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How (super) rough is the glassy phase of a crystalline surface with a disordered substrate?

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Abstract. We discuss the behaviour of a crystalline surface with a disordered substrate. We focus on the possible existence of a *super-rough* glassy phase, with height–height correlation functions which vary as the square logarithm of the distance. With numerical simulations we establish the presence of such a behaviour, that does not seem to be connected to finite-size effects. We comment on the variational approach, and suggest that a more general extension of the method could be needed to fully explain the behaviour of the model.

1. Introduction

Recently two letters [1, 2] (and a related comment [2]) have stressed, by obtaining new numerical results, the interest of a problem that can be described in the first instance as that of the surface of a crystal deposited on a disordered substrate.

The model has a long history. Renormalization-group ideas were applied at first [3–5], while more recently the Mézard and Parisi [6] variational approximation has lead to the drawing of a quite different picture [7–9].

The relevant universality class describes many and different physical situations. The first one, which we have already quoted, is the model of a crystal deposited on a disordered substrate. A second one is a two-dimensional array of flux lines with the magnetic field parallel to the superconducting plane in the presence of random pinning. Close to the phase transition (whose existence is predicted by renormalization-group and variational theory) the two models are expected to have the same critical behaviour. The universality class is that of the 2D Sine–Gordon model with random phases.

Let us define our system. The dynamical variables of the model are the integral displacements $d(x, y)$ of the surface from a disordered bidimensional substrate. The variables x and y take integral values from 1 to L. The number of points of the lattice is $S = L^2$. The displacements $d(x, y)$ take positive, negative or zero integral values. The disordered substrate is characterized by quenched random heights $\rho(x, y)$ in the range $(-\frac{a}{2}, +\frac{a}{2})$, where a is the elementary step of the surface columns (and will be 1 in the numerical simulations). The total height of the surface on the elementary (x, y) square is

$$h(x, y) \equiv ad(x, y) + \rho(x, y). \tag{1}$$

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The Hamiltonian of the system is

$$H \equiv \frac{\kappa}{2} \sum_{x,y=0}^{L} \left[(h(x,y) - h(x+1,y))^2 + (h(x,y) - h(x,y+1))^2 \right] \tag{2}$$

where, in the numerical simulations, we will put the surface tension κ equal to 2. The partition function will be defined as

$$Z_\rho \equiv \sum_{\{d(x,y)\}} \mathrm{e}^{-\beta H} . \tag{3}$$

We will consider a quenched substrate, i.e. the free energy F will be defined as

$$F \equiv -\overline{\log Z_\rho} . \tag{4}$$

Here we will mainly discuss the height–height correlation function, which we define as

$$C(d) = \left\langle \left(h(\vec{r}_0 + \vec{d}) - h(\vec{r}_0) \right)^2 \right\rangle \tag{5}$$

where we only take the two-dimensional vector $\vec{d}$ of the form $(d, 0)$ or $(0, d)$, and by $\langle \cdot \rangle$ we denote collectively the average over the different realizations of the noise, over the different origins and the thermal average.

In the Gaussian model with integral variables and no disorder, the surface is rough for $T > T_R$ [10]. In the warm phase the $C(d)$ of (5) behaves as $\log(d)$. When $T < T_R$ the surface becomes flat, glued to the ordered bulk.

When one considers the case of a disordered substrate the situation is far less easy to analyse. The traditional approach to the problem is the one based on renormalization-group ideas, while only recently the variational approximation approach by Mézard and Parisi [6] has been applied to the problem. The results one obtains in the two approaches have something in common. Both approaches find that there is a transition at $T = T_R = \frac{\kappa}{\pi}$. In the high-$T$ phase thermal fluctuations make the quenched disorder irrelevant, and the systems behaves as the pure model. Here correlations behave logarithmically, i.e.

$$C_{T>T_R}(d) \simeq \frac{T}{\kappa\pi} \log(d) . \tag{6}$$

The differences come for $T < T_R$. In the renormalization-group approach [3–5] one gets a new $\log^2 d$ dominant contribution. Here one finds that

$$C^{(RG)}_{T<T_R}(d) \simeq a_1 \log(d) + a_2 \log^2 d \tag{7}$$

where a_1 is non-universal, and a_2 is

$$a_2 \equiv \left(\frac{T_R - T}{T_R} \right)^2 \frac{2}{\pi^2} . \tag{8}$$

The presence of such a *super-rough* phase (where by super-rough we imply a $\log^2 d$ behaviour of the height–height correlation functions) is indeed an interesting potential implication of the presence of quenched disorder. Such a behaviour would imply that the low-T phase is rougher than the high-T phase, which is quite unusual. At high T, thermal fluctuations are able to carry the surface away from the deep (but not deep enough) potential wells due to the quenched disorder. So the roughening is the same as for the pure model. At low T the surface gets glued to the bulk. In the ordered case this makes the surface smooth, since the bulk is ordered. But in the presence of the quenched disordered substrate this effect does not smooth the surface, but, on the contrary, forces it to follow a very rough potential landscape. This mechanism could force a super-rough behaviour.

The application of the variational approximation [6] to this system [7–9] does not lead to the presence of a $\log^2 d$ term, but to a behaviour similar to the one of the high-T phase, with a slope of the logarithmic term which freezes at the critical point

$$C^{(VAR)}_{T<T_R}(d) \simeq \frac{T_R}{\kappa\pi}\log(d)\,. \tag{9}$$

In section 3 we will try to argue that in some sense this is an intrinsic limit of a too straightforward application of the variational approximation (originally discussed for systems with continuous replica-symmetry breaking [6]) to systems with a single-step broken replica symmetry, and we will suggest that a more complex approach could be needed in order to get a fair picture of this kind of system.

A numerical analysis of [2, 1] made the mystery even greater. Systems which should belong to the same universality class seem to show a very different behaviour. Reference [2] was unable to detect any signature of the glass transition when measuring static quantities in a continuum random phase model, which, as we mentioned, should belong to the same universality class of our discrete model (but see the comment [2]). The authors of [1] study the model we have defined before, and numerically seem to detect a picture compatible with the variational ansatz. The approach suggested from Cule and Shapir seemed to us interesting, and worth pursuing further. It has motivated us to run further simulations and more analysis of the numerical data, and to look more closely at the theoretical problem of selecting the correct analytic approach.

2. Numerical simulations

We have run our numerical simulations on the APE parallel computer [11]. Our code, written in a high level language and very elementary, ran at 20% of the theoretical maximal speed. The clear limit was the memory to floating point unit bandwidth, which our way of writing the problem was limiting us to 25% of the theoretical efficiency. It would surely be possible, and not very difficult, to rewrite the code to obtain an efficiency close to 50%. Our code was running at a sustained performance close to one Gflops on an APE *tube* (with a theoretical optimal performance close to 5 Gflops).

Our program was truly parallel, in the sense that each lattice was divided among many processors. For example, on an APE *tube*, which has 128 processors arranged in a three-dimensional tubular shape of $2 \times 2 \times 32$ we were running a single lattice on four processors, and we were running in parallel 32 different random substrates in the third processor direction. With this approach the smallest lattice we could simulate is 4×4. Our actual runs have all been using $L = 64$ and $L = 128$, simulating 256 different substrate realizations and by evolving two uncoupled replicas of the system in each random substrate (with a total of 512 systems). The average over the disorder was taken over 256 such realizations of the random quenched substrate.

We have started from a high value of T, running simulations for decreasing T values. For $L = 128$ we have used temperatures of 0.9, 0.8, 0.7, 0.65, 0.6, 0.45 and 0.35, while for $L = 64$ we have used the values 1.0, 0.95, 0.9, 0.85, 0.8, 0.75, 0.7, 0.65, 0.6, 0.55, 0.50, 0.45, 0.40, 0.35 and 0.30. At each T value our run started from the last configuration of the higher T value. We have been very conservative in requesting a long thermalization. At each T value we have added for $L = 64$ 0.5 million full Monte Carlo sweeps of the lattice (0.7 million for $L = 128$), and then we measured the correlation functions 100 times during 100 000 further lattice sweeps. That turned out to guarantee a good statistical determination of the correlation functions. To check in more detail we have chosen two T values, one in

the warm phase and one in the cold phase, i.e. $T = 0.60$ and $T = 0.35$ for $L = 64$. On this lattice, starting from the final configurations, we have first added a series of 100 000 more lattice sweeps, and measured expectation values again. Then we have repeated the procedure (all the measurements and the statistical analysis) by doubling the added run (i.e. with 200 000 added sweeps), and by doubling it again (with 400 000 added sweeps), and again (with 800 000 added sweeps). For both T values all results were compatible, and no transient effects were detected. The data points for the $L = 128$ are always very similar to the ones on the smaller lattice, in all our range of temperatures. The dynamics was a simple Metropolis Monte Carlo simulation.

Let us note that all our numerical data are fully compatible (even if based on larger lattices and better statistics), as far as we have been able to check, with the data of [1]. What differs here is the analysis of the data, and the fact that a more extensive data sample allows us to look in better detail at the relevant quantities. Here we will detect a small effect, and the high statistics we have is crucial to being sure it is significant. We stress the importance of comparing the full set of correlation functions, at all distances, with the lattice form computed on the same value of the lattice size L. We also believe it is important to use the discrete form both for picking up the logarithmic behaviour and for picking up the super-rough behaviour which is dominated by a squared logarithm.

The lattice Gaussian propagator, which reproduces, in the continuum limit, the logarithmic behaviour, is

$$P_L(d) \equiv \frac{1}{2L^2} \sum_{n_1=1}^{L-1} \sum_{n_2=0}^{L-1} \frac{1 - \cos\left(\frac{2\pi d n_1}{L}\right)}{2 - \cos\left(\frac{2\pi n_1}{L}\right) - \cos\left(\frac{2\pi n_2}{L}\right)} \simeq_{L \gg 1} \frac{\log(d)}{2\pi} . \tag{10}$$

As we have already stressed we also need a lattice transcription of the squared logarithmic term. It is natural to take

$$P_L^{(2)}(d) \equiv P_L(d)^2 . \tag{11}$$

These are indeed the terms we have used to fit our numerical data and to try to distinguish a logarithmic behaviour from a different asymptotic law.

In the following we will be comparing two possible behaviours of the correlation function $C(d)$. One is the Gaussian scaling

$$C(d) = a_0 + a_1 P_L(d) \tag{12}$$

while the second includes a quadratic term, i.e.

$$C(d) = a_0 + a_1 P_L(d) + a_2 P_L^{(2)} . \tag{13}$$

We stress that we are using the form (13) (and specifically we choose $P_L^{(2)}$ for describing the lattice squared logarithmic dependence) as an educated, reasonable guess, and that it does not originate from an analytic calculation. The three coefficients depend on T.

In the high-T phase, the Gaussian fit to the correct lattice propagator is very successful, and the non-Gaussian best fit gives a nonlinear contribution compatible with zero. In this region we do not encounter any problem.

In the following we will discuss the low-T region, and we will use as an example the temperature $T = 0.45$. In figure 1 we plot the measured correlation function $C(d)$ versus the lattice Gaussian propagator, at $T = 0.45$ on a lattice of size $L = 128$. A linear fit looks quite satisfactory at this level. The discrepancy at short distances is not necessarily worrying, since we expect short distance modifications to the asymptotic behaviour. We note for future comparison that here the best fit gives

$$C_{(linear)}^{(all\ points)}(d) = -0.02 + 0.62 P_L(d) \tag{14}$$

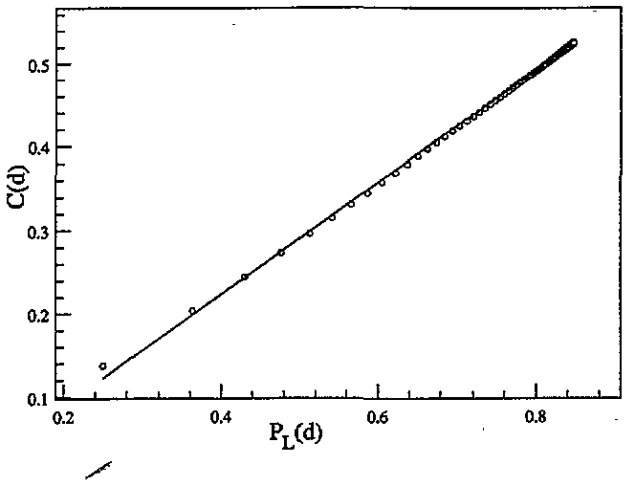

Figure 1. The measured correlation function $C(d)$ versus the lattice Gaussian propagator, at $T \approx 0.45$ on a lattice of size $L = 128$. The straight line is our best fit to a linear behaviour, by using all distance data points.

by using all data points in the fit. Let us now note that in this fit and in all the following except for the quadratic one (equation (17)) the errors (which we have estimated by a jack-knife approach) are very small, of the order or smaller than one per cent. All the best fits have been found to be exact minimization of the χ^2 function, since in all cases it is quadratic in the parameters. The estimated linear coefficient is exactly what one finds in the variational approach (since the lattice propagator is equal, in the continuum limit, to (constant $+ \frac{1}{2\pi}\log(r)$)). A quadratic fit works very well here, but since it has one more parameter than the linear fit let us ignore this fact for a moment. The quadratic fit of (17), with three free parameters and discarding 10 distance points, has, on the contrary, a very large error, but we report it for the indications it gives about the reliability of the value we quote for the quadratic coefficient (see the following discussion). Fitting including distance points starting, for example, from $d = 4$ would give an accurate determination of all parameters.

As a next step in figure 2 we plot $C(d)$ divided by the lattice propagator $P_L(d)$ as a function of $P_L(d)$. Linearity of this quantity as a function of $P_L(d)$ implies the presence of a $\log^2$ term in $C(d)$. The effect is very clear, and the evidence for the presence of such a contribution is unambiguous. We find here that

$$\left(\frac{C(d)}{P_L(d)}\right)^{(all\ points)}_{(linear)} = 0.52 + 0.12 P_L(d) \tag{15}$$

again by using data points from all distances.

The only concern we are left with is that in the previous analysis we have used all distance points, while we are trying to resolve a long distance behaviour. We have to be careful not to be mislead by short distance artifacts, which could obscure the true long distance behaviour. In order to play safe, in figure 3 we plot both $C(d)$ and $\frac{C(d)}{P_L(d)}$ as a function of $P_L(d)$ for distances larger than 10 lattice units, and our best fits are done using only these distance points. In this case we fit $C(d)$ both to the linear and to the quadratic form. We get

$$C^{(d>10)}_{(linear)}(d) = -0.06 + 0.69 P_L(d) \tag{16}$$

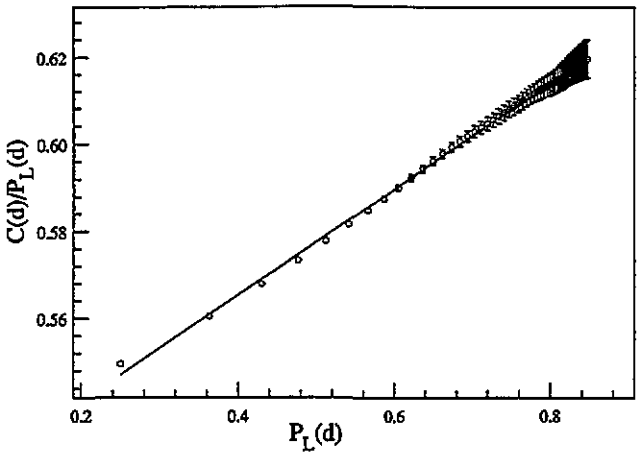

Figure 2. The measured correlation function $C(d)$ divided by the lattice Gaussian propagator versus the lattice Gaussian propagator, at $T = 0.45$ on a lattice of size $L = 128$. The straight line is our best fit to a linear behaviour, by using all distance data points.

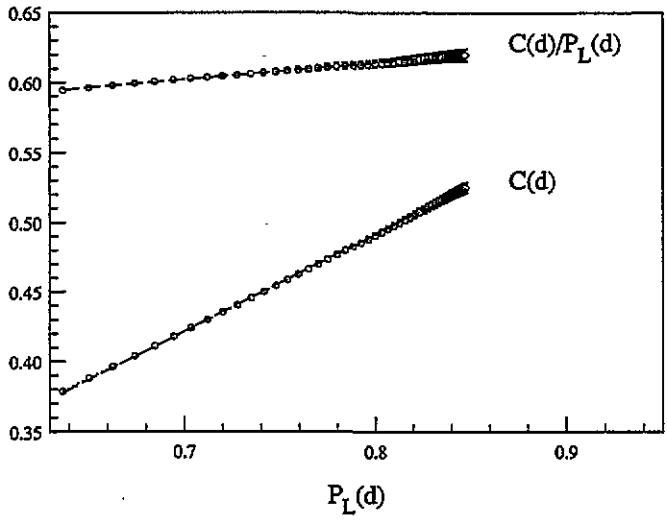

Figure 3. The measured correlation function $C(d)$ and the measured correlation function divided by the lattice Gaussian propagator versus the lattice Gaussian propagator, at $T = 0.45$ on a lattice of size $L = 128$, after discarding the first ten distance points. The straight continuous lines are our best fits to a linear behaviour, while the dotted line is the best fit to a quadratic behaviour of the function $C(d)$.

that is very similar to our previous fit, and

$$C^{(d>10)}_{(quadratic)}(d) = -0.014 + 0.56 P_L(d) + 0.093 P^{(2)}_L(d)\,. \tag{17}$$

The most remarkable result is for the ratio we get

$$\left(\frac{C(d)}{P_L(d)}\right)^{(d>10)}_{(linear)} = (0.52 \pm .01) + (0.12 \pm .02) P_L(d) \tag{18}$$

with a very small χ^2 and in complete agreement with what we got by fitting all data points.

Two comments about two remarkable facts are in order. First, the linear coefficient of the best fit for the ratio is equal to the quadratic coefficient of the best fit for $C(d)$, and the constant coefficient in the ratio fit is equal to the linear coefficient of the quadratic fit to $C(d)$. Second, discarding ten short distance points does not change the results for the linear and the quadratic contribution. We are definitely not looking at a short distance effect. The variational approximation predicts a short to long distance crossover in the coefficient of the logarithmic term. Even if from our numerical simulation we cannot reach conclusions about the short distance region, the same analysis done previously shows that the effect we are measuring is a genuine long distance one, and cannot be exclusively due to this transient behaviour. Let us also notice that the reader could think that since the error on the different points of the divided $C(d)$ of figure 3 are quite large the slope has to be compatible with zero. This is not true since the data points (different correlation functions for different d values) are highly correlated, and the error over the slope has to be estimated directly. We have presented evidence that the value of the slope is non-zero.

The fit to the form (13) gives a very good result both in the warm phase (where it coincides with the Gaussian fit) and in the cold phase. The presence of a lattice term corresponding to a continuum $\log^2 d$ behaviour accounts very well for our numerical data. In figure 4 we show the coefficients a_1 and a_2 from our best fits in all the temperature range we have explored (here we use all distance points). The full curves are only a visual aid, smoothly joining the numerical data points. The coefficient of the nonlinear term $P_L^{(2)}$ becomes sizeably different from zero close to the critical temperature $T_c = \frac{2}{\pi}$. The effect is quite clear and convincing. The coefficient a_1 is not the one of the $\log(d)$ term in the continuum limit, that is renormalized by a contribution coming from the $P_L^{(2)}(d)$ term. We find that the coefficient of the continuum $\log^2$ term is in the order of 5 times smaller than the universal value we would expect from the RG computations. This is a fact that will have to be understood in better detail. The linear dependence of a_1 over T with the correct coefficient in the high-T phase, where $a_2 = 0$, is very clear.

We believe that the previous evidence clearly shows that the ansatz of a purely Gaussian

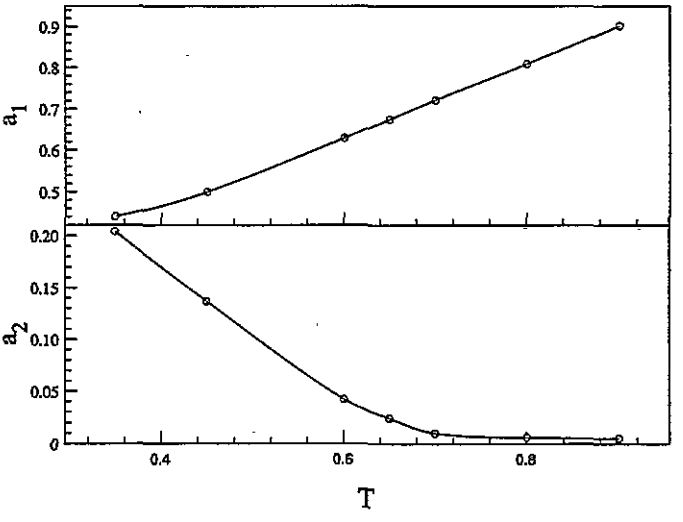

Figure 4. The coefficients a_1 and a_2 from our best fits to the form (13) versus the temperature T in all the temperature range we have explored. Here $L = 128$. Results for $L = 64$ (not shown) are very similar.

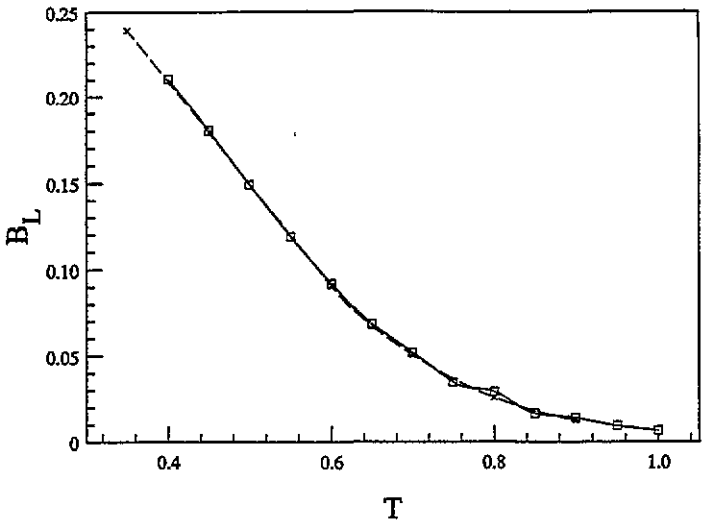

Figure 5. The Binder parameter $B_L^{(\Delta)}$ as a function of T for the two values of the lattice size, $L = 64$ and $L = 128$.

probability distribution does not explain the behaviour of the system for $T < T_R$, while the hypothesis of a super-rough phase, with a $\log^2 d$ behaviour of the correlation functions, matches the numerical findings very well. In order to gather more information about this glassy phase we have looked at the probability distribution of

$$\Delta \equiv h - h' \tag{19}$$

where h' is a first neighbour of h. In order to monitor the shape of the probability distribution we plot in figure 5 the related Binder parameter defined as

$$B_L^{(\Delta)}(T) \equiv \frac{1}{2}\left(3 - \frac{\langle \Delta^4 \rangle}{\langle \Delta^2 \rangle^2}\right). \tag{20}$$

B_L is zero for a Gaussian distribution, and 1 for a δ-function. In our measurement it is very small in the warm phase, calling again for a very Gaussian behaviour. On the contrary in the low-T phase we get a non-trivial shape. Here B_L is definitely non-zero, non-one, and in our T range does not seem to depend on L. This again shows that in the cold phase there is a non-trivial behaviour. A value of B_L which is non-trivial (non-0 and non-1) and does not depend on L is reminiscent of a Kosterlitz–Thouless situation. Further analysis will be required to reach a better understanding of the characteristic features of the low-T phase.

3. Some comments on the variational approach

We have already argued that the numerical results presented above do not coincide with the analytical predictions either of the renormalization-group or of the Gaussian variational approach. From the qualitative standpoint, the disagreement is even stronger with the latter since it predicts that the asymptotic correlation function grows only logarithmically with the distance. Consequently, one has a right to wonder how much the Gaussian variational approach is trustworthy. Some general remarks on this issue will be given in this section.

As argued by Mézard and Parisi in their original paper [6], the Gaussian variational theory (GVT) is exact for the theory of an N-component field $\phi(x)$ in the limit $N \to \infty$

(while the model considered in this paper corresponds to $N = 1$). This may be easily understood by noticing that the GVT coincides with the Hartree–Fock partial resummation of the graphs due to the interaction potential between the replicas [6]. If the quenched potential $V(x, \vec{\phi})$ seen at point x by the field $\vec{\phi}$ is itself a Gaussian variable of zero mean and variance $\overline{V(x, \vec{\phi})V(x', \vec{\phi}')} = \delta(x-x')\mathcal{R}(\vec{\phi}-\vec{\phi}')$ that is, with a purely local interaction, then the tadpole contribution to the self-energy $\sigma^{ab}(k)$ between two different replicas a and b will not depend upon the momentum k and will only result in renormalization of the mass term. When the solution of the variational equations turns out to be consistent with a continuously replica broken mass term $\sigma(u)$ (where $0 < u < 1$ is the distance between the replicas), this is not a serious limitation and non-trivial exponents may be found [6, 8, 9], related to the small-u behaviour of $\sigma(u)$. On the contrary, when the solution consists of a finite number of breaking steps as in the present case, there is no such small k-small u crossover, and the full propagator is proportional to the bare propagator at small k (when $\sigma(0) = 0$). This explains why the one-step solution found in [8, 9] necessarily leads to a logarithmic growth of the correlation function which corresponds to the free behaviour, the only non-trivial prediction being the freezing of the coefficient of proportionality under T_R (see equations (6) and (9)). Obviously the fact that the correct solution is the one broken at one step is very non-trivial.

An important example where the Gaussian ansatz leads to erroneous results is the random field Ising model (RFIM). Recently, Mézard and Young proposed a general method of adding momentum-dependent contributions to the self-energy $\sigma^{ab}(k)$ by considering a self-consistent expansion in $1/N$ of the variational free energy [12]. Applying this method to the RFIM, they were able to show that the new graphs at $O(1/N)$ improved the Gaussian ansatz and were sufficient to break the so-called dimensional reduction coming from the usual perturbation theory, and which, of course, held at the Gaussian level. Such an approach could also be used to improve our theoretical understanding of the model studied in this paper. It suffers, however, from a mathematical difficulty related to the absence of solutions $\sigma^{ab}(k)$ with a finite number of steps of breaking, forcing one to look for a fully broken mass $\sigma(k, u)$. So far, no solution has been found in the case of the RFIM and one would probably have to face the same difficulties for the random Sine–Gordon model.

Beyond the quantitative calculation of the critical exponents, an important feature of the GVT is that it leads to a simple determination of the phase diagram of the model studied here. In this respect, the figures 4 and 5 seem to indicate that the distribution of the height differences Δ defined in (19) differs from a Gaussian even at temperatures higher than the usual theoretical prediction $T_R = \frac{\kappa}{\pi}$. As the two curves for the sizes $L = 64$ and $L = 128$ coincide quite well, finite-size effects can apparently not account for this discrepancy. Some preliminary analytical results we have obtained using the GVT above T_R hint at a possible dynamical transition [13] at a temperature T_d ($T_d > T_R$) whose value depends on the amount of disorder given by the variance of the quenched displacement field $d(x, y)$ (see the introduction). If this were so, there would already exist, at the temperature T_d, an exponentially large number (in L^2) of metastable states and the system would only partially 'thermalize' in these traps. Both numerical and analytical work is currently in progress to investigate this important issue.

4. Conclusions

The results we have obtained describe a very complex picture. A super-rough behaviour does indeed seem to exist, implying that the GVT does not fully account for the behaviour

of the model. Here we are discussing very small effects, so we cannot completely exclude that we are not looking at a transient behaviour, but that does not seem likely. On the other hand the coefficient of such a nonlinear term seems to be, far beyond the statistical and systematic error, different from the one obtained with an RG computation. Also, the Binder parameter looks non-trivial even in the beginning of the to-be warm phase (that is maybe not the warm phase yet), suggesting the presence of a complex scenario also for temperatures T on the order of 0.8.

We have argued that from a theoretical viewpoint we have some understanding of what is happening. We hope we will succeed in deepening this understanding in the near future.

Acknowledgments

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Note added. After this work was completed we received an interesting paper by J Kierfeld [14], which discusses the possible replica-symmetry breaking solutions to the renormalization-group equations. The instability of the replica-symmetric solution, noticed in [15], is discussed in the context of a large sector of admissible solutions. In this scenario a non-zero coefficient for the square logarithmic contribution, different from the one predicted by replica-symmetric RG, seems a plausible issue.

Obviously, the fact that the correct solution is a one-step breaking is non-trivial. We would, however, like to underline that dimension $D = 2$ plays a special role in this respect. Both the choice of the interaction potential and the dimension of the space influence the nature of the RSB variational ansatz (either one-step or continuous). It has been found [6] that $D = 2$ is the borderline between the one-step solution and the continuous one and that the crossover between the two regimes is smooth. In other words, when $D \to 2$, the slope of the continuous fully broken solution goes to infinity and the solution becomes one-step like. Therefore, it seems that at $D = 2$ all solutions have either a true one-step or an almost one-step behaviour.

We have also run some numerical simulations in the cold phase with a cold start (in order to be sure we are not measuring effects due to trapping in metastable states visited thanks to the slow cooling). In this way we have reproduced the results discussed in the letter, making clearer the fact that we really have thermalized our system. We thank D Cule and Y Shapir for friendly advice on this matter.

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