^2 = (\Delta l)^2 / L^2 \tag{4}$$

(fluctuation-dissipation theorem).

Monte Carlo data for $\Delta l^2/L^2$ as a function of the temperature T are depicted in figure 1. Any value is calculated as an average over 1000 configurations each obtained after five complete sweeps through the lattice. In the same way, all other calculated quantities discussed below are obtained.

The most singular part at $T \approx T_c$ defines the critical exponents α', α and amplitudes A below and above T_c:

$$\left.\begin{array}{ll} c \simeq A_-(-t)^{-\alpha'} & T \uparrow T_c \\ c \simeq A_+ t^{-\alpha} & T \downarrow T_c \end{array}\right\} (t = T/T_c - 1). \tag{5}$$

For the case $\alpha = \alpha' = 0$, a logarithmic dependence on t is defined by

$$\Delta l^2/L^2 \simeq a^{(\prime)} \log|t| \qquad \text{for } T \to T_c^{\pm}. \tag{5'}$$

A linear c against $\log|t|$ plot (figure 2(a)) shows that a logarithmic dependence, equation (5'), is consistent with the Monte Carlo data, in contrast to a power law (figure 2(b)).

As a result,

$$\alpha' = \alpha = 0 \qquad a' = 0.61 \pm 0.02 \qquad a = 0.59 \pm 0.04. \tag{5''}$$

Moreover, a shift of the low and high temperature curves of

$$\Delta c = c(T_c + \delta) - c(T_c - \delta) \simeq (0.32 \pm 0.07)\varepsilon^2/k_B T^2 \tag{5'''}$$

for small finite δ is observed.

The deviation of the logarithmic dependence corresponding to equation (8) close to T_c is caused by the finite-size effect. We have obtained for the square lattice loop gas with $L = 10$, 20, 40 and 80 and periodic boundary conditions approximately

$$|T_{dev} - T_c|/T_c = (0.9 \pm 0.06)/L. \tag{6}$$

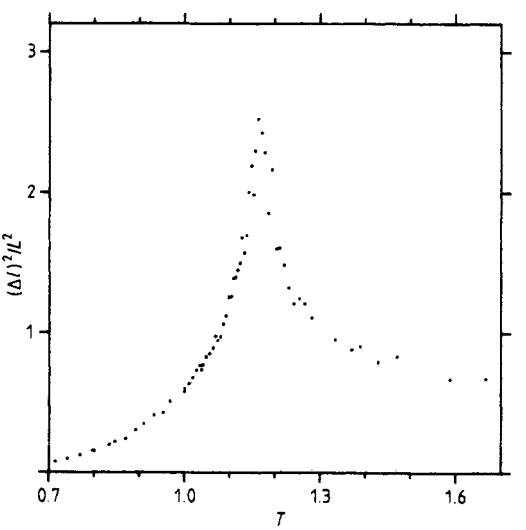

Figure 1. Temperature dependence of the mean-square total loop length fluctuations $(\Delta l)^2/L^2 = \langle (l - \langle l \rangle)^2 \rangle / L^2$ (i.e. $k_B T^2 \times$ specific heat per site, (4)) of the LG on a square lattice with $L = 80$ with periodic boundary conditions, near the critical point.

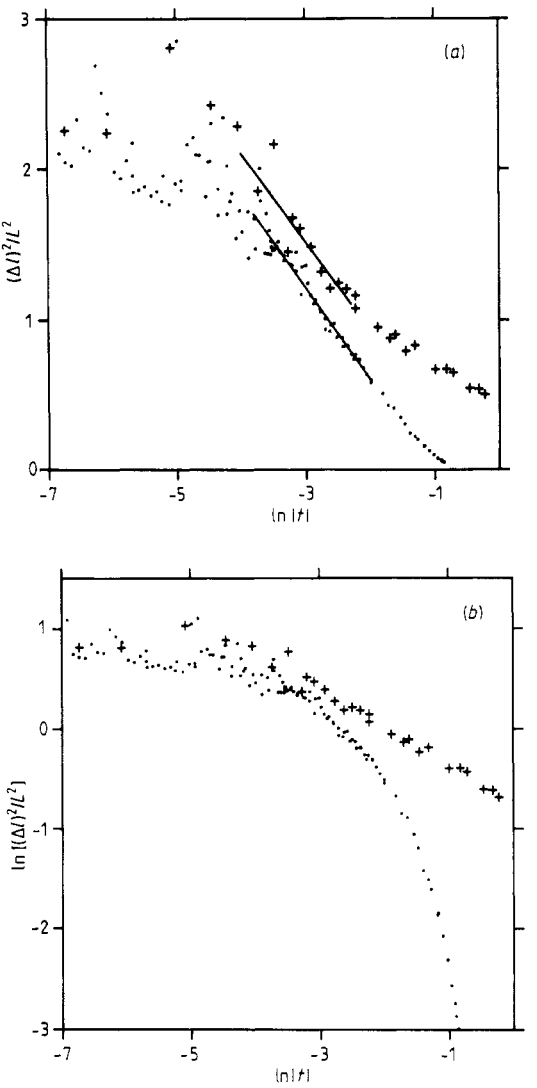

Figure 2. Semi-logarithmic plot of $(\Delta l)^2/L^2$ against $\ln|t|$ ($t = T/T_c - 1$), for $t < 0$ (●) and $t > 0$ (+), respectively (*a*). The lines represent an optimised linear fit within the 'critical window' below and above T_c, respectively, and yield $\alpha' = \alpha = 0$, the values of the prefactors (5') $a' = 0.61 \pm 0.02$ ($t < 0$) and $a = 0.59 \pm 0.04$ ($t > 0$) ($a'_{\text{Ising}} = a_{\text{Ising}} = 2/\pi = 0.636$), respectively, and a constant shift $\Delta C = 0.32 \pm 0.07$(*a*). A corresponding log-log plot does not show any apparent linear behaviour (*b*), in agreement with $\alpha' = \alpha = 0$.

A finite exponent α or α', equation (5), would show up in a linear portion of the log c against $\log|t|$ plot. As shown in figure 2(*b*), no linear dependence is observed.

3. Order parameter and susceptibility

An order parameter of the self-avoiding loop gas model can be defined from the close analogy to the Ising model in its line graph representation of the high temperature

expansion mentioned above. The Ising graphs can be viewed as closed lines (loops) with allowed crossings (i.e. with a crossing energy $\varepsilon_c = 0$; in contrast, $\varepsilon_c = \infty$ for the loop gas model). The Ising order parameter, i.e. the magnetisation m, is defined by the statistical average $\langle s \rangle$ of the site-averaged spin s:

$$m = \langle s \rangle = \left\langle \frac{1}{N} \sum_{i=1}^{N} s_i \right\rangle \qquad N = L^2.$$

In general, the loops separate regions of opposite spins $s_i = \pm 1$, and divide the whole lattice into an exterior (v_{ex} with $s_i = +1$) and an interior (v_{in} with $s_i = -1$) part, respectively. Therefore

$$s = (v_{ex} - v_{in})/(v_{ex} + v_{in}).$$

Introducing a magnetic field H by

$$Z(h) = \sum_c \exp(-\beta l(c) + hs) \qquad h = \beta H \tag{7}$$

it follows that

$$m = \frac{1}{N} \frac{\partial}{\partial h} \ln Z. \tag{8}$$

The response of the spins to an applied infinitesimally small external magnetic field H defines the susceptibility χ

$$\chi = \frac{1}{N} \frac{\partial m}{\partial H} = \beta \langle (s - \langle s \rangle)^2 \rangle = \beta \Delta m^2 \tag{9}$$

again from the fluctuation–dissipation theorem. An analysis of $m(T)$ close to T_c yields

$$m \simeq B(T_c - T)^{\beta} \tag{8'}$$

where β is the critical exponent of the magnetisation. In calculating $\langle s \rangle$ for finite systems at $h = 0$ and close to T_c, and starting with $\langle s \rangle > 0$, it occurs from time to time that 'wrong' magnetisation directions $\langle s \rangle < 0$ contribute to the average value of m. Thus, $|\langle s \rangle|$ underestimates the magnetisation value of the infinite lattice. For very large lattice sizes L, 'wrong' magnetisation directions occur very rarely even for long calculation times τ. Note that $m = \lim_{\tau \to \infty} \lim_{L \to \infty} \langle s \rangle$ defines the magnetisation for the infinite system whereas for the opposite order of limits, $\lim_{L \to \infty} \lim_{\tau \to \infty} \langle s \rangle \ (\tau, L) = 0$ at *all* temperatures.

We have analysed the quantities $|\langle s \rangle|$ and $\langle |s| \rangle$, for which, evidently

$$|\langle s \rangle| < \langle |s| \rangle \tag{10}$$

holds. Numerically, equality holds for (10) everywhere except very close to and above the critical point T_c. In figure 3, Monte Carlo results for the order parameter m are plotted against T. To evaluate β we have plotted in figure 4 data from a 80×80 lattice in a log m against log$|t|$ graph. The linear fit has been achieved by statistically weighting the m values using the mean-square deviation of m which is proportional to $\chi^{-1/2}$ (where χ is the susceptibility):

$$m^{(W)} = (1/\chi^{1/2}) \langle s \rangle.$$

We have obtained for an 80×80 lattice

$$\beta = 0.115 \pm 0.002 \qquad B = 1.17 \pm 0.01. \tag{8''}$$

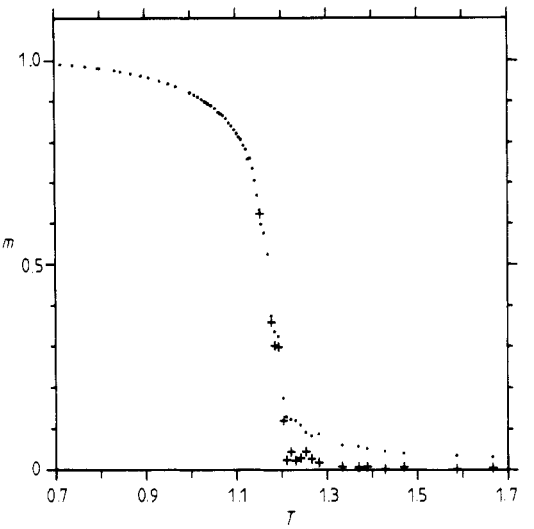

Figure 3. Temperature dependence of the order parameter m of the LG on a square lattice with $L = 80$ with periodic boundary conditions, near the critical point. The points (●) denote sampling of the absolute values of s, $\langle|s|\rangle$, whereas the crosses (+) denote $|\langle s\rangle|$. For convenience the latter have been drawn only in the case for $\langle|s|\rangle - |\langle s\rangle| > 0.002$.

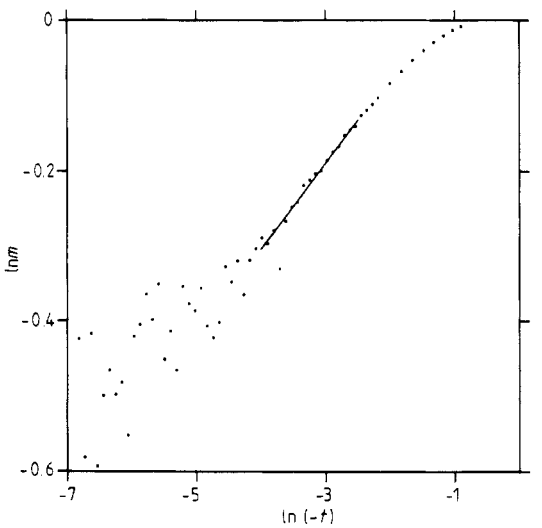

Figure 4. Log-log plot of the order parameter, ln m against $\ln(-t)$ for $L = 80$. The optimised linear fit yields $\beta_{80} = 0.115 \pm 0.002$, $B = 1.17 \pm 0.01$ (equation (8″)). Apparently the deviation of β from the expected Ising value is caused by finite-size effects.

The finite-size effect is illustrated for $L = 10, 20, 40$ and 80 in figure 5. The $(L = \infty)$ extrapolated values for the exponent β and the amplitude B are

$$\beta = 0.124 \pm 0.002 \qquad B = 1.19 \pm 0.001 \tag{8‴}$$

compatible with the Ising values $\beta = 0.125$ and $B = 1.22$. The Monte Carlo results for the susceptibility for the 80×80 lattice are shown in figure 6. A remarkable linear

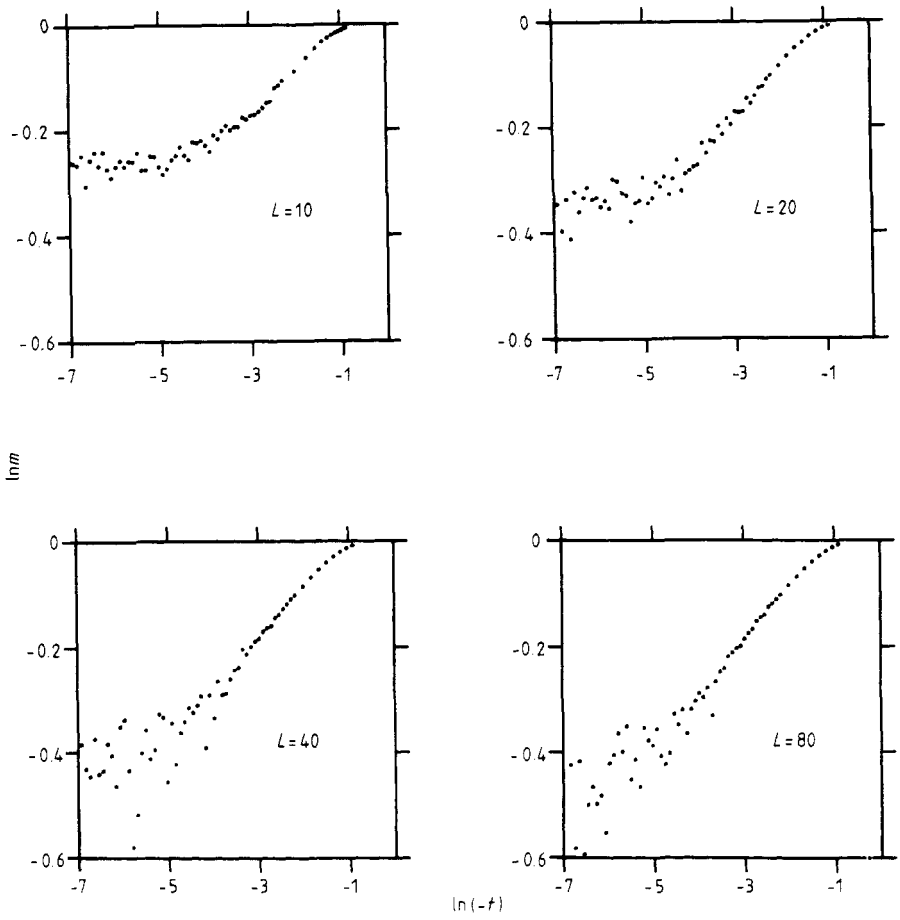

Figure 5. Log-log plots of the order parameter ln m against $\ln(-t)$ for $L = 10$, 20, 40 and 80. An extrapolation of the β values for the lattice sizes $L = 10$, 20, 40 and 80 gives $\beta_\infty = 0.124 \pm 0.002$ and $B_\infty = 1.19 \pm 0.001$.

behaviour is obtained if $\ln(\Delta m^2/L^2)$ is plotted against $\ln(T_c/T - 1)$ instead of $\ln(T/T_c - 1)$, cf figure 7. A simple fit within the critical window yielded sufficiently accurate values for the exponents γ, γ' and amplitudes $C_\mp$ defined by

$$\begin{aligned} (\Delta m)^2 &= C_-(-t)^{-\gamma'} \qquad (T \uparrow T_c) \\ &\quad C_+ t^{-\gamma} \qquad (T \downarrow T_c). \end{aligned} \tag{11}$$

We have obtained

$$\begin{aligned} \gamma' &= 1.77 \pm 0.03 \qquad C_- = 0.024 \pm 0.003 \\ &= 1.70 \pm 0.08 \qquad C_+ = 1.3 \pm 0.1. \end{aligned} \tag{11'}$$

Again, the critical exponents coincide, within error limits, with the Ising values ($\gamma'_{is} = \gamma_{is} = 1.75$). Interestingly, the LT critical amplitude C_- is equal to the Ising value C_-^{Ising} whereas the HT value $C_+ \simeq 0.8\ C_+^{Ising}$. The deviation of the latter from the Ising value can be understood qualitatively in terms of the stronger effect of the non-crossing property of the LG at higher loop densities, i.e. on the HT side of T_c.

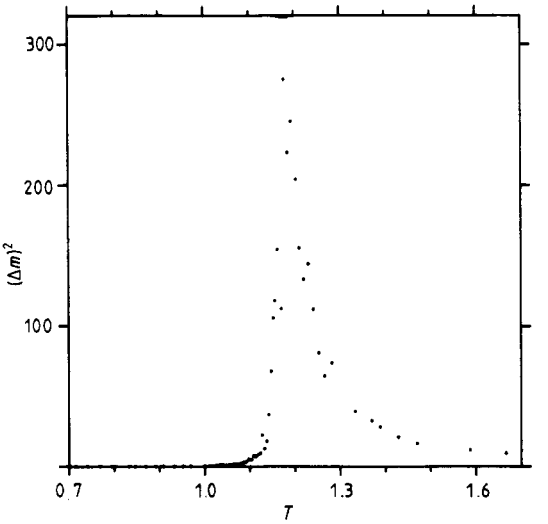

Figure 6. Temperature dependence of the mean-square order parameter fluctuations Δm^2 (9) of the LG on a square lattice with $L = 80$ with periodic boundary conditions.

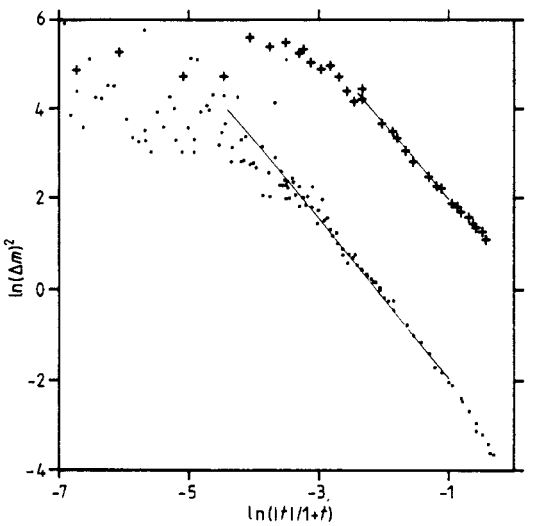

Figure 7. Log-log plot of $(\Delta l)^2/L^2$ (susceptibility): $\ln[(\Delta l)^2/L^2]$ against $\ln[|t|/(1+t)]$, for $t>0$ (+) and for $t<0$ (●) respectively, for $L=80$. The linear fits yield $\gamma' = 1.77 \pm 0.03$, $C_- = 0.024 \pm 0.003$ ($t<0$) and $\gamma = 1.70 \pm 0.08$, $C_+ = 1.3 \pm 0.1$ ($t>0$). Note the enlarged critical window in a $t/(1+t)$ ($=1-T_c/T$) plot (compared with a $t(=T/T_c-1)$ plot).

4. Critical isotherm

Using the definition of the magnetic field (7), the critical isotherm $m(h, T = T_c)$ scales, for small values of $|h|$, as

$$m \simeq D|h|^{1/\delta}. \tag{12}$$

To determine the critical exponent δ and the amplitude D, we have plotted log m against log $|h|$ at $T = T_c$ in figure 8. The linear regime within the 'critical window' is

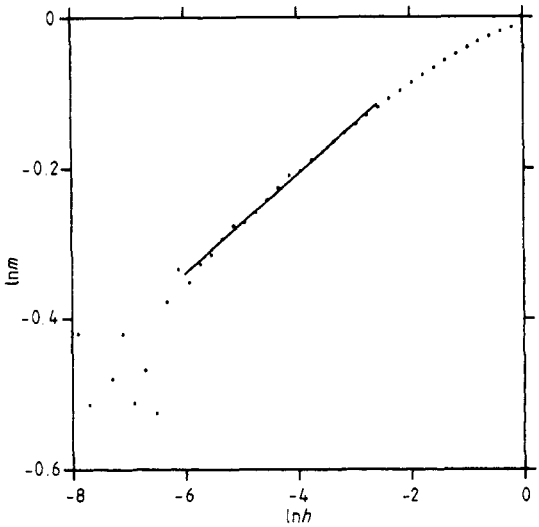

Figure 8. Log-log plot of the critical isotherm $m(h, t=0)$ for $L=80$. The linear fit yields $\delta = 15.1 \pm 0.2$, $D = 1.06 \pm 0.01$.

rather narrow. The analysis of a linear fit gives

$$\delta = 15.1 \pm 0.2 \qquad D = 1.06 \pm 0.01. \tag{12'}$$

For the Ising model, $\delta = 15$, $D^{is} = 1.06$.

5. Conclusions

As the main result, the 2D Ising-like *critical exponents* have been established for the LG model with $m = 1$ on the square lattice, using the critical window method and an accurate value of T_c. The *critical amplitudes* assume Ising-like values below T_c but deviate slightly from the latter above T_c. The numerical results are summarised in table 1.

Moreover, finite-size effects for the order parameter have been studied for the (linear) lattice sizes $L = 10, 20, 40, 80$ and periodic boundary conditions. A confirmation and sharpening of the previous results has been obtained.

Acknowledgments

This work was supported by the Deutsche Forschungsgemeinschaft under contract Schr 4/10-1 and Sfb 6-TP A7/2. The calculations were performed on the VAX 11/780 of the Fachbereich Physik der Freien Universität Berlin and on the Cray 1M of the Berlin Konrad-Zuse Rechenzentrum.

Note added in proof. The methods of this paper have been used to investigate random surfaces on the cubic lattice [11].

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