

Influence of quenched dilution on the quasi-long-range ordered phase of the 2d XY model

B. Berche^{1,a}, A.I. Fariñas-Sánchez^{1,2}, Yu. Holovatch^{3,4}, and R. Paredes V.²

¹ Laboratoire de Physique des Matériaux, Université Henri Poincaré, Nancy 1, 54506 Vandœuvre les Nancy Cedex, France

² Centro de Física, Instituto Venezolano de Investigaciones Científicas, Apartado 21827, Caracas 1020A, Venezuela

³ Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, 1 Svientsitskii Str., Lviv, 79011 Ukraine

⁴ Ivan Franko National University of Lviv, 12 Drahomanov Str., Lviv, 79005 Ukraine

Received 7 July 2003 / Received in final form 9 September 2003

Published online 28 October 2003 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2003

Abstract. The influence of non magnetic impurities in the 2d XY model is investigated through Monte Carlo (MC) simulations. The general picture of the transition is fully understood from the Harris criterion which predicts that the universality class is unchanged, and the Berezinskii-Kosterlitz-Thouless description of the topological transition remains valid. We nevertheless address here the question about the influence of dilution on the quasi-long-range order at low temperatures. In particular, we study the asymptotic of the pair correlation function and report the MC estimates for the critical exponent η at different dilutions. In the weak dilution region, our MC calculations are further supported by simple spin-wave-like calculations.

PACS. 05.50.+q Lattice theory and statistics (Ising, Potts, etc.) – 64.60.Fr Equilibrium properties near critical points, critical exponents – 75.10.Hk Classical spin models

1 Introduction

From general scaling arguments, the Harris criterion predicts that Gaussian disorder (coupled to the energy density) is an irrelevant perturbation at the fixed point of any pure system when the exponent α which governs the singular behaviour of the specific heat of the pure model in the vicinity of the critical point is negative [1]. The critical behaviour of the random system is thus governed by the pure fixed point and the universality class of the model remains unchanged.

From this point of view, the 2d XY model is probably the one where the influence of quenched disorder is essentially trivial, and nothing special is expected, since it displays a critical behaviour described by essential singularities. On the other hand, the transition of the 2d XY model is not conventional and has very interesting features which make the question of the influence of disorder worth studying. Indeed, the transition, first described by Berezinskii [2] and Kosterlitz and Thouless [3,4], is governed by the condensation of topological defects. The symmetry of the XY model being continuous, there is no spontaneous order in the system (in 2d) at any non zero temperature according to Mermin-Wagner theorem [5,6]. Nevertheless at very low temperatures, the spin-wave approximation which assumes that the disorientation $\theta_{\mathbf{r}} - \theta_{\mathbf{r}+\boldsymbol{\mu}}$ between neighbouring spins ($\boldsymbol{\mu}$ denotes the unit lattice

spacing) remains small, captures the essential features of the behaviour of the system, leading to an algebraic decay of the correlation function [7]

$$\langle \boldsymbol{\sigma}(\mathbf{r}) \cdot \boldsymbol{\sigma}(\mathbf{r} + \mathbf{R}) \rangle \sim |\mathbf{R}|^{-\eta(T)}, \quad (1)$$

(where $\boldsymbol{\sigma}(\mathbf{r})$ are two-component unit vectors), and, as a consequence, to the absence of magnetization and to an infinite susceptibility. The correlation function exponent, $\eta(T)$, continuously increases with temperature. The model is said to have a low temperature phase with *quasi-long-range* order. At *high temperatures* on the other hand, a high temperature series expansion leads to a more conventional exponential decay of the correlation function. It is clear from these two extreme behaviours that something must happen in between and that the model undergoes a transition in the intermediate regime. The scenario proposed by Kosterlitz and Thouless (KT) is based on the existence of vortices, which are localized defects where the field $\theta_{\mathbf{r}}$ (the angle between spin $\boldsymbol{\sigma}(\mathbf{r})$ and some arbitrary reference direction) may become singular at some points. The energy carried by such defects increases logarithmically with the system size, and thus they are constrained to be associated in pairs which nevertheless amplify the disordering of the system, leading to an effective increase of the temperature. The vortices appear in increasing number in the system when the temperature increases, and the transition temperature is reached when the pairs break, leaving the system totally

^a e-mail: berche@lpm.u-nancy.fr

disordered. In the high temperature phase, the approach to the critical point T_c , (also referred to as KT temperature, T_{KT}), is described by essential singularities, for instance, the correlation length and the susceptibility behave as $\xi(t) \sim \exp(-bt^{-\sigma})$, $\chi(t) \sim \xi^{2-\eta}$, $t = |T - T_{KT}|$, with $\eta = \frac{1}{4}$ and $\sigma = \frac{1}{2}$ (for reviews, see e.g. [8–12]).

From the hyperscaling relation $\alpha = 2 - \nu d$, and from the fact that the correlation length has an essential singularity at the critical point, one deduces a non typical value for the exponent of the specific heat, $\alpha = -\infty$, which implies, according to the Harris criterion, that the adjunction of thermal randomness (i.e. coupled to the energy density) does not modify the general scenario described above. All along the transition line, the KT universality class might be recovered (that is an exponent $\eta(T_{KT}) = \frac{1}{4}$ for the correlation function decay). Let us specify the case of site dilution for example. The original Hamiltonian of the pure $2d$ XY model,

$$H_0 = -J \sum_{\mathbf{r}} \sum_{\mu} \boldsymbol{\sigma}(\mathbf{r}) \cdot \boldsymbol{\sigma}(\mathbf{r} + \boldsymbol{\mu}), \quad (2)$$

where $\boldsymbol{\sigma}(\mathbf{r}) \cdot \boldsymbol{\sigma}(\mathbf{r} + \boldsymbol{\mu})$ denotes the scalar product and the spins $\boldsymbol{\sigma}(\mathbf{r})$ are located at the lattice sites \mathbf{r} of a square lattice Λ , is modified by the introduction of a set of occupation variables $c_{\mathbf{r}}$ which take the values 0 (with probability $1-p$) or 1 (with probability p) depending on the fact that site \mathbf{r} is empty or occupied by a spin,

$$\begin{aligned} \mathcal{P}[c_{\mathbf{r}}] &= \prod_{\mathbf{r}} P(c_{\mathbf{r}}) \\ &= \prod_{\mathbf{r}} [p\delta(c_{\mathbf{r}} - 1) + (1-p)\delta(c_{\mathbf{r}})]. \end{aligned} \quad (3)$$

Thus the Hamiltonian of the diluted $2d$ XY model reads:

$$H = -J \sum_{\mathbf{r}} \sum_{\mu} c_{\mathbf{r}} c_{\mathbf{r}+\boldsymbol{\mu}} \boldsymbol{\sigma}(\mathbf{r}) \cdot \boldsymbol{\sigma}(\mathbf{r} + \boldsymbol{\mu}). \quad (4)$$

Altogether, one expects a phase diagram starting from the pure system critical temperature $k_B T_{KT}/J \simeq 0.893$ [13] at $p = 1$, and decreasing up to a transition at zero temperature at the site percolation threshold of the $2d$ square lattice, $p_c \simeq 0.59$, since no transition at all takes place in the system when there is no more percolating cluster of spins. The question which remains interesting is to understand the exact role of the impurities. Of course, the adjunction of impurities would first decrease the transition temperature through the usual dilution effect which, at a mean field approximation decreases the average coordination number. But in the same time, the number of vortices (and thus also their disordering consequences) will possibly decrease. Also their interactions between each other and the interactions between vortices and impurities might play some role. This question has been partly discussed in references [14,15] and we essentially address here the question of the role of impurities at low temperature, where the spin-wave approximation should give reliable results.

2 Determination of the phase diagram of the diluted model

The determination of the phase diagram is performed using a fit of the order parameter profile inside a finite system to the functional expression predicted by a convenient conformal mapping, valid at a scale-invariant critical point. By extension it is also valid in the *whole low-temperature phase* of the XY model which displays scale-invariant algebraic correlation functions. This method has been applied with success to the case of the pure XY model [16–18] and should provide here also reliable results. The order parameter vanishes in the bulk of the system at any temperature in the XY model, unless symmetry breaking fields are applied along some boundaries $\partial\Lambda$ for example. The magnetization profile $\langle \boldsymbol{\sigma}(\mathbf{r}) \cdot \boldsymbol{\sigma}_{\partial\Lambda} \rangle$ thus obeys a general covariance law under conformal transformations. The case of a square geometry with fixed spins along its four edges is particularly easy to implement in Monte Carlo simulations. There, the effect of the Schwarz-Christoffel conformal mapping is just to define a rescaled distance variable, called $\kappa(w)$ (here and in the following, w stands for the complex variable associated to the point \mathbf{r}), in terms of which one recovers inside the square with fixed boundary conditions, a simple power law for the profile:

$$\langle \boldsymbol{\sigma}(w) \cdot \boldsymbol{\sigma}_{\partial\Lambda} \rangle \sim [\kappa(w)]^{-\frac{1}{2}\eta}, \quad (5)$$

with

$$\kappa(w) = \text{Im} \left[\text{sn} \frac{2Kw}{L} \right] \times \left| \text{cn} \frac{2Kw}{L} \text{dn} \frac{2Kw}{L} \right|^{-1/2}. \quad (6)$$

Here, $\text{cn} x$, $\text{dn} x$ and $\text{sn} x$ are the Jacobi elliptic functions [19], L the linear size of the lattice Λ and $K \equiv K(k)$ (the complete elliptic integral of the first kind) and k are constants related to the aspect ratio of the system. For more details, the reader is referred to reference [18]. The main advantage of this technique is that one lattice size is in principle sufficient (provided it is large enough), since the shape effects are included in the conformal mapping and the method is not much sensitive to finite-size effects. The effect of discretization of the lattice is only apparent at the scale of a few lattice spacings. One more advantage is the fact that all the information encoded in the profile is used, since all the points w inside the square are taken into account in the fit. The strategy to obtain the phase diagram is summarised in the following:

i) Perform simulations on a small system (32×32) for several dilutions (from $p = 0.50$ to 1.00 every 0.05) and several temperatures (from $k_B T/J = 0.05$ to 1.25 every 0.05).

ii) Fit the data to equation (5) (from now on, we use the notation $m(w)$ for $\langle \boldsymbol{\sigma}(w) \cdot \boldsymbol{\sigma}_{\partial\Lambda} \rangle$), compute from a least-square fit the sum of deviation squares, χ^2 , per degree of freedom (d.o.f.).

iii) Plot the chi-square per degree of freedom, $\chi^2/\text{d.o.f.}$, as a function of temperature for all dilutions. It should keep a small value (the better the disorder statistics the smaller the expected value) in the scale-invariant

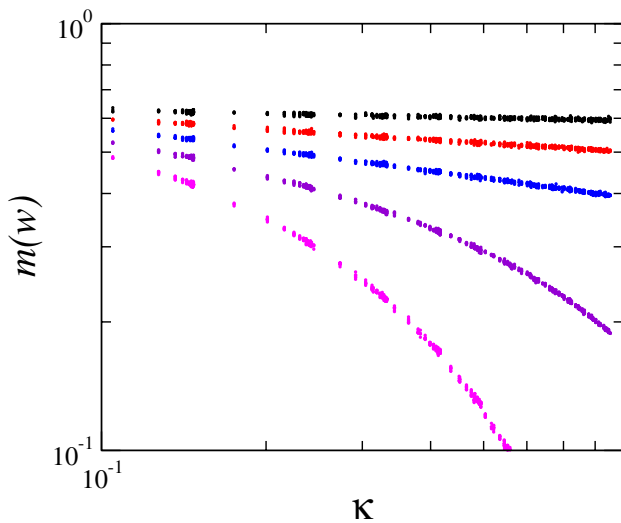


Fig. 1. Order parameter profile for several temperatures ($k_B T/J = 0.1; 0.3; 0.5; 0.7$ and 0.9 from top to bottom) at a dilution $p = 0.80$ as a function of the rescaled variable $\kappa(w)$. The transition is below $k_B T/J = 0.5$.

phase and then increase sharply in the paramagnetic phase where expression (5) is no longer valid.

iv) Report on the phase diagram the temperature where the $\chi^2/d.o.f.$ starts to increase sharply, and which is the estimate of the critical temperature at a given dilution. The results will be refined later when larger lattices will be considered in order to investigate the universality class at the transition.

We may also mention here a few comments about the technical details: we use a Wolff algorithm [20] and each sample is thermalized by 10^4 Wolff iterations, and 10^4 other sweeps are used for computation of the physical quantities. The average over disorder realizations is performed over 10^4 samples. One iteration takes of the order of $1 \mu s$ of CPU time per spin on a standard processor, so one simulation needs around $200 \times L^2$ seconds (and here we have 23 temperatures times 10 dilutions). For more precise estimates to be described later, we also performed simulations for sizes 64×64 (with 4×10^4 samples for disorder average, so one simulation takes $8000 \times L^2$ seconds) and 128×128 (with 2×10^4 samples for disorder average, or $4000 \times L^2$ seconds for one simulation).

In order to illustrate the above mentioned programme, we first show in Figure 1 the behaviour of the order parameter profile for several temperatures at a dilution $p = 0.80$ as a function of the rescaled variable $\kappa(w)$ on a log-log scale. It is particularly clear that the data fit quite nicely to a power law at low temperatures while this type of fit completely breaks down at higher temperatures.

A 3d plot of the χ^2 in the temperature-dilution plane is then presented in Figure 2. For the sake of clarity, a cutoff at 0.5 was introduced in order to avoid too large χ^2 at high temperatures. The low temperature phase with quasi-long-range order extends in the whole region in the (p, T) plane where the χ^2 is close to zero, revealing that equation (5) nicely fits the numerical data. The phase di-

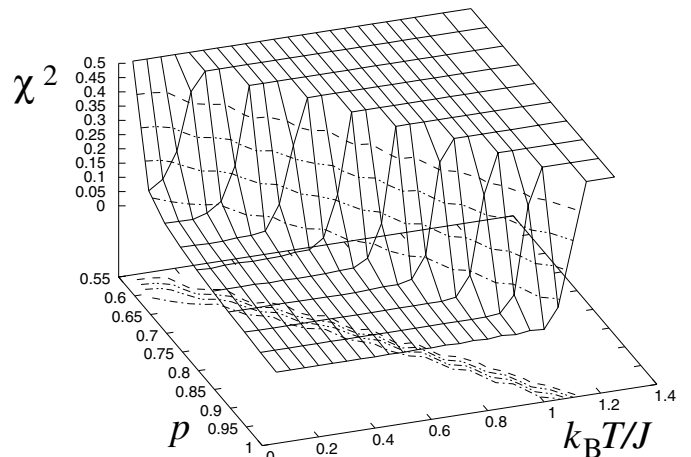


Fig. 2. 3d plot of the χ^2 (to get it per d.o.f., one has to divide by L^2) as a function of temperature and dilution for a system of size 32×32 .

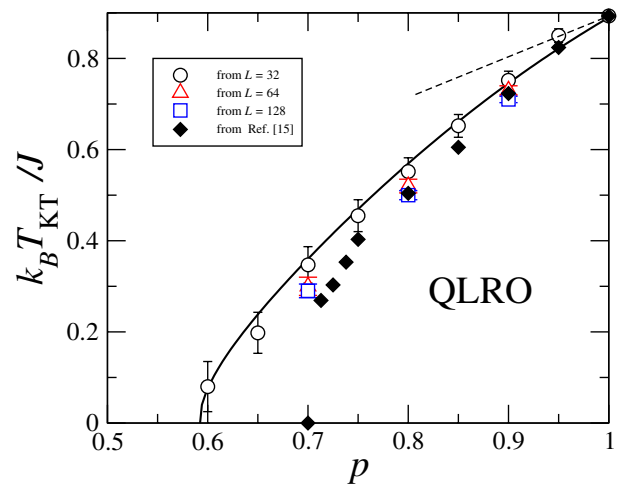


Fig. 3. Phase diagram of the 2d dilute XY model. The data points correspond to the results obtained after fitting the order parameter to the conformal expression. They correspond to the temperature where the χ^2 has a sudden increase. The error bars are estimated empirically. Three different sizes are represented and the solid line is only a guide for the eyes. The full symbols also reported were taken from the work of Leonel et al. [15]. Dashed line shows the mean field prediction.

agram which can be deduced from these data is shown in Figure 3 where the data from larger system sizes are also reported, as well as previous results [15]. As expected, as a result of the influence of dilution, the transition temperature decreases from the pure system value at $p = 1$ and it vanishes at the percolation threshold of site percolation on the square lattice.

A simple standard mean field argument for dilution in the low impurity concentration regime (p close to 1) gives the beginning of the transition line in the vicinity of the pure system. The coordination number z on the lattice with zero impurity concentration becomes pz when only a (small) fraction $1 - p$ of sites is unoccupied (this is of course correct only to leading order in

the close neighbourhood of $p = 1$, since the problem under interest here is *site dilution* and not *bond dilution*) and thus the transition temperature may be estimated by $k_B T_{KT}(p)/J = p k_B T_{KT}(p=1)/J \simeq 0.893p$. This transition curve is shown in dashed line in Figure 3 and fits correctly only the first point at $p = 0.95$.

In the vicinity of the percolation threshold, one would expect that the transition temperature increases with the fraction of sites belonging to the percolating cluster. From this argument a power-law behaviour would follow, $T_c \sim (p - p_c)^{5/36}$, with the exponent of the order parameter in $2d$ percolation (see for example Refs. [21, 22]). We cannot check this behaviour in the present model where we essentially focus on smaller dilutions (p closer to 1) and we did not perform enough simulations close to the percolation threshold.

3 Low temperature behaviour of the diluted XY model

In this section, we address the question of the behaviour of the diluted XY model at low temperatures and of the universality class along the transition line. More precisely, does the spin-wave description provide the correct behaviour at low temperatures in the presence of dilution, and does one recover the Kosterlitz-Thouless universality class at the transition temperature between the phase with quasi-long-range order and the paramagnetic phase?

First of all, in order to bring reliable arguments, we have to produce more precise data at larger sizes to approach the thermodynamic limit. We performed simulations for systems of sizes $L = 64$ and 128 , but only for a few temperatures in the vicinity of the transition (estimated from the previous results for the system of size $L = 32$) and for three dilutions, $p = 0.70, 0.80$ and 0.90 . The data are shown in Figure 4. On the left we plot the η exponent obtained from a least square fit of $\ln m(w)$ vs $\ln \kappa(w)$ and on the right, we show the corresponding $\chi^2/d.o.f.$ The vertical stripe in each figure is a rough estimate of the transition temperature, where η takes its KT value $\frac{1}{4}$ and $\chi^2/d.o.f.$ is at the edge of the plateau region (which means that order parameter density profiles are still fitted by power laws, i.e. the system is still critical). The larger the system size, the smaller the value of T where the $\chi^2/d.o.f.$ increases and the sharper the increase (note the logarithmic scale on the vertical axis). We also notice that the absolute value of the $\chi^2/d.o.f.$ in the quasi-long-range ordered phase is meaningless, since it is strongly dependent on the number of disorder realisations. Here the smaller value is obtained for $L = 64$ where 40000 samples were produced while only 20000 were realized at $L = 128$. The horizontal scale has been chosen identical for all three figures, since it facilitates the comparison and makes obvious the role of dilution.

Let us now discuss the low temperature limit. There, a spin-wave calculation (given in the appendix), based on the assumption that the spin disorientation remains small and allows to expand the cos in the definition of the Hamiltonian, shows that the correlation function exponent is

Table 1. Comparison between the Monte Carlo results and the spin-wave approximation for the $2d$ dilute XY model. The numerical data were obtained by fitting the density profile inside a square of size $L = 128$. For comparison, the results of the spin-wave approximation of the corresponding pure system are also presented.

p	$k_B T/J$	η_{MC}	$\eta_{SW}^{\text{diluted}}$	η_{SW}^{pure}
0.96	0.04	0.007(2)	0.0069	0.0064
--	0.08	0.016(2)	0.0138	0.0127
--	0.12	0.024(2)	0.0208	0.0191
--	0.16	0.032(2)	0.0277	0.0255
0.92	0.04	0.009(2)	0.0076	0.0064
--	0.08	0.018(2)	0.0152	0.0127
--	0.12	0.027(2)	0.0227	0.0191
--	0.16	0.036(2)	0.0303	0.0255
0.88	0.04	0.010(2)	0.0084	0.0064
--	0.08	0.021(2)	0.0168	0.0127
--	0.12	0.032(2)	0.0251	0.0191
--	0.16	0.043(2)	0.0355	0.0255

simply modified by a “rescaling” of temperature due to the presence of the impurities. While the pure model exponent in the spin-wave approximation is given by

$$\eta_{SW}^{\text{pure}} = \frac{k_B T}{2\pi J}, \quad (7)$$

we get in the case of the disordered system

$$\eta_{SW}^{\text{diluted}} = \frac{k_B T}{2\pi J(1 - 2(1 - p))}. \quad (8)$$

Within the spin-wave approximation, the η -exponent still varies linearly with temperature at low temperatures, but as expected, it increases faster in the disordered model. The role of impurities is simply described by an augmented effective temperature. We also note that the value of the coefficient, $k_B/2\pi J(1 - 2(1 - p))$, is not simply obtained from a replacement of the nearest-neighbour coupling J by its average pJ in the low dilution limit.

A comparison with numerical results (in Tab. 1) deduced from Monte Carlo simulations shows that the spin-wave approximation fits correctly the numerical results at very low temperature and low empty sites concentration. It is worth noticing that the numerical data were obtained on a finite system, and that increasing the system size still decreases slightly the resulting exponent (see Fig. 4).

4 Conclusions

We have performed an extensive Monte Carlo study of the critical behaviour in the quasi-long-range ordered phase of the two-dimensional diluted XY model. According to

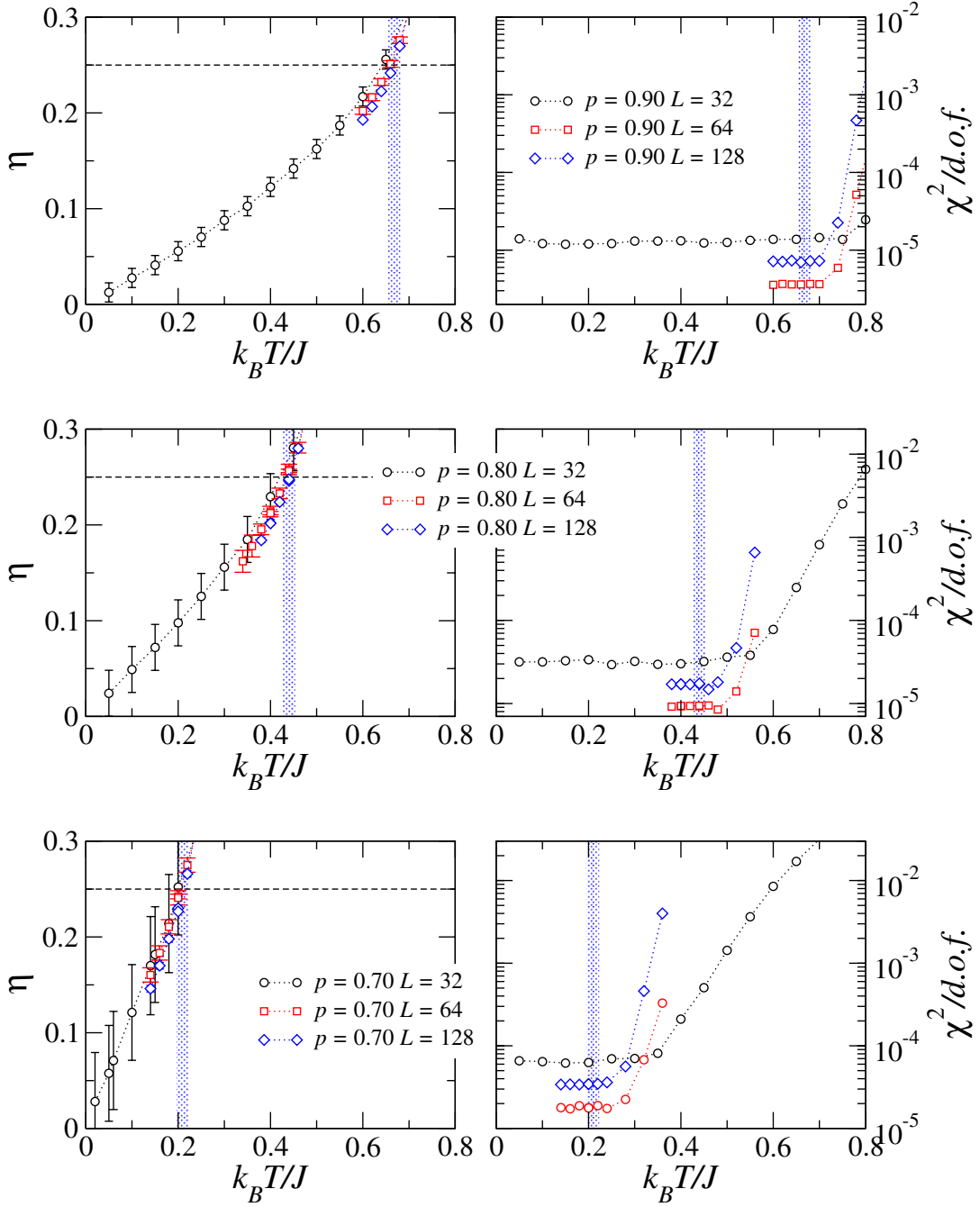


Fig. 4. Plot of the exponent η as a function of the temperature (left) for three different dilutions. The figures on the right give the $\chi^2/d.o.f.$ corresponding to the fit of the order parameter profiles. The vertical stripe materialises the transition temperature where the $\chi^2/d.o.f.$ suddenly increases (logarithmic scale).

the Harris criterion, one expects weak disorder to be irrelevant at the Kosterlitz-Thouless transition where the pure model exhibits essential singularities. The numerical results confirm this picture, since at the transition temperature, we observe from Figure 4 that the η exponent is compatible with the constant value $\frac{1}{4}$.

We also obtained the approximate spin-wave solution which describes the properties of the diluted model at very low temperatures. The presence of non magnetic impurities produces an effective increase of the temperature,

but does not completely suppress the transition before the percolation threshold is reached, as it was suspected in reference [15] where a zero-temperature transition was reported at $p \simeq 0.70$. The argument reported in reference [15] was that impurities, when located in the vicinity of a pair, produce a repulsive interaction between vortices which facilitates pair unbinding. This scenario, together with dilution effect, enhances the disordering of the system but is not sufficient to prevent quasi-long-range ordering at impurity concentrations above the percolation

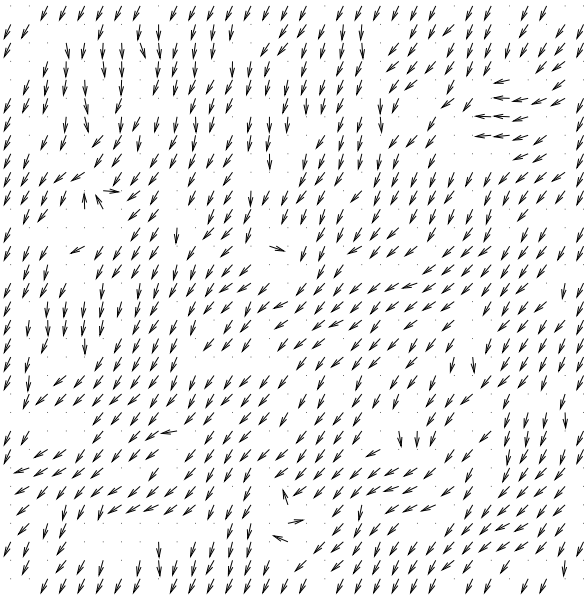


Fig. 5. Typical configuration for a system of size 32×32 , $p = 0.70$ at low temperature $k_B T/J = 0.05$.

threshold. As an example, a typical configuration at low temperature is shown in Figure 5 for a system of size 32×32 at $p = 0.70$.

In conclusion, one should stress that the behaviour of the model in the low temperature critical phase is in full agreement with what might be expected from general relevance arguments.

This work is supported by the French-Venezuelan PCP program ‘Fluides pétroliers’ and by the French-Ukrainian cooperation Dnipro project. The authors gratefully acknowledge both programs for their support. Support from the CINES under project c20020622309 is also gratefully acknowledged. B.B. warmly thanks C. Chatelain for his friendly technical cooperation and Yu.H. acknowledges useful discussions with V. Tkachuk.

Appendix: spin-wave calculation at low temperature

In this appendix, we present the result of a spin-wave calculation valid in the low temperature limit. First, we rewrite the Hamiltonian (4) of the diluted $2d$ XY model for the case of arbitrary short-range ferromagnetic interaction potential $J(|\mathbf{r}|)$:

$$H = -\frac{1}{2} \sum_{\mathbf{r} \neq \mathbf{r}'} J(|\mathbf{r} - \mathbf{r}'|) \cos(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'}) c_{\mathbf{r}} c_{\mathbf{r}'}. \quad (9)$$

Here, $\cos(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})$ stands for a scalar product of two-component unit vectors $\boldsymbol{\sigma}(\mathbf{r})$ directed by angles $\theta_{\mathbf{r}}$, $\theta_{\mathbf{r}'}$ (cf. Eq. (2)). Expanding $\cos(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})$ in (9) for small difference

in directions of spins one gets the Hamiltonian (9) in the spin-wave approximation:

$$\begin{aligned} H &\simeq H' + \frac{1}{4} \sum_{\mathbf{r} \neq \mathbf{r}'} J(|\mathbf{r} - \mathbf{r}'|) (\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})^2 c_{\mathbf{r}} c_{\mathbf{r}'} \\ &\equiv H' + H_1. \end{aligned} \quad (10)$$

The term H' in the Hamiltonian (10) will be further absorbed into the energy reference point, whereas to rewrite the remaining part H_1 we pass to the Fourier-transformed angle variables and the interaction potential. Taking the periodic boundary conditions we define the Fourier-transformed quantities as:

$$\theta_{\mathbf{r}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \theta_{\mathbf{k}}, \quad \theta_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{-i\mathbf{k} \cdot \mathbf{r}} \theta_{\mathbf{r}}. \quad (11)$$

$$J(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \nu(\mathbf{k}), \quad \nu(\mathbf{k}) = \sum_{\mathbf{r}} e^{-i\mathbf{k} \cdot \mathbf{r}} J(\mathbf{r}). \quad (12)$$

In (11), (12) $\sum_{\mathbf{r}}$ spans N sites of the lattice whereas $\sum_{\mathbf{k}}$ is within the first Brillouin zone. Written in the Fourier-transformed variables the Hamiltonian H_1 reads:

$$\begin{aligned} H_1 &= \frac{1}{2} \sum_{\mathbf{q}, \mathbf{k}_1, \mathbf{k}_2} S(\mathbf{q} + \mathbf{k}_1 + \mathbf{k}_2) S(-\mathbf{q}) \nu(\mathbf{q}) \theta_{\mathbf{k}_1} \theta_{\mathbf{k}_2} \\ &\quad - \frac{1}{2} \sum_{\mathbf{q}, \mathbf{k}_1, \mathbf{k}_2} S(\mathbf{q} + \mathbf{k}_1) S(\mathbf{k}_2 - \mathbf{q}) \nu(\mathbf{q}) \theta_{\mathbf{k}_1} \theta_{\mathbf{k}_2}, \end{aligned} \quad (13)$$

with

$$S(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{r}} e^{i\mathbf{q} \cdot \mathbf{r}} c_{\mathbf{r}}. \quad (14)$$

Let us single out in (13) the Hamiltonian of the pure $2d$ XY model. To this end let us introduce variables $\rho(\mathbf{q})$ which may serve to show deviation of $S(\mathbf{q})$ from the Kronecker’s delta $\delta(\mathbf{q})$:

$$S(\mathbf{q}) = \delta(\mathbf{q}) - \rho(\mathbf{q}), \quad (15)$$

with

$$\rho(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{r}} e^{i\mathbf{q} \cdot \mathbf{r}} (1 - c_{\mathbf{r}}). \quad (16)$$

Denoting a configurational average with the distribution function (3) by $\overline{(\dots)}$ we get for the two first moments of the random variable $c_{\mathbf{r}}$: $\overline{c_{\mathbf{r}}} = \sum_{c_{\mathbf{r}}=0,1} P(c_{\mathbf{r}}) c_{\mathbf{r}} = p$ and $\overline{c_{\mathbf{r}} c_{\mathbf{r}'}} = p^2$ for $\mathbf{r} \neq \mathbf{r}'$, or p for $\mathbf{r} = \mathbf{r}'$. Here, we remember that p is the concentration of the occupied sites $c_{\mathbf{r}} = 1$ and that $\mathcal{P}[c_{\mathbf{r}}] = \prod_{\mathbf{r}} P(c_{\mathbf{r}})$. This leads to the following values for the first two moments of $\rho(\mathbf{q})$ (note, that due to (9) $\mathbf{r} \neq \mathbf{r}'$): $\overline{\rho(\mathbf{q})} = (1 - p) \delta(\mathbf{q})$ and $\overline{\rho(\mathbf{q}) \rho(\mathbf{q}')}$ = $(1 - p)^2 \delta(\mathbf{q}) \delta(\mathbf{q}')$. Considering the concentration of empty sites $(1 - p)$ to be small we take it as an expansion parameter and further we keep only linear in $\rho(\mathbf{q})$ contributions. For the Hamiltonian (9) we get:

$$\begin{aligned} H &= H_0 - \frac{1}{2} \sum_{\mathbf{k}_1, \mathbf{k}_2} \left[\nu(\mathbf{k}_1 + \mathbf{k}_2) + \nu(0) - \nu(\mathbf{k}_1) \right. \\ &\quad \left. - \nu(\mathbf{k}_2) \right] \rho(\mathbf{k}_1 + \mathbf{k}_2) \theta_{\mathbf{k}_1} \theta_{\mathbf{k}_2} + O(\rho^2) \end{aligned} \quad (17)$$

where H_0 stands for the Hamiltonian of the undiluted system:

$$H_0 = \frac{1}{2} \sum_{\mathbf{k}} \left[\nu(0) - \nu(\mathbf{k}) \right] \theta_{\mathbf{k}} \theta_{-\mathbf{k}}. \quad (18)$$

For the nearest neighbour interaction and square lattice with a lattice constant $a = |\boldsymbol{\mu}|$ we have $J(\mathbf{r}) = J$ for $|\mathbf{r}| = a$ and 0 for $|\mathbf{r}| \neq a$,

$$\nu(\mathbf{k}) = 2J(\cos(k_x a) + \cos(k_y a)) \simeq 4J - J|\mathbf{k}|^2 a^2 + \dots \quad (19)$$

Subsequently, the Hamiltonian (17) reads:

$$H \simeq \frac{1}{2} \sum_{\mathbf{k}} J|\mathbf{k}|^2 a^2 \theta_{\mathbf{k}} \theta_{-\mathbf{k}} + \sum_{\mathbf{k}_1, \mathbf{k}_2} J a^2 (\mathbf{k}_1 \cdot \mathbf{k}_2) \rho(\mathbf{k}_1 + \mathbf{k}_2) \theta_{\mathbf{k}_1} \theta_{\mathbf{k}_2}, \quad (20)$$

with a scalar product $\mathbf{k}_1 \cdot \mathbf{k}_2$.

For a given configuration of disorder, the configurationally-dependent partition function Z_{conf} is defined by:

$$Z_{\text{conf}} = \text{Sp}_{\theta} e^{-\beta H}, \quad (21)$$

where Sp_{θ} means integration over spin degrees of freedom on each site (and $\beta = (k_B T)^{-1}$):

$$\text{Sp}_{\theta}(\dots) = \prod_{\mathbf{r}} \int_{-\pi}^{\pi} \frac{d\theta_{\mathbf{r}}}{2\pi} (\dots). \quad (22)$$

For a given configuration of occupied and empty sites, let us define a thermodynamic averaging by:

$$\langle (\dots) \rangle = \frac{1}{Z_{\text{conf}}} \text{Sp}_{\theta} e^{-\beta H} (\dots). \quad (23)$$

Considering the quenched dilution (i.e. the case when magnetic and non-magnetic sites are fixed on their places) one gets the observables by averaging thermodynamically averaged quantities with respect to different configurations of disorder [23]. Now, the pair correlation function is defined as

$$G_2(|\mathbf{r}_2 - \mathbf{r}_1|) = \overline{\langle c_{\mathbf{r}_2} c_{\mathbf{r}_1} \cos(\theta_{\mathbf{r}_2} - \theta_{\mathbf{r}_1}) \rangle} \simeq \frac{1}{Z_{\text{conf}}} \text{Sp}_{\theta} e^{-\beta H} c_{\mathbf{r}_2} c_{\mathbf{r}_1} \left(1 - \frac{1}{2} (\theta_{\mathbf{r}_2} - \theta_{\mathbf{r}_1})^2 \right). \quad (24)$$

As far as we keep only linear in $\rho(\mathbf{q})$ terms, we may decouple configurational averaging in (24) and write the pair correlation function as:

$$G_2(|\mathbf{r}_2 - \mathbf{r}_1|) \simeq \frac{\text{Sp}_{\theta} e^{-\beta \overline{H}} \overline{c_{\mathbf{r}_2} c_{\mathbf{r}_1}} \left(1 - (\theta_{\mathbf{r}_2} - \theta_{\mathbf{r}_1})^2 / 2 \right)}{\text{Sp}_{\theta} e^{-\beta \overline{H}}}. \quad (25)$$

For the configurationally averaged value of the Hamiltonian \overline{H} one gets:

$$\begin{aligned} \overline{H} &= \frac{1}{2} \sum_{\mathbf{k}} J|\mathbf{k}|^2 a^2 \theta_{\mathbf{k}} \theta_{-\mathbf{k}} + \sum_{\mathbf{k}_1, \mathbf{k}_2} J a^2 \mathbf{k}_1 \cdot \mathbf{k}_2 \overline{\rho(\mathbf{k}_1 + \mathbf{k}_2)} \theta_{\mathbf{k}_1} \theta_{\mathbf{k}_2} \\ &= \frac{1}{2} \sum_{\mathbf{k}} J|\mathbf{k}|^2 a^2 \theta_{\mathbf{k}} \theta_{-\mathbf{k}} \\ &\quad + \sum_{\mathbf{k}_1, \mathbf{k}_2} J a^2 \mathbf{k}_1 \cdot \mathbf{k}_2 \delta(\mathbf{k}_1 + \mathbf{k}_2) (1-p) \theta_{\mathbf{k}_1} \theta_{\mathbf{k}_2} \\ &= \frac{1}{2} [1 - 2(1-p)] \sum_{\mathbf{k}} J|\mathbf{k}|^2 a^2 \theta_{\mathbf{k}} \theta_{-\mathbf{k}} \\ &= [1 - 2(1-p)] H_0. \end{aligned} \quad (26)$$

Then the formula for the pair correlation function (25) reads:

$$G_2(|\mathbf{r}_2 - \mathbf{r}_1|) = \text{const.} \times \text{Sp}_{\theta} e^{-\beta' H_0} \left(1 - (\theta_{\mathbf{r}_2} - \theta_{\mathbf{r}_1})^2 / 2 \right) / \text{Sp}_{\theta} e^{-\beta' H_0}, \quad (27)$$

with

$$\text{const.} = 1 - 2(1-p), \quad (28)$$

$$\beta' = [1 - 2(1-p)]\beta. \quad (29)$$

Formula (27) for the pair correlation function of the diluted 2d XY model has the form of the spin-wave approximated pair correlation function of the pure system. It differs only by a constant (28) which renormalizes also the temperature β (29). Taking that in the spin-wave approximation the pair correlation function critical exponent for the pure system equals [7]:

$$\eta_{SW}^{\text{pure}} = \frac{1}{2\pi J \beta} \quad (30)$$

one gets the exponent for the diluted system substituting in (30) temperature β by β' (29):

$$\eta_{SW}^{\text{diluted}} = \frac{1}{2\pi J \beta (1 - 2(1-p))}. \quad (31)$$

References

1. A.B. Harris, J. Phys. C **7**, 1671 (1974)
2. V.L. Berezinskii, Sov. Phys. JETP **32**, 493 (1971)
3. J.M. Kosterlitz, D.J. Thouless, J. Phys. C **6**, 1181 (1973)
4. J.M. Kosterlitz, J. Phys. C **7**, 1046 (1974)
5. N.D. Mermin, H. Wagner, Phys. Rev. Lett. **22**, 1133 (1966)
6. P.C. Hohenberg, Phys. Rev. **158**, 383 (1967)
7. F. Wegner, Z. Phys. **206**, 465 (1967)
8. J.M. Kosterlitz, D.J. Thouless, Prog. Low Temp. Phys. **78**, 371 (1978)
9. D.R. Nelson, in *Phase Transitions and Critical Phenomena*, edited by C. Domb, J.L. Lebowitz, (Academic Press, London 1983), p. 1

10. C. Itzykson, J.M. Drouffe, *Statistical field theory*, (Cambridge University Press, Cambridge 1989), Vol. 1
11. Z. Gulácsi, M. Gulácsi, *Adv. Phys.* **47**, 1 (1998)
12. P.M. Chaikin, T.C. Lubensky, *Principles of Condensed Matter Physics* (Cambridge University Press, Cambridge 1995)
13. M. Hasenbuch, K. Pinn, *J. Phys. A* **30**, 63 (1997)
14. L.A.S. Mól, A.R. Pereira, A.S.T. Pires, *Phys. Rev. B* **66**, 052415 (2002), arXiv e-print [cond-mat/0208523](#)
15. S.A. Leonel, P. Zimmermann Coura, A.R. Pereira, L.A.S. Mól, B.V. Costa, *Phys. Rev. B* **67**, 104426 (2003), arXiv e-print [cond-mat/0210210](#)
16. I. Reš, J. Straley, *Phys. Rev. B* **61**, 14425 (2000)
17. B. Berche, A.I. Fariñas-Sánchez, R. Paredes V., *Europhys. Lett.* **60**, 539 (2002), arXiv e-print [cond-mat/0208521](#)
18. B. Berche, *J. Phys. A* **36**, 585 (2003), arXiv e-print [cond-mat/0211584](#)
19. *Handbook of mathematical functions*, edited by M. Abramowitz, I. Stegun (National Bureau of Standards, 1964)
20. U. Wolff, *Nucl. Phys. B* **322**, 759 (1989)
21. K. Kato, S. Todo, K. Harada, N. Kawashima, S. Miyashita, H. Takayama, *Phys. Rev. Lett.* **84**, 4204 (2000), arXiv e-print [cond-mat/9905379](#)
22. A.W. Sandvik, *Phys. Rev. B* **66**, 024418 (2002), arXiv e-print [cond-mat/0110510](#)
23. R. Brout, *Phys. Rev.* **115**, 824 (1959)