J. Phys. A: Math. Gen. **16** (1983) 4073–4081. Printed in Great Britain

Numerical study of self-avoiding loops on d-dimensional hypercubic lattices

M Karowski†, H J Thun†, W Helfrich‡ and Franz S Rys‡

† Institut für Theorie der Elementarteilchen, Freie Universität Berlin, Arnimallee 14, D-1000 Berlin 33, Germany

‡ Institut für Theorie der Kondensierten Materie, Freie Universität Berlin, Arnimallee 14, D-1000 Berlin 33, Germany

Received 9 March 1983, in final form 22 June 1983

Abstract. The loop gas in $d = 2, 3, 4$ and 5 dimensions and with multiplicities $m = 0, 1, 1.5, 2, 3$ and 4 is investigated by the Monte Carlo method. The critical temperatures and approximate values for the critical exponent ν corresponding to second-order phase transitions are obtained for $d = 2$ and 3.

1. Introduction

The statistical behaviour of self-avoiding loops, i.e. non-intersecting closed lines in thermal equilibrium, has been studied recently in the context of defect-line mediated phase transitions in various dimensions (Rys and Helfrich 1982) and the equilibrium polymerisation of sulphur (Wheeler *et al* 1980, Duplantier and Pfeuty (1982). The loops are thermally created, their energy being proportional to the total length of all loops in the configuration. Hence the statistical weight of a loop configuration equals x^l where $x = e^{-\beta}$, and β is proportional to the inverse temperature, $\beta = \varepsilon/(k_B T)$. On a hypercubic lattice l denotes the total number of links constituting the loops and ε is the energy of a single link. Furthermore, a loop multiplicity m is introduced which allows a multiple counting of each of the loops, e.g. $m = 1$ for polymer rings and $m = 2$ for polar dislocation loops in three dimensions (Rys and Helfrich 1982). In another context, quantum field theories can be expressed by systems of loops (Symanzik 1969, Brydges *et al* 1982, Karowski *et al* 1983).

In equilibrium statistical mechanics a system of self-avoiding loops is described by the partition function

$$Z = \sum_c m^s x^l \tag{1}$$

where the sum extends over all allowed configurations c of self-avoiding loops on a given domain L^d of $\mathbb{R}^d$. For mathematical convenience, the problem is formulated on a regular lattice. The number of loops of a configuration is denoted by s, and l is their total length in units of the lattice spacing. The loop multiplicity m plays the role of a loop fugacity whereas x stands for the monomer fugacity. For generic values of m, Z is the partition function of a 'gas' of thermally created closed self-avoiding lines. Any phase transition shows up in a singularity of the free energy density $f(m, T) = -(k_B T \ln Z) L^{-d}$ in the thermodynamic limit $L \to \infty$.

Despite the difficulties of the underlying mathematical problem, due to the non-Markovian nature of the excluded volume problem, much progress has been made as regards single and dilute polymer chains (Flory 1967, de Gennes 1972, 1979). The few studies of closed polymers were restricted to a single ring (des Cloizeaux 1981, Baumgärtner 1982). The critical exponent of the radius of gyration, ν, of the ring appears to be equal to that of the chain. In our description the ring polymer corresponds to the loop gas in the limit $m \to 0$. Studying a low-temperature series expansion of the loop gas in terms of the parameter x, one of us (Rys 1983) calculated for $m = 0$ the critical value x_c and the exponent of the specific heat, α. The latter agrees with the value derived from ν on the basis of hyperscaling (see below). Unfortunately, the use of this method was quite unsuccessful for any case $m > 0$ (Rys 1981). A mean-field theory for the loop gas on a lattice with $m > 0$ has been proposed, characterising the critical point by the first appearance of one or more infinite loops (Helfrich 1983). An additional argument for the existence of a critical point relies on the fact that the analogous loop gas model with $m = 1$ on a honeycomb lattice is equivalent to the Ising model at zero magnetic field on that lattice (Nienhuis 1982). However, for the self-avoiding loop gas on other lattices with $m > 0$, the existence of critical points and, if they exist, their nature remain open questions.

In this work we present a numerical analysis of the equilibrium loop gas problem. Applying a novel computer simulation technique which will be described in more detail in a separate publication (Karowski *et al* 1983), we investigate several cases of the loop gas on finite lattices in $d = 2$ and 3 dimensions. Some preliminary results for four and five dimensions are also obtained. The linear size L of the considered hypercubic lattices ranges from 4 to 50 for $d = 2$ and from 4 to 12 for $d = 3$. We mainly concentrate on multiplicities $m = 0$ and 1 but also report some results for $m = 1.5$, 2, 3 and 4.

In § 2 we give a short description of the Monte Carlo method. In § 3 we present our main results. Using finite-size scaling arguments (Fisher 1971, Binder 1976) we evaluate the critical temperatures from the positions of the maxima of the specific heat. In conjunction with an analysis of the heights of these maxima as a function of the lattice size, we also obtain estimates for the critical exponent α.

In § 4 we discuss the distribution of the loop sizes for various temperatures and multiplicities. The nature of a 'change-over' from small loops to large ones apparently depends on the values of m; there is a qualitative difference between the cases $m < 2$ and $m > 2$ for $d = 2$. Concluding remarks follow in § 5.

2. Monte Carlo simulation

A detailed description of the Monte Carlo method (Metropolis *et al* 1953, Friedberg and Cameron 1970) to construct loop gas configurations on a lattice will be given in a separate publication (Karowski *et al* 1983). Here we only sketch the main ideas. Our variant of the heat bath method generates samples of equilibrium ensembles of configurations of loops which are self-avoiding by construction. For simplicity we illustrate it only for the case of multiplicity $m = 1$.

Starting from an arbitrary allowed configuration c of loops with total length l, a new one c' with length l' is proposed (which differs from the old one only by a local change). In our updating procedure we sequentially sweep the plaquettes of the entire lattice. At each of the L^d lattice points we look in turn at $d(d-1)/2$ plaquettes. In

a given plaquette we make a local change of the present configuration. The four possible types (up to rotation) of such changes are depicted in figure 1. One has to

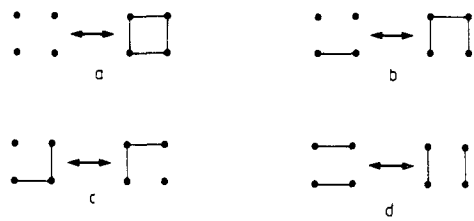


Figure 1. Local changes of loop configurations within a plaquette.

make sure, however, that the global configuration remains self-avoiding (no crossings and branchings). In a thermal cycle we start at low temperature from the empty lattice for loop gas configurations (multiplicity $m > 0$), and from one small square for the one-loop case ($m = 0$), respectively. In the latter case we have to exclude local changes of the types a and d in figure 1. We decide to take the new configuration c', if a pseudo-random number (equally distributed in the unit interval) is less than $e^{-\beta l'}(e^{-\beta l'} + e^{-\beta l})^{-1}$, otherwise we retain the old one. Since every allowed configuration can in principle be attained after sufficiently many iterations the 'ergodic condition' is satisfied. Obviously a large set of configurations with a probability distribution proportional to the Boltzmann factor $e^{-\beta l}$ is stable under this procedure. Moreover, starting from an arbitrary initial configuration, we expect to reach such an equilibrium set after an appropriate 'warming up' period. From this sequence we select a subset of configurations which are separated by so many single steps that their correlation seems negligible.

Then the thermal average value of a variable A

$$\langle A \rangle = \sum_c A(c)\, e^{-\beta l}/Z \tag{2}$$

is approximated by

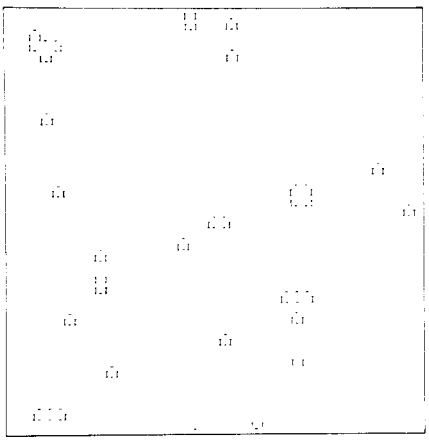
$$\langle A \rangle \approx \sum_{c_i} A(c_i) / \sum_{c_i} 1 \tag{3}$$

where now the sum extends only over a sufficiently large sample of configurations c_i constructed above.

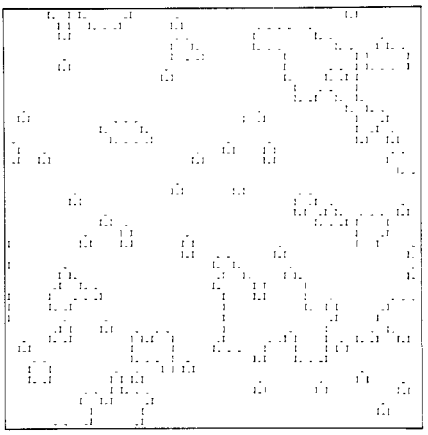
3. Critical behaviour of loop gas systems

We consider loop gas systems on hypercubic lattices with periodic boundary conditions. For fixed dimension d, multiplicity m and lattice size L we 'measure' the average length $\langle l \rangle$ (proportional to the energy) and the fluctuation $\langle \Delta l^2 \rangle = \langle l^2 \rangle - \langle l \rangle^2$ (proportional to the specific heat) in a so-called thermal cycle: $\beta = \beta_1,\ \beta_1 - \delta\beta, \ldots, \beta_2,\ \beta_2 + \delta\beta, \ldots, \beta_1$ (cf Creutz *et al* 1979).

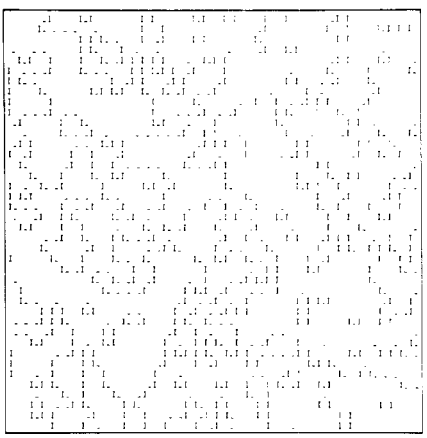
Figure 2(*a*) shows a typical configuration on a 40×40 lattice with periodic boundary conditions at low temperature ($\beta = 1.16$). There are only a few small loops. Around



(*a*)



(*b*)



(*c*)

Figure 2. Three typical loop gas configurations for multiplicity $m = 1$ on a 40×40 lattice with periodic boundary conditions. The temperatures are: (*a*) far below ($\beta = 1.16$), (*b*) close to ($\beta = 0.86$) and (*c*) far above ($\beta = 0.56$) the critical point.

$\beta \approx 0.86$, $\langle l \rangle$ grows rapidly with temperature and $\langle \Delta l^2 \rangle$ has a maximum. The single configurations show strong fluctuations: some of them contain loops of medium size, others also comprise rather large ones (cf figure 2(*b*)). For high temperatures the energy approaches its asymptotic value and the specific heat decreases again. Figure 2(*c*) is a typical example for a high temperature configuration ($\beta = 0.56$) where the lattice is filled with many loops, among them a very large one. (In this regime only few configurations contain more than one very long loop.)

The characteristic dependence on β of $\langle l \rangle$ and $\langle \Delta l^2 \rangle$ is displayed in figure 3 for a 5×5 lattice and multiplicity $m = 1$. Since the corresponding data for other lattice sizes and multiplicities and for dimensions $d = 3, 4$ and 5 look similar we refrain from presenting them in the same manner. Instead, in figures 4(*a*) and 4(*b*) we have plotted fits for $\langle \Delta l^2 \rangle / L^d$ against β for $m = 1$ for several lattice sizes L in 2 and 3 dimensions, respectively. The peaks are interpreted as the remainders of the singular behaviour of the specific heat

$$C(\beta) \sim |\beta - \beta_{\text{crit}}|^{-\alpha} \tag{4}$$

of an infinite system at a second-order phase transition. We observe the typical shift

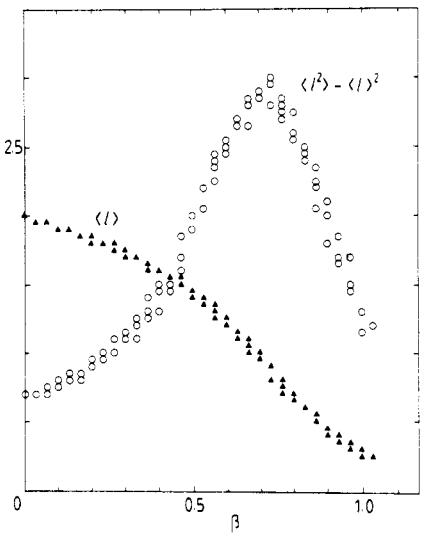


Figure 3. The average energy $\langle l\rangle$ and the length fluctuation $\langle l^2\rangle - \langle l\rangle^2$ against β for a loop gas of multiplicity $m = 1$ on a 5×5 lattice. The thermal cycle runs from $\beta = 1.02$ to $\beta = 0$ in steps of $\delta\beta = 0.01$. For each temperature (in both directions) a sample of 4000 configurations has been taken.

of the locations of the maxima according to finite size corrections (Fisher 1971, Binder 1976)

$$\beta_{\max} \approx \beta_{\text{crit}} - aL^{-\lambda} \tag{5}$$

for $L \to \infty$.

We also notice that with increasing lattice size the peaks of the specific heat are higher and sharper. On an infinite lattice the correlation length diverges as $\xi \sim |\beta - \beta_{\text{crit}}|^{-\nu}$. Finite-size corrections set in when the correlation length ξ becomes comparable to the lattice size: $\xi \approx L$. The positions of the maxima $\beta_{\max}$ as functions of the lattice size L are plotted in figure 5 together with least squares fits according to (5) with $\lambda = 1.25$ and 1.6 for $d = 2$ and 3, respectively. Using the relation $\lambda = 1/\nu$ (which was checked in the case of the Ising model (Fisher 1971, Binder 1976)) we obtain first estimates of the critical exponent ν. Assuming a further finite-size scaling relationship (Fisher 1971, Binder 1976)

$$C_{\max} \sim L^{\alpha/\nu} \tag{6}$$

and hyperscaling, $d\nu = 2 - \alpha$, we get slightly higher values for ν. However, the case $d = 2$, $m = 1$ is compatible with a logarithmic increase of $C_{\max}$, too. At present we cannot decide whether the above finite-size relations may be unambiguously applied to the self-avoiding loop gas. In a subsequent publication we shall concentrate on the determination of additional quantities revealing the critical behaviour.

Our results for the critical inverse temperature β_{crit} and estimates for the critical exponent ν are collected in table 1. For multiplicity $m = 0$ we find good agreement with results obtained by other methods on the polymer problem (Flory 1967, de Gennes 1972, 1979, Rys 1983, Sykes *et al* 1972, Aragão de Carvalho and Caracciolo 1983†). Our values $\beta_{\text{crit}} = 0.963$ and $\beta_{\text{crit}} = 1.54$ for two and three dimensions compare

† We thank B Berg for bringing this reference to our attention after completion of our manuscript.

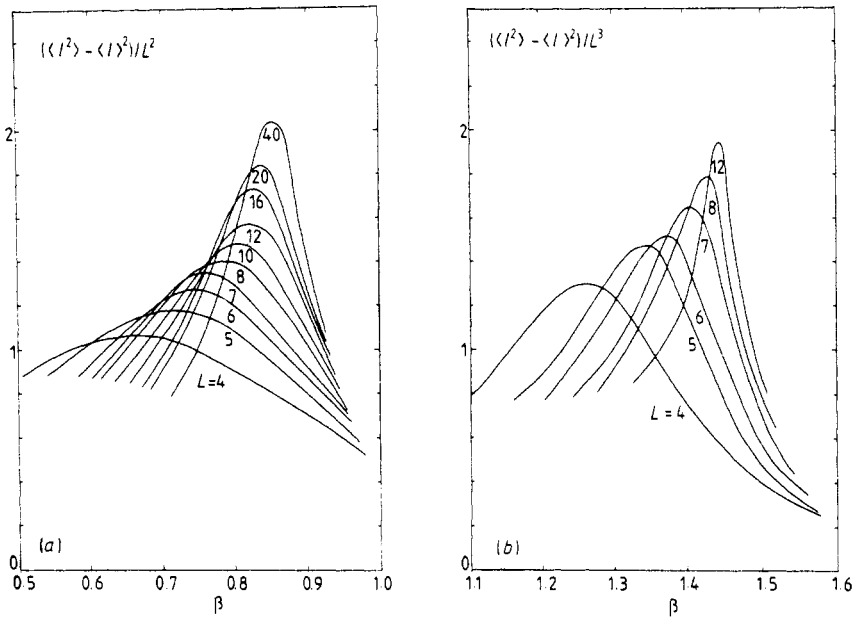


Figure 4. The average length fluctuation density $(\langle l^2\rangle - \langle l\rangle^2)/L^d$ against β for multiplicity $m = 1$ for various lattice sizes L in (a) $d = 2$ and (b) $d = 3$ dimensions. The curves are fits to Monte Carlo data collected in several thermal cycles. Suitable samples (from 1000 up to 8000 configurations depending on the lattice size and the temperature regime) have been taken into account.

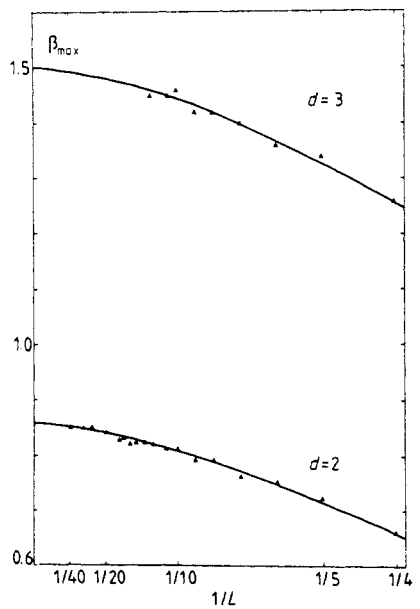


Figure 5. Fits to the values β_{max} obtained from figure 4 (and from some additional lattice sizes) for $m = 1$. The extrapolation $L \to \infty$ gives the critical inverse temperature $\beta_{crit} = 0.86$ and 1.50 for $d = 2$ and 3, respectively.

Table 1. Monte Carlo results for self-avoiding loop gas systems in d dimensions for multiplicities m: critical inverse temperatures β_{crit} and some estimates for the critical exponent ν.

d	2	2	2	2	2	3	3	4	5
m	0	1	1.5	2	4	0	1	1	1
β_{crit}	0.963	0.86	0.8	0.8	(0.8)	1.54	1.50	1.9	(2)
ν	0.75–0.85	0.8–1.0	?	?	?	0.55–0.65	0.6–0.7	?	?

closely with those results. The loop gas calculations with non-zero m values, on the other hand, give novel results for the critical inverse temperature β_{crit} and the critical exponent ν. As mentioned before, most calculations were performed for dimensions $d = 2$ and 3 and $m = 0$ and 1; the other results are very preliminary.

4. Loop distributions

As mentioned before, the critical behaviour of a loop gas seems to be related to the appearance of very large loops (probably of infinite size on an infinite lattice, cf figure 2). This can be investigated more quantitatively by means of the loop distribution function $\langle s(l)\rangle$ where $s(l)$ is the number of loops of length l in a configuration. Figure 6(a) shows the first moment of the loop distribution function, $l\langle s(l)\rangle$ for dimension $d = 2$, multiplicity $m = 1$, and three typical temperatures: far below, close to, and far above the critical temperature. Obviously, the critical temperature separates two regions of different behaviour. At the low temperature side only small loops appear and the whole energy is shared by them. This picture changes rather abruptly when the critical temperature is passed. Then most of the energy resides in large loops. The second maximum of the high temperature curve seems to indicate the existence of infinitely large loops in an infinite system. This behaviour is typical also for other dimensions and sufficiently low multiplicities. However, in two dimensions and for multiplicities $m > 2$ the second maximum of the loop distribution at high temperatures is absent (cf figure 6(c)) indicating that very large loops do not dominate. In figure 6(b) the case $m = 2$, $d = 2$ is shown which looks marginal. It is not clear whether the (still present) peaks in the specific heat signal a critical behaviour for loop gases with multiplicities $m > 2$ in two dimensions.

5. Conclusion

By means of Monte Carlo simulations we studied self-avoiding loop gas systems with various multiplicities on hypercubic lattices in several dimensions. We found second-order phase transitions. The most extensive data were obtained for dimensions two and three, and for multiplicities zero and one. For multiplicity zero which correspond to the one-loop (or polymer) problem our values of β_{crit} and ν are in good agreement with those obtained by other methods. The investigations for non-zero multiplicities, however, to our knowledge are novel. They furnish fairly accurate critical temperatures but so far only crude values for the critical exponent of the correlation length.

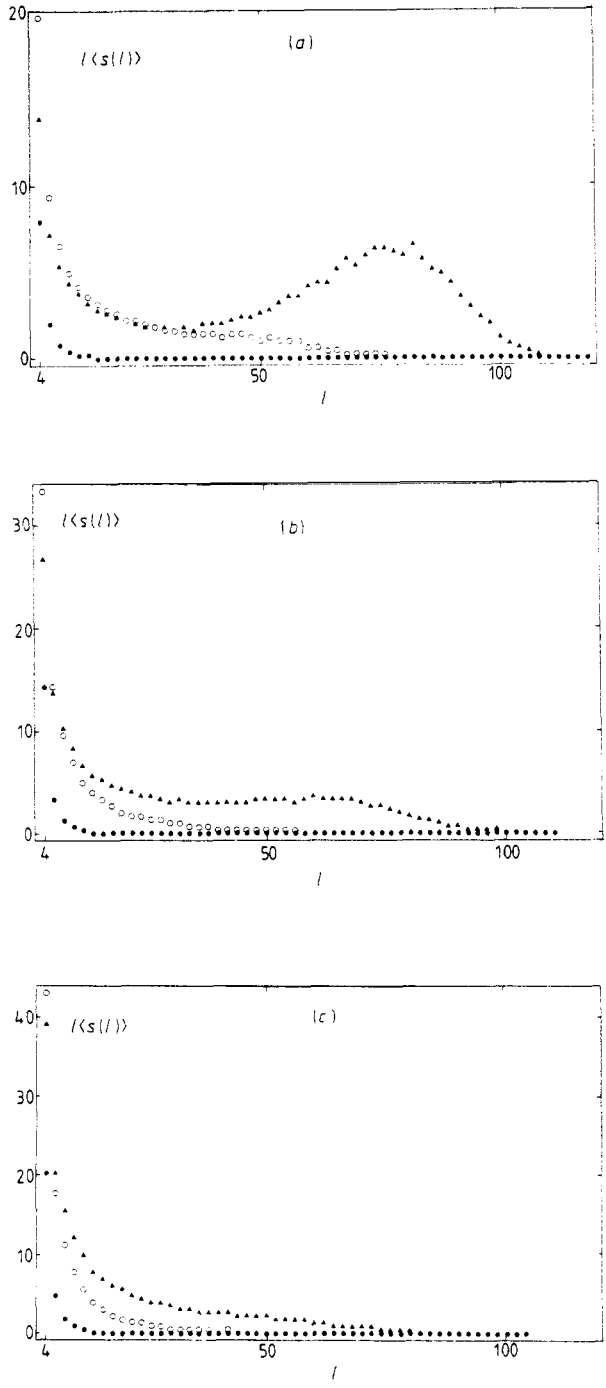


Figure 6. Loop distributions for loop gas systems on a 12×12 lattice for temperatures far above, close to, and far below the critical value. We have plotted the function $l\langle s(l)\rangle$ against l where $s(l)$ is the number of loops of length l in a configuration. The average has been taken over samples of 10 000 configurations. (*a*), (*b*) and (*c*) correspond to multiplicity 1, 2 and 3, respectively. ▲, $\beta = 0.42$; ○, $\beta = 0.82$; ●, $\beta = 1.22$.

Acknowledgment

We gratefully acknowledge useful discussions with B Schroer. Two of us (MK and HJT) thank R Schrader for his collaboration in the development of the present Monte Carlo program. One of us (HJT) thanks E Tränkle for advice in the numerical analysis of the data. This work was supported by the Deutsche Forschungsgemeinschaft under contracts Schr 160/7-1 and He 952/9-2.

References

Aragão de Carvalho C and Caracciolo S 1983 *J. Physique* **44** 323
Baumgärtner A 1982 *J. Chem. Phys.* **76** 4275
Binder K 1976 *Phase Transitions and Critical Phenomena* ed C Domb and M S Green vol 5B, ch 1 (New York: Academic)
Brydges D, Fröhlich J and Spencer T 1982 *Commun. Math. Phys.* **82** 123
des Cloizeaux J 1981 *J. Physique Lett.* **42** L433
Creutz M, Jacobs L and Rebbi C 1979 *Phys. Rev.* D **20** 1915
Duplantier B and Pfeuty P 1982 *J. Phys. A: Math. Gen.* **15** L127
Fisher M E 1971 *Proc. Int. School of Physics 'Enrico Fermi', Varenna Course LI* ed M S Green (New York: Academic)
Flory P J 1967 *Principles of Polymer Chemistry* (Ithaca, NY: Cornell University Press)
Friedberg R and Cameron J E 1970 *J. Chem. Phys.* **52** 6049
de Gennes P G 1972 *Phys. Lett.* **38A** 339
—— 1979 *Scaling Concepts in Polymer Physics* (Ithaca, NY: Cornell University Press)
Helfrich W 1983 *J. Physique* **44** 13
Karowski M, Schrader R and Thun H J 1983 to be published
Metropolis N, Rosenbluth A W, Rosenbluth M N, Teller A H and Teller E 1953 *J. Chem. Phys.* **27** 1087
Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
Rys F S 1981 *Preprint, TKM Dez. 81/33* Freie Universität Berlin
—— 1983 to be published
Rys F S and Helfrich W 1982 *J. Phys. A: Math. Gen.* **15** 599
Sykes M F, Watts M G and Roberts P D 1972 *J. Phys. A: Gen. Phys.* **5** 653
Symanzik K 1969 *Proc. Int. School of Physics 'Enrico Fermi', Varenna Course XLV* ed R Jost (New York: Academic)
Wheeler J C, Kennedy S J and Pfeuty P 1980 *Phys. Rev. Lett.* **45** 1748