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LETTER TO THE EDITOR

Is there a glassy phase in two dimensions?

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Abstract. The lattice gas model is studied as a function of dimensionality by a combination of analytical and numerical techniques. It is shown that for $d \leq 2$ the order-disorder transition density ρ_c is higher than the maximal filling density for a random filling process ρ_r , while for $d \geq 3$, $\rho_r > \rho_c$. The existence of a disordered metastable phase with $\rho > \rho_c$ is discussed in view of these results.

Phase transitions are often described by simple lattice models, whose main advantage is mathematical tractability. These models are chosen so that they share with the physical system the basic symmetries; the hope is that such models will fall into the same universality class (in the sense of renormalisation group) as the system to be described, so that results obtained in the lattice model (for universal quantities) can be carried over to the physical system.

Hard core lattice gas models are simple systems with Ising-like variables, which are believed to describe the solid-fluid transition [1]. Indeed, there is considerable evidence suggesting that the structure of the solid and fluid phases is determined primarily by the short-range repulsive intermolecular forces. The long-range attractive component is relatively weak and can be treated as a perturbation [2].

The model is defined by the Hamiltonian

$$H = \beta \sum_{\langle i,j \rangle} s_i s_j \quad (1)$$

with $s_i = 0$, the Hamiltonian (1) for empty (occupied) sites i on a d -dimensional lattice, i, j running over all nearest-neighbour pairs on the lattice, and $\beta \rightarrow \infty$. The system described by the partition function at density ρ :

$$Z = \text{Tr} \exp\left(-H + \mu \sum s_i\right) \quad (2)$$

with μ related to ρ by $(1/N) \partial \ln Z / \partial \mu = \rho$, undergoes a phase transition from a (disordered) fluid to a (ordered) solid one at a critical density ρ_c which depends on the dimension d , type of lattice and interaction range.

Lattice gas models appear in another context under the name of random sequential adsorption (RSA) models. The latter are irreversible dynamical models: particles are adsorbed at random at the sites of a lattice until no additional particles can be added. The density at which this happens is denoted by ρ_r . There are many one-, two- and three-dimensional systems which realise this process [3]. These models have been studied by several authors [4].

In this letter we will discuss the relation between ρ_r and ρ_c . Our physical motivation for this is related to the glass phase. It is known that a fluid ($T > T_c$), can be quenched (to $T < T_c$) to form a metastable phase which is fluid-like (disordered) despite the low temperature. In our model the analogue of temperature is density. Low density corresponds to high temperature. As ρ grows and approaches the closest packing density, the equivalent temperature tends to zero. The solid-fluid transition at $T = T_c$ is described by the order-disorder transition at $\rho = \rho_c$. The quenching procedure can be described by the RSA process. This assumption is intuitively reasonable but certainly not rigorous. The RSA phase is a disordered phase for all values of ρ for which it exists ($\rho < \rho_r$). Therefore whenever $\rho_r > \rho_c$, we can obtain by the RSA process a glassy phase. If $\rho_r < \rho_c$, this is impossible, at least in this framework. We will find that for $d < 3$ the latter relation holds, so that there is no glassy phase. There are two possible responses to such a situation. One is that for low dimensions the above framework is simply not appropriate to describing the metastable phase. The second (more intuitive) is to conclude that this phase does not exist below three dimensions.

The densities ρ_r and ρ_c depend on the details of the lattice and interactions. Even the order of the transition may change as a function of the range of the interaction. However, from an examination of ρ_r, ρ_c for several cases, it seems that the main conclusions above are quite universal.

To establish the above results we proceed in three steps. First, we consider $d = 1$. The fluid phase extends in this case up to[†] $\rho_c = 1$. The one-dimensional RSA models have maximal coverage densities depending on the interaction, from 0.864 66... for nearest-neighbour exclusion to 0.7476... for hard rods [4]. Thus, for $d = 1, \rho_c > \rho_r$ for all models.

Next we consider the opposite limit of large d . First simplicity we confine the discussion to the cubic lattice; the generalisation to other cases is simple.

We have shown recently [5] that the maximal coverage of the RSA process is well approximated in this case by (in this part we use absolute ρ):

$$\rho_r(d) \approx \frac{\ln 2d}{2d}. \quad (3)$$

For $d \geq 2$ the error in the estimate (3) is less than 5%. The convergence to the asymptotic limit (3) is extremely fast. We still need an estimate for $\rho_c(d)$, which can be obtained in the following way[‡]. The d -dimensional cubic lattice can be divided into two sublattices A, B , so that the Hamiltonian (1) takes the form

$$H = \beta \sum_{i \in A} s_i^A X_i^A \quad (4)$$

where

$$X_i^A = \frac{1}{2d} \sum_{(i,j)} s_j^B \quad (5)$$

and the sum over j runs over the $2d$ nearest neighbours of the site $i \in A$.

The order parameter of this lattice gas system is $m = \rho^A - \rho^B$. We would like to estimate the maximal $\rho = \rho^A + \rho^B$ for which $m = 0$. The assumption we make to simplify things is that the d different directions on the lattice effectively decouple for large d ,

[†] All densities are in units of closest packing unless stated otherwise.

[‡] Actually, we will obtain an upper bound on ρ_c which becomes exact at large d .

or in more practical terms we assume that the sites j in (5) (which are nearest neighbours of i), satisfy $\langle s_j^B s_k^B \rangle = (\rho^B)^2$ ($j \neq k$). This assumption is essentially equivalent to the one made in [5]. The good agreement with numerical results there as well as heuristic arguments are its main justifications.

The main advantage of X (5) is its narrow statistics. Since $s^2 = s$, it is obvious that if $\mu^B = \rho^B$ then the standard deviation is $\sigma^B = \sqrt{\rho^B(1-\rho^B)}$. X^A is an average over $2d$ independent (by assumption) s and therefore, in the limit of large d we have $\mu^X = \rho^B$ and $\sigma^X = \sqrt{\rho^B(1-\rho^B)}/2d$ or

$$\frac{\mu^X}{\sigma^X} = \sqrt{\frac{2d\rho^B}{1-\rho^B}} \tag{6}$$

For large d , $\rho^B \ll 1$ near the transition point (see below), and therefore $\mu^X/\sigma^X \approx \sqrt{2d\rho^B}$. By (4), X^A serves as a background for s^A . For $2d\rho^B \leq 1$, the X distribution is wide by (6), and there is no problem in having $\rho^A = \rho^B$. Consider, however, the region $2d\rho^B \gg 1$. The X variable becomes then ‘classical’—its fluctuations are small. The $\langle s^A \rangle$ average can then be estimated by $\langle s_i^A \rangle = P(s_i^A = 1) = P(X_i^A = 0)$, where the last equality holds because $\beta \rightarrow \infty$. $P(X_i^A = 0)$ is given by $[1 - P(s^B = 1)]^{2d}$. Of course, $P(s^B = 1) = \rho^B$, so that finally $\rho^A = (1 - \rho^B)^{2d}$. The disordered phase with $\rho^A = \rho^B$ can exist only up to the critical density

$$\rho_0 = (1 - \rho_0)^{2d} \tag{7}$$

Increasing ρ^B above ρ_0 necessarily creates a non-zero m : ρ^A cannot follow ρ^B because of the relation between them, and the distribution of X is much narrower than the difference m . The fluctuations of X are too small to change these ‘classical’ conclusions. Thus we get an upper limit on ρ_c :

$$\rho_c \leq \rho_0(d) \tag{8}$$

For large d , equation (7) has the form $\exp(-2d\rho_0) = \rho_0$, which has the solution

$$\rho_0 = \frac{1}{2d} (\ln 2d - \ln \ln 2d + \dots) \tag{9}$$

Several remarks concerning (9) are in order. $2d\rho_0 \approx \ln 2d$ for large d , thus the distribution of X (6) is indeed narrow and the approximation leading to (8) is justified, so the procedure is at least self-consistent. We expect (8) to break as d becomes small. Numerically we find that it holds for $d \geq 3$. For very large d , the inequality (8) becomes an equality. The meaning of ‘very large’ in this context is that $\ln 2d \gg 1$, so that the asymptotic result sets in at much higher dimensions than in the corresponding RSA problem [5]. Equation (9) has a form curiously similar to the RSA result (3), although the two were obtained from completely orthogonal arguments. The difference between the two has negative sign (so that $\rho_c \leq \rho_0 < \rho_r$); it becomes negligible at large enough d , for which ρ_r and ρ_c coincide.

To summarise, we found that contrary to the $d = 1$ case, for $d \rightarrow \infty$ the inequality is $\rho_c < \rho_r$. There have to be one or more points where the two densities cross. The third step in the argument is establishing that this crossover occurs at $2 < d < 3$. This was checked numerically for several lattices. The results for ρ_r were obtained by the graphical series method of [5] and MC simulations, and compared with known results for ρ_c [1, 6, 7]. The results are presented in table 1.

Table 1. Values of ρ_c and ρ_r for several different models.

Model	d	ρ_c	ρ_r
SL1	2	0.736 (2)	0.7282 (1)
SL2	2	>0.92	0.7480 (6)
SL3	2	0.30 (2)	0.6985 (10)
TL1	2	0.829...	0.6939 (5)
TL2	2	0.684 (15)	0.5965 (10)
TL3	2	0.80 (3)	0.6692 (15)
TL4	2	0.79 (2)	0.5655 (10)
HD	2	0.76 (1)	0.603 (1)
SC	3	0.426 (10)	0.608 (1)
BCC	3	0.354 (10)	0.594 (1)
FCC	3	0.48 (2)	0.628 (4)
SC	4	0.30 (3)	0.528 (2)

In table 1 different models on the same lattice are denoted by the range of the interaction. The abbreviations are : SL = square, TL = triangular, HD = hard discs, SC = simple cubic etc. Note that the HD model is a continuum one. The TL1 model is the hard hexagon model on the triangular lattice with nearest-neighbour exclusion, which has been exactly solved by Baxter [6]. The numbers in parentheses denote the uncertainties in the last digits. In all cases, for $d = 2$ $\rho_c > \rho_r$ while for $d = 3$ $\rho_r > \rho_c$, although the nature (order) of the transition is different in different cases. At this stage it is natural to ask what is the origin of the universality we find. We do not know, but there are several ways to think about this problem which might help. The first† is that the nature of the ordered phase is peculiar in two dimension [8, 9]. For example, the XY model [10] exhibits an infinite correlation length for all $T < T_c$. Making the analogy to our context, this would seem to mean that there are long correlations for $\rho > \rho_c$, which would make the existence of a disordered phase as the RSA phase impossible. Note also the universality of the behaviour of ρ_c, ρ_r discussed above. The estimates (3), (8), (9) can be easily extended to other lattices and interactions, with essentially the same formulae. Thus for example $\rho_c \rightarrow \rho_r$ from below as $d \rightarrow \infty$. The issue of universality will be discussed elsewhere [11].

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