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Statistical mechanics of non-intersecting line systems†

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Abstract. Statistical assemblies of non-intersecting closed lines (loops) with a variable loop multiplicity are considered which may have relevance for defect models of certain phase transitions. A loop gas model on a lattice is formulated and shown to be formally equivalent to an m-anisotropc n-vector model in the limit $n = 0$. In two dimensions, the equivalence with the eight-vertex model in a field is discussed. In a few special cases the novel model is equivalent to known ones.

1. Introduction

Assemblies of lines play an important role in various physical problems. As an example, a system of linear polymers in solution is represented by non-intersecting, polar (i.e. oriented) or non-polar, open or closed lines. The statistical description is quite non-trivial due to the non-Markovian character of the excluded-volume effect even in the absence of any further interaction. The one-chain problem was formulated some time ago (Flory 1953, Edwards 1965). de Gennes (1972) showed its equivalence with the field theory of the n-vector model in the limit $n = 0$, and des Cloizeaux (1975) generalised it to treat polymers at finite densities. A particularly elegant formulation of the $n = 0$ formalism was given by Sarma (1975) which will be used in a modified version to describe our problem. Up to date, the single chain, dilute and semi-dilute solutions, as well as polydisperse systems can be described satisfactorily (Burch and Moore 1976, Witten and Schäfer 1978, de Gennes 1980, Rys 1980).

Another example is the description of certain 'melting transitions' in three dimensions involving liquid crystalline states; especially, the smectic A to nematic (AN) transition was considered by one of us (Helfrich 1978, 1980). In these cases closed dislocation lines which do not intersect and are polar, i.e. have multiplicity two, are thought to break up a periodicity. Assemblies of thermally generated loops were considered and the phase transition was attributed to the appearance of infinite lines at the critical temperature. Very recently, the defect theory of the AN transition was treated in some detail by Nelson and Toner (1981).

In the present note we study a statistical lattice model of non-intersecting thermal loops of multiplicity z ('loop gas'). The low-temperature expansion (LTE) of the partition function may be written as

$$Z_N = \sum_{s,l} g_N(s, l) z^s \, e^{-\beta \varepsilon l}. \tag{1}$$

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Here s is the number of loops of a given configuration, l the total number of nearest-neighbour bonds forming the loops, ε the chemical potential per line element, i.e. the energy of creation in the case of defect lines. β is the inverse temperature, z denotes the loop multiplicity and may be regarded as the loop fugacity, and $g_N(s, l)$ is the number of configurations of s non-intersecting (but otherwise non-interacting) loops of a total length l on a lattice with N lattice points.

Among others the following systems of non-intersecting closed lines can be described by the loop gas model (1).

For $z = 1$: thermally created non-polar loops or thermally equilibrated *ring* polymers (if the density of *chains* is negligible).

For $z = 2$: polar loops, which may be instrumental in the aforementioned melting transitions.

For $z = 4$: dislocation loops with multiplicity four involving two pairs of equivalent Burgers vectors, which could describe more complex melting phenomena.

In § 2, a formal equivalence of the low-temperature expansion of the loop gas partition function with the corresponding high-temperature expansion of an *m-anisotropic n*-vector model in the limit $n = 0$ ('m-anisotropic ($n = 0$)-vector model') is shown. It differs from a relationship between a system of loops of multiplicity n and the *isotropic* n-vector model for $n > 0$ (Helfrich and Müller 1980) which is characterised by a 'soft' line repulsion and does not describe the 'hard' excluded-volume effect.

In both descriptions there is no elastic interaction of the lines. For the case of defect lines this approximation is expected to be good in the presence of sufficient mutual screening (Helfrich 1978).

In § 3, some special cases are discussed. On a two-dimensional square lattice, the loop gas with $z = 1$ is equivalent to the eight-vertex model in a staggered (or, alternatively, in a direct) field. Moreover, the critical behaviour of the loop gas is discussed in the dilute limit (one-loop) case and for lattices with coordination number 3. In § 4 some final remarks are made.

2. Equivalence with the m-anisotropic ($n = 0$)-vector model

The loop gas model for integer valued multiplicities z is formally related to a spin-anisotropic n-vector model in the $n = 0$ limit. We consider an n-vector Hamiltonian with an anisotropic nearest-neighbour coupling constant $J^{(\alpha)}$ ($\alpha = 1, \ldots, n$)

$$\mathscr{H} = -\sum_{\substack{\langle ij \rangle \\ \alpha}} J^{(\alpha)} S_i^{(\alpha)} S_j^{(\alpha)} \tag{2}$$

where $S_i^{(\alpha)}$ is the αth component of an n-component spin vector $\boldsymbol{S}_i$ at lattice site i, normalised by $\|\boldsymbol{S}_i\| = \sqrt{n}$. Using the method of Sarma (1975) (which was developed for isotropic couplings only) we set:

$$\begin{aligned} J^{(\alpha)} &= J \qquad \text{for } \alpha = 1, \ldots, m \\ &= \lambda J \qquad \text{for } \alpha = m+1, \ldots, n. \end{aligned} \tag{3}$$

In the limit $n = 0$, the high-temperature expansion (HTE) graphs of the partition function are given by assemblies of closed non-intersecting loops with weight factors $m(1 - \lambda^k)$ for each loop where k is the number of line elements of the loop. In Sarma's isotropic case the weight factors all vanish as $\lambda = 1$. On the other hand, for $\lambda = 0$, they are all equal to m. Therefore, the HTE of the m-anisotropic ($n=0$)-vector model for $\lambda=0$ reads

$$Z_N^{(m)}=\sum_{s,l} g_N(s,l)m^s(\beta_0 J)^l \tag{4}$$

where $g_N(s,l)$ has the same meaning as in equation (1). Upon setting

$$\beta_0 J=\mathrm{e}^{-\beta\varepsilon} \tag{5}$$

the LTE of the partition function of the loop gas with a positive integer-valued fugacity $z=m>0$ is obtained. Due to this formal equivalence the critical behaviour of the loop gas *below* T_c is expected to be given by the critical behaviour of the m-anisotropic ($n=0$)-vector model for $\lambda=0$ *above* T_c in a certain neighbourhood of the critical temperature T_c.

3. Special cases

3.1.

In two dimensions, the simple loop gas with $z=1$ on a square lattice corresponds to the eight-vertex model in a staggered field (Nagle (1974), for a definition see Baxter (1971, 1972), Fan and Wu (1970)) with the following choice of the vertex energies

$$\begin{aligned}&\varepsilon_1=\ldots=\varepsilon_6=\varepsilon \qquad \varepsilon_7=0 \qquad \varepsilon_8=\infty\\&\varepsilon_1'=\ldots=\varepsilon_6'=\varepsilon \qquad \varepsilon_7'=\infty \qquad \varepsilon_8'=0\end{aligned} \tag{6}$$

on sublattices A and A' respectively. If bonds are placed on all *out*going arrows from vertices on the sublattice A and on all *in*going arrows to vertices on the sublattice A', then to every configuration of the eight-vertex model with the energies (6) corresponds one, and only one, loop gas configuration, the loops being formed by the bonds. For $m=1$, both models are therefore equivalent. Exact solutions of the eight-vertex model in a staggered field are known only for cases in which the free fermion condition (FFC) is satisfied (Hsue *et al* 1975)

$$\begin{aligned}&\omega_1\omega_2+\omega_3\omega_4=\omega_5\omega_6+\omega_7\omega_8\\&\omega_1'\omega_2'+\omega_3'\omega_4'=\omega_5'\omega_6'+\omega_7'\omega_8'\end{aligned} \tag{7}$$

where

$$\omega_i^{(\prime)}=\mathrm{e}^{-\beta\varepsilon_i^{(\prime)}} \qquad i=1,\ldots,8.$$

This condition cannot be fulfilled for all values of β if line intersections are not allowed, i.e. for

$$\omega_7'=\omega_8=0.$$

On the other hand, if the latter condition is replaced by

$$\omega_7'=\omega_8=\omega_1^2$$

the lines can cross freely and thus the graphs are identical to those of the single-bond Ising HTE graphs. Indeed, for this case, the FFC condition is fulfilled for all β and the solution displays Ising-like critical behaviour. It may be noted that an alternative bond assignment gives an equivalence of the $z=1$ loop gas with an eight-vertex model in a *direct* field.

3.2.

For small values of z, $Z_N - 1$ and thus the free energy of the loop gas is proportional to z (neglecting higher powers in z). After dividing by z, and passing to the limit $z = 0$ the generating function of the one-loop problem (corresponding to the low-loop density limit) is obtained. The critical behaviour is governed by the $n = 0$ critical exponents; for instance, the specific heat exponent is given for $d = 3$ by

$$\alpha(d = 3, n = 0) = 0.264 \ldots$$

as calculated, e.g. by Zinn-Justin and Le Guillou (1980), by renormalisation group methods. Incidentally, an analysis by the ratio method (Rys 1981) of the data for the three-dimensional n-vector model (English *et al* 1979) agrees well with this value.

3.3.

On lattices with coordination number 3 the Ising HTE graphs of the partition function consist of non-intersecting closed loops only. Therefore, for this particular case, the loop gas model with $z = 1$ is equivalent in the sense of equation (5) to the Ising model. In particular, the specific heat for the two-dimensional honeycomb lattice diverges logarithmically at the critical temperature.

4. Final remarks

We have studied the statistical behaviour of multiply counted non-intersecting loops on a lattice. The aim is to deal with the effect of the excluded volume which is known to be important in the statistical theory of dilute and semi-dilute polymer systems. As pointed out above, the phase transition of the loop gas may have relevance for certain melting phenomena, e.g. the AN transition of smectics. The loop gas model, although equivalent to known models in special cases (Ising model, eight-vertex model in an external field), has not been treated in the general case up to date. It may feature interesting critical and crossover phenomena. Among the unsolved problems we mention the dependence on z of the critical exponents, the question of the existence of an order parameter at low temperatures, and the behaviour at high multiplicities z.

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