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Rigorous bounds for 2D disordered Ising models

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Résumé. — Nous développons une méthode améliorant de façon systématique les bornes recuites (pour l'énergie libre et l'état fondamental) et l'appliquons aux modèles d'Ising désordonnés. Cette méthode prend en compte les effets géométriques de frustration et conduit, à la suite d'un procédé d'optimisation, à des bornes dont le comportement critique diffère de celui du modèle pur. Les lignes critiques déduites de cette étude s'avèrent être des expressions algébriques simples en accord remarquable avec les résultats exacts déjà connus.

Abstract. — A method systematically improving the annealed bounds (for the free energy and the ground state energy) is presented and illustrated by the example of disordered Ising models. An optimization procedure leads to new bounds for which the critical behaviour differs from the pure model behaviour. Geometrical effects, such as frustration, can also be included in this method. We obtain simple expressions for the critical lines which agree remarkably well with previously known exact results.

1. Introduction.

Because of the complexity of the disordered systems it is natural to develop methods which use as much as possible the known results available for pure models, with, of course, a special emphasis on the exact results. Apart from very few exceptions, the analytical approaches for two (or more than two) finite dimensional models are either rigorous inequalities or approximation schemes whose validity is difficult to judge. It is the aim of this paper to present a method in which those two aspects are combined.

This method applies to all disordered systems once an exact solution is available for the corresponding pure model (even on a restricted region of the parameter space). Here, we apply it to two 2D disordered Ising models : the dilute bond model and the spin glass model.

A relevant quantity for these problems is the quenched average $\langle \ln Z \rangle$ of the logarithm of the partition function. The well-known annealed bound for this quantity follows from the convexity of the

logarithm

$$\langle \ln Z \rangle \leq \ln \langle Z \rangle. \quad (1)$$

This « simple annealed » bound is certainly also a good approximation of the true free energy in the high temperature region. However, since it amounts to replacing the high temperature variables $\tanh(\beta J_{ij})$ by their mean values, one cannot expect a critical behaviour different from the pure model one. Furthermore such an approximation scheme does not take into account some essential physical effects (such as frustration [1]) which become relevant at low temperatures.

Our method is a systematic improvement of the annealed scheme leading to rigorous bounds which have the two following properties :

- i) a « bootstrap type » optimization process leads to a modification of the critical behaviour which amounts to a Fisher renormalization [2] of the exponents ;
- ii) geometrical effects are explicitly taken into

account (such as frustration on a plaquette in the spin glass case).

2. Method.

Let us consider an elementary cell α of the lattice (which can be a single bond, a plaquette or any bigger pattern) and denote by W_α its associated Boltzmann weight. For a fixed configuration of bonds, the partition function reads :

$$Z[\{J_{ij}\}] = \sum_{\{\sigma\}} \prod_{\alpha} W_{\alpha}[\{J_{ij}\}]. \quad (2)$$

The usual annealed approximation (1) amounts to choosing a single bond as elementary cell α and to replace W_α by its mean value $\langle W_\alpha \rangle$.

Let us introduce an arbitrary positive function $f(\{J_{ij}^{(\alpha)}\})$ of all the bonds which lie in the elementary cell, being the same for all the cells. One can write :

$$\ln Z = - \sum_{\alpha} \ln f[\{J_{ij}^{\alpha}\}] + \ln \sum_{\{\sigma\}} \prod_{\alpha} f W_{\alpha}. \quad (3)$$

The Boltzmann weight for each cell has thus been replaced by $f W_\alpha$. Now one can obtain an upper bound on $\langle \ln Z \rangle$ by exactly averaging the first term in the sum and using the annealed procedure for the new weight $f W_\alpha$:

$$- N_{\alpha} \langle \ln f \rangle + \ln \sum_{\{\sigma\}} \prod_{\alpha} \langle f W_{\alpha} \rangle \quad (4)$$

where N_{α} is the number of elementary cells α .

This upper bound, that we denote by $\ln Z_f$, depends on the particular choice for the function f . The best of all these bounds is given by :

$$\langle \ln Z \rangle \leq \min_{\{f\}} \ln Z_f \quad (5)$$

where the minimum is taken over all positive functions. In this bound the original disordered model has been replaced by a pure one, with an effective Boltzmann weight $\langle f W_{\alpha} \rangle$. This method can be used in practice whenever some exact piece of information can be found for this new pure model. In this respect the choice of function f can be restricted in order to keep, or make, the model solvable.

To be explicit we now illustrate these general ideas by the example of the random bond Ising model on the triangular lattice, with a probability distribution $P(J_{ij})$ of the couplings. We introduce three different types of rigorous bounds, corresponding to different choices for α and f .

2.1 TYPE-I BOUND. — In this case one chooses each bond J_{ij} to be the elementary cell α , which is the simplest possible choice. W then reads :

$$W = e^{\beta J_{ij} \sigma_i \sigma_j}. \quad (6)$$

The optimized bound is then given by (5) with

$$\frac{1}{N} \ln Z_f = \ln 2 - 3 \langle \ln f \rangle + 3 \ln \langle f c \rangle + F_1\left(\frac{\langle t f c \rangle}{\langle f c \rangle}\right) \quad (7)$$

where $t = \tanh \beta J_{ij}$ and $c = \cosh \beta J_{ij}$ and we have suppressed the indices i, j when not explicitly needed. $F_1(\tau)$ is a function which can be deduced from the Onsager-Houtappel [3] solution of the triangular Ising model

$$F_1(\tau) = \frac{1}{8 \pi^2} \int_0^{2\pi} \int_0^{2\pi} dq_1 dq_2 \ln [(1 + \tau^2)^3 + 8 \tau^3 - 2 \tau (1 - \tau^2)^2 (\cos q_1 + \cos q_2 + \cos (q_1 + q_2))]. \quad (8)$$

In the particular case where $P(J_{ij})$ takes only two values :

$$P(J_{ij}) = p \delta(J_{ij} - J) + (1 - p) \delta(J_{ij} + J) \quad (\text{spin glass}) \quad (9a)$$

$$P(J_{ij}) = p \delta(J_{ij} - J) + (1 - p) \delta(J_{ij}) \quad (\text{dilute model}) \quad (9b)$$

one can always choose the function f to be :

$$f(J_{ij}) = \begin{cases} 1 & \text{if } J_{ij} = J \\ \lambda & \text{otherwise.} \end{cases} \quad (10)$$

Minimization with respect to f simply amounts to fixing λ by :

$$\left. \frac{\partial}{\partial \lambda} \ln Z_f \right|_{\lambda=\lambda^*} = 0 \quad (11)$$

the optimized bound (7) being $\ln Z_f$ taken for this value λ^* of λ . We thus see that we make use of the exact solution of the pure model, both to determine the optimum value λ^* of λ and to compute the bound itself, using λ^* . The equation of the critical variety for this bound is simply given by :

$$\left. \frac{\langle t f c \rangle}{\langle f c \rangle} \right|_{\lambda=\lambda^*} = t_c \quad (12)$$

where t_c is the critical value of the pure model ($t_c = 2 - \sqrt{3}$ for the triangular lattice). A straightforward calculation shows that this « bootstrap » procedure modifies the original critical behaviour of the pure model (logarithmic singularity) into a cusplike behaviour. More generally, for a pure model with a non-zero exponent α , the thermal exponent of the optimized bound is :

$$\alpha' = - \frac{\alpha}{1 - \alpha} \quad (< 0 \text{ in general}). \quad (13)$$

This is precisely a Fisher-type renormalization in the presence of an external constraint.

This last result is reminiscent of the approximations of the spin glass problem developed by Syozi [4]. In this approach, one treats on the same footing the thermodynamical and disordered averages, by introducing a grand partition function Ξ which depends on the temperature and on some chemical potential μ . The mean concentration p of bonds $J_{ij} = J$ is then determined as :

$$p = \frac{\partial \ln \Xi}{\partial \mu}. \quad (14)$$

We notice that in the particular cases of binary probability distribution (9), where the function f reduces to a single parameter λ , equation (11) is somewhat similar to (14) (λ playing the role of μ).

However, let us point out the following differences with Syozi-type effective medium approaches :

i) for continuous probability distribution, instead of a minimization with respect to a single variable (chemical potential), we minimize in a whole functional space ;

ii) our method is a *controlled* approximation scheme in the sense that we obtain *rigorous bounds* on the free energy.

2.2 TYPE-II BOUND. — We now choose the hatched triangle depicted in figure 1 as the elementary cell α . The Boltzmann weight associated with each cell α can be written as :

$$W_\alpha = \phi(1 + \tau_1 \sigma_2 \sigma_3 + \tau_2 \sigma_1 \sigma_3 + \tau_3 \sigma_2 \sigma_1) \quad (15)$$

where

$$\phi = c_1 c_2 c_3 (1 + t_1 t_2 t_3)$$

$$\tau_i = \frac{t_i + t_j t_k}{1 + t_i t_j t_k}$$

with $t_i = \tanh \beta J_i$ (see Fig. 1).

Fig. 1. — The three coupling constants and the elementary cell of the anisotropic triangular Ising model.

For this type-II bound, we do not use any optimization scheme but make a particular choice for f , which is naturally suggested by equation (15), namely $f = \phi^{-1}$. The remarkable point is that averaging the new Boltzmann weight $\langle f W \rangle$ still leads to an exactly solvable model for the triangular case. This leads to :

$$\frac{\langle \ln Z \rangle}{N} \leq \ln 2 + \langle \ln \phi \rangle + F_2(\langle \tau_i \rangle) \quad (16)$$

where F_2 has a very simple expression in terms of the τ_i variables [5] (all the $\langle \tau_i \rangle$ are equal) :

$$F_2(\tau) = \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} dq_1 dq_2 \ln [1 + 3\tau^2 + 2\tau(\tau - 1)(\cos q_1 + \cos q_2 + \cos(q_1 + q_2))] \quad (17)$$

The critical variety for (16) is :

$$\langle \tau_i \rangle = 1/3 \quad (18)$$

and the critical behaviour for this type-II bound is, of course, the same as the pure one.

Clearly, this bound is not only simple to obtain, but is also well suited to take frustration effects inside each elementary cell into account. Indeed the dominant high temperature contribution of each elementary plaquette $\langle \ln \phi \rangle$ is averaged exactly (however, correlations effects between different frustrated plaquettes are ignored).

2.3 TYPE-III BOUNDS. — Type-III approximation generalizes both types I and II : in the case of spin glasses, it takes account of the frustration of each elementary cell in an optimal way.

The arbitrary function $f(\tau_1, \tau_2, \tau_3)$ now depends on the three couplings of an elementary triangle. In Z_f is still an exactly anisotropic solvable model :

$$\frac{\ln Z_f}{N} = -\ln 2 + \langle \ln \phi \rangle - \langle \ln f\phi \rangle + \ln \langle f\phi \rangle + F_2\left(\frac{\langle f\phi\tau_1 \rangle}{\langle f\phi \rangle}, \frac{\langle f\phi\tau_2 \rangle}{\langle f\phi \rangle}, \frac{\langle f\phi\tau_3 \rangle}{\langle f\phi \rangle}\right) \quad (19)$$

where F_2 is the anisotropic version of (17) (see [5]) :

$$F_2(\tau_1, \tau_2, \tau_3) = \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} dq_1 dq_2 \ln (1 + \tau_1^2 + \tau_2^2 + \tau_3^2 + 2(\tau_3 \tau_2 - \tau_1) \cos q_1 + 2(\tau_1 \tau_3 - \tau_2) \cos q_2 + 2(\tau_1 \tau_2 - \tau_3) \cos(q_1 + q_2)). \quad (20)$$

Minimization with respect to f can be achieved by a functional derivation of $\ln Z_f$. This leads to the following simple (and symmetric) function, at the minimum :

$$f\phi = \frac{1}{\gamma + \delta(\tau_1 + \tau_2 + \tau_3)} \quad (21)$$

where γ, δ are given by the relation :

$$\langle f\phi \rangle = 1 \quad (\text{normalization})$$

$$\delta = \frac{\partial}{\partial \tau_i} F_2 \Big|_{(\langle f\phi\tau_1 \rangle, \langle f\phi\tau_2 \rangle, \langle f\phi\tau_3 \rangle)} \quad (22)$$

and the critical variety is now :

$$\langle f\phi\tau_i \rangle = 1/3. \quad (23)$$

In the high temperature limit $f\phi$ goes to 1 and we recover the type-II bound. The type-III bound is however always better than both type-I and type-II, and has the same critical exponent α' as type-I.

3. Results.

In this section we detail the applications of our 3 types of bounds for dilute Ising models and for Ising $\pm J$ spin glass.

3.1 DILUTE ISING MODEL. — In this case we concentrate on the phase diagram for the binary distribution (9b).

Critical curves for type-I and III approximations are given in figure 2 for the triangular lattice. The two approximations give almost indistinguishable curves, except at very low temperatures (where, as we shall see, type-III only is in agreement with the known exact p_c). Moreover, type-III is extremely close to real space RG calculations [6] or effective medium-type approximations [7].

Exact results available for this critical curve are the following [8] :

i) in the low temperature limit, p_c is the threshold of the percolation problem of the triangular lattice, given by :

$$p_c^3 - 3p_c + 1 = 0 \quad (24a)$$

namely

$$p_c = 2 \sin \frac{\pi}{18} = 0.3473... \quad (24b)$$

The asymptotic behaviour near $p = p_c$ can be obtained exactly from some duality arguments [8] and, in the case of the triangular lattice, is given by :

$$\left. \frac{dT}{dp} \right|_{p=p_c} = - \frac{2 \ln 2}{p_c} = - 3.9917... \quad (25)$$

ii) In the pure limit $p \rightarrow 1$ the critical value is $t_c = 2 - \sqrt{3}$ and the slope is given by [8] :

$$\left. \frac{1}{T_c} \frac{dT_c}{dp} \right|_{p=1} = \frac{12}{11} \frac{3\sqrt{3} - 4}{\ln 3} = 1.1878. \quad (26)$$

The observed agreement with numerical results fully justifies the comparison of the analytical expressions for the type-III critical curve with this exact

Fig. 2. — The paramagnetic-ferromagnetic (P/F) critical curve for the triangular dilute Ising model in the (p, T) plane, for type I and type III approximations. An enlargement of the low temperature region is also represented.

Fig. 2bis. — The type I P/F curve for the dilute Ising model on the square lattice.

information. Equation (23) reads :

$$\frac{p^3}{3(1+\tau)} + \frac{3p^2(1-p)}{3+a} + \frac{3p(1-p)^2}{3+t} + \frac{(1-p)^3}{3} - \frac{1}{4} = 0 \quad (27)$$

with $\tau = t/1 - t + t^2$ and $a = 2t + t^2$.

Straightforward calculation shows that this equation is in complete agreement with p_c , t_c and the slope $\left. \frac{dp}{dT} \right|_{p=1}$. Equation (27) leads to an asymptotic beha-

viour at low temperatures given by :

$$\left. \frac{dt}{dp} \right|_{p=p_c} \simeq -4.07...$$

The constant is different from the exact one but is very close to it (less than 2 %).

For such an approximation scheme, agreement in the pure limit is not surprising. On the other hand, it is remarkable to notice that equation (27), which was deduced from the exact solution of a free fermion model, completely coincides in the low temperature limit with the equation (24a) which is a consequence of a star triangle relation on the percolation model (or equivalently q -Potts model in the limit $q \rightarrow 1$).

The type-I bound can be extended in a straightforward way to the case of the square lattice. (We display the corresponding critical curve in Fig. 2bis).

$$p = 1 - \frac{1 + \sqrt{2}}{2\sqrt{2}} \left(1 - \frac{\sqrt{2} - 1}{t} \right).$$

This curve also gives the exactly known $p_c = \frac{1}{2}$ and $\left. \frac{dt}{dp} \right|_{p=1} = 8 - 6\sqrt{2}$ slope, and is in remarkable agreement with RG calculations [9].

3.2 $\pm J$ SPIN GLASSES. — We consider now the binary distribution of equation (9a).

3.2.1 Critical varieties. — The critical curves for the triangular Ising model are plotted in figure 3. They correspond to the simple annealed (I), type I, II, III bounds. We have also plotted Nishimori's line where the exact internal energy is known (and

Fig. 3. — The P/F critical curves for the triangular $\pm J$ Ising spin glass in the (p, T) plane, for the simple annealed SA, type (I), types (II), (III) approximations. Nishimori's line N is also represented and the corresponding value for p^* is given.

is not singular [10]) and imposes constraints on the structure of the phase diagram. The type-III critical line is given by

$$\frac{p^3}{3(1+\tau)} + \frac{3p^2(1-p)}{3+b} + \frac{3p(1-p)^2}{3-\tau} + \frac{(1-p)^3}{3(1-b)} = 1 \quad (28)$$

with $b = t/(1+t+t^2)$ and $\tau = t/(1-t+t^2)$. Types I and III are certainly closer to the true ferromagnetic/paramagnetic (F/P) critical curve than the simple annealed and the type-II lines. In the pure limit, types I and III agree with the exact values $t_c = 2 - \sqrt{3}$ and $\left. \frac{1}{T_c} \frac{dT_c}{dp} \right|_{p=1} = \frac{3}{\ln 3}$ [11]. Type-I and -III

curves are very close to each other and differ only in the low temperature regions where the reentrance feature of type-I (already noticed by many authors [4]) is lost when frustration effects are taken into account. Finally, as discussed in [12], a precise location of Nishimori's line should shed some light on the value of p_c . Indeed Nishimori has shown the existence of the following topological constraint for the F/P transition line. Let us consider the intersection point (p^*, t^*) of Nishimori's line and the true F/P line : one has, for the true p_c at $T = 0$,

$$p_c \geq p^*. \quad (29)$$

Fortunately enough, the intersection of Nishimori's line and both types I and III are extremely close so that one can safely estimate the lower bound p^* to be $p^* \simeq 0.8$. On the square lattice the same analysis for type-I bound leads to the lower bound $p^* \simeq 0.87$ on p_c , in good agreement with numerical simulations which give $p_c \simeq 0.9$ [13, 14].

3.2.2 Upper and lower bounds of the quenched free energy. — Our approximation scheme gives a set of better and better lower bounds for the quenched free energy of the triangular random Ising model. We now choose to explicitly display the results in two regions of particular interest in the phase diagram : Nishimori's line and $p = 1/2$.

Restricted to Nishimori's line at $\tanh \beta J = 2p - 1$, there exist two upper bounds that provide a test of the accuracy of the method. Figure 4 gives the different upper and lower bounds for the free energy of the model restricted to Nishimori's line. The two upper bounds are related to the knowledge of the exact internal energy and to the exact calculation of $\ln \langle 1/Z \rangle$, respectively. The lower bounds correspond to the simple annealed and type I, II, III bounds. The true quenched free energy lies in the hatched region. One remarks again that types I and III give rather close results.

Another region of special interest is $p = 1/2$. We display, in figure 5, the lower bounds on the free energy as a function of the temperature for $p = 1/2$. For low temperatures the behaviour of type II is

Fig. 4. — Bounds for the free energy of the triangular Ising model on Nishimori's line as function of p . Lower bounds : simple annealed SA, types (I), (II), (III). Upper bounds : internal energy U (dashed dotted line), and $\ln \langle 1/Z \rangle$ (dashed line). The true free energy lies in the hatched region.

Fig. 5. — Lower bounds on the free energy as a function of the temperature T for $p = 1/2$ (Triangular Ising Model) : simple annealed SA, type II. We also give the bound obtained by considering a bigger pattern made of three hatched triangles.

greatly improved as compared with the « simple annealed » approximation.

3.2.3 Lower bounds on the ground state energy. — As remarked by Vannimenus and Toulouse [14], a lower bound F_A on the free energy provides, at the same time, a lower bound on the ground state energy :

$$E_0(p) \geq \max_T F_A(p, T). \quad (30)$$

Furthermore, a simple counting argument for the frustration of the plaquettes on the triangular lattice gives another lower bound [15] :

$$\frac{E_0(p)}{NJ} \geq -3 + 2(3p^2(1-p) + (1-p)^3). \quad (31)$$

Fig. 6. — Bounds for the ground state energy of the triangular Ising model : the lower bound of Toulouse and Vannimenus (dotted line), the simple annealed SA and type-II lower bounds. Type-III is very close to type (II) and is not represented. We also give the ferromagnetic upper bound E^* .

Figure 6 shows bound (30) for the sample annealed and type-II cases, together with (31). We have also indicated the obvious ferromagnetic upper bound :

$$\frac{E_0(p)}{NJ} \leq -3(2p-1). \quad (32)$$

One remarks that type-II bound has two different regimes :

- i) for low frustration ($p \gtrsim 0.8$) the maximum value of the free energy is reached at $T = 0$ and (30) coincides exactly with (31);
- ii) for higher frustration ($0.2 \leq p \leq 0.8$) the temperature for which the maximum is reached in (30) changes abruptly so that type-II bound splits off from (31) when (31) becomes worse than the simple annealed bound.

Here again the entropy of this bound remains positive for p not too far from 0 or 1. This is in contrast with the simple annealed approximation and in this region this could provide an approximation of the ground state entropy.

4. Comments and speculations.

It has been shown that the usual annealed bound can be efficiently improved by using a simple systematic optimization scheme and by including geometrical effects (such as frustration effects).

For the dilute Ising model, for instance, simple algebraic expressions are obtained for the critical curves which are in remarkable agreement with both known exact results and available simulations.

The leading idea was to make the maximum use of exact information available on pure models in

order to get rigorous bounds for the corresponding disordered model. Here we have dealt with the situation where the pure case is an *integrable* model.

This idea can be easily generalized : let us suppose for example that some exact information is available only on a submanifold of the parameter space (partition function on the critical variety and disorder variety of the two-dimensional pure Potts model, $\langle 1/Z \rangle$ on Nishimori's line for Ising spin glass and Potts glass [12]). It is then possible, using the function f , introduced above by (3), to bring the effective parameters back on this submanifold and thus to obtain an exact bound on the free energy.

As an illustration of these ideas, one can make use of the upper bound recently derived [12] for the free energy restricted to Nishimori's line. One can extend this bound in the whole parameter space, to get for

the binary distribution (9a) :

$$F \leq T(N_L - N) \ln 2 + N_L(1 - 2p)J + TN_L((1 - p) \ln(1 - p) + p \ln p). \quad (33)$$

Moreover these ideas could also apply when only numerical data are available (Monte Carlo simulations, ...). Another field of application for such an idea is the estimation of the Lyapounov exponent of a product of random matrices [16].

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