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**Cluster Expansion Technique for
Coexistence Phenomena away from
the Critical Point.**

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CANDIDATE

Pierluigi Contucci

SUPERVISOR

Prof. Giovanni Gallavotti

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TRIESTE

Questa tesi é il frutto di un lavoro paziente e disciplinato. La dedico ai miei genitori che, pur avendomi rivelato con l'esempio il segreto di queste virtù, raramente mi hanno visto paziente e disciplinato.

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Introduction

The main body of rigorous results in statistical mechanics and constructive quantum field theory is obtained by applying techniques which can be essentially grouped in two fundamental and in some sense complementary classes: perturbation methods and convexity methods.

The perturbations method applies to theories which can be interpreted, by means of small parameter, close to linear or exactly soluble ones.

The other method applies to theories which have a definite sign in the sense that hold for them some properties like global positivity, monotonicity, convexity etc. This last method is generally not affected by limited parameter range and is used to establish existence of limits, like the infinite volume one, for the observables of the theory or their sign in that limit. The theorems obtained in this way give informations on consistency of the theory or on the presence of fundamental phenomena like phase transitions; but in spite of their elegance they are unable to say, at least directly, something about the mutual functional dependence for those observables which is essential for the experimental test.

Perturbative methods fill exactly this lack giving detailed properties of the theory like analyticity in the coupling constants and estimates for the radius of convergence; a fundamental point for the method to be rigorous and not only formal, is that all the estimates for finite size system have to be uniform in their

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size. These well posed expansions are usually known as cluster expansions.

Cluster expansions originated with the work of Mayer and Montroll ^[1] in 1941, and Kirkwood and Salsburg in 1953 ^[2], but the power and the wideness of applications of this tool was fully recognised only after some decade with the works by Gallavotti, Martin-Löf, Miracle-Solé in 1971 ^[3] in classical statistical mechanics, and by Glimm, Jaffe, Spencer in 1973 ^[4,5] in constructive quantum field theory.

Although these works use the same conceptual strategy, they contain special features depending on the field its was applied. Only recently it has been realised that with the notion of polymers model it is possible to unify these various forms and formalize in an abstract way this techniques.

In the nature of rigorous perturbative method there is a limited parameter range; the conceptual reason is that for a field theory with nontrivial phase structure cannot exist a unique suitable cluster expansion. In the Ising model for instance the high and low temperature expansions are defined by completely different expansions; if the dimension is greater than one, it is not possible to have the convergence of one of them in the entire phase space because that would imply the absence of critical point.

A problem emerges naturally: how close to the critical point can we go with cluster expansion techniques? This thesis is a possible investigation on this subject.

Actually, in order to avoid misunderstanding, the question needs some specifications. The point is that one cannot establish a priori an abstract threshold as the "good" one, since every problem has its own degree of tolerance depending on conceptual and practical reasons like the theoretical meaning of the given model, and the details of experimental results which have been obtained in the

given context. So we can divide the problem in two steps: first try to give the best possible estimates in the general formalism with the polymers language and then to test the result in an explicit example trying to take advantage from its particular feature. As concrete case we have chosen the problem of surface tension in two dimensional Ising model.

The exposition is organised as follows. In the first chapter we introduce the abstract polymer model: it is defined by a partition function which is a sum of products of the activities of some elementary objects called polymers. In order to establish convergence theorems in our abstract expansion we formulate two requirements which guarantee that the elements we have to sum have to be not too big and not too many. Using an algebraic method and introducing a formal derivation, we establish our basic recursive functional equation of “Kirkwood-Salsburg” type. Since it lives in a Banach space we exploit the freedom in the choice of (equivalent) norms. This optimization is reflected in the radius of convergence for the considered expansion and in the estimates of critical parameters which generally follow from them in the explicit problems of statistical mechanics and constructive quantum field theory. Our optimization procedure leads to a result which is, so far, the best estimate obtained in such general context.

In the second chapter we treat the problem of surface tension in two-dimensional Ising model following the method in Ref. [3]. With duality methods we map the low temperature regime in the general polymers formalism and improve the previous general bound exploiting some peculiar features of Z^2 . In the so found temperature range (which estimates from above the critical β to within 25%), we observe that the model exhibit the phase separation phenomenon rigorously expressed by some theorems which enables one to give a suitable expression

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for the surface tension.

Finally we study the infinite volume limit for the so found formula. We use the same ideas of Ref. [3] with slightly modified and improved lemmas; in this way we are able to stay in the wider temperature range previously established and to prove inside the well known Onsager value for the surface tension.

Chapter 1

The cluster expansion technique for abstract polymer models.

As explained in the introduction, cluster expansion techniques have been used in many different contexts. In each of them they appear with different and special ad hoc features. A natural process of generalization has been developed in the last decade [6,7] and a kind of axiomatic structure has been singled out; in this way, in the study of a particular problem, one has only to check that it is possible to map the problem in the abstract formulation and verify that the axioms hold. The entire set of theorems will follow automatically without any extra work.

The models we can study with this general formalism are usually known, for historical reasons, as polymer models. They are defined by a partition function in a volume V :

$$Z(V) = \sum_{\substack{\text{polymer} \\ \text{families}}} \prod_{\gamma \in \text{family}} z(\gamma) \quad (1.1)$$

where the function $z(\gamma)$ is the activity of the polymer γ and characterizes the model together with the space on which one performs the sum.

The meaning of the axioms is related to the possibility of defining the “free energy density” i.e. the $\frac{1}{V} \log(Z(V))$ in the infinite volume as expansion in the activity: in order the sum be convergent the activity has to be sufficiently small, and the cardinality of the space on which the sum is performed has to be normalizable

with the volume.

There are essentially two approaches to the proof of convergence: one is based on the use of Kirkwood-Salsburg type of equations ^{[8][9][3]}, while the other relies on combinatorics counting of trees of a graph ^{[10][11][4]}.

We follow the first method because it is particularly suitable for the general optimization procedure which we are looking for. The Banach structure on which the functional equations live is defined by a norm: the degree of freedom in this definition can be optimised and produce, in the last analysis, estimates for critical parameters.

1.1 The definition of polymer model.

We start with a set P_1 of object γ_k , $k = 1, 2, \dots$, called polymers. One has to think of this set as an alphabet. The collections of r -polymers, i.e. the elements of the r -fold Cartesian product $P_r = P_1 \times P_1 \times \dots \times P_1$ r -times, will be the space of r -words; we will denote them by $X = \gamma_1, \dots, \gamma_r$ with $N(X) \equiv r$. The fundamental notion for polymer models is the notion of incompatibility. One can define it by a reflexive and symmetric relation on P_2 represented by a characteristic function:

$$f(\gamma, \gamma') = \begin{cases} 1, & \text{if } \gamma, \gamma' \text{ compatible;} \\ 0, & \text{otherwise.} \end{cases} \quad (1.2)$$

In addition to the compatibility the following two primitive notions for a polymer will be introduced. The activity $z(\gamma)$ is a function from P_1 to the complex numbers, and the volume $|\gamma|$ is a function from P_1 to nonnegative real numbers with the order preserving property with respect to an assigned partial order in P_1 .

Two subset of P_r are important for the polymer expansion, namely the completely compatible r -polymers D_r and the incompatible r -polymers C_r . In order

to easily visualize the structure of these two sets we can represent a r -polymer X as a r -vertex graph. Each vertex represent one $\gamma_i \in X$. The graph is constructed connecting two vertices by a line if the two corresponding polymers are not compatible. In this picture the r -graph without lines are the elements of D_r and the path-connected r -graph are the elements of C_r . We set by definition

$$C_1 = D_1 = P_1. \quad (1.3)$$

Furthermore $D_0 = P_0 = \emptyset$ and

$$D = \bigcup_{k=0}^{\infty} D_k \quad C = \bigcup_{k=1}^{\infty} C_k \quad P = \bigcup_{k=0}^{\infty} P_k. \quad (1.4)$$

It will be of great importance the distinction between the spaces introduced and their quotient to respect the permutation group; we will indicate these modified sets overposing a hat, e.g. \hat{P}_k, \hat{D} etc., and their elements putting them inside the parenthesis, e.g. $(\gamma_1, \dots, \gamma_r) \in \hat{D}_r$. The difference is essentially seen in the typical sums:

$$\frac{1}{r!} \sum_{\gamma_1, \dots, \gamma_r \in D_r} z(\gamma_1) \cdots z(\gamma_r) = \sum_{(\gamma_1, \dots, \gamma_r) \in \hat{D}_r} z(\gamma_1) \cdots z(\gamma_r) \quad (1.5)$$

and

$$\sum_{\gamma_1, \dots, \gamma_r \in P_r} z(\gamma_1) \cdots z(\gamma_r) = \sum_{(\gamma_1, \dots, \gamma_r) \in \hat{P}_r} \frac{r!}{r_1! \cdots r_n!} z(\gamma_1) \cdots z(\gamma_r) \quad (1.6)$$

where r_i is the multiplicity of γ_i in $\gamma_1, \dots, \gamma_r$.

The whole set of informations contained in a r -polymer can be split in this way in two complementary part: the combinatoric part which refer the topological nature of the associated graph, and the analytic part which refer the functional properties of its activity.

Now defining

$$z^X = \prod_{\gamma \in X} z(\gamma). \quad (1.7)$$

with $z(\emptyset) \equiv 1$, and

$$f^X = \prod_{(\gamma_i, \gamma_j) \in X \times X} f(\gamma_i, \gamma_j) \quad (1.8)$$

with $f(\emptyset, \emptyset) \equiv 1$, we introduce the notion of partition function Z for a given set of polymers P_1 :

$$Z = \sum_{X \in \mathcal{D}} \frac{1}{N(X)!} z^X = \sum_{X \in \widehat{\mathcal{D}}} z^X = \sum_{X \in \widehat{\mathcal{P}}} z^X f^X. \quad (1.9)$$

If P_1 is a finite set the previous sum is finite. In the infinite case, which will correspond to the infinite volume limit in some explicit case, there are obviously problems of convergence which will require some additional properties to control the expansions; we examine all these problems in the section 1.3 after the study of a resummation procedure which we allow to express the logarithm of the partition function in terms of activities and to derive the recursive functional equations of Kirkwood-Salsburg type.

1.2 The algebraic method.

We are now interested in a formal algebraic relation between the partition function and its logarithm. The method we use in order to derive this relation is a very powerful tool introduced some decade ago in the study of statistical mechanical properties for ordinary gas; it can be found in a completely abstract formulation in Ref. [8].

We consider the set of finite configurations $X = (\gamma_1, \dots, \gamma_n)$, i.e. those elements of $\widehat{\mathcal{P}}$ with $N(X) = \sum_{\gamma} X(\gamma) < \infty$, where $X(\gamma)$ is the multiplicity of γ in X .

A natural definition of sum can be introduced by $(X_1 + X_2)(\gamma) = X_1(\gamma) + X_2(\gamma)$. We also consider the space F of functions of configurations $\phi(X)$ such that $\sup_{N(X)=n} |\phi(X)| < \infty$ for all n , and its subspaces F_0 and F_1 defined by $\phi(\emptyset) = 0$ and $\phi(\emptyset) = 1$ respectively. We define in F a convolution product by

$$(\phi_1 * \phi_2)(X) = \sum_{X_1+X_2=X} \phi_1(X_1)\phi_2(X_2). \quad (1.10)$$

The sum is obviously finite since X is finite and $\phi_1 * \phi_2 \in F$. The corresponding exponential can be defined for $\phi \in F_0$:

$$(\text{Exp}\phi)(X) = \sum_{n \geq 0} \frac{\phi^{n*}}{n!} = \mathbb{I}(X) + \sum_{n \geq 1} \frac{1}{n!} \sum_{X_1+\dots+X_n=X} \phi(X_1)\cdots\phi(X_n) \quad (1.11)$$

where $\phi^{0*} = \mathbb{I}(X)$ is defined to be 1 if $X = \emptyset$ and 0 otherwise. We also define the corresponding logarithmic function for $\phi \in F_1$; posing $\phi = \mathbb{I} + \phi_0$ with $\phi_0 \in F_0$ we have:

$$(\text{Log}\phi)(X) = \sum_{n \geq 1} \frac{(-1)^{n+1}}{n} \phi_0^{n*} = \sum_{n \geq 1} \frac{(-1)^{n+1}}{n} \sum_{X_1+\dots+X_n=X} \phi_0(X_1)\cdots\phi_0(X_n). \quad (1.12)$$

The reason for introducing the convolution product is the property:

$$\sum_{X \in \hat{P}} (\phi_1 * \phi_2)(X)z^X = \left(\sum_{X \in \hat{P}} \phi_1(X)z^X \right) \left(\sum_{X \in \hat{P}} \phi_2(X)z^X \right) \quad (1.13)$$

and then

$$\sum_{X \in \hat{P}} (\text{Exp}\phi)(X)z^X = \exp\left(\sum_{X \in \hat{P}} \phi(X)z^X \right) \quad (1.14)$$

if $\phi \in F_0$.

For the estimates we will derive it will be of great importance a "derivation" formalism defined by:

$$(D_X\phi)(Y) = \phi(X+Y) \frac{(X+Y)!}{Y!} \quad (1.15)$$

with $X! = \prod_{\gamma} X(\gamma)!$. In terms of it one can prove the usual rules like the Taylor formula

$$\sum_{X \in \widehat{P}} \phi(X)(u+v)^X = \sum_{X \in \widehat{P}} \frac{u^X}{X!} \sum_{Y \in \widehat{P}} (D_X \phi)(Y)v^Y \quad (1.16)$$

and the Leibnitz rule

$$D_{\gamma}(\phi_1 * \phi_2) = (D_{\gamma}\phi_1) * \phi_2 + \phi_1 * (D_{\gamma}\phi_2). \quad (1.17)$$

We can now derive our main algebraic relation. Observing that the ϕ defined by $\phi(X) = z^X f^X$ belong to F_1 we define $\phi^T = \text{Log} \phi$, so that $\phi = \text{Exp} \phi^T$. Then

$$Z = \sum_{X \in \widehat{P}} \phi(X) = \exp\left(\sum_{X \in \widehat{P}} \phi^T(X)\right). \quad (1.18)$$

The explicit formula for ϕ^T is [3]:

$$\phi^T(\gamma_1, \dots, \gamma_r) = \frac{n(X)}{X!} z^X \quad (1.19)$$

with $n(X) = n_+(X) - n_-(X)$ and $n_{\pm}(X)$ is the number of subgraphs of X in C_r which contain an even (resp. odd) number of lines. So we can finally write:

$$\log Z = \sum_{X \in \widehat{C}} \frac{n(X)}{X!} z^X. \quad (1.20)$$

1.3 Convergence of the polymer expansion.

An optimised norm.

With the algebraic and differential language introduced in the previous section we can easily derive estimates for ϕ^T .

We use the method of functional equations of “Kirkwood-Salsburg” type. There is no unique way to formulate the problem with this approach; one could say that the “art of the job” is the right choice between the various possibilities of formulation. We follow the line which can be found in Ref. [3] and we try to optimize it.

Our optimization procedure can be understood in the general abstract framework commonly used to describe these mathematical structures [8]. The functional equations describing our problem live in a Banach space; the (equivalent) norms defining that structure have some degree of freedom which we can exploit to optimize it. This optimization will be reflected in the radius of convergence for the considered expansion and in the estimates of critical parameters which generally follow from them in the explicit problems of statistical mechanics and constructive quantum field theory.

In order to establish convergence in our abstract polymer expansion we have to formulate two requirements whose meaning can be roughly explained saying that the elements we have to sum have to be not too big and not too many.

Defining $N(\gamma, x)$ as the number of γ -incompatible polymers in P_1 which have a volume between x and $x + 1$, one introduces two axiomatic estimates:

A1 (Entropy Estimate). There exist a constant μ such that

$$N(\gamma, x) \leq |\gamma| \mu^x \quad \forall \quad \gamma \in P_1 \quad (1.21)$$

A2 (Energy Estimate). There exist a constant $\lambda < 1$ such that

$$|z(\gamma)| \leq \lambda^{|\gamma|} \quad \forall \quad \gamma \in P_1 \quad (1.22)$$

The problem of thermodynamic limit is now reflected in the number of elements of P_1 . We are interested only in uniform estimates in this number. We start with the

definition of correlation function $\varrho(X)$ which is the probability that the polymers in X are present:

$$\varrho(X) = \frac{\sum_{Y \in \widehat{P}} \phi(X + Y)}{\sum_{Y \in \widehat{P}} \phi(Y)} = \sum_{Y \in \widehat{P}} (\phi^{-1} * D_X \phi)(Y) = \sum_{Y \in \widehat{P}} \Delta_X(Y) \quad (1.23)$$

(we remind that ϕ^{-1} defined by $\phi^{-1} * \phi = 1$ is well defined if $\phi(\emptyset) \neq 0$) where $\Delta_X(Y)$ is defined by:

$$\Delta_X(Y) = (\phi^{-1} * D_X \phi)(Y) = \sum_{Y_1 + Y_2 = Y} \phi^{-1}(Y_1) \phi(X + Y_2). \quad (1.24)$$

We can now derive the recursive equation for $\Delta_X(Y)$.

From (1.24) is easy to see that $\Delta_X(Y) = 0$ if X is not in D , i.e. when there are inside incompatible polymers. Consider $\Delta_{\gamma+X}(Y)$ for $\gamma + X \in D$. From the definition it follows that

$$\begin{aligned} \phi(\gamma + X + Y_2) &= z(\gamma) \phi(X + Y_2) \prod_{\gamma' \in Y_2} (1 + g(\gamma, \gamma')) \\ &= z(\gamma) \phi(X + Y_2) \sum_{S \subseteq Y_2}^{\gamma} (-1)^{N(S)}. \end{aligned} \quad (1.25)$$

if Y_2 is without “multiplicities”, and the overposed γ means that the sum is over sets S (the empty set have to be included) all of whose elements are incompatible with γ . We obtain:

$$\begin{aligned} \Delta_{\gamma+X}(Y) &= \sum_{Y_1 + Y_2 = Y} \phi^{-1}(Y_1) \phi(\gamma + X + Y_2) \\ &= z(\gamma) \sum_{Y_1 + Y_2 = Y} \phi^{-1}(Y_1) \phi(X + Y_2) \sum_{S \subseteq Y_2}^{\gamma} (-1)^{N(S)}. \end{aligned} \quad (1.26)$$

since the only contributing Y_2 are those without multiplicities. Posing $Y_2 = S + Y_3$ and interchanging the sums we obtain:

$$\begin{aligned} \Delta_{\gamma+X}(Y) &= z(\gamma) \sum_{S \subseteq Y}^{\gamma} (-1)^{N(S)} \sum_{Y_1 + Y_3 = Y - S} \phi^{-1}(Y_1) \phi(X + S + Y_3) \\ &= z(\gamma) \sum_{S \subseteq Y}^{\gamma} (-1)^{N(S)} \Delta_{X+S}(Y - S). \end{aligned} \quad (1.27)$$

We observe that this equation determine $\Delta_X(Y)$ with $N(X) + N(Y) = m + 1$ in terms of $\Delta_X(Y)$ with $N(X) + N(Y) = m$ for $m = 0, 1, \dots$, successively. This is exactly what we need in order to obtain convergence estimates. We define the Banach structure by the m -norm depending on an optimization parameter x :

$$I_m(x) = \sup_{\substack{\gamma_1, \dots, \gamma_m \\ m \geq n \geq 1}} \sum_{\substack{Y \\ N(Y)=m-n}} |\Delta_{\gamma_1, \dots, \gamma_m}(Y)| (\lambda^{-1} e^{-x})^{\sum |\gamma_i|} \quad (1.28)$$

We can now deduce from (1.27) and from A1, A2:

$$\begin{aligned} & \sum_{\substack{Y \\ N(Y)+N(X)=m}} |\Delta_{\gamma+X}(Y)| (\lambda^{-1} e^{-x})^{|\gamma|+|X|} \leq \\ & \leq \sum_{\substack{Y \\ N(Y)+N(X)=m}} \sum_{S \subseteq Y}^\gamma |\Delta_{X+S}(Y-S)| (\lambda^{-1} e^{-x})^{|\gamma|+|X|} \lambda^{|\gamma|} \leq \\ & \leq \sum_S^\gamma \sum_{\substack{Y \\ N(Y)=m-N(X)}} |\Delta_{X+S}(Y-S)| (\lambda^{-1} e^{-x})^{|X|+|S|} e^{-x|\gamma|} (\lambda e^x)^{|S|} \leq \\ & \leq I_m(x) e^{-x|\gamma|} \sum_S^\gamma (\lambda e^x)^{|S|}. \end{aligned} \quad (1.29)$$

Since the only contributing S are those without multiplicities we can transform the last sum in:

$$\sum_S^\gamma (\lambda e^x)^{|S|} = \sum_{n \geq 0} \frac{1}{n!} \left(\sum_{\sigma \in P_1}^\gamma (\lambda e^x)^{|\sigma|} \right)^n \leq \exp(|\gamma| \sum_{l \geq 1} (\mu \lambda e^x)^l) = \exp(|\gamma| \frac{\mu \lambda e^x}{1 - \mu \lambda e^x}) \quad (1.30)$$

if

$$\mu \lambda e^x < 1 \quad (1.31)$$

where we have supposed, without restriction, that the minimum size of a polymer is 1. The fact that we have extended to infinity the previous sum in l corresponds to consider the thermodynamic limit; the resulting estimates are uniform in the volume. We can conclude that:

$$I_{m+1}(x) \leq I_m(x) \exp\left(-x + \frac{\mu \lambda e^x}{1 - \mu \lambda e^x}\right). \quad (1.32)$$

It's clear that for the m -norm to be a contraction and the expansion to be convergent the argument in the exponential has to be negative:

$$-x + \frac{\mu\lambda e^x}{1 - \mu\lambda e^x} \leq 0 \quad (1.33)$$

or

$$\mu\lambda \leq \frac{x}{1+x} e^{-x}$$

and in order to optimize the choice of x we have to find the positive value of x that maximize the right hand side. A simple calculation give $x = \frac{(\sqrt{5}-1)}{2}$ as solution for the first variation vanishing condition $x^2 + x - 1 = 0$.

The final general estimate is:

$$\lambda < \frac{1}{\mu} \frac{x}{1+x} e^{-x} \Big|_{x=\frac{(\sqrt{5}-1)}{2}} \quad (1.34)$$

since, of course, this estimate is stronger than the optimized version of the (1.31). A result numerically identical has been obtained with different method in Ref. [7] and with the same method but in a slightly different context in Ref. [12]; it is, so far, the best estimate obtained in a so general context.

One could take advantage from an eventual inequality $|\gamma| \geq \underline{m}$; in this case the (1.33) becomes

$$-x + \frac{(\mu\lambda e^x)^{\underline{m}}}{1 - \mu\lambda e^x} \leq 0 \quad (1.35)$$

but since it is not exactly optimizable as function of μ we will use it only in the concrete case that we will examine in the next chapter.

One can see ^{[8][7][13][12]} that in the range (1.34) the polymer expansion converges absolutely as a power series in the $z(\lambda)$ for every finite P_1 , and the convergence for $\frac{1}{V} \log(Z(V))$ is uniform in the volume; in this abstract case the volume is defined as $V = \sup_{\gamma \in P_1} |\gamma|$. Furthermore standard theorems on analytic functions, in particular Vitali theorem, imply analyticity of thermodynamic functions.

Chapter 2

The surface tension problem in two-dimensional Ising model

The history of the surface tension for the Ising model starts with the fundamental work by Onsager ^[14]. He gave, in this paper, the first definition and, at the same time, the first calculation for it with a simple and ingenious method: one considers instead of a ferromagnetic Ising model with coupling $+1$ an antiferromagnetic model with coupling -1 , and cylindrical boundary condition. According to the parity of the number of the spin in the periodic direction the phase structure have to change: if this parity is odd there is going to be somewhere a mismatch at low temperature (in more recent terminology we said the model is frustrated) in the arrangement of the spin as if one puts together two oppositely magnetized phase in the ferromagnetic case. Therefore one will be able to interpret the difference in the free energy when the parity is odd and when it is even as due to the phase separation and therefore as a surface tension. In this way Onsager obtained:

$$\tau(\beta) = -2\beta - \log(\tanh(\beta)). \quad (2.1)$$

Only in 1971 ^[15] it has been proved that the Onsager's value coincides , for β large enough, with that computed using a different definition based on a detailed microscopic description of the separation of the phase and of the line of separation which we are going to consider.

In this chapter we expose the duality method and map the low temperature regime in the general polymers formalism. After some definitions we improve the general polymer estimate, taking advantage of the structure of closed contours in the lattice; in particular the fact that they have a minimum side of 4 units implies good improvements since it eliminates the first three terms in a geometric sum. In the range so found we prove the validity of some theorems stating in a rigorous form the phase separation phenomenon. Finally with a simplified expression for surface tension we prove its existence in the infinite volume limit using an improved version of the proof in Ref. [16].

2.1 Notations and definitions.

Let Θ be a finite subset of the infinite square lattice Z^2 . The Ising model in the “box” Θ is defined by associating to each point $x \in \Theta$ a spin variable σ_x taking values ± 1 . We will suppose that the spins on the boundary of Θ are fixed and we denote by $\underline{\tau}$ the array specifying their values. In this way to each configuration defined by $\underline{\sigma}$, $\underline{\tau}$ we associate the usual weight:

$$\tilde{w}_{\underline{\tau}}(\underline{\sigma}) = \exp\left(\beta \sum_{\langle x,y \rangle} \sigma_x \sigma_y\right) \quad (2.2)$$

where the sum runs over all pairs of nearest neighbors in Θ , including the boundary.

From the first pioneering work by Peierls in 1936 [17] up to more recent work [18,15], one has realised that, for the purpose of investigating the system at low temperature it is very convenient to use the duality transformation method. It consists essentially in a representation in terms of contours in the dual lattice of a spin configuration for assigned boundary condition: one draws a line on the

lattice bond which separate opposite spin. The set of lines thus obtained splits into several components and, at each vertex of the $(1/2, 1/2)$ -shifted lattice will end 0,2,4 lines excluding the points in the boundary. In order to map this formalism in the polymer language it is useful to transform this set of lines in selfavoiding contours; this is simply done cutting the overlapping lines along a fixed diagonal direction (for instance: \nearrow). We obtain in this way a family of edge-selfavoiding contours $(\gamma_1, \dots, \gamma_n)$ some of which start and end at the fixed segments of the boundary, the others being closed and lying "inside" Θ . We stress that for a given $\underline{\tau}$ we have a one to one correspondence between $\underline{\sigma}$ and $(\gamma_1, \dots, \gamma_n)$.

It is straightforward now to rewrite the thermodynamics in terms of contours:

$$\sum_{\langle x,y \rangle} \sigma_x \sigma_y = \text{no. of bonds in } \Theta - 2 \sum_1^n |\gamma_i| \quad (2.3)$$

and from (2.3)

$$w_{\underline{\tau}}(\gamma_1, \dots, \gamma_n) = \exp(-2\beta \sum_1^n |\gamma_i|) \quad (2.4)$$

so that the partition function will be

$$Z(\mathcal{M}^{\underline{\tau}}(\Theta), \beta) = \sum_{(\gamma_1, \dots, \gamma_n) \in \mathcal{M}^{\underline{\tau}}(\Theta)} \exp(-2\beta \sum_1^n |\gamma_i|) \quad (2.5)$$

where $\mathcal{M}^{\underline{\tau}}(\Theta)$ is the set of allowed configurations of contours, called ensemble, which correspond to the set of spin configurations.

More generally we will consider partition functions for any assigned ensemble \mathcal{M} , for example it will be important the canonical ensemble $\mathcal{M}^{\underline{\tau}}(\Theta, m)$ of allowed configurations with a given magnetization $\sum_{x \in \Theta} \sigma_x = m|\Theta|$.

In the following we will consider, instead of the infinite planar lattice Z^2 , an infinitely long cylinder $\Omega_{\infty, N}$ with sectional perimeter N . In this way we will obtain periodic boundary condition in the horizontal direction; in particular our box will

be a cylindrical region $\Omega \in \Omega_{\infty, N}$ with flat top and bottom and with height N^δ for some $\delta > 1$. For it, the four boundary conditions $+$ on the top and $-$ at the bottom etc, will be denoted by $+, -$ etc. We will refer as “big” to the contours which go around the cylinder; for each of the defined b.c. they have a given parity. A subscript 0 will indicate that a given ensemble have a minimal number of such contour compatible with the right parity. So, for instance, $\mathcal{M}_0^{++}(\Omega)$ will be the ensemble with $+, +$ b.c. and without “big” contour. Finally we will also have the occasion to consider the ensemble of “c-small” contours in Ω defined by the restriction of having a length bounded by $c \log |\Omega| = c \log N^{1+\delta}$.

The definition of surface tension used in our approach is based on the microscopic description of the phase separation phenomenon. A basic property of the partition function of any well posed thermodynamic model is the extensivity of its logarithm. E.g. $|\Omega|^{-1} \log Z(\mathcal{M}^{+-}(\Omega, m), \beta) \rightarrow -\beta f(\beta, m)$ as $\Omega \nearrow \Omega_{\infty, \infty}$, where $f(\beta, m)$ is the limiting free energy density. In this picture, surface effects are manifested in terms proportional to the measure of surface between interacting phases in the corrections to $\log Z + |\Omega| \beta f(\beta, m)$. For the ensemble $\mathcal{M}^{+-}(\Omega, m)$, where there is typically one surface between the two phases and one at each end of the cylinder, one would expect to have an asymptotic relation:

$$\log Z(\mathcal{M}^{+-}(\Omega, m), \beta) = -|\Omega| \beta f(\beta, m) + N\tau + 2N\tau' + o(N) \quad (2.6)$$

τ being the surface tension between the two phases and τ' the one between each phase and the fixed spins. In order to extract τ we can compare the (2.6) to the corresponding expression expected for an ensemble consisting only of one phase like $\mathcal{M}^{++}(\Omega, m^*)$ where m^* is the value of the corresponding spontaneous magnetization:

$$\log Z(\mathcal{M}^{++}(\Omega, m^*), \beta) = -|\Omega| \beta f(\beta, m^*) + 2N\tau' + o(N) \quad (2.7)$$

where we have supposed that in this last ensemble there is not going to be, typically, any big contour and that for symmetry reasons the contributions from the bases in (2.6) and (2.7) are the same. Furthermore, for symmetry reasons it have to result that $f(\beta, m^*) = f(\beta, -m^*)$ and posing $m = \alpha m^* + (1 - \alpha)(-m^*)$, $0 < \alpha < 1$ it should be $f(\beta, m) = \alpha f(\beta, m^*) + (1 - \alpha)f(\beta, -m^*) = f(\beta, m^*)$. This should allow the definition:

$$\tau = \lim_{N \rightarrow \infty} \frac{1}{N} \log \frac{Z(\mathcal{M}^{+-}(\Omega, m), \beta)}{Z(\mathcal{M}^{++}(\Omega, m^*), \beta)} \quad (2.8)$$

In the following sections we will prove that all our assumptions are correct and that the defined limit exist.

2.2 Cluster expansion for contours in two-dimensional lattice.

As previously explained, we have now to check that our problem can be mapped into the general polymers formalism; in order to do that we first have to show the correspondence between the underlying conceptual structure and then to show that our case verifies the axioms.

This is easily done comparing the (2.5) with the general (1.1). The contours have the role of polymers, the incompatibility is simply the overlap between edge and the volume $|\gamma|$ of a polymer is the number of its edge which trivially verifies the order preserving property with respect to the set inclusion. The activity is $z(\gamma) = \exp(-2\beta|\gamma|)$. This last identification permits an immediate test of the Energy Estimate axiom which give

$$\lambda = \exp(-2\beta). \quad (2.9)$$

The Entropy Estimate axiom is easily verified too: the number of contours γ -incompatible are simply $|\gamma|$ -times the contours which intersect a given point. The estimate which gives how many such contours exist for a given length l is μ^l where μ is the connective constant for the two-dimensional lattice. It is trivial to see that in this case $\mu \leq 3$. Much less trivial is to improve this bound; we will base our final estimate on a bound for the connective constant which can be found in Ref. [19].

Now we can improve the general bound (1.34) taking advantage from the peculiar structure of our polymers. Since the minimum size of closed contours is 4 we can rewrite the (1.30) with $l \geq 4$; this change will produce good results because it eliminates the first three terms, the biggest ones, in a geometric sum. The (1.35) became:

$$-x + \frac{(\mu\lambda e^x)^4}{1 - \mu\lambda e^x} \leq 0. \quad (2.10)$$

This form is not explicitly solvable as the general one but we can optimize the choice of x numerically, with the help of a computer, using the value for μ given in Ref. [19]; we have obtained

$$\beta > \bar{\beta} = 0.55$$

which can be compared with the general estimate (1.34)

$$\beta > 1.04$$

The $\bar{\beta}$ gives an estimate from above of the critical β ($\beta_c \simeq 0.44$) to within 25%. It will be our landmark in all what follow.

It would be easy now [3] to prove some fundamental estimate for ϕ^T which are useful for convergence theorems and which we will use in the next section in order to establish the theorems on the phase separation.

If $\beta > \bar{\beta}$

$$\sum_X |\phi^T(\gamma + X)| \leq a \exp(-b\beta) \exp(-c\beta|\gamma|) \quad (2.11)$$

and

$$\sum_{\substack{X \ni p \\ X \ni q}} |\phi^T(X)| \leq a' \exp(-b'\beta) \exp(-c'\beta)^{d(p,q)} \quad (2.12)$$

where the a,b etc. are positive constants.

2.3 The phase separation.

This section contains three theorems which study the phase separation phenomenon; they are essentially a rigorous form of the droplet theory of phase transition [20]. The proofs, which we do not report, are essentially those that can be found in Ref. [16]. One has only to use our improved estimates of cluster expansion, in particular the (2.11) and (2.12). In the following we will denote differently functions of β which have different asymptotic behaviour as $\beta \rightarrow \infty$. For instance $\delta(\beta)$, $\eta(\beta)$, $\xi(\beta)$ will be functions of β which approach zero exponentially as $\beta \rightarrow \infty$; $a(\beta)$, $b(\beta)$, $d(\beta)$ will approach zero as a power. Finally if we are not interested in the asymptotic behaviour we will write $A(\beta)$, $B(\beta)$, $D(\beta)$. Let us now discuss in detail in what sense we have phase separation in the ensemble $\mathcal{M}^{+-}(\Omega, m)$. Consider the set of configurations $\tilde{\mathcal{M}}_0^{+-}(\Omega, m) \subset \mathcal{M}^{+-}(\Omega, m)$ consisting of those $X \in \mathcal{M}^{+-}(\Omega, m)$ such that the conditions 1-4 below are verified:

1. X contain just one big contour λ and λ is such that:

$$|\lambda| \leq N(1 + \beta/\bar{\beta}). \quad (2.13)$$

2. Calling Ω_λ the region above the big contour λ associated to X we have:

(for some p with $0 < p < 1$)

$$||\Omega_\lambda| - \alpha|\Omega|| \leq \chi(\beta)|\Omega|^p. \quad (2.14)$$

3. Calling m^+ the average magnetization of the configuration in Ω_λ we have:

$$|m^+|\Omega_\lambda| - m^*\alpha|\Omega|| \leq \chi(\beta)|\Omega|^p. \quad (2.15)$$

4. The total length of the c-large contours is bounded by $Nd(\beta)$

As essentially proved in Ref. [9] and reformulated in Ref. [16] the following result holds:

Th. I. If $\beta > \bar{\beta}$ and $0 < \alpha < 1$, $\delta > 1$

$$\lim_{N \rightarrow \infty} \frac{Z(\tilde{\mathcal{M}}_0^{+-}(\Omega, m), \beta)}{Z(\mathcal{M}^{+-}(\Omega, m), \beta)} = 1 \quad (2.16)$$

provided the functions $\chi(\beta)$, $d(\beta)$ and the parameter p are “suitably” ^[16,3] chosen.

From the physical point of view this theorem says that the typical configurations (i.e. with probability approaching one in the infinite volume) of our system look like two seas of up and down spins, the first on the top of the other, separated by a rather well defined surface λ at height $\sim (1 - \alpha)H$. On each of these seas there are small holes of opposite sign which produce an average magnetization $\sim m^*$.

The following simple and physically deep result establish that the probability of “minimal” ensemble (having a minimal number of big contours) approach one in the thermodynamic limit.

Th. II. If $\beta > \bar{\beta}$

$$\lim_{N \rightarrow \infty} \frac{Z(\mathcal{M}_0^{b.c.})}{Z(\mathcal{M}^{b.c.})} = 1 \quad (2.17)$$

Using the two probabilistic estimates (2.16), (2.17) we can simplify the surface tension formula to:

$$\tau = \lim_{N \rightarrow \infty} \frac{1}{N} \log \frac{Z(\tilde{\mathcal{M}}_0^{+-}(\Omega, m), \beta)}{Z(\mathcal{M}_0^{++}(\Omega, m^*), \beta)}. \quad (2.18)$$

This last expression is very difficult to handle because the canonical sum have the fixed magnetization constraint. A possible way to solve this difficulty is to evaluate the probability in the simpler gran canonical ensemble and to estimate the probability of canonical ensemble in the gran canonical one; since it holds indeed

$$\frac{Z(\tilde{\mathcal{M}}_0^{+-}(\Omega, m), \beta)}{Z(\mathcal{M}_0^{++}(\Omega, m^*), \beta)} = \frac{Z(\tilde{\mathcal{M}}_0^{+-}(\Omega, m), \beta)}{Z(\mathcal{M}_0^{++}(\Omega), \beta)} \frac{Z(\mathcal{M}_0^{++}(\Omega), \beta)}{Z(\mathcal{M}_0^{++}(\Omega, m^*), \beta)} \quad (2.19)$$

if we have a suitable upper bound on the last ratio we can interchange the two partition functions in the (2.18). Suitable in this case means that their logarithm differ by an amount small compared to the order $\sim N$. The estimate which we are looking for is:

Th. III. If $\beta > \bar{\beta}$

$$\frac{Z(\mathcal{M}_0^{++}(\Omega), \beta)}{Z(\mathcal{M}_0^{++}(\Omega, m^*), \beta)} \leq D(\beta)^{-1} |\Omega|^{1/2} \exp(R(\beta)N^{1/2}). \quad (2.20)$$

This transforms the (2.18) in:

$$\tau = \lim_{N \rightarrow \infty} \frac{1}{N} \log \frac{Z(\tilde{\mathcal{M}}_0^{+-}(\Omega, m), \beta)}{Z(\mathcal{M}_0^{++}(\Omega, \beta))}. \quad (2.21)$$

2.4 The surface tension.

In Ref. [3] it has been proved that the (2.21) can be transformed in simpler object, and at the end, the surface tension will appear as the thermodynamic limit of a

partition function of the ensemble of big contours λ , each one having a weight of the form $\exp(-2\beta|\lambda| + \nu(\lambda, \beta))$ with $|\nu(\lambda, \beta)| \leq a|\lambda|e^{-b\beta}$ with a, b positive constants. To do that one needs only to use the (2.11), (2.12) and the theorems of previous section.

The proof of the existence of the limit (2.21) needs some modification since we need a more accurate lemma to adapt to the wider range of temperature on which we are working.

Following Ref. [3] one have:

$$\tau = \lim_{N \rightarrow \infty} N^{-1} \log \sum_{(\lambda)} \exp(-2\beta|\lambda| - \nu(\lambda, \beta)) \quad (2.22)$$

where the sum is over the class of vertical congruence of big contours compatible with $\tilde{\mathcal{M}}_0^{+-}(\Omega, m)$ and where

$$\nu(\lambda, \beta) = \sum_{\substack{X \ni \lambda \\ X \subset \Omega_{\infty, N}}} \phi^T(X). \quad (2.23)$$

To show that the limit (2.22) exist we will prove a weak form of the subadditivity property for the function

$$S_N(\beta) = \log \sum_{(\lambda)} \exp(-2\beta|\lambda| - \nu(\lambda, \beta)). \quad (2.24)$$

We start observing that if $\beta > \bar{\beta}$ the λ appearing in the sum are bounded by $2N$ thanks to the property 1 of the ensemble $\tilde{\mathcal{M}}_0^{+-}(\Omega, m)$. This gives us the possibility of founding a column C in the original lattice Ω_N with the following properties :

(a) The strip of width one immediately to the right of C only contains one horizontal step of λ .

(b) The strip of width $2N^{1/3}$ centered at C contains a portion of λ at most $N^{1/2}$ long.

These properties can be proved as follows. Define N_s and N_m the number of columns with, respectively, intersection simple or multiple with λ . It is easily seen that a multiple column consumes at least 5 units in the length of λ ; at least three step are in fact consumed in the horizontal direction and two in the vertical direction in order to connect the horizontal ones. Hence $5N_m + N_s \leq |\lambda| \leq 2N$ which gives $N_s \geq 3/4N$. This bound, which trivially prove the (a), is essential to prove the (b). Consider now for each simple step the strip of width $2N^{1/3}$ centered at its left end, and let L be the shortest length of λ contained in any of these strips. Let M be the maximal cardinality of a family of disjoint such strips; it is easy to see that if the strips of this family are widened to $4N^{1/3}$ their union will contain all simple steps. Hence $M \cdot 4N^{1/3} \geq N_s \geq 3/4N$. Moreover, $LM \leq |\lambda| \leq 2N$, so $L \leq 2N/M \leq 11N^{1/3} < N^{1/2}$ if N is large. This prove the (b).

Using the property (a) we can now construct a mapping F which associates to any pair $(\lambda_N, \lambda_{N'})$ coming from $S_N(\beta)$ and $S_{N'}(\beta)$ a $\lambda_{N+N'}$ in $S_{N+N'}(\beta)$; we cut λ_N and $\lambda_{N'}$ at some C_N and $C_{N'}$ as described above and join them together in the given order on a cylinder with circumference $N + N'$ to a closed path $\lambda_{N+N'}$. The property (a) says that the so constructed $\lambda_{N+N'}$ is an allowed contour in $S_{N+N'}(\beta)$. Considering that the mapping F can have a $N \cdot N'$ degeneracy and using the property (b) one can prove ^[3] with cluster expansion techniques that $\nu(\lambda, \beta)$ is weakly additive:

if $\beta > \bar{\beta}$

$$|\nu(\lambda_{N+N'}, \beta) - \nu(\lambda_N, \beta) - \nu(\lambda_{N'}, \beta)| \leq c(N^{1/2} + N'^{1/2}) \quad (2.25)$$

and hence in the same range

$$S_{N+N'}(\beta) = (NN')^{-1} \exp(-c(N^{1/2} + N'^{1/2})) S_N(\beta) S_{N'}(\beta). \quad (2.26)$$

from which the existence of the limit (2.22) immediately follows in the range $\beta > \bar{\beta}$. Using the result in Ref. [15] which establishes the identity of (2.22) and (2.1), our final result became:

if $\beta > \bar{\beta}$

$$\tau = \lim_{N \rightarrow \infty} N^{-1} \log \frac{Z(\mathcal{M}^{+-}(\Omega, m), \beta)}{Z(\mathcal{M}^{++}(\Omega, m^*), \beta)} = -2\beta - \log(\tanh(\beta)). \quad (2.27)$$

2.5 Comments.

The knowledge of the two-dimensional Ising model can be considered one of the most satisfactory in the entire field of statistical mechanics. Our simple result is not intended to add some basic progress to that knowledge: it simply provides further support to the conjecture that in the coexistence phase, i.e. for $\beta \geq \beta_c$ as it has been proved in Ref. [21], it is possible to produce phase separation with the Onsager value for the surface tension.

It can be interesting to compare our result with the one obtained in Ref. [22]. One can find in that reference the elegant theorem which establishes the abstract existence of the limit (2.8) at any value of the temperature simply using duality property and Griffith's inequalities. Our result is in some sense complementary to that one since we have a complete functional control of phase equation in a slightly smaller range.

Conclusions

As explained in the introduction, the present work was motivated by the interest of investigating theories with rigorous perturbative methods in a range of parameters as wide as possible; in this way one can first obtain good estimates for critical parameters and consequently the knowledge of phase equations in a wide phase space range. One underlying problem which emerges directly from this analysis is whether cluster expansions are suitable methods in order to obtain indications on the order of magnitude of critical values for those parameters which control phase transitions.

The analysis done in this thesis gives, in our opinion, some indications which suggest a positive answer to the previous question.

We have in fact obtained, in the examined problem, an estimate from above of the critical beta to within 25%. Our conviction is not based on this percentage which can be or cannot be a satisfactory result according to the context on which it is considered; it rather relies on the fact that we have obtained such a result without drastic changes in the old strategy which was intended only to establish the phase separation phenomenon and the functional dependence of surface tension for large enough beta, no matter how large.

Summing up we have explored only few possibilities for optimization procedures: the general one in the polymer context with the optimization of the norm,

its improvement in the particular contours case in Z^2 , and finally the remake of the series of theorems and lemmas of Ref. [3] trying to obtain better estimates.

A less naive procedure, possibly a subject of further investigations, could be performed giving up the particular Kirkwood-Salsburg type equations considered in our case; they are not, of course, the only possible iterative equations suitable to establish convergence theorems and, may be, one could take advantage considering an entire class of them with the appropriate norms and finally take the best.

Since the first application of cluster expansion methods many weak points have been pointed out, and many attempts have been done to find alternative ways to obtain the same results [23,24]. This dissatisfaction, actually not commonly accepted, is relative to the fact that while both the problems treated and the results obtained have a clear physical meaning the intermediate steps have not and also to the fact that the entire cluster expansion technique seems a very cumbersome machinery.

Without enter in the details of this debate we observe only that up to now, in spite of the fact that some of the alternative ways to cluster expansion avoid the mentioned problems, the power and the generality of this technique have not yet been reached by none of them.

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