UWThPh-1982-15

LOCAL COEXISTENCE OF DIFFERENT PHASES

Heide Narnhofer

Institut für Theoretische Physik
Universität Wien

Abstract

Under intuitively reasonable assumptions it is shown that in two dimensions different phases cannot exist locally. In three dimensions we discuss the possibility of local coexistence of districts with different magnetization for the Heisenberg ferromagnet and show that an interaction that breaks rotational invariance is necessary for this phenomenon.

1. Introduction

By now there exists quite an extended literature on the existence or nonexistence of more than one equilibrium state, especially when these states correspond to the spontaneous breaking of an internal symmetry. Much less is known about the local coexistence of phases (where we count different extremal equilibrium states obtained by the action of symmetry-automorphisms as different phases) though this is a phenomenon frequently observed in nature.

We will concentrate on the ferromagnet. Here the stable state of a ferromagnet without magnetic field consists of ferromagnetic domains of some magnetization and between these domains we find the Bloch walls, in which the magnetization gradually switches from one direction into the other and whose size is e.g. for ferrum about 300 lattice points. The explanation is given by the interplay of the magnetostatic energy and the exchange energy, which consists of a large isotropic part giving rise to ferromagnetism and a small anisotropic part. The magnetostatic energy favours the existence of several domains such that the total macroscopic magnetization is zero, whereas the anisotropic energy is necessary to keep the interface finite since the switching of the magnetizations runs over unfavoured directions [1,2].

We want to translate these properties into the language of equilibrium states, i.e. states satisfying the KMS-condition. These states describe correlations of finite length. Thus we will only obtain states that are not invariant under space translations if the Bloch walls are of finite size and the observables we consider are located in the Bloch walls and their neighbourhood.

We describe our system as the quasilocal C^*-algebra over the lattice. Its time evolution is given by a Hamiltonian consisting of the three parts:

shortrange isotropic energy $\quad - \sum_{x,y} J(x-y)\, \vec{\sigma}_x \vec{\sigma}_y$

magnetostitic energy $\quad \sum \frac{x^i y^i}{|x-y|} \sigma_x^i \sigma_y^j - \frac{1}{3} \frac{\sigma_x^i \sigma_y^i}{|x-y|^3}$

the shortrange anisotropic energy, which can be chosen to be

$$-\sum M(x-y)\,\sigma^z_x\,\sigma^z_y$$

or for cubic invariance $$-\sum M(x,y,u,v)\,\sigma^i_x\,\sigma^i_y\,\sigma^i_u\,\sigma^i_v\,.$$

The heuristic arguments correspond to the following fact: The shortrange isotropic interaction is able to give rise to extremal invariant states, for which rotational symmetry is broken.

Adding the longrange magnetostatic interactions in three dimensions it can give rise to different extremal KMS-states but under suitable assumptions on clustering properties of these states (which are known to be satisfied for translation invariant states) they must be translation invariant (i.e. we know that the Bloch walls are infinitely extended but we do not know whether the correlations in the Bloch walls are the same as in a uniformly magnetized sample). Already for the Ising model the anisotropic part is known to produce states that are not translationally invariant. Thus it can be taken to be responsible for the finite Bloch walls of the Heisenberg ferromagnet.

We want to repeat the results and methods used for the study of symmetry breaking: With the appropriate assumptions on the shortrange interaction we know that in one dimension only one equilibrium state can exist. In two dimensions a discrete symmetry can be broken (as it happens for the Ising model), for breaking a continuous symmetry (as for the Heisenberg magnet without anisotropic part) three dimensions are necessary. The proofs are either based on the idea of Mermin-Wagner [3]: they concentrate on the generator of the symmetry and use Bogoliubov's inequality [4]. The other possibility is to follow an idea of Araki [5] and to estimate the relative entropy. This relative entropy $S(\omega_1|\omega_2)$ has to be infinite if the two states differ globally and thus correspond to different representations. If, therefore, we are able to show that the relative entropy is bounded from above for two extremal KMS-states ω_1 and ω_2, these states have necessarily to coincide since extremal KMS-states are either equal or disjoint.

In [5] the relative entropy between two KMS-states for a system with sufficiently decreasing potential was estimated to be of surface size, thus bounded in one dimension. In [6] Fröhlich and Pfister used the idea of the gauge group to estimate the relative entropy over a finite though increasing region and obtained by perturbation estimates an optimal result [7] for the absence of the breakdown of a continuous symmetry in two dimensions.

We will assume that extremal KMS-states that are not translation invariant are obtained as limits of Gibbs states with non-uniform boundary conditions. The way how we choose these boundary conditions is dictated by our knowledge how we can obtain extremal translation invariant KMS-states, i.e. we choose two different but for a homogeneous state sufficiently strong boundary conditions in the two half-spaces. It seems rather plausible to assume that such states should be good candidates to lead to states that are not space translation invariant.

Our results are the following:

a) In two dimensions we cannot construct locally coexisting phases. (This is in correspondence with the concrete result for the Ising model where a partition in two different half-spaces is only possible for dimensions higher or equal to three [8,9,10,11].)

b) If the two states correspond to the spontaneous breakdown of a continuous symmetry then the construction also fails in three dimensions.

c) If we take the magnetostatic interaction into account but ignore the anisotropic one we observe: Let $\omega \circ \gamma_{\alpha_\pm}$ be two translationally invariant extremal KMS-states corresponding to the breaking of the gauge symmetry γ_α of rotation. If for a non-homogeneous state $\bar{\omega}$ $\bar{\omega}_{x \to \pm\infty}(\sigma_x)$ converges to $\omega \circ \gamma_{\alpha_\pm}(\sigma_x)$ as fast as $1/|x|^2$ then the relative entropy between spatially translated states remains finite. Thus $\bar{\omega}$ should equal both $\omega \circ \gamma_{\alpha_+}$ and $\omega \circ \gamma_{\alpha_-}$ which is impossible.

We have to remember that our method can only exclude locally coexisting phases. What is missing are estimates on the critical temperature. But nevertheless it is satisfying that heuristic arguments based on the energy are in agreement with the discussion on the level of the KMS-condition.

2. The Relative Entropy

Unfortunately the definition of relative entropy varies in the literature so that it is sometimes positive and sometimes negative definite. We follow the definition in [12]. If the two states ω_1 and ω_2 correspond to the density matrices ρ_1 and ρ_2 then

$$S(\omega_1|\omega_2) = \mathrm{Tr}\, \rho_2(\ln \rho_2 - \ln \rho_1) .$$

The generalization to states on Von Neumann algebras reads [13]: Let ω_1 and ω_2 be two faithful normal states on a Von Neumann algebra M with modular operators $\Delta_1 = e^{-H_1}$ and $\Delta_2 = e^{-H_2}$ then

$$S(\omega_1|\omega_2) = \omega_2(\log \Delta_2 - \log \Delta_1) = \omega_2(H_1 - H_2) .$$

We will use the following properties of the relative entropy:

1. $S(\omega_1|\omega_2) \geq 0$.
2. Let ω correspond to the automorphism group τ_t and the GNS-vector Ω, and ω^P correspond to the perturbed automorphism group τ_t^P, then

$$S(\omega^P|\omega) = \log ||e^{H/2}\, e^{-\frac{H+P}{2}}\, \Omega||^2 - \omega(P)$$

$$S(\omega|\omega^P) = - \log ||e^{H/2}\, e^{-\frac{H+P}{2}}\, \Omega||^2 + \omega^P(P) .$$

3. $0 \leq S(\omega|\omega^P) + S(\omega^P|\omega) = \omega^P(P) - \omega(P)$.

3. Absence of Coexisting Phases in Two Dimensions

We assume that there are already two different KMS-states. They may belong to a broken discrete symmetry or may differ completely. The Gibbs condition tells us [14,15] that these two states can be obtained as limit of local equilibrium states (= Gibbs states)

$$\omega_{1,2}(A) = \frac{\mathrm{Tr}\, e^{-H_\Lambda - P_{\Lambda,1,2}} A}{\mathrm{Tr}\, e^{-H_\Lambda - P_{\Lambda,1,2}}} \qquad \forall\, A \in A(\Lambda)\ ,$$

where H_Λ is the restriction of the Hamiltonian to the region Λ and P_Λ represents the interaction of the region Λ with the outside and thus depends on the state. For shortrange interactions P_Λ is of surface size. But unfortunately there is not sufficient further information about the structure of this P_Λ. Therefore we will assume that if the KMS-state is translationally invariant, it is obtained as limit of Gibbs states with P_Λ concentrated and homogeneous on the surface, i.e.

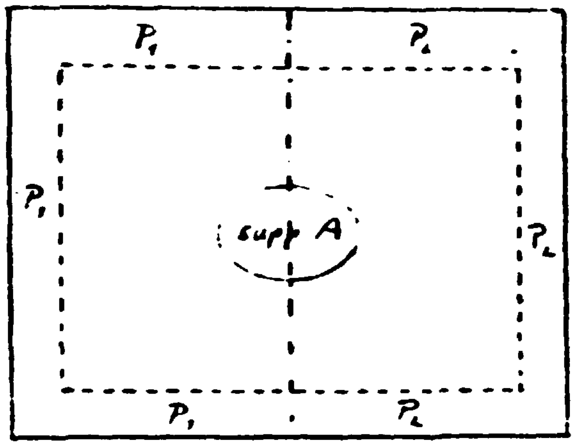
$$\omega_{1,2}(A) = \lim_{\Lambda\to\infty} \frac{\mathrm{Tr}\, e^{-H_\Lambda - \sum_{x\in\bar\Lambda} \tau_x P_{1,2}} A}{\mathrm{Tr}\, e^{-H_\Lambda - \sum_{x\in\bar\Lambda} \tau_x P_{1,2}}}$$

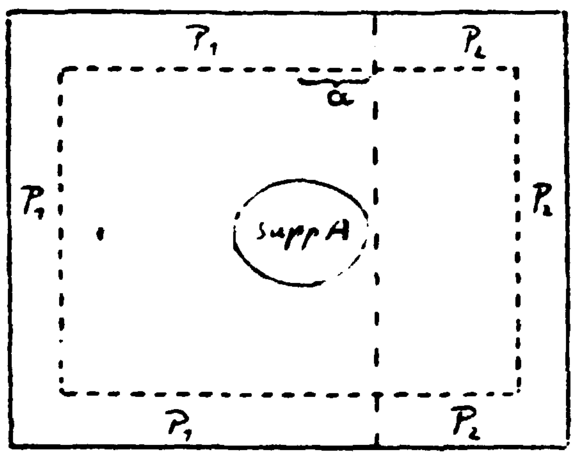
where $\bar\Lambda$ is the surface of Λ and τ_x space translations and P_i some local operator.

It should be noted that by this method the pure equilibrium states for the Ising model are obtained: Here P is chosen to be the interaction term with the spin outside of the region Λ fixed. If the pure translationally invariant states ω_1 and ω_2 can be obtained by P_1 and P_2 the natural possibility to construct locally coexisting phases is to consider the limit

$$\omega(A) = \lim_{\Lambda\to\infty} \frac{\mathrm{Tr}\, e^{-H_\Lambda - \sum_{x\in\bar\Lambda_+} \tau_x P_1 - \sum_{x\in\bar\Lambda_-} \tau_x P_2} A}{\mathrm{Tr}\, e^{-H_\Lambda - \sum_{x\in\bar\Lambda_+} \tau_x P_1 - \sum_{x\in\bar\Lambda_-} \tau_x P_2}}$$

where $\bar{\Lambda}_+$ and $\bar{\Lambda}_-$ are the surfaces of Λ in the right resp. the left half-space. The spatially translated state is obtained in a similar way, only the division into right ans left half-space is now shifted.





Thus the boundary condition differs only in a finite interval and therefore

$$S(\omega \circ \tau_a | \omega) \leq 2|a| \; ||P_1 - P_2||$$

and stays bounded in two dimensions. Therefore the limit cannot be space-dependent.

4. Local Coexisting Phases for the Heisenberg Ferromagnet

We concentrate now on the Heisenberg ferromagnet and neglect first the anisotropic part and the longrange part of the interaction. Therefore rotation is a gauge automorphism group $\gamma(\alpha)$

$$\gamma(\alpha)\ J(x-y)(\vec{\sigma}_x\cdot\vec{\sigma}_y) = J(x-y)(\vec{\sigma}_x\cdot\vec{\sigma}_y)\ .$$

We assume that ω is an extremal KMS-state. Let

$$\omega(A) = \lim_{\Lambda\to\infty} \frac{\mathrm{Tr}\ e^{-H_\Lambda - P_\Lambda} A}{\mathrm{Tr}\ e^{-H_\Lambda - P_\Lambda}}\ .$$

A natural way to obtain the transformed state $\omega\circ\gamma(\alpha)$ would be to consider

$$\omega\circ\gamma(\alpha)(A) = \lim_{\Lambda\to\infty} \frac{\mathrm{Tr}\ e^{-H_\Lambda - \gamma(-\alpha)P_\Lambda} A}{\mathrm{Tr}\ e^{-H_\Lambda - \gamma(-\alpha)P_\Lambda}}\ .$$

Unfortunately our knowledge on P_Λ is too poor to obtain sufficient estimates on $\omega(2P_\Lambda - \gamma(-\alpha)P_\Lambda - \gamma(+\alpha)P_\Lambda)$.

In [6] it was shown how to change the strategy to obtain better estimates on the relative entropy. Fröhlich and Pfister consider a space dependent gauge transformation, namely

$$\omega\circ\gamma(\alpha)(A) = \lim_{\Lambda\to\infty} \frac{\mathrm{Tr}\ e^{-H_\Lambda - P_\Lambda}\ \gamma_\Lambda(\alpha)\cdot A}{\mathrm{Tr}\ e^{-H_\Lambda - P_\Lambda}}$$

where Λ are cubes of diameter 4L and

$$\gamma_\Lambda(\alpha) = \bigotimes \gamma_x(\alpha(x))$$

with

$$\alpha(x) = \alpha \qquad \text{for} \qquad |x_i| \leq L\ ,$$

$$\alpha(x) = \frac{L-k}{L}\,\alpha \qquad \text{for} \qquad \max(|x_i|) = L + k\ .$$

Therefore

$$\omega \circ \gamma(\alpha)(A) = \lim_{L\to\infty} \frac{\mathrm{Tr}\; e^{-H_L - W_L(\alpha)} A}{\mathrm{Tr}\; e^{-H_L - W_L(\alpha)}}$$

with

$$W_L(\alpha) = P_{\Lambda_L} - \sum_{x,y} \gamma_y(\alpha(x) - \alpha(y))\; J(x-y)\; \vec{\sigma}_x\, \vec{\sigma}_y\ .$$

__Remark__: If one prefers that W_L is really a surface term where the diameter of the surface is kept fixed as Λ goes to ∞ this is possible but the arguments to get sufficient estimates on the relative entropy become somewhat involved and we believe that the above choice of W_L is physically satisfying.

Now we can estimate [6] in two dimensions that

$$0 \le S(\omega_\Lambda \circ \gamma_\Lambda(\alpha)|\omega_\Lambda) + S(\omega_\Lambda|\omega_\Lambda \circ \gamma_\Lambda(\alpha)) = \omega(W_L(\alpha) + W_L(-\alpha) - 2W_L(0)) \le$$

$$\sum\sum_{x,y\in\bar{\Lambda}} \frac{\alpha^2}{L^2}\, |J(x-y)|(x-y)^2 + O(\tfrac{1}{L}) = \sum_y \alpha^2 \;\; J(y)^2\cdot c + O(\tfrac{1}{L})\ .$$

Therefore in two dimensions broken symmetry cannot occur if J decreases sufficiently fast.

We are interested whether in three dimensions different phases can exist locally, i.e. if a state exists, that tends to the pure state ω for $x_1 \to -\infty$ and to $\omega \circ \gamma(\alpha)$ for $x_1 \to +\infty$. Therefore, led by the above choice of W_L we consider the limit

$$\bar{\omega}(A) = \lim_{\Lambda\to\infty} \frac{\mathrm{Tr}\; e^{-H_\Lambda - P_\Lambda - \sum_{x_1,y_1>0} \gamma_y(\alpha(x)-\alpha(y))\, J(x-y)\, \vec{\sigma}_x\, \vec{\sigma}_y} A}{\mathrm{Tr}\; [\cdot]}$$

whereas the translated state is obtained as

$$\bar{\omega}(\tau_a A) = \lim \omega_a(A) \doteq \lim_{\Lambda \to \infty} \frac{\mathrm{Tr}\, e^{-H_\Lambda - P_\Lambda - \sum_{x_\parallel, y_\parallel > a} \gamma_y(\alpha(x)-\alpha(y)) J(x-y)\, \vec{\sigma}_x \vec{\sigma}_y} A}{\mathrm{Tr}\,[\cdot]} .$$

We estimate as in the two dimensional case where the relevant sum runs over $x, y \in \bar{\Lambda}$, $0 \leq x_\parallel \leq a$, thus the sum over x is again essentially two-dimensional and therefore we obtain from the previous result

$$S(\omega_{\Lambda,a} | \omega_\Lambda) \leq c ,$$

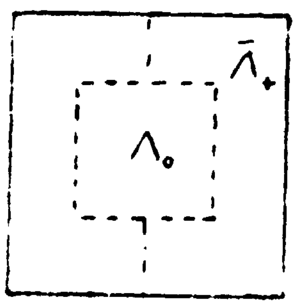
therefore the shortrange interaction is unable to produce space dependent KMS-states.

We will take now into account the longrange magnetostatic interaction. Evidently the above estimate fails. But we should remember that the argument with the relative entropy is a rather delicate one: Certainly we can always change the boundary conditions in such a way that the relative entropy grows faster than allowed, but since the relative entropy is not continuous but only lower semicontinuous it can still drop to 0 in the limit $\Lambda \to \infty$. On the other hand we must vary the boundary conditions with reasonable strength so that at least our physical intuition should tell us that this variation should cover the effect that should lead to the new equilibrium state. Our choice of the "surface" term is

$$\sum_{y \in \bar{\Lambda}_+, x \in \Lambda_0} [J(x-y) + \bar{J}(x-y)]\, \sigma_x (1 - \gamma_y(\alpha(y)) \sigma_y +$$

$$+ \sum_{y \in \bar{\Lambda}_+, x \in \bar{\Lambda}_+} [J(x-y) + \bar{J}(x-y)]\, \sigma_x (1 - \gamma_y(\alpha(y) - \alpha(x)) \sigma_y$$

where $\bar{J}$ is the tensor corresponding to the magnetostatic interaction, Λ_0 is the inside of the considered region and $\bar{\Lambda}_+$ the surface of the right half-space:



We ignore interaction between the right and the left surface. But since in any case the new equilibrium state cannot be obtained by a locally varying gauge transformation we feel that this transformation should not be taken too serious leading to a large contribution of differently oriented spins in the interface.

With this choice of boundary conditions we estimate

$$S(\omega \circ \tau_a|\omega) \leq \omega\Big(\sum_{x\in\Lambda_0, y\in\bar{\Lambda}_+, 0\leq y_1\leq a} (J + \bar{J})\, \sigma_x(1 - \gamma_y(\alpha(y))\sigma_y)\Big) +$$

$$+ \omega\Big(\sum_{x\in\bar{\Lambda}_+, y\in\bar{\Lambda}_+, 0\leq y_1\leq a} (J + \bar{J})\, \sigma_x(1 - \gamma_y(\alpha(y)) - \alpha(x)))\sigma_y\Big) .$$

We concentrate on the effect of the longrange interaction, thus we have to consider terms of the type (i,j fixed)

$$\frac{(x-y)_i(x-y)_j}{|x-y|^5}\, \omega(\sigma_x^i\, \sigma_y^j - \sigma_x^i\, \gamma(\alpha(y))\sigma_y^j) \underset{\substack{0\leq y_1\leq a \\ |x_1|\to\infty}}{=} \frac{(x-y)_i(x-y)_j}{|x-y|^5}\, \omega(\sigma_x^i) \cdot$$

$$\cdot\, [\omega(\sigma_y^j) - \omega(\gamma(\alpha(y))\sigma_y^j)] + O\Big(\frac{1}{|x-y|^5}\Big)$$

if we assume that cluster properties are unchanged with respect to uniformly magnetized states. The last term is sufficiently decreasing, therefore after summation over x and y the contribution to the relative entropy stays bounded. We concentrate on the first term that decreases as $1/|x-y|^3$ and is therefore not summable. But we can improve our estimate by considering the desired properties of our limit state.

A. Let us assume that the two half-spaces correspond to spin up and spin down. Then $\lim_{x_1\to+\infty} \omega(\sigma_x) = -\lim_{x_1\to-\infty} \omega(\sigma_x)$. If we assume that our interface lies really in the middle of the sample (which we should do since we are interested in the behaviour in the Bloch walls) the conditional convergence makes the relative entropy bounded, thus excludes the possibility of such a state.

B. In general different orientations of the spins are possible, thus we have to look for a more subtle argument. Now we use some convexity properties of the relative entropy and estimate for the longrange effects

$$S(\omega_a|\omega) + S(\omega|\omega_a) \leq \sum_{0 \leq y_1 \leq a,\, x \in \Lambda_0} \bar{J}(x-y)\omega(\sigma_x \sigma_y - \sigma_x \, \gamma(\alpha(y)\sigma_y)) -$$

$$- \sum_{0 \leq y_1 \leq a,\, x \in \Lambda_0} \bar{J}(x-y)\omega_a(\sigma_x \sigma_y - \sigma_x \, \gamma(\alpha(y)\sigma_y)) \, .$$

ω_a will be approximately $\omega \circ \tau_a$ for local observables. We assume now that

$$\omega_a(\sigma_x \, \sigma_y) = \omega(\sigma_x) \, \omega_a(\sigma_y) + O\left(\frac{1}{|x-y|^2}\right) = \omega(\sigma_x) \, \omega(\sigma_{y-a}) + O\left(\frac{1}{|x-y|^2}\right) .$$

Thus the effective range is again $1/|x-y|^5$ and insufficient to produce breaking of translation invariance.

We want to repeat that our estimates depend on uncontrolled assumptions on our states. Nevertheless we feel it as worthwhile to translate heuristic arguments on the expectation value of the energy, which essentially work on the macroscopic level, onto arguments on the microscopic level of the KMS-structure of states.

5. The Anisotropic Contribution

The anisotropic contribution breaks rotational symmetry. Thus we work with a system that is similar to the Ising model, and here we already know, that not translationally invariant states are possible in three dimensions. Thus we can take it to be responsible for the existence of magnetic domains with interfaces of finite size. Another problem remains and cannot be answered on this level: For the Ising model in three dimensions there is some numerical evidence but no proof that the critical temperature corresponding to locally coexisting phases lies below the critical temperature corresponding to spontaneous magnetization. Now the anisotropic contribution in ferromagnets is rather small and insufficient to produce magnetization at relevant temperatures. Therefore it is still possible that only the interplay of longrange interaction and anisotropic interaction can produce the coexisting phases. Since our argument does not refer to a special temperature it is evidently too weak to give information in this direction.

Acknowledgement

I want to thank Prof. R. Haag who turned my interest to this problem and Prof. W. Thirring for many critical and stimulating discussions.

Remark

After finishing this manuscript we received the preprint "On the Statistical Mechanics of Surfaces" by J. Fröhlich et al., which deals with similar problems [16].

References

[1] Ch. Kittel, Introduction to Solid State Physics, New York 1967 (Einführung in die Festkörperphysik, Oldenburg, München 1969).

[2] L.D. Landau, E.M. Lifschitz, L.P. Pitajewski, Lehrbuch der theoretischen Physik IX, Akademie Verlag, Berlin 1980.

[3] N.D. Mermin, H. Wagner, Phys. Rev. Lett. 17, 1133 (1966)

[4] C.A. Bonato, J.F. Perez, A. Klein, The Mermin-Wagner Phenomenon and Cluster Properties, preprint, Univ. de Sao Paulo (1981).

[5] H. Araki, P.D.F. Jon, CMP 35, 1 (1974).

[6] J. Fröhlich, C. Pfister, CMP 81, 277 (1981).

[7] H. Kunz, C.E. Pfister, CMP 46, 245 (1976).

[8] G. Gallavotti, CMP 27, 103 (1972).

[9] A. Messager, S. Miracle Sole, J. Stat. Phys. 17, 245 (1977).

[10] R.L. Dobrushin, Theory Probab. Its Appl. 18, 253 (1973).

[11] H. Beijeren, CMP 40, 1 (1975).

[12] W. Thirring, Lehrbuch der Mathematischen Physik IV, Springer, Wien 1980.

[13] O. Bratteli, D.W. Robinson, Operator Algebras and Quantum Statistical Mechanics II, Springer, New York 1981.

[14] H. Araki, CMP 14, 120 (1969).

[15] H. Narnhofer, Thermodynamical Phases and Surface Effects, preprint (1981).

[16] J. Fröhlich, C.E. Pfister and T. Spencer, On the Statistical Mechanics of Surfaces, preprint IHES (1982).