HAL open science

Influence of disorder on the low temperature behaviour of two-dimensional spin models with continuous symmetry

Oleksandr Kapikranian

To cite this version:

Oleksandr Kapikranian. Influence of disorder on the low temperature behaviour of two-dimensional spin models with continuous symmetry. Condensed Matter [cond-mat]. Université Henri Poincaré - Nancy I, 2009. English. NNT : . tel-00374650

HAL Id: tel-00374650

https://theses.hal.science/tel-00374650v1

Submitted on 9 Apr 2009

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

FACULTE DES SCIENCES ET TECHNIQUES

U.F.R Science & Techniques de la Matière et des Procédés
Ecole Doctorale Energie Mécanique et Matériaux
Formation Doctorale Physique et Chimie de la Matière et des Matériaux

National Academy of Sciences of Ukraine

Institute for Condensed Matter Physics

Thèse

présentée pour l'obtention du titre de

Docteur de l'Université Henri Poincaré, Nancy-I

en Sciences Physiques

par **Oleksandr KAPIKRANIAN**

Influence du désordre sur le comportement à basse température de modèles de spins de symétrie continue à deux dimensions

Influence of disorder on the low-temperature behaviour of two-dimensional spin models with continuous symmetry

Membres du jury:

Rapporteurs:	M. Dominique MOUHANNA	Maître de Conférence, U.P.M.C., Paris VI
	M. Ihor STASYUK	Professeur, I.C.M.P., Lviv (Ukraine)
Examinateurs:	M. Bertrand DELAMOTTE	Chercheur CNRS, U.P.M.C., Paris VI
	M. Ihor MRYGLOD	Professeur, I.C.M.P., Lviv (Ukraine)
	M. Bertrand BERCHE	Professeur, U.H.P., Nancy I (Codirecteur de thèse)
	M. Yurij HOLOVATCH	Professeur, I.C.M.P., Lviv (Ukraine) (Codirecteur de thèse)

Laboratoire de Physique des Matériaux
Faculté des Sciences & Techniques -54500 Vandoeuvre-les-Nancy

I am sincerely gratefull to all those people who happened to be in any connection to me and my work during my PhD program in the Institute for condensed matter physics of the National academy of sciences of Ukraine and Laboratoire de Physique des Matériaux, Université Henri Poincaré; their constant help, advices, attention to my work, understanding, and, not less important, their help with the arrangment of bureaucratic questions, and finally their warm personal treatment, all that spread well beyond their professional duties.

The two people without whom this work whould not be possible to appear at all should be acknowledged especially. These are of course my scientific supervisors, Yurij Holovatch and Bertrand Berche. All mentioned above surely concerns them as well, and their qualities of scientists, teachers, great scientific supervisors have been well known long before I actually met them. However, I whould like to personally mention one their common feature which impressed me the most. Not the formal outcome written on paper, no matter how important it is, seems to be the most important aim for them, but rather those human relationships which arise from the search of this result. It is probably the real essence of science as well as of any other branch of human activity in general. Such their position resulted in the fact that during the past three years I acquired along with some professional skills priceless life expirience which will stay with me under any circumstances.

THANK YOU!

(I also thank to all people who showed any interest to my work and came with their questions, remarks and suggestions which very often happened to be of use.)

Contents

INTRODUCTION **8**

1 LITERATURE OVERVIEW **16**

1.1 Spin models of continuous symmetry 16

1.1.1 Topological defects 16

1.1.2 Two-dimensional XY model 18

1.1.3 Vortices in two-dimensional XY model 22

1.2 Structural disorder 24

1.2.1 Quenched and annealed disorder 24

1.2.2 Disorder in two-dimensional XY model 26

1.3 Conclusions 30

2 TWO-DIMENSIONAL XY MODEL WITH DISORDER **32**

2.1 Quenched dilution 33

2.1.1 Configurational averaging 33

2.1.2 Self-averaging 35

2.2 Spin-wave approximation 36

2.2.1 Spin-wave Hamiltonian 36

2.2.2 Fourier transformation on a two-dimensional lattice . 38

2.2.3 Disorder configuration inhomogeneity parameter . . 41

2.2.4 Free energy of a weakly diluted model 44

2.3 Pair correlation function of spins 48

2.3.1 Expansion in the disorder configuration inhomogeneity parameter 48

2.3.2 Pair correlation function asymptotic behaviour . . . 55
2.3.3 Expansion in $\rho_{\mathbf{q}}$ 60
2.3.4 Pair correlation function self-averaging 62
2.3.5 Comparison to the Monte Carlo simulation results . 63
2.4 Conclusions 66

3 TOPOLOGICAL DEFECTS IN PRESENCE OF DISORDER 68
3.1 Villain model with nonmagnetic impurities 69
3.1.1 Villain model as a low-temperature limit of the $2D$ XY model 69
3.1.2 Diluted Villain model Hamiltonian 72
3.1.3 Topological defects in the Villain model 77
3.2 Topological defects and nonmagnetic impurities interaction . 89
3.2.1 Microscopic approach of the Villain model Hamiltonian 89
3.2.2 Kosterlitz-Thouless phenomenological model 93
3.3 BKT transition temperature reduction in presence of disorder 96
3.4 Conclusions 101

4 LATTICE FINITENESS INFLUENCE ON THE PROPERTIES OF TWO-DIMENSIONAL SPIN MODELS OF CONTINUOUS SYMMETRY 104
4.1 Residual magnetization in a finite $2D$ XY model with quenched disorder 105
4.1.1 Magnetization probability distribution function . . . 105
4.1.2 Ring functions 108
4.1.3 Mean magnetization and its moments in presence of disorder 111
4.2 Quasi-long-range ordering in a finite two-dimensional Heisenberg model 114
4.3 Conclusions 121

CONCLUSIONS **124**

THE LIST OF LITERATURE SOURCES **128**

INTRODUCTION

Low-dimensional physical models were originally introduced as a purely mathematical abstraction with the intention to find some exact solutions to the models which do not allow analytical solutions in the usual "physical" dimensions ($d = 3$). With respect to the modern development of the experimental physics they however obtain quite practical use. The practical applications again stimulate theoretical researches of the influence of any kinds of structure imperfections or lattice finiteness on the now well known behaviour of the ideal models. The investigation of these problems has a great practical value, since such phenomena inevitably appear in real physical samples. Since the present work concerns ferromagnetic lattice spin models, it is natural to consider as structural defects "quenched" nonmagnetic impurities introduced in the initial regular lattice [1, 2].

Spin models of *continuous symmetry* can possess also defects of another kind: *topological defects* [3–5] which in despite of their name are not something artificially brought but deeply connected to the nature of these models. Present in higher dimensions as well these special excitations of the ground state have especially remarkable impact in two dimensions. For example, in the classical two-dimensional XY model topological defects (also called *vortices* in the context of this model) behave themselves similarly to the two-dimensional neutral gas of particles with Coulomb interaction and cause a phase transition (*Berezinskii-Kosterlitz-Thouless transition* (BKT) [6, 7]) with features similar to the insulator-conductor transition in the two-dimensional electrolyte [8, 9].

The classical two-dimensional XY model presents a beautiful exam-

ple of topological defects influence on the critical behaviour. One of the exact results for the model formulated in the Mermin-Wagner-Hohenberg theorem [10, 11] and $1/q^2$ Bogolyubov theorem [12] states the absence of spontaneous magnetization for non-zero temperatures, but at low temperatures the model exhibits so called *quasi-long-range order* which cannot be described by such a usual order parameter as magnetization. One of the interesting consequences of the quasi-long-range ordering is a remarkable residual magnetization in a system of a finite size L which vanishes with a power law as L increases [13, 14]. At the critical temperature, T_{BKT}, topological defects reach a "conducting" state destroying the quasi-long-range order and leaving the system magnetically completely disordered.

It is well known that introduction of additional disorder (positional disorder, for example) can significantly reflect in the model properties and even change the character of the critical behaviour. Although disorder is irrelevant (Harris criterium [15]) at the very BKT transition point, i.e. it does not change the universal critical exponents, there are important disorder effects such as changes in the critical temperature T_{BKT} and non-universal (at $T < T_{\mathrm{BKT}}$) value of the temperature-dependent exponent of the spin pair correlation function which defines the residual magnetization scaling behaviour too. A highly important question is also the question of the topological and structural defects interaction.

Due to the absence of an exact solution the two-dimensional XY model requires approximate approaches, among which one should remark the following:

- *spin-wave approximation* [16] which allows for a precise enough analytical estimation of all important physical characteristics of the system at low temperatures; this approximation neglects topological defects, so it fails at higher temperatures when the influence of vortices becomes visible and does not describe the BKT transition;

- *Villain model* [17, 18] which apart from its importance as an alternative model possessing vortices and a BKT transition and having the Hamiltonian convenient for analytical purposes, can serve as a low-temperature approximation to the $2D$ XY model; the Villain model describes topological defects as well as spin-wave excitations;

- *Kosterlitz-Thouless phenomenological model* [7, 8] based on the continuous elastic medium approximation an artificial intoduction of topological defects; not being derived from the microscopic $2D$ XY model Hamiltonian, it still gives correct qualitative picture of its universal critical behaviour (at T_{BKT}).

Subject actuality. The problem of the influence of structural disorder on the behaviour of magnetic models, first formulated almost fifty years ago (see, for example, [1, 2]), has become the subject of a sufficient number of theoretical works since that time. Somehow, the two-dimensional XY model remained a bit aside these researches, very fruitful for other spin models (as Ising and Heisenberg models, see [19] for references), mostly because of the fact that quenched disorder does not change qualitatively the critical behaviour of this model according to the Harris criterium [15]. However, it is known that the model has some highly interesting analytically accessible properties of the low temperature phase (see, for example, [8, 14, 16]) of a non-universal character which thus can depend on the presence of disorder [20]. Paradoxically, the first steps in the investigation of these questions were made only quite recently [21, 22], mostly by Monte Carlo simulations [20, 22–27], but neither the experimental nor the analytic results [20, 24] can be considered as exhaustive enough; for example, no approximate analytic estimation of the critical temperature reduction caused by disorder (registered in the computer simulations [20, 26]) has been made before our research started. With our research we hope at least to contribute to a partial filling of these white spots.

Research connection with scientific programs, plans, themes. The thesis is prepared in the Institute for condensed matter physics of the NAS of Ukraine and in Laboratoire de Physique des Matériaux, Université Henri Poincaré, Nancy 1 according to the plans of the following themes: № 0105U002081 "Peculiarities of the condensed systems critical behaviour under the influence of an external field, structural disorder, frustration, and anisotropy" (2005-2007), № 0107U002081 "Development and application of the analytic theory and computer experiment methods to the description of transport phenomena in ion-electronic systems" (2007-2011); under support of the grant "Allocation de these en co-tutelle MESR", french-german PhD program Collège doctoral Franco-Allemand "Statistical Physics of Complex Systems", and CNRS (France) - NASU (Ukraine) cooperation project «Critical behaviour of structurally disordered and frustrated systems» (2005-2007).

Goal and tasks of the research. The *object of study* are classical two-dimensional spin models of continuous symmetry with lattice defects (non-magnetic impurities) distributed randomly on the lattice sites (quenched disorder). The *subject of study* is a research of the disorder and lattice finiteness influence on the behaviour of such models. The *goal of study* is to obtain quantitative characteristics of the behaviour of the models under consideration (for example, the pair correlation function decay exponent, the critical temperature) as functions of the nonmagnetic dilution concentration. As the *method of study* we use both analytical computations on the basis of the given models with the help of functional integration method [28–30] and Monte Carlo simulations with the Wolff algorithm [31].

Scientific novelty of the results. In the thesis the temperature-dependent pair correlation function exponent as a function of structural defects concentration is obtained and the result accords with the Monte Carlo simulations data better than the previously existing estimates. The

exponent of the residual spontaneous magnetization decay with the lattice size is obtained as well and it appears to be connected with the pair correlation function exponent as expected from the finite-size scaling theory. Within the approximate approaches explored in the work an argument in favor of the pair correlation function self-averaging is given at low temperatures.

For the first time non-magnetic impurities are explored in the context of the Villain model and the interaction between structural and topological defects is found from the microscopic Hamiltonian. A similar type of interaction is obtained in the frame of the Kosterlitz-Thouless phenomenological model through a procedure more appropriate for the lattice structure description than the methods previously used by other researchers. The estimates of the topological and structural defects interaction found for the Villain and Kosterlitz-Thouless models agree with each other as well as with the presently available computer experiment results.

On the basis of the results for the structural and topological defects interaction an analytical estimation of the topological phase transition (BKT transition) critical temperature reduction due to nonmagnetic dilution is given for the first time. The result obtained is in fair agreement with the available Monte carlo data.

The behaviour of the pair correlation function of a finite two-dimensional Heisenberg model is estimated in the low-temperature limit.

The spontaneous magnetization probability distribution in a finite two-dimensional XY model with quenched disorder is investigated in Monte Carlo simulations and analytically.

Practical value of the results. The results presented in the thesis can be useful for experimental researches of magnetic materials with two-dimensional XY model properties (layered magnets and ultrathin magnetic films with planar anisotropy).

Personal contribution of the researcher. In the papers written

with co-authors the contribution of the author includes:

- the pair correlation function and residual magnetization (for a finite lattice) behaviour estimation for the two-dimensional XY model in the spin-wave approximation [32–34];
- the diluted Villain model derivation from the diluted two-dimensional XY model in the low-temperature limit and the structural and topological defects interaction estimation from the microscopic diluted Villain model Hamiltonian [35, 37];
- the analytical estimation of the interaction between structural and topological defects in the phenomenological Kosterlitz-Thouless model [35];
- the analytical estimation of the BKT transition critical temperature reduction due to structural disorder [35];
- interpretation of the magnetization probability distribution functions in a finite two-dimensional XY model with disorder obtained in Monte Carlo simulations [33, 34];
- participation in Monte Carlo simulations [32–34];
- the pair correlation function behaviour in a finite two-dimensional Heisenberg model in the low-temperature limit [36].

Thesis results approbation. The results of the thesis have been reported and discussed at the following scientific meetings: "Statistical Physics and Low Dimensional Systems 2006: Atelier des groupes Physique Statistique et Surface et Spectroscopies du LPM" (Nancy, 17th-19th May 2006), "2nd International Conference on Quantum Electrodynamics and Statistical Physics (QEDSP2006)" (Kharkiv, 19th-23rd September 2006), "Statistical Physics and Low Dimensional Systems 2007: Atelier des groupes

Physique Statistique et Surface et Spectroscopies du LPM" (Nancy, 23rd-25th May 2007), "The 32nd Conference of the Middle European Cooperation in Statistical Physics (MECO32)" (Ladek Zdroj, Poland, 16th-18th April 2007), "Christmas discussions 2008" (Lviv, 4th-5th January 2008), "VII-th All-ukrainian seminar-school and competition of young scientists in the field of statistical physics and condensed matter – 2008" (Lviv, 5th-6th June 2008); and also in numerous seminars of the Condensed matter statistical theory section of the Institute for condensed matter physics of the National academy of sciences of Ukraine, of the theoretical group at Laboratoire de Physique des Matériaux (Université Henri Poincaré, Nancy 1), and in a seminar in the Theoretical Physics Institute in Leipzig (Germany).

Publications. Five papers [32–36], one preprint [37], and four conference abstracts [38–41] have been published on the materials of the thesis.

Chapter 1

LITERATURE OVERVIEW

In this chapter an overview of the main literature concerning spin models of continuous symmetry, especially the two-dimensional XY model, and with respect to the structural disorder influence is given.

1.1 Spin models of continuous symmetry

1.1.1 Topological defects

Presence of topological defects and their possible influence on the critical properties attract special attention to the spin models of continuous symmetry [3, 5]. For the first time topological defects drew the attention of researchers in the field of phase transitions and critical phenomena in connection to the extremely unusual behaviour of the two-dimensional XY model [6, 7]. The topological phase transition in this model gives the most profound example of the influence of topological defects on the critical properties of spin models with continuous symmetry. However, other similar models show interesting effects of a topological nature as well.

In a general case the Hamiltonian of a classical spin model of continuous symmetry can be written as:

$$H = -\sum_{\mathbf{r},\mathbf{r}'} J(\mathbf{r},\mathbf{r}')\mathbf{S}_{\mathbf{r}}\mathbf{S}_{\mathbf{r}'} , \tag{1.1}$$

where the sums span all the lattice sites, $\mathbf{S_r}$ is the value of a spin on the site $\mathbf{r}$, and $J(\mathbf{r}, \mathbf{r}')$ is the spin coupling for the sites $\mathbf{r}$ and $\mathbf{r}'$. Such models, as one knowns, can properly describe properties of a number of magnetic materials. Depending on the number of components of spins one distinguishes: XY model ($\mathbf{S_r} = (S^x_\mathbf{r}, S^y_\mathbf{r})$), Heisenberg model ($\mathbf{S_r} = (S^x_\mathbf{r}, S^y_\mathbf{r}, S^z_\mathbf{r})$), N-vector model ($\mathbf{S_r} = (S^1_\mathbf{r}, S^2_\mathbf{r}, \ldots, S^N_\mathbf{r})$).

In order to difine in a simple way what a topological defects is let us say that a topological defect is such a spin configuration that is characterized by some region (the core) of strong spin disorientation and the remaining area where the spin orientation changes slowly from one site to another (see fig.1.1). Of course, the above description is very loose, for a mathematical definition one should refer to [3, 42]. Topological defects have specific names in different models, for example, *vortices* in the two-dimensional XY model, or *hedgehogs* in the three-dimensional Heisenberg model [3].

The case of the two-dimensional XY model (also sometimes referred to as $O(2)$ model or the plane rotators model) will be discussed later in detail. For the moment let us mention the interesting effects caused by the presence of topological defects in other models described by a Hamiltonian of the form (1.1).

The three-dimensional XY model in contrast to its two-dimensional realization exhibits a more familiar ferromagnetic-paramagnetic phase transition picture with long-range order appearance [43, 44]. But there are works which present results in favor of the crucial role of topological defects (called *vortex strings* in this context) in the phase transition in this model (see, for example, [45]).

Another well known continuous symmetry spin model – the Heisenberg model (also called $O(3)$ model) – has quite different properties in $2D$ and $3D$ as well. In three dimensions the model undergoes a phase transition from the magnetically ordered state with a nonzero order parameter to the state of disorder [43]. Although the critical properties can

be described properly within the frames of the theories that do not take into account topological excitations, there are strong evidences about an essential influence of topological defects on the model behaviour [47–49]. Some works claim complete impossibility of the phase transition occurrence if topological defects are excluded (that can be artificially achieved in Monte Carlo simulations using unfavourable chemical potential associated to the topological defects) [47, 48], others only mention the change of critical exponents in this case [49].

The two-dimensional Heisenberg model behaviour remains in some sense a controversial question even today. Topological defects that can exist in this model are called *instantons* [46]. The previously mentioned Mermin-Wagner-Hohenberg theorem [10, 11] denies the very possibility of long-rang ordering at any nonzero temperature (in the thermodynamic limit), but the early high-temperature expansions [50] were in favor of a phase transition in the Hesinberg model in two dimensions as well as in the $2D$ XY model. In the two-dimensional XY model case these results were subsequently supported by the discovery of the BKT transition. In contrast to this, the $2D$ Heisenberg model has not received any subsequent evidences for a phase transition, and the Polyakov renorm-group analysis [46, 51] claimed absence of any phase transition at nonzero temperature. That conclusion has become generally accepted, although there are alternative opinions (see, for example, [5, 52]) in favour of a phase transition similar to that in the two-dimensional model.

1.1.2 Two-dimensional XY model

As it is definitely known today, topological defects play a crucial role in the critical behaviour of the two-dimensional XY model and related models [4, 42]. One of the exact results for spin models of continuous symmetry in one and two dimensions is the *Mermin-Wagner-Hohenberg theorem* [10, 11] which denies existence of any spontaneous magnetization at

nonzero temperature. This property is caused by the fact that in an infinite lattice with dimensions less than three, spin-wave excitations destroy any long-range order even at arbitrary small temperatures. But the spin pair correlation function behaves in a different way in $1D$ and $2D$ systems, although it decays to zero with distance in both cases. The spin-wave approximation applicable in the low-temperature limit ($T \to 0$) gives the following asymptotic forms of the pair correlation function as a function of the distance R in the XY model in different dimensions [16, 42]:

$$G_2(R) \underset{R\to\infty}{\sim} \begin{cases} \text{const} \ , & d \geq 3 \ ; \\ R^{-\eta} \ , & d = 2 \ ; \\ e^{-\alpha R} \ , & d = 1 \ . \end{cases} \tag{1.2}$$

It is obvious that the two-dimensional case is very particular. Although the correlations decay with distance, so one can not speak about long-range ordering, they decay algebraically that is much slower than in the case of a usual magnetic disorder (which can be observed in the same model in $1D$, for example). This phenomenon is called *quasi-long-range ordering.*

The Hamiltonian of the two-dimensional XY model with the nearest neighbours interaction writes as:

$$H \ = \ - \ J \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \left(S^x_{\mathbf{r}} S^x_{\mathbf{r}'} + S^y_{\mathbf{r}} S^y_{\mathbf{r}'} \right) \ , \tag{1.3}$$

where the sum spans all the nearest neighbour pairs in a square lattice, and J is the coupling constant.

Besides possible description of the properties of such an important physical object as the superfluid helium, the two-dimensional model can also apply to more closely related real physical systems such as magnets with planar anisotropy. Of course, low dimensionality restricts its application to so called quasi-two-dimensional magnets [55] such as layered magnets (three-dimensional structures with weak interplane interaction) and ultrathin magnetic films. Although the mentioned materials should

be described by three-component Heisenberg spins rather than by two-component XY spins [55], easy plane spin anisotropy and weak interplane coupling draw their properties closely to those typical for the $2D$ XY model [55–57].

Another interesting subject is the investigation of stability and behaviour of vortices (similar to those in the $2D$ XY model) in the two-dimensional Heisenberg model with easy-plane anisotropy [54, 68, 70]. The researches show qualitative resemblance to the $2D$ XY model behaviour in a wide interval of the disorder parameter values [56–58].

Features of the $2D$ XY model behaviour can be observed in some temperature region even in so unlike (in the sense of its symmetry) model as the two-dimensional clock model with $q > 4$ [4, 59].

So, on one hand, the two-dimensional XY model really has a great practical value describing (at least qualitatively) an important class of magnetic materials, and, on the other hand, it is highly interesting from the fundamental theoretical point of view revealing the most profound topological defects influence. It is moreover accessible for analytical researches.

It is convenient to investigate the low-temperature phase of the $2D$ XY model analytically in the spin-wave approximation which is supposed to be quantitatively reliable in the low-temperature limit and also gives qualitatively correct results in the whole quasi-long-range ordering phase [18].

The spin-wave approximation means the substitution of the scalar product of spins in the Hamiltonian (1.3) with an approximate expansion up to the quadratic term in the angle $\left(\widehat{\mathbf{S}_{\mathbf{r}}, \mathbf{S}_{\mathbf{r}'}}\right)$ between the spins [16]:

$$S^x_{\mathbf{r}} S^x_{\mathbf{r}'} \; + \; S^y_{\mathbf{r}} S^y_{\mathbf{r}'} \; = \; \cos\left(\widehat{\mathbf{S}_{\mathbf{r}}, \mathbf{S}_{\mathbf{r}'}}\right) \; \to \; 1 \; - \; \frac{1}{2}\left(\widehat{\mathbf{S}_{\mathbf{r}}, \mathbf{S}_{\mathbf{r}'}}\right)^2 \; . \qquad (1.4)$$

Such a substitution is acceptable only at low enough temperatures when the neighbouring spins are oriented almost in the same direction.

In the spin-wave approximation the Hamiltonian (1.3) can be diagonalized and the model admits analytical solution. The pair correlation function of spins shows a power law decay with distance [16]:

$$\langle \mathbf{S_r}, \mathbf{S_{r+R}} \rangle \ \sim \ R^{-\eta(T)} \tag{1.5}$$

with the non-universal temperature-dependent exponent

$$\eta(T) \ = \ \frac{k_B T}{2\pi J} \ , \tag{1.6}$$

where k_B – the Boltzman constant. Divergence of the magnetic susceptibility in the low-temperature phase follows from the above result as well [16].

The finite two-dimensional XY model possesses some residual spontaneous magnetization which goes to zero as the lattice size increases [13, 14, 60]. The spontaneous magnetization can be defined as:

$$\langle m \rangle \ = \ \frac{1}{N} \left\langle \sqrt{\left(\sum_{\mathbf{r}} \mathbf{S_r} \right)^2} \right\rangle \ . \tag{1.7}$$

This decay is so slow that spontaneous magnetization can be observed even in macroscopic magnetic samples [13, 14]. The spin-wave approximation gives a power law vanishing of the magnetization with the lattice size $N = L \times L$ (L is the linear size):

$$\langle m \rangle \ = \ N^{-\eta(T)/4} \ , \tag{1.8}$$

with the exponent η defined by (1.6).

But the thermodynamically averaged value of the magnetization alone does not contain in itself the complete information about the finite system properties. As the researches [60, 62] suggest important scientific value has the form of the magnetization probability distribution which appears to be non-Gaussian and non-universal (in the sense of its independence of the system size and exponent η). This is a consequence of the quasi-long-range correlation in the system and accord well with the fact that the correlation length ξ is divergent in the low-temperature phase [42].

1.1.3 Vortices in two-dimensional XY model

The spin-wave approximation describes the behaviour of the model quantitatively correct only in the limit of low temperatures. This is so because according to the Kosterlitz-Thouless theory [7] at low temperatures topological defects are closely bound in neutral vortex-antivortex pairs which insufficiently disturb the spin field and thus in fact do not show themselves in the model properties. As the temperature increases the mean distance between the vortices in the bound pairs becomes larger and their influence on the model behaviour correspondingly increases, but somehow the spin-wave theory continues to give qualitatively correct results for the pair correlation function and other physical characteristics behaviour in the system in the whole low-temperature phase, only the real temperature should be replaced with some effective value [8, 18].

In spite of such a wide temperature region of its applicability (at least for a qualitative description) the spin-wave approximation does not give any information about the most exciting phenomenon in the two-dimensional XY model – the Berezinskii-Kosterlitz-Thouless transition. The model described by the spin-wave Hamiltonian remains quasi-long-range ordered at any finite temperature and no phase transition occurs [16].

Spin vortices (topological defects) (see fig.1.1) introduced by Kosterlitz and Thouless to explain the unusual phase transition on a phenomenological level [7] later received a firm support of their existence and importance both in experimental (meaning Monte Carlo experiments) [13, 71] and theoretical [17, 18] researches. As great achievement, in the topic one should consider the approximate model proposed by Villain [17] and subsequently called with his name. Within this frame the vortex spin configurations and their $2D$-Coulomb-like interaction can be analytically obtained directly from the microscopic Hamiltonian. Although the Villain model can be formally considered as an independent model with a specifically defined Hamiltonian possessing together with the $2D$ XY model spin vortices

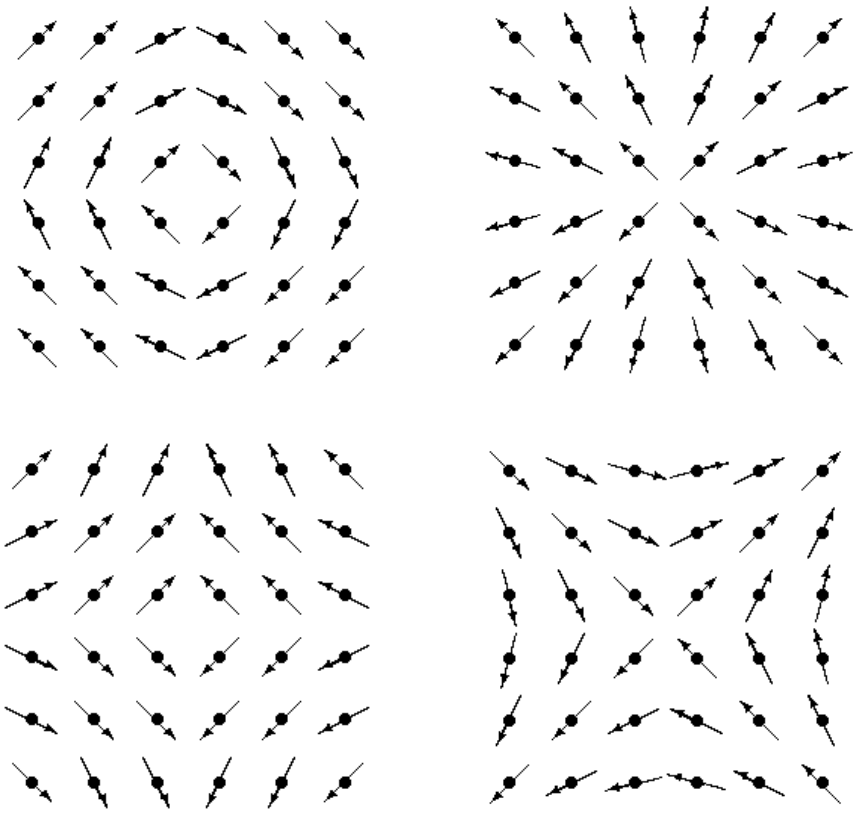

Figure 1.1: Examples of vortices with topological charges equal to $+1$ (top) and -1 (bottom) in the two-dimensional XY model.

and a topological phase transition, in the low-temperature limit it can be mathematically derived from the $2D$ XY model Hamiltonian [18]. Thus, at least at low temperatures, one can be confident with the fact that the Villain model vortices are equivalent to those of the two-dimensional XY model (though at higher temperatures their behaviour can differ because the difference in their critical temperature values (non-universal property) are remarkably different [66]). In fig.1.1 some examples of the vortices with diverse topological charges are presented (vortices with the same charges are topologically equivalent though they differ visually). The researches suggest that real influence on the model behaviour can make only vortices with charges with the absolute value equal to one [18], topological defects with higher values of the charge are energetically unfavourable.

According to the Kosterlitz-Thouless theory [7] the phase transition in the $2D$ XY model has features of the insulator-conductor transition in the two-dimensional Coulomb gas [9]. The mean distance between the vortices bound in pairs increases with temperature and finally at some critical value T_{BKT} dissociation of such pairs happens. The resulting gas of free topological defects ruins any quasi-long-range ordering in the system.

1.2 Structural disorder

1.2.1 Quenched and annealed disorder

The concept of disorder in the context of condensed matter physics is very broad and can apply in fact almost to any physical system [76–78]. Our research concerns lattice spin models of continuous symmetry and this defines the circle of possible types of disorder that can be added to this models. For example, in the two-dimensional XY model one can study disorder in the form of a random phase shift (for example, [79, 81]), random local field (for example, [80, 81]), random anisotropy (for example, [82, 83]) or random coupling constant (for example, [27, 100]). But perhaps the most typical kind of disorder in magnetic systems is the positional disorder which means that some sites in the lattice are randomly occupied by nonmagnetic ions [1, 2]. Such a model of disorder describes appropriately defects in real magnetic materials. Already in the first profound works devoted to this problem [2] an idea about configurational averaging (averaging over all the possible realizations of disorder) of observable physical quantities arised. Mazo [84] showed that the free energy of a physical system depending not only on dynamical variables (atomic spins in our case) but also on random variables (nonmagnetic impurities positions, for example), with some fixed probability distribution function, should be the averaged value of the free energy as a function of the random variables.

The described situation corresponds to *nonequilibrium* impurities distribution defined phenomenologically. This kind of disorder is called *quenched disorder* and it reflects the situation in real physical samples properly, since the relaxation time of such impurities is usually very large compared to the timescale of the spin relaxation. A specific property of the quenched disorder influence on the behaviour of magnetic systems is the existence of the *percolation threshold* [1, 85, 86].

However, there is also another type of positional disorder which is called *annealed* in contrast to the quenched one (see, for example, [88, 89]). In this case the positions of nonmagnetic ions are defined by the thermodynamic equilibrium state and their distribution is at equilibrium. From the mathematical point of view this means that the free energy of the system is the logarithm of the configurationally averaged partition function. When computing other thermodynamical quantities the averaging over the variables describing the impurities positions should be added to the trace over the spin variables. In fact, annealed disorder is equivalent to the lattice-gas magnetic models.

There are some works devoted to the research of the impurities relaxation dynamics, i.e. the transition from the quenched to annealed disorder (see, for example, [90]). Another link between two different types of disorder can be seen in the works that suggest to study quenched disorder through some fictitious system with annealed disorder constructed in such a way that it has the properties analogous to the properties of the initial system (see [91]).

When dealing with quenched disorder, attention should be paid to the self-averaging property of the system physical quantities [92–94]. In the case when a quantity is non-self-averaging, its configurational average obtained on the basis of a finite set of disorder realizations will not represent properly its real observable value.

1.2.2 Disorder in two-dimensional XY model

Since our study mostly concerns quenched disorder, let us give only a very brief excursus to the works on the influence of annealed disorder on the two-dimensional XY model behaviour. $2D$ XY model is used in particular to describe ^{3}He-^{4}He mixture in two dimensions [95, 96] and realizes the classical two-dimensional ferromagnetic lattice gas model [98]. The existence of the quasi-long-range ordering at low temperatures in this model is proved rigorously [101] and supported by Monte Carlo simulations [97]. The critical temperature decreases as the nonmagnetic impurities concentration increases [97]. There are also convincing evidences about a first order phase transition which occurs at some values of the dilution concentration in this model [98–100]. This phenomenon appears only for annealed disorder and does not have place in the model with quenched disorder [20, 26].

Quenched disorder in the two-dimensional XY model causes reduction of the critical temperature which, as a function of nonmagnetic sites concentration, decreases with concentration and turns to zero at some finite critical value of concentration [20, 26] (see fig.1.2). Today there are practically no doubts that this critical concentration coincides with the percolation threshold [20, 26] (which is $c \simeq 0.59$ [105] for the square lattice which is usually considered). Thus the quasi-long-range ordering phase exists until there is an infinite percolation cluster in the system. Ones the concentration of magnetic sites reaches the percolation threshold any ordering becomes impossible. Before our research started no analytical estimation of the critical temperature of a diluted $2D$ XY model as a function of dilution concentration existed in the literature.

According to the Harris criterium [15], universal critical exponents of the $2D$ XY model at the BKT transition remain unchanged by quenched structural disorder. Obviously, this is true only for such dilution concentrations at which an infinite percolation cluster exists. Thus the value of

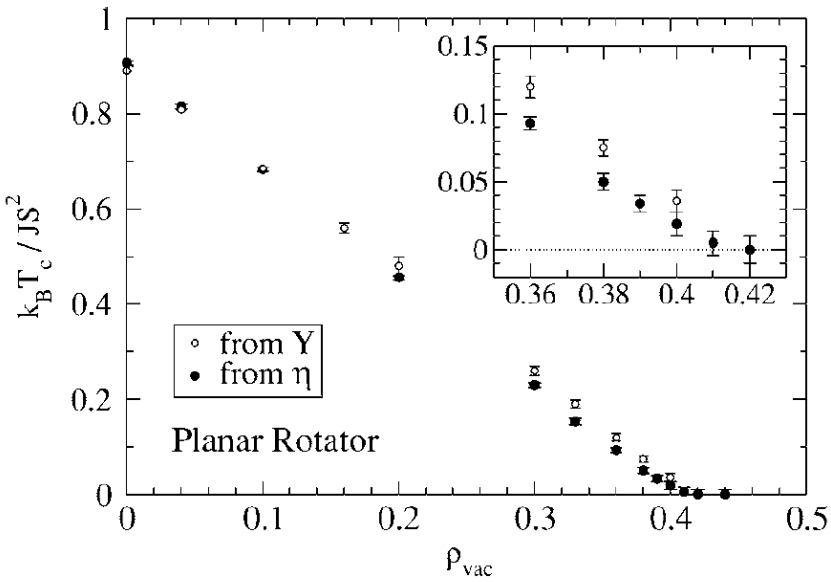

Figure 1.2: Phase diagram quoted from [26]: $2D$ XY model critical temperature as a function of nonmagnetic sites concentration observed in Monte Carlo simulations. The insert shows the vicinity of the percolation threshold.

the pair correlation function exponent at the critical point which is universal ($\eta(T_{\mathrm{BKT}}) = 1/4$ [8]) remains the same in the model with disorder. However, in the low-temperature phase the exponent η depends on the temperature and coupling constant [16], thus it is not universal. As the researches show in the model with structural disorder the exponent η also depends on the nonmagnetic impurities concentration increasing with the dilution concentration [20].

The residual spontaneous magnetization behaviour in a finite two-dimensional XY model with quenched disorder stayed unexplored until very recently.

Finally, one of the most crucial questions concerning nonmagnetic dilution in the $2D$ XY model is the form of the interaction between nonmagnetic impurities and topological defects present in the system. The knowledge of this interaction can be of use in calculating the critical tem-

perature reduction connected with the dilution and also is important itself concerning the possible applications in nanotechnology [104].

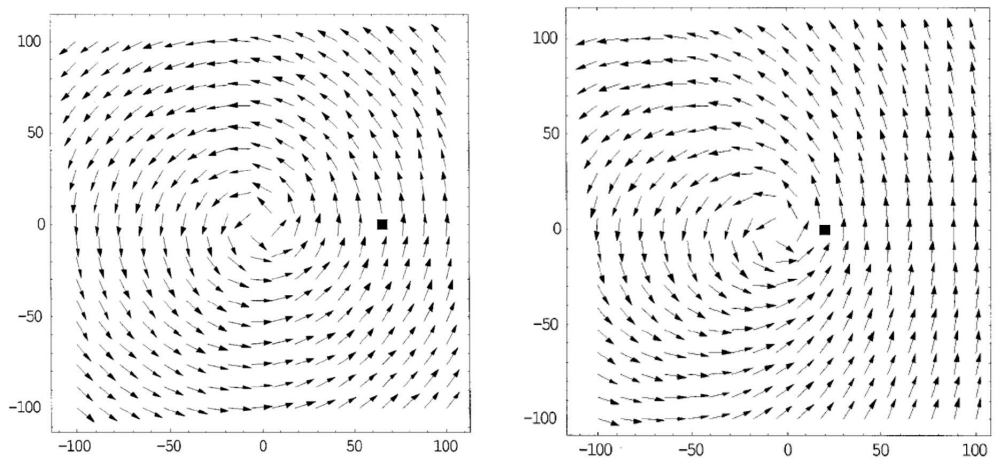

Figure 1.3: A spin vortex centered in (0,0) with a nonmagnetic vacancy in (5,0) (left) and (1,0) (right) obtained through energy minimization of the spin field [21].

The first paper [21] devoted to the research of the interaction between a spin vacancy and a topological defect suggested a repulsive form of the interaction due to the incorrect estimation scheme. It was based upon the continuous elastic medium approximation with artificially introduced topological defect configurations (the Kosterlitz-Thouless model), and a spin vacancy was presented in this model by some cutout area removed from the continuous spin field. In fig.1.3 quoted from [21] one can see a spin configuration obtained by a minimization of the energy of the spin field (vortex structure was guaranteed by antisymmetric boundary conditions) with a spin vacancy (a cutout) at the distance of five (left) and one (right) lattice constants from the vortex center (on the right side there is a visible distortion of the initial vortex form which looks like a "screening" of the spin field behind the vacancy). The energy of the vortex with a vacancy situated closer to its center has a greater value, so it is energetically preferable for a vortex to keep away from a spin vacancy.

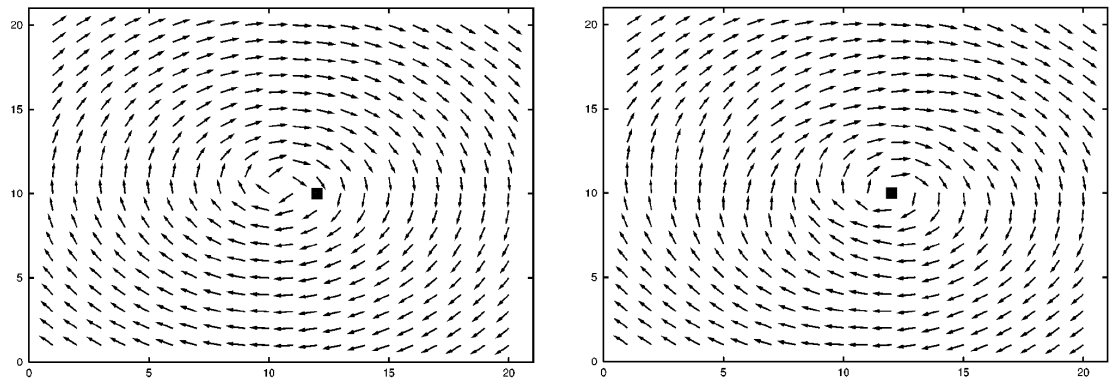

Figure 1.4: Spin dynamics simulation results for a vortex spin configuration with a nonmagnetic vacancy [24]. Comparison of the initial configuration (left) with the configuration obtained after 150 time steps (right) suggests an attractive interaction between the vacancy and the vortex center.

However, Monte Carlo and spin dynamics simulations strongly suggested the opposite picture of interaction [24]: vacancies attract topological defects and pin them (see fig.1.4). Calculations redone with the crucial assumption about the vortex configuration unchanged by the presence of a vacancy leaded to a qualitatively correct result [24]. Of course, speaking rigorously, such an assumption is not completely true, it is an approximation needed to avoid physically incorrect consequences when substituting the discrete lattice with a continuous spin field. One can assume that the truth is somewhere in between: the spin field changes due to the presence of a vacancy but only locally and not so globally as it appears in fig. 1.3. Another disadvantage of the study [24] can be seen in the dependence of the interaction result on the way one chooses the "vacancy" cutout form, i.e. on its area which is somewhat indefinite and moreover is not linked to the microscopic structure of the lattice (the coordination number, for example).

Attractive form of the interaction between structural and topological defects is supported by the studies of other model possessing vortices as well [23].

1.3 Conclusions

The presented overview reveals great theoretical and practical value of the research of the influence of positional disorder on the behaviour of two-dimensional spin models of continuous symmetry (and especially the $2D$ XY model), and in the same time it shows the insufficiency of such researches remaining for today. Particularly interesting seems the question of the lattice finiteness influence on such models behaviour which has never been investigated in combination with structural disorder. The form of the interaction between structural defects and spin vortices is important also from the point of view of the modern nanotechnology development and search of new data storage methods, since vortex structures are often observed in nanostructured magnetic thin films (see [104], for example).

The described situation opens an intriguing field for scientific research which the present thesis tries to cover at least partially.

Chapter 2

TWO-DIMENSIONAL XY MODEL WITH DISORDER

This chapter presents a study of the influence of structural disorder on the behaviour of the two-dimensional XY model at temperatures sufficiently lower than the Berezinskii-Kosterlitz-Thouless transition temperature. In this interval of temperatures one can with good precision neglect the impact of the topological defects present in the system, so the spin-wave approximation can be of use. We will present an original perturbation theory: expansion in the parameter which characterizes dilution (several alternative candidates for such a parameter are proposed). Our attention will be mainly focused on the pair correlation function behaviour which is one of the most interesting characteristics of the two-dimensional XY model. Together with the analytical treatment a series of Monte Carlo simulations were performed for the $2D$ XY model with different concentrations of dilution; the results of these simulations are presented in this chapter as well. We will compare the computer experiment data to the analytical results. The most essential results of this chapter were published in [32–34, 37–41].

2.1 Quenched dilution

2.1.1 Configurational averaging

Herein, quenched dilution (disorder) in a ferromagnetic system means random replacement of some fraction of magnetic lattice sites with nonmagnetic impurities (spin vacancies). The mathematical description deals with the "occupation numbers":

$$c_{\mathbf{r}} = \begin{cases} 1 \ , & \text{if site } \mathbf{r} \text{ has a spin ;} \\ 0 \ , & \text{if site } \mathbf{r} \text{ is empty .} \end{cases} \tag{2.1}$$

Setting a certain set of the variables $\{c_{\mathbf{r}}\}$ any disorder configuration can be realized with a given dilution concentration. We will deal with uncorrelated random disorder, i.e. the occupation probability for a site is independent of the other sites states. Thus, to obtain such a disorder configuration with the concentration c of magnetic sites (and concentration $1-c$ of nonmagnetic impurities respectively) it is enough to set the probability $P(c_{\mathbf{r}})$ for the site $\mathbf{r}$ to be empty or occupied by a spin:

$$P(c_{\mathbf{r}}) = \begin{cases} \mathrm{c} \ , & \text{if } \mathrm{c}_{\mathbf{r}} = 1 \ ; \\ 1-\mathrm{c} \ , & \text{if } \mathrm{c}_{\mathbf{r}} = 0 \ . \end{cases} \tag{2.2}$$

Following [2], we distinguish quenched disorder (when the impurities are filled randomly in the system) and annealed disorder when nonmagnetic sites are in their thermodynamic equilibrium positions. In fact, such annealed disorder is nothing else but another formulation of a lattice-gas ferromagnetic model [97] where spin sites have a space degree of freedom: their position in the lattice. In the annealed disorder case the partition function of the system should be averaged for all the possible realizations of disorder, this just means inclusion of the magnetic sites space coordinates into the trace. Contrary, according to [2, 84] when dealing with quenched disorder such averaging can be and should be done only for observable

physical quantities such as the free energy or, for example, the spin pair correlation function.

The present research is restricted to the uncorrelated quenched disorder consideration, so hereafter speaking about disorder/dilution we will always mean quenched impurities distribution (except where something else is explicitely stated). The configurationally averaged physical quantities will be of importance. A dash over an expression, $\overline{(\ldots)}$, will denote configurational averaging; mathematically it can be defined as:

$$\begin{aligned}\overline{(\ldots)} &= \sum_{c_{\mathbf{r}_1}=0,1} \cdots \sum_{c_{\mathbf{r}_N}=0,1} \left[\prod_{\mathbf{r}} P(c_{\mathbf{r}})\right] (\ldots) \\ &= \sum_{c_{\mathbf{r}_1}=0,1} \cdots \sum_{c_{\mathbf{r}_N}=0,1} \left[\prod_{\mathbf{r}} (c\delta_{1-c_{\mathbf{r}},0} + (1-c)\delta_{c_{\mathbf{r}},0})\right] (\ldots) \ . \quad (2.3)\end{aligned}$$

Sometimes quantities averaged in such a way will be called configurational averages (in analogy with thermodynamical averages) but mostly we will implicitly mean configurationally averaged values when speaking about observable physical quantities. For example, the free energy of the system which is an observable quantity and thus has to be averaged over all possible configurations of disorder will be given by the expression:

$$F_{\text{dis}} = -T\,\overline{\ln Z_{\text{conf}}} \quad (2.4)$$

where T – the temperature in energy units, and Z_{conf} – the configurationally dependent partition function which depends on the particular disorder realization and generally is given by the expression:

$$Z_{\text{conf}} = \text{Tr}\ e^{-H(\{c_{\mathbf{r}}\})/T} \quad (2.5)$$

with $H(\{c_{\mathbf{r}}\})$ being the system Hamiltonian dependent on the occupation numbers (2.1) along with the spin variables, and Tr(...) meaning only integration over the spin degrees of freedom.

Another important characteristic, the pair correlation function of spins, averaged over disorder configurations has the form:

$$G(\mathbf{R}) \;=\; \overline{c_{\mathbf{r}}c_{\mathbf{r}+\mathbf{R}}\langle \mathbf{S}_{\mathbf{r}}\mathbf{S}_{\mathbf{r}+\mathbf{R}}\rangle} \;=\; \overline{\frac{c_{\mathbf{r}}c_{\mathbf{r}+\mathbf{R}}}{Z_{\mathrm{conf}}}\,\mathrm{Tr}\; e^{-H(\{c_{\mathbf{r}}\})/T}\mathbf{S}_{\mathbf{r}}\mathbf{S}_{\mathbf{r}+\mathbf{R}}}\;. \tag{2.6}$$

2.1.2 Self-averaging

Systems with quenched disorder can be characterized by such a property as self-averaging [92]. In the previous subsection the configurational averaging procedure was defined, but the practical value of such an averaged quantity is related to the form of its probability distribution over different realizations of disorder. The value of an arbitrary physical quantity X in a system with disorder depends on the exact form of the disorder configuration, thus, it is a random quantity described by the probability distribution function $P(X,N)$ dependent on the size N of the system. If one desires to describe the system with the configurational average $\overline{X}$ one should check the relative variance of the distribution $P(X,N)$:

$$R_X(N) \;=\; \frac{\overline{X^2} \;-\; \overline{X}^2}{\overline{X}^2}\;. \tag{2.7}$$

If the relative variance of a macroscopic quantity X goes to zero, $R_X \to 0$, in the thermodynamic limit ($N \to \infty$) then one says that X is self-averaging and thus the system can be described explicitly by the configurational average $\overline{X}$. If R_X goes with $N \to \infty$ to a finite constant value then the system is said to be non-self-averaging. When $R_X \to 0$ there are different degrees of self-averaging which can be distinguished depending on the form of the decay of R_X. When $R_X \sim N^{-1}$ one says about strong self-averaging, and if $R_X \sim N^{-z}$ $(0 < z < 1)$ the self-averaging is weak.

Beyond the critical region the additivity property along with the central limit theorem automatically lead to a strong self-averaging, i. e. $R_X \sim N^{-1}$ (this is true for additive quantities, of course). However, at the

critical point the situation becomes more complicated because of the long-range critical correlations; it has been shown by the renormalization group technic [92] that in the case of relevant disorder (when disorder influences the critical behaviour, according to the Harris criterium) the self-averaging is lost at the critical point. Though at the very critical point of the BKT transition in the $2D$ XY model disorder is irrelevant according to the Harris criterium [15], the whole low-temperature phase ($T < T_{\mathrm{BKT}}$) is critical, and there disorder has visible influence on the properties of the model, for example, the nonuniversal pair correlation function exponent depends on the dilution concentration [20]. This poses an important task of finding along with the configurationally averaged values of physical quantities like (2.4) and (2.6) their relative variances (2.7).

2.2 Spin-wave approximation

2.2.1 Spin-wave Hamiltonian

A spin in the model (1.3) has a fixed length (we choose it equal to one), thus, in fact, each site is described by a single degree of freedom. Instead of the two spin components, $S^x_{\mathbf{r}}$ and $S^y_{\mathbf{r}}$, let us introduce a single variable which describes rotation of a spin in two-dimensional space; the angle between the spin and an arbitrary fixed reference direction in the plain of its rotation can serve as such a variable. Introducing in this way the angle variables $\theta_{\mathbf{r}}$ the scalar product $S^x_{\mathbf{r}}S^x_{\mathbf{r}'} + S^y_{\mathbf{r}}S^y_{\mathbf{r}'}$ can be rewritten as a cosine of the angle difference between the two spins: $\cos(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})$. The Hamiltonian (1.3) then writes as:

$$H \;=\; -\,J\sum_{\mathbf{r}}\sum_{\alpha=x,y}\cos(\theta_{\mathbf{r}+\mathbf{a}_\alpha} - \theta_{\mathbf{r}})\ , \tag{2.8}$$

where $\mathbf{a}_x$, $\mathbf{a}_y$ – the elementary cell basis.

The Hamiltonian of the two-dimensional XY model with quenched

disorder can be written using the occupation numbers (2.1):

$$H \;=\; -\,J\sum_{\mathbf{r}}\sum_{\alpha=x,y}\cos(\theta_{\mathbf{r}+\mathbf{a}_\alpha}-\theta_{\mathbf{r}})\;c_{\mathbf{r}+\mathbf{a}_\alpha}c_{\mathbf{r}}\;. \tag{2.9}$$

It is obvious that (2.9) as well as (2.8) is minimal when all spins are parallel. Considering low temperatures one can obtain satisfactory results by taking into account only low energy excitations which are small deviations from the ground state. In this case the difference between the angles $\theta_{\mathbf{r}}$ on neighbouring sites remains small and the cosine can be expanded in a Taylor series around the energy minimum:

$$\cos\left(\theta_{\mathbf{r}+\mathbf{a}_\alpha}-\theta_{\mathbf{r}}\right)\;\rightarrow\;1-\frac{1}{2}\left(\theta_{\mathbf{r}+\mathbf{a}_\alpha}-\theta_{\mathbf{r}}\right)^2\;. \tag{2.10}$$

The Hamiltonian (2.9) will write as:

$$H\;\simeq\;H_0\;+\;H_{\mathrm{sw}},$$

where

$$H_{\mathrm{sw}}\;=\;\frac{1}{2}\,J\sum_{\mathbf{r}}\sum_{\alpha=x,y}\left(\theta_{\mathbf{r}+\mathbf{a}_\alpha}-\theta_{\mathbf{r}}\right)^2\;c_{\mathbf{r}+\mathbf{a}_\alpha}c_{\mathbf{r}} \tag{2.11}$$

will be referred of as the "spin-wave" Hamiltonian, and according to (2.2) H_0 can be written with good precision as:

$$H_0\;=\;-\,J\sum_{\mathbf{r}}\sum_{\alpha=x,y}c_{\mathbf{r}+\mathbf{a}_\alpha}c_{\mathbf{r}}\;\simeq\;-\,2Jc^2\;.$$

H_0 does not depend on the spin degrees of freedom, and thus reduces to a constant added to the free energy:

$$F\;\simeq\;F_{\mathrm{sw}}\;+\;2Jc^2$$

$\left(F_{\mathrm{sw}}\;=\;-T\ln\left(\mathrm{Tr}\;e^{-H_{\mathrm{sw}}/T}\right)\right)$, and does not enter the observable physical quantities such as the spin pair correlation function, for example.

The trace, $\mathrm{Tr}\ldots$, over the spin degrees of freedom can be defined in terms of the angle variables $\theta_{\mathbf{r}}$ as a functional integral:

$$\mathrm{Tr}_\theta \ldots = \left[\prod_{\mathbf{r}} \int_{-\pi}^{\pi} \frac{d\theta_{\mathbf{r}}}{2\pi}\right] \ldots \ . \tag{2.12}$$

The coefficient $1/(2\pi)$ appears from the normalization: $\mathrm{Tr}_\theta 1 = 1$. To obtain a thermodynamic average in the spin-wave approximation we will use the following formula:

$$\langle \ldots \rangle = \frac{\mathrm{Tr}_\theta \left[e^{-\beta H_{\mathrm{sw}}} \ \ldots\right]}{\mathrm{Tr}_\theta \ e^{-\beta H_{\mathrm{sw}}}} \ . \tag{2.13}$$

Of course, any observable quantity which characterizes the diluted model (2.11) along with the thermodynamical averaging should be averaged over the configurations of disorder according to the formula (2.3):

$$\overline{\langle \ \ldots \ \rangle} = \overline{\left(\frac{\mathrm{Tr}_\theta \left[e^{-\beta H_{\mathrm{sw}}} \ \ldots\right]}{\mathrm{Tr}_\theta \ e^{-\beta H_{\mathrm{sw}}}}\right)} \ . \tag{2.14}$$

The dependence of the Hamiltonian H_{sw} on the occupation numbers, Eq. (2.11), puts a nontrivial problem which will require approximate approaches.

2.2.2 Fourier transformation on a two-dimensional lattice

In the pure model case (Eq. (2.8)) the spin-wave approximation (2.10) allows to find an analytic solution of the model by passing to the Fourier variables $\theta_{\mathbf{k}}$ according to the transformation formulas:

$$\theta_{\mathbf{r}} = \tfrac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{kr}} \theta_{\mathbf{k}} \ , \qquad \theta_{\mathbf{k}} = \tfrac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\mathbf{kr}} \theta_{\mathbf{r}} \ , \tag{2.15}$$

where the sum over $\mathbf{k}$ spans N sites of the reciprocal lattice within the first Brillouin zone (N is the number of sites in the original lattice). In terms of the variables $\theta_{\mathbf{k}}$ the Hamiltonian (2.8) has a diagonal form (decomposes

into a sum of terms each of which depends on a single wave-vector $\mathbf{k}$) and is written as [16]:

$$H_{\rm sw}^{\rm p} \;=\; \frac{J}{2}\sum_{\mathbf{k}}\sum_{\alpha=x,y} K_\alpha^2(\mathbf{k})\;\theta_{\mathbf{k}}\theta_{-\mathbf{k}}\;, \tag{2.16}$$

where $K_\alpha(\mathbf{k}) \;\equiv\; 2\sin\frac{\mathbf{k}\mathbf{a}_\alpha}{2}$.

Although the Hamiltonian with quenched impurities, Eq. (2.11), cannot be diagonalized in such a way, we apply the Fourier transformation (2.15) since our approach will be based on an extraction of the diagonal part in (2.11) which will correspond to the undiluted system (2.16).

Before calculating any thermodynamical quantities with the Hamiltonian written in the Fourier variables on should express the trace (2.12) in terms of $\theta_{\mathbf{k}}$ too. This can be done with the help of the well known formula for the change of variables in a multiple integral [106]:

$$\begin{aligned}&\int\ldots\int f(x_1,\ldots,x_n)\;dx_1\ldots dx_n \\ &=\int\ldots\int f(x_1(\xi_1,\ldots,\xi_n),\ldots x_n(\xi_1,\ldots,\xi_n))\;\mid\mathcal{J}\mid\;d\xi_1\ldots d\xi_n\;,\end{aligned} \tag{2.17}$$

where x_i are the initial variables, ξ_i are the new variables, and $\mathcal{J} = \det(\partial x_i/\partial\xi_j)$ is the transformation Jacobian. The transformation (2.15) is linear , thus one can conclude straightforwardly that the Jacobian is constant and can be put outside the integral.

Obviously, $\theta_{\mathbf{k}}$ are complex quantities: $\theta_{\mathbf{k}} = \theta_{\mathbf{k}}^c + i\theta_{\mathbf{k}}^s$, and from the first look it seems that one has too many new variables than one needs; however, it is easy to see that not all of them are independent because $\theta_{-\mathbf{k}} = \theta_{\mathbf{k}}^*$. To exclude the extra variables we will consider only $\theta_{\mathbf{k}}$ with $\mathbf{k}$ within one arbitrary half of the first Brillouin zone (for example, $\left(0\le k_x\le\frac{\pi}{a}, 0<k_y\le\frac{\pi}{a}\right)\bigcup\left(0<k_x\le\frac{\pi}{a}, -\frac{\pi}{a}\le k_y\le 0\right)$, see fig. 2.1) and we will denote this domain as B_+, and the rest of the 1st Brillouin zone will be denoted as B_- (the point $\mathbf{k}=0$ will be considered separately).

Then, the Hamiltonian (2.16) will read as:

$$\begin{aligned} H^{\mathrm{p}}_{\mathrm{sw}} &= \frac{J}{2}\sum_{\mathbf{k}\in B_+}\sum_{\alpha=x,y} K^2_\alpha(\mathbf{k})\ \theta_{\mathbf{k}}\theta_{-\mathbf{k}} \ + \ \frac{J}{2}\sum_{\mathbf{k}\in B_-}\sum_{\alpha=x,y} K^2_\alpha(\mathbf{k})\ \theta_{\mathbf{k}}\theta_{-\mathbf{k}} \\ &= \frac{J}{2}\sum_{\mathbf{k}\in B_+}\sum_{\alpha=x,y} K^2_\alpha(\mathbf{k})\ \theta_{\mathbf{k}}\theta_{-\mathbf{k}} \ + \ \frac{J}{2}\sum_{\mathbf{k}\in B_+}\sum_{\alpha=x,y} K^2_\alpha(-\mathbf{k})\ \theta_{-\mathbf{k}}\theta_{\mathbf{k}} \\ &= J\sum_{\mathbf{k}\in B_+}\sum_{\alpha=x,y} K^2_\alpha(\mathbf{k})\ |\theta_{\mathbf{k}}|^2\ , \end{aligned} \tag{2.18}$$

where $|\theta_{\mathbf{k}}| = \sqrt{\theta_{\mathbf{k}}\theta_{-\mathbf{k}}} = \sqrt{(\theta^c_{\mathbf{k}})^2 + (\theta^s_{\mathbf{k}})^2}$. Let us note that $\theta_{\mathbf{k}}$ with $\mathbf{k} = 0$ does not enter the Hamiltonian

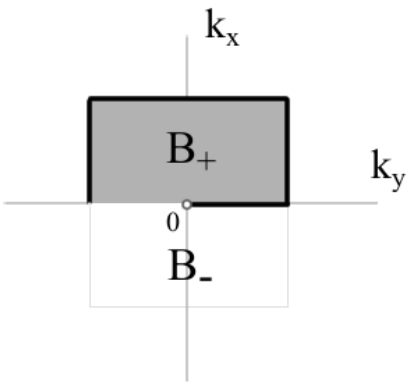

Figure 2.1: The division of the 1st Brillouin zone into two equal parts: if $\mathbf{k} \in B_+$ then $-\mathbf{k} \in B_-$.

The trace $\mathrm{Tr}_\theta \ldots$, Eq. (2.12), can be written in the Fourier variables as the functional integral:

$$\mathrm{Tr}_\theta \ldots = |\ \mathcal{J}\ | \int_{-N\frac{\pi}{a}}^{N\frac{\pi}{a}} d\theta_0 \left(\prod_{\mathbf{k}\in B_+} \int_{-\infty}^{\infty} d\theta^c_{\mathbf{k}} \int_{-\infty}^{\infty} d\theta^s_{\mathbf{k}} \right) \ldots\ . \tag{2.19}$$

Expansion of the boundaries of the integration over $\theta^c_{\mathbf{k}}$ and $\theta^s_{\mathbf{k}}$ in (2.19) is possible owing to the fact that the trace operation always acts on an expression containing the Boltzman factor $e^{-\beta H^{\mathrm{p}}_{\mathrm{sw}}}$ which is not vanishing at low temperatures ($\beta \to \infty$) only for small values of $\theta^c_{\mathbf{k}}$, $\theta^s_{\mathbf{k}}$ (see (2.18)).

The absolute value of the Jacobian $\mathcal{J}$ can be found by comparing the trace $\mathrm{Tr}_\theta\ e^{-\beta\sum_{\mathbf{r}}\theta_{\mathbf{r}}^2}$ calculated in the variables $\theta_{\mathbf{r}}$ and in the Fourier-transformed variables $\theta_{\mathbf{k}}$. It is easy to check that $\sum_{\mathbf{r}}\theta_{\mathbf{r}}^2 = \sum_{\mathbf{k}}|\theta_{\mathbf{k}}|^2 = \theta_0^2 + 2\sum_{\mathbf{k}\in B^+}|\theta_{\mathbf{k}}|^2$, and thus,

$$\prod_{\mathbf{r}}\left(\int_{-\infty}^{\infty}\frac{d\theta_{\mathbf{r}}}{2\pi}\ e^{-\beta\theta_{\mathbf{r}}^2}\right)$$
$$= \mid \mathcal{J} \mid \int_{-\infty}^{\infty} d\theta_0\ e^{-\beta\theta_0^2}\prod_{\mathbf{k}\in B_+}\left(\int_{-\infty}^{\infty} d\theta_{\mathbf{k}}^c\ e^{-2\beta(\theta_{\mathbf{k}}^c)^2}\int_{-\infty}^{\infty} d\theta_{\mathbf{k}}^s e^{-2\beta(\theta_{\mathbf{k}}^s)^2}\right)$$

which leads to

$$\mid \mathcal{J} \mid = \frac{2^{\frac{N-1}{2}}}{(2\pi)^N}\ . \tag{2.20}$$

Now, one can draw the finale expression of the functional integral $\mathrm{Tr}_\theta\ldots$ in the Fourier variables $\theta_{\mathbf{k}}$:

$$\mathrm{Tr}_\theta\ldots = \int_{-N\frac{\pi}{a}}^{N\frac{\pi}{a}}\frac{d\theta_0}{2\pi}\left(\prod_{\mathbf{k}\in B_+} 2\int_{-\infty}^{\infty}\frac{d\theta_{\mathbf{k}}^c}{2\pi}\int_{-\infty}^{\infty}\frac{d\theta_{\mathbf{k}}^s}{2\pi}\right)\ldots\ . \tag{2.21}$$

2.2.3 Disorder configuration inhomogeneity parameter

The nonmagnetic sites density can be written as:

$$\rho(\mathbf{r}) = \sum_{\mathbf{r}'}(1-c_{\mathbf{r}'})\delta_{\mathbf{r},\mathbf{r}'}\ , \tag{2.22}$$

where

$$\delta_{\mathbf{r},\mathbf{r}'} = \begin{cases} 1\ , & \text{if } \mathbf{r}=\mathbf{r}'\ ; \\ 0\ , & \text{if } \mathbf{r}\neq\mathbf{r}'\ . \end{cases} \tag{2.23}$$

is the Kroneker symbol which can be represented as:

$$\delta_{\mathbf{r},\mathbf{r}'} = \frac{1}{N}\sum_{\mathbf{q}} e^{i\mathbf{q}(\mathbf{r}'-\mathbf{r})}\ , \tag{2.24}$$

where the sum over $\mathbf{q}$ spans sites of the reciprocal lattice within the 1st Brillouin zone. Inserting (2.24) into (2.22) one obtains:

$$\rho(\mathbf{r}) \;=\; \sum_{\mathbf{q}} e^{-i\mathbf{q}\mathbf{r}} \frac{1}{N} \sum_{\mathbf{r}'} e^{i\mathbf{q}\mathbf{r}'} (1 - c_{\mathbf{r}'}) \;. \tag{2.25}$$

The Fourier transform of the impurities density,

$$\rho_{\mathbf{q}} \;=\; \frac{1}{N} \sum_{\mathbf{r}} e^{i\mathbf{q}\mathbf{r}} (1 - c_{\mathbf{r}}) \;, \tag{2.26}$$

can serve as a parameter which characterizes the dilution (2.1) in the inverse space. In the limiting case when there is no dilution (all $c_{\mathbf{r}} = 1$) $\rho_{\mathbf{q}} = 0$ for any $\mathbf{q}$.

It is easy to see that ρ_0 is the concentration of nonmagnetic sites, $1 - c$, if one neglects the fluctuation of this concentration in different realizations of disorder. Due to the random distribution of nonmagnetic impurities in the lattice it is statistically not preferable to come across essential inhomogeneities of the impurities local density, so all $\rho_{\mathbf{q}}$ with $\mathbf{q} \neq 0$ have small absolute values. In other words, $\rho_{\mathbf{q}}$ does not differ essentially from its configurationally averaged value (see (2.3)):

$$\overline{\rho_{\mathbf{q}}} \;=\; (1 - c)\delta_{\mathbf{q},0} \;. \tag{2.27}$$

A deviation of $\rho_{\mathbf{q}}$ from its averaged value (2.27),

$$\Delta\rho_{\mathbf{q}} \;=\; \rho_{\mathbf{q}} \;-\; \overline{\rho_{\mathbf{q}}} \;=\; \frac{1}{N} \sum_{\mathbf{r}} e^{i\mathbf{q}\mathbf{r}} (c - c_{\mathbf{r}}) \;, \tag{2.28}$$

will be called the disorder configuration inhomogeneity parameter or briefly just "disorder parameter", since it characterizes the fluctuation of $\rho_{\mathbf{q}}$ connected with the random character (disorder) of the dilution. Let us imagine the situation when the nonmagnetic sites which make the fraction $1 - c$ of all the sites form some regular structure, then $\rho_{\mathbf{q}}$ can be written as:

$$\rho_{\mathbf{q}} \;=\; (1 - \mathrm{c}) \left[\frac{1}{(1 - \mathrm{c})N} \sum_{\tilde{\mathbf{r}}} e^{i\mathbf{q}\tilde{\mathbf{r}}} \right] \;, \tag{2.29}$$

where the sum over $\tilde{\mathbf{r}}$ spans the empty sites only. The expression in the brackets in (2.29) is just a Kroneker symbol $\delta_{\mathbf{q},0}$, thus, in this particular case, when the impurities are ordered in some sense, the equalities $\rho_{\mathbf{q}} = \overline{\rho_{\mathbf{q}}}$ and $\Delta\rho_{\mathbf{q}} = 0$ hold.

Let us rewrite the spin-wave Hamiltonian of the diluted model (2.11) in the Fourier-transformed variables $\theta_{\mathbf{k}}$, Eq. (2.15), and $\rho_{\mathbf{q}}$, Eq. (2.26):

$$\begin{aligned} H_{\rm sw} \;=\; H^{\rm p}_{\rm sw} \;-\; \frac{J}{2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha}\theta_{\mathbf{k}}\theta_{\mathbf{k}'}\left(1-e^{-ik_\alpha a}-e^{-ik'_\alpha a}+e^{-i(k_\alpha+k'_\alpha)a}\right) \\ \times\left[\sum_{\mathbf{q}}\rho_{\mathbf{q}}\,\left(1+e^{-iq_\alpha a}\right)\frac{1}{N}\sum_{\mathbf{r}}e^{-i(\mathbf{k}+\mathbf{k}'+\mathbf{q})\mathbf{r}}\right. \\ \left.-\sum_{\mathbf{q}}\sum_{\mathbf{q}'}\rho_{\mathbf{q}}\rho_{\mathbf{q}'}\,e^{-iq'_\alpha a}\frac{1}{N}\sum_{\mathbf{r}}e^{-i(\mathbf{k}+\mathbf{k}'+\mathbf{q}+\mathbf{q}')\mathbf{r}}\right], \end{aligned}$$

where $H^{\rm p}_{\rm sw}$ is the Hamiltonian of the pure model (2.16). Since $\frac{1}{N}\sum_{\mathbf{r}}e^{-i(\mathbf{k}+\mathbf{k}'+\mathbf{q})\mathbf{r}} = \delta_{\mathbf{k}+\mathbf{k}'+\mathbf{q},0}$ and $\frac{1}{N}\sum_{\mathbf{r}}e^{-i(\mathbf{k}+\mathbf{k}'+\mathbf{q}+\mathbf{q}')\mathbf{r}} = \delta_{\mathbf{k}+\mathbf{k}'+\mathbf{q}+\mathbf{q}',0}$, we have

$$\begin{aligned} H_{\rm sw} \;=\; H^{\rm p}_{\rm sw} \;+\; J\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha}\cos\tfrac{(k_\alpha+k'_\alpha)a}{2}\;\rho_{-\mathbf{k}-\mathbf{k}'}\;K_\alpha(\mathbf{k})K_\alpha(\mathbf{k}')\;\theta_{\mathbf{k}}\theta_{\mathbf{k}'} \\ -\frac{J}{2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha}e^{i\frac{(k_\alpha+k'_\alpha)a}{2}}\left[\sum_{\mathbf{q}}e^{iq_\alpha a}\;\rho_{\mathbf{q}}\;\rho_{-\mathbf{k}-\mathbf{k}'-\mathbf{q}}\right]K_\alpha(\mathbf{k})K_\alpha(\mathbf{k}')\;\theta_{\mathbf{k}}\theta_{\mathbf{k}'} \end{aligned} \tag{2.30}$$

with

$$K_\alpha(\mathbf{k}) \;\equiv\; 2\sin\tfrac{k_\alpha a}{2}\;. \tag{2.31}$$

Also we will use the Hamiltonian (2.30) written through the disorder parameter $\Delta\rho_{\mathbf{q}}$:

$$\begin{aligned} H_{\rm sw} = H_{\Delta\rho=0} + {\rm c}J\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha}\cos\tfrac{(k_\alpha+k'_\alpha)a}{2}\Delta\rho_{-\mathbf{k}-\mathbf{k}'}\;K_\alpha(\mathbf{k})K_\alpha(\mathbf{k}')\theta_{\mathbf{k}}\theta_{\mathbf{k}'} \\ -\frac{J}{2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha}e^{i\frac{(k_\alpha+k'_\alpha)a}{2}}\left[\sum_{\mathbf{q}}e^{iq_\alpha a}\Delta\rho_{\mathbf{q}}\Delta\rho_{-\mathbf{k}-\mathbf{k}'-\mathbf{q}}\right]K_\alpha(\mathbf{k})K_\alpha(\mathbf{k}')\theta_{\mathbf{k}}\theta_{\mathbf{k}'}\;, \end{aligned} \tag{2.32}$$

where

$$H_{\Delta\rho=0} \;=\; \frac{c^2 J}{2} \sum_{\mathbf{k}} \sum_{\alpha=x,y} K_\alpha^2(\mathbf{k})\; \theta_{\mathbf{k}} \theta_{-\mathbf{k}} \tag{2.33}$$

is the Hamiltonian of the undiluted model (2.16) with the renormalized coupling constant $c^2 J$ (c is the concentration of magnetic sites).

2.2.4 Free energy of a weakly diluted model

Let us estimate the free energy (2.4) of a system described by the Hamiltonian (2.30). The configuration-dependent partition function will write in this case as:

$$Z_{\text{conf}} \;=\; \text{Tr}_\theta\; e^{-\beta(H_{\text{sw}}^{\text{p}} + H_\rho + H_{\rho^2})}\;, \tag{2.34}$$

where notions H_ρ and H_{ρ^2} were introduced for the linear and quadratic in ρ parts of the Hamiltonian (2.30) respectively. Multiplying and dividing (2.34) by the partition function of the pure model Z_{pure} we have:

$$Z_{\text{conf}} \;=\; Z_{\text{pure}}\, \frac{\text{Tr}_\theta\; e^{-\beta(H_{\text{sw}}^{\text{p}} + H_\rho + H_{\rho^2})}}{\text{Tr}_\theta\; e^{-\beta H_{\text{sw}}^{\text{p}}}}\;,$$

and thus one can write:

$$Z_{\text{conf}} \;=\; Z_{\text{pure}}\, \left\langle e^{-\beta(H_\rho + H_{\rho^2})} \right\rangle_{\text{p}}\;, \tag{2.35}$$

where $\langle \ldots \rangle_{\text{p}}$ denotes the thermodynamic averaging with the undiluted model Hamiltonian (2.16). Then, the configurationally averaged free energy (2.4) can be expressed as:

$$F_{\text{sw}} \;=\; F_{\text{sw}}^{\text{p}} \;-\; \frac{1}{\beta}\, \overline{\ln \left\langle e^{-\beta(H_\rho + H_{\rho^2})} \right\rangle_{\text{p}}}\;, \tag{2.36}$$

where F_{sw}^{p} is the free energy of the pure model (2.16).

Expanding the configuration-dependent expression into the Taylor series in powers of $\rho_{\mathbf{q}}$ one arrives at:

$$\overline{\ln \left\langle e^{-\beta(H_\rho + H_{\rho^2})} \right\rangle_{\text{p}}} \;=\; \overline{\ln \left(1 + \sum_{l=1}^{\infty} \frac{(-\beta)^l}{l!} \left\langle (H_\rho + H_{\rho^2})^l \right\rangle_{\text{p}} \right)} \;=$$

$$\sum_{m=1}^{\infty}\frac{(-1)^{m-1}}{m}\sum_{l_1=1}^{\infty}\ldots\sum_{l_m=1}^{\infty}\frac{(-\beta)^{l_1+\ldots+l_m}}{l_1!\ldots l_m!}\overline{\langle(H_\rho+H_{\rho^2})^{l_1}\rangle_{\rm p}\ldots\langle(H_\rho+H_{\rho^2})^{l_m}\rangle_{\rm p}}\ .$$

The configurational averaging procedure acts on the variables $\rho_{\mathbf{q}}$, so the problem reduces to the estimation of averages of the type: $\overline{\rho_{\mathbf{q}_1}\ldots\rho_{\mathbf{q}_n}}$ $(n=1,\ldots,\infty)$. The expression for $\overline{\rho_{\mathbf{q}}}$ has already been written once, Eq. (2.27); it is also not difficult to find that:

$$\overline{\rho_{\mathbf{q_1}}\rho_{\mathbf{q_2}}} \;=\; \left[(1-c)-(1-c)^2\right]\frac{1}{N}\delta_{\mathbf{q_1}+\mathbf{q_2},0} \;+\; (1-c)^2\;\delta_{\mathbf{q_1},0}\;\delta_{\mathbf{q_2},0}\ , \quad (2.37)$$

$$\begin{aligned}\overline{\rho_{\mathbf{q_1}}\rho_{\mathbf{q_2}}\rho_{\mathbf{q_3}}} \;&=\; \left[(1-c)-3(1-c)^2+2(1-c)^3\right]\;\frac{1}{N^2}\;\delta_{\mathbf{q_1}+\mathbf{q_2}+\mathbf{q_3},0}\\ &+\left[(1-c)^2-(1-c)^3\right]\frac{1}{N}\Big(\delta_{\mathbf{q_1},0}\delta_{\mathbf{q_2}+\mathbf{q_3},0}+\delta_{\mathbf{q_2},0}\delta_{\mathbf{q_1}+\mathbf{q_3},0}+\delta_{\mathbf{q_3},0}\delta_{\mathbf{q_1}+\mathbf{q_2},0}\Big)\\ &+(1-c)^3\;\delta_{\mathbf{q_1},0}\;\delta_{\mathbf{q_2},0}\;\delta_{\mathbf{q_3},0}\ . \qquad (2.38)\end{aligned}$$

Considering low concentrations of nonmagnetic sites (weak dilution) one can keep in (2.37) and (2.38) only terms linear in $(1-c)$. Then, it is easy to generalize:

$$\overline{\rho_{\mathbf{q_1}}\ldots\rho_{\mathbf{q_n}}} \;\simeq\; (1-c)\;\frac{1}{N^{n-1}}\;\delta_{\mathbf{q_1}+\ldots+\mathbf{q_n},0}\ . \qquad (2.39)$$

According to the expressions drawn, the terms containing any powers of H_{ρ^2} will vanish, since they will include sums of the type: $\sum_{\mathbf{q}} e^{iq_\alpha a}$ (see (2.30)) which give zero. Then, one can write:

$$\begin{aligned}&\overline{\ln\left\langle e^{-\beta(H_\rho+H_{\rho^2})}\right\rangle_{\rm p}}\\ &\quad=\sum_{m=1}^{\infty}\frac{(-1)^{m-1}}{m}\sum_{l_1=1}^{\infty}\ldots\sum_{l_m=1}^{\infty}\frac{(-\beta)^{l_1+\ldots+l_m}}{l_1!\ldots l_m!}\overline{\left\langle H_\rho^{l_1}\right\rangle_{\rm p}\ldots\left\langle H_\rho^{l_m}\right\rangle_{\rm p}}\ .\end{aligned}$$

The thermodynamic averages $\left\langle H_\rho^l\right\rangle_{\rm p}$ will obviously lead to the calculation of the quantities $\left\langle\theta_{\mathbf{k}_1}\theta_{\mathbf{k}_2}\ldots\theta_{\mathbf{k}_{2l-1}}\theta_{\mathbf{k}_{2l}}\right\rangle_{\rm p}$ which can be written as (see Eq. (2.60–2.62)): $\left\langle\theta_{\mathbf{k}_1}\theta_{\mathbf{k}_2}\ldots\theta_{\mathbf{k}_{2l-1}}\theta_{\mathbf{k}_{2l}}\right\rangle_{\rm p} \;=\; \delta_{\mathbf{k}_1+\mathbf{k}_2+\ldots+\mathbf{k}_{2l-1}+\mathbf{k}_{2l},0}$ $\times\ \left\langle\theta_{\mathbf{k}_1}\theta_{\mathbf{k}_2}\ldots\theta_{\mathbf{k}_{2l-1}}\theta_{\mathbf{k}_{2l}}\right\rangle_{\rm p}$. Thus, we arrive at the expression:

$$\overline{\ln\left\langle e^{-\beta(H_\rho+H_{\rho^2})}\right\rangle_{\rm p}}$$

$$= (1-c)N\sum_{m=1}^{\infty}\frac{(-1)^{m-1}}{m}\sum_{l_1=1}^{\infty}\dots\sum_{l_m=1}^{\infty}\frac{(-\beta)^{l_1+\dots+l_m}}{l_1!\dots l_m!}\left\langle H^{l_1}_{\rho=\frac{1}{N}}\right\rangle_{\rm p}\dots\left\langle H^{l_m}_{\rho=\frac{1}{N}}\right\rangle_{\rm p},$$

where $H_{\rho=\frac{1}{N}}$ is the part H_ρ of the Hamiltonian (2.30) with $\rho_{\mathbf{k}+\mathbf{k}'}=1/N$:

$$H_{\rho=\frac{1}{N}} \;=\; \frac{J}{N}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha}\cos\tfrac{(k_\alpha+k'_\alpha)a}{2}\;K_\alpha(\mathbf{k})K_\alpha(\mathbf{k}')\;\theta_{\mathbf{k}}\theta_{\mathbf{k}'}\;. \qquad (2.40)$$

Collecting the series we get the free energy (2.36):

$$F_{\rm sw} \;=\; F^{\rm p}_{\rm sw} \;-\; (1-c)N\,\frac{1}{\beta}\,\ln\left\langle e^{-\beta H_{\rho=\frac{1}{N}}}\right\rangle_{\rm p}\;. \qquad (2.41)$$

Going back to the direct space and expressing the quantity $H_{\rho=\frac{1}{N}}$ in the angle variables $\theta_{\mathbf{r}}$ we have:

$$H_{\rho=\frac{1}{N}} \;=\; -\frac{J}{2}\left((\theta_{\mathbf{a}_x}-\theta_0)^2+(\theta_{\mathbf{a}_y}-\theta_0)^2+(\theta_{-\mathbf{a}_x}-\theta_0)^2+(\theta_{-\mathbf{a}_y}-\theta_0)^2\right)\;,$$

i.e. the energy for one single spin vacancy (empty site) in the coordinate system origin. Thus, one can write:

$$-\frac{1}{\beta}\,\ln\left\langle e^{-\beta H_{\rho=\frac{1}{N}}}\right\rangle_{\rm p} \;=\; F_{\rho=\frac{1}{N}} \;-\; F^{\rm p}_{\rm sw} \;\equiv\; \Delta F_{\rho=\frac{1}{N}}\;,$$

where $F_{\rho=\frac{1}{N}}$ is the free energy of the model (2.11) with one single spin vacancy at the origin, and $F^{\rm p}_{\rm sw}$ is the free energy of the pure model. So,

$$F_{\rm sw} \;=\; F^{\rm p}_{\rm sw} \;+\; (1-c)N\;\Delta F_{\rho=\frac{1}{N}}\;. \qquad (2.42)$$

As one can conclude, our assumption of the dilution concentration $1-c$ smallness led to the reduction of the initial problem to a calculation of the free energy of a system with one single vacancy. In other words, the nonmagnetic impurities almost do not "feel" each other being present in small concentrations.

It is not difficult to find the analytical expression for the free energy of the pure model, $F^{\rm p}_{\rm sw}$, using the Hamiltonian (2.16) diagonalized in the Fourier variables. From the partition function,

$$\begin{aligned} Z_{\rm pure} &= \prod_{\mathbf{k}\in B_+} \left(2\int_{-\infty}^{\infty} \frac{d\theta^c_{\mathbf{k}}}{2\pi} \int_{-\infty}^{\infty} \frac{d\theta^s_{\mathbf{k}}}{2\pi}\, e^{-\beta J \sum_\alpha K^2_\alpha(\mathbf{k})\left[(\theta^c_{\mathbf{k}})^2+(\theta^s_{\mathbf{k}})^2\right]} \right) \\ &= \prod_{\mathbf{k}\in B_+} \frac{1}{2\pi\beta J \sum_\alpha K^2_\alpha(\mathbf{k})} = \prod_{\mathbf{k}\neq 0} \left(2\pi\beta J \sum_\alpha K^2_\alpha(\mathbf{k}) \right)^{-1/2} , \end{aligned} \tag{2.43}$$

we find the free energy:

$$F^{\rm p}_{\rm sw} = \frac{T}{2} \sum_{\mathbf{k}\neq 0} \ln \left(2\pi \frac{J}{T} \sum_\alpha K^2_\alpha(\mathbf{k}) \right) , \tag{2.44}$$

where the sum covers the 1st Brillouin zone except $\mathbf{k} \neq 0$, $K_\alpha(\mathbf{k})$ was defined in (2.31), and T is the temperature expressed in the energy units.

The difference between the free energies of the "single-vacancy" and pure models, $\Delta F_{\rho=\frac{1}{N}}$, can be estimated approximately expanding the expression

$$-\frac{1}{\beta} \ln \left\langle e^{-\beta H_{\rho=\frac{1}{N}}} \right\rangle_{\rm p}$$

in powers of $H_{\rho=\frac{1}{N}}$. Obviously, the influence of a single spin vacancy on the infinite system is infinitesimally small, thus $H_{\rho=\frac{1}{N}}$ can be considered as a weak perturbation and the first several terms in the perturbation expansion are enough to have a nice result. Note that the same result could be obtained directly in the expansion in $\rho_{\mathbf{q}}$ keeping the corresponding order terms and neglecting the rest. We emphasize that such a procedure cannot be considered as the perturbation expansion in the dilution concentration $1-c$, since any term in the expansion gives its own contribution linear in $1-c$ (Eq. (2.39)). In the following subsection similar expansion will be applied to estimate the spin pair correlation function.

2.3 Pair correlation function of spins

2.3.1 Expansion in the disorder configuration inhomogeneity parameter

The configurationally average spin pair correlation function (2.6) of the model (2.11) can be written in the angle variables $\theta_{\mathbf{r}}$ as:

$$G(\mathbf{R}) \;=\; c^2 \overline{\left\langle \cos\,(\theta_{\mathbf{r}+\mathbf{R}} - \theta_{\mathbf{r}}) \right\rangle} \;, \tag{2.45}$$

where c^2 is the probability that the sites $\mathbf{r}$ and $\mathbf{r}+\mathbf{R}$ are not empty. Passing to the Fourier variables $\theta_{\mathbf{k}}$ according to the formula (2.15), (2.45) can be written as:

$$G(\mathbf{R}) \;=\; c^2 \overline{\left\langle \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}} \theta_{\mathbf{k}} \right\rangle} \tag{2.46}$$

with $\eta_{\mathbf{k}} \;=\; \eta^c_{\mathbf{k}} \;+\; i\,\eta^s_{\mathbf{k}}$,

$$\begin{aligned} \eta^c_{\mathbf{k}} \;&=\; \tfrac{1}{\sqrt{N}}\,(\cos \mathbf{k}(\mathbf{r}+\mathbf{R}) \;-\; \cos \mathbf{k}\mathbf{r}) \;, \\ \eta^s_{\mathbf{k}} \;&=\; \tfrac{1}{\sqrt{N}}\,(\sin \mathbf{k}(\mathbf{r}+\mathbf{R}) \;-\; \sin \mathbf{k}\mathbf{r}) \;. \end{aligned} \tag{2.47}$$

The expression (2.46) is correct due to the property: $\theta^c_{-\mathbf{k}} = \theta^c_{\mathbf{k}},\;\; \theta^s_{-\mathbf{k}} = -\theta^s_{\mathbf{k}}$, $\eta^c_{-\mathbf{k}} = \eta^c_{\mathbf{k}},\;\; \eta^s_{-\mathbf{k}} = -\eta^s_{\mathbf{k}}$.

The occupation numbers $c_{\mathbf{r}}$ enter the thermodynamic average (2.46) through the Fourier-transform of the impurities density $\rho_{\mathbf{k}}$ in the Hamiltonian (2.30) or through the disorder configuration inhomogeneity parameter $\Delta\rho_{\mathbf{k}}$ in the Hamiltonian written in the form (2.32). In order to find the configurationally averaged value of the pair correlation function (2.46) one has to expand the expression (2.46) into a series in powers of $\rho_{\mathbf{k}}$ or $\Delta\rho_{\mathbf{k}}$. The result of the expansion in $\rho_{\mathbf{k}}$ which corresponds to the perturbation theory for a weak dilution will be found in the next subsection. Herein, we will obtain the result of the expansion which we expect to be more reliable at stronger concentrations of dilution. As the parameter of such

an expansion we take the disorder configuration inhomogeneity parameter $\Delta\rho_{\mathbf{k}}$ which is supposed to be small for the most probable configurations of disorder at any concentrations of dilution. As one will convince afterwards, comparing the results of both expansions (calculated up to the third order) with the Monte Carlo simulation data, the expansion in $\Delta\rho_{\mathbf{k}}$ will really better describe the stronger dilution region of the phase diagram. Although the convergence of this expansion (as well as of the expansion in $\rho_{\mathbf{k}}$) remains questionable one can notice similarity with the well known perturbation theory for the sum over the wave-vector $\mathbf{k}$ (a sum over $\mathbf{k}$ will correspond to each power of $\rho_{\mathbf{k}}$ or $\Delta\rho_{\mathbf{k}}$ in our expansions) which is of the order of the ratio between the effective interaction volume and the elementary cell volume, a^{-3} [107, 108].

Let us introduce the following designations in the Hamiltonian (2.32):

$$H_{\rm sw} \;=\; H_{\Delta\rho=0} \;+\; H_{\Delta\rho} \;+\; H_{(\Delta\rho)^2}\;, \tag{2.48}$$

$$H_{\Delta\rho} \;=\; \mathrm{c}J\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha}\cos\tfrac{(k_\alpha+k'_\alpha)a}{2}\Delta\rho_{-\mathbf{k}-\mathbf{k}'}K_\alpha(\mathbf{k})K_\alpha(\mathbf{k}')\theta_{\mathbf{k}}\theta_{\mathbf{k}'}, \tag{2.49}$$

$$H_{(\Delta\rho)^2} \;=\; -\frac{J}{2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha}e^{i\frac{(k_\alpha+k'_\alpha)a}{2}}\left[\sum_{\mathbf{q}}e^{iq_\alpha a}\;\Delta\rho_{\mathbf{q}}\;\Delta\rho_{-\mathbf{k}-\mathbf{k}'-\mathbf{q}}\right]$$

$$\times\; K_\alpha(\mathbf{k})K_\alpha(\mathbf{k}')\;\theta_{\mathbf{k}}\theta_{\mathbf{k}'}\;. \tag{2.50}$$

In order to realize the configurational averaging operation in (2.46) we expand $\left\langle\cos\sum_{\mathbf{k}\neq0}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\right\rangle$ in powers of the disorder parameter $\Delta\rho_{\mathbf{k}}$:

$$\left\langle\cos\sum_{\mathbf{k}\neq0}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\right\rangle \;=\; \left\langle\cos\sum_{\mathbf{k}\neq0}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\right\rangle_{\Delta\rho=0} \tag{2.51}$$

$$+\;\sum_{\mathbf{k}}\left[\frac{\partial\left\langle\cos\sum_{\mathbf{k}\neq0}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\right\rangle}{\partial\Delta\rho_{\mathbf{k}}}\right]_{\Delta\rho=0}\Delta\rho_{\mathbf{k}}$$

$$+\frac{1}{2!}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\left[\frac{\partial^2\left\langle\cos\sum_{\mathbf{k}\neq 0}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\right\rangle}{\partial\Delta\rho_{\mathbf{k}}\partial\Delta\rho_{\mathbf{k}'}}\right]_{\Delta\rho=0}\Delta\rho_{\mathbf{k}}\Delta\rho_{\mathbf{k}'}$$

$$+\frac{1}{3!}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{k}''}\left[\frac{\partial^3\left\langle\cos\sum_{\mathbf{k}\neq 0}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\right\rangle}{\partial\Delta\rho_{\mathbf{k}}\partial\Delta\rho_{\mathbf{k}'}\partial\Delta\rho_{\mathbf{k}''}}\right]_{\Delta\rho=0}\Delta\rho_{\mathbf{k}}\Delta\rho_{\mathbf{k}'}\Delta\rho_{\mathbf{k}''}\ ,$$

where $\langle\ldots\rangle_{\Delta\rho=0}$ denotes the thermodynamic averaging with the Hamiltonian $H_{\Delta\rho=0}$, (2.33).

In our research we take into account only the terms up to the third order in the expansion (2.51). As it was mentioned before, $\Delta\rho_{\mathbf{k}}$ can be considered as a small parameter in the case of a random non-correlated disorder. One can call the expansion (2.51) the perturbation theory for the unperturbed Hamiltonian (2.33).

Now, (2.46) can be averaged over the configurations of disorder noting that:

$$\begin{aligned}
\overline{\Delta\rho_{\mathbf{q}}} &= 0\ ,\\
\overline{\Delta\rho_{\mathbf{q}}\Delta\rho_{\mathbf{q}'}} &= c(1-c)\,\frac{1}{N}\,\delta_{\mathbf{q}+\mathbf{q}',0}\ ,\\
\overline{\Delta\rho_{\mathbf{q}}\Delta\rho_{\mathbf{q}'}\Delta\rho_{\mathbf{q}''}} &= -\,c(1-3c+2c^2)\,\frac{1}{N^2}\,\delta_{\mathbf{q}+\mathbf{q}'+\mathbf{q}'',0}\ .
\end{aligned}\tag{2.52}$$

The spin pair correlation function (2.46) can be also written in the form:

$$G(\mathbf{R}) = c^2\frac{\overline{\left\langle e^{-\beta(H_{\Delta\rho}+H_{(\Delta\rho)^2})}\cos\sum_{\mathbf{k}\neq 0}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\right\rangle_{\Delta\rho=0}}}{\left\langle e^{-\beta(H_{\Delta\rho}+H_{(\Delta\rho)^2})}\right\rangle_{\Delta\rho=0}}\ .\tag{2.53}$$

The expansion (2.51) is equivalent to the expansion of the expression above in powers of $H_{\Delta\rho}$ and $H_{(\Delta\rho)^2}$ where the terms up to the third order in $\Delta\rho_{\mathbf{k}}$ are kept only. The terms of the expansion containing $H_{(\Delta\rho)^2}$ will vanish after the configurational averaging, since they will contain the sums $\sum_{\mathbf{q}} e^{iq_\alpha a}$ which give zeros. The terms linear in $\Delta\rho_{\mathbf{k}}$ will disappear as well

(see (2.52)), thus:

$$
\begin{aligned}
G(\mathbf{R}) \;=\; & c^2 \Big\langle \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle_{\Delta\rho=0} \\
& \times \Bigg\{ 1 \;+\; \frac{\beta^2}{2} \left(\frac{\Big\langle \overline{H^2_{\Delta\rho}} \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle_{\Delta\rho=0}}{\langle \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \rangle_{\Delta\rho=0}} \;-\; \Big\langle \overline{H^2_{\Delta\rho}} \Big\rangle_{\Delta\rho=0} \right) \\
& - \beta^2 \left(\frac{\overline{\Big\langle H_{\Delta\rho} \Big\rangle_{\Delta\rho=0} \Big\langle H_{\Delta\rho} \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle}_{\Delta\rho=0}}{\Big\langle \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle_{\Delta\rho=0}} \;-\; \overline{\Big\langle H_{\Delta\rho} \Big\rangle}^2_{\Delta\rho=0} \right) \\
& + \frac{\beta^3}{2} \left(\frac{\overline{\Big\langle H^2_{\Delta\rho} \Big\rangle_{\Delta\rho=0} \Big\langle H_{\Delta\rho} \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle}_{\Delta\rho=0}}{\Big\langle \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle_{\Delta\rho=0}} \;-\; \overline{\Big\langle H^2_{\Delta\rho} \Big\rangle_{\Delta\rho=0} \Big\langle H_{\Delta\rho} \Big\rangle}_{\Delta\rho=0} \right) \\
& + \frac{\beta^3}{2} \left(\frac{\overline{\Big\langle H_{\Delta\rho} \Big\rangle_{\Delta\rho=0} \Big\langle H^2_{\Delta\rho} \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle}_{\Delta\rho=0}}{\Big\langle \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle_{\Delta\rho=0}} \;-\; \overline{\Big\langle H_{\Delta\rho} \Big\rangle_{\Delta\rho=0} \Big\langle H^2_{\Delta\rho} \Big\rangle}_{\Delta\rho=0} \right) \\
& - \beta^3 \left(\frac{\overline{\Big\langle H_{\Delta\rho} \Big\rangle^2_{\Delta\rho=0} \Big\langle H_{\Delta\rho} \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle}_{\Delta\rho=0}}{\Big\langle \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle_{\Delta\rho=0}} \;-\; \overline{\Big\langle H_{\Delta\rho} \Big\rangle^3}_{\Delta\rho=0} \right) \\
& - \frac{\beta^3}{6} \left(\frac{\Big\langle \overline{H^3_{\Delta\rho}} \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle_{\Delta\rho=0}}{\langle \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \rangle_{\Delta\rho=0}} \;-\; \Big\langle \overline{H^3_{\Delta\rho}} \Big\rangle_{\Delta\rho=0} \right) \Bigg\} \;. \qquad (2.54)
\end{aligned}
$$

Let us find $\Big\langle \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle_{\Delta\rho=0}$ first:

$$
\begin{aligned}
\Big\langle \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle_{\Delta\rho=0} \;=\; & Re \Big\langle e^{i \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}}} \Big\rangle_{\Delta\rho=0} \\
= \; Re \; & \frac{\displaystyle\prod_{\mathbf{k}\in B_+} \left(2 \int_{-\infty}^{\infty} \frac{d\theta^c_{\mathbf{k}}}{2\pi} \int_{-\infty}^{\infty} \frac{d\theta^s_{\mathbf{k}}}{2\pi} \; e^{-\beta c^2 J \sum_\alpha K^2_\alpha(\mathbf{k}) \left[(\theta^c_{\mathbf{k}})^2 + (\theta^s_{\mathbf{k}})^2 \right] + i2(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}} + \eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}})} \right)}{\displaystyle\prod_{\mathbf{k}\in B_+} \left(2 \int_{-\infty}^{\infty} \frac{d\theta^c_{\mathbf{k}}}{2\pi} \int_{-\infty}^{\infty} \frac{d\theta^s_{\mathbf{k}}}{2\pi} \; e^{-\beta c^2 J \sum_\alpha K^2_\alpha(\mathbf{k}) [(\theta^c_{\mathbf{k}})^2 + (\theta^s_{\mathbf{k}})^2]} \right)} \\
= \; \exp & \left\{ -\frac{1}{2\beta c^2 J} \sum_{\mathbf{k}\neq 0} \frac{|\eta_{\mathbf{k}}|^2}{\gamma_{\mathbf{k}}} \right\} \;, \qquad (2.55)
\end{aligned}
$$

where the following notation was applied:

$$
\gamma_{\mathbf{k}} \;\equiv\; \sum_\alpha K^2_\alpha(\mathbf{k}) \;=\; K^2_x(\mathbf{k}) \;+\; K^2_y(\mathbf{k}) \;. \qquad (2.56)
$$

The thermodynamical averaging in $\left\langle H^m_{\Delta\rho} \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0}$ concerns the variables $\theta_{\mathbf{k}}$, so, regarding the form of $H_{\Delta\rho}$ (Eq. (2.49)), the problem reduces to the estimation of the averages of the type $\left\langle \theta_{\mathbf{k}_1}\theta_{\mathbf{k}'_1} \cdots \theta_{\mathbf{k}_{2m}}\theta_{\mathbf{k}'_{2m}} \times \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0}$. Obviously, one can write:

$$\left\langle \theta_{\mathbf{k}_1}\theta_{\mathbf{k}'_1} \cdots \theta_{\mathbf{k}_{2m}}\theta_{\mathbf{k}'_{2m}} \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0}$$
$$= (-1)^m \left\langle \frac{\partial}{\partial\eta_{\mathbf{k}_1}} \frac{\partial}{\partial\eta_{\mathbf{k}'_1}} \cdots \frac{\partial}{\partial\eta_{\mathbf{k}_{2m}}} \frac{\partial}{\partial\eta_{\mathbf{k}'_{2m}}} \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0} ,$$

where the short notation is introduced: $\frac{\partial}{\partial\eta_{\mathbf{k}}} \equiv \frac{\partial}{\partial\eta^c_{\mathbf{k}}} - i\frac{\partial}{\partial\eta^s_{\mathbf{k}}}$. The operations of the differentiation with respect to the parameter $\eta_{\mathbf{k}}$ and thermodynamical averaging can be reversed:

$$\left\langle \theta_{\mathbf{k}_1}\theta_{\mathbf{k}'_1} \cdots \theta_{\mathbf{k}_{2m}}\theta_{\mathbf{k}'_{2m}} \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0}$$
$$= (-1)^m \frac{\partial}{\partial\eta_{\mathbf{k}_1}} \frac{\partial}{\partial\eta_{\mathbf{k}'_1}} \cdots \frac{\partial}{\partial\eta_{\mathbf{k}_{2m}}} \frac{\partial}{\partial\eta_{\mathbf{k}'_{2m}}} \left\langle \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0} .$$

Using the result (2.55) and the equality: $\frac{\partial\eta_{\mathbf{k}}}{\partial\eta_{\mathbf{k}'}} = 2\delta_{\mathbf{k},\mathbf{k}'}$ (which is easily deduced from the property: $\eta^c_{-\mathbf{k}} = \eta^c_{\mathbf{k}}$, $\eta^s_{-\mathbf{k}} = -\eta^s_{\mathbf{k}}$) we get:

$$\left\langle \theta_{\mathbf{k}}\theta_{\mathbf{k}'} \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0} \tag{2.57}$$
$$= \left\langle \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0} \left\{ -\frac{1}{(\beta c^2 J)^2} \frac{\eta_{-\mathbf{k}}\eta_{-\mathbf{k}'}}{\gamma_{\mathbf{k}}\gamma_{\mathbf{k}'}} + \frac{1}{\beta c^2 J} \frac{\delta_{\mathbf{k}+\mathbf{k}',0}}{\gamma_{\mathbf{k}}} \right\} ,$$

$$\left\langle \theta_{\mathbf{k}_1}\theta_{\mathbf{k}_2}\theta_{\mathbf{k}_3}\theta_{\mathbf{k}_4} \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0} \tag{2.58}$$

$$
\begin{aligned}
&= \left\langle \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0} \left\{ \frac{1}{(\beta c^2 J)^4} \frac{\eta_{-\mathbf{k}_1}\eta_{-\mathbf{k}_2}\eta_{-\mathbf{k}_3}\eta_{-\mathbf{k}_4}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_2}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_4}}} \right. \\
&- \frac{1}{(\beta c^2 J)^3} \left(\frac{\delta_{\mathbf{k_1}+\mathbf{k_2},0}\eta_{-\mathbf{k}_3}\eta_{-\mathbf{k}_4}}{\gamma_{\mathbf{k_2}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_4}}} + \frac{\delta_{\mathbf{k_1}+\mathbf{k_3},0}\eta_{-\mathbf{k}_2}\eta_{-\mathbf{k}_4}}{\gamma_{\mathbf{k_2}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_4}}} + \frac{\delta_{\mathbf{k_1}+\mathbf{k_4},0}\eta_{-\mathbf{k}_2}\eta_{-\mathbf{k}_3}}{\gamma_{\mathbf{k_2}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_4}}} \right. \\
&\qquad \left. + \frac{\delta_{\mathbf{k_2}+\mathbf{k_3},0}\eta_{-\mathbf{k}_1}\eta_{-\mathbf{k}_4}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_2}}\gamma_{\mathbf{k_4}}} + \frac{\delta_{\mathbf{k_2}+\mathbf{k_4},0}\eta_{-\mathbf{k}_1}\eta_{-\mathbf{k}_3}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_2}}\gamma_{\mathbf{k_3}}} + \frac{\delta_{\mathbf{k_3}+\mathbf{k_4},0}\eta_{-\mathbf{k}_1}\eta_{-\mathbf{k}_2}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_2}}\gamma_{\mathbf{k_3}}} \right) \\
&\left. + \frac{1}{(\beta c^2 J)^2} \left(\frac{\delta_{\mathbf{k_1}+\mathbf{k_2},0}\delta_{\mathbf{k_3}+\mathbf{k_4},0}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_2}}} + \frac{\delta_{\mathbf{k_1}+\mathbf{k_3},0}\delta_{\mathbf{k_2}+\mathbf{k_4},0}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_2}}} + \frac{\delta_{\mathbf{k_1}+\mathbf{k_4},0}\delta_{\mathbf{k_2}+\mathbf{k_3},0}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_2}}} \right) \right\}
\end{aligned}
$$

and

$$
\begin{aligned}
&\left\langle \theta_{\mathbf{k}_1}\theta_{\mathbf{k}_2}\theta_{\mathbf{k}_3}\theta_{\mathbf{k}_4}\theta_{\mathbf{k}_5}\theta_{\mathbf{k}_6} \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0} \qquad (2.59) \\
&= \left\langle \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0} \left\{ -\frac{1}{(\beta c^2 J)^6} \frac{\eta_{-\mathbf{k}_1}\eta_{-\mathbf{k}_2}\eta_{-\mathbf{k}_3}\eta_{-\mathbf{k}_4}\eta_{-\mathbf{k}_5}\eta_{-\mathbf{k}_6}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_2}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_4}}\gamma_{\mathbf{k_5}}\gamma_{\mathbf{k_6}}} \right. \\
&\qquad + \frac{1}{(\beta c^2 J)^5} \left(\overbrace{\frac{\delta_{\mathbf{k_1}+\mathbf{k_2},0}\eta_{-\mathbf{k}_3}\eta_{-\mathbf{k}_4}\eta_{-\mathbf{k}_5}\eta_{-\mathbf{k}_6}}{\gamma_{\mathbf{k_2}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_4}}\gamma_{\mathbf{k_5}}\gamma_{\mathbf{k_6}}} + \cdots}^{15} \right) \\
&\qquad - \frac{1}{(\beta c^2 J)^4} \left(\overbrace{\frac{\delta_{\mathbf{k_1}+\mathbf{k_2},0}\delta_{\mathbf{k_3}+\mathbf{k_4},0}\eta_{-\mathbf{k}_5}\eta_{-\mathbf{k}_6}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_5}}\gamma_{\mathbf{k_6}}} + \cdots}^{45} \right) \\
&\qquad \left. + \frac{1}{(\beta c^2 J)^3} \left(\overbrace{\frac{\delta_{\mathbf{k_1}+\mathbf{k_2},0}\delta_{\mathbf{k_3}+\mathbf{k_4},0}\delta_{\mathbf{k_5}+\mathbf{k_6},0}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_5}}} + \cdots}^{15} \right) \right\},
\end{aligned}
$$

in the last expression the sums in the brackets span all the possible combinations of the wave-vectors in the Kroneker symbols (the numbers over the brackets report the number of terms inside the brackets).

One instantly gets the averages $\langle \theta_{\mathbf{k}}\theta_{\mathbf{k}'} \rangle_{\Delta\rho=0}$, $\langle \theta_{\mathbf{k}_1}\theta_{\mathbf{k}_2}\theta_{\mathbf{k}_3}\theta_{\mathbf{k}_4} \rangle_{\Delta\rho=0}$ and $\langle \theta_{\mathbf{k}_1}\theta_{\mathbf{k}_2}\theta_{\mathbf{k}_3}\theta_{\mathbf{k}_4}\theta_{\mathbf{k}_5}\theta_{\mathbf{k}_6} \rangle_{\Delta\rho=0}$ from (2.57)-(2.59) putting all $\eta_{\mathbf{k}}$ equal to zero:

$$\langle\theta_{\mathbf{k}}\theta_{\mathbf{k}'}\rangle_{\Delta\rho=0} \;=\; \frac{1}{\beta c^2 J}\frac{\delta_{\mathbf{k}+\mathbf{k}',0}}{\gamma_{\mathbf{k}}}\;, \tag{2.60}$$

$$\begin{aligned}\langle\theta_{\mathbf{k}_1}\theta_{\mathbf{k}_2}\theta_{\mathbf{k}_3}\theta_{\mathbf{k}_4}\rangle_{\Delta\rho=0} \;=\; \frac{1}{(\beta c^2 J)^2}\Bigg\{&\frac{\delta_{\mathbf{k}_1+\mathbf{k}_2,0}\delta_{\mathbf{k}_3+\mathbf{k}_4,0}}{\gamma_{\mathbf{k}_1}\gamma_{\mathbf{k}_2}}\\ &+\frac{\delta_{\mathbf{k}_1+\mathbf{k}_3,0}\delta_{\mathbf{k}_2+\mathbf{k}_4,0}}{\gamma_{\mathbf{k}_1}\gamma_{\mathbf{k}_2}}+\frac{\delta_{\mathbf{k}_1+\mathbf{k}_4,0}\delta_{\mathbf{k}_2+\mathbf{k}_3,0}}{\gamma_{\mathbf{k}_1}\gamma_{\mathbf{k}_2}}\Bigg\}\;,\end{aligned} \tag{2.61}$$

$$\begin{aligned}&\langle\theta_{\mathbf{k}_1}\theta_{\mathbf{k}_2}\theta_{\mathbf{k}_3}\theta_{\mathbf{k}_4}\theta_{\mathbf{k}_5}\theta_{\mathbf{k}_6}\rangle_{\Delta\rho=0}\\ &= \frac{1}{(\beta c^2 J)^3}\left(\overbrace{\frac{\delta_{\mathbf{k}_1+\mathbf{k}_2,0}\delta_{\mathbf{k}_3+\mathbf{k}_4,0}\delta_{\mathbf{k}_5+\mathbf{k}_6,0}}{\gamma_{\mathbf{k}_1}\gamma_{\mathbf{k}_3}\gamma_{\mathbf{k}_5}}+\cdots}^{15}\right).\end{aligned} \tag{2.62}$$

Substituting the equalities obtained above, (2.55), (2.57)-(2.62), and the expressions for the configurational averaging (2.52) into the expansion (2.54), the spin pair correlation function (2.46) can be brought to the following form:

$$\begin{aligned}G(\mathbf{R}) \;=\; c^2\exp\left\{-\frac{1}{2\beta c^2 J}\sum_{\mathbf{k}\neq 0}\frac{|\eta_{\mathbf{k}}|^2}{\gamma_{\mathbf{k}}}\right\}\Bigg(1\;-\;\frac{1}{\beta c^2 J}\\ \times\Bigg\{\frac{1-c}{c}\,\frac{2}{N}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\alpha,\beta}\cos\frac{(k_\alpha+k'_\alpha)a}{2}\cos\frac{(k_\beta+k'_\beta)a}{2}\frac{K_\alpha(\mathbf{k})K_\beta(\mathbf{k})}{\gamma_{\mathbf{k}}}\frac{K_\alpha(\mathbf{k}')K_\beta(\mathbf{k}')}{\gamma_{\mathbf{k}'}}\frac{|\eta_{\mathbf{k}}|^2}{\gamma_{\mathbf{k}}}\\ +\frac{1-3c+2c^2}{c^2}\Bigg[\frac{4}{N^2}\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''}\sum_{\alpha,\beta,\gamma}\cos\frac{(k_\alpha+k'_\alpha)a}{2}\cos\frac{(k'_\beta+k''_\beta)a}{2}\cos\frac{(k''_\gamma-k_\gamma)a}{2}\\ \times\frac{K_\alpha(\mathbf{k})K_\gamma(\mathbf{k})}{\gamma_{\mathbf{k}}}\frac{K_\alpha(\mathbf{k}')K_\beta(\mathbf{k}')}{\gamma_{\mathbf{k}'}}\frac{K_\beta(\mathbf{k}'')K_\gamma(\mathbf{k}'')}{\gamma_{\mathbf{k}''}}\frac{|\eta_{\mathbf{k}}|^2}{\gamma_{\mathbf{k}}}+\sum_{\mathbf{k}\neq 0}\frac{|\eta_{\mathbf{k}}|^2}{\gamma_{\mathbf{k}}}\Bigg]\Bigg\}\Bigg)\,.\end{aligned} \tag{2.63}$$

In the expression above we neglected the terms containing powers of temperature, $1/\beta$, higher than the first, since we are dealing with the low-temperature region. We neglected the terms vanishing in the thermodynamic limit as well. The expression in the parentheses has the form of

the first two orders of the Taylor expansion of an exponent; in the low-temperature limit, $1/\beta \to 0$, which we consider it can be replaced by the exponent:

$$
\begin{aligned}
G(\mathbf{R}) \;=\; c^2 \exp\Bigg\{ & -\frac{1}{2\beta c^2 J}\sum_{\mathbf{k}\neq 0}\frac{|\eta_{\mathbf{k}}|^2}{\gamma_{\mathbf{k}}} \;-\; \frac{1}{\beta c^2 J} \\
& \times \Bigg\{ \frac{1-c}{c}\,\frac{2}{N}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\alpha,\beta}\cos\tfrac{(k_\alpha+k'_\alpha)a}{2}\cos\tfrac{(k_\beta+k'_\beta)a}{2}\,\frac{K_\alpha(\mathbf{k})K_\beta(\mathbf{k})}{\gamma_{\mathbf{k}}}\,\frac{K_\alpha(\mathbf{k}')K_\beta(\mathbf{k}')}{\gamma_{\mathbf{k}'}}\,\frac{|\eta_{\mathbf{k}}|^2}{\gamma_{\mathbf{k}}} \\
& + \frac{1-3c+2c^2}{c^2}\Bigg[\frac{4}{N^2}\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''}\sum_{\alpha,\beta,\gamma}\cos\tfrac{(k_\alpha+k'_\alpha)a}{2}\cos\tfrac{(k'_\beta+k''_\beta)a}{2}\cos\tfrac{(k''_\gamma-k_\gamma)a}{2} \\
& \times \frac{K_\alpha(\mathbf{k})K_\gamma(\mathbf{k})}{\gamma_{\mathbf{k}}}\,\frac{K_\alpha(\mathbf{k}')K_\beta(\mathbf{k}')}{\gamma_{\mathbf{k}'}}\,\frac{K_\beta(\mathbf{k}'')K_\gamma(\mathbf{k}'')}{\gamma_{\mathbf{k}''}}\,\frac{|\eta_{\mathbf{k}}|^2}{\gamma_{\mathbf{k}}} \;+\; \sum_{\mathbf{k}\neq 0}\frac{|\eta_{\mathbf{k}}|^2}{\gamma_{\mathbf{k}}}\Bigg]\Bigg\}\Bigg\}\,.
\end{aligned}
\tag{2.64}
$$

The expression (2.64) is a result of the thermodynamic and configurational averaging of the pair correlation function expansion in the disorder configuration inhomogeneity parameter up to the third order. The first term in the exponent argument corresponds to the zeroth order of the expansion; the first order contribution is zero, since $\overline{\Delta\rho_{\mathbf{k}}} = 0$; the terms with the coefficients $\frac{1-c}{c}$ and $\frac{1-3c+2c^2}{c^2}$ correspond to the contributions of the second and third orders respectively.

2.3.2 Pair correlation function asymptotic behaviour

It is not difficult to convince ourself that for $\eta_{\mathbf{k}}$ defined by the equalities (2.47):

$$
|\eta_{\mathbf{k}}|^2 \;=\; \frac{4}{N}\sin^2\tfrac{\mathbf{kR}}{2}\,. \tag{2.65}
$$

Substituting (2.65) into the result (2.64) of the third order expansion in the disorder parameter, we get:

$$
G(\mathbf{R}) \;=\; c^2 \exp\Bigg\{ -\frac{1}{\beta c^2 J}\Bigg(S_0(\mathbf{R}) \;+\; \frac{1-c}{c}\,S_1(\mathbf{R})
$$

$$- \frac{1-3c+2c^2}{c^2} \left[S_2(\mathbf{R}) \; + \; 2 \; S_0(\mathbf{R}) \right] \Bigg) \Bigg\} \; , \qquad (2.66)$$

where we used the following notations:

$$S_0(\mathbf{R}) \;\equiv\; \frac{2}{N} \sum_{\mathbf{k}\neq 0} \frac{\sin^2 \frac{\mathbf{kR}}{2}}{\gamma_{\mathbf{k}}} \; , \qquad (2.67)$$

$$S_1(\mathbf{R}) \;\equiv\; \frac{8}{N^2} \sum_{\mathbf{k}\neq 0} \sum_{\mathbf{k}'} \sum_{\alpha,\beta} \cos \tfrac{(k_\alpha + k'_\alpha)a}{2} \cos \tfrac{(k_\beta + k'_\beta)a}{2}$$
$$\times \; \frac{K_\alpha(\mathbf{k}) K_\beta(\mathbf{k})}{\gamma_{\mathbf{k}}} \; \frac{K_\alpha(\mathbf{k}') K_\beta(\mathbf{k}')}{\gamma_{\mathbf{k}'}} \; \frac{\sin^2 \frac{\mathbf{kR}}{2}}{\gamma_{\mathbf{k}}} \; , \qquad (2.68)$$

$$S_2(\mathbf{R}) \;\equiv\; \frac{16}{N^2} \sum_{\mathbf{k}\neq 0} \sum_{\mathbf{k}'} \sum_{\mathbf{k}''} \sum_{\alpha,\beta,\gamma} \cos \tfrac{(k_\alpha + k'_\alpha)a}{2} \; \cos \tfrac{(k'_\beta + k''_\beta)a}{2} \; \cos \tfrac{(k''_\gamma - k_\gamma)a}{2}$$
$$\times \; \frac{K_\alpha(\mathbf{k}) K_\gamma(\mathbf{k})}{\gamma_{\mathbf{k}}} \; \frac{K_\alpha(\mathbf{k}') K_\beta(\mathbf{k}')}{\gamma_{\mathbf{k}'}} \; \frac{K_\beta(\mathbf{k}'') K_\gamma(\mathbf{k}'')}{\gamma_{\mathbf{k}''}} \; \frac{\sin^2 \frac{\mathbf{kR}}{2}}{\gamma_{\mathbf{k}}} \; . \qquad (2.69)$$

We are interested in the asymptotic behaviour of the pair correlation function at large distances R. Thus, the next step should be the evaluation of the asymptotic form of the sums (2.67)-(2.69) in the limits: $R \to \infty$, $N \to \infty$. Let us commence with $S_0(\mathbf{R})$; when $R < \infty$, the expression under the sum is finite everywhere (including the point $\mathbf{k} = 0$), so, in the thermodynamic limit one can pass in (2.67) from summation to integration over the 1st Brilouin zone according to the rule:

$$\sum_{\mathbf{k}} \;\to\; \frac{Na^2}{(2\pi)^2} \int d\mathbf{k} + o(N^{-1}) \; ,$$

Then,

$$S_0(\mathbf{R}) \;=\; \frac{a^2}{2\pi^2} \int d\mathbf{k} \frac{\sin^2 \frac{\mathbf{kR}}{2}}{\gamma_{\mathbf{k}}} \; .$$

Since $\gamma_{\mathbf{k}} = 0$ for $\mathbf{k} = 0$, it is not difficult to notice that the integral diverges with $R \to \infty$. The form of this divergence is defined by the pole of $\frac{1}{\gamma_{\mathbf{k}}}$ at $\mathbf{k} = 0$, so the asymptotic behaviour of the integral will not change if one

expands $\gamma_{\mathbf{k}}$ around $\mathbf{k}=0$: $\gamma_{\mathbf{k}} \simeq a^2|\mathbf{k}|^2$. We have:

$$S_0(\mathbf{R}) \;\simeq\; \frac{1}{2\pi^2}\int d\mathbf{k}\frac{\sin^2\frac{\mathbf{kR}}{2}}{|\mathbf{k}|^2}\;, \qquad R\to\infty\;. \tag{2.70}$$

Introducing the polar coordinates $k=\sqrt{k_x^2+k_y^2}$, $\varphi=\arctan\frac{k_y}{k_x}$, one can rewrite (2.70) as:

$$S_0(\mathbf{R}) \;=\; \frac{1}{2\pi^2}\int_0^{\frac{2\sqrt{\pi}}{a}} dk\int_0^{2\pi} d\varphi\frac{1}{k}\sin^2\left(\tfrac{kR}{2}\cos\varphi\right)\;, \tag{2.71}$$

where we changed the integration domain: $-\pi/a<k_x<\pi/a$, $-\pi/a<k_y<\pi/a$, to the equal by area domain: $0<k<2\sqrt{\pi}/a$, $0<\varphi<2\pi$, and the vector $\mathbf{R}$ was chosen parallel to the Ok_x axis.

After the change of the variable: $\frac{kR}{2}\to x$ let us split the domain of integration in the following way:

$$\int_0^{\frac{R\sqrt{\pi}}{a}} dx \quad\to\quad \int_0^{\varepsilon} dx \;+\; \int_{\varepsilon}^{\frac{R\sqrt{\pi}}{a}} dx\;,$$

where ε is chosen in such a way that it is possible within the interval $(0,\varepsilon)$ to expand:
$\sin^2(x\cos\varphi)\simeq x^2\cos^2\varphi$. Then,

$$S_0(\mathbf{R}) = \frac{1}{2\pi^2}\int_0^{\varepsilon} xdx\int_0^{2\pi} d\varphi\cos^2\varphi + \frac{1}{2\pi^2}\int_{\varepsilon}^{\frac{R\sqrt{\pi}}{a}} dx\int_0^{2\pi} d\varphi\frac{\sin^2(x\cos\varphi)}{x}\;.$$

The first term is small and independent of R, so it can be neglected when investigating the asymptotic form of $S_0(\mathbf{R})$. Expressing: $\sin^2(x\cos\varphi)=\frac{1}{2}(1-\cos(2x\cos\varphi))$, we get:

$$S_0(\mathbf{R}) \;=\; \frac{1}{4\pi^2}\int_{\varepsilon}^{R\sqrt{\pi}}\frac{dx}{x}\int_0^{2\pi} d\varphi \;-\; \frac{1}{4\pi^2}\int_{\varepsilon}^{\frac{R\sqrt{\pi}}{a}} dx\int_0^{2\pi} d\varphi\frac{\cos(2x\cos\varphi)}{x}\;.$$

One notices that the integral with respect to x in the second term reduces in the limit $R\to\infty$ to the integral cosine $\mathrm{Ci}(\varepsilon)=-\int_{\varepsilon}^{\infty}\frac{\cos x}{x}dx$ [109] which

is a function of ε only, so the asymptotic behaviour is determined by the first term, and finally:

$$S_0(\mathbf{R}) \simeq \frac{1}{2\pi}\ln(R/a)\ , \qquad R\to\infty\ . \tag{2.72}$$

This result allows for the immediate evaluation of the asymptotic behaviour of the pair correlation function in the pure model (2.16). Let us use (2.55) putting $c=1$, then:

$$G_{\rm pure}(\mathbf{R}) = \exp\left\{-\frac{1}{\beta J}S_0(\mathbf{R})\right\} \simeq \left(\frac{R}{a}\right)^{-\frac{1}{2\pi\beta J}}\ . \tag{2.73}$$

Thus, we have recovered the well known result [16] for the temperature-dependent exponent of the pair correlation function of the $2D$ XY model: $\eta_{\rm pure} = 1/(2\pi\beta J)$. In order to obtain the exponent $\eta_{\rm dis}$ of the model with quenched disorder one should evaluate the asymptotic behaviour of the sums $S_1(\mathbf{R})$ and $S_2(\mathbf{R})$ in (2.66) as well. The mentioned behaviour is determined again by the region of small $|\mathbf{k}|$. In (2.68) let us expand: $\cos\frac{(k_\alpha+k'_\alpha)}{2} \simeq \cos\frac{k'_\alpha}{2}$, $\cos\frac{(k_\beta+k'_\beta)}{2} \simeq \cos\frac{k'_\beta}{2}$, $K_\alpha(\mathbf{k}) \simeq ak_\alpha$, $K_\beta(\mathbf{k}) \simeq ak_\beta$, $\gamma_{\mathbf{k}} \simeq a^2|\mathbf{k}|^2$ (the higher order terms do not contribute to the asymptotic behaviour for $R\to\infty$):

$$\begin{aligned} S_1(\mathbf{R}) &\simeq \frac{8}{N^2}\sum_{\mathbf{k}\neq 0}\sum_{\mathbf{k}'\neq 0}\sum_{\alpha,\beta}\cos\tfrac{k'_\alpha a}{2}\cos\tfrac{k'_\beta a}{2}\,\frac{k_\alpha k_\beta}{|\mathbf{k}|^2}\,\frac{K_\alpha(\mathbf{k}')K_\beta(\mathbf{k}')}{\gamma_{\mathbf{k}'}}\,\frac{\sin^2\frac{\mathbf{kR}}{2}}{a^2|\mathbf{k}|^2} \\ &= \frac{2}{N}\sum_{\mathbf{k}\neq 0}\frac{\sin^2\frac{\mathbf{kR}}{2}}{a^2|\mathbf{k}|^2}\,\frac{4}{N}\sum_{\mathbf{k}'\neq 0}\cos^2\tfrac{k'_x a}{2}\,\frac{K_x^2(\mathbf{k}')}{\gamma_{\mathbf{k}'}} \\ &\simeq S_0(\mathbf{R})\,\frac{4}{N}\sum_{\mathbf{k}'\neq 0}\cos^2\tfrac{k'_x a}{2}\,\frac{K_x^2(\mathbf{k}')}{\gamma_{\mathbf{k}'}}, \end{aligned} \tag{2.74}$$

since the terms containing the product k_xk_y vanished after the averaging. The coefficient in front of $S_0(\mathbf{R})$ in (2.74) converges rapidly to a constant value when $N\to\infty$ and can be estimated with any desirable precision by

a simple numerical summation (with the help of a computer code):

$$\frac{4}{N}\sum_{\mathbf{k}'\neq 0}\cos^2\tfrac{k'_x a}{2}\,\frac{K_x^2(\mathbf{k}')}{\gamma_{\mathbf{k}'}} \;=\; 0.727^{1}\;. \tag{2.75}$$

So, from (2.72) we finally obtain:

$$S_1(\mathbf{R}) \;\simeq\; 0.727\,\frac{1}{2\pi}\ln(R/a)\;, \qquad R\to\infty\;. \tag{2.76}$$

In a similar way, expanding (2.69) for small $|\mathbf{k}|$:

$$S_2(\mathbf{R}) \;\simeq\; S_0(\mathbf{R})\,\frac{8}{N^2}\sum_{\mathbf{k}'\neq 0}\sum_{\mathbf{k}''\neq 0}\sum_{\alpha}\cos\tfrac{(k'_\alpha+k''_\alpha)a}{2}\cos\tfrac{k''_x a}{2}\cos\tfrac{k''_x a}{2}$$
$$\times\frac{K_x(\mathbf{k}')K_\alpha(\mathbf{k}')}{\gamma_{\mathbf{k}'}}\;\frac{K_x(\mathbf{k}'')K_\alpha(\mathbf{k}'')}{\gamma_{\mathbf{k}''}}\;.$$

Expressing $\cos\frac{(k'_\alpha+k''_\alpha)a}{2}=\cos\frac{k'_\alpha a}{2}\cos\frac{k''_\alpha a}{2}-\sin\frac{k'_\alpha a}{2}\sin\frac{k''_\alpha a}{2}$, we get:

$$S_2(\mathbf{R})\simeq S_0(\mathbf{R})\frac{1}{2}\left\{\left(\frac{4}{N}\sum_{\mathbf{k}'\neq 0}\cos^2\tfrac{k'_x a}{2}\,\frac{K_x^2(\mathbf{k}')}{\gamma_{\mathbf{k}'}}\right)^2-\left(\frac{2}{N}\sum_{\mathbf{k}'\neq 0}\sin k'_x a\,\frac{K_x^2(\mathbf{k}')}{\gamma_{\mathbf{k}'}}\right)^2\right.$$
$$\left.-\left(\frac{2}{N}\sum_{\mathbf{k}'\neq 0}\sin k'_x a\,\frac{K_y^2(\mathbf{k}')}{\gamma_{\mathbf{k}'}}\right)^2+\left(\frac{4}{N}\sum_{\mathbf{k}'\neq 0}\cos\tfrac{k'_x a}{2}\cos\tfrac{k'_y a}{2}\,\frac{K_x(\mathbf{k}')K_y(\mathbf{k}')}{\gamma_{\mathbf{k}'}}\right)^2\right\}\;.$$

Numerical summation suggests that all the terms in the braces except the first one vanish in the thermodynamical limit $N\to\infty$. Thus,

$$S_2(\mathbf{R}) \;\simeq\; \frac{(0.727)^2}{2}\,S_0(\mathbf{R}) \;=\; 0.264\,S_0(\mathbf{R})\;,$$

and finally, using (2.72):

$$S_2(\mathbf{R}) \;\simeq\; 0.264\,\frac{1}{2\pi}\ln(R/a)\;, \qquad R\to\infty\;. \tag{2.77}$$

[1]The sum (2.75) and similar sums hereafter span the sites of the inverse lattice within the 1st Brillouin zone (except the point $\mathbf{k}=0$); we say about rapid convergence of the sums, since (2.75), for example, differs only by the value of the order of 10^{-11} for $N=1000$ and $N=10000$. However, for our purposes it is quite enough to write down the result up to the third figure after the decimal point.

Substituting (2.72), (2.76) and (2.77) into (2.66), we have:

$$G(\mathbf{R}) \simeq \left(\frac{R}{a}\right)^{-\eta_{\rm dis}} \tag{2.78}$$

with the pair correlation function exponent dependent on the magnetic sites concentration c:

$$\eta_{\rm dis} = \frac{1}{2\pi\beta J}\left(\frac{1}{c^2} + 0.727\,\frac{1-c}{c^3} - 2.264\,\frac{1-3c+2c^2}{c^4}\right) . \tag{2.79}$$

The first term in the parentheses corresponds to the zeroth order of the expansion in the disorder parameter; the first order contribution is zero; the second and third terms in the parentheses correspond to the second and third order of the expansion respectively.

2.3.3 Expansion in $\rho_{\mathbf{q}}$

At small concentrations of nonmagnetic impurities one can consider their contribution to the Hamiltonian (2.30) as a perturbation and expand the spin pair correlation function (2.46) in $\rho_{\mathbf{q}}$ instead of $\Delta\rho_{\mathbf{q}}$. Again we only take into account the terms up to the third order:

$$\begin{aligned}
G(\mathbf{R}) \;=\; & c^2\Big\langle \cos\sum_{\mathbf{k}\neq 0}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\Big\rangle_p \Bigg\{ 1 - \beta\left(\frac{\Big\langle\overline{H_\rho}\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\Big\rangle_p}{\langle\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\rangle_p} - \Big\langle\overline{H_\rho}\Big\rangle_p\right) \\
& + \frac{\beta^2}{2}\left(\frac{\Big\langle\overline{H_\rho^2}\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\Big\rangle_p}{\langle\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\rangle_p} - \Big\langle\overline{H_\rho^2}\Big\rangle_p\right) - \beta^2\left(\frac{\Big\langle\overline{H_\rho}\Big\rangle_p\Big\langle\overline{H_\rho}\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\Big\rangle_p}{\Big\langle\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\Big\rangle_p} - \Big\langle\overline{H_\rho}\Big\rangle_p^2\right) \\
& + \frac{\beta^3}{2}\left(\frac{\Big\langle\overline{H_\rho^2}\Big\rangle_p\Big\langle\overline{H_\rho}\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\Big\rangle_p}{\Big\langle\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\Big\rangle_p} - \Big\langle\overline{H_\rho^2}\Big\rangle_p\Big\langle\overline{H_\rho}\Big\rangle_p\right) \\
& + \frac{\beta^3}{2}\left(\frac{\Big\langle\overline{H_\rho}\Big\rangle_p\Big\langle\overline{H_\rho^2}\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\Big\rangle_p}{\Big\langle\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\Big\rangle_p} - \Big\langle\overline{H_\rho}\Big\rangle_p\Big\langle\overline{H_\rho^2}\Big\rangle_p\right) \\
& - \beta^3\left(\frac{\Big\langle\overline{H_\rho}\Big\rangle_p^2\Big\langle\overline{H_\rho}\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\Big\rangle_p}{\Big\langle\cos\sum_{\mathbf{k}}\eta_{\mathbf{k}}\theta_{\mathbf{k}}\Big\rangle_p} - \Big\langle\overline{H_\rho}\Big\rangle^3_{\Delta\rho=0}\right)
\end{aligned}$$

$$- \frac{\beta^3}{6} \left(\frac{\left\langle \overline{H_\rho^3} \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}} \theta_{\mathbf{k}} \right\rangle_p}{\left\langle \cos \sum_{\mathbf{k}} \eta_{\mathbf{k}} \theta_{\mathbf{k}} \right\rangle_p} - \left\langle \overline{H_\rho^3} \right\rangle_p \right) \Bigg\} , \tag{2.80}$$

where we denoted the thermodynamical averaging with the undiluted model Hamiltoian (2.16) as $\langle \ldots \rangle_p$. Using (2.39) and (2.55), (2.57)-(2.62) with $c = 1$, in the limit $\beta \to \infty$ we have:

$$G(\mathbf{R}) \simeq c^2 \exp \Bigg\{ - \frac{1}{\beta J} \Bigg(S_0(\mathbf{R}) + \underbrace{(1-c)\, 2S_1(\mathbf{R})}_{\text{1st order}} + \underbrace{(1-c)\, S_1(\mathbf{R})}_{\text{2nd order}} + \underbrace{(1-c) \left[S_2(\mathbf{R}) + 2\, S_0(\mathbf{R}) \right]}_{\text{3rd order}} \Bigg) \Bigg\} ,$$

where the correspondence of the terms to the orders of the expansion is noted. The asymptotic behaviour of the sums $S_0(\mathbf{R})$, $S_1(\mathbf{R})$ and $S_2(\mathbf{R})$ for large R is given by the expressions (2.72), (2.76) and (2.77), thus,

$$G(\mathbf{R}) \simeq \left(\frac{R}{a} \right)^{-\eta_{\text{dis}}} \tag{2.81}$$

with the pair correlation function exponent:

$$\eta_{\text{dis}} = \frac{1}{2\pi\beta J} \left(1 + \underbrace{2\,(1-c)}_{\text{1st order}} + \underbrace{0.727\,(1-c)}_{\text{2nd order}} + \underbrace{2.264\,(1-c)}_{\text{3rd order}} \right) . \tag{2.82}$$

Please note that the mentioned orders correspond to the powers of $\rho_{\mathbf{q}}$ in the expansion, not to the powers of the dilution concentration $1-c$. As it has been remarked before, any power of $\rho_{\mathbf{q}}$ gives its own contribution linear in $1-c$, the higher order contributions are neglected in (2.82), since we have used an approximate equality (2.39). We will compare (2.82) to the result of the expansion in $\Delta\rho_{\mathbf{q}}$, Eq. (2.79), later comparing both analytical results to the Monte Carlo simulation data.

2.3.4 Pair correlation function self-averaging

In order to make any conclusions about the self-averaging of the configuration-dependent pair correlation function,

$$G_{\rm conf}(\mathbf{R}) \;=\; c^2 \left\langle \cos(\theta_{\mathbf{r}+\mathbf{R}} - \theta_{\mathbf{r}}) \right\rangle \;, \tag{2.83}$$

one has to find the relative variance,

$$R_G \;=\; \frac{\overline{G^2_{\rm conf}} \;-\; \overline{G_{\rm conf}}^2}{\overline{G_{\rm conf}}^2} \;. \tag{2.84}$$

We will evaluate this quantity within the second order approximation of the expansion in $\Delta\rho_{\mathbf{q}}$. The pair correlation function, $\overline{G_{\rm conf}} = G(\mathbf{R})$, already estimated in the third order approximation of the perturbation expansion (Eq. (2.66)), in the second order approximation has the form:

$$\overline{G_{\rm conf}} \;=\; c^2 \exp\left\{ -\frac{1}{\beta c^2 J}\left(S_0(\mathbf{R}) \;+\; \frac{1-c}{c}\, S_1(\mathbf{R}) \right) \right\} . \tag{2.85}$$

Thus, it remains to evaluate the quantity:

$$\overline{G^2_{\rm conf}(\mathbf{R})} \;=\; c^4 \overline{\left\langle \cos(\theta_{\mathbf{r}+\mathbf{R}} - \theta_{\mathbf{r}}) \right\rangle^2} \;, \tag{2.86}$$

which in the second order approximation will write as:

$$\begin{aligned}
\overline{G^2_{\rm conf}} \;=\; & c^4 \Big\langle \cos \sum_{\mathbf{k}\neq 0} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \Big\rangle^2_{\Delta\rho=0} \\
& \times \Bigg\{ 1 \;+\; \beta^2 \left(\frac{\left\langle \overline{H^2_{\Delta\rho}} \cos\sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0}}{\left\langle \cos\sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0}} \;-\; \left\langle \overline{H^2_{\Delta\rho}} \right\rangle_{\Delta\rho=0} \right) \\
& - 3\beta^2 \left(\frac{\left\langle \overline{H_{\Delta\rho}} \right\rangle_{\Delta\rho=0} \left\langle \overline{H_{\Delta\rho}} \cos\sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0}}{\left\langle \cos\sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0}} \;-\; \left\langle \overline{H_{\Delta\rho}} \right\rangle^2_{\Delta\rho=0} \right) \\
& + \beta^2 \left(\frac{\overline{\left\langle H_{\Delta\rho} \cos\sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle^2_{\Delta\rho=0}}}{\left\langle \cos\sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle^2_{\Delta\rho=0}} \;-\; \frac{\overline{\left\langle H_{\Delta\rho} \right\rangle_{\Delta\rho=0} \left\langle H_{\Delta\rho} \cos\sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0}}}{\left\langle \cos\sum_{\mathbf{k}} \eta_{\mathbf{k}}\theta_{\mathbf{k}} \right\rangle_{\Delta\rho=0}} \right) \Bigg\} .
\end{aligned}$$

Applying the results obtained in the previous subsections, we find:

$$\overline{G^2_{\rm conf}} \;=\; c^2 \exp\left\{ -\frac{2}{\beta c^2 J}\left(S_0(\mathbf{R}) \;+\; \frac{1-c}{c}\, S_1(\mathbf{R}) \right) \right\} . \qquad (2.87)$$

Substituting (2.85) and (2.87) into (2.84), we obtain immediately:

$$R_G \;=\; 0 \; . \qquad (2.88)$$

Note that the result (2.88) is obtained in the thermodynamic limit $N \to \infty$, so, it is rather impossible to say something about the scaling form of the relative variance, $R_G(N)$.

Formally our result allows to claim the self-averaging of the pair correlation function, although it should be clearly realized that (2.88) was estimated in the second order approximation of the expansion in the disorder parameter and the whole analytical approach is based on the assumption that the temperature is low. The question about the self-averaging property of the pair correlation function at higher temperatures remains open.

2.3.5 Comparison to the Monte Carlo simulation results

In order to check the results of our analytical approach we have performed a series of Monte Carlo simulations of the two-dimensional XY model with different concentrations of nonmagnetic dilution and at different temperatures. We used the Wolff cluster algorithm [31], periodic boundary conditions, 10000 Monte Carlo sweeps for thermalization and the same number of sweeps for the measurements.

We explored the following lattice sizes: 16×16, 32×32, 64×64, 128×128 and 256×256. The pair correlation function exponent $\eta(T)$ was obtained through the residual magnetization scaling behaviour:

$$M_T(L) \sim L^{-x_\sigma(T)} \; , \quad x_\sigma(T) = \frac{1}{2}\eta(T) \; , \qquad (2.89)$$

the last relation is true for a two-dimensional lattice ($L = \sqrt{N}$ is the linear size of the system). We implicitly assume here that the universality remains unchanged for a diluted system and the exponent $\eta(T)$ which stands in the scaling relation (2.89) is the same as the one in the pair correlation function decay, $G_2(R) \sim R^{-\eta(T)}$, just like in the undiluted model. The residual magnetization behaviour will be discussed in detail in Chapter 4.

Our choice of such indirect way of estimation of the pair correlation function exponent is caused by the difficulties with the pair correlation function measurement in Monte Carlo simulation due to its possible non-self-averaging. Although just in the previous subsection we put arguments in favor of the self-averaging property of this particular physical quantity at low temperatures, those arguments were obtained through an approximate method and do not remove the problem completely, moreover we explored a wide range of temperatures in our computer simulations including those close the transition temperature. Non-self-averaging of a physical quantity results in such an unpleasant fact that the configuration average of the quantity cannot be evaluated reliably enough on the basis of an incomplete set of random realizations of disorder as we deal with in the Monte Carlo simulations; in this case such an incomplete configurational averaging leads rather to the most probable value than to the real configurational average (see, for example, [114]).

Global quantities such as magnetization undergo less fluctuations when switching between diffirent disorder realizations than the local quantities such as the pair correlation function, but even in this case there is a risk of non-self-averaging which may impact the result of the Monte Carlo simulations. However, the researches of two and three dimensional systems suggest (see, for example, [93, 94, 115]) that usually the number of disorder realizations of order of a thousand is enough for reliable configurational averages. In our simulations we used 1000 realizations of disorder.

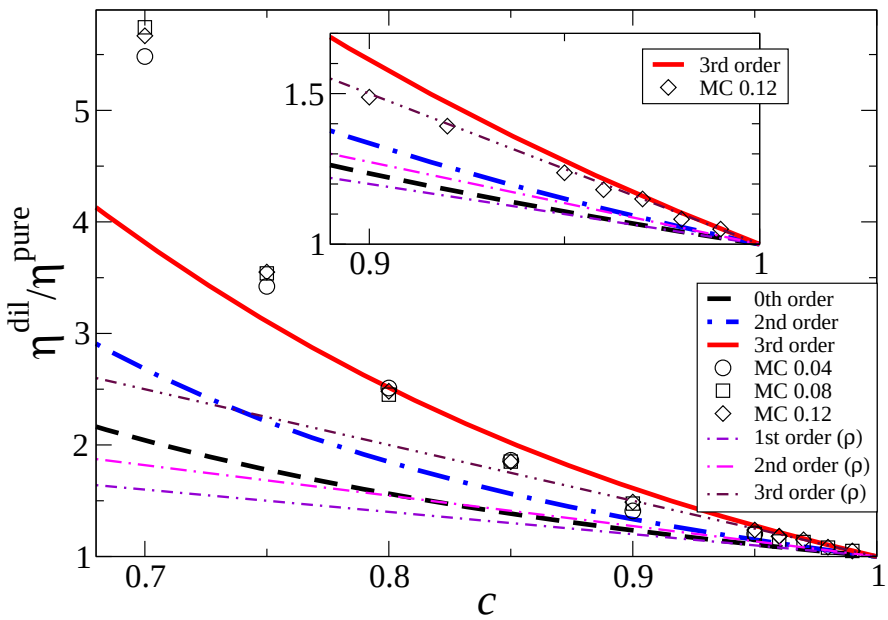

Figure 2.2: Comparison of the results for the ratio $\eta^{\mathrm{dil}}/\eta^{\mathrm{reg}}$ as a function of the magnetic sites concentration c obtained from different orders of the perturbation expansions in ρ and $\Delta\rho$ and in the Monte Carlo simulations. The figures in front of the "MC" symbols mean the relative temperature k_BT/J values taken in the computer simulations.

In fig. 2.2 we show for comparison in the same plot the Monte Carlo simulation outputs and the results of the expansions in $\rho_{\mathbf{q}}$ and $\Delta\rho_{\mathbf{q}}$ to different orders. Though the every next order of both expansions (at least up to the third order) seems to come closer to the "experimental data", the differences between the different orders of the expansions do not allow to say about their rapid convergence. However, this is not surprising, since similar expansions in other problems of condensed matter physics often happen to be divergent (for example, the field-theoretical expansions, see [67]), but they still can be succesfully used applying some special technics. We also conclude that the results of the corresponding orders of the two expansions (except the zeroth order) coincide in the small dilution concentration $(1-c)$ limit, but differ significantly at stronger dilutions and the expansion in $\Delta\rho_{\mathbf{q}}$ seems to be closer to the Monte Carlo points

within that range as we predicted.

Anyway, comparing the analytical curves and the Monte Carlo simulation results in fig. 2.2 one can conclude about good accordance of our analytical approach with the computer experiments in the range from $c = 0.75$ to $c = 1$ at low temperatures, at least up to the third orders in the expansions in $\rho_{\mathbf{q}}$ and $\Delta\rho_{\mathbf{q}}$.

2.4 Conclusions

The main result of this chapter is the analytic estimation of the spin pair correlation function behaviour of the two-dimensional XY model with quenched disorder (random nonmagnetic dilution) at low temperatures through a perturbation expansion in the parameter characterizing disorder. Moreover, we have explored two different candidates for the perturbation theory parameter: 1) the Fourier-transform of the nonmagnetic impurities local density which was assumed small for low concentrations of dilution; 2) the deviation of the dilution density Fourier-transform from its average (over all possible realizations of disorder) value which is expected to be small for a macroscopic system. Both expansions show also some analogy with the perturbation theory for the sum over $\mathbf{k}$ which corresponds to the expansion in the effective-interaction-volume-to-elementary-cell-volume ratio ($\sim a^{-3}$). Both expansions lead to a power law decay of the pair correlation function for large distances (like in the pure model), but with a different nonuniversal exponent $\eta(T)$. Structural disorder causes increase of the pair correlation function decay exponent at low temperatures. Since it is known that the value of this exponent at the critical point of the BKT transition ($\eta(T_{\mathrm{BKT}}) = 1/4$) remains unchanged in the presence of disorder, one can already deduce that the critical temperature T_{BKT} should decrease in a diluted system (which is understood even intuitively).

Also we have realized a number of Monte Carlo simulations of the

two-dimensional XY model with different concentrations of nonmagnetic dilution in order to check our analytical approach. The comparison of the first three orders results of the two perturbation expansions, (2.79) and (2.82), to the pair correlation function exponent observed in the Monte Carlo simulations shows better accordance between theoretical and numerical results with every next order (at least up to the third order terms) (see fig.2.2), although the convergence of these expansions is questionable. In the weak dilution limit the pair correlation function exponent behaviours estimated from the two expansions of the corresponding order (except the 0th order) coincide, but in the region of stronger dilutions the expansion in the disorder configuration inhomogeneity parameter seems to come closer to the "experimental" data (see fig.2.2) (as it was expected from the very beginning).

Besides the configurationally averaged value of the pair correlation function we have found with the help of our perturbation theory the relative variance (2.84) of the configurationally dependent pair correlation function which happened to be a zero in the thermodynamic limit. Although it does not fit completely the definition of the self-averaging of a physical quantity this result is definitely in favor of the self-averaging of the pair correlation function.

Chapter 3

TOPOLOGICAL DEFECTS IN PRESENCE OF DISORDER

In this chapter the influence of nonmagnetic impurities on the behaviour of the topological defects present in the two-dimensional XY model will be studied explicitly. Such impurities being distributed randomly in the system make an example of structural disorder. In our research we will use mainly the Villain model which allows for a direct estimation of the energy of the topological defects and their interaction from the microscopic Hamiltonian of the model. The Villain model being alone a specific spin model possessing topological defects and a BKT transition with its own critical temperature can also be considered as a low-temperature approximation of the two-dimensional XY model. First of all we will focus on the energy of interaction between topological defects and nonmagnetic impurities (spin vacancies) brought into the lattice. Besides the Villain model we will make use of the phenomenological Kosterlitz-Thouless model based on the continuous medium approximation. The results obtained in both models will agree with each other as well as with other available researches of this problem. Finally, we will conclude with an approximate estimation of the critical temperature reduction due to the presence of nonmagnetic dilution. The main results of this chapter were published in [35, 37, 40, 41].

3.1 Villain model with nonmagnetic impurities

3.1.1 Villain model as a low-temperature limit of the two-dimensional XY model

As it is known for today, the Villain model [17] can be derived in the low temperature approximation from the two-dimensional XY model [18]. We are going to use the same derivation scheme in order to obtain explicitly the expressions describing the Villain model with nonmagnetic impurities starting from the model (2.9). For our convenience we consider the Hamiltonian

$$H = -J \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} [\ \cos(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'}) - 1\ ]\ c_{\mathbf{r}} c_{\mathbf{r}'} \tag{3.1}$$

equivalent to (2.9); the sum spans all the pairs of nearest neighbours. The corresponding configuration-dependent partition function reads as:

$$Z = \left(\prod_{\mathbf{r}} \int_{-\pi}^{\pi} \frac{d\theta_{\mathbf{r}}}{2\pi} \right) \exp \left[\sum_{\langle \mathbf{r},\mathbf{r}' \rangle} V(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})\ c_{\mathbf{r}} c_{\mathbf{r}'} \right] , \tag{3.2}$$

where $V(\theta) = K\,[\ \cos\theta - 1\ ]$ and $K = \beta J$.

As we have shown in the previous subsection, the spin-wave approximation applicable at low temperatures leads to the solution which obviously misses the topological defects which are supposed to cause the BKT transition, thus, in the spin-wave approximation the model possesses quasi-long-range ordering at any temperature. Further we will see that the existence of topological defects in the two-dimensional XY model is connected to the periodicity of the potential $V(\theta)$ with respect to its argument change by 2π. Obviously, this periodicity is lost when replacing the cosine in $V(\theta)$ by its approximate quadratic form valid only in the vicinity of the maximum at $\theta = 0$. As a matter of fact, $V(\theta)$ has an infinite number

of maxima at the points: $\theta = 2\pi m$, $m = 0, \pm 1, \pm 2, \ldots, \pm\infty$, and the Villain approximation means the change:

$$e^{V(\theta)} \rightarrow \sum_{m=-\infty}^{+\infty} e^{-\beta J(\theta - 2\pi m)^2} \tag{3.3}$$

which in contrast to the spin-wave approximation: $e^{V(\theta)} \rightarrow e^{-\beta J\theta^2}$, recovers the initial periodic symmetry of the $2D$ XY model.

As the first step of the derivation we expand the Boltzmann factor in the partition function (3.2) in a Fourier series:

$$\exp\left[\sum_{\langle \mathbf{r},\mathbf{r}'\rangle} V(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})\ c_{\mathbf{r}} c_{\mathbf{r}'}\right] = \prod_{\langle \mathbf{r},\mathbf{r}'\rangle} \sum_{s=-\infty}^{+\infty} \Theta(s)\ e^{is(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})}\ e^{\widetilde{V}(s) c_{\mathbf{r}} c_{\mathbf{r}'}}\ , \tag{3.4}$$

where the Fourier-transform has been written in the form $\Theta(s)\ e^{\widetilde{V}(s) c_{\mathbf{r}} c_{\mathbf{r}'}}$ with $\Theta(s) = c_{\mathbf{r}} c_{\mathbf{r}'} + (1 - c_{\mathbf{r}} c_{\mathbf{r}'})\delta_{s,0}$ which insures the equality when $c_{\mathbf{r}} c_{\mathbf{r}'} = 0$. The Fourier variable s conjugate to $\theta_{\mathbf{r}} - \theta_{\mathbf{r}'}$ is a function of two lattice sites: $s = s(\mathbf{r}, \mathbf{r}')$.

The central point of the derivation is the Poisson summation formula [110] application:

$$\sum_{s=-\infty}^{\infty} g(s) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} d\phi\ g(\phi)\ e^{-2\pi i \phi m}\ , \tag{3.5}$$

which is usually used in order improve the convergence of slowly convergent series. Thus, we can already predict that the result should be rapidly convergent. Applying (3.5) to the sum over s in (3.4) we can write the partition function (3.2) as:

$$Z = \left(\prod_{\mathbf{r}} \int_{-\pi}^{\pi} \frac{d\theta_{\mathbf{r}}}{2\pi}\right) \sum_{m_{\mathbf{r},\mathbf{r}'}=-\infty}^{+\infty} \Theta(m_{\mathbf{r},\mathbf{r}'})\ e^{\sum_{\langle \mathbf{r},\mathbf{r}'\rangle} V_0(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'} - 2\pi m_{\mathbf{r},\mathbf{r}'})\ c_{\mathbf{r}} c_{\mathbf{r}'}}\ , \tag{3.6}$$

where

$$e^{V_0(\theta)} = \int_{-\infty}^{\infty} d\phi\ e^{\widetilde{V}(\phi)}\ e^{i\phi\theta}\ . \tag{3.7}$$

For the moment we have not done any specific assumption, so the expression written above is a result of exact mathematical transformation. Now, let us consider low temperatures, i.e. $K \to \infty$. Then, the Fourier-transform

$$\begin{aligned} e^{\widetilde{V}(s)} &= \frac{1}{2\pi}\int_0^{2\pi} d\theta\; e^{-is\theta}\; e^{K(\cos\theta-1)} \;=\; e^{-K} I_s(K) \\ &\simeq \frac{1}{\sqrt{2\pi K}}\, e^{-s^2/(2K)}\;, \quad K\to\infty\;, \end{aligned} \tag{3.8}$$

where we used the well known result for the modified Bessel function $I_s(K)$ asymptotic behaviour for $K \to \infty$ [109]. Substituting (3.8) into (3.7) we find

$$e^{V_0(\theta)} \simeq e^{-K\theta^2/2}\;, \quad K\to\infty\;. \tag{3.9}$$

As a consequence, the partition function (3.6) will write in the low temperature limit:

$$Z = \sum_{m_{\mathbf{r},\mathbf{r}'}=-\infty}^{+\infty} \Theta(m_{\mathbf{r},\mathbf{r}'}) \left(\prod_{\mathbf{r}} \int_{-\pi}^{\pi} \frac{d\theta_{\mathbf{r}}}{2\pi}\right)\; e^{-\frac{K}{2}\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}(\theta_{\mathbf{r}}-\theta_{\mathbf{r}'}-2\pi m_{\mathbf{r},\mathbf{r}'})^2 c_{\mathbf{r}} c_{\mathbf{r}'}}\;. \tag{3.10}$$

But, as far as the integration boundaries with respect to the angle variables $\theta_{\mathbf{k}}$ remain $(-\pi,\pi)$, all the terms with $m_{\mathbf{r},\mathbf{r}'} \neq 0$ give vanishing contribution to the integral in comparison to the term $m_{\mathbf{r},\mathbf{r}'} = 0$. Thus, (3.10) remains equivalent to the spin-wave approximation. In order to expand the integration domain to infinity let us use the equality [17]:

$$\int_{-\pi}^{\pi} f(\varphi)d\varphi \;=\; \lim_{\varepsilon\to 0} 2\sqrt{\beta\pi\varepsilon}\int_{-\infty}^{\infty} e^{-\beta\varepsilon\varphi^2} f(\varphi)d\varphi\;, \tag{3.11}$$

true for any periodic function $f(\varphi) = f(\varphi + 2\pi)$. (3.11) can be easily checked by passing to the Fourier variables:

$$f(\varphi) = \sum_{s=-\infty}^{\infty} e^{is\varphi}F(s)\;, \qquad F(s) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-is\varphi} f(\varphi)d\varphi$$

Then, the left hand side of (3.11) simply gives $2\pi F(0)$. Integrating term by term the right hand side:

$$\sum_{s=-\infty}^{\infty} F(s) \lim_{\varepsilon\to 0} 2\sqrt{\beta\pi\varepsilon} \int_{-\infty}^{\infty} e^{-\beta\varepsilon\varphi^2+is\varphi} d\varphi \;=\; 2\pi \sum_{s=-\infty}^{\infty} F(s) \lim_{\varepsilon\to 0} e^{-s^2/(4\beta\varepsilon)} \;,$$

and taking the limit $\varepsilon \to 0$, we get $2\pi F(0)$ again.

Finally, we come to the partition function of the Villain model with nonmagnetic dilution [35]:

$$Z = \sum_{m(\mathbf{r},\mathbf{r}')=-\infty}^{+\infty} \Theta(m_{\mathbf{r},\mathbf{r}'}) \left(\prod_{\mathbf{r}} \int_{-\infty}^{\infty} \frac{d\theta_{\mathbf{r}}}{2\pi} \right) e^{-\beta H_{\mathrm{Vill}}}, \tag{3.12}$$

with the Hamiltonian

$$H_{\mathrm{Vill}} = \frac{J}{2} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} (\theta_{\mathbf{r}} - \theta_{\mathbf{r}'} - 2\pi m_{\mathbf{r},\mathbf{r}'})^2 c_{\mathbf{r}} c_{\mathbf{r}'} + \varepsilon \sum_{\mathbf{r}} \theta_{\mathbf{r}}^2 \;. \tag{3.13}$$

Putting all $c_{\mathbf{r}}$ equal to 1 we get the well known Hamiltonian of the undiluted Villain model [17]. Although, being strict, on should apply the limit $\varepsilon \to 0$ only after the functional integration with respect to the variables $\theta_{\mathbf{k}}$, hereafter we will not consider the second term when investigating the properties of the Hamiltonian (3.13).

3.1.2 Diluted Villain model Hamiltonian

The spin-wave approximation allows for an analytic solution of the pure $2D$ XY model through the Hamiltonian diagonalization in the Fourier variables, as was mentioned before. It is also known [17] that the undiluted Villain model Hamiltonian can be diagonalized (with respect to the spin-wave variables) in a similar way. But, in the case of the Villain model, the Fourier transformation should concern the discrete variables $m_{\mathbf{r},\mathbf{r}'}$ as well. Considering the sum in (3.13), we deal only with $m_{\mathbf{r},\mathbf{r}'}$ for $\mathbf{r}$ and $\mathbf{r}'$ being the nearest neighbours: $\mathbf{r}' = \mathbf{r} + \mathbf{a}_\alpha$, $\alpha = x, y$ ($\mathbf{a}_x = (a, 0)$, $\mathbf{a}_y = (0, a)$ are

the vectors of a unit cell), so, when applying the Fourier transformation, one can consider the two separate sets of "one-site" quantities $m_{\mathbf{r},\mathbf{r}+\mathbf{a}_x} \equiv m(\mathbf{r}+\frac{\mathbf{a}_x}{2})$ and $m_{\mathbf{r},\mathbf{r}+\mathbf{a}_y} \equiv m(\mathbf{r}+\frac{\mathbf{a}_y}{2})$ defined at the point shifted from the sites of the initial lattice by the vectors $\frac{\mathbf{a}_x}{2}$ and $\frac{\mathbf{a}_y}{2}$ respectively. Then, in addition to (2.15) we can write the transformation law:

$$m_{\mathbf{r},\mathbf{r}+\mathbf{a}_\alpha} = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}} e^{-i\mathbf{q}(\mathbf{r}+\frac{\mathbf{a}_\alpha}{2})} m^\alpha_{\mathbf{q}} \ , \quad m^\alpha_{\mathbf{q}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{r}} e^{i\mathbf{q}(\mathbf{r}+\frac{\mathbf{a}_\alpha}{2})} m_{\mathbf{r},\mathbf{r}+\mathbf{a}_\alpha} \ , \tag{3.14}$$

where $\alpha = x, y$, i.e. we have two independent Fourier transformations for the bonds along the Ox and Oy axes.

The Hamiltonian (3.13) can be written through (2.15), (3.14) and (2.26) as:

$$\begin{aligned} H_{\text{Vill}} \ = \ H^{\text{p}}_{\text{Vill}} \ &- \ \frac{J}{2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha} \left\{ \left(e^{i\frac{k_\alpha a}{2}} - e^{-i\frac{k_\alpha a}{2}}\right)\left(e^{i\frac{k'_\alpha a}{2}} - e^{-i\frac{k'_\alpha a}{2}}\right)\theta_{\mathbf{k}}\theta_{\mathbf{k}'} \right. \\ &- \ \left. 4\pi\left(e^{i\frac{k_\alpha a}{2}} - e^{-i\frac{k_\alpha a}{2}}\right)\theta_{\mathbf{k}} m^\alpha_{\mathbf{k}'} \ + \ 4\pi^2 m^\alpha_{\mathbf{k}} m^\alpha_{\mathbf{k}'} \right\} e^{-i\frac{(k_\alpha+k'_\alpha)a}{2}} \\ &\times \ \left[\sum_{\mathbf{q}} \rho_{\mathbf{q}} \ \left(1+e^{-iq_\alpha a}\right)\frac{1}{N}\sum_{\mathbf{r}} e^{-i(\mathbf{k}+\mathbf{k}'+\mathbf{q})\mathbf{r}} \right. \\ &- \ \left. \sum_{\mathbf{q}}\sum_{\mathbf{q}'} \rho_{\mathbf{q}}\rho_{\mathbf{q}'} \ e^{-iq'_\alpha a}\frac{1}{N}\sum_{\mathbf{r}} e^{-i(\mathbf{k}+\mathbf{k}'+\mathbf{q}+\mathbf{q}')\mathbf{r}} \right] , \end{aligned} \tag{3.15}$$

where $H^{\text{p}}_{\text{Vill}}$ is the Hamiltonian of the undiluted Villain model. Introducing special notations H^{ρ}_{Vill} and $H^{\rho^2}_{\text{Vill}}$ for the two parts of the Hamiltonian respectively linear and quadratic in ρ:

$$H_{\text{Vill}} \ = \ H^{\text{p}}_{\text{Vill}} \ + \ H^{\rho}_{\text{Vill}} \ + \ H^{\rho^2}_{\text{Vill}} \ . \tag{3.16}$$

Since $\frac{1}{N}\sum_{\mathbf{r}} e^{-i(\mathbf{k}+\mathbf{k}'+\mathbf{q})\mathbf{r}} = \delta_{\mathbf{k}+\mathbf{k}'+\mathbf{q},0}$ and $\frac{1}{N}\sum_{\mathbf{r}} e^{-i(\mathbf{k}+\mathbf{k}'+\mathbf{q}+\mathbf{q}')\mathbf{r}} = \delta_{\mathbf{k}+\mathbf{k}'+\mathbf{q}+\mathbf{q}',0}$, from (3.15) we get:

$$H^{\rho}_{\text{Vill}} \ = \ \frac{J}{2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha} \ 2\cos\frac{(k_\alpha+k'_\alpha)a}{2} \ \rho_{-\mathbf{k}-\mathbf{k}'} \left\{ K_\alpha(\mathbf{k})K_\alpha(\mathbf{k}')\theta_{\mathbf{k}}\theta_{\mathbf{k}'} \right.$$

$$+ 4\pi i K_\alpha(\mathbf{k})\theta_{\mathbf{k}} m^\alpha_{\mathbf{k}'} \; - \; 4\pi^2 m^\alpha_{\mathbf{k}} m^\alpha_{\mathbf{k}'} \Bigg\} \, , \tag{3.17}$$

where $K_\alpha(\mathbf{k}) \equiv 2\sin\frac{k_\alpha a}{2}$. In a similar way we get:

$$H^{\rho^2}_{\text{Vill}} \; = \; -\frac{J}{2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha} e^{i\frac{(k_\alpha+k'_\alpha)a}{2}} \left[\sum_{\mathbf{q}} e^{iq_\alpha a} \; \rho_{\mathbf{q}} \; \rho_{-\mathbf{k}-\mathbf{k}'-\mathbf{q}}\right] \tag{3.18}$$
$$\times\Bigg\{K_\alpha(\mathbf{k})K_\alpha(\mathbf{k}')\theta_{\mathbf{k}}\theta_{\mathbf{k}'} \; + \; 4\pi i K_\alpha(\mathbf{k})\theta_{\mathbf{k}} m^\alpha_{\mathbf{k}'} \; - \; 4\pi^2 m^\alpha_{\mathbf{k}} m^\alpha_{\mathbf{k}'} \Bigg\} \, .$$

The undiluted Villain model Hamiltonian, $H^{\text{p}}_{\text{Vill}}$, written in the Fourier variables has the form:

$$H^{\text{p}}_{\text{Vill}} = \frac{J}{2}\sum_{\mathbf{k}}\sum_{\alpha} \Bigg\{K^2_\alpha(\mathbf{k})\theta_{\mathbf{k}}\theta_{-\mathbf{k}} + 4\pi i K_\alpha(\mathbf{k})\theta_{\mathbf{k}} m^\alpha_{-\mathbf{k}} - 4\pi^2 m^\alpha_{\mathbf{k}} m^\alpha_{-\mathbf{k}}\Bigg\}. \tag{3.19}$$

One can get rid of the cross-term in (3.19) depending both on the angle variables $\theta_{\mathbf{k}}$ and discrete variables $m^\alpha_{\mathbf{k}}$ by the change of the angle variables:

$$\theta_{\mathbf{k}} \; = \; \varphi_{\mathbf{k}} \; - \; 2\pi i \frac{\sum_\alpha K_\alpha(\mathbf{k}) m^\alpha_{\mathbf{k}}}{\sum_\gamma K^2_\gamma(\mathbf{k})} \; \equiv \; \varphi_{\mathbf{k}} \; + \; \widetilde{\theta}_{\mathbf{k}} \; . \tag{3.20}$$

Substituting (3.20) into (3.19) we get:

$$H^{\text{p}}_{\text{Vill}} \; = \; \frac{J}{2}\sum_{\mathbf{k}}\sum_{\alpha} K^2_\alpha(\mathbf{k})\varphi_{\mathbf{k}}\varphi_{-\mathbf{k}} \tag{3.21}$$
$$- \; 2\pi^2 J \sum_{\mathbf{k}} \frac{\left(K_y(\mathbf{k})m^x_{\mathbf{k}} - K_x(\mathbf{k})m^y_{\mathbf{k}}\right)\left(K_y(-\mathbf{k})m^x_{-\mathbf{k}} - K_x(-\mathbf{k})m^y_{-\mathbf{k}}\right)}{K^2_x(\mathbf{k}) \; + \; K^2_y(\mathbf{k})} \; .$$

The first term has the form that fits exactly that of the spin-wave Hamiltonian (2.16) but is written through the variables $\varphi_{\mathbf{k}}$. The second part depends exclusively on the discrete variables $m^\alpha_{\mathbf{k}}$; it will be shown below that it describes the topological defects (vortices) present in the system. Let us denote the spin-wave and the vortex parts of the Hamiltonian (3.21)

as $H^{\rm p}_{\rm sw}$ and $H^{\rm p}_{\rm vort}$ respectively: $H^{\rm p}_{\rm Vill} = H^{\rm p}_{\rm sw} + H^{\rm p}_{\rm vort}$. Introducing instead of $m^\alpha_{\mathbf{k}}$ the variables

$$q_{\mathbf{k}} \;=\; i\,(K_x(\mathbf{k})m^y_{\mathbf{k}} - K_y(\mathbf{k})m^x_{\mathbf{k}}) \;\;, \tag{3.22}$$

the vortex part of the undiluted Villain model Hamiltonian can be written as:

$$H^{\rm p}_{\rm vort} \;=\; 2\pi^2 J \sum_{\mathbf{k}\neq 0} \frac{q_{\mathbf{k}} q_{-\mathbf{k}}}{\gamma_{\mathbf{k}}} \;\;, \tag{3.23}$$

where $\gamma_{\mathbf{k}} = K^2_x(\mathbf{k}) \;+\; K^2_y(\mathbf{k})$.

Unfortunately, it is not possible to split in a similar way the diluted Villain model Hamiltonian (3.17) into parts depending exclusively on $\varphi_{\mathbf{k}}$ and $q_{\mathbf{k}}$. Instead of this one has:

$$H^\rho_{\rm Vill} \;=\; H^\rho_{\rm sw} \;+\; H^\rho_{\rm vort} \;+\; H^\rho_{\rm sw,vort} \;\;, \tag{3.24}$$

where

$$H^\rho_{\rm sw} \;=\; J \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \rho_{-\mathbf{k}-\mathbf{k}'} \left(\sum_\alpha \cos\tfrac{(k_\alpha+k'_\alpha)a}{2}\; K_\alpha(\mathbf{k}) K_\alpha(\mathbf{k}') \right) \varphi_{\mathbf{k}} \varphi_{\mathbf{k}'} \tag{3.25}$$

coincides with the form of the $2D$ XY model spin-wave Hamiltonian part linear in $\rho_{\mathbf{q}}$, (2.30), and

$$\begin{aligned} H^\rho_{\rm vort} \;&=\; 4\pi^2 J \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \rho_{-\mathbf{k}-\mathbf{k}'} \\ &\times \left(\frac{\cos\frac{(k_x+k'_x)a}{2} K_y(\mathbf{k}) K_y(\mathbf{k}') + \cos\frac{(k_y+k'_y)a}{2} K_x(\mathbf{k}) K_x(\mathbf{k}')}{\left(K^2_x(\mathbf{k}) + K^2_y(\mathbf{k})\right)\left(K^2_x(\mathbf{k}') + K^2_y(\mathbf{k}')\right)} \right) q_{\mathbf{k}} q_{\mathbf{k}'} \;\;, \end{aligned} \tag{3.26}$$

and the cross-term dependent on the vortex degrees of freedom as well as on the spin-wave ones,

$$\begin{aligned} H^\rho_{\rm sw,vort} \;&=\; 4\pi J \sum_{\mathbf{k}} \sum_{\mathbf{k}'} \rho_{-\mathbf{k}-\mathbf{k}'} \\ &\times \left(\frac{\cos\frac{(k_x+k'_x)a}{2} K_x(\mathbf{k}) K_y(\mathbf{k}') - \cos\frac{(k_y+k'_y)a}{2} K_y(\mathbf{k}) K_x(\mathbf{k}')}{K^2_x(\mathbf{k}') + K^2_y(\mathbf{k}')} \right) \varphi_{\mathbf{k}} q_{\mathbf{k}'} \;\;. \end{aligned} \tag{3.27}$$

The term quadratic in $\rho_{\mathbf{q}}$ in the Hamiltonian (3.18) can be expressed in a similar way:

$$H_{\text{Vill}}^{\rho^2} \;=\; H_{\text{sw}}^{\rho^2} \;+\; H_{\text{vort}}^{\rho^2} \;+\; H_{\text{sw,vort}}^{\rho^2}\;, \tag{3.28}$$

where

$$H_{\text{sw}}^{\rho^2} = -\frac{J}{2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\alpha} e^{i\frac{(k_\alpha+k'_\alpha)a}{2}}\left[\sum_{\mathbf{q}} e^{iq_\alpha a}\;\rho_{\mathbf{q}}\rho_{-\mathbf{k}-\mathbf{k}'-\mathbf{q}}\right] K_\alpha(\mathbf{k})K_\alpha(\mathbf{k}')\varphi_{\mathbf{k}}\varphi_{\mathbf{k}'} \tag{3.29}$$

is the same as the quadratic in $\rho_{\mathbf{q}}$ part of the spin-wave Hamiltonian of the diluted two-dimensional XY model (2.30), and

$$\begin{aligned} H_{\text{vort}}^{\rho^2} \;&=\; -2\pi^2 J\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{q}}\rho_{\mathbf{q}}\rho_{-\mathbf{k}-\mathbf{k}'-\mathbf{q}} \\ &\times\left(\frac{e^{i\left(\frac{(k_x+k'_x)}{2}+q_x\right)a}K_y(\mathbf{k})K_y(\mathbf{k}') + e^{i\left(\frac{(k_y+k'_y)}{2}+q_y\right)a}K_x(\mathbf{k})K_x(\mathbf{k}')}{\left(K_x^2(\mathbf{k})+K_y^2(\mathbf{k})\right)\left(K_x^2(\mathbf{k}')+K_y^2(\mathbf{k}')\right)}\right)q_{\mathbf{k}}q_{\mathbf{k}'}, \end{aligned} \tag{3.30}$$

and

$$\begin{aligned} H_{\text{sw,vort}}^{\rho^2} \;&=\; -2\pi J\sum_{\mathbf{k}}\sum_{\mathbf{k}'}\sum_{\mathbf{q}}\rho_{\mathbf{q}}\rho_{-\mathbf{k}-\mathbf{k}'-\mathbf{q}} \\ &\times\left(\frac{e^{i\left(\frac{(k_x+k'_x)}{2}+q_x\right)a}K_x(\mathbf{k})K_y(\mathbf{k}') - e^{i\left(\frac{(k_y+k'_y)}{2}+q_y\right)a}K_y(\mathbf{k})K_x(\mathbf{k}')}{K_x^2(\mathbf{k}')+K_y^2(\mathbf{k}')}\right)\varphi_{\mathbf{k}}q_{\mathbf{k}'}. \end{aligned} \tag{3.31}$$

The part (3.26) of the diluted Villain model Hamiltonian describes the interaction of isolated nonmagnetic impurities with the topological defects (vortices) in the system, and (3.27) describes the combined interaction with the vortices as well as with the spin-wave excitations. The explicit form of these interaction energies will be written a bit later. The terms (3.29), (3.30) and (3.31) are responsable for the interaction between the nonmagnetic impurities in the presence of spin-wave and vortex excitations of the ground state. Since we consider uncorrelated disorder, it can be shown that actually only those impurities can interact which are placed at the neighbouring sites. Thus, for the case of a weak dilution when the

concentration of impurities is sufficiently small and the probability to meet two impurities on neighbouring sites is low, it is enough to consider only those contributions to the Hamiltonian linear in $\rho_{\mathbf{q}}$.

3.1.3 Topological defects in the Villain model

In order to find the quantity which corresponds in the direct space to the Fourier-transform $q_{\mathbf{k}}$ that stands in the vortex part of the Villain model Hamiltonian let us come back to the direct lattice according to the formula (3.14):

$$q_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} \left\{ iK_x(\mathbf{k}) e^{i\left(\mathbf{r}+\frac{\mathbf{a}_y}{2}\right)} m_{\mathbf{r},\mathbf{r}+\mathbf{a}_y} - iK_y(\mathbf{k}) e^{i\left(\mathbf{r}+\frac{\mathbf{a}_x}{2}\right)} m_{\mathbf{r},\mathbf{r}+\mathbf{a}_x} \right\} . \tag{3.32}$$

Obviously, one can write: $iK_\alpha(\mathbf{k}) = 2i \sin \frac{k_\alpha a}{2} = e^{i\frac{k_\alpha a}{2}} - e^{-i\frac{k_\alpha a}{2}}$. Then,

$$\begin{aligned} q_{\mathbf{k}} = & \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\mathbf{k}\left(\mathbf{r}+\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2}\right)} m_{\mathbf{r},\mathbf{r}+\mathbf{a}_y} - \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\mathbf{k}\left(\mathbf{r}-\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2}\right)} m_{\mathbf{r},\mathbf{r}+\mathbf{a}_y} \\ & - \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\mathbf{k}\left(\mathbf{r}+\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2}\right)} m_{\mathbf{r},\mathbf{r}+\mathbf{a}_x} + \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\mathbf{k}\left(\mathbf{r}+\frac{\mathbf{a}_x}{2}-\frac{\mathbf{a}_y}{2}\right)} m_{\mathbf{r},\mathbf{r}+\mathbf{a}_x} . \end{aligned} \tag{3.33}$$

Since at zero temperature we have from the Hamiltonian (3.13) minimum condition: $m_{\mathbf{r},\mathbf{r}'} = (\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})/2\pi$, it is obvious that $m_{\mathbf{r},\mathbf{r}'} = -m_{\mathbf{r}',\mathbf{r}}$. So, we can make the change: $m_{\mathbf{r},\mathbf{r}+\mathbf{a}_y} = -m_{\mathbf{r}+\mathbf{a}_y,\mathbf{r}}$, $m_{\mathbf{r},\mathbf{r}+\mathbf{a}_x} = -m_{\mathbf{r}+\mathbf{a}_x,\mathbf{r}}$ in the second and third terms in (3.33). Also we can change the summation variables in the second and the fourth terms: $\mathbf{r} \to \mathbf{r} + \mathbf{a}_x$ and $\mathbf{r} \to \mathbf{r} + \mathbf{a}_y$ respectively. After such transformations (3.33) will written as:

$$\begin{aligned} q_{\mathbf{k}} = & \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{i\mathbf{k}\left(\mathbf{r}+\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2}\right)} \Big\{ m_{\mathbf{r},\mathbf{r}+\mathbf{a}_y} + m_{\mathbf{r}+\mathbf{a}_y,\mathbf{r}+\mathbf{a}_x+\mathbf{a}_y} \\ & + m_{\mathbf{r}+\mathbf{a}_x+\mathbf{a}_y,\mathbf{r}+\mathbf{a}_x} + m_{\mathbf{r}+\mathbf{a}_x,\mathbf{r}} \Big\} . \end{aligned} \tag{3.34}$$

Introducing the vectors $\mathbf{R} = \mathbf{r} + \frac{\mathbf{a}_x}{2} + \frac{\mathbf{a}_y}{2}$ which define the sites of the so called dual lattice, we write:

$$q_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{i\mathbf{k}\mathbf{R}} \Big\{ m_{\mathbf{R}-\frac{\mathbf{a}_x}{2}-\frac{\mathbf{a}_y}{2},\mathbf{R}-\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2}} + m_{\mathbf{R}-\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2},\mathbf{R}+\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2}} + m_{\mathbf{R}+\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2},\mathbf{R}+\frac{\mathbf{a}_x}{2}-\frac{\mathbf{a}_y}{2}} + m_{\mathbf{R}+\frac{\mathbf{a}_x}{2}-\frac{\mathbf{a}_y}{2},\mathbf{R}-\frac{\mathbf{a}_x}{2}-\frac{\mathbf{a}_y}{2}} \Big\} . \quad (3.35)$$

Thus, $q_{\mathbf{k}}$ is the Fourier-transform of the quantity

$$q(\mathbf{R}) = m_{\mathbf{R}-\frac{\mathbf{a}_x}{2}-\frac{\mathbf{a}_y}{2},\mathbf{R}-\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2}} + m_{\mathbf{R}-\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2},\mathbf{R}+\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2}} + m_{\mathbf{R}+\frac{\mathbf{a}_x}{2}+\frac{\mathbf{a}_y}{2},\mathbf{R}+\frac{\mathbf{a}_x}{2}-\frac{\mathbf{a}_y}{2}} + m_{\mathbf{R}+\frac{\mathbf{a}_x}{2}-\frac{\mathbf{a}_y}{2},\mathbf{R}-\frac{\mathbf{a}_x}{2}-\frac{\mathbf{a}_y}{2}} , \quad (3.36)$$

defined on the sites of the dual lattice (see fig. 3.1); it is called topological charge or charge/strength of the vortex.

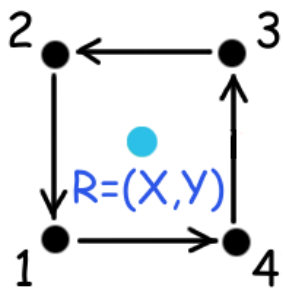

Figure 3.1: Topological charge defined on the sites $\mathbf{R}$ of the dual lattice: $q(\mathbf{R}) = m_{1,2} + m_{2,3} + m_{3,4} + m_{4,1}$, where $1 \equiv \mathbf{R} - \frac{\mathbf{a}_x}{2} - \frac{\mathbf{a}_y}{2}$, $2 \equiv \mathbf{R} - \frac{\mathbf{a}_x}{2} + \frac{\mathbf{a}_y}{2}$, $3 \equiv \mathbf{R} + \frac{\mathbf{a}_x}{2} + \frac{\mathbf{a}_y}{2}$, $4 \equiv \mathbf{R} + \frac{\mathbf{a}_x}{2} - \frac{\mathbf{a}_y}{2}$ are the sites of the initial lattice.

The vortex part (3.23) of the undiluted Villain model Hamiltonian can be written through the topological charges $q(\mathbf{R})$ as [17]:

$$H^{\mathrm{p}}_{\mathrm{vort}} = \sum_{\mathbf{R}} \sum_{\mathbf{R}'} V^{\mathrm{p}}_{qq}(\mathbf{R}-\mathbf{R}') q(\mathbf{R}) q(\mathbf{R}') + V^{\mathrm{p}}_{qq}(0) \left(\sum_{\mathbf{R}} q(\mathbf{R}) \right)^2 , \quad (3.37)$$

where the interaction energy of the two topological charges placed at sites $\mathbf{R}$ and $\mathbf{R}'$ is

$$V^{\mathrm{p}}_{qq}(\mathbf{R}-\mathbf{R}') = -2\pi^2 J \frac{2}{N} \sum_{\mathbf{k}\neq 0} \frac{\sin^2 \frac{\mathbf{k}(\mathbf{R}-\mathbf{R}')}{2}}{\gamma_{\mathbf{k}}} . \quad (3.38)$$

We already have evaluated the asymptotic behaviour of a sum of this type, (2.67), for large values of the argument $\mathbf{R}-\mathbf{R}'$: (2.72). Thus, the interaction energy of the two topological charges (vortices) $q(\mathbf{R})$ and $q(\mathbf{R}')$ is

$$V_{qq}^{\mathrm{p}}(\mathbf{R}-\mathbf{R}') \;\simeq\; -\,\pi J \ln \frac{|\mathbf{R}-\mathbf{R}'|}{a}\;, \qquad \mathbf{R}-\mathbf{R}' \to \infty\;. \tag{3.39}$$

The form of the expression (3.39) coincides with the interaction energy of the two Coulomb particles with charges $+\pi J$ in two dimensions [9]. This explains the name "charge" for the quantities $q(\mathbf{R})$. The potential $V_{qq}^{\mathrm{p}}(0)$ in (3.37) diverges with the system size N:

$$V_{qq}^{\mathrm{p}}(0) \;=\; 2\pi^2 J \frac{1}{N}\sum_{\mathbf{k}\neq 0}\frac{1}{\gamma_{\mathbf{k}}} \;\simeq\; \pi J \int_{\frac{2\sqrt{\pi}}{a\sqrt{N}}}^{\frac{2\sqrt{\pi}}{a}} \frac{dk}{k} \;\to\; \infty\;, \quad N\to\infty\;, \tag{3.40}$$

but the second term in (3.37) disappears in the case of a "neutral" system of topological charges: $\sum_{\mathbf{R}} q(\mathbf{R}) = 0$. Note that for a system of charges defined by (3.36) its neutrality follows automatically from the periodic boundary conditions.

According to Villain [17] the vortex part (3.37) of the Hamiltonian of the undiluted Villain model can be expressed with sufficient precision as:

$$H_{\mathrm{vort}}^{\mathrm{p}} \;=\; -\,\pi J \sum_{\mathbf{R}}\sum_{\mathbf{R}'\neq\mathbf{R}} q(\mathbf{R})q(\mathbf{R}') \ln\frac{|\mathbf{R}-\mathbf{R}'|}{a} \;+\; \frac{\pi^2 J}{2}\sum_{\mathbf{R}}\left(q(\mathbf{R})\right)^2\;. \tag{3.41}$$

Thus, (3.41) is equivalent to the Hamiltonian of a two-dimensional electroneutral system of Coulomb charges. The complete Hamiltonian (3.21) of the pure Villain model can be written in the direct space as:

$$\begin{aligned} H_{\mathrm{Vill}}^{\mathrm{p}} \;=\; \frac{J}{2}\sum_{\mathbf{r}}\sum_{\alpha}\left(\varphi_{\mathbf{r}}-\varphi_{\mathbf{r}+\mathbf{a}_\alpha}\right)^2 \;&-\; \pi J \sum_{\mathbf{R}}\sum_{\mathbf{R}'\neq\mathbf{R}} q(\mathbf{R})q(\mathbf{R}') \ln\frac{|\mathbf{R}-\mathbf{R}'|}{a} \\ &+\; \pi^2\frac{J}{2}\sum_{\mathbf{R}}\left(q(\mathbf{R})\right)^2\;, \end{aligned} \tag{3.42}$$

where the variable describing the spin-wave excitations,

$$\varphi_{\mathbf{r}} \;=\; \frac{1}{\sqrt{N}}\sum_{\mathbf{r}} e^{-i\mathbf{kr}}\varphi_{\mathbf{k}} \;=\; \theta_{\mathbf{r}} \;-\; \widetilde{\theta}_{\mathbf{r}}\;, \tag{3.43}$$

(see 3.20), is the angle between the spin on the site $\mathbf{r}$ and a certain direction defined by the angle

$$\widetilde{\theta}_{\mathbf{r}} \;=\; \frac{1}{\sqrt{N}}\sum_{\mathbf{r}} e^{-i\mathbf{kr}}\widetilde{\theta}_{\mathbf{k}}\;, \tag{3.44}$$

where $\widetilde{\theta}_{\mathbf{k}}$ is defined by (3.20). So,

$$\widetilde{\theta}_{\mathbf{r}} \;=\; -\,\frac{i\pi}{\sqrt{N}}\sum_{\mathbf{r}} \frac{m^x_{\mathbf{k}}\sin\frac{k_x a}{2} \;+\; m^y_{\mathbf{k}}\sin\frac{k_y a}{2}}{\sin^2\frac{k_x a}{2} \;+\; \sin^2\frac{k_y a}{2}}\; e^{-i\mathbf{kr}} \tag{3.45}$$

depends on the variables $m^{\alpha}_{\mathbf{k}}$ which are related to the topological charges. We are going to show below that the angle field $\widetilde{\theta}_{\mathbf{r}}$ describes vortex excitations of the ground state (topological defects).

Let us find the form of $\widetilde{\theta}_{\mathbf{r}}$ as a function of topological charges $q(\mathbf{R})$. For this purpose in (3.45) we pass from the variables $m^{\alpha}_{\mathbf{k}}$ to $m_{\mathbf{r},\mathbf{r}+\mathbf{a}_\alpha}$ according to (3.14) and express all the exponents under the sum through the Euler formula: $e^{\pm ix} = \cos x \pm i\sin x$. Then,

$$\widetilde{\theta}_{\mathbf{r}} \;=\; \frac{\pi}{2}\sum_{\mathbf{r}'}\left\{ m_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_x} P_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_x}(\mathbf{r}) \;+\; m_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_y} P_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_y}(\mathbf{r}) \right\}\;, \tag{3.46}$$

where we used the following notations:

$$P_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_x}(\mathbf{r}) \equiv \frac{1}{N}\sum_{\mathbf{k}} \frac{[\cos k_x(x'-x) - \cos k_x(x'+a-x)]\cos k_y(y'-y)}{\sin^2\frac{k_x a}{2} \;+\; \sin^2\frac{k_y a}{2}}\;, \tag{3.47}$$

$$P_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_y}(\mathbf{r}) \equiv \frac{1}{N}\sum_{\mathbf{k}} \frac{[\cos k_y(y'-y) - \cos k_y(y'+a-y)]\cos k_x(x'-x)}{\sin^2\frac{k_x a}{2} \;+\; \sin^2\frac{k_y a}{2}} \tag{3.48}$$

($\mathbf{r} = (x,y)$, $\mathbf{r}' = (x',y')$). Obviously, $P_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_x}(\mathbf{r}) = -P_{\mathbf{r}'+\mathbf{a}_x,\mathbf{r}'}(\mathbf{r})$, $P_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_y}(\mathbf{r}) = -P_{\mathbf{r}'+\mathbf{a}_y,\mathbf{r}'}(\mathbf{r})$. Before we noted the property: $m_{\mathbf{r},\mathbf{r}'} = -m_{\mathbf{r}',\mathbf{r}}$. Thus, we are

allowed to rewrite (3.46) as:

$$\widetilde{\theta}_{\mathbf{r}} = \frac{\pi}{4}\sum_{\mathbf{r}'}\Big\{ m_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_y} P_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_y}(\mathbf{r}) + m_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_x} P_{\mathbf{r}',\mathbf{r}'+\mathbf{a}_x}(\mathbf{r}) + m_{\mathbf{r}'+\mathbf{a}_y,\mathbf{r}'} P_{\mathbf{r}'+\mathbf{a}_y,\mathbf{r}'}(\mathbf{r}) + m_{\mathbf{r}'+\mathbf{a}_x,\mathbf{r}'} P_{\mathbf{r}'+\mathbf{a}_x,\mathbf{r}'}(\mathbf{r}) \Big\} . \tag{3.49}$$

Changing the summation indexes in the second and the third term: $\mathbf{r} \to \mathbf{r}+\mathbf{a}_y$ and $\mathbf{r} \to \mathbf{r}+\mathbf{a}_x$ respectively, and passing to the sites of the dual lattice $\mathbf{R} = (X,Y) = \mathbf{r} + \frac{\mathbf{a}_x}{2} + \frac{\mathbf{a}_y}{2}$ (see fig. 3.1), we get:

$$\widetilde{\theta}_{\mathbf{r}} = \frac{\pi}{4}\sum_{\mathbf{R}} \{P_{1,2}(\mathbf{r})m_{1,2} + P_{2,3}(\mathbf{r})m_{2,3} + P_{3,4}(\mathbf{r})m_{3,4} + P_{4,1}(\mathbf{r})m_{4,1}\} , \tag{3.50}$$

where indexes 1-4 are functions of $\mathbf{R}$: $1 \equiv \mathbf{R} - \frac{\mathbf{a}_x}{2} - \frac{\mathbf{a}_y}{2}$, $2 \equiv \mathbf{R} - \frac{\mathbf{a}_x}{2} + \frac{\mathbf{a}_y}{2}$, $3 \equiv \mathbf{R} + \frac{\mathbf{a}_x}{2} + \frac{\mathbf{a}_y}{2}$, $4 \equiv \mathbf{R} + \frac{\mathbf{a}_x}{2} - \frac{\mathbf{a}_y}{2}$. The coefficients in front of the discrete variables $m_{i,j}$ can be written as:

$$\begin{aligned}
P_{1,2}(\mathbf{r}) &= -I_{sc}(Y-y, X-x) - I_{ss}(X-x, Y-y) , \\
P_{2,3}(\mathbf{r}) &= -I_{sc}(X-x, Y-y) + I_{ss}(X-x, Y-y) , \\
P_{3,4}(\mathbf{r}) &= I_{sc}(Y-y, X-x) - I_{ss}(X-x, Y-y) , \\
P_{4,1}(\mathbf{r}) &= I_{sc}(X-x, Y-y) + I_{ss}(X-x, Y-y) ,
\end{aligned}$$

where

$$I_{sc}(X,Y) = \frac{1}{N}\sum_{k_x}\sum_{k_y} \frac{\sin\frac{k_x a}{2}\cos\frac{k_y a}{2}}{\sin^2\frac{k_x a}{2} + \sin^2\frac{k_y a}{2}} \sin k_x X \cos k_y Y , \tag{3.51}$$

$$I_{ss}(X,Y) = \frac{1}{N}\sum_{k_x}\sum_{k_y} \frac{\sin\frac{k_x a}{2}\sin\frac{k_y a}{2}}{\sin^2\frac{k_x a}{2} + \sin^2\frac{k_y a}{2}} \sin k_x X \sin k_y Y . \tag{3.52}$$

Now, let us write down the definition of a topological defect in terms of the Villain model. Obviously, the ground state of the system is realized when all $\theta_{\mathbf{r}} = \text{const}$ and all $m_{\mathbf{r},\mathbf{r}'} = 0$. A topological defect (vortex) with the charge q on the site $\mathbf{R}$ of the dual lattice is such a distorsion of the

ground state of the spins with the minimal possible energy for which the following condition is fulfilled:

$$\sum_{\langle \mathbf{r},\mathbf{r}' \rangle \in L} (\theta_{\mathbf{r}} - \theta_{\mathbf{r}'}) \;=\; q \;, \tag{3.53}$$

where the sum spans the bonds which form an arbitrary closed path L enclosing the point $\mathbf{R}$. Obviously, the minimal energy state of the system for the fixed values of $m_{\mathbf{r},\mathbf{r}'}$ will happen when $\theta_{\mathbf{r}} - \theta_{\mathbf{r}'} = 2\pi m_{\mathbf{r},\mathbf{r}'}$. So, a topological excitation of the ground state is completely defined (up to a simultaneous rotation of all spins) by the discrete variables $m_{\mathbf{r},\mathbf{r}'}$, and one can write:

$$\sum_{\langle \mathbf{r},\mathbf{r}' \rangle \in L} m_{\mathbf{r},\mathbf{r}'} \;=\; \sum_{\mathbf{R} \in V} q(\mathbf{R}) \;, \tag{3.54}$$

where the sum on the right side spans the topological charges within the area V enclosed by the path L. The equality (3.54) is a generalisation of (3.36). Some examples of isolated topological defects with different values of the charge can be seen in fig. 1.1. It is visible that such spin configurations have a common feature: when going counterclockwise around the vortex origin a full circle the angle variable undergoes a jump by $2\pi q$ where q is the vortex charge. For an isolated vortex there can be defined a line (the exact form of which is arbitrary) going from the vortex origin $\mathbf{R}$ to infinity along which the angle variable jump happens (see fig. 3.2). In order to insure the condition (3.54) one should put $m_{\mathbf{r},\mathbf{r}'}$ equal to zero for all the bond $(\mathbf{r}, \mathbf{r}')$ except those which cross the defined line and for which $m_{\mathbf{r},\mathbf{r}'} = \pm q$ (where the sign depends on the direction of the crossing).

We already have shown that a system of topological defects is neutral by definition in the Villain model with periodic boundary conditions (the sum over all the topological charges gives zero). For the neutral pair of vortices $q(\mathbf{R})$ and $-q(\mathbf{R}')$ the line of the angle variable jump must connect their origins $\mathbf{R}$ and $\mathbf{R}'$ (see fig. 3.3) in order to insure the condition (3.54).

Now, considering the vortex excitations field (3.50) far enough from the

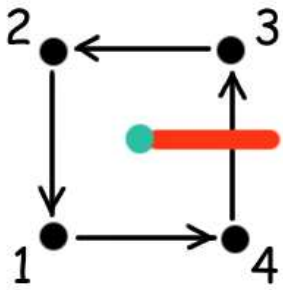

Figure 3.2: The topological charge q. All $m_{\mathbf{r},\mathbf{r}'} = 0$ except those which cross the line of the angle variable jump (thick red line): $m_{1,2} = 0$, $m_{2,3} = 0$, $m_{3,4} = q$, $m_{4,1} = 0$.

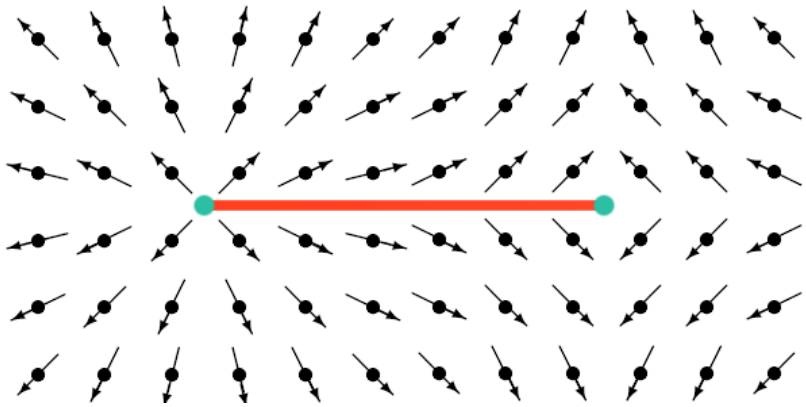

Figure 3.3: The angle variable jump line which connects the origins of the vortices bound in a neutral pair.

topological defects origins, $|\mathbf{R} - \mathbf{r}| \to \infty$, one can use the asymptotic form of the sums (3.68), (3.83). Since for a discrete lattice $X = la$, $Y = na$ (where a is the lattice constant), and l, n are integers: $\sin \frac{\pi}{a} X = \sin l\pi = 0$, $\sin \frac{\pi}{a} Y = \sin n\pi = 0$. Then, (3.50) will reads as:

$$\begin{aligned}
\widetilde{\theta}_{\mathbf{r}} \;=\; & \frac{a}{2} \sum_{\mathbf{R}} \frac{(m_{3,4} \;-\; m_{1,2})(Y-y)}{(X-x)^2 \;+\; (Y-y)^2} \left(1 - e^{-\frac{\pi}{a}(X-x)} \cos \tfrac{\pi}{a}(Y-y)\right) \\
& + \frac{a}{2} \sum_{\mathbf{R}} \frac{(m_{4,1} \;-\; m_{2,3})(X-x)}{(X-x)^2 \;+\; (Y-y)^2} \left(1 - e^{-\frac{\pi}{a}(Y-y)} \cos \tfrac{\pi}{a}(X-x)\right) \\
& - 0.17 \, \frac{a^2}{4\pi^2} \sum_{\mathbf{R}} \frac{(m_{1,2} + m_{3,4}) - (m_{2,3} + m_{4,1})}{(X-x)(Y-y)}
\end{aligned}$$

$$\times \left(1 - \cos\tfrac{\pi}{a}(X - x)\right)\left(1 - \cos\tfrac{\pi}{a}(Y - y)\right) \ . \tag{3.55}$$

Let us consider, for example, a neutral pair of vortices with charges $+q$ and $-q$ centred at the points $\mathbf{R}_+ = (X_+, Y_0)$ and $\mathbf{R}_- = (X_-, Y_0)$ respectively. Only $m_{\mathbf{r},\mathbf{r}'}$ corresponding to the bonds $(\mathbf{r}, \mathbf{r}')$ which cross the straight line l joining the origins of the topological defects and parallel to the axes Ox (see fig. 3.4) are nonzero.

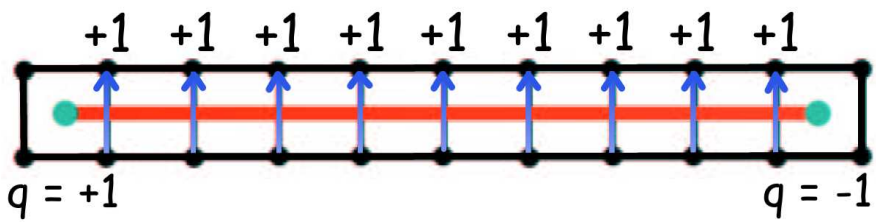

Figure 3.4: A pair of vortices with topological charges q and $-q$. The arrows mark the bonds for which $m_{\mathbf{r},\mathbf{r}'} = q$ (and, thus, $m_{\mathbf{r}',\mathbf{r}} = -q$), the rest of $m_{\mathbf{r},\mathbf{r}'}$ are zero.

So, for the dual lattice sites which are situated on the line l: $m_{1,2} = -q$, $m_{2,3} = 0$, $m_{3,4} = +q$, $m_{4,1} = 0$ in the sums in (3.55); all the rest $m_{\mathbf{r},\mathbf{r}'}$ are equal to zero. It immediately follows that the second term in (3.55) is zero, since it contains $m_{2,3}$ and $m_{4,1}$ only. In the third term all the terms in the sum turn to zero except the two corresponding to the sites $\mathbf{R}_+$ and $\mathbf{R}_-$, so it can be written as:

$$- \ 0.17\,\frac{qa^2}{4\pi^2}\left(\frac{\left(1 - \cos\frac{\pi}{a}(X_+ - x)\right)\left(1 - \cos\frac{\pi}{a}(Y_+ - y)\right)}{(X_+ - x)(Y_+ - y)} - \frac{\left(1 - \cos\frac{\pi}{a}(X_- - x)\right)\left(1 - \cos\frac{\pi}{a}(Y_- - y)\right)}{(X_- - x)(Y_- - y)}\right) .$$

We will not write this third term hereafter as it will become clear that it gives a vanishing contribution at a sufficient distance from the vortices origins. So, we are interested in the form of the spin field corresponding to a neutral vortex pair far from the origins of the topological defects. In

the limit $X_+ - x$, $Y_+ - y$, $X_- - x$, $Y_- - y \to \infty$ we can write (3.55) as:

$$\widetilde{\theta}_{\mathbf{r}} \simeq q \sum_{\mathbf{R}\in l} \frac{a(Y-y)}{(X-x)^2 + (Y-y)^2} , \tag{3.56}$$

where the sum already spans the dual lattice sites which lay on the line l only. When the distance between the origins of the topological defects, $|\mathbf{R}_+ - \mathbf{R}_-|$, is large enough, one can use an integral instead of the sum in (3.56):

$$\begin{aligned} \widetilde{\theta}_{\mathbf{r}} &= q \int_{X_+}^{X_-} dX \frac{Y_0 - y}{(X-x)^2 + (Y_0-y)^2} \\ &= q \arctan \frac{y - Y_0}{x - X_+} - q \arctan \frac{y - Y_0}{x - X_-} . \end{aligned}$$

Generalising the above result for an arbitrary number of topological defects, we may write the vortex excitations field as:

$$\widetilde{\theta}_{\mathbf{r}} = \sum_{\mathbf{R}} q(\mathbf{R}) \arctan \frac{y - Y}{x - X} , \tag{3.57}$$

where the sum spans the topological charges in the system.

Evaluation of some important integrals

Let us find the form of the functions:

$$I_{sc}(X,Y) \equiv \frac{1}{N} \sum_{k_x} \sum_{k_y} \frac{\sin\frac{k_x a}{2} \cos\frac{k_y a}{2}}{\sin^2\frac{k_x a}{2} + \sin^2\frac{k_y a}{2}} \sin k_x X \cos k_y Y , \tag{3.58}$$

$$I_{ss}(X,Y) \equiv \frac{1}{N} \sum_{k_x} \sum_{k_y} \frac{\sin\frac{k_x a}{2} \sin\frac{k_y a}{2}}{\sin^2\frac{k_x a}{2} + \sin^2\frac{k_y a}{2}} \sin k_x X \sin k_y Y , \tag{3.59}$$

containing sums which span the dual lattice sites within the 1st Brillouin zone for large values of their arguments X, Y. First of all we pass from sums to integrals in the thermodynamic limit $N \to \infty$:

$$I_{sc}(X,Y) = 4\frac{a^2}{(2\pi)^2} \int_0^{\frac{\pi}{a}} dk_x \int_0^{\frac{\pi}{a}} dk_y \frac{\sin\frac{k_x a}{2} \cos\frac{k_y a}{2}}{\sin^2\frac{k_x a}{2} + \sin^2\frac{k_y a}{2}} \sin k_x X \cos k_y Y , \tag{3.60}$$

$$I_{ss}(X,Y) \;=\; 4\frac{a^2}{(2\pi)^2}\int_0^{\frac{\pi}{a}} dk_x \int_0^{\frac{\pi}{a}} dk_y \frac{\sin\frac{k_x a}{2}\sin\frac{k_y a}{2}}{\sin^2\frac{k_x a}{2}+\sin^2\frac{k_y a}{2}}\sin k_x X \sin k_y Y \;, \tag{3.61}$$

where due to the fact that the functions in the integrals are even it was possible to reduce the integration domain to one quarter of the 1st Brillouin zone ($0 < k_x < \pi/a$, $0 < k_y < \pi/a$) just multiplying the result by 4. Changing the variable in the integral (3.60): $k_y \to y/Y$, we get:

$$I_{sc}(X,Y) \;=\; 4\frac{a^2}{(2\pi)^2}\int_0^{\frac{\pi}{a}} dk_x \int_0^{\frac{\pi}{a}Y} \frac{dy}{Y}\frac{\sin\frac{k_x a}{2}\cos\frac{ya}{2Y}}{\sin^2\frac{k_x a}{2}+\sin^2\frac{ya}{2Y}}\sin k_x X \cos y \;. \tag{3.62}$$

Then, in the limit $Y \to \infty$ one can write:

$$\begin{aligned} I_{sc}(X,Y) \;&\simeq\; 4\frac{a^2}{(2\pi)^2}\int_0^{\frac{\pi}{a}} dk_x \int_0^{\frac{\pi}{a}Y} \frac{dy}{Y}\,\frac{\sin\frac{k_x a}{2}\sin k_x X\cos y}{\sin^2\frac{k_x a}{2}+\left(\frac{ya}{2Y}\right)^2} \\ &=\; \frac{4Y}{\pi^2}\int_0^{\frac{\pi}{a}} dk_x \sin\frac{k_x a}{2}\sin k_x X \int_0^{\frac{\pi}{a}Y} \frac{\cos y\; dy}{y^2+\left(2\frac{Y}{a}\sin\frac{k_x a}{2}\right)^2} \;. \end{aligned} \tag{3.63}$$

We will get the integral with respect to y from the known formula [111]:

$$\int_0^\infty \frac{\cos my}{y^2+a^2}\,dy \;=\; \frac{\pi}{2|a|}\,e^{-|ma|} \qquad (a>0)\;, \tag{3.64}$$

then,

$$I_{sc}(X,Y) \;=\; \frac{a}{\pi}\int_0^{\frac{\pi}{a}} e^{-2\frac{Y}{a}\sin\frac{k_x a}{2}}\sin k_x X\; dk_x \;. \tag{3.65}$$

Since $Y \to \infty$, the function under the sign of an integral is vanishing everywhere except $k_x \to 0$, so we apply the Taylor expansion up to the quadratic order: $\sin\frac{k_x a}{2} \simeq \frac{k_x a}{2}$. The integral

$$I_{sc}(X,Y) \;=\; \frac{a}{\pi}\int_0^{\frac{\pi}{a}} e^{-Yk_x}\sin k_x X\; dk_x \tag{3.66}$$

is given by the formula [112]:

$$\int e^{ax}\sin bx\; dx \;=\; \frac{e^{ax}}{a^2+b^2}\left(a\sin bx - b\cos bx\right) \;. \tag{3.67}$$

Finally, we obtain:

$$I_{sc}(X,Y) \;=\; \frac{a}{\pi}\frac{X}{X^2+Y^2} \;+\; \frac{a}{\pi}\frac{e^{-\frac{\pi}{a}Y}}{X^2+Y^2}\left(Y\sin\frac{\pi}{a}X - X\cos\frac{\pi}{a}X\right) \;. \tag{3.68}$$

Although (3.68) was obtained from the assumption that $Y \to \infty$, we have serious reasons to claim that this estimation is good in a more general case when at least one of the arguments X or Y is sufficiently large, in other words, when $\sqrt{X^2+Y^2} \to \infty$. In order to convince the reader let us show explicitly that (3.68) gives the correct asymptotic behaviour of the integral (3.60) in the case: $X \to \infty$, $Y = 0$. Then, (3.60) writes as:

$$I_{sc}(X,0) \;=\; 4\frac{a^2}{(2\pi)^2}\int_0^{\frac{\pi}{a}} dk_x \int_0^{\frac{\pi}{a}} dk_y \frac{\sin\frac{k_x a}{2}\cos\frac{k_y a}{2}}{\sin^2\frac{k_x a}{2}+\sin^2\frac{k_y a}{2}}\sin k_x X \;, \tag{3.69}$$

and after the integration with respect to k_y it will look as:

$$I_{sc}(X,0) \;=\; \frac{2a}{\pi^2}\int_0^{\frac{\pi}{a}} dk_x \arctan\left[\frac{1}{\sin\frac{k_x a}{2}}\right]\sin k_x X \;. \tag{3.70}$$

After the change of the variable $k_x \to x/X$:

$$I_{sc}(X,0) \;=\; \frac{2a}{\pi^2}\,\frac{1}{X}\int_0^{\frac{\pi}{a}X} \arctan\left[\frac{1}{\sin\frac{ax}{2X}}\right]\sin x\; dx \;, \tag{3.71}$$

where in the limit $X \to \infty$: $\arctan\left[\frac{1}{\sin\frac{ax}{2X}}\right] \simeq \pi/2$. Then, finally,

$$I_{sc}(X,0) \;=\; \frac{a}{\pi}\,\frac{1}{X}\left(1-\cos\left[\pi\frac{X}{a}\right]\right) \;. \tag{3.72}$$

It is obvious that the same result follows from (3.68) for $Y = 0$.

In order to discover the behaviour of the integral (3.61) for large values of its arguments, we note that the expression $\frac{\sin\frac{k_x a}{2}\sin\frac{k_y a}{2}}{\sin^2\frac{k_x a}{2}+\sin^2\frac{k_y a}{2}}$ is slowly varying and finite in the whole domain of integration, so the rapidly oscillating functions $\sin k_x X$, $\sin k_y Y$ can be replaced in the limit $X, Y \to \infty$ by their mean values in the integration domain:

$$\frac{a}{\pi}\int_0^{\frac{\pi}{a}} \sin k_x X\; dk_x \;=\; \frac{\pi}{a}\left(1-\cos\pi\frac{X}{a}\right) \;, \tag{3.73}$$

$$\frac{a}{\pi}\int_0^{\frac{\pi}{a}} \sin k_y Y \; dk_y \;=\; \frac{\pi}{a}\left(1-\cos\pi\frac{Y}{a}\right) \;. \tag{3.74}$$

Then, the integral (3.61) will write as:

$$\begin{aligned} I_{ss}(X,Y) \;&\simeq\; \frac{a^2}{\pi^2}\frac{\left(1-\cos\pi\frac{X}{a}\right)\left(1-\cos\pi\frac{Y}{a}\right)}{XY} \\ &\times\; \frac{a^2}{\pi^2}\int_0^{\frac{\pi}{a}} dk_x \int_0^{\frac{\pi}{a}} dk_y \frac{\sin\frac{k_x a}{2}\sin\frac{k_y a}{2}}{\sin^2\frac{k_x a}{2}+\sin^2\frac{k_y a}{2}} \;, \end{aligned} \tag{3.75}$$

and the problem is reduced to the evaluation of the integral:

$$I \;=\; \frac{a^2}{\pi^2}\int_0^{\frac{\pi}{a}} dk_x \int_0^{\frac{\pi}{a}} dk_y \frac{\sin\frac{k_x a}{2}\sin\frac{k_y a}{2}}{\sin^2\frac{k_x a}{2}+\sin^2\frac{k_y a}{2}} \;, \tag{3.76}$$

which after the change of variables: $k_x \to x = \sin^2\frac{k_x a}{2}$, $k_y \to y = \sin^2\frac{k_y a}{2}$, can be written as:

$$I \;=\; \frac{1}{\pi^2}\int_0^1 \frac{dx}{\sqrt{1-x}}\int_0^1 \frac{dy}{\sqrt{1-y}}\,\frac{1}{x+y} \;. \tag{3.77}$$

Integrating with respect to y, we have:

$$I \;=\; \frac{1}{\pi^2}\int_0^1 \frac{dx}{\sqrt{1-x^2}}\ln\frac{\sqrt{1+x}+1}{\sqrt{1+x}-1} \;\equiv\; \frac{1}{\pi^2}\int_0^1 dx\frac{dV}{dx}\ln U \;, \tag{3.78}$$

where the following notions were introduced: $\frac{dV}{dx} = \frac{1}{\sqrt{1-x^2}}$, $U = \frac{\sqrt{1+x}+1}{\sqrt{1+x}-1}$. Integrating by parts, we get:

$$I \;=\; \frac{1}{\pi^2}V\ln U\Big|_0^1 \;-\; \frac{1}{\pi^2}\int_0^1 \frac{V}{U}\frac{dU}{dx}dx \;. \tag{3.79}$$

Since $V = \arcsin x$ and $\frac{dU}{dx} = \frac{1}{\left(\sqrt{1+x}-1\right)^2}$, finally:

$$I \;=\; \frac{1}{2\pi}\ln\frac{\sqrt{2}+1}{\sqrt{2}-1} \;-\; \frac{1}{\pi^2}\int_0^1 \frac{\arcsin x}{x}\,dx \;. \tag{3.80}$$

Thus,

$$\begin{aligned} I_{ss}(X,Y) \;&\simeq\; \frac{a^2}{\pi^2}\frac{\left(1-\cos\pi\frac{X}{a}\right)\left(1-\cos\pi\frac{Y}{a}\right)}{XY} \\ &\times\; \left(\frac{1}{2\pi}\ln\frac{\sqrt{2}+1}{\sqrt{2}-1} \;-\; \frac{1}{\pi^2}\int_0^1 \frac{\arcsin x}{x}\,dx\right) \;. \end{aligned} \tag{3.81}$$

The integral in the parentheses can be presented with the series [112]:

$$\int \frac{\arcsin x}{x}\, dx \;=\; x \;+\; \frac{1}{2\cdot 3\cdot 3}\, x^3 \;+\; \frac{1\cdot 3}{2\cdot 4\cdot 5\cdot 5}\, x^5 \;+\; \ldots\;, \qquad (3.82)$$

which converges very rapidly for $x = 1$. With a high enough degree of precision one can write:

$$I_{ss}(X,Y) \;\simeq\; 0.17\, \frac{a^2}{\pi^2} \frac{\left(1-\cos\pi\frac{X}{a}\right)\left(1-\cos\pi\frac{Y}{a}\right)}{XY}\;. \qquad (3.83)$$

3.2 Topological defects and nonmagnetic impurities interaction

3.2.1 Microscopic approach of the Villain model Hamiltonian

The interaction between the nonmagnetic impurities and the topological defects in the Villain model is described by the terms (3.26), (3.27), (3.30), (3.31) of the Hamiltonian (3.16). In the direct space the mentioned expressions will read as:

$$H^{\rho}_{\text{vort}} \;=\; \sum_{\mathbf{r}} (1-c_{\mathbf{r}}) \sum_{\mathbf{R}} \sum_{\mathbf{R}'} q(\mathbf{R}) q(\mathbf{R}') V^{\rho}_{qq}(\mathbf{R}-\mathbf{r}, \mathbf{R}'-\mathbf{r})\;, \qquad (3.84)$$

$$H^{\rho}_{\text{sw,vort}} \;=\; \sum_{\mathbf{r}} (1-c_{\mathbf{r}}) \sum_{\mathbf{R}} \sum_{\mathbf{r}'} q(\mathbf{R}) \varphi_{\mathbf{r}'} V^{\rho}_{q\varphi}(\mathbf{R}-\mathbf{r}, \mathbf{r}'-\mathbf{r})\;, \qquad (3.85)$$

where

$$V^{\rho}_{qq}(\mathbf{R}-\mathbf{r}, \mathbf{R}'-\mathbf{r}) \;=\; 4\pi^2 J \frac{1}{N^2} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} e^{i\mathbf{k}(\mathbf{R}-\mathbf{r})}\; e^{i\mathbf{k}'(\mathbf{R}'-\mathbf{r})} \qquad (3.86)$$
$$\times\; \frac{\cos\frac{(k_x+k'_x)a}{2} K_y(\mathbf{k}) K_y(\mathbf{k}') + \cos\frac{(k_y+k'_y)a}{2} K_x(\mathbf{k}) K_x(\mathbf{k}')}{\left(K_x^2(\mathbf{k}) + K_y^2(\mathbf{k})\right)\left(K_x^2(\mathbf{k}') + K_y^2(\mathbf{k}')\right)}$$

is the interaction energy of the pair of unit charge vortices with their origins on the sites $\mathbf{R}$ and $\mathbf{R}'$ of the dual lattice and a nonmagnetic impurity (spin

vacancy) on the site $\mathbf{r}$ of the direct lattice,

$$V^{\rho}_{q\varphi}(\mathbf{R}-\mathbf{r},\mathbf{r}'-\mathbf{r}) \;=\; 4\pi J\frac{1}{N^2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'} e^{i\mathbf{k}(\mathbf{R}-\mathbf{r})}\; e^{i\mathbf{k}'(\mathbf{R}'-\mathbf{r})} \tag{3.87}$$
$$\times\;\frac{\cos\frac{(k_x+k'_x)a}{2}K_x(\mathbf{k})K_y(\mathbf{k}')-\cos\frac{(k_y+k'_y)a}{2}K_y(\mathbf{k})K_x(\mathbf{k}')}{K_x^2(\mathbf{k}')+K_y^2(\mathbf{k}')}$$

is the energy of the interaction between the unit charge topological defect on the site $\mathbf{R}$ of the dual lattice, the spin-wave variable φ on the site $\mathbf{r}'$ of the initial lattice, and a nonmagnetic impurity on the site $\mathbf{r}$ of the initial lattice.

The contributions (3.30), (3.31), quadratic in ρ, correspond to the interaction between impurities on different sites in the presence of topological and spin-wave excitations of the ground state. In the direct space they write as:

$$H^{\rho^2}_{\text{vort}} \;=\; \sum_{\mathbf{r}}\sum_{\mathbf{r}'}(1-c_{\mathbf{r}})(1-c_{\mathbf{r}'})\sum_{\mathbf{R}}\sum_{\mathbf{R}'} q(\mathbf{R})q(\mathbf{R}')V^{\rho^2}_{qq}(\mathbf{r},\mathbf{r}',\mathbf{R},\mathbf{R}')\;, \tag{3.88}$$

$$H^{\rho^2}_{\text{sw,vort}} \;=\; \sum_{\mathbf{r}}\sum_{\mathbf{r}'}(1-c_{\mathbf{r}})(1-c_{\mathbf{r}'})\sum_{\mathbf{R}}\sum_{\mathbf{r}''} q(\mathbf{R})\varphi_{\mathbf{r}''}V^{\rho^2}_{q\varphi}(\mathbf{r},\mathbf{r}',\mathbf{R},\mathbf{r}'')\;. \tag{3.89}$$

It can be shown that this interaction can concern only those impurities which are placed at neighbouring sites. So,

$$V^{\rho^2}_{qq}(\mathbf{r},\mathbf{r}',\mathbf{R},\mathbf{R}') \;=\; -2\pi^2 J\frac{1}{N^3}\sum_{\mathbf{k}}\sum_{\mathbf{k}'} e^{i\mathbf{k}(\mathbf{R}-\mathbf{r})}\; e^{i\mathbf{k}'(\mathbf{R}'-\mathbf{r}')}$$
$$\times\sum_{\mathbf{q}} e^{i\mathbf{q}(\mathbf{r}-\mathbf{r}')}\frac{e^{i\left(\frac{k_x+k'_x}{2}+q_x\right)a}K_y(\mathbf{k})K_y(\mathbf{k}')+e^{i\left(\frac{k_y+k'_y}{2}+q_y\right)a}K_x(\mathbf{k})K_x(\mathbf{k}')}{\left(K_x^2(\mathbf{k})+K_y^2(\mathbf{k})\right)\left(K_x^2(\mathbf{k}')+K_y^2(\mathbf{k}')\right)}\;,$$

and

$$V^{\rho^2}_{q\varphi}(\mathbf{r},\mathbf{r}',\mathbf{R},\mathbf{r}'') \;=\; -2\pi J\frac{1}{N^3}\sum_{\mathbf{k}}\sum_{\mathbf{k}'} e^{i\mathbf{k}(\mathbf{R}-\mathbf{r})}\; e^{i\mathbf{k}'(\mathbf{r}''-\mathbf{r}')}$$
$$\times\sum_{\mathbf{q}} e^{i\mathbf{q}(\mathbf{r}-\mathbf{r}')}\frac{e^{i\left(\frac{k_x+k'_x}{2}+q_x\right)a}K_x(\mathbf{k})K_y(\mathbf{k}')-e^{i\left(\frac{k_y+k'_y}{2}+q_y\right)a}K_y(\mathbf{k})K_x(\mathbf{k}')}{K_x^2(\mathbf{k}')+K_y^2(\mathbf{k}')}\;.$$

The sums $\frac{1}{N}\sum_{\mathbf{q}} e^{i\mathbf{q}(\mathbf{r}+\mathbf{a}_\alpha-\mathbf{r}')}$ give the Kronecker symbols $\delta_{\mathbf{r}+\mathbf{a}_\alpha,\mathbf{r}'}$, thus,

$$V_{qq}^{\rho^2}(\mathbf{r},\mathbf{r}',\mathbf{R},\mathbf{R}') = -2\pi^2 J\frac{1}{N^2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'} e^{i\mathbf{k}(\mathbf{R}-\mathbf{r})}\, e^{i\mathbf{k}'(\mathbf{R}'-\mathbf{r}')} \times \frac{\delta_{\mathbf{r}+\mathbf{a}_x,\mathbf{r}'}K_y(\mathbf{k})K_y(\mathbf{k}') + \delta_{\mathbf{r}+\mathbf{a}_y,\mathbf{r}'}K_x(\mathbf{k})K_x(\mathbf{k}')}{\left(K_x^2(\mathbf{k})+K_y^2(\mathbf{k})\right)\left(K_x^2(\mathbf{k}')+K_y^2(\mathbf{k}')\right)}\,, \tag{3.90}$$

and

$$V_{q\varphi}^{\rho^2}(\mathbf{r},\mathbf{r}',\mathbf{R},\mathbf{r}'') = -2\pi J\frac{1}{N^2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'} e^{i\mathbf{k}(\mathbf{R}-\mathbf{r})}\, e^{i\mathbf{k}'(\mathbf{r}''-\mathbf{r}')} \times \frac{\delta_{\mathbf{r}+\mathbf{a}_x,\mathbf{r}'}K_x(\mathbf{k})K_y(\mathbf{k}') - \delta_{\mathbf{r}+\mathbf{a}_y,\mathbf{r}'}K_y(\mathbf{k})K_x(\mathbf{k}')}{K_x^2(\mathbf{k}')+K_y^2(\mathbf{k}')}\,. \tag{3.91}$$

Indeed, the expressions (3.90) and (3.91) are nonzero only in the case when the sites $\mathbf{r}$ and $\mathbf{r}'$ are nearest neighbours.

Since herein we consider small concentrations of dilution, the probability for a pair of impurities to occur at neibouring sites is small, so within the frame of our work we will focus on the form of the expressions (3.86) and (3.87) only.

Applying the Euler formula and the formula for a cosine of the product of arguments, one can write (3.86), (3.87) through the sums (3.58), (3.59) as:

$$\begin{aligned} V_{qq}^{\rho}(\mathbf{R}-\mathbf{r},\mathbf{R}'-\mathbf{r}) = -\pi^2 J\Big\{ & I_{\rm sc}(X-x,Y-y)I_{\rm sc}(X'-x,Y'-y) \\ & + I_{\rm sc}(Y-y,X-x)I_{\rm sc}(Y'-y,X'-x) \\ & - 2I_{\rm ss}(X-x,Y-y)I_{\rm ss}(X'-x,Y'-y)\Big\} \end{aligned} \tag{3.92}$$

$$\begin{aligned} V_{q\varphi}^{\rho}(\mathbf{R}-\mathbf{r},\mathbf{r}'-\mathbf{r}) = \pi J\Big\{ & \left(\delta_{\mathbf{r}-\mathbf{a}_x,\mathbf{r}'} - \delta_{\mathbf{r}+\mathbf{a}_x,\mathbf{r}'}\right) I_{\rm sc}(Y-y,X-x) \\ & + \left(\delta_{\mathbf{r}+\mathbf{a}_y,\mathbf{r}'} - \delta_{\mathbf{r}-\mathbf{a}_y,\mathbf{r}'}\right) I_{\rm sc}(X-x,Y-y) \\ & - \left(\delta_{\mathbf{r}+\mathbf{a}_x,\mathbf{r}'} + \delta_{\mathbf{r}-\mathbf{a}_x,\mathbf{r}'}\right) I_{\rm ss}(X-x,Y-y) \\ & - \left(\delta_{\mathbf{r}+\mathbf{a}_y,\mathbf{r}'} + \delta_{\mathbf{r}-\mathbf{a}_y,\mathbf{r}'}\right) I_{\rm ss}(X-x,Y-y)\Big\} \end{aligned} \tag{3.93}$$

Knowing the asymptotic behaviour of the sums (3.68), (3.68), we can write (3.92) and (3.93) as:

$$
\begin{aligned}
&V^{\rho}_{qq}(\mathbf{R}-\mathbf{r},\mathbf{R}'-\mathbf{r}) \qquad (3.94)\\
&= -\,a^2 J\Bigg\{\frac{(X-x)(X'-x)}{((X-x)^2+(Y-y)^2)\,((X'-x)^2+(Y'-y)^2)}\\
&\quad\times\left(1-e^{-\frac{\pi}{a}(Y-y)}\cos\tfrac{\pi}{a}(X-x)\right)\left(1-e^{-\frac{\pi}{a}(Y'-y)}\cos\tfrac{\pi}{a}(X'-x)\right)\\
&\qquad+\frac{(Y-y)(Y'-y)}{((X-x)^2+(Y-y)^2)\,((X'-x)^2+(Y'-y)^2)}\\
&\quad\times\left(1-e^{-\frac{\pi}{a}(X-x)}\cos\tfrac{\pi}{a}(Y-y)\right)\left(1-e^{-\frac{\pi}{a}(X'-x)}\cos\tfrac{\pi}{a}(Y'-y)\right)\\
&\qquad-2(0.17)^2\frac{a^2}{\pi^2}\,\frac{\left(1-\cos\frac{\pi}{a}(X-x)\right)\left(1-\cos\frac{\pi}{a}(Y-y)\right)}{(X-x)(X'-x)(Y-y)(Y'-y)}\\
&\qquad\times\left(1-\cos\tfrac{\pi}{a}(X'-x)\right)\left(1-\cos\tfrac{\pi}{a}(Y'-y)\right)\Bigg\}\,,
\end{aligned}
$$

$$
\begin{aligned}
&V^{\rho}_{q\varphi}(\mathbf{R}-\mathbf{r},\mathbf{r}'-\mathbf{r}) \qquad (3.95)\\
&= aJ\Bigg\{(\delta_{\mathbf{r}-\mathbf{a}_x,\mathbf{r}'}-\delta_{\mathbf{r}+\mathbf{a}_x,\mathbf{r}'})\,\frac{(Y-y)\left(1-e^{-\frac{\pi}{a}(X-x)}\cos\frac{\pi}{a}(Y-y)\right)}{(X-x)^2+(Y-y)^2}\\
&\quad+\left(\delta_{\mathbf{r}+\mathbf{a}_y,\mathbf{r}'}-\delta_{\mathbf{r}-\mathbf{a}_y,\mathbf{r}'}\right)\frac{(X-x)\left(1-e^{-\frac{\pi}{a}(Y-y)}\cos\frac{\pi}{a}(X-x)\right)}{(X-x)^2+(Y-y)^2}\\
&\quad-\left(\delta_{\mathbf{r}+\mathbf{a}_x,\mathbf{r}'}+\delta_{\mathbf{r}-\mathbf{a}_x,\mathbf{r}'}+\delta_{\mathbf{r}+\mathbf{a}_y,\mathbf{r}'}+\delta_{\mathbf{r}-\mathbf{a}_y,\mathbf{r}'}\right)\\
&\qquad\times 0.17\,\frac{a}{\pi}\,\frac{\left(1-\cos\frac{\pi}{a}(X-x)\right)\left(1-\cos\frac{\pi}{a}(Y-y)\right)}{(X-x)(Y-y)}\Bigg\}\,.
\end{aligned}
$$

Neglecting the last term in (3.94) which has a small coefficient $(0.17)^2/\pi^2$ as prefactor and considering large distances $X-x$, $Y-y$, $X'-x$, $Y'-y$ $\to\infty$, we arrive at the result:

$$
\begin{aligned}
&V^{\rho}_{qq}(\mathbf{R}-\mathbf{r},\mathbf{R}'-\mathbf{r}) \qquad (3.96)\\
&\quad= -\,a^2 J\frac{(X-x)(X'-x)+(Y-y)(Y'-y)}{((X-x)^2+(Y-y)^2)\,((X'-x)^2+(Y'-y)^2)}\,,
\end{aligned}
$$

which accords perfectly with the one obtained in the following subsection in terms of the phenomenological Kosterlitz-Thouless model.

3.2.2 Kosterlitz-Thouless phenomenological model

The Kosterlitz-Thouless model [7] built in a phenomenological way to explain the $2D$ XY model specific behaviour by the topological defects influence can be used as an alternative to the Villain model. This model is based on the continuous elastic medium approximation in which one deals with a continuous spin field instead of the discrete lattice of the $2D$ XY model (i.e. the lattice constant $a \to 0$). The spin variable $\theta_{\mathbf{r}}$ defined on the sites of a discrete lattice transforms into the field $\theta(\mathbf{r})$ defined at any point of the two-dimensional space. The energy of such a field (which is called in analogy with the elastic medium theory as *elastic energy*) is given by definition by the spin-wave Hamiltonian in which integration over the continuous domain is used instead of the sum over the lattice:

$$E_{\text{el}} \;=\; \frac{1}{2}J\int d\mathbf{r}(\nabla\theta(\mathbf{r}))^2 \;. \tag{3.97}$$

However, the elastic energy (3.97) alone can describe the system only when $\theta(\mathbf{r})$ and its gradient $\nabla\theta(\mathbf{r})$ are continuous fields, i.e. they do not contain any singularities. The topological defects (vortices) are in fact such singularities of the field $\theta(\mathbf{r})$ and its gradient.

By definition [7], a vortex with its origin at the point $\mathbf{R}$ is such a configuration of the spin field $\theta(\mathbf{r})$ which satisfies at the same time the elastic energy (3.97) (computed for the entire system except the very vicinity of the vortex origin $\mathbf{R}$) minimum condition and the special topological constrain:

$$\oint_L d\theta \;=\; 2\pi q \;, \tag{3.98}$$

where L is an arbitrary path enclosing the point $\mathbf{R}$, and q is called the vortex charge or strength. The field $\theta(\mathbf{r})$ satisfying the above conditions

has the from [42]:

$$\theta(\mathbf{r}) \;=\; q \arctan \frac{y-Y}{x-X} \;+\; \text{const} \;, \tag{3.99}$$

where $\mathbf{r} = (x, y)$ is the reference point, and $\mathbf{R} = (X, Y)$ is the vortex origin. It is not difficult to find from (3.99) the gradient:

$$\nabla\theta(\mathbf{r}) \;=\; \frac{q}{\sqrt{(x-X)^2 + (y-Y)^2}}\, \mathbf{e}_\varphi \;, \tag{3.100}$$

where

$$\mathbf{e}_\varphi \;=\; (-\sin\varphi, \cos\varphi) \;, \qquad \varphi \;=\; \arctan \frac{y-Y}{x-X} \;. \tag{3.101}$$

The gradient at the point $\mathbf{r}$ is always directed perpedicular to the radius-vector $\mathbf{r}$ drawn from the vortex origin. The vortex is completely defined by its charge q, since the constant addend (3.99) does not enter the gradient (3.100) and thus does not change the energy (3.97).

The total energy of a system possessing a topological defect consists of its elastic energy (3.97) computed for the whole system except some area around the vortex origin which is called the vortex core and the energy of that very core:

$$E \;=\; E_{\text{core}} \;+\; E_{\text{el}} \;. \tag{3.102}$$

The evaluation of the energy E_{core} is a nontrivial task and, obviously, it requires microscopic consideration of the lattice structure. However, we omit this question in our research only stating that the core energy is finite and does not depend on the system size. Hereafter we do not mention the core energies of the vortices considering only the elastic part of the energy, but keeping in mind that the vortex cores are always excluded from the integration in (3.97) and the total energy must contain the core energies as well.

The energy of the system with one single vortex defined by the equation (3.99),

$$E_{\text{el}}^{\text{pure}} \;=\; q^2 J\pi \int_A^L \frac{dr}{r} \;=\; q^2 J\pi \ln(L/A) \tag{3.103}$$

(A is the vortex core radius), diverges with the system linear size L. The energy of the system with the very same topological defect and a nonmagnetic impurity (spin vacancy) at the point r sufficiently far from the vortex origin can be evaluated by subtracting from the energy (3.103) the energy corresponding to the four bonds (for a square lattice) associated with the empty site:

$$\begin{aligned} E_{\rm el}^{\rm dil} &= E_{\rm el}^{\rm pure} - E_{\rm vac} = E_{\rm el}^{\rm pure} - \frac{1}{2} J \sum_{\alpha=x,y} [(\nabla\theta \cdot \mathbf{a}_\alpha)^2 + (-\nabla\theta \cdot \mathbf{a}_\alpha)^2] \\ &= E_{\rm el}^{\rm pure} - \frac{1}{2} q^2 J \frac{a^2}{r^2} \left\{ 2\sin^2\varphi + 2\cos^2\varphi \right\} = E_{\rm el}^{\rm pure} - Jq^2 \left(a/r\right)^2 \ . \end{aligned} \tag{3.104}$$

Thus, the interaction between a nonmagnetic impurity and a vortex appears to be attractive decaying with their separation as a power law and it depends on the absolute value of the topological charge but not on its sign. This is in good accordance with [23, 24] and our own result obtained in the Villain model. Of course, the result (3.104) is obtained with the assumption that the nonmagnetic site does not influence the vortex configuration (3.99). The validity of this approximation is reliably argued in [24]. Our result (3.104) is in fact very close to those of [24], but we have reasons to claim that our approach is more adequate, since the lattice structure has not been taken into account in [24] and the coefficient in front of the interaction energy was not set reliably.

We go beyond the single-vortex-vacancy interaction and consider a nonmagnetic impurity in a system with a pair of vortices with the charges q and q'. The spin field of such a system is presented by a superposition of the separate single vortex fields: $\theta(\mathbf{r}) + \theta'(\mathbf{r})$, where $\theta(\mathbf{r})$ and $\theta'(\mathbf{r})$ are the fields of the vortices q and q' respectively. It is known [42] that for such a system without spin vacancies the energy has the form:

$$E_{\rm el}^{\rm pure} = -2\pi J q q' \ln(R/A) + \pi J (q+q')^2 \ln(L/A) \ , \tag{3.105}$$

where R is the vortices separation. Note that the second term divergent with the system size L vanishes in the case of a neutral vortex pair ($q' = -q$).

Let the polar coordinates of the impurity be (r, φ) in the coordinate system centered in the origin of the vortex q and (r', φ') in the coordinate system centered in the origin of the vortex q'. Then, the first vortex field can be expressed as: $\theta = q\varphi + \text{const}$, and the field of the second vortex will be: $\theta' = q'\varphi' + \text{const}'$. The corresponding gradients are: $\nabla\theta = \frac{q}{r}(-\sin\varphi, \cos\varphi)$, $\nabla\theta' = \frac{q'}{r'}(-\sin\varphi', \cos\varphi')$. Then, the energy of the system reads as:

$$E_{\text{el}}^{\text{dil}} = E_{\text{el}}^{\text{pure}} - \frac{1}{2}J\sum_{i=1}^{4}\left(\nabla\theta^{(1)}\cdot\mathbf{a}_i + \nabla\theta^{(2)}\cdot\mathbf{a}_i\right)^2 \tag{3.106}$$

with $\mathbf{a}_1 = (a, 0)$, $\mathbf{a}_2 = (0, a)$, $\mathbf{a}_3 = (-a, 0)$, $\mathbf{a}_4 = (0, -a)$. Finally, we get:

$$E_{\text{el}}^{\text{dil}} = E_{\text{el}}^{\text{pure}} - Ja^2\left((q/r)^2 + (q'/r')^2 + 2(q/r)(q'/r')\cos(\varphi - \varphi')\right) . \tag{3.107}$$

It is not difficult to generalise the above result for a system with an arbitrary number of topological defects and a nonmagnetic impurity at the point $\mathbf{r}$:

$$\begin{aligned} E_{\text{el}}^{\text{dil}} &= E_{\text{el}}^{\text{pure}} - E_{\text{vac}}(\mathbf{r}) \qquad (3.108)\\ &= E_{\text{el}}^{\text{pure}} - J\sum_{\mathbf{R}}\sum_{\mathbf{R}'} q(\mathbf{R})q(\mathbf{R}')\frac{a^2}{|\mathbf{R}-\mathbf{r}||\mathbf{R}'-\mathbf{r}|}\frac{(\mathbf{R}-\mathbf{r})(\mathbf{R}'-\mathbf{r})}{|\mathbf{R}-\mathbf{r}||\mathbf{R}'-\mathbf{r}|} , \end{aligned}$$

where the sums with respect to $\mathbf{R}$ and $\mathbf{R}'$ span the topological defects in the system.

3.3 BKT transition temperature reduction in presence of disorder

The preceding subsections presented research of the form of interaction between nonmagnetic impurities and topological defects in the Villain model

as well as in the phenomenological Kosterlitz-Thouless model. Below we will use the obtained results for the evaluation of the critical temperature reduction due to the quenched nonmagnetic dilution applying appropriate simple approximations to each of these models.

Let us consider a system possessing topological defects and quenched nonmagnetic impurities. Its elastic energy can be written as:

$$E_{\rm el}^{\rm dil} = E_{\rm el}^{\rm pure} + \sum_{\mathbf{r}_{\rm vac}} E_{\rm vac}(\mathbf{r}) \ , \tag{3.109}$$

where $E_{\rm el}^{\rm pure}$ is the energy of the same system without impurities and $E_{\rm vac}(\mathbf{r})$ is the energy associated with a vacancy on the site $\mathbf{r}$ which is obviously negative and according to (3.108) has the form:

$$E_{\rm vac}(\mathbf{r}) \ = \ - \ J \sum_{\mathbf{R}} \sum_{\mathbf{R}'} q(\mathbf{R}) q(\mathbf{R}') \frac{a^2}{|\mathbf{R}-\mathbf{r}||\mathbf{R}'-\mathbf{r}|} \frac{(\mathbf{R}-\mathbf{r})(\mathbf{R}'-\mathbf{r})}{|\mathbf{R}-\mathbf{r}||\mathbf{R}'-\mathbf{r}|} \ , \tag{3.110}$$

Strictly speaking, (3.109) is not an exact expression, since the result (3.110) was obtained for a single isolated impurity. The energy of the two impurities placed on neighbouring sites is not equal to the sum of the energies of each impurity alone, since they have one common bond. Nevertheless, (3.109) can be considered as a good approximation in the case of a weak dilution. In the continuous limit one can write (3.109) as:

$$E_{\rm el}^{\rm dil} = E_{\rm el}^{\rm pure} + \int d\mathbf{r} \rho_{\rm vac}(\mathbf{r}) E_{\rm vac}(\mathbf{r}) \ , \tag{3.111}$$

where the impurities density

$$\rho_{\rm vac}(\mathbf{r}) = \sum_{\mathbf{r}'} \delta(\mathbf{r}-\mathbf{r}')(1-c_{\mathbf{r}}) \tag{3.112}$$

was introduced; δ is the delta-function, and $c_{\mathbf{r}}$ are the occupation numbers (2.1).

The energy (3.111) can be used in order to estimate the BKT transition temperature, $T_{\rm BKT}$. Let us consider an ideal system consisting only of

one neutral pair of vortices with charges with absolute values equal to one [46]. Spin-wave excitations are not taken into account, since they do not affect the topological phase transition. Thus, such a simplistic system will have only one degree of freedom which is the distance between the vortices, R. The BKT transition temperature can be approximately estimated as the temperature at which the vortex pair dissociate, i.e. when the thermodynamical average of the squared distance R^2 diverges [46]:

$$\left\langle R^2 \right\rangle = \frac{\int_a^\infty R^3 e^{-\beta E_{\rm el}(R)} dR}{\int_a^\infty R e^{-\beta E_{\rm el}(R)} dR} \to \infty \ . \tag{3.113}$$

In the undiluted system it happens at the temperature $kT_{\rm BKT}/J \simeq \pi/2$, since $E_{\rm el}^{\rm pure}(R) = 2\pi J \ln(R/a)$ and it is easy to check that $\left\langle R^2 \right\rangle = a^2(\pi\beta J - 1)/(\pi\beta J - 2)$.

The best estimations of the transition temperatures in the two-dimensional XY model and in the Villain model available for today state: $kT_{\rm BKT}^{\rm XY}/J \simeq 0.893$ and $kT_{\rm BKT}^{\rm Vill}/J \simeq 1.503$ [66]. Thus, the described method of estimation rather seems to give a result closer to the BKT transition temperature of the Villain model than to that of the $2D$ XY model. The difference between the two models is probably caused by the different behaviour of the vortices at temperatures closer to the transition temperature. We will apply the above scheme to estimate the transition temperature of the diluted Villain model.

We will estimate the BKT transition temperature as the temperature at which the average squared separation (3.113) with the energy $E_{\rm el}(R)$ given by (3.111) diverges. In principle, this result should be configuration-dependent (depend on the realization of disorder) and is practically inaccessible, but we are going to make an approximation which simplifies the problem essentially. Let us replace the actual impurities density (3.112) with an approximate form which we expect to discribe well the real dilution. Since we consider uncorrelated quenched disorder, the impurities are distributed in the system completely randomly, so there is no reason for

different parts of the system to be more or less diluted than the rest. This means that the random fluctuations of the local impurities density can be neglected to some extent, though it denies the very possibility to see any possible effects originating from these fluctuations. We replace the density (3.112) with the "smeared" density:

$$\rho(\mathbf{r}) \simeq (1-c)N/(a^2N) = (1-c)/a^2$$

which is simply the total number of empty sites devided by the system volume. Then, the integral in (3.111) can be calculated easily and we get: $E_{\rm el}(R) = [1-2(1-c)]2\pi J \ln(R/a)$. It immediately follows that the critical temperature of the system with concentration of dilution $1-c$ is $kT^{\rm dil}_{\rm BKT}/J = [1-2(1-c)]\pi/2$, or, normalizing by the pure model critical temperature,

$$T^{\rm dil}_{\rm BKT}/T^{\rm pure}_{\rm BKT} = 1-2(1-c)\ . \tag{3.114}$$

The critical temperature decreases with the concentration of nonmagnetic impurities as one could naturally expect because of the mean coordination number reduction. Although our derivation was based on the assumption about weak dilution, the result (3.114) still predicts the extinction of the BKT transition (critical temperature turns to zero) at the concentration of magnetic sites $c \leq 0.5$. Being qualitatively correct this prediction differs however from the real site percolation threshold value for the square lattice, $c \simeq 0.59$ [105].

The above consideration concerned the phenomenological Kosterlitz-Thouless model. Further we show that the same result can be found for the Villain model within the appropriate approximation. In this case the neglect of the local impurities density fluctuations means that we put $\Delta\rho_{\mathbf{q}} = 0$, or

$$\rho(\mathbf{k}+\mathbf{k}') = (1-c)\delta_{\mathbf{k}+\mathbf{k}',0}\ . \tag{3.115}$$

This can be considered as the zeroth order approximation of the perturbation expansion in the disorder configuration inhomogeneity parameter.

It leads to the following result for the interaction energy of vortices:

$$H_{\mathrm{Vort}}^{\mathrm{dil}} = 2\pi\left[1-2(1-c)\right] J \sum_{\mathbf{k}\neq\mathbf{0}} \frac{q_{\mathbf{k}} q_{-\mathbf{k}}}{\sum_{\gamma} K_{\gamma}^{2}(\mathbf{k})} \ . \tag{3.116}$$

As a consequence, the same value (3.114) of the critical temperature is obtained.

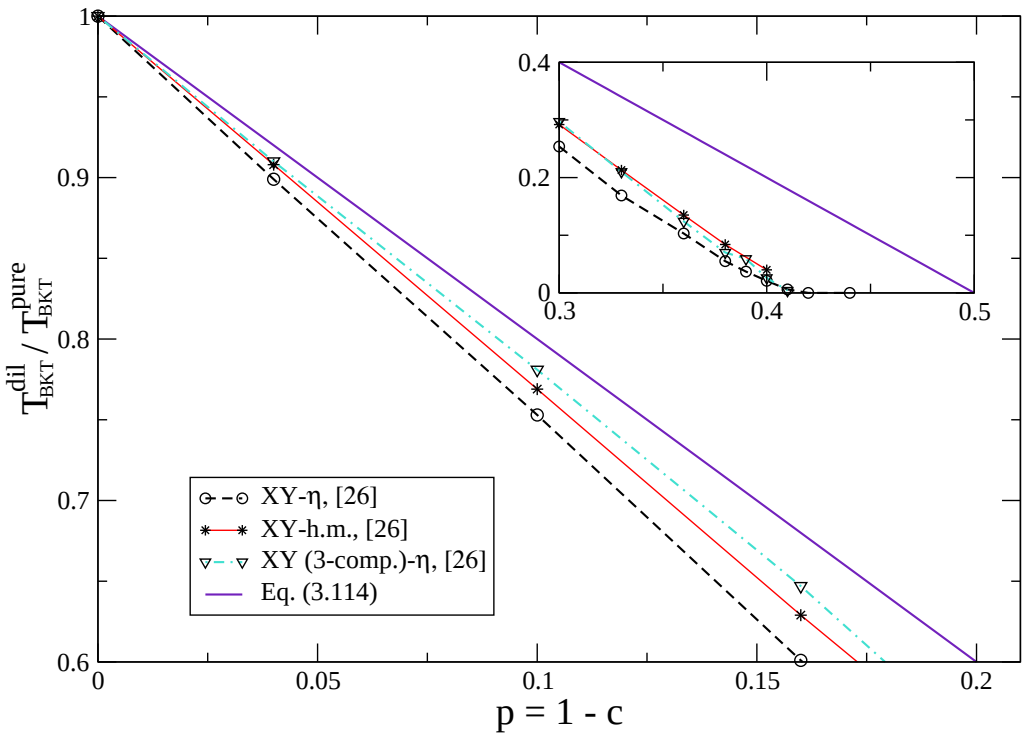

Figure 3.5: The phase diagram of the $2D$ XY model with quenched dilution of concentration $p = 1 - c$ (c is the concentration of magnetic sites). The Monte Carlo simulation results [26] are compared to our analytical prediction (3.114). The insert shows the vicinity of the percolation threshold.

Let us compare the result (3.114) obtained analytically with the critical temperature values observed in Monte Carlo simulations of a diluted $2D$ XY model available today. We compare our result with the phase diagram $(c, T_{\mathrm{BKT}}(c))$ [26]) (fig. 3.5). Those simulations covered the two variants of the XY model: with two-component and three-component spins (the third component still does not take part in the interaction, of course).

Since our estimate concerns rather the Villain model than the $2D$ XY, it is better to compare not the absolute values of the critical temperatures but the ratio (3.114) which we expect to be close for the models with the same topological mechanism of a phase transition. In [26] the transition temperature of the three-component $2D$ XY model was identified from the pair correlation function exponent $\eta(T)$ behaviour ($\eta(T_{\mathrm{BKT}}) = 1/4$). For the two-component $2D$ XY model the helicity modulus jump was used to identify the BKT transition temperature along with the mentioned method. Although the Monte Carlo data differ significantly even within the same model for different methods of critical temperature measurement, we see that our result seems to give an overestimated value of the transition temperature and this disagreement becomes more crucial at stronger dilutions. First of all one should recall that the whole analytic treatment was based on the assumption of dilution weakness, but since a systematic deviation between our prediction and the computer simulation results is notable even at low concentrations of dilution, one has to suppose that this must be the consequence of the impurities local density fluctuations which were neglected in our derivation. So, these fluctuations seem to show themselves in the increase of the effective temperature.

3.4 Conclusions

In this chapter analytical results for the structural and topological defects interaction energy were obtained, within the frame of the Villain model as well as from the phenomenological Kosterlitz-Thouless model. These two approaches together realize in fact the complete set of possible analytical tools applicable to this interaction research. The result we found in the Kosterlitz-Thouless model shows attractive interaction between non-magnetic impurities and topological defects according well with the other researches of this problem [24] which suffered however from the vague va-

cancy representation in the continuous medium approximation. We got rid of this uncertainty by taking the microscopic lattice structure into account. However, the most significant point of the chapter was the involving of the Villain model which has never been studied before in the context of the structural disorder researches. The asymptotic form of the vortex-impurity interaction found in this model coincides with the result of the Kosterlitz-Thouless model, but is obviously more reliable since it comes from the microscopic Hamiltonian and thus confirms the Kosterlitz-Thouless model approach. Moreover, the Villain model reveals much more about the impurities behaviour, for example, it says also about a combined interaction involving not only the vacancy and the vortices but also the spin-waves. Needless to say that this result would never be found in the Kosterlitz-Thouless model which do not take spin-wave excitations into account at all.

The results obtained for the energy of the interaction between structural and topological defects were used for the critical temperature reduction estimation caused by the quenched disorder. Although it was possible to obtain such an estimate only neglecting the fluctuations of the local impurities density, the final result accords with the accessible Monte Carlo simulation data, especially at low enough dilution concentrations. A deviation from the computer experiment results becomes significant for stronger dilution which we explain by the influence of the mentioned local impurities density fluctuations.

Chapter 4

LATTICE FINITENESS INFLUENCE ON THE PROPERTIES OF TWO-DIMENSIONAL SPIN MODELS OF CONTINUOUS SYMMETRY

In this chapter the lattice finiteness influence on the properties of the two-dimensional XY and Heisenberg models is studied. In the case of the $2D$ XY model we are interested in the change of the behaviour of a finite system (already well studied in the undiluted case) caused by quenched nonmagnetic dilution. In a finite $2D$ Heisenberg model the low temperature behaviour is still interesting even in the context of the undiluted model, since it lacks for researches due to the common opinion that no phase transition can occur in this model at nonzero temperature. Nevertheless, the Heisenberg model considered on a finite $2D$ lattice exhibits features very similar to those of the $2D$ XY model. Our research covers both computer simulations and analytical computations. The main results of this chapter were published in [33, 34, 36]

4.1 Residual magnetization in a finite $2D$ XY model with quenched disorder

4.1.1 Magnetization probability distribution function

The pair correlation function exponent estimation in the Monte Carlo simulations of Chapter 2 was based on the mean residual magnetization scaling behaviour. However, the very form of the residual magnetization distribution in a system of a finite size is of a great theoretical interest. As it was mentioned in Chapter 1, in the undiluted $2D$ XY model this distribution is of a non-Gaussian universal form. In presence of disorder one can naturally expect some dependence of this distribution form on the dilution concentration.

Let us define the instantaneous magnetization which is a function of the microscopic state of the system as the sum of all the spins devided by the total number of lattice sites:

$$m = \frac{1}{N} \left| \sum_{\mathbf{r}} c_{\mathbf{r}} \mathbf{S}_{\mathbf{r}} \right| \ . \tag{4.1}$$

One should notice that within the above definition the total magnetization in the ground state is equal to the concentration of magnetic sites c multiplied by the absolute value of the magnetic moment of a single spin (which is chosen equal to one in our case).

The probability to observe the equilibrium system in a state with a particular value of the magnetization (4.1) is given by the probability distribution function $P_{\text{conf}}(m)$ which is obviously dependent on the configuration of disorder.

The mean value of the magnetization defined in a usual way by the thermodynamic averaging operation with the diluted $2D$ XY model Hamiltonian (2.9):

$$\langle m \rangle = \frac{\text{Tr}\left(m e^{-\beta H}\right)}{\text{Tr}\ e^{-\beta H}} \ , \tag{4.2}$$

can be alternatively written in terms of the magnetization probability distribution function:

$$\langle m \rangle = \int_0^1 m P_{\text{conf}}(m) dm \ . \tag{4.3}$$

We define the p-th moment of magnetization as:

$$M_p \equiv \langle m^p \rangle = \frac{\text{Tr}\left(m^p e^{-\beta H}\right)}{\text{Tr}\ e^{-\beta H}} \ , \tag{4.4}$$

or, in terms of the magnetization probability distribution function:

$$M_p \equiv \langle m^p \rangle = \int_0^1 m^p P_{\text{conf}}(m) dm \ . \tag{4.5}$$

It is worth stating for complete clarity that the magnetization probability distribution function $P_{\text{conf}}(m)$ is a thermodynamic quantity, i.e. it depends on the macroscopic state of the system and m plays the role of a parameter. It becomes clear when writing the magnetization probability distribution function of the quantity m through its moments [113]:

$$P_{\text{conf}}(m) = \int_{-\infty}^{\infty} \frac{dx}{2\pi} e^{imx} \sum_{p=0}^{\infty} \frac{(-ix)^p}{p!} M_p \ . \tag{4.6}$$

Thus, the pairs of equations (4.2)/(4.4) and (4.3)/(4.5) are just alternative definitions of the same physical quantities.

It is quite obvious that the mean magnetization and its moments are configuration-dependent quantities, so to obtain their observable values one should average (4.2) and (4.4) over all possible realizations of disorder. Then, using the magnetization probability distibution function, they can be written as:

$$\overline{\langle m \rangle} = \int_0^1 m P(m) dm \tag{4.7}$$

and

$$\overline{M_p} = \int_0^1 m^p P(m) dm \ , \tag{4.8}$$

where $P(m) = \overline{P_{\text{conf}}(m)}$ is the configurationally averaged magnetization probability distribution function.

The outputs of the Monte Carlo simulations mentioned in Chapter 2 can be presented in the most explicit form by the magnetization probability distribution function for each realization of disorder (in those simulations we used 1000 random disorder realizations). The procedure of configurational averaging of the magnetization probability distribution functions observed in the Monte Carlo simulations is illustrated in fig. 4.1. One average curve $P(m)$ is drawn on the basis of the curves $P_{\text{conf}}(m)$.

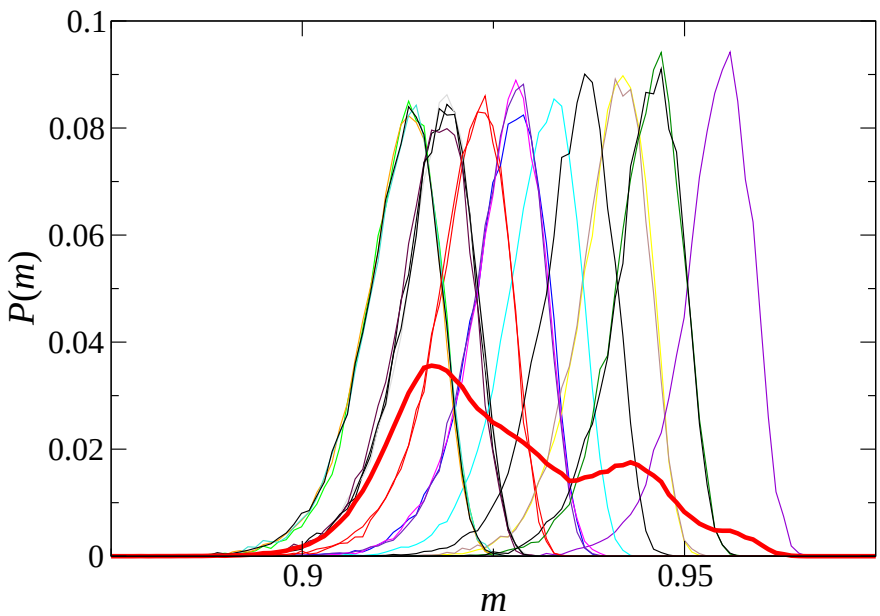

Figure 4.1: The magnetization probability distribution functions obtained for 20 different realizations of disorder in a system of the size $L = 16$ with concentration $c = 0.95$ of magnetic sites at the temperature $k_BT/J = 0.1$. The thick line represents the magnetisation probability distribution function averaged over the twenty realizations of disorder.

Probably the most remarkable features of the magnetization probability distribution function of the pure $2D$ XY model is its non-Gaussian form and universality in the sense of independence of its form on the system size and the critical exponent η. Those features have been observed in computer simulations as well as analytically [60, 62].

Fig. 4.2 presents configurationally averaged simulation results for the

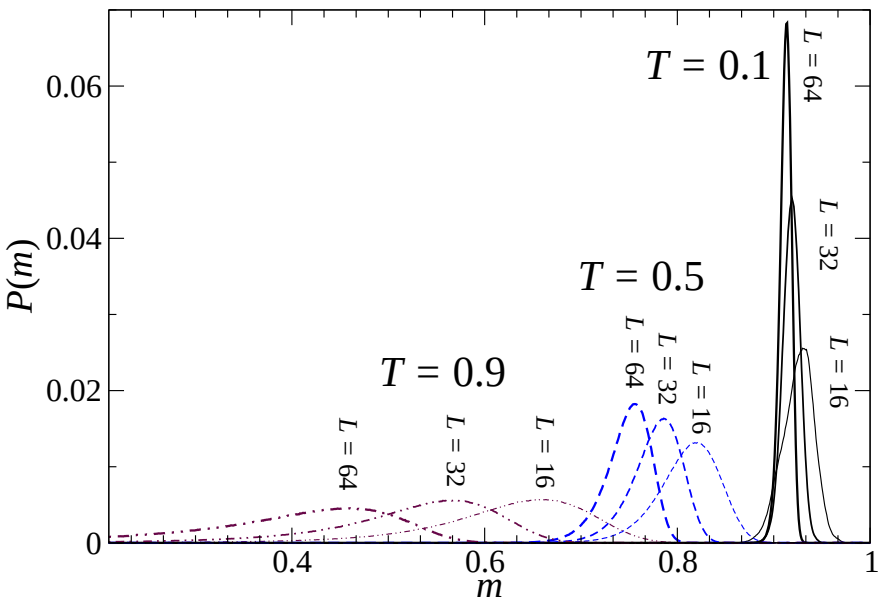

Figure 4.2: The form of the magnetization probability distribution functions averaged over 10^3 realizations of disorder ($c = 0.95$) at the temperatures $k_BT/J = 0.1$ ($T/T_{BKT}(c) \simeq 0.12$), 0.5 ($T/T_{BKT}(c) \simeq 0.60$) and 0.9 ($T/T_{BKT}(c) \simeq 1.07$) for the system of the sizes $L = 16$, 32, 64.

magnetization probability distribution function in the $2D$ XY model with fraction of magnetic sites $c = 0.95$ at three different values of the temperature. The immediate conclusion is that the distribution peak (and thus the mean value of m as well) decreases with the lattice size. The curves for lower temperatures show clearly non-Gaussian character just like in the case without dilution [60, 62].

4.1.2 Ring functions

Another way to represent the magnetization probability distribution measured in Monte Carlo simulations taking into account also the orientation of the magnetization is to draw the ring function which is obtained when one plots in the plane (m_x, m_y) (where m_x, m_y are the two conponents of the magnetization vector) the points corresponding to each measurement (see fig. 4.3). In fact, the ring function is just a bit more detailed form of

the magnetization probability distribution function.

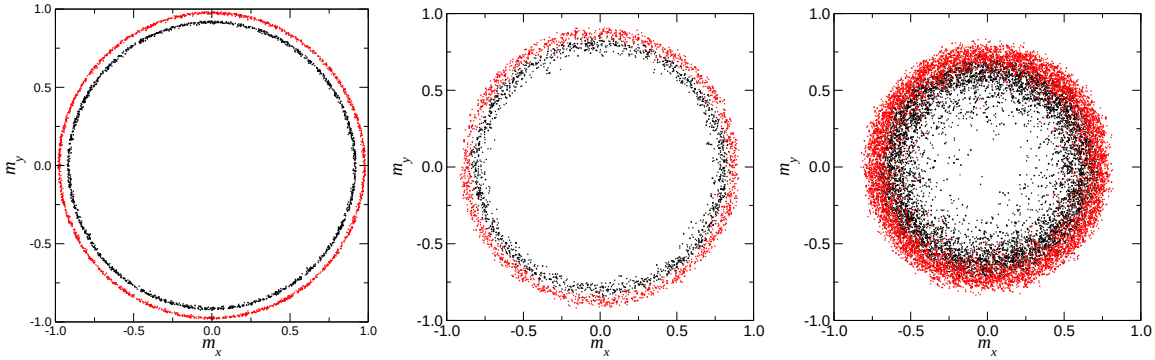

Figure 4.3: The ring functions obtained for the system of the size $L = 16$ with concentration $c = 0.95$ of magnetic sites at the temperature (left to right) $k_BT/J = 0.1$, 0.5, and 0.9. The outer rings (in red color) represent the correspondingm model without dilution.

Since the Wolff algorithm [31] that we use is a cluster algorithm, different measurement are practically not correlated in contrast to the Metropolis algorithm where the measurements correlate.

We are interested in the temperature dependence of the ring function of the diluted $2D$ XY system of a finite size with the given concentration of nonmagnetic impurities. For this purpose three different ring functions for the three values of temperature: $k_BT/J = 0.1$, 0.5 and 0.9, for a system of the size $L = 16$ are plotted in fig. 4.3. The outer rings (in red color) represent the undiluted system with analogous parameters.

Since we consider the magnetization per site and not per spin (N in (4.1) is the total number of sites both magnetic and nonmagnetic), it is obvious that its mean value in the system without dilution will be greater than the corresponding value in the diluted system with the same parameters. The stronger the dilution is, the smaller the radius of the most probable values region becomes. This feature is quite trivial and can be easily eliminated by a proper normalization of magnetization for each given dilution concentration, but the quenched non-magnetic dilution also initi-

ates other much more interesting features of the ring functions.

One of the most remarkable features is the dependence of the width of the ring function (or its variance) on the temperature. It is well seen in fig. 4.4 that the width grows as the temperature increases and tends to a delta-function when $T \to 0$. This feature is also well known from the Monte Carlo simulations and analytical researches of the undiluted two-dimensional XY model [60, 62]. The ring function of the diluted model as well as of the pure one has a distinct non-Gaussian form which can be noticed in the visible asymmetry density of the points in the regions inside and outside the peak.

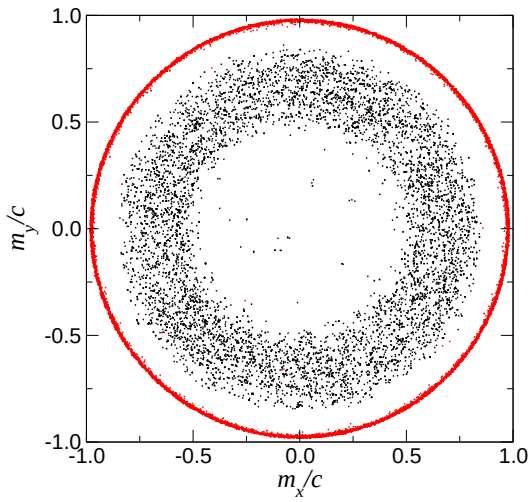

Figure 4.4: The ring function of the system of size $L = 16$ with concentration $c = 0.70$ of magnetic sites at temperature $k_BT/J = 0.1$. The outer ring represents the simulation of the analogous system without dilution.

In fig. 4.3 the behaviours of the undiluted system and the system with concentration $c = 0.95$ of magnetic sites seem to be allmost equivalent. But the dilution impact becomes more profound as the dilution concentration increases. The ring function of the system of the size $L = 16$ at the temperature $k_BT/J = 0.1$ but with much stronger dilution $c = 0.70$ is presented in fig. 4.4. It should be compared with the first plot on the left in fig. 4.3 which corresponds to the same temperature value. One can

see that nonmagnetic dilution essentially affects the distribution from: the peak position as well as the variance. Thus, theoretical description of such a behaviour is an interesting challenge for the analytic theory.

4.1.3 Mean magnetization and its moments in presence of disorder

In Chapter 2 we used the residual magnetization scaling behaviour (2.89) to estimate the pair correlation function exponent of the diluted model implicitly understanding that this relation does not change in presence of disorder. In this section we will show explicitly within the spin-wave approximation and the perturbation theory proposed in Chapter 2 that the scaling form (2.89) is valid indeed in the model with dilution.

The magnetization probability distibution in presence of disorder discussed in the previous section also requires a theoretical description, so along with the mean magnetization value we will evaluate the moments of magnetization (which allow to examine the distribution form) as well.

For analytic treatment the magnetization (4.1) should be written in angle variables $\theta_{\mathbf{r}}$:

$$m = \frac{1}{N} \sum_{\mathbf{r}} c_{\mathbf{r}} \cos(\theta_{\mathbf{r}} - \overline{\theta}) \ , \tag{4.9}$$

where $\overline{\theta} \equiv \frac{1}{N} \sum_{\mathbf{r}} \theta_{\mathbf{r}}$ is the arithmetic mean of $\theta_{\mathbf{r}}$ for the entire system.

Since we are looking for observable physical quantities, we should average the magnetization moments over all the possible realizations of disorder:

$$\overline{M_p} \equiv \overline{\langle m^p \rangle} = \frac{1}{N^p} \sum_{\mathbf{r_1},\ldots\mathbf{r_p}} \overline{\left\langle c_{\mathbf{r_1}} \cdots c_{\mathbf{r_p}} \cos\psi_{\mathbf{r_1}} \cdots \cos\psi_{\mathbf{r_p}} \right\rangle} \ ,$$

where the notation $\psi_{\mathbf{r}} = \theta_{\mathbf{r}} - \overline{\theta}$ was introduced. Note that the 1st moment,

$$\overline{M_1} = \frac{1}{N} \sum_{\mathbf{r}} \overline{\langle c_{\mathbf{r}} \cos\psi_{\mathbf{r}} \rangle} = \overline{\langle c_0 \cos\psi_0 \rangle} \ ,$$

is just the mean magnetization $\overline{\langle m\rangle}$.

Replacing the pruduct of cosines by a sum, the $(n+1)$-th moment can be written as:

$$\overline{M_{n+1}} \;=\; \frac{1}{2^n N^n}\sum_{\mathbf{r_1},\ldots\mathbf{r_n}}\sum_{\alpha_i=\pm 1}\overline{\langle c_0 c_{\mathbf{r_1}}\cdots\cos\left(\psi_0+\sum_{i=1}^n\alpha_i\psi_{\mathbf{r_i}}\right)\rangle}\;. \quad (4.10)$$

The expression under the sign of a sum in (4.10) will be written in the Fourier variables as:

$$\begin{aligned}&\overline{\langle c_0 c_{\mathbf{r_1}}\cdots c_{\mathbf{r_n}}\cos(\psi_0+\alpha_1\psi_{\mathbf{r_1}}\cdots+\alpha_n\psi_{\mathbf{r_n}})\rangle}\\ &=\overline{\left\langle c_0 c_{\mathbf{r_1}}\cdots c_{\mathbf{r_n}}\cos\tfrac{1}{\sqrt{N}}\textstyle\sum_{\mathbf{k}}\left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}}+\eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle}\end{aligned}$$

with

$$\begin{aligned}\eta^c_{\mathbf{k}} &= 1+\alpha_1\cos\mathbf{kr_1}+\cdots+\alpha_n\cos\mathbf{kr_n}\;,\\ \eta^s_{\mathbf{k}} &= -\left(\alpha_1\sin\mathbf{kr_1}+\cdots+\alpha_n\sin\mathbf{kr_n}\right)\;. \end{aligned}\quad (4.11)$$

Applying to (4.10) the expansion in the disorder configuration inhomogeneity parameter $\Delta\rho$ (analogous to (2.51)) and using the configuratinal averages (2.52), we get:

$$\begin{aligned}\overline{M_{n+1}} &= \frac{c^{n+1}}{2^n N^n}\sum_{\mathbf{r_1},\ldots\mathbf{r_n}}\sum_{\alpha_i=\pm 1}\langle\cos\left(\psi_0+\textstyle\sum_{i=1}^n\alpha_i\psi_{\mathbf{r_i}}\right)\rangle_*\\ &\times\Bigg[\;1-\frac{1}{\beta J}\Bigg(\frac{1-c}{4c^3}\frac{1}{N^2}\sum_{\mathbf{k},\mathbf{k}'}\frac{g_{\mathbf{k},\mathbf{k}'}g_{\mathbf{k}',\mathbf{k}}}{\gamma_{\mathbf{k}}}+\frac{1-3c+2c^2}{c^4}\\ &\times\left(\frac{1}{2N}\sum_{\mathbf{k}}\frac{1}{\gamma_{\mathbf{k}}}-\frac{1}{4N^3}\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''}g_{\mathbf{k},\mathbf{k}'}g_{\mathbf{k}',\mathbf{k}''}g_{\mathbf{k}'',\mathbf{k}}\frac{1}{\gamma_{\mathbf{k}}}\right)\Bigg)\\ &\qquad\times\left(n+1+2\textstyle\sum_{i<j}\alpha_i\alpha_j\cos\mathbf{k}(\mathbf{r_i}-\mathbf{r_j})\right)\Bigg]\;,\end{aligned}\quad (4.12)$$

where $g_{\mathbf{k},\mathbf{k}'}\equiv(\gamma_{\mathbf{k}+\mathbf{k}'}-\gamma_{\mathbf{k}}-\gamma_{\mathbf{k}'})/\gamma_{\mathbf{k}}$. Then, using (2.55), in the low-temperature limit one can write:

$$\langle\cos(\psi_0+\alpha_1\psi_{\mathbf{r_1}}\cdots+\alpha_n\psi_{\mathbf{r_n}})\rangle_* \;\approx\; 1 \quad (4.13)$$

$$-\tfrac{1}{4c^2\beta JN}\sum_{\mathbf{k}\neq 0}\tfrac{1}{\gamma_{\mathbf{k}}}\left(n+1+2\sum_{i<j}\alpha_i\alpha_j\cos\mathbf{k}(\mathbf{r_i}-\mathbf{r_j})\right)\ .$$

Substituting the above expression into (4.12), it then becomes possible to sum it up with respect to α_i using the obvious equalities:

$$\sum_{\alpha_i=\pm 1}\alpha_i=0\ ,\quad \alpha_i^2=1\ .$$

The $(n+1)$-th moment of magnetization then reads:

$$\begin{aligned}\overline{M_{n+1}}=c^{n+1}\Bigg[1-\frac{n+1}{\beta J}\Bigg(&\frac{1}{4c^2}\frac{1}{N}\sum_{\mathbf{k}\neq 0}\tfrac{1}{\gamma_{\mathbf{k}}}\\ &-\frac{1-c}{4c^3}\frac{1}{N^2}\sum_{\mathbf{k},\mathbf{k}'}g_{\mathbf{k},\mathbf{k}'}g_{\mathbf{k}',\mathbf{k}}\tfrac{1}{\gamma_{\mathbf{k}}}+\frac{1-3c+2c^2}{2c^4}\\ &\times\left(\frac{1}{N}\sum_{\mathbf{k}}\tfrac{1}{\gamma_{\mathbf{k}}}-\frac{1}{2N^3}\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''}g_{-\mathbf{k},\mathbf{k}'}g_{\mathbf{k}',\mathbf{k}''}g_{\mathbf{k}'',\mathbf{k}}\tfrac{1}{\gamma_{\mathbf{k}}}\right)\Bigg)\Bigg]\ .\end{aligned}\tag{4.14}$$

In the limit $N\to\infty$ the sums in (4.14) have the following asymptotic behaviour:

$$\begin{aligned}&\frac{1}{N}\sum_{\mathbf{k}}\tfrac{1}{\gamma_{\mathbf{k}}}\simeq \text{const}+\frac{1}{2\pi}\ln N,\\ &\frac{1}{N^2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'}g_{\mathbf{k},\mathbf{k}'}g_{\mathbf{k}',\mathbf{k}}\tfrac{1}{\gamma_{\mathbf{k}}}\simeq \text{const}'+\frac{0.73}{2\pi}\ln N,\\ &\frac{1}{N^3}\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''}g_{-\mathbf{k},\mathbf{k}'}g_{\mathbf{k}',\mathbf{k}''}g_{\mathbf{k}'',\mathbf{k}}\tfrac{1}{\gamma_{\mathbf{k}}}\simeq \text{const}''-\frac{0.27}{2\pi}\ln N\ .\end{aligned}$$

Now, in the low-temperature limit the p-th moment of magnetization can be expressed in the form:

$$\overline{M_p}\approx c^p N^{-\frac{p}{4}\eta^{\text{dil}}}\tag{4.15}$$

with the exponent η^{dil} given by Eq. (2.79). The formula (4.15) can be also written as:

$$\overline{M_p} \approx \overline{M_1}^p \ . \tag{4.16}$$

Since any moment of magnetization $\overline{M_p}$ can be expressed trivially through $\overline{M_1}$ in our approximation, there is no multifractality, and (4.16) does not recover the result of the work [62]:

$$M_n = M_1^n \left(1 \ + \frac{1}{(\beta J)^2} \ \frac{n(n-1)}{16N^2} \sum_{\mathbf{q}\neq 0} \frac{1}{\gamma_{\mathbf{q}}^2} \ + \ ... \right) \ .$$

The reason of this is the fact that we have neglected in our derivation the terms containing higher powers of the temperature, $1/(\beta J)$, than one. In fact, our result (4.16) corresponds to a delta-function-like probability distribution (zero variance) which is true only the low-temperature limit.

Nevertheless, the mean magnetization value predicted by (4.15) with $p = 1$:

$$\overline{\langle m \rangle} \approx c N^{-\frac{1}{4}\eta^{\mathrm{dil}}} \ , \tag{4.17}$$

supports the scaling form (2.89) and accords with the Monte Carlo simulations.

4.2 Quasi-long-range ordering in a finite two-dimensional Heisenberg model

In this section we investigate the low-temperature behaviour of the pair correlation function of a finite size two-dimensional Heisenberg model. Our research is based on the assumption that a finite $2D$ Heisenberg model possesses some spontaneous magnetization, although it should vanish in the thermodynamic limit according to the Mermin-Wagner-Hohenberg [10, 11]. Such an assumption has quite reasonable argumentation: transition to the ordered ground state (all spins in the same direction) of a finite lattice

should be continuous. So, at sufficiently low temperature the system must exhibit some finite magnetization which increases approaching $T = 0$.

According to the assumption made, all the spins $\mathbf{S_r} = (S^x_{\mathbf{r}}, S^y_{\mathbf{r}}, S^z_{\mathbf{r}})$ standing in the Hamiltonian (1.1) of the two-dimensional Heisenberg model of the size $N = L \times L$ with the ferromagnetic nearest neighbours interaction, $J(\mathbf{r} - \mathbf{r}') = J\delta_{|\mathbf{r}-\mathbf{r}'|,a}$, $(J > 0)$:

$$H = -\frac{1}{2} J \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \left(S^x_{\mathbf{r}} S^x_{\mathbf{r}'} + S^y_{\mathbf{r}} S^y_{\mathbf{r}'} + S^z_{\mathbf{r}} S^z_{\mathbf{r}'} \right) \ , \tag{4.18}$$

are pointing more less in the same direction if the temperature is sufficiently small. This approximation which is reffered to hereafter simply as the low-temperature approximation is clearly more restricting than the ordinary spin-wave approximation which only assumes the nearest neighbours to be oriented in the same way.

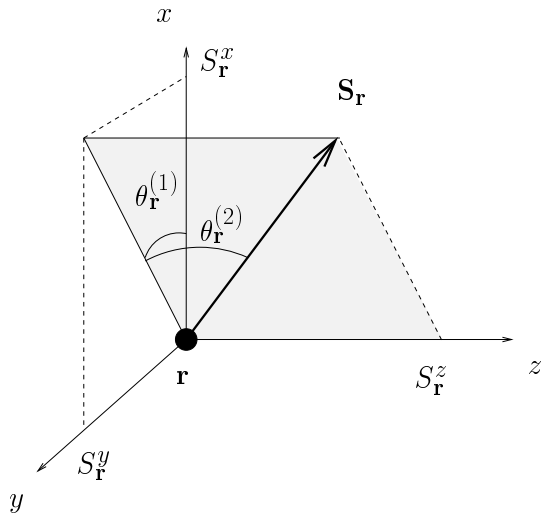

Figure 4.5: The angle variables $\theta^{(1)}_{\mathbf{r}}$ and $\theta^{(2)}_{\mathbf{r}}$ used to describe the state of the spin $\mathbf{S_r}$ placed at the site $\mathbf{r}$.

Let us pass to the angle coordinates $\theta^{(1)}_{\mathbf{r}}$, $\theta^{(2)}_{\mathbf{r}}$ (see fig. 4.5) defined by

the following relations to the Cartesian ones:

$$\begin{aligned} S^x_{\mathbf{r}} &= \cos\theta^{(1)}_{\mathbf{r}} \cos\theta^{(2)}_{\mathbf{r}} \ , \\ S^y_{\mathbf{r}} &= \sin\theta^{(1)}_{\mathbf{r}} \cos\theta^{(2)}_{\mathbf{r}} \ , \\ S^z_{\mathbf{r}} &= \sin\theta^{(2)}_{\mathbf{r}} \ , \end{aligned} \tag{4.19}$$

where $-\pi \leq \theta^{(1)} < \pi$, $-\frac{\pi}{2} \leq \theta^{(2)} < \frac{\pi}{2}$. The chosen variables are modified spherical coordinates φ, θ: $\theta^{(1)}_{\mathbf{r}} = \varphi$, $\theta^{(2)}_{\mathbf{r}} = \theta - \pi/2$. Considering the angles $\theta^{(1)}_{\mathbf{r}}$, $\theta^{(2)}_{\mathbf{r}}$ small at low enough temperatures, the scalar product of the two spins in (4.18):

$$\begin{aligned} S^x_{\mathbf{r}} S^y_{\mathbf{r}'} + S^y_{\mathbf{r}} S^y_{\mathbf{r}'} + S^z_{\mathbf{r}} S^z_{\mathbf{r}'} &= \cos(\theta^{(1)}_{\mathbf{r}} - \theta^{(1)}_{\mathbf{r}'}) \cos(\theta^{(2)}_{\mathbf{r}} - \theta^{(2)}_{\mathbf{r}'}) \\ &+ \left(1 - \cos(\theta^{(1)}_{\mathbf{r}} - \theta^{(1)}_{\mathbf{r}'})\right) \sin\theta^{(2)}_{\mathbf{r}} \sin\theta^{(2)}_{\mathbf{r}'} \ , \end{aligned} \tag{4.20}$$

can be expressed as:

$$S^x_1 S^x_2 + S^y_1 S^y_2 + S^z_1 S^z_2 \approx 1 - \frac{1}{2}(\theta^{(1)}_1 - \theta^{(1)}_2)^2 - \frac{1}{2}(\theta^{(2)}_1 - \theta^{(2)}_2)^2 \ , \tag{4.21}$$

and the Hamiltonian (4.18) takes the form

$$H = H_0 + H^{XY}_1(\{\theta^{(1)}\}) + H^{XY}_1(\{\theta^{(2)}\}) \ , \tag{4.22}$$

where

$$H^{XY}_1(\{\theta\}) = \frac{1}{4} \sum_{\mathbf{r}} \sum_{\mathbf{r}'} J(\mathbf{r} - \mathbf{r}') \left(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'}\right)^2 \tag{4.23}$$

is the $2D$ XY model Hamiltonian in the spin-wave approximation [16]. H_0 is nothing more than a trivial shift in the energy scale.

The spin pair correlation function under the assumption of small values of $\theta^{(1)}_{\mathbf{r}}$ and $\theta^{(2)}_{\mathbf{r}}$ writes as:

$$G_2(R) = \langle \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\mathbf{R}} \rangle \approx \left\langle \cos(\theta^{(1)}_{\mathbf{r}} - \theta^{(1)}_{\mathbf{r}+\mathbf{R}}) \cos(\theta^{(2)}_{\mathbf{r}} - \theta^{(2)}_{\mathbf{r}+\mathbf{R}}) \right\rangle \ . \tag{4.24}$$

where the brackets designate thermodynamical averaging:

$$\langle ... \rangle = \frac{1}{Z} \mathrm{Tr}\,(... \ e^{-\beta H}), \qquad \text{де} \quad Z = \mathrm{Tr}\ e^{-\beta H}$$

and

$$\mathrm{Tr}\ldots = \prod_{\mathbf{r}} \frac{1}{4\pi} \int_{-\pi}^{\pi} d\theta_{\mathbf{r}}^{(1)} \int_{-\pi/2}^{\pi/2} d\theta_{\mathbf{r}}^{(2)} \cos\theta_{\mathbf{r}}^{(2)} \ldots \ . \tag{4.25}$$

Due to the separation of variables $\theta_{\mathbf{r}}^{(1)}$ and $\theta_{\mathbf{r}}^{(2)}$ in the integral in (4.24) the pair correlation function can be written in the following form:

$$G_2(R) \ = \ G_2^{(1)}(R) \times G_2^{(2)}(R) \ , \tag{4.26}$$

where

$$G_2^{(1)}(R) = \frac{1}{Z_1}(2\pi)^{-N} \left(\prod_{\mathbf{r}'} \int_{-\pi}^{\pi} d\theta_{\mathbf{r}'}^{(1)} \right) e^{-\beta H_1^{XY}(\{\theta^{(1)}\})} \cos(\theta_{\mathbf{r}}^{(1)} - \theta_{\mathbf{r}+\mathbf{R}}^{(1)}) \ , \tag{4.27}$$

and

$$G_2^{(2)}(R) = \frac{1}{Z_2} 2^{-N} \left(\prod_{\mathbf{r}'} \int_{-\pi/2}^{\pi/2} d\theta_{\mathbf{r}'}^{(2)} \cos\theta_{\mathbf{r}'}^{(2)} \right) e^{-\beta H_1^{XY}(\{\theta^{(2)}\})} \cos(\theta_{\mathbf{r}}^{(2)} - \theta_{\mathbf{r}+\mathbf{R}}^{(2)}) \ . \tag{4.28}$$

Z_1 and Z_2 appear from the separation of the variables $\theta_{\mathbf{r}}^{(1)}$ and $\theta_{\mathbf{r}}^{(2)}$ respectively in the partition function: $Z = Z_1 Z_2$.

Now, it is enough to evaluate the asymptotic behaviour of the functions $G_2^{(1)}(R)$ and $G_2^{(2)}(R)$ in the limit $R/a \to \infty$ to know the pair correlation function behaviour at large distances. It is easy to notice that $G_2^{(1)}(R)$ has the same form as the pair correlation function of the $2D$ XY model which asymptotic behaviour is well known. Thus, our task reduces to the evaluation of $G_2^{(2)}(R)$ in the limit $R/a \to \infty$. For this purpose we pass to the Fourier variables:

$$\theta_{\mathbf{r}}^{(2)} = \frac{1}{L} \sum_{\mathbf{k}} \ e^{i\mathbf{kr}} \theta_{\mathbf{k}}, \quad \theta_{\mathbf{k}} = \frac{1}{L} \sum_{\mathbf{r}} \ e^{-i\mathbf{kr}} \theta_{\mathbf{r}}^{(2)}, \tag{4.29}$$

where $\mathbf{r}$ spans the sites of a square lattice of the size $L \times L$, and $\mathbf{k}$ spans the sites of the inverse lattice within the 1st Brillouin zone. Then, the Hamiltonian (4.23) writes as:

$$H_1^{XY}(\{\theta\}) = J \sum_{\mathbf{k} \neq 0} \gamma_{\mathbf{k}} \theta_{\mathbf{k}} \theta_{-\mathbf{k}}$$

with $\gamma_{\mathbf{k}} \equiv 2 - \cos k_x - \cos k_y$. The Jacobian of the transformation, $\prod_{\mathbf{r}} \cos\theta_{\mathbf{r}}^{(2)}$, in (4.28) can be replace in the low-temperature limit by the expression $\exp\left[-\frac{1}{2}\sum_{\mathbf{r}}(\theta_{\mathbf{r}}^{(2)})^2\right]$ and written in the Fourier variables using the equality: $\sum_{\mathbf{r}}(\theta_{\mathbf{r}}^{(2)})^2 = \sum_{\mathbf{k}}\theta_{\mathbf{k}}\theta_{-\mathbf{k}}$. The cosine $\cos(\theta_{\mathbf{r}}^{(2)} - \theta_{\mathbf{r}+\mathbf{R}}^{(2)})$ in (4.28) can be represented in the Fourier variables as the real part of $\exp\left[\frac{i}{L}\sum_{\mathbf{k}}(e^{i\mathbf{k}(\mathbf{r}+\mathbf{R})} - e^{i\mathbf{k}\mathbf{r}})\theta_{\mathbf{k}}\right]$.

So, (4.28) leads to a product of the integrals of the type $\int d\theta e^{-a\theta^2+b\theta}$ which can be immediately calculated expanding the integration boundaries to infinity (it is acceptable in the low-temperature limit). The integration gives:

$$G_2^{(2)}(R) = \exp\left(-\frac{1}{\beta JN}\sum_{\mathbf{k}}\frac{\sin^2\frac{\mathbf{kR}}{2}}{\gamma_{\mathbf{k}} + \frac{1}{2\beta J}}\right) . \tag{4.30}$$

In order to obtain the explicit form of (4.30) as a function of temperature $1/(\beta J)$ and distance R/a when its both arguments are sufficiently large, we expand $\gamma_{\mathbf{k}}$ for small $\mathbf{k}$-s: $\gamma_{\mathbf{k}} \simeq k^2/2$ and replace the sum with an integral in the polar coordinates ($\frac{1}{2}\mathbf{kR} = \frac{1}{2}kR\cos\varphi \equiv z\cos\varphi$):

$$I(R) \equiv \frac{1}{N}\sum_{\mathbf{k}}\frac{\sin^2\frac{\mathbf{kR}}{2}}{\gamma_{\mathbf{k}} + \frac{1}{2\beta J}} = \frac{1}{2\pi^2}\int_0^{\frac{\sqrt{\pi}}{a}R}\frac{zdz}{z^2 + \frac{(R/a)^2}{4\beta J}}\int_0^{2\pi} d\varphi \sin^2(z\cos\varphi) . \tag{4.31}$$

In the limit $\frac{(R/a)^2}{4\beta J} \gg 1$ $\sin^2(z\cos\varphi)$ can be replace by its mean value over the integration domain, $\frac{1}{2}$, which leads to $I(R) \approx \frac{1}{2\pi}\ln(4\pi\beta J)$. In the opposite case, $\frac{(R/a)^2}{4\beta J} \ll 1$, we choose a finite parameter $\varepsilon < 1$ in such a way that $\frac{(R/a)^2}{4\beta J}/\varepsilon^2 \ll 1$ and split the integration with respect to z in $I(R)$ into two parts: $\int_0^{\varepsilon} + \int_{\varepsilon}^{\frac{\sqrt{\pi}}{a}R}$. The first part vanishes after the cosine expansion and term by term integration in the limiting case we consider. The second part exhibits the following behaviour: $\frac{1}{2\pi}\ln(R/a)$. So,

$$G_2^{(2)}(R) \simeq \begin{cases} (R/a)^{-\frac{1}{2\pi\beta J}} & \text{for} \quad \frac{(R/a)^2}{4\beta J} \ll 1; \\ (4\pi\beta J)^{-\frac{1}{2\pi\beta J}} & \text{for} \quad \frac{(R/a)^2}{4\beta J} \gg 1 . \end{cases} \tag{4.32}$$

We see that $G_2^{(2)}(R)$ is either constant with respect to R or equivalent

to the $2D$ XY model pair correlation function depending on the value of $\frac{(R/a)^2}{4\beta J}$.

Finally, substituting (4.32) into (4.26) we get the following pair correlation function behaviour for a finite two-dimensional Heisenberg model at sufficiently low temperatures:

$$G_2(R) \simeq \begin{cases} (R/a)^{-2\eta^{XY}} & \text{for} \quad \frac{(R/a)^2}{4\beta J} \ll 1 \ ; \\ (4\pi\beta J)^{-\eta^{XY}} \, (R/a)^{-\eta^{XY}} & \text{for} \quad \frac{(R/a)^2}{4\beta J} \gg 1 \ , \end{cases} \tag{4.33}$$

where η^{XY} is the exponent of the $2D$ XY model pair correlation function decay, Eq. (1.6).

At this point we should clarify which of the two asymptotic forms obtained, (4.33), is physically correct. Though we consider large distances, the limit $R/a \to \infty$ remains in fact practically unrichable in a finite system, since its value is limited by the lattice size: $R/a < L$. On the other hand, the lower the temperature is, the bigger the spontaneous magnetization value becomes, and thus the more reliable our approximation is. So the limit $\beta J \to \infty$ is our case. This leads to the conclusion that it is the case $\frac{(R/a)^2}{4\beta J} \ll 1$ in (4.33) which is physically correct. So, we can claim that in the low-temperature limit the pair correlation function of a finite two-dimensional Heisenberg model decays with the distance according to a power law with the exponent two times greater that that of the $2D$ XY model:

$$G_2(R) \simeq (R/a)^{-2\eta^{XY}} \ . \tag{4.34}$$

In order to check the analytical result we have performed a series of Monte Carlo simulations of the Heisenberg model on two-dimensional lattices of different sizes at different temperatures. The simulation was based on the Wolff cluster algorithm [31]. The pair correlation function exponent η was obtained from the scaling behaviour of the three physical quantities: magnetization, $M \sim L^{-\frac{1}{2}\eta(T)}$ (see fig. 4.6); pair correlation function, $G_2(L/2) \sim L^{-\eta(T)}$; and magnetic susceptibility: $\chi \sim L^{2-\eta(T)}$ (see fig. 4.6).

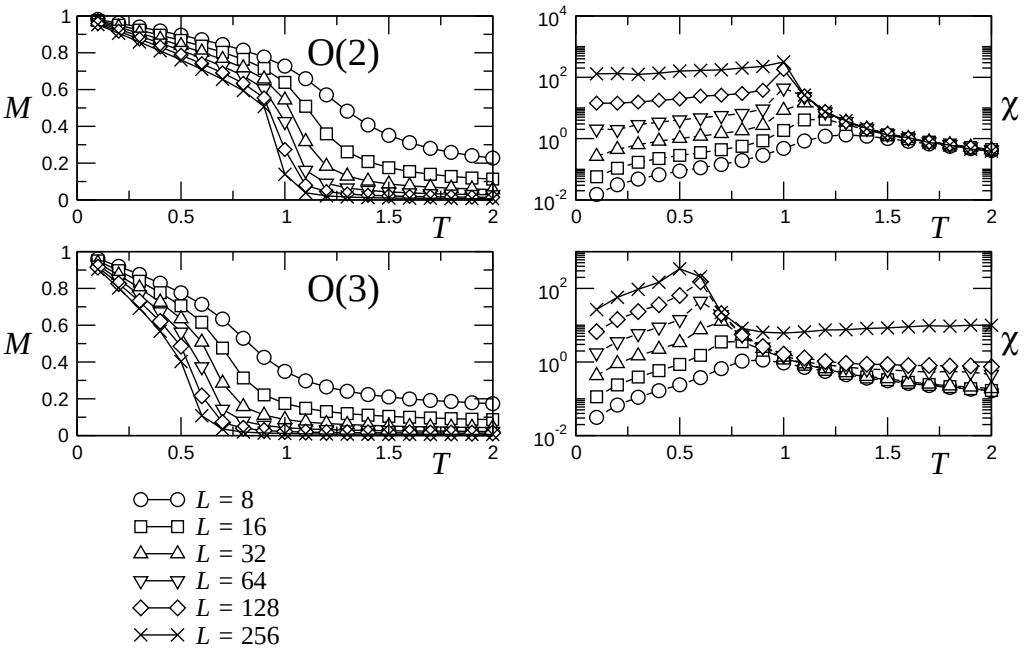

Figure 4.6: The Monte Carlo simulation results for the temperature behaviour of the magnetization (left) and magnetic susceptibility (right) of the two-dimensional XY ($O(2)$) (top) and Heisenberg ($O(3)$) (bottom) models on lattices of different sizes.

The power law scaling behaviour found in all three cases suggests about a quasi-long-range-like ordering in a finite $2D$ Heisenberg model. The lattice size varied in our simulations from $N = 8\times8$ to $N = 256\times256$ for each value of the temperature (see fig. 4.6). The estimates of the exponent $\eta(T)$ obtained from the scaling of different quantities are plotted in fig. 4.7. The majority of the experimental points comes from the magnetization measurements, since reliable measurement of magnetic susceptibility and pair correlation function requires longer times of simulation. The temperature range of the computer simulations was between 10^{-9} and 10^{0}.

In spite of the restricting low-temperature approximation the result $\eta = 2\eta^{XY}$ seems to accord very well with the Monte Carlo simulations of the corresponding model in a wide range of temperatures. Only a few last experimental points on the high temperature side start to deviate from this prediction.

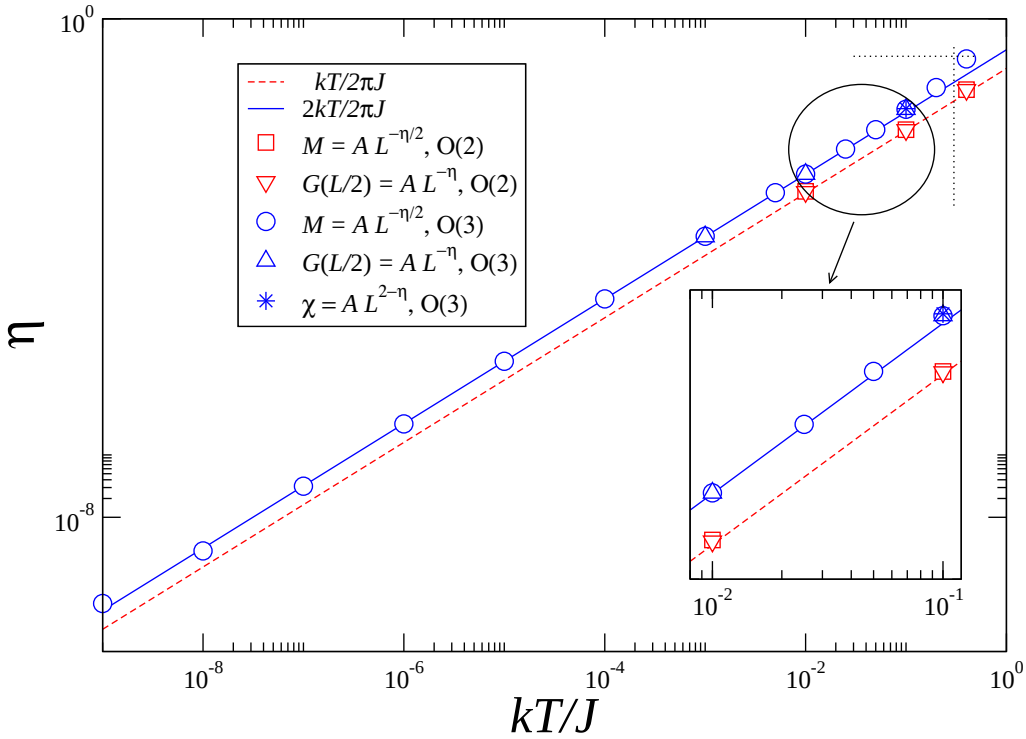

Figure 4.7: The comparison between the results for the exponent η of the two-dimensional Heisenberg model obtained in the Monte Carlo simulations and analytically within the low-temperature approximation. The corresponding exponent of the $2D$ XY model is plotted for comparison (dashed line).

4.3 Conclusions

In this section several different aspects of the lattice finiteness influence on the well known properties of the two-dimensional spin models of continuous symmetry were studied.

Firstly, it was the residual spontaneous magnetization probability distribution function research in the $2D$ XY model with structural disorder. We have investigated the probability distributions observed in the Monte Carlo simulations at different values of the temperature and dilution concentration presenting the results in the most explicit possible form: as ring functions (fig.4.3,4.4). Together with the Monte Carlo simulations analyt-

ical calculations were taken in the spin-wave approximation. The results for the mean magnetization and its moments obtained through the perturbation expansion in the disorder configuration inhomogeneity parameter up to the third order support a scaling of the magnetization with an exponent related to the pair correlation function exponent (found in the same approximation), but cannot explain the distribution variance dependence on the dilution concentration observed in the Monte Carlo simulations. This a bit disappointing fact has place because of the neglect of terms of higher order powers of temperature.

Secondly, basing on an assumption about quasi-long-range ordering existence in a finite (!) two-dimensional Heisenberg model at low enough temperatures, the asymptotic behaviour of the pair correlation function of spins was studied and appeared to be a power law decay with the exponent two times larger than the corresponding exponent of the $2D$ XY model (found in the SWA). Such a result for the model which in the thermodynamic limit does not exhibit any ordering is a purely finite-size effect. The analytic result is reliably confirmed in Monte Carlo simulations of the Heisenberg model realized for different sizes in a wide interval of low temperatures.

CONCLUSIONS

Although the present thesis, devoted to the changes in the behaviour of the two-dimensional spin models of continuous symmetry caused by quenched structural disorder and lattice finiteness, does not pretend to give a completely explicit answer to every question posed, but makes a profound and diverse research which shifts the knowledge of the mentioned problem one step forward comparing to the situation described in the literature overview (Chapter 1).

Let us remind briefly the main results and conclusions of the research which can be found in a more explicit form in Conclusions after the corresponding chapters.

1. The pair correlation function of the two-dimensional XY model with nonmagnetic quenched dilution was estimated in the spin-wave approximation on the basis of the perturbation expansion in the disorder configuration inhomogeneity parameter. The behaviour observed is a power law decay with distance (just like in the pure model) which indicates about quasi-long-range ordering. However, the pair correlation function exponent in a diluted model has a nontrivial dependence on the dilution concentration, to be more specific it increases with the concentration of nonmagnetic impurities. The result obtained from the perturbation expansion up to the third order terms shows nice accordance with the Monte Carlo simulations performed on purpose to check the reliability of the analytical approach. Analytic arguments in favor of the pair correlation function self-averaging in the low-temperature phase were also presented.

2. The analytic form of the interaction between topological defects (vor-

tices) and nonmagnetic impurities found in the phenomenological Kosterlitz-Thouless model is attractive (in agreement with other researches of this problem [23, 24]) but advantageously differs by its correct lattice structure representation. The result is generalized for an arbitrary number of topological defects in the system.

3. The form of the interaction between nonmagnetic impurities and topological defects was also investigated within the Villain model which gives much more appropriate description that the phenomenological Kosterlitz-Thouless model. The diluted Villain model Hamiltonian was obtained in the low-temperature limit from the diluted $2D$ XY model Hamiltonian according to a scheme analogous to the one applicable in the pure case [18]. Along with the separate interactions as "impurity-vortices" and "impurity-spin-waves" interaction the Hamiltonian obtained describes a combined interaction between an impurity, topological and spin-wave excitations of the ground state. The asymptotic form of the interaction between an impurity and vortices coincides with the corresponding result found in the Kosterlitz-Thouless model. So, the two estimates obtained in the two different models describing topological defects support each other.

4. From the expressions for the interaction energy of nonmagnetic impurities and topological defects obtained both in the Villain and Kosterlitz-Thouless models an analytical estimate of the critical temperature reduction due to nonmagnetic dilution was made for the first time. The analytic result accords to some extent with the available Monte Carlo phase diagrams.

5. The probability distribution functions of the spontaneous magnetization in a finite two-dimensional XY model with quenched nonmagnetic dilution observed in Monte Carlo simulations were represented in a form of ring function and showed nontrivial dependence on the concentration of nonmagnetic impurities. An important observation has been made that the width of these distributions increases with the concentration of mag-

netic sites.

6. The analytical calculation of the mean spontaneous magnetization in a finite $2D$ XY model with disorder within the spin-wave approximation leads to a power law dependence on the linear size of the system with an exponent two times less than the pair correlation function exponent which confirms the scaling relation proven for the pure model. An analogous estimation of the moments of magnetization unfortunately does not give the desirable analytical description of the probability distribution form dependence on the concentration because of the neglect of higher powers of temperature.

7. The analytical result for the pair correlation function of the two-dimensional Heisenberg model of finite size obtained in the low-temperature limit shows power law decay (indication of quasi-long-range ordering) with an exponent twice bigger than the analogous exponent (estimated in the SWA) of the $2D$ XY model. The Monte Carlo simulations of the $2D$ Heisenberg model for a variety of system sizes within a wide interval of low temperatures supports the analytical result.

THE LIST OF LITERATURE SOURCES

[1] Sato H. Remarks on magnetically dilute systems / H. Sato, A. Arrott, R. Kikuchi // J. Phys. Chem. Solids. – 1959. – **10**. – P. 19–34.

[2] Brout R. Statistical mechanical theory of a random ferromagnetic system / R. Brout // Phys. Rev. – 1959. – **115**, № 4. – P. 824–835.

[3] Mermin N. D. The topological theory of defects in ordered media / N. D. Mermin // Rev. Mod. Phys. – 1979. – **51**, №3. – P. 591–648.

[4] Nelson D. R. Defects and geometry in condensed matter physics / D. R. Nelson. – Cambridge: Cambridge University Press, 2002.

[5] Kenna R. Homotopy in statistical physics / R. Kenna // Condensed Matter Physics. – 2006. – **9**. – P. 283–304.

[6] Berezinskii V. L. / V. L. Berezinskii // Sov. Phys. JETP. – 1971. – **32**. – P. 493.

[7] Kosterlitz J. M. Ordering, metastability and phase transitions in two-dimensional systems / J. M. Kosterlitz, D. J. Thouless // J. Phys. C: Solid State Phys. – 1973. – **6**. – P. 1181–1203.

[8] Kosterlitz J. M. The critical properties of the two-dimensional xy model / J. M. Kosterlitz // J. Phys. C: Solid State Phys. – 1974. – **7**. – P. 1046–1060.

[9] Minnhagen P. The two-dimensional Coulomb gas, vortex unbinding,

and superfluid-superconducting films / P. Minnhagen // Rev. Mod. Phys. – 1987. – **59**, №4. – P. 1001–1066.

[10] Mermin N. D. Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic Heisenberg models / N. D. Mermin, H. Wagner // Phys. Rev. Lett. – 1966. – **22**. – P. 1133–1136.

[11] Hohenberg P. C. Existence of long-range order in one and two dimensions / P. C. Hohenberg // Phys. Rev. – 1967. – **158**, №2. – P. 383–386.

[12] Bogolyubov N.N. Selected works, v.3 / N.N. Bogolyubov. – Kiev, 1970.

[13] Tobochnik J. Monte Carlo study of the planar spin model / J. Tobochnik, G. V. Chester // Phys. Rev. B. – 1979. – **20**, No. 9. – P. 3761–3769.

[14] Bramwell S. T. Magnetization: A characterisitc of the Kosterlitz-Thouless-Berezinskii transition / S. T. Bramwell, P. C. W. Holdsworth // Phys. Rev. B. – 1994. – **49**, №13. – P. 8811–8814.

[15] Harris A. B. Effect of random defects on the critical behaviour of Ising model / A. B. Harris // J. Phys. C: Solid State Phys. – 1974. – **7**. – P. 1671–1692.

[16] Wegner F. Spin-ordering in a planar classical Heisenberg model / F. Wegner // Z. Phys. – 1967. – **206**. – P. 465–470.

[17] Villain J. Theory of one- and two-dimensional magnets with an easy magnetization plane. II. The planar, classical, two-dimensional magnet / J. Villain // Le Journal de Physique. – 1975. – **36**. – P. 581–590.

[18] José J. V. Renormalization, vortices, and symmetry-breaking perturbations in the two-dimensional planar model / J. V. José, L. P.

Kadanoff, S. Kirkpatrick, D. R. Nelson // Phys. Rev. B. – 1977. – **16**, №3. – P. 1217–1241.

[19] Hilbert S. Disorder in diluted spin systems / S. Hilbert, W. Nolting // Phys. Rev. B. – 2004. – **70**. – P. 165203.

[20] Berche B. Influence of quenched dilution on the quasi-long-range ordered phase of the 2d XY model / B. Berche, A. I. Fariñas-Sánchez, Yu. Holovatch, R. Paredes V. // Eur. Phys. J. B. – 2005. – **36**. – P. 91–98.

[21] Mól L. A. S. Planar vortex in two-dimensional XY ferromagnets with a nonmagnetic impurity potential / L. A. S. Mól, A. R. Pereira, A. S. T. Pires // Phys. Rev. B. – 2002. – **66**. – P. 052415.

[22] Leonel S. A. Monte Carlo study of the critical temperature for the planar rotator model with nonmagnetic impurities / S. A. Leonel, P. Z. Coura, A. R. Pereira, L. A. S. Mól, B. V. Costa // Phys. Rev. B. – 2003. – **67**. – P. 104426.

[23] Wysin G. M. Vortex-vacancy interactions in two-dimensional easy-plane magnets / G. M. Wysin // Phys. Rev. B. – 2003. – **68**. – P. 184411.

[24] Pereira A. R. Vortex behavior near a spin vacancy in two-dimensional XY magnets / A. R. Pereira, L. A. S. Mól, S. A. Leonel, P. Z. Coura, B. V. Costa // Phys. Rev. B. – 2003. – **68**. – P. 132409.

[25] Pereira A. R. Vortex motion induced by lattice defects in two-dimensional easy-plane magnets / A. R. Pereira, S. A. Leonel, P. Z. Coura, B. V. Costa // Phys. Rev. B. – 2005. – **71**. – P. 014403.

[26] Wysin G. M. Extinction of the Berezinskii-Kosterlitz-Thouless phase transition by nonmagnetic disorder in planar symmetry spin models

/ G. M. Wysin, A. R. Pereira, I. A. Marques, S. A. Leonel, P. Z. Coura // Phys. Rev. B. – 2005. – **72**. – P. 094418.

[27] Surungan T. Kosterlitz-Thouless transition in planar spin models with bond dilution / T. Surungan, Yu. Okabe // Phys. Rev. B. – 2005. – **71**. – P. 184438.

[28] Amit D. J. Field theory, the renormalization group, and critical phenomena / D. J. Amit. – World Scientific, 1984. – 394 p.

[29] Kleinert H. Critical properties of ϕ^4-theories / H. Kleinert, V. Schulte-Frohlinde. – World Scientific, 2001. – 489 p.

[30] Рудавський Ю. К. Функціональні інтеграли та їх застосування: Навч. посібник / Ю. К. Рудавський. – Львів: Видавництво Національного університету «Львівська політехніка», 2002. – 312 с.

[31] Wolff U. Collective Monte Carlo updating for spin systems / U. Wolff // Phys. Rev. Lett. – 1989. – **62**, No.4. – P. 361–364.

[32] Kapikranian O. Perturbation expansion for the diluted two-dimensional XY model / O. Kapikranian, B. Berche, Yu. Holovatch // Phys. Lett. A. – 2007. – **366**. – P. 150–154.

[33] Kapikranian O. The $2D$ XY model on a finite lattice with structural disorder: quasi-long-range ordering under realistic conditions / O. Kapikranian, B. Berche, Yu. Holovatch // Eur. Phys. J. B. – 2007. – **56**. – P. 94–105.

[34] Kapikranian O. Finite size induced phenomena in 2D classical spin models / O. Kapikranian, B. Berche, Yu. Holovatch // Problems of Atomic Science and Technology, Ser. Nuclear Physics. – 2007. – № 3 (2). – P. 376–379.

[35] Kapikranian O. Interplay of topological and structural defects in the two-dimensional XY model / O. Kapikranian, B. Berche, Yu. Holovatch // Phys. Lett. A. – 2008. – **372**. – P. 5716–5721.

[36] Kapikranian O. Quasi-long-range ordering in a finite-size 2D classical Heisenberg model / O. Kapikranian, B. Berche, Yu. Holovatch // J. Phys. A: Math. Theor. – 2007. – **40**. – P. 3741–3748.

[37] Kapikranian O. Topological and structural defects in the two-dimensional XY model / Kapikranian O. – Lviv: Institute for condensed matter physics, 2008. – 19 p. – (Preprint; ICMP–08–11U).

[38] Kapikranian O. The low-temperature phase of the disordered finite-size $2D$ XY model. In "Book of abstracts: 2nd International Conference on Quantum Electrodynamics and Statistical Physics (QEDSP2006)"/ O. Kapikranian, B. Berche, Yu. Holovatch. – Kharkov: NSC KIPT, 2006. – 212 p.

[39] Kapikranian O. Influence of disorder on the 2D XY model properties. In "MECO32: The 32nd Conference of the Middle European Cooperation in Statistical Physics. Abstracts" / O. Kapikranian, B. Berche, Yu. Holovatch. – Ladek Zdrój, 2007. – 78 p.

[40] Капікранян О. Є. Вихори та немагнітні домішки у двовимірній XY-моделі (анотація) / О. Є. Капікранян // Journal of Physical Studies. – 2008. – Vol. 12, No. 1. – P. 1998.

[41] Капікранян О. Вплив замороженого структурного безладу на поведінку двовимірних спінових моделей неперервної симетрії. У збірці тез "VII Всеукраїнська школа-семінар і конкурс молодих вчених у галузі статистичної фізики та конденсованої речовини – 2008". – Львів: ІФКС НАНУ, 2008. - 45 с.

[42] Chaikin P. M. Principles of condensed matter physics / P. M. Chaikin, T. C. Lubensky. – Cambridge: Cambridge University Press, 1995. – 699 p.

[43] Stanley H. E. Introduction to Phase Transitions and Critical Phenomena – Oxford University Press, 1987. – 336 p.

[44] Ma Sh. Modern Theory of Critical Phenomena – Westview Press, 2000. – 561 p.

[45] Kohring G. Role of vortex strings in the three-dimensional O(2) model / G. Kohring, R. E. Shrock, P. Wills // Phys. Rev. Lett. – 1986. – **57**, №11. – P. 1358–1361.

[46] Izyumov Yu. A., Skryabin Yu. N. Statistical Mechanics of Magnetically Ordered Systems – Springer, 1988. – 312 p.

[47] Lau M. Role of topological defects in the phase transition of the three-dimensional Heisenberg model / M. Lau, C. Dasgupta // J. Phys. A: Math. Gen. – 1988. – **21**. – P. L51–L57.

[48] Lau M. Numerical investigation of the role of topological defects in the three-dimensional Heisenberg transition / M. Lau, C. Dasgupta // Phys. Rev. B. – 1989. – **39**, No. 10. – P. 7212–7222.

[49] Kamal M. New O(3) transition in three dimensions / M. Kamal, G. Murthy // Phys. Rev. Lett. – 1993. – **71**, №12. – P. 1911–1914.

[50] Stanley H. E. Possibility of a phase transition for the two-dimensional Heisenberg model / H. E. Stanley, T. A. Kaplan // Phys. Rev. Lett. – 1966. – **17**, №17. – P. 913–915.

[51] Polyakov A. M. Interaction of goldstone particles in two dimensions. Application to ferromagnets and massive Yang-Mills fields // A. M. Polyakov / Phys. Lett. B. – 1975. – **59**, №1. – P. 79–81.

[52] Patrascioiu A. Superinstantons and the reliability of perturbation theory in non-abelian models // A. Patrascioiu, E. Seiler / Phys. Rev. Lett. – 1995. – **74**, №11. – P. 1920–1923.

[53] Antunes N. D. Role of pointlike topological excitations at criticality: From vortices to global monopoles / N. D. Antunes, L. M. A. Bettencourt, M. Kunz // Phys. Rev. E. – 2002. – **65**. – P. 066117.

[54] Borisov A. B. Spiral vortices in a two-dimensional ferromagnet / A. B. Borisov, I. G. Bostrem, A. S. Ovchinnikov // Phys. Rev. B. – 2005. – **72**. – P. 134423.

[55] Hikami Sh. Phase transition of quasi-two dimensional planar system / Sh. Hikami, T. Tsuneto // Prog. Theor. Phys. – 1980. – **63**, №2. – P. 387–401.

[56] Kawabata C. Monte Carlo simulation of the two-dimensional classical Heisenberg model with easy-plane anisotropy / C. Kawabata, A. R. Bishop // Solid State Communications. – 1982. – **42**, №8. – P. 595–600.

[57] Cuccoli A. Two-dimensional XXZ model on a square lattice: A Monte Carlo simulation / A. Cuccoli, V. Tognetti, R. Vaia // Phys. Rev. B. – 1995. – **52**, №14. – P. 10221–10231.

[58] Lee K. W. Monte Carlo study of the Kosterlitz-Thouless transition in the Heisenberg model with antisymmetric exchange interactions / K. W. Lee, Ch. E. Lee // Phys. Rev. B. – 2005. – **72**. – P. 054439.

[59] Challa M. S. S. Critical behavior of the six-state clock model in two dimensions / M. S. S. Challa, D. P. Landau // Phys. Rev. B. – 1986. – **33**, №1. – P. 437–443.

[60] Archambault P. Magnetic fluctuations in a finite two-dimensional XY model / P. Archambault, S. T. Bramwell, P. C. W. Holdsworth // J. Phys. A: Math. Gen. – 1997. – **30**. – P. 8363—8378.

[61] Chung S. G. Essential finite-size effect in the two-dimensional XY model / S. G. Chung // Phys. Rev. B. – 1999. – **60**, №16. – P. 11761–11 764.

[62] Bramwell S. T. Magnetic fluctuations in the classical XY model: The origin of an exponential tail in a complex system / S. T. Bramwell, J.-Y. Fortin, P. C. W. Holdsworth et al. // Phys. Rev. E. – 2001. – **63**. – P. 041106.

[63] Palma G. Finite size scaling in the two-dimensional XY model and generalized universality / G. Palma, T. Meyer, R. Labbé // Phys. Rev. E. – 2002. – **66**. – P. 026108.

[64] Amit D. J. Renormalisation group analysis of the phase transition in the 2D Coulomb gas, Sine-Gordon theory and XY-model / D. J. Amit, Ya. Y. Goldschmidt, G. Grinstein // J. Phys. A: Math. Gen. – 1980. – **13**. – P. 585–620.

[65] Minnhagen P. New renormalization equations for the Kosterlitz-Thouless transition / P. Minnhagen // Phys. Rev. B. – 1985. – **32**, №5. – P. 3088–3102.

[66] Hasenbusch M. Computing the roughening transition of Ising and solid-on-solid models by BCSOS model matching / M. Hasenbusch K. Pinn // J. Phys. A: Math. Gen. – 1997. – **30**. – P. 63–80.

[67] Zinn-Justin J. Quantum field theory and critical phenomena / J. Zinn-Justin – Oxford: Oxford University Press, 1996. – 1008 p.

[68] Gouvêa M. E. Vortices in the classical two-dimensional anisotropic Heisenberg model / M. E. Gouvêa, G. M. Wysin, A. R. Bishop // Phys. Rev. B. – 1989. – **39**, №16. – P. 11840–11849.

[69] Gouvêa M. E. Numerical study of vortices in a two-dimensional XY model with in-plane magnetic field / M. E. Gouvêa, G. M. Wysin, A. S. T. Pires // Phys. Rev. B. – 1997. – **55**, №21. – P. 14144–14147.

[70] Wysin G. M. Instability of in-plane vortices in two-dimensional easy-plane ferromagnets / G. M. Wysin // Phys. Rev. B. – 1994. – **49**, №13. – P. 8780–8789.

[71] Ota S. B. Vortices in the 2d classical XY-model: a microcanonical Monte Carlo simulation study / S. B. Ota, S. Ota // Phys. Lett. A. – 1995. – **206**. – P. 133-136.

[72] Moore M. A. Additional evidence for a phase transition in the plane-rotator and classical Heisenber models for two-dimensional lattices / M. A. Moore // Phys. Rev. Lett. – 1969. – **23**, №15. – P. 861–863.

[73] Patrascioiu A. The difference between Abelian and Non-Abelian models: Fact and fancy / A. Patrascioiu, E. Seiler. – arXiv:math-ph/9903038v1, 1999. – 22 p.

[74] Levanyuk A. P. The two-dimensional Heisenberg ferromagnet with various types of interactions: temperature dependence of magnetic parameters / A. P. Levanyuk, N. Garcia // J. Phys: Condens. Matter. – 1992. – **4**. – P. 10277–10294.

[75] Govéa M. E. The two dimensional classical anisotropic Heisenberg ferromagnetic model with nearest- and next-nearest neighbor interactions / M. E. Govéa, A. S. T. Pires // Eur. Phys. J. B. – 2002. – **25**. – P. 147–153.

[76] Ziman J. M. Models of disorder. The theoretical physics of homogeneously disordered systems / J. M. Ziman – Cambridge: Cambridge University Press, 1979. – 592 p.

[77] Order, disorder and criticality: Advanced problems of phase transition theory / [edited by Yurij Holovatch]. – Singapore: World Scientific, 2004. – 304 p.

[78] Order, disorder and criticality: Advanced problems of phase transition theory, vol. 2 / [edited by Yurij Holovatch]. – Singapore: World Scientific, 2007. – 308 p.

[79] Tang L.-H. Vortex statistics in a disordered two-dimensional XY model / L.-H. Tang // Phys. Rev. B. – 1996. – **54**, №5. – P. 3350–3366.

[80] Cardy J. L. Random symmetry-breaking fields and the XY model / J. L. Cardy, S. Ostlund // Phys. Rev. B. – 1982. – **25**, №11. – P. 6899– 6909.

[81] Scheidl S. XY models with disorder and symmetry-breaking fields in two dimensions / S. Scheidl, M. Lehnen // Phys. Rev. B. – 1998. – **58**, №13. – P. 8667–8682.

[82] Reed P. Critical properties of the two-dimensional planar spin model in the presence of p-fold random anisotropy / P. Reed // J. Phys. A Math. Gen. – 1991. – **24**. – P. L1299–L1304.

[83] Denholm D. R. Monte Carlo studies of two-dimensional random-anisotropy magnets / D. R. Denholm, T. J. Sluckin // Phys. Rev. B. – 1993. – **48**, №2. – P. 901–912.

[84] Mazo R. M. Free energy of a system with random elements / R. M. Mazo // Jour. of Chem. Phys. – 1963. – **39**, № 5. – P. 1224–1225.

[85] Rushbrooke G. S. On the magnetically dilute Heisenberg and Ising ferromagnetics // G. S. Rushbrooke, D. J. Morgan / Molecular Physics. – 1961. – **4**, №1. – P. 1-15.

[86] Coopersmith M. Threshold concentration for the existence of ferromagnetism in dilute alloys // M. Coopersmith, R. Brout / J. Phys. Chem. Solids. – 1961. – **17**, №3/4. – P. 254–258.

[87] Morgan D. J. On the magnetically dilute Heisenberg and Ising ferromagnetics II. High-temperature expansions // D. J. Morgan, G. S. Rushbrooke / Molecular Physics. – 1961. – **4**, №4. – P. 291-303.

[88] Rapaport D. C. The Ising ferromagnet with impurities : a series expansion approach: I // D. C. Rapaport / J. Phys. C: Solid State Phys. – 1972. – **5**. – P. 1830–1858.

[89] Syozi I. A statistical model for the dilute ferromagnet // I. Syozi, S. Miyazima / Prog. Theor. Phys. – 1966. – **36**, №6. – P. 1083–1094.

[90] Aharony A. From spin glass to spin liquid : Dynamics of a simple model / A. Aharony, B. A. Huberman // J. Phys. C: Solid State Phys. – 1979. – **9**. – P. L465–L468.

[91] Morita T. Statistical mechanics of quenched solid solutions with application to magnetically dilute alloys // T. Morita / Jour. Math. Phys. – 1964. – **5**, №10. – P. 1401–1405.

[92] Aharony A. Absence of Self-Averaging and Universal Fluctuations in Random Systems near Critical Points / A. Aharony, A. B. Harris // Phys. Rev. Lett. – 1996. – **77**, № 18. – P. 3700–3703.

[93] Wiseman S. Finite-size scaling and lack of self-averaging in critical disordered systems / S. Wiseman, E. Domany // Phys. Rev. Lett. – 1998. – **81**. – P. 22.

[94] Wiseman S. Self-averaging, distribution of pseudocritical temperatures, and finite size scaling in critical disordered systems / S. Wiseman, E. Domany // Phys. Rev. E. – 1998. – **58**. – P. 2938.

[95] Berker A. N. Superfluidity and phase separation in helium films / A. N. Berker, D. R. Nelson // Phys. Rev. B. – 1979. – **19**, №5. – P. 2488–2503.

[96] Cardy J. L. Phase diagram of a model for ^{3}He-^{4}He mixtures in two dimensions / J. L. Cardy, D. J. Scalapino // Phys. Rev. B. – **19**, №3. – P. 1428–1436.

[97] Chamati H. Berezinskii-Kosterlitz-Thouless transition in two-dimensional lattice gas models / H. Chamati, S. Romano // Phys. Rev. B – 2006. – **73**. – P. 184424.

[98] Chamati H. First-order phase transitions in classical lattice gas spin models / H. Chamati, S. Romano // Phys. Rev. B – 2007. – **75**. – P. 184413.

[99] van Enter A. C. D. First-order transitions for some generalized XY models / A. C. D. van Enter, S. Romano, V. A. Zagrebnov // J. Phys. A: Math. Gen. – 2006. – **39**. – P. L439–L445.

[100] Korshunov S. E. Disorder-induced first-order transition in superconducting films / S. E. Korshunov // Phys. Rev. B. – 1992. – **46**, №10. – P. 6615–6617.

[101] Gruber C. Berezinski–Kosterlitz–Thouless Order in Two-Dimensional O(2)-Ferrofluid // C. Gruber, H. Tamura, V. A. Zagrebnov // Journal of Statistical Physics. – **106**, №5/6. – P. 875–893.

[102] Paula F. M. Contribution of impurity-pinned vortices to the response function in a randomly diluted easyplane ferromagnet on a square

lattice / F. M. Paula, A. R. Pereira, G. M. Wysin // Phys. Rev. B. – 2005. – **72**. – P. 094425.

[103] Paula F. M. Diluted planar ferromagnets: nonlinear excitations on a non-simply connected manifold / F. M. Paula, A. R. Pereira, L. A. S. Mól // Phys. Lett. A. – 2004. – **329**. – P. 155–161.

[104] Pereira A. R. Inhomogeneous states in permalloy nanodisks with point defects / A. R. Pereira // Phys. Rev. B. – 2005. – **71**. – P. 224404.

[105] Gebele T. Site percolation threshold for square lattice / T. Gebele // J. Phys. A: Math. Gen. – 1984. – **17**, №2. – P. L51–L54.

[106] Фихтенгольц Г. М. *Курс дифференциального и интегрального исчисления* - Москва: издательство «Наука» - 1966. - т. III. - с. 388.

[107] Вакс В. Г. Термодинамика идеального ферромагнетика / В. Г. Вакс, А. И. Ларкин, С. А. Пикин // Журн. экспер. и теорет. физики. - 1967. - **53**, вып. 1 (7). - С. 281-299.

[108] Vakarchuk I. A. Free energy of the amorphous ferromagnets with Heisenberg exchange interaction and liquid-like disorder / I. A. Vakarchuk, Yu. K. Rudavskii, G. V. Ponedilok // Phys. Stat. sol. B - 1985. - **128**, № 2. - P. 231-242.

[109] Handbook of Mathematical Functions With Formulas, Graphs, and Mathematical Tables / Edited by M. Abramowitz and I. A. Stegun. – National Bureau of Standards, Applied Mathematics Series 55, 1972. – 1046 p.

[110] Dictionary of analysis, calculus, and differential equations (Comprehensive dictionary of mathematics) / [edited by] D. N. Clark. – CRC Press LLC, 2000. – 257 p.

[111] Tallarida R. J. Pocket Book of Integrals and Mathematical Formulas (3rd Edition) / R. J. Tallarida. – Chapman and Hall / CRC, 1999. – 285 p.

[112] Bronstein I. N., Semendyaev N. A., Handbook of Mathematics for Engineers and Technical Institute Students – Nauka, Moscow, 1981.

[113] Gnedenko B. The theory of probability / B. Gnedenko. – Moskow: Mir Publishers, 1975. – 392 p.

[114] Derrida B. On correlation functions in random magnets / B. Derrida, H. Hilhorst // J. Phys. C: Solid State Phys. – 1981. – **14**. – P. L539–L544.

[115] Berche P. E. Bond dilution in the 3D Ising model: a Monte Carlo study / P. E. Berche, C. Chatelain, B. Berche, W. Janke // Eur. Phys. J. B - 2004. - **38**. - P. 463.