

Gas of self-avoiding loops on the brickwork lattice

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1998 J. Phys. A: Math. Gen. 31 1685

(<http://iopscience.iop.org/0305-4470/31/7/005>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.104

The article was downloaded on 02/06/2010 at 07:22

Please note that [terms and conditions apply](#).

Gas of self-avoiding loops on the brickwork lattice

F Eghbal†, D P Foster† and H Orland‡

† Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, 2 ave A Chauvin, 95302 Cergy-Pontoise, France

‡ Service de Physique Théorique, CE Saclay, Orme des Merisiers, 91911 Gif-sur-Yvette, France

Received 19 September 1997

Abstract. An exact calculation of the phase diagram for a loop-gas model on the brickwork lattice is presented. The model includes a bending energy. In the dense limit, where all the lattice sites are occupied, a phase transition occurring at an asymmetric Lifshitz tricritical point is observed as the temperature associated with the bending energy is varied. Various critical exponents are calculated. At lower densities, two lines of transitions (in the Ising universality class) are observed, terminated by a tricritical point, where there is a change in the modulation of the correlation function. To each tricritical point an associated disorder line is found.

1. Introduction

Models of closed loops on lattices in two dimensions have attracted considerable attention [1]. In a theoretical context they arise naturally as high-temperature expansions of spin models and they are closely related to integrable systems such as vertex models [2]. Loops on a lattice may also be regarded as simple models for (short) ring polymers in solution [3, 4]. The segments of the loop are then regarded as monomers, or small clusters of monomers. While realistic systems are three-dimensional, the two-dimensional case provides rich critical behaviour, and it may be hoped that some features hold in higher dimensions. Solid-on-solid models used in the study of roughening transitions in three-dimensional growth may also be mapped onto various two-dimensional loop-gas models [1].

In this paper a model of loops is studied, consisting of self-avoiding rings with a bending energy. We are mainly interested in the effects of varying the density of monomers on the lattice and temperature. The model is defined as follows. Each bond of the lattice is either occupied by a monomer or empty. Each monomer placed on the lattice connects to two others such that the only allowed configurations consist of closed self-avoiding loops. An energy penalty ϵ is associated with each turn. The density of lattice bonds occupied is allowed to change, and the model is studied in the grand canonical ensemble by introducing a fugacity K for each monomer.

On the square lattice, and in the limit that the lattice is maximally occupied (all the sites visited) this model corresponds to the so-called F-model [5, 17], which exhibits an infinite-order phase transition as the bending energy, or equivalently temperature, is varied. At low temperatures corners are expelled from the bulk, while at high temperatures there is a proliferation of corners.

A qualitatively similar transition is seen in a model of a single Hamiltonian walk on the square lattice with a bending energy [6]. The Hamiltonian walk may be thought of as the

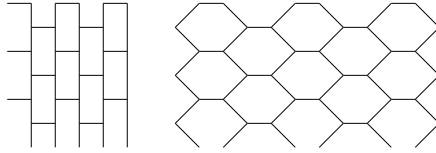


Figure 1. The BW and the corresponding honeycomb lattice.

limit of an interacting self-avoiding walk where the attractive nearest-neighbour monomer–monomer interactions are strong enough to exclude any lattice vacancies. In the other limit, the non-interacting self-avoiding walk, it is known that the bending energy is irrelevant [3, 4]; it changes the effective size of a monomer without changing the critical behaviour. At low enough densities we expect that for the loop-gas model the bending energy will also be irrelevant in this sense.

One therefore expects that between zero density (bending interaction irrelevant) and density one (bending interaction relevant) there should be a ‘critical’ density corresponding to a change of behaviour.

In this paper we study the loop-gas model on the brickwork (BW) lattice. The BW lattice corresponds to a square lattice with half the horizontal bonds removed, giving rise to the ‘brick wall’ motif, see figure 1. The BW lattice is topologically identical to the hexagonal lattice.

At density one we find a qualitatively similar phase transition to that on the standard square lattice in that there is a low-temperature phase in which the corners are expelled from the bulk and a high-temperature phase where there is a finite density of corners in the bulk. The details of the transition are, however, very different: the transition occurs at a tricritical Lifschitz point and the high-temperature phase is modulated and critical. Such a phase transition is reminiscent of the Pokrovsky–Talapov transition [7]. In this limit our model is equivalent to a modified KDP model on the hexagonal lattice [8, 9]. The existence of a modulated phase at $\rho = 1$ implies the existence of lines of disorder in the phase diagram [10], along which the correlation functions change from modulated at high densities to monotonic at low densities.

As the density is reduced the tricritical point is extended into a line of critical points in the Ising universality class which terminates at zero temperature at a critical density of about 0.8. For $K < 1$, or at low density, another line of critical points is observed, again in the Ising universality class; our model in this region is essentially the Ising model on the hexagonal lattice with one of the three couplings different from the other two.

The remainder of this paper is organized as follows. In section 2, the grand canonical partition function (and other relevant quantities) is calculated by expressing it first in terms of Grassman integrals, which are then exactly computed in the thermodynamic limit. In section 3 the $K \rightarrow \infty$ ($\rho \rightarrow 1$) limit is discussed, along with the nature of the low and high temperature phases. In section 4 the phase boundaries and lines of disorder are found and the different aspects of the phase diagram discussed. Section 5 is devoted to final discussions and conclusions.

2. The model

We consider a two-dimensional gas of loops on a BW lattice. The loops are self-avoiding, and we assign a fugacity K to each occupied link. This BW lattice can be visualized as a honeycomb (HC) lattice (see figure 1), and we associate a weight of $e^{-\beta\varepsilon}$ (where $\beta = 1/T$

is the inverse temperature) to each corner of a loop or equivalently $\lambda = e^{-2\beta\varepsilon}$ to horizontal links. This model is a straightforward extension of the F-model to the BW lattice. The aim of this paper is to calculate the phase diagram and properties of this system as a function of the site density ρ (or equivalently bond fugacity K) and temperature. The grand canonical partition function Z of the system is given by:

$$Z = \sum_{N=0}^{\Omega} K^N Z_N \tag{1}$$

$$= e^{-\beta\Omega f(K,T)} \tag{2}$$

where $\Omega = L^2$ is the total number of sites of the lattice of linear dimension L , and Z_N is the N -site partition function. As usual, the canonical partition function at site density $\rho = N/\Omega$ can be obtained through (1) by:

$$Z_N = \oint \frac{dK}{K} e^{-\Omega[\rho \log K - \beta f(K,T)]} \tag{3}$$

$$= e^{-\beta\Omega f_c(\rho,T)}. \tag{4}$$

In the thermodynamic limit, we have the usual relation

$$\rho = K \frac{\partial}{\partial K} \log Z. \tag{5}$$

The loop gas can be identified with the graphs of the high-temperature expansion of an Ising model on a BW lattice, with a weight K per vertical bond and $\lambda^2 K$ per horizontal bond. This identification holds provided that $K \leq 1$. However, the solution follows for any value of K .

Using the results of Houtappel [11, 12], we have, for any K :

$$f(K, T) = \frac{1}{16\pi^2} \int_0^\pi dk_x \int_0^\pi dk_y \log(a_1 K^4 + a_2 K^2 + a_3) \tag{6}$$

where

$$a1 = 1 + 4\lambda^4 \cos^2 k_y - 4\lambda^2 \cos k_x \cos k_y, \tag{7}$$

$$a2 = 2 - 4 \cos^2 k_y + 4\lambda^2 \cos k_x \cos k_y \tag{8}$$

$$a3 = 1. \tag{9}$$

This result, as well as the correlation functions, can be easily obtained by using Grassman variables. Following Samuel [14, 13], the partition function Z can be represented as a Grassman integral

$$Z = \int D\psi D\varphi e^{-A} \tag{10}$$

where

$$\begin{aligned} A = - \sum_{m,n} & (\psi_3^{m,n} \psi_1^{m,n} + \psi_4^{m,n} \psi_2^{m,n} + \varphi_3^{m,n} \varphi_1^{m,n} + \varphi_4^{m,n} \varphi_2^{m,n} + \lambda(\psi_1^{m,n} \psi_2^{m,n} + \psi_3^{m,n} \psi_4^{m,n} \\ & + \psi_2^{m,n} \psi_3^{m,n} + \psi_1^{m,n} \psi_4^{m,n} \varphi_1^{m,n} \varphi_2^{m,n} + \varphi_3^{m,n} \varphi_4^{m,n} + \varphi_2^{m,n} \varphi_3^{m,n} + \varphi_1^{m,n} \varphi_4^{m,n}) \\ & + K(\lambda^2 \varphi_3^{m,n} \psi_1^{m,n} + \psi_4^{m,n+1} \varphi_2^{m,n} + \varphi_4^{m,n} \psi_2^{m-1,n}) \end{aligned} \tag{11}$$

and $\psi_1^{m,n}, \psi_2^{m,n}, \psi_3^{m,n}, \psi_4^{m,n}$ are fermionic fields attached to each lattice site (m, n) . The fermion integral can be performed and the grand potential (6) can be recovered. In addition, the generic correlation functions read:

$$G(m, n) = (-1)^m \frac{1}{4\pi^2} \int_0^\pi dk_x \int_0^\pi dk_y \frac{e^{i(mk_x + nk_y)}}{a_1 K^4 + a_2 K^2 + a_3}. \tag{12}$$

The actual correlation functions contain regular multiplication factors which do not modify the long-distance behaviour.

Integration over k_x can be performed and gives:

$$f(K, T) = \frac{1}{8\pi} \int_0^\pi dk_y \log \frac{a + \sqrt{a^2 - b^2}}{2} \quad (13)$$

$$G(m, n) = (-1)^m \int_0^\pi \frac{dk_y}{2\pi} \frac{e^{ink_y}}{\sqrt{a^2 - b^2}} \left(\frac{\sqrt{a^2 - b^2} - a}{b} \right)^m \quad (14)$$

where

$$a = (1 + 4\lambda^4 \cos^2 k_y)K^4 + (2 - 4\cos^2 k_y)K^2 + 1 \quad (15)$$

$$b = -4\lambda^2 \cos k_y K^2 (K^2 - 1). \quad (16)$$

The canonical free energy (at bond density $\rho = N/\Omega$) is given by:

$$f_c(\rho, T) = \rho \log K - f \quad (17)$$

where K is determined as a function of ρ through:

$$\frac{\rho}{K} = \frac{1}{8\pi} \int_0^\pi dk_y \frac{1}{g(K, T, k_y)} \frac{\partial g(K, T, k_y)}{\partial K} \quad (18)$$

and

$$g = \frac{a + \sqrt{a^2 - b^2}}{2}. \quad (19)$$

In the following, we will work in the grand canonical ensemble, and transpose the results to the canonical ensemble when necessary. We first consider the fully packed lattice ($\rho = 1$) and then discuss the dilute case.

3. The fully packed lattice

By analogy with polymer theory, it is interesting to consider the case where all lattice sites are visited once and only once by the loops. This is the non-connected version of Hamiltonian path model, with a penalty factor λ per corner. From equation (18), we see that $\rho = 1$ for $K = \infty$. We are thus led to study equation (17) in the limit when $K \rightarrow \infty$. One obtains:

$$f_c = -\frac{1}{4\pi\beta} \int_0^\pi dk_x \int_0^\pi dk_y \log(1 + 4\lambda^4 \cos^2 k_y - 4\lambda^2 \cos k_x \cos k_y). \quad (20)$$

As usual we identify the critical points of the system from the zeros of the argument of the log in the above equation. It may be seen that no zeros exist for $\lambda < 1/\sqrt{2}$ and that for $\lambda \geq 1/\sqrt{2}$ zeros exist at:

$$\begin{aligned} k_x &= 0 \\ \cos k_y &= \frac{1}{2\lambda^2}. \end{aligned} \quad (21)$$

This implies that the whole region $\lambda \geq 1/\sqrt{2}$ is critical, with a temperature-dependent critical wavevector. We therefore identify $\lambda = 1/\sqrt{2}$ with a tricritical Lifshitz point, and the region $\lambda \geq 1/\sqrt{2}$ as a Lifshitz line of critical points. Using the definition $\lambda = \exp -\varepsilon/T$, the corresponding temperature for the tricritical point is $T_c = 2\varepsilon/\log 2$.

The integration over k_x in equation (20) may be carried out explicitly, giving:

$$f_c = -\frac{1}{4\pi\beta} \int_0^\pi dk_y \log \left(\frac{1 + 4\lambda^4 \cos^2 k_y + |1 - 4\lambda^4 \cos^2 k_y|}{2} \right) \quad (22)$$

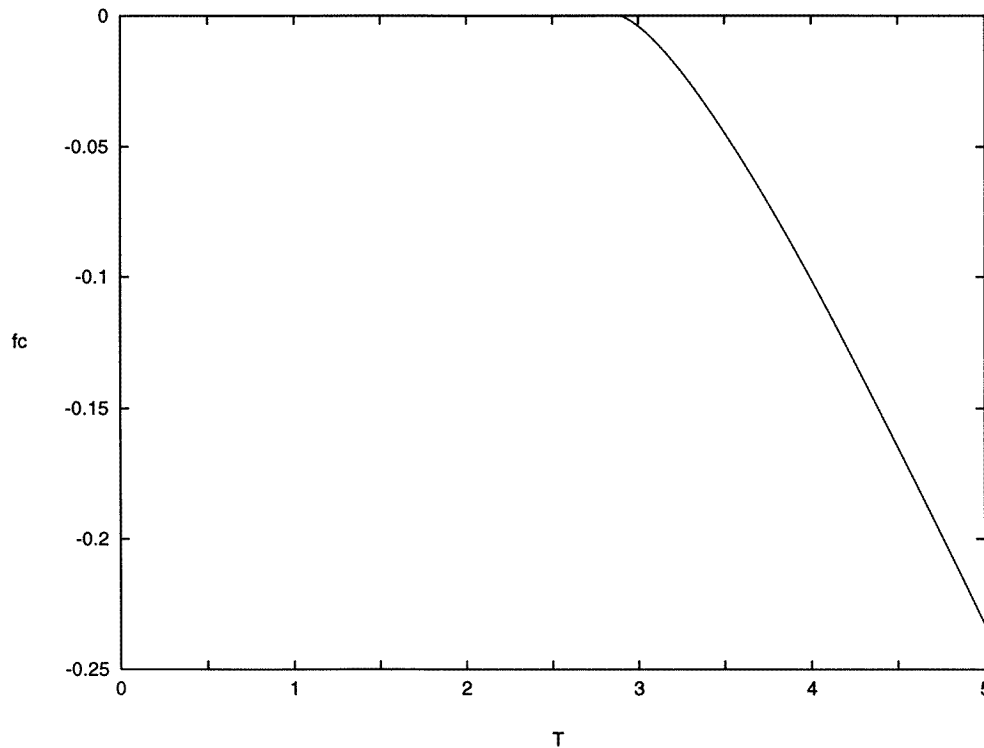


Figure 2. The free energy as a function of temperature for the fully packed model.

or

$$f_c = -\frac{1}{2} \int_0^{\arccos(1/2\lambda^2)} dk_y \log(4\lambda^4 \cos^2 k_y) \quad \text{for } T \geq T_c \quad (23)$$

$$\equiv 0 \quad \text{for } T \leq T_c. \quad (24)$$

This form is similar to the models studied in [7, 8] (see figure 2).

It is natural to define the average number density of corners n_c as the order parameter for this transition. Indeed, we find (see figure 3),

$$n_c = \frac{2}{\pi} \arccos\left(\frac{1}{2\lambda^2}\right) \quad \text{for } T \geq T_c \quad (25)$$

$$\equiv 0 \quad \text{for } T \leq T_c. \quad (26)$$

The critical behaviour of the order parameter is given by $n_c \sim \delta T^{1/2}$ as $T \rightarrow T_c$ so that the critical exponent β is equal to $\frac{1}{2}$. The low-temperature phase is completely frozen, consisting of straight vertical lines, with all the corners rejected to the outer boundary. The high-temperature phase is modulated in the y -direction with a wavevector given by equation (21)

The same critical behaviour is also seen in the zero-temperature phase diagram of the frustrated Ising model on the triangular lattice with appropriately chosen coupling constants [8, 9]. This model may be mapped onto a tiling consisting of three types of lozenge [9]. One lozenge has a lower energy than the other two. At zero temperature, the tiling must be perfect. One rapidly realizes that the only way of introducing a lozenge of higher energy is to introduce an infinite line of them. Identifying the side of a lozenge with the bisector

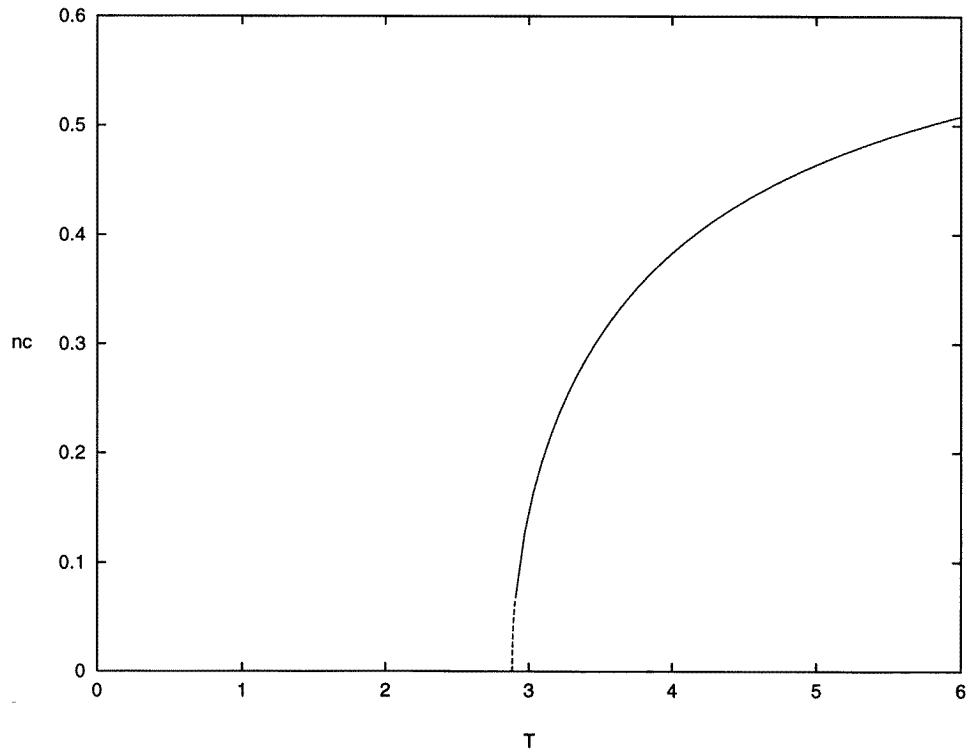


Figure 3. The average number of corners as a function of temperature for the fully packed model.

of an occupied bond on the dual hexagonal lattice, our loop model may be seen as being equivalent to this lozenge tiling (see figure 4). At non-zero temperature (as defined in our model) a defect line may be seen as a restricted SOS interface crossing the lattice. The energy needed to create one such line is $E = 2\varepsilon L$ and the entropy is $S = L \log 2$. When the associated free energy, $F_1 = L(2\varepsilon - T \log 2)$, becomes negative, defect lines (and hence corners) proliferate. This defines the critical temperature as $T_c = 2\varepsilon / \log 2$, consistent with the tricritical temperature found analytically above.

In the high-temperature phase, where these lines proliferate, we give a simple physical argument for the observed modulation in the correlation functions. The free energy F_1 is simply the chemical potential for creating one such line. When a finite density of lines is present, the reduction of entropy must be taken into account [15], yielding an effective repulsion between them. The total free energy for N lines, per occupied bond, is:

$$F_N = -F_1 N + c \sum_{i=1}^N \frac{T}{d_i^2} \quad (27)$$

where d_i is the distance between lines i and $i + 1$. Minimizing F_N with respect to the d_i , subject to the constraint $\sum_i d_i = L$, gives all the d_i equal and given by:

$$d_i \sim \frac{1}{\sqrt{T \log 2 - 2\varepsilon}} \quad (28)$$

explaining the form of the temperature dependence of the modulation wavevector, equation (21).

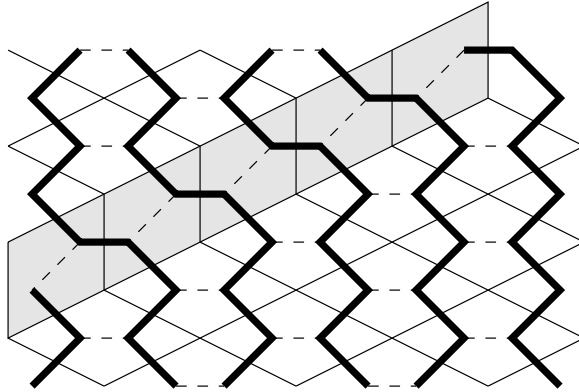


Figure 4. The mapping between the loop-gas and lozenge model: the shaded region shows an infinite line of defects.

Close to the tricritical Lifshitz point, the free energy scales as

$$f \sim \frac{4}{\pi T_c^3} (\delta T)^{3/2} \quad (29)$$

from which we obtain the specific-heat critical exponent $\alpha = \frac{1}{2}$.

Along the Lifshitz line, the critical behaviour of the correlation functions can be analysed; a generic correlation function is given by

$$G(\mathbf{r}) = \frac{1}{4\pi^2} \int_0^\pi \int_0^\pi d^2k \frac{e^{-i\mathbf{k}\cdot\mathbf{r}}}{1 + 4\lambda^4 \cos^2 k_y - 4\lambda^2 \cos k_x \cos k_y} \quad (30)$$

up to a regular multiplication factor.

Away from the tricritical point, i.e. $\lambda > 1/\sqrt{2}$, we may develop around the critical wavevector $(0, k)$ defined in equation (21). Setting $k_x = q_x$ and $k_y = k + q_y$, this becomes:

$$G(x, y) \sim e^{-iky} \int dq_x \int dq_y \frac{e^{-iq\cdot r}}{q_x^2 + (4\lambda^4 - 1)q_y^2}. \quad (31)$$

The exponential prefactor gives the expected spatial modulation in the y -direction, and the correlation function has a logarithmic behaviour at large distances.

Around the tricritical point, the critical wavevector vanishes as well as the coefficient of the q_y^2 term, and the expansion must be carried to the next order:

$$G(x, y) \sim \int dq_x \int dq_y \frac{e^{-iq\cdot r}}{\mu^2 + q_x^2 - \mu q_y^2 + q_y^4/4} \quad (32)$$

where $\mu = 2\lambda^2 - 1$. Therefore, the correlation functions have anisotropic scaling, with critical exponents $\nu_x = 1$ and $\nu_y = \frac{1}{2}$.

4. The dilute lattice

We now move to the dilute case $\rho < 1$.

4.1. Critical lines

As the density ρ or the fugacity K is lowered, the tricritical Lifshitz point extends into a critical line. This line can be obtained from the zeros of the logarithm of equation (6)

$$\begin{aligned} k_x &= 0 \\ k_y &= 0 \\ K &= \frac{1}{\sqrt{1 - 2\lambda^2}}. \end{aligned} \quad (33)$$

This critical line exists for $K \geq 1$. In the $\rho - T$ plane, its equation close to the fully packed case $\rho = 1$ is given by

$$\rho \simeq 1 + 2\varepsilon \frac{\delta T}{T_c^2} \quad (34)$$

where $T_c = 2\varepsilon / \log 2$ is the Lifshitz tricritical temperature.

For $K \leq 1$, there exists another critical line given by

$$\begin{aligned} k_x &= 0 \\ k_y &= \pi \\ K &= \frac{1}{\sqrt{1 + 2\lambda^2}}. \end{aligned} \quad (35)$$

In this region ($K < 1$), the fugacity can be identified with the $\tanh \beta J_1$ of a regular anisotropic Ising model on a HC lattice. Similarly, the second coupling is given by $\lambda^2 K = \tanh \beta J_2$.

It can be easily seen that both lines correspond to the two-dimensional Ising universality class: $\nu = 1$. Note that since the problem is formulated as a loop gas, the correlation functions do not correspond to the spin correlation functions of the Ising model; here we have $\eta = 0$.

The phase diagram in the $K - T$ plane is shown in figure 5. Using equation (18), we find the phase diagram in the $\rho - T$ plane (see figure 6). One can identify a high-density transition line and a low-density transition line. The high-density line ends at $\rho_c \simeq 0.8185$ and the low-density one ends at $\rho_c \simeq 0.19$.

The two critical lines merge at $K = 1$, where three phases become critical simultaneously, defining a tricritical point. This is manifested in the $\rho - T$ plane by a jump in the critical density ρ at $K = 1$. As usual, for zero-temperature tricritical points, observables develop essential singularities.

4.2. Disorder line

From equation (14), it is easily seen that the correlation functions change from oscillating (in the x -direction) for $K > 1$ to monotonic for $K < 1$. These two regimes must therefore be separated by a line where the short-distance correlation changes from oscillating to non-oscillating. This line $K = 1$, which passes through the tricritical point ($K = 1, T = 0$), is called a disorder line [10]. According to the definition of Garel and Maillard [16], this is a line of disorder points of the first kind (with zero correlation length).

We have seen that at $\rho = 1$, there is a Lifshitz critical point separating a frozen low-temperature phase from a modulated (in the y -direction) high-temperature phase. At lower densities, the correlation functions are not modulated. This happens separately for each value of k_x . Following Garel and Maillard [16], we define the disorder line as the line for

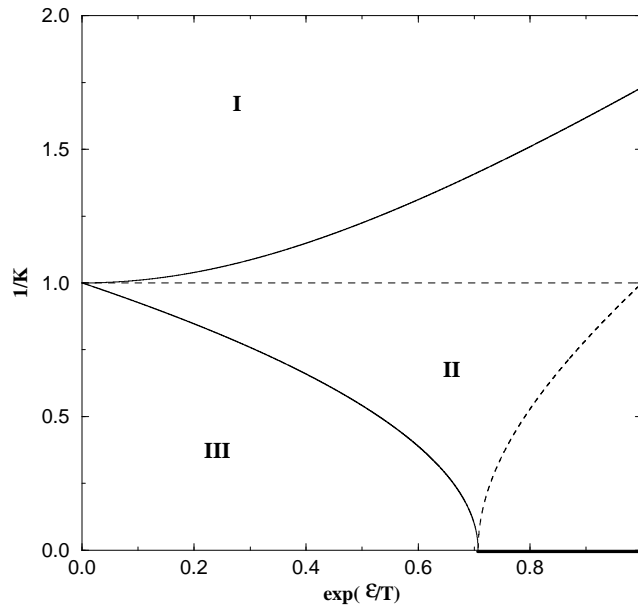


Figure 5. Phase diagram of the loop gas in the $K - T$ plane; the full curves denote the phase boundaries; the heavy line represents the Lifshitz line; the broken curves correspond to the disorder lines. The three phases are defined in the text.

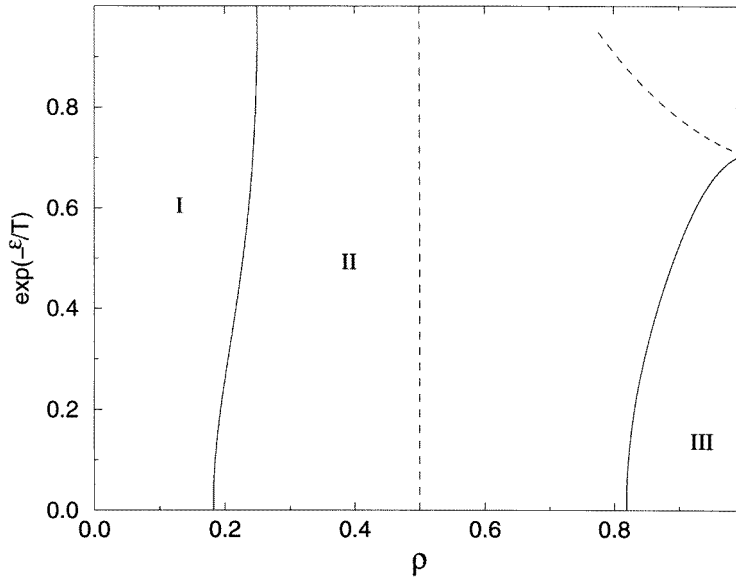


Figure 6. Phase diagram of the loop gas in the $\rho - T$ plane; the full curves denote the phase boundaries; the heavy line represents the Lifshitz line; the broken curves correspond to the disorder lines. The three phases are defined in the text.

which the first mode ($k_x = 0$) changes behaviour:

$$K = \frac{1}{\sqrt{2\lambda^2 - 1}}. \quad (36)$$

This line is defined in the high-temperature region $\lambda > 1/\sqrt{2}$ only, and corresponds to a line of disorder points of the second kind.

5. Conclusion

In this paper, a loop-gas model on a BW lattice was considered. An energetic penalty was included for each corner. At $\rho = 1$ we observed a phase transition from a low-temperature frozen (corner free) phase to a high-temperature phase modulated in the y -direction. The phase transition occurs at a tricritical Lifshitz point, where $\nu_x = 1$, $\nu_y = \frac{1}{2}$. The whole high-temperature phase is critical. These results are reminiscent of a phase transition of the Pokrovsky–Talapov type. This behaviour is completely different from the critical behaviour of the analogously defined model on the square lattice at $\rho = 1$ (the F-model). This is due to the combination of two effects; the BW lattice automatically imposes self-avoidance without the inclusion of additional fugacities, and the BW lattice is intrinsically asymmetric.

The phase diagram is given in the $K - T$ (and equivalently the $\rho - T$) plane. Two lines of critical points were observed corresponding to high- and low-density phase transitions. The high-density phase transition is to a phase modulated in the x -direction, and the low-density phase corresponds to the usual Ising transition. Both transitions are in the Ising universality class and meet at $T = 0$ at another tricritical point.

While the model studied is simple, the resulting phase diagram is surprisingly complex. In the formalism chosen, it is not clear how to characterize the different finite-density phase transitions in terms of the loop-model observables.

References

- [1] Nienhuis B 1987 *Phase Transitions and Critical Phenomena* vol 11, ed C Domb and J L Lebowitz (New York: Academic)
- [2] Baxter R J 1982 *Exactly Solved Models in Statistical Physics* (New York: Academic)
- [3] de Gennes P-G G 1979 *Scaling Concepts in Polymer Physics* (Ithaca, NY: Cornell University Press)
- [4] des Cloizeaux J and Jannink G 1990 *Polymers in Solution, their Modelling and Structure* (Oxford: Clarendon)
- [5] Lieb E M and Wu F Y 1972 *Phase Transitions and Critical Phenomena* vol 1, ed C Domb and M S Green (New York: Academic)
- [6] Flory J P 1956 *Proc. R. Soc. A* **234** 60
- [7] Pokrovsky V L and Talapov A L 1979 *Phys. Rev. Lett.* **42** 65–7
- [8] Wu F Y 1968 *Phys. Rev.* **168** 539–43
- [9] Blöte H W J and Hilhorst H J 1982 *J. Phys. A: Math. Gen.* **15** L631–7
- [10] Stephenson J 1969 *Can. J. Phys.* **47** 2621
Stephenson J 1970a *Can. J. Phys.* **48** 1724
Stephenson J 1970b *Can. J. Phys.* **48** 2118
Stephenson J 1970c *J. Math. Phys.* **11** 420
- [11] Houtappel R M F 1950 *Physica* **16** 425
- [12] Syozi I 1972 *Phase Transitions and Critical Phenomena* vol 1, ed C Domb and M S Green (New York: Academic)
- [13] Dotsenko V S and Dotsenko V S 1983 *Adv. Phys.* **32** 129–72
- [14] Samuel S 1980 *J. Math. Phys.* **21** 2806–14
- [15] Helfrich W 1978 *Z. Naturforsch.* a **33** 305
- [16] Garel T and Maillard J M 1986 *J. Phys. C: Solid State Phys.* **19** L505–11
- [17] Saleur H 1986 *J. Phys. A: Math. Gen.* **19** 2409–23