The Phase Separation Line in the Two-Dimensional Ising Model and Its Relationship with the Nonfree-Random-Walk Problem.

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Recently some research has been devoted to the problem of the microscopic definition of the surface of separation between two phases ([1]). Most of the published results have been obtained for the two-dimensional Ising model ([2]).

In this case it has been proven that the problem of studying the line of phase separation is equivalent to the study of ensembles $U_q(N)$ of edge self-avoiding random walks λ lying on a strip of a square lattice with, as base, a segment of $N+1$ lattice points. By edge self-avoiding random walks we mean random walks which may return to lattice points which have been passed previously, but may not repeat a previous step, neither in the same nor in the opposite direction. The ensemble $U_q(N)$ contains all random walks which start at the origin and end at the point $R=(N, q)$ (see Fig. 1). If a random walk λ belongs to $U_q(N)$, its statistical weight in this ensemble is ([2])

$$W(\lambda)=\frac{1}{U_q(N)}\exp\left[-\beta|\lambda|-\mu(\lambda)\right]. \tag{1}$$

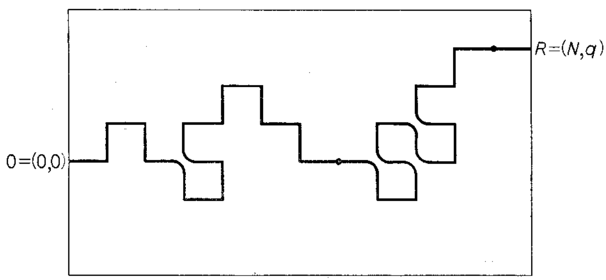

Fig. 1. – A phase separation line on a lattice with a base of 13 lattice points, drawn as a random walk.

([1]) R. A. MINLOS and YA. SINAÏ: *Math. USSR Sbornik*, **2**, 355 (1967).
([2]) G. GALLAVOTTI and A. MARTIN-LÖF: *Comm. Math. Phys.*, **25**, 87 (1972); D. ABRAHAM, G. GALLAVOTTI and A. MARTIN-LÖF: *Lett. Nuovo Cimento*, **2**, 143 (1971).

$|\lambda|$ is the length of λ, $\mu(\lambda)$ is a function which describes the interaction of λ with the pure phases which are separated by it. $U_q(N)$ takes care of the normalization of $W(\lambda)$.

As the statistical weight of a random walk is not only determined by its length but also by its geometrical shape (unless $\mu(\lambda) \equiv 0$), we call $U_q(N)$ an ensemble of non-free random walks.

The function $\mu(\lambda)$ has some nice properties which are qualitatively equivalent to the following:

(2) $$\mu(\lambda) = \sum_{\boldsymbol{r},\boldsymbol{r}'\in\lambda} \phi(\boldsymbol{r}-\boldsymbol{r}') .$$

$\sum_{\boldsymbol{r},\boldsymbol{r}'}$ runs over the centres of the unit segments the union of which builds λ. For the function $\phi(\boldsymbol{r})$, which also depends on β, the following inequality holds:

(3) $$|\phi(\boldsymbol{r})| \leqslant D(\beta) \exp[-k\beta|\boldsymbol{r}|] \qquad (k>0) ,$$

where $D(\beta) \xrightarrow[\beta\to\infty]{} 0$ exponentially fast.

An important quantity is

(4) $$P_N(s) = \frac{1}{U_0(N)} \sum_{\lambda\ni(N/2,s)} W(\lambda) ,$$

i.e. the probability that a random walk from $(0, 0)$ to $(N, 0)$ passes through the point $(N/2, s)$.

A relevant and physically important question is whether

(5) $$\lim_{N\to\infty} P_N(s) = 0 \qquad (s \text{ fixed}) .$$

If this were true it would mean that the line of separation stays away from any fixed region. Hence if one considers correlation functions locally, like $\langle\sigma_x\rangle$, $\langle\sigma_x\sigma_y\rangle$, $\langle\sigma_x\sigma_y\sigma_z\rangle$, ... where x, y, z, ... are points fixed at a finite distance from the centre $(N/2, 0)$, one finds that they are a linear combination of the correlation functions of the two coexisting pure phases with coefficients α and $1-\alpha$, where α is the probability that λ passes above the point where the observations are made ([3]). This would imply that the correlation functions, even when observed locally, would be translationally invariant.

Another problem, which is closely related to the one we mentioned above, is the following.

Let $U(N)$ be the ensemble which is the union of all $U_q(N)$, in which the random walks again have a statistical weight which is given by (1) with the only difference that the normalization constant is changed into $U(N)$ in accordance with the ensemble. Let $\tilde{P}_N(q)$ be the probability in this ensemble that a random walk which starts at 0 ends at (N, q).

Then the question arises whether or not

(6) $$\lim_{N\to\infty} \tilde{P}_N(q) = \lim_{N\to\infty} \frac{U_q(N)}{U(N)} = 0 \text{ for all } q .$$

In the case of free random walks this problem has been treated by HAMMERSLEY ([4]).

([3]) See also G. GALLAVOTTI and R. S. MIRACLE: *Phys. Rev.*, **5** B, 2555 (1972).

([4]) J. M. HAMMERSLEY: *Proc. Camb. Phil. Soc.*, **57**, 516 (1961) (pag. 519 and 521).

We have found a rigorous proof of both conjectures (5) and (6) for large β in the case that $W(\lambda)$ is given by (1) under conditions (2) and (3).

In the following we will sketch the proof in the simplified case that the ensembles $U(N)$ and $U_q(N)$ are replaced by $\bar{U}(N) \subset U(N)$ and $\bar{U}_q(N) \subset U_q(N)$, which only contain the lines λ which do not « go back », *i.e.* which, thought as random walks, are only allowed to step forward, upward and downward. Any $\lambda \in \bar{U}(N)$ can be described by a sequence of nonzero indexed integers $(s_{x_1}, \ldots, s_{x_n})$ telling us the positions $x_1 < x_2 < \ldots < x_n$ of the jumps of λ and their magnitudes $s_{x_1}, \ldots, s_{x_n}$. An example is given in Fig. 2 which

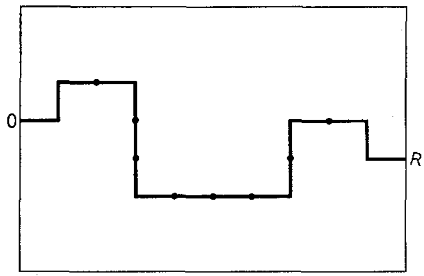

Fig. 2. – The phase separation line on a lattice with a base of 10 lattice points which corresponds to the sequence $(1_1, -3_3, 2_7, -1_9)$.

shows the line on a strip with a base of eleven lattice points corresponding to the sequence $(1_1, -3_3, 2_7, -1_9)$. If we define

$$\psi(s_{x_1}, \ldots, s_{x_n}) = \frac{\mu(s_{x_1}, \ldots, s_{x_n}) - \mu(0)}{\beta}, \tag{7}$$

where $\mu(0)$ is the interaction of a straight line from $(0, 0)$ to $(N, 0)$ with the pure phases, and

$$\Psi(s_{x_1}, \ldots, s_{x_n}) = \psi(s_{x_1}, \ldots, s_{x_n}) - \sum_{i=1}^{n} \psi(s_{x_i}), \tag{8}$$

we may rewrite (1) for the ensemble $\bar{U}(N)$ as

$$\bar{W}(\lambda) = \bar{W}(s_{x_1}, \ldots, s_{x_n}) = \frac{\exp[-(\beta N + \mu(0))]}{\bar{U}(N)} \exp\left[-\beta\left(\sum_i (|s_{x_i}| + \psi(s_{x_i})) + \Psi(s_{x_1}, \ldots, s_{x_n})\right)\right]. \tag{9}$$

We can interpret $\bar{U}(N)$ as the grand canonical ensemble of a multicomponent one-dimensional lattice gas of $N+1$ cells.

The component particles correspond to jumps of different lengths. The activity of a particle of type s_i is $\exp[-\beta(|s_i| + \psi(s_i))]$, the interaction energy of a configuration is $\Psi(s_{x_1}, \ldots, s_{x_n})$. From (2), (3) one may derive that this interaction can be expressed by means of a small short-ranged interparticle potential (with pair potential, three-body, four-body, etc. components). At the same time for large β the activities become very small. Hence we may expect that the systems behave qualitatively as a perfect gas, for we may expect that the Mayer expansion converges. Therefore no qualitative difference should exist between the ensembles $\bar{U}(N)$, $\bar{U}_q(N)$ and the corresponding perfect-gas ensembles which one obtains by replacing in (1) $\mu(\lambda)$ by zero. For this perfect gas the statistical properties can be evaluated exactly and one easily finds (using the same symbols as in (5), (6)) that $P_N(q) \sim \tilde{P}_N(q) \sim O(1/\sqrt{N})$ as $N \to \infty$.

To show that the properties of $\bar{U}_N$, $\bar{U}_q(N)$ are close to the properties of the corresponding perfect-gas ensembles one can use the technique based on the Mayer expansion and the Kirkwood-Salsburg equations. These techniques, as is well known, enable one to estimate the deviations from the perfect-gas (or free-random-walk) behaviour. As already mentioned this program has been carried out ([5]) and leads to the results for a suitable $c > 0$ (β-independent)

$$P_N(q),\, \tilde{P}_N(q) \sim \frac{1}{\sqrt{N}} \qquad \text{if } \frac{|q|(\log N)^c}{\sqrt{N}} \xrightarrow[N\to\infty]{} 0 . \tag{10}$$

A much simpler proof can be provided if one only wants to prove (6) for the ensemble $\bar{U}(N)$ ([6]). One may define $\bar{U}(N, L) \subset \bar{U}(N)$ as the ensemble which consists of only those lines λ which contain at least one jump of length s with $|s| = L'$ for each integer $0 < L' \leqslant L$. It is easy to see that

$$\frac{\bar{U}(N, L_0)}{\bar{U}(N)} = 1 - O(1/\sqrt{N}) \qquad (N \to \infty) , \tag{11}$$

where $L_0 = c(\beta)\log N$, with $c(\beta)$ a well-chosen constant depending on β.

This implies that it is sufficient to prove (6) for the ensemble $\bar{U}(N, L_0)$ instead of the complete ensemble $\bar{U}(N)$. Now there is a 1-1 correspondence between each line λ belonging to $\bar{U}_q(N, L_0)$ and a set V_λ of L_0 lines $\lambda'(\lambda, L)$, with $L = 1, 2, ..., L_0$, belonging to $\bar{U}(N, L_0)$, where $\lambda'(\lambda, L)$ is the line one obtains by reversing in λ the direction of the first jump of length $+$ or $-$ L one encounters as one walks along λ, starting at the origin.

As the reversal of direction of just one jump causes only a minor change in the shape of λ, it does not change the value of $W(\lambda)$ appreciably in most cases, hence for most λ's $\sum W(\lambda')$ over all $\lambda' \in V_\lambda$ will about be equal to $L_0 W(\lambda)$.

In fact one can show rigorously that

$$\bar{U}(N, L_0) > \sum_{\lambda \in \bar{U}_q(N, L_0)} \sum_{\lambda' \in V_\lambda} W(\lambda') > \alpha L_0 \sum_{\lambda \in \bar{U}_q(N, L_0)} W(\lambda) \tag{12}$$

with $\alpha > 0$ and independent of N.

From this it follows that

$$\frac{\bar{U}_q(N)}{\bar{U}(N)} \leqslant \frac{1}{\alpha c(\beta) \log N} . \tag{13}$$

The above estimate is too weak to draw any conclusions about the asymptotic behaviour of $\tilde{P}_N(q)$ as $N \to \infty$, also it seems to be very hard to prove (5) in a similar manner. On the other hand, the β-region where it can be proven with this technique is much larger than the β-region where (5), (6) are proven with the aid of the Kirkwood-Salsburg equations.

The proofs of (5), (6) that one can provide for the complete ensembles $U(N)$ and $U_q(N)$ are essentially the same as the ones we described above, the main differences

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([5]) G. GALLAVOTTI: *The phase separation line in the two-dimensional Ising model*, preprint.

([6]) H. VAN BEIJEREN: to appear.

lying in the fact that one has to define still more and more complicated kinds of lattice-gas particles.

An interesting question to study would be under which conditions on ϕ the results (5), (6) and also (10), (13) stay true. *E.g.* one would naturally conjecture that, if $\phi(\boldsymbol{r})$ is short ranged (say $\phi(\boldsymbol{r}) \leqslant \exp[-\varkappa|\boldsymbol{r}|]$) but β-independent), (5), (6) should still hold (this is « natural » in so far as one-dimensional lattice gases with short-range interactions should have no phase transitions).

Finally we mention that the analogous problems in 3 dimensions (here $U_0(N)$ is replaced by a set of polyedrical surfaces on the lattices with boundary fixed on a square in the plane $z = 0$) should have completely different solutions, at least at large β. In this case intuitive arguments [7] suggest that the phase separation plane has a non-vanishing probability to pass through a point in the middle of the $(z = q)$-plane, so there would be a possibility to have a locally translationally noninvariant situation.

A fascinating question arises at this point: Let $\beta_c = 1/kT_c$, where T_c is the three-dimensional Ising-model critical temperature. Is it possible that for not too large β, say for $\beta_c < \beta < \tilde{\beta}_c$, the results (5), (6) hold also in 3 dimensions?

If this were the case one would have a second phase transition: For $T_c < T < \tilde{T}_c$ the phase separation surface would show fluctuations in shape which stay coherent over macroscopic distances.

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[7] L. LANDAU and E. LIFSHITZ: *Physique statistique* (Moscow, 1967), p. 576.