Eur. Phys. J. B **31**, 525–531 (2003)
DOI: 10.1140/epjb/e2003-00062-2

THE EUROPEAN PHYSICAL JOURNAL B

Monte Carlo simulations of the classical two-dimensional discrete frustrated ϕ^4 model

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Received 16 December 2002 / Received in final form 17 January 2003
Published online 6 March 2003 –

Abstract. The classical two-dimensional discrete frustrated ϕ^4 model is studied by Monte Carlo simulations. The correlation function is obtained for two values of a parameter d that determines the frustration in the model. The ground state is a ferro-phase for $d = -0.35$ and a commensurate phase with period $N = 6$ for $d = -0.45$. Mean field predicts that at higher temperature the system enters a para-phase *via* an incommensurate state, in both cases. Monte Carlo data for $d = -0.45$ show two phase transitions with a floating-incommensurate phase between them. The phase transition at higher temperature is of the Kosterlitz-Thouless type. Analysis of the data for $d = -0.35$ shows only a single phase transition between the floating-fluid phase and the ferro-phase within the numerical error.

PACS. 64.70.Rh Commensurate-incommensurate transitions – 63.70.+h Statistical mechanics of lattice vibrations and displacive phase transitions

1 Introduction

One of the microscopic origins of the spatially modulated structures is given by the competing interactions between the particles. The Frenkel-Kontorova model, the axial next-nearest-neighbour Ising (ANNNI) model, and the discrete frustrated ϕ^4 (DIFFOUR) model provide basic microscopic Hamiltonians for the systems of this class. These models have been studied extensively, specially the first two [1,2]. Competing interactions lead to the appearance of incommensurate and commensurate regions in the phase diagrams of these models. The order parameter in these systems is a vector that determines the amplitude and the phase of modulation. For the incommensurate state, the free energy is degenerate in the phase of modulation. The two-dimensional case is of special interest here, since there is no long-range order in such planar systems if the order parameter has more than one component [3]. A nonmonotonic algebraic decay of correlations appears instead of the usual incommensurate state [2].

The correlation function in two-dimensional systems with competing interactions has at least three possible types of behaviour, as found in the spin models [2]. The disordered phase shows an exponential monotonic or modulated ($q \neq 0$) fall-off of the correlation function:

$$C(r) = \langle S(0)S(r)\rangle \sim \exp(-r/\xi)\cos(qr). \qquad (1)$$

The case $q \neq 0$ is usually called floating-fluid phase. An algebraical decay of correlations at $r \to \infty$ is a property of the floating-incommensurate (FIC) or floating-solid phase:

$$C(r) \sim r^{-\eta}\cos(qr + \varphi). \qquad (2)$$

Finally, a commensurate phase with locked-in wavevector q_0 is not destroyed by the fluctuations in two-dimensional case. Therefore the correlation function in this case takes the form

$$C(r) \sim \cos(q_0 r). \qquad (3)$$

The commensurate case includes the ferro-phase also ($q_0 = 0$).

One should note that in the two-dimensional case the phase transition from the para-phase to the FIC-phase is believed to be related with the formation and dissociation of the dislocations or vortices [2]. This scenario of a phase transition can be described by the Kosterlitz-Thouless theory which is basic for the two-dimensional XY universality class [4–6]. The power law dependence of $C(r)$ for this universality class appears everywhere below the critical temperature, down to $T = 0$ or to another phase transition (to a commensurate state, for example). The critical index η is equal to 0.25 in the point of the phase transition (T_c) and decreases for decreasing temperature as $\eta(T) = 0.25 - C\sqrt{T_c - T}$, where C is a constant ($\eta \sim T$ for $T \to 0$). The thermal dependence of the correlation length above the transition point is of the form $\xi \sim \exp(b/\sqrt{T - T_c})$, where b is a constant.

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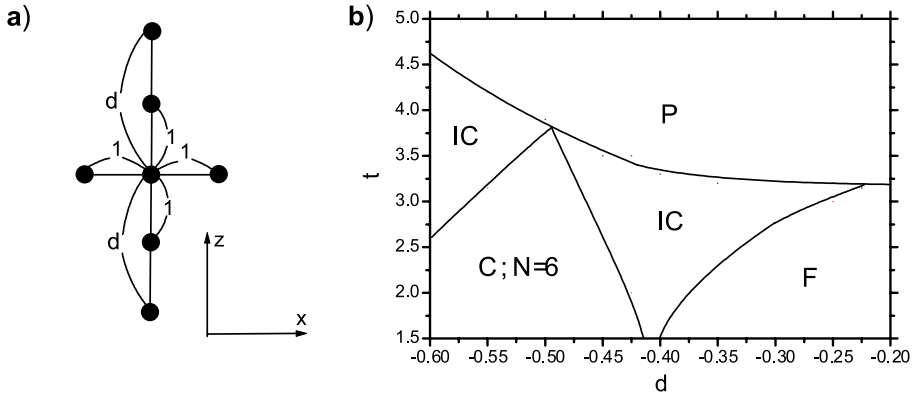

Fig. 1. a) Scheme of interactions in the two-dimensional DIFFOUR model. b) Mean-field phase diagram of the two-dimensional DIFFOUR model for the parameter $a = 5$ (t is the temperature hereafter). P-para-phase, F-ferro-phase, IC-incommensurate phase, C-commensurate phase. There are also narrow regions of the commensurate phases in the area of the incommensurate phase not shown in the picture.

One of the well studied spin models with competing interactions is the ANNNI model. The ANNNI model is a spin lattice model with ± 1 classical spins, ferromagnetic nearest-neighbours interaction J_1 in all directions and antiferromagnetic next-nearest-neighbour interaction J_2 in a single direction. The ANNNI model in two dimensions has been studied by numerous methods [1,2]. The ground state of this model at zero temperature is a ferromagnetic phase for $-J_2/J_1 < 0.5$ and a $\langle 2 \rangle$ phase (two spins up and two spins down $\uparrow\uparrow\downarrow\downarrow$) for $-J_2/J_1 > 0.5$. Obviously, an FIC-phase can appear only at finite temperature between the paramagnetic phase and the $\langle 2 \rangle$ phase for $-J_2/J_1 > 0.5$. The behaviour of the model was studied by transfer-matrix calculations and finite-size-scaling analysis [7], Monte Carlo simulations [8,9], dynamical Monte Carlo method [10], fermion approximation [11] and its modification [12], the interface free energy method [13]. Some of these results seem to indicate a Kosterlitz-Thouless [4] type of the phase transition from the paramagnetic to the FIC-phase and a Pokrovsky-Talapov [14] type of phase transition from this phase to $\langle 2 \rangle$. The latter scenario implies a square-root power law change of the wavevector with respect to temperature near the transition to the $\langle 2 \rangle$ phase. One should point out that the one-dimensional quantum ANNNI model studied in [15] also reveals all phases and types of the phase transitions mentioned above. The approximations give a spread of the phase transition temperature over a rather wide region. On the other hand, other calculations predict an FIC-phase with a width comparable to that spread. The recent results on a cluster heat bath simulation [9] of systems of about 64×128 atoms demonstrate that the FIC region is at least 2 times smaller than the previous papers predicted [7]. Further, the nonequilibrium relaxation method [16] for 6400×6400 systems does not predict any area for the FIC-phase at all, so that even the presence of this phase was questioned.

In this paper we consider the classical two-dimensional DIFFOUR, which has continuous variables and competing interactions in one direction. The DIFFOUR model was introduced in [17] as a displacement translationally invariant model for the incommensurate phases. Instead of ± 1 spins, this model considers double-well anharmonic 2-4 oscillators at the nodes of a lattice. Similarly, there is a harmonic nearest-neighbour and next-nearest-neighbour coupling. The potential energy can be written as

$$V = -\frac{a}{2}\sum_i u_i^2 + \frac{a}{4}\sum_i u_i^4 + \frac{1}{2}\sum_{i,j}(u_i - u_j)^2\sigma_{ij} + \frac{d}{2}\sum_{i,j}(u_i - u_j)^2\sigma'_{ij}. \quad (4)$$

Here $\sigma_{ij} = 1$ for the nearest neighbours and $\sigma_{ij} = 0$ otherwise, while $\sigma'_{ij} = 1$ for the next-nearest-neighbours in the direction z (see Fig. 1a). The phase diagram for the analogous three-dimensional model is presented in [18]. The system has commensurate and incommensurate regions in the phase diagram for $d < 0$ *i.e.* with competing interactions.

The ANNNI model can be considered as a limiting case of the DIFFOUR model ($a \to +\infty$). It corresponds to the order-disorder limit of the latter model. In the other limit ($a \to +0$) of the DIFFOUR model the ground state may be an incommensurate phase which is reached *via* a displacive transformation [19]. Furthermore, the greater freedom in the DIFFOUR model could also possibly lead to the existence of a broader the FIC-phase than in the ANNNI model. In view of the unclear situation in the latter we want to study the existence of FIC-phase in the DIFFOUR model. We shall do this using Monte Carlo simulations. The mean-field phase diagram can easily be determined and is presented in Figure 1b.

Correlation functions of the model are analyzed for certain parameters; their behaviour is always one of the three scenarios mentioned above (1, 2, 3). An FIC-phase has been found. Indications of the Kosterlitz-Thouless scenario of the phase transition from the floating-fluid to the FIC-phase are discussed. The transition to the ferro-phase occurs *via* the floating-fluid phase. Surprisingly, the period of this phase *increases* as temperature decreases.

2 Algorithm

We study the two-dimensional DIFFOUR model using the Monte Carlo method. The difficulty of the simulation of the models with competing interactions is in the complexity of their configuration space which usually has many deep almost degenerate local minima. Then, it is difficult to overcome a potential barrier and to change the period of the modulation. This situation can lead to an unacceptably long computation time using conventional Monte Carlo schemes, particularly for large systems. Special algorithms should be used to achieve a reasonable result [9,16].

In this paper, we use the "local-heating" algorithm which worked well for the three-dimensional DIFFOUR model [18]. The idea is to modify the potential energy in certain regions of the system to allow an easier switch between local minima. Actually, the temperature of the system is not changed but the constants of the potential energy are modified. However, for the largest part of the system its potential energy is still determined by (4). The regions with a modified potential energy are not included in the calculation of the physical quantities (order parameter, correlation functions), while the usual Metropolis algorithm for Monte Carlo sampling is applied to the whole system.

We use periodic boundary conditions and the following modification of the potential energy:

$$V = -\frac{a}{2}\sum_i \theta_i u_i^2 + \frac{a}{4}\sum_i \theta_i u_i^4 + \frac{1}{4}\sum_{i,j}(\theta_i+\theta_j)(u_i-u_j)^2\sigma_{ij} + \frac{d}{4}\sum_{i,j}\theta_{(i+j)/2}(u_i-u_j)^2\sigma'_{ij},$$

$$\theta_i = (1 + l_1(\exp\left[-(x_i^2+z_i^2)/l_2^2\right] + \exp[-((N_x-x_i)^2+(N_z-z_i)^2)/l_2^2]))^{-1}, l_1 > 0. \quad (5)$$

N_x and N_z are the sizes of the lattice along the x and z-directions, respectively. The new coefficients θ_i (5) mean that their values in the vicinity of the lines $x_i = 0$ and $z_i = 0$ are smoothly decreased. Parameters l_1, l_2 determine the height and the width of this decrease, respectively. The change of the parameters mimics a local heating of the corresponding regions. The idea of this procedure is to put these parts of the system in a para-phase and to destroy the local modulation phase. If the profile $\theta(x,z)$ is smooth enough, the phases of modulation at the two sides of the heated line are in an ideal case independent and can randomly fluctuate. The whole system may change the period of the modulation now. Use of "local heating" leads to faster thermalization of the system.

Additionally we realised that it is useful to simulate the systems with a larger size along the x direction. The possible explanation is that once the period is changed at some x, it is relatively easy for this change to spread to the whole system. The probability for this initial change is proportional to the x-size.

We calculate the correlation function as follows:

$$C(\boldsymbol{r}) = \langle u(\boldsymbol{r}')u(\boldsymbol{r}'+\boldsymbol{r})\rangle|_{\boldsymbol{r}'}. \quad (6)$$

Here $\langle\rangle|_{\boldsymbol{r}'}$ means an ensemble average. We consider two functions $C_x = C(\boldsymbol{r} = r_x)$ (along x axis) and $C_z = C(\boldsymbol{r} = r_z)$ (along z axis) hereafter. The presence of the heated regions is taken into account as follows. We add data to the point $\boldsymbol{r}$ of correlation function (6) if there is no "local heated" region between $\boldsymbol{r}$ and $\boldsymbol{r}'$ and add data to the point $\boldsymbol{r}-\boldsymbol{r}'$ otherwise. If one of the points $\boldsymbol{r}$ or $\boldsymbol{r}'$ appears to be in the "local heated" region the data are not included in the calculation of the correlation function. This procedure reduces the influence of the finite-size effects. The data for the correlation function appear to be reliable even for distances larger than half the system size.

We check whether the approach of the "local heating" algorithm by changing the size of the system and by starting with various initial distributions of atom's displacements is reasonable. One should use large enough sizes of the system since it is difficult to distinguish exponential and power law decay of correlations. The situation becomes worse when we deal with modulated structures with large modulation period. We found that an optimal size for the present algorithm is about 200×100. The total number of Monte Carlo samplings for the given parameters of the model a, d and temperature t is about $10^{10} \div 10^{11}$. Parameters of "local heating" are varied in a region $2 \lesssim l_1, l_2 \lesssim 4$. We have checked that a two-times increase of the slab size in the x or z-direction does almost not change the exponents of power or exponential decaying or the period of the modulation within the numerical accuracy. The result does not depend on the initial configuration of the system. Thus, we believe that the presented algorithm allows us to perform accurate numerical simulations.

3 Results and their analysis

We present here detailed results for two values of the parameter d at $a = 5$: $d = -0.45$ and $d = -0.35$. We choose these values of the parameter d since at least the mean-field approximation predicts various ground states for zero temperature (commensurate phase with $N = 6$ for $d = -0.45$ and ferro-phase for $d = -0.35$, see Fig. 1b). The parameter value $a = 5$ of the DIFFOUR model (4) is used since the amplitude of modulation then has a value comparable with the value of $C(0)$. It makes the analysis of the data easier. We have found that the modulation amplitude is much less than the value $C(0)$ for larger values of a (for example, at $a \gtrsim 20$). The mean-field approach for the DIFFOUR model confirms these observations.

The correlation functions C_z and C_x are calculated at several values of the temperature. The results for C_z are presented in Figures 2, 3 for $d = -0.45$ and $d = -0.35$, respectively. Typical dependencies of C_x for both values of the parameter d are shown in Figure 4. We use a log-log scale for the C_x functions. The most informative dependencies here are C_z (Figs. 2, 3). Qualitatively the behaviour of the functions C_x and C_z is different: non-monotonic and monotonic dependence on the distance, respectively. We believe that the influence of the finite-size effects starts at $x \gtrsim 100$ and at $z \gtrsim 70$ and we do not

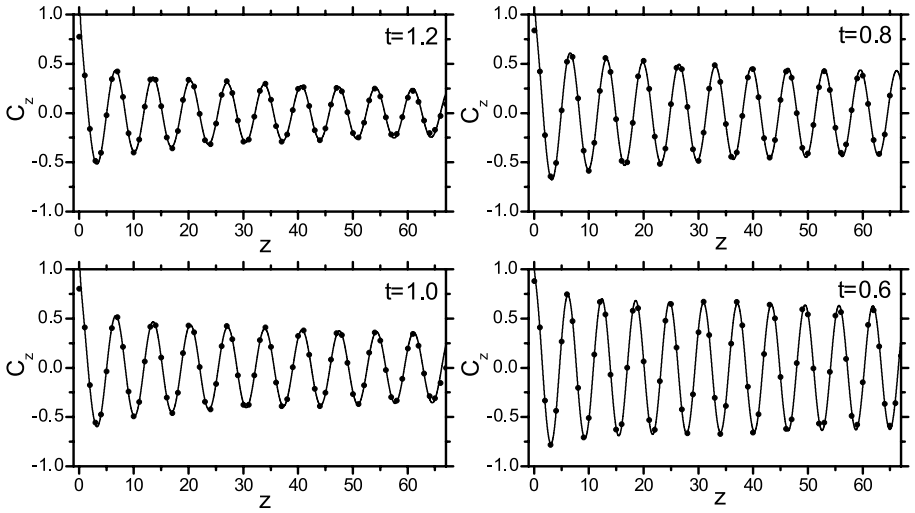

Fig. 2. The correlation function C_z for various temperatures: $t = 1.2$, $t = 1.0$, $t = 0.8$ and $t = 0.6$. Parameters of the DIFFOUR model are $a = 5$, $d = -0.45$. Dots - Monte Carlo results, solid lines - results of fitting by non-monotonic power law decay (2). The Kosterlitz-Thouless like phase transition takes place at $t_1 \approx 1.2$ (index $\eta = 0.25$).

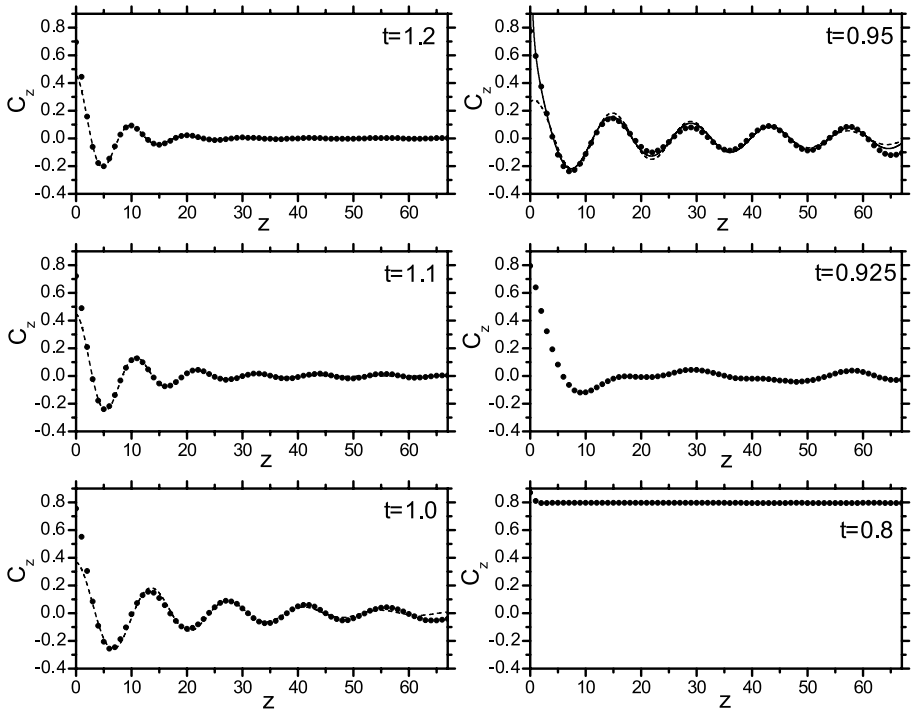

Fig. 3. The correlation function C_z for various temperatures: $t = 1.2$, $t = 1.1$, $t = 1.0$, $t = 0.95$, $t = 0.925$ and $t = 0.8$. Parameters of the DIFFOUR model are $a = 5$, $d = -0.35$. Dots: Monte Carlo results, dashed lines: results of fitting by non-monotonic exponential decay (1). Solid line: result of the fitting at $t = 0.95$ by non-monotonic power law decay (2): index η is approximately equal to 0.5. Single phase transition from floating-fluid phase to the ferro-phase takes place at $t_c \approx 0.91$.

consider these regions in the analysis of the data. The error bar for C_x and C_z at moderate values of temperature for $d = -0.45$ and $d = -0.35$ is about a few percent and becomes larger at lower temperatures.

We analyze the obtained results by fitting the data for C_z (Figs. 2, 3) using one of the functions (1, 2). We also try to find a power law decay for C_x (Fig. 4) if it is possible.

3.1 Case d = −0.45

We start with the case $d = -0.45$ (Fig. 2). We look for the possibility of a phase transition from the para-phase to the FIC-phase. The dependencies of the correlation functions C_z at $t \gtrsim 1.2$ can be fitted by equation (1), *i.e.* by non-monotonic exponential decay. There is no power law decay for C_x either for these values of temperature. Thus,

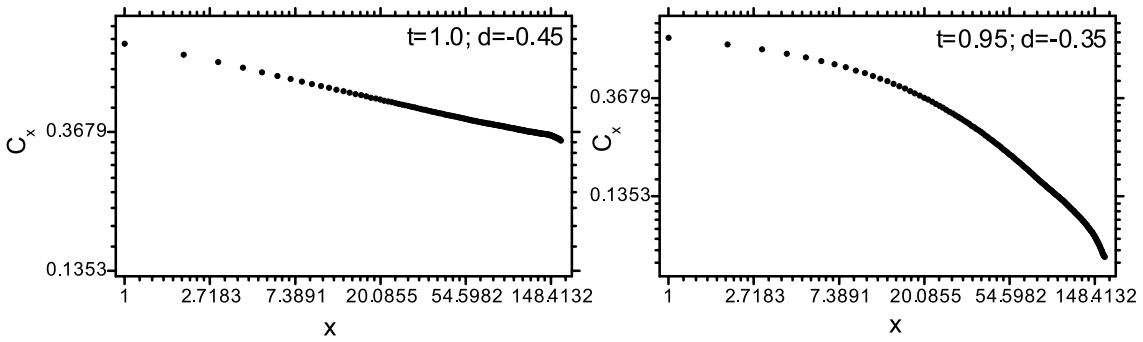

Fig. 4. Typical dependencies of the correlation function C_x for $d = -0.45$ and $d = -0.35$ (temperatures are equal to $t = 1.0$ and $t = 0.95$, respectively). Logarithmic scale is used for both axes. Results are obtained by Monte Carlo simulations.

we conclude that it is floating-fluid phase at $t > 1.2$ and $d = -0.45$.

One can fit the dependencies C_z in the vicinity of the $t \sim 1.2$ by nonmonotonic power law decay (2). The results of this fitting are presented in Figure 2 by solid lines. It is possible also to find a power law decay for C_x. This region is believed to be close to the possible point of the phase transition from the floating-fluid phase to the FIC-phase. The value of the index η is approximately equal to 0.25 at the temperature $t_1 \approx 1.2$. This coincides with the condition of the Kosterlitz-Thouless phase transition. One can find, that data for C_z (Fig. 2) for the region $0.55 < t < 1.2$ can also be fitted by a non-monotonic power law dependence (2) with index η depending on temperature. We plot the dependence of the $(0.25 - \eta(t))^2$ on $t_1 - t$ for the $t < 1.2$ (Fig. 5a). One sees a linear dependence, which is a feature of the Kosterlitz-Thouless type behaviour [4,6]. Thus, the phase transition from the floating-fluid phase to the FIC-phase at $t_1 \approx 1.2$ is believed to be of Kosterlitz-Thouless type. The data for C_x at $0.55 < t < 1.2$ can also be fitted by a monotonic power law decay. Typical dependence of C_x for this temperature region is presented in Figure 4 ($t = 1.0$). In our calculations, the indices η for C_x and C_z do not coincide (the difference is about $10-20\%$). Although, we don't know whether this difference is of physical or numerical origin, we rather attribute it to finite-size effects in simulations. Nevertheless, we use here the index η obtained from the data of fitting in the z direction, *i.e.* by equation (2) for analysis of the data.

We also show in Figure 5b how the wavevector changes as a function of temperature. We find that the modulation period is equal to $N = 6$ at $t \leq 0.55$. The appearance of the domain walls (discommensurations – small regions with pseudo-period $N \neq 6$) can be seen at $t \gtrsim 0.55$. It prevents the system to get a commensurate modulation period ($N = 6$). The point $t_2 \approx 0.55$ is supposed to be the point of the phase transition from the FIC-phase to the commensurate phase with period $N = 6$ (see Fig. 5b). This picture is similar to that for the two-dimensional ANNNI model [9] for the transition from the FIC-phase to the $\langle 2 \rangle$ phase. One should note that the accuracy of our results is not sufficient to determine whether the phase transition from FIC-phase to the $\langle 2 \rangle$ phase is of Pokrovsky-Talapov type or not (Fig. 5). Present results are in agreement with previous conclusions by Schulz and Haldane *et al.* that only commensurate phase with sufficiently small periodicity can transform into a FIC-phase [20,21]. It is also possible that narrow commensurate regions exist in the temperature range $0.55 < t < 1.2$. Study of this problem demands more accurate methods of numerical simulations and analysis of the data.

3.2 Case d = −0.35

Before presenting the numerical results, let us stress several features of the $d = -0.35$ situation. The mean-field predicts two transitions: from the para-phase to an incommensurate one, and than to the ferro-phase. The three-dimensional DIFFOUR model indeed behaves so at certain parameters [18]. On the other hand, the ANNNI model does not show two transitions; there is only a single transition from the floating-fluid (disordered) to the ferro-phase. For the present system, because of the relatively small value $a = 5$, the modulation is much more pronounced and falls off slower than in the ANNNI model. As well, the mean-field region for the incommensurate phase is quite wide. Therefore one could expect a transition from a floating-fluid to an FIC-phase for $d = -0.35$. Surprisingly, we did not found evidence for this; qualitatively the result coincides with that of the ANNNI model.

Results for the case $d = -0.35$ for C_z are presented in Figure 3. Data for $t \gtrsim 1.0$ can be fitted by non-monotonic exponential decay (1). Results of fitting C_z are shown in Figure 3 by dashed lines. We have performed a detailed studies of the region $1.0 < t < 0.8$ (part of them is shown in Fig. 3). Since the period of the modulation is more than 14 in this region it is difficult to distinguish whether there is a non-monotonic power law decay or not. Besides, the fluctuations in this region are increased and our algorithm does not allow us to judge the type of decay of the correlations. We try to fit these dependencies by exponential and power law decay. The results for $t = 0.95$ are presented in Figure 3 by dashed and solid lines, respectively. Both dependencies show agreement with Monte Carlo results within the numerical error. The index η for power law decay is found to be about 0.5. Thus, we believe that there is no Kosterlitz-Thouless phase transition for $d = -0.35$ since there is no agreement with a power law decay (2)

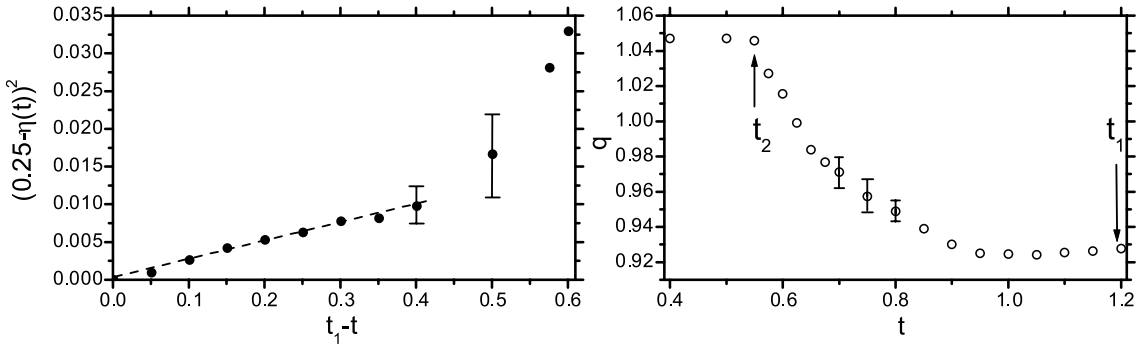

Fig. 5. a) Dependence of the function $(0.25 - \eta(t))^2$ on the $t_1 - t$ below the point of the phase transition from floating-fluid phase to the FIC-phase (parameters of the model $a = 5$, $d = -0.45$). Dots are the results of the analysis of the Monte Carlo data (Fig. 2), dashed line is a linear approximation in the vicinity of the phase transition. b) Dependence of the wavevector q on the temperature t (parameters of the model $a = 5$, $d = -0.45$). Dots are the results of the analysis of the Monte Carlo data (Fig. 2). t_1 and t_2 are the temperatures of the phase transitions from the floating-fluid phase to the FIC-phase and from the FIC-phase to the commensurate phase with period $N = 6$, respectively.

with the exponent value $\eta = 0.25$ in this temperature region. One can see that the period of the modulation is increased, while the amplitude of modulation is decreased. This situation is opposite to the case $d = -0.45$. A typical result for the C_x is presented in Figure 4 ($t = 0.95$). It is difficult to find power law decay in the region $1.0 < t < 0.8$ for C_x. Certainly, there is no index $\eta = 0.25$ in this case either. It is difficult to obtain clear dependence of correlations decay in the vicinity of the phase transition point due to increase of fluctuations and strong influence of the finite-size effects (see Fig. 3, $t = 0.925$). Thus, we conjecture that there is only one second order phase transition for $d = -0.35$ from the floating-fluid phase into the ferro-phase. We estimate the temperature of this phase transition to be $t_c \approx 0.91$. We would like to note that one can suggest a transition from floating-fluid phase to a ferro-phase *via* a phase with monotonic exponential decay of correlations with $q = 0$ (1) and the existence of a disorder line by analogy with the ANNNI model [7]. This phase may exist in a very narrow temperature region at given parameters of the model and data for $t = 0.925$ confirm this. The question of the presence of a disorder line in the phase diagram of the two-dimensional DIFFOUR model needs an additional study.

4 Conclusions

In conclusion, we have studied the DIFFOUR model in two dimensions by Monte Carlo simulations. The classical DIFFOUR model has two parameters a and d, where the latter one is the effective constant of the competition of the interactions. Two sets of parameters of the model have been considered here in detail: $a = 5, d = -0.45$ and $a = 5, d = -0.35$. A "local heating" algorithm has been used for numerical simulations. This algorithm uses modifications of the constants and parameters of the potential energy of the DIFFOUR model. Correlation functions in both directions have been calculated for analysis of the behaviour of the model.

We have found that correlation functions for the $a = 5, d = -0.45$ can be fitted by a non-monotonic exponential decay at $t > 1.2$ and by non-monotonic power law decay at temperatures $0.55 < t < 1.2$. The phase transition at $t_1 \approx 1.2$ of Kosterlitz-Thouless type is believed to take place with $\eta = 0.25$ from the floating-fluid phase to the FIC-phase. The dependence of the index $\eta(t)$ below the point of the phase transition has a square root of $t_1 - t$ behaviour in agreement with the Kosterlitz-Thouless theory. The ground state of the model at $t < 0.55$ ($a = 5, d = -0.45$) is a commensurate phase with modulation period $N = 6$. The second phase transition at these parameters of the model from FIC-phase to the commensurate one occurs at $t_2 \approx 0.55$.

The correlation functions for the case $a = 5, d = -0.35$ can be fitted by a non-monotonic exponential decay for $t > 0.95$. Dependencies at $t \sim 0.95$ can be fitted by non-monotonic power law decay also but with $\eta > 0.25$. Numerical data do not allow us to distinguish exponential from power law decay for this case since the period of modulation is too large. Nevertheless, we believe that there is no FIC-phase in this case and only one phase transition from the floating-fluid phase to the ferro-phase, at $t_c \approx 0.91$. The ground state of the model for $t < 0.9$ is a ferro-phase.

We would like to point out that the results of the Monte Carlo simulations (Figs. 2, 3) and the mean-field data (Fig. 1) are different. Mean-field approximation predicts an incommensurate phase, while Monte Carlo results show a FIC-phase with power law decay of correlations. Mean-field theory predicts two phase transitions for $d = -0.35$ and a region of the incommensurate phase, while Monte Carlo simulations show only one phase transition from the floating-fluid phase to the ferro-phase. Nevertheless, the low-temperature phase (ferro-phase for $d = -0.35$ and commensurate phase with period $N = 6$ for $d = -0.45$) is predicted correctly in the mean-field approximation, as in the limit $t = 0$ fluctuations are absent and the mean-field result is exact.

This work was supported by INTAS project for young scientists (grant YSF 2001/1 - 135).

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