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The 2D XY model on a finite lattice with structural disorder: quasi-long-range ordering under realistic conditions

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Abstract. We present an analytic approach to study concurrent influence of quenched non-magnetic site-dilution and finiteness of the lattice on the 2D XY model. Two significant deeply connected features of this spin model are: a special type of ordering (quasi-long-range order) below a certain temperature and a size-dependent mean value of magnetisation in the low-temperature phase that goes to zero (according to the Mermin-Wagner-Hohenberg theorem) in the thermodynamic limit. We focus our attention on the asymptotic behaviour of the spin-spin correlation function and the probability distribution of magnetisation. The analytic approach is based on the spin-wave approximation valid for the low-temperature regime and an expansion in the parameters which characterise the deviation from completely homogeneous configuration of impurities. We further support the analytic considerations by Monte Carlo simulations performed for different concentrations of impurities and compare analytic and MC results. We present as the main quantitative result of the work the exponent of the spin-spin correlation function power law decay. It is non universal depending not only on temperature as in the pure model but also on concentration of magnetic sites. This exponent characterises also the vanishing of magnetisation with increasing lattice size.

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1 Introduction

The quasi-long-range ordering (QLRO) is a special feature of a number of important many-particle systems including two-dimensional solids, magnets, Bose fluids, liquid crystals [1–3]. As it is known by now the 2D XY model serves as an archetype capturing special features of QLRO in these systems. Here we will focus on this particular model keeping in mind that the results can be generalised for some other similar models. The regular model, described by the Hamiltonian

$$H_{\rm reg} = -\frac{1}{2}\sum_{\mathbf{r}}\sum_{\mathbf{r}'} J(\mathbf{r}-\mathbf{r}')\left(S^x_{\mathbf{r}}S^x_{\mathbf{r}'} + S^y_{\mathbf{r}}S^y_{\mathbf{r}'}\right), \quad (1)$$

has been investigated in great detail, and although most of its properties are known, no exact solution was found. In (1) $\mathbf{r}$ and $\mathbf{r}'$ span sites of a two-dimensional lattice, $J(\mathbf{r})$ is the nearest neighbours interaction potential, $S^x_{\mathbf{r}}$, $S^y_{\mathbf{r}}$ are the components of a classical "spin" $\mathbf{S}_{\mathbf{r}}$, the coefficient 1/2 stands to prevent double count of each bond. We restrict ourselves to the case of 2-component spins (also called planar rotator model [4]). The spin-wave approximation (SWA) applied by Wegner [5] to analyse the 2D XY model leads to a result very close to recent Monte Carlo computations in the region of low enough temperatures. In particular, the presence of a special type of ordering — the QLRO — manifests itself in the power law decay of the spin-spin correlation function:

$$\langle \mathbf{S}_{\mathbf{r}}\mathbf{S}_{\mathbf{r}+\mathbf{R}}\rangle \sim R^{-\eta^{\rm reg}}, \quad (2)$$

where R is the distance between the spins. The exponent $\eta^{\rm reg}$ given by the SWA is non-universal:

$$\eta^{\rm reg} = kT/(2\pi J). \quad (3)$$

The detailed description of properties of the model given by Berezinskii [6], and Kosterlitz and Thouless (BKT) [7,8] is based on the hypothesis that certain local spin configurations, named topological defects, are responsible for the QLRO and the behaviour of the system near the transition to the QLRO phase (the BKT transition) at the temperature T_{BKT}. The intuitive analogy with the transition in electrolytes was used in those works. A further analytical basement for this approach can be found in the work of Villain [9].

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There are two important aspects which differ the ideal 2D XY model from the systems that can be met in nature: real physical systems *are always finite* and *possess structural defects*. The finite size effect already has been widely explored in the pure (undiluted) XY model. The interest of this question is that in any 2D XY system of finite size, magnetisation is non-vanishing [10] and goes to zero only when the lattice becomes infinite as it should be according to the Mermin-Wagner-Hohenberg theorem [11,12].

The decay of the magnetisation has a power law form (below the BKT transition temperature) that can be easily found in the SWA [13,14]:

$$\langle m \rangle \sim N^{-\frac{\eta^{\mathrm{reg}}}{4}}, \tag{4}$$

with the same η^{reg}, equation (3), that stands in the correlation function (2). Here, N is the total number of spins. The same result can be obtained also from the finite size scaling (FSS) (see e.g. Ref. [15] in a similar context.).

The recent works of Bramwell et al. [14,16,17] give deep analysis of the magnetisation probability distribution which they claim to be non-Gaussian and of universal form, independent of both system size and critical exponent η^{reg}.

Structural disorder as site- or bond-dilution deserves much attention since it moves an ideal model closer towards true physical systems which can be found in nature. However the number of works dedicated to this aspect in the 2D XY model is not mirrored in the great importance of the topic. Harris criterion [18] implies that energy-coupled disorder has no effect on the universal properties (e.g. the critical exponents) *at the transition temperature*. The BKT universality class (and in particular the celebrated $\eta(T_{BKT}) = 1/4$) is thus unchanged by the introduction of quenched disorder, but one can expect highly non-trivial dependence of the low-temperature characteristics, like the spin-spin correlation function, on the concentration of spin-vacancies [19].

A non-magnetic site can change the interaction between topological defects which are responsible as it was mentioned above for the QLRO [20–22]. The character of this influence is not completely clear up to now, for example, the question: when the QLRO disappears as the concentration of vacant sites increases, has got different answers [19,22,23]. As it appears now, the most convincing scenario is that the QLRO remains up to concentrations very close to the percolation threshold [19,23]. However we do not touch this question focusing mostly on the region far from the percolation threshold.

In this paper we investigate the concurrent influence of quenched site-dilution and finite size of the lattice on the properties of the 2D XY model. These two modifications together present a nice approach to investigation of real physical systems. To quantify the disorder-induced changes in the QLRO phase we pay attention to the spin-spin correlation function exponent of the 2D XY model with quenched site-dilution, η^{dil}. It describes not only the decay of the correlation function with the distance but also the vanishing of the magnetisation in a finite system with increase of the lattice size and the divergence of the susceptibility in the same limit. The analytic approach we use here relies on the SWA and a perturbation expansion and is verified by MC simulations.

Also we will perform Monte Carlo simulations for a wide range of 2D XY-spin systems of different sizes at different temperatures and with different concentrations of impurities. Systems explored in computer experiments are always finite, thus they possess a non-vanishing mean value of magnetisation. The instantaneous magnetisation, which is the scalar value of the total sum of the spins divided by the number of sites, measured in a given state from the thermodynamical ensemble of states of the system is distributed with a certain law. The form of this distribution is the point of our interest as well.

The structure of the paper is the following: in the second section we give a description of the model and calculate analytically the spin-spin correlation function combining the SWA and perturbation expansion, we support the result by MC simulations. In Section 3 more details about MC simulations can be found. The results are presented in the form of ring functions and probability distribution functions of magnetisation. We analyse the plots and add an analytic calculation of the moments of magnetisation. We discuss the analytic and MC results and sketch the plans of future work in Conclusions and give two appendices with technical details of the calculations. Some of our results have been announced in [24].

2 The spin-spin correlation function

In this section we give description of the diluted 2D XY model and explain the expansion applied to analyse the asymptotic behaviour of the spin-spin correlation function in the low temperature limit. The comparison with our Monte Carlo results is added to support the analytic approach.

2.1 The model

The regular 2D XY model (5) is equally described in the angle variables $\theta_{\mathbf{r}}$'s that are the angles between the spins and a certain fixed direction by the Hamiltonian

$$H_{\mathrm{reg}} = -\frac{1}{2}\sum_{\mathbf{r}}\sum_{\mathbf{r}'} J(\mathbf{r}-\mathbf{r}')\cos(\theta_{\mathbf{r}}-\theta_{\mathbf{r}'}), \tag{5}$$

since $S^x_{\mathbf{r}}S^x_{\mathbf{r}'} + S^y_{\mathbf{r}}S^y_{\mathbf{r}'} = \cos(\theta_{\mathbf{r}}-\theta_{\mathbf{r}'})$ for unit length spins. All the notations are the same as in (1).

We define a set of occupation numbers $c_{\mathbf{r}}$'s that introduce disorder into the lattice:

$$c_{\mathbf{r}} = \begin{cases} 1, \text{ if the site } \mathbf{r} \text{ has a spin;} \\ 0, \text{ if the site } \mathbf{r} \text{ is empty.} \end{cases} \tag{6}$$

The Hamiltonian modified with these numbers,

$$H = -\frac{1}{2}\sum_{\mathbf{r}}\sum_{\mathbf{r}'} J(\mathbf{r}-\mathbf{r}')\cos(\theta_{\mathbf{r}}-\theta_{\mathbf{r}'})c_{\mathbf{r}}c_{\mathbf{r}'}, \tag{7}$$

will describe the model on a lattice with dilution. Setting a certain sequence of numbers $\{c_{\mathbf{r}}\}$ we are able to realize any configuration of lattice dilution with any desirable concentration of magnetic sites $c = \overline{c_{\mathbf{r}}}$. We are interested in some thermodynamical quantities which are dependent in this case on the configuration of impurities. To obtain observable values we will average the quantities of interest over all the possible configurations of non-magnetic sites; this is referred to as quenched disorder in the literature as in contrast to annealed disorder when magnetic and non-magnetic sites are in equilibrium and the configurational averaging has to be made already in the partition function [25]. We denote the configurational averaging as $\overline{(...)}$:

$$\overline{(...)} = \prod_{\mathbf{r}} \sum_{c_{\mathbf{r}}=0,1} [c\delta_{1-c_{\mathbf{r}},0} + (1-c)\delta_{c_{\mathbf{r}},0}](...) \tag{8}$$

($\delta_{i,j}$ are Kroneker deltas), here and below index $\mathbf{r}$ in sums and products spans all sites of a 2D square lattice.

Since we restrict ourselves to the low temperature phase of the model we assume that the directions of spins on neighboring sites do not differ essentially. This approximation is based on the fact that we expect then that on a finite system, the spin orientations will not differ significantly from their ground state value when $T \to 0$. This allows us to pass to the SWA replacing $\cos(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})$ in the Hamiltonian with a quadratic form $1 - (\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})^2/2$. Nevertheless we cannot give a bound (in terms of temperature nor in terms of dilution) for the validity of such an approximation, but all the main features of the model are preserved in the low temperature limit in the Hamiltonian

$$H = H_0 + \frac{1}{4}\sum_{\mathbf{r}}\sum_{\mathbf{r}'} J(\mathbf{r}-\mathbf{r}')\left(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'}\right)^2 c_{\mathbf{r}} c_{\mathbf{r}'} \tag{9}$$

where the first term in the expression can be regarded just as a shift in the energy scale, from now on we denote the second term by H for simplicity.

Using Fourier transformation of the variables:

$$\theta_{\mathbf{r}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{kr}}\theta_{\mathbf{k}}, \quad \theta_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{r}} e^{-i\mathbf{kr}}\theta_{\mathbf{r}}, \tag{10}$$

$$J(\mathbf{r}) = \frac{1}{N}\sum_{\mathbf{q}} e^{i\mathbf{qr}}\nu(\mathbf{q}), \quad \nu(\mathbf{q}) = \sum_{\mathbf{r}} e^{-i\mathbf{qr}} J(\mathbf{r}),$$

where $\mathbf{k}$ runs over the 1st Brillouin zone, one arrives at:

$$H = c^2 H_{\mathrm{reg}} + H_\rho + H_{\rho^2}, \tag{11}$$

with

$$H_\rho \equiv -cJ\sum_{\mathbf{k},\mathbf{k}'} \gamma_{\mathbf{k}} g_{\mathbf{k},\mathbf{k}'} \rho_{\mathbf{k}+\mathbf{k}'} \theta_{\mathbf{k}}\theta_{\mathbf{k}'} \tag{12}$$

$$H_{\rho^2} \equiv J\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} (2-\gamma_{\mathbf{q}}) \times \left[\rho_{-\mathbf{k}-\mathbf{k}'-\mathbf{q}}\rho_{\mathbf{q}} - \rho_{-\mathbf{k}-\mathbf{q}}\rho_{-\mathbf{k}'+\mathbf{q}}\right]\theta_{\mathbf{k}}\theta_{\mathbf{k}'} \tag{13}$$

where

$$\rho_{\mathbf{q}} \equiv \frac{1}{N}\sum_{\mathbf{r}} e^{-i\mathbf{qr}}(c_{\mathbf{r}} - c), \tag{14}$$

$$g_{\mathbf{k},\mathbf{k}'} \equiv \frac{\gamma_{\mathbf{k}+\mathbf{k}'} - \gamma_{\mathbf{k}} - \gamma_{\mathbf{k}'}}{\gamma_{\mathbf{k}}}, \tag{15}$$

$$\gamma_{\mathbf{k}} = 2 - \cos k_x a - \cos k_y a. \tag{16}$$

The last relation is true for a square lattice with spacing a and the nearest neighbours interaction of strength J. It is important to stress that the first term in the Hamiltonian can be regarded as the SWA Hamiltonian of the model on a pure (undiluted) lattice with a renormalised coupling. We can use it and write thermodynamical averaging with respect to the Gibbs distribution as

$$\langle ... \rangle = \left\langle ...\ e^{-\beta(H_\rho + H_{\rho^2})}\right\rangle_* \left\langle e^{-\beta(H_\rho + H_{\rho^2})}\right\rangle_*^{-1}, \tag{17}$$

where the notation $\langle ... \rangle_*$ is used for thermodynamical averaging with the Hamiltonian of the pure system:

$$\langle ... \rangle_* = \frac{\mathrm{Tr}\left(...\ e^{-c^2\beta H_{\mathrm{reg}}}\right)}{\mathrm{Tr}\ e^{-c^2\beta H_{\mathrm{reg}}}}, \tag{18}$$

$$\mathrm{Tr}\ (...) \equiv \left(\prod_{\mathbf{k}\in B/2}\int_{-\infty}^{+\infty} d\theta_{\mathbf{k}}^c \int_{-\infty}^{+\infty} d\theta_{\mathbf{k}}^s\right)(...),$$

where $\theta_{\mathbf{r}}^c \equiv \Re\theta_{\mathbf{r}}$, $\theta_{\mathbf{r}}^s \equiv \Im\theta_{\mathbf{r}}$, and in order to keep the same number N of variables the product has to be taken over a half of the 1st Brillouin zone which we have denoted as $B/2$. It was possible to extend the integration region to $(-\infty, +\infty)$ because of the Gaussian form of the Boltzmann factor that stands in the integrals.

2.2 The expansion in $\{\rho_{\mathbf{q}}\}$

Let us note, that the transformation (11) of the Hamiltonian (9) is exact, although it looks like a perturbation expansion in ρ. In the forthcoming calculations in order to perform configurational averaging we expand any thermodynamical quantity of interest $\langle F(\{\rho_{\mathbf{q}}\})\rangle$ in terms of functional variables $\rho_{\mathbf{k}}$'s, equation (14):

$$\langle F(\{\rho_{\mathbf{q}}\})\rangle = \langle F(\{0\})\rangle + \sum_{\mathbf{k}} f_1(\mathbf{k})\rho_{\mathbf{k}} + \sum_{\mathbf{k},\mathbf{k}'} f_2(\mathbf{k},\mathbf{k}')\rho_{\mathbf{k}}\rho_{\mathbf{k}'} + \sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''} f_3(\mathbf{k},\mathbf{k}',\mathbf{k}'')\rho_{\mathbf{k}}\rho_{\mathbf{k}'}\rho_{\mathbf{k}''} + ... \tag{19}$$

Since $\rho_{\mathbf{k}}$'s characterize the deviation from the completely homogeneous disorder in the Hamiltonian they can be considered as parameters of perturbation. Note that a power of ρ corresponds to the number of sums over $\mathbf{k}$ in (19). A classification of the perturbation theory series with respect to the number of sums over $\mathbf{k}$ corresponds to the expansion in the ratio of the volume of effective interaction to the elementary cell volume [26]. Taking this ratio to be small means that it is valid for the short-range interacting systems, which holds for our problem. As far as we

don't make any assumption about weakness of disorder, we may expect that accordance of results of this expansion with the MC simulations should not be very sensitive to the value of dilution $(1-c)$ (but of course still far enough from the percolation threshold where the whole approach fails).

In the calculations presented below we limit ourselves to the third order term in the expansion. Then it is not difficult to perform averaging over configurations of disorder using the equalities:

$$\begin{aligned} \overline{\rho_{\mathbf{q}}} &= 0, \\ \overline{\rho_{\mathbf{q}}\rho_{\mathbf{q}'}} &= c(1-c)\frac{1}{N}\delta_{\mathbf{q}+\mathbf{q}',0}, \\ \overline{\rho_{\mathbf{q}}\rho_{\mathbf{q}'}\rho_{\mathbf{q}''}} &= c(1-3c+2c^2)\frac{1}{N^2}\delta_{\mathbf{q}+\mathbf{q}'+\mathbf{q}'',0} \end{aligned} \tag{20}$$

which can be obtained easily from (8).

2.3 The asymptotic behaviour of the spin-spin correlation function

The spin-spin correlation function of the diluted 2D XY model,

$$G_2(R) = \overline{\langle c_{\mathbf{r}} c_{\mathbf{r}+\mathbf{R}} \cos(\theta_{\mathbf{r}+\mathbf{R}} - \theta_{\mathbf{r}})\rangle}, \tag{21}$$

can be written in the Fourier variables (10) as

$$\overline{\left\langle c_{\mathbf{r}} c_{\mathbf{r}+\mathbf{R}} \cos \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} (\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}} + \eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}) \right\rangle}$$

with

$$\begin{aligned} \eta^c_{\mathbf{k}} &= \cos \mathbf{kr} - \cos \mathbf{k}(\mathbf{r}+\mathbf{R}), \\ \eta^s_{\mathbf{k}} &= -(\sin \mathbf{kr} - \sin \mathbf{k}(\mathbf{r}+\mathbf{R})). \end{aligned} \tag{22}$$

Writing the expansion (19) and applying the equalities (20) we arrive (see appendix A) at the next expression:

$$\begin{aligned} G_2(R) = c^2 &\langle \cos(\theta_{\mathbf{r}+\mathbf{R}} - \theta_{\mathbf{r}})\rangle_* \\ &\times \Bigg[1 - \frac{1-c}{c^3}\,\frac{1}{\beta J}\frac{1}{N^2}\sum_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}',\mathbf{k}} \frac{\sin^2\frac{\mathbf{kR}}{2}}{\gamma_{\mathbf{k}}} \\ &+ \frac{1-3c+2c^2}{c^4}\,\frac{1}{\beta J}\Bigg(\frac{2}{N}\sum_{\mathbf{k}} \frac{\sin^2\frac{\mathbf{kR}}{2}}{\gamma_{\mathbf{k}}} \\ &- \frac{1}{N^3}\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''} g_{-\mathbf{k},\mathbf{k}'} g_{\mathbf{k}',\mathbf{k}''} g_{\mathbf{k}'',\mathbf{k}} \frac{\sin^2\frac{\mathbf{kR}}{2}}{\gamma_{\mathbf{k}}} \Bigg)\Bigg]. \end{aligned} \tag{23}$$

Since equation (23) is already configurationally averaged it does not contain the ρ's anymore, so the correspondence with the orders of the expansion (19) is not obvious. Let us explain the origin of each term. The unity corresponds to the zeroth-order in ρ, the first-order term is identically vanishing as follows from (20), and the second- and third-order terms in ρ can be distinguished by their coefficients that are clear from (20). The second-order term contains two sums according to the expansion (19). At the same time the third-order term contains, except the triple sum, a sum over one $\mathbf{k}$: the summation over two remaining $\mathbf{k}$'s was possible to carry out explicitly in this particular case.

For our purpose it is enough to get the leading asymptotics of the sums that stand in the expression (23) when $N \to \infty$ and $R \to \infty$ (see Appendix B):

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

Inserting these expressions in (23) it is possible to write the pair correlation function for small enough temperatures in the power law form:

$$G_2(R) \approx c^2 (R/a)^{-\eta^{\text{dil}}}. \tag{24}$$

Reminding the spin-spin correlation function exponent of the pure system, η^{reg}, given in the SWA by equation (3), we write

$$\eta^{\text{dil}} = \eta^{\text{reg}}\left(\frac{1}{c^2} + 0.73\frac{1-c}{c^3} - 2.27\frac{(1-3c+2c^2)}{c^4}\right). \tag{25}$$

In fact, as it can be seen from Appendix B, this result is true not only in the thermodynamic limit but also for a system of finite large enough size N. The first term in the brackets, $1/c^2$, corresponds to the zeroth order of the ρ-expansion, the first-order term is identically vanishing as was already noted before, the second and third terms in the brackets correspond to the second- and third-order terms of the ρ-expansion respectively. In the next subsection we evaluate formula (25) and compare this result with the MC experiments.

2.4 Comparison with the Monte Carlo results for the exponent of the spin-spin correlation function

In order to check equation (25), we have performed simulations of 2D XY-spins using Wolff cluster Monte Carlo algorithm [27]. We only mention here the main features of the simulations used in order to obtain the exponent η^{dil}.

The system size is typically varying from $L = 16$ to $L = 256$. Illustrations will be usually given for the smaller sizes, and FSS extrapolations require the whole set of sizes. We discard typically 10^5 sweeps for thermalization, and the measurements are performed with typically 10^5 production sweeps.

The boundary conditions are chosen periodic and the critical exponent $\eta(T)$ of the correlation function *is measured indirectly through the finite-size scaling behaviour of the magnetisation* rather than through the space dependence of the correlation function:

$$M_T(L) \sim L^{-x_\sigma(T)}, \quad x_\sigma(T) = \frac{1}{2}\eta(T), \tag{26}$$

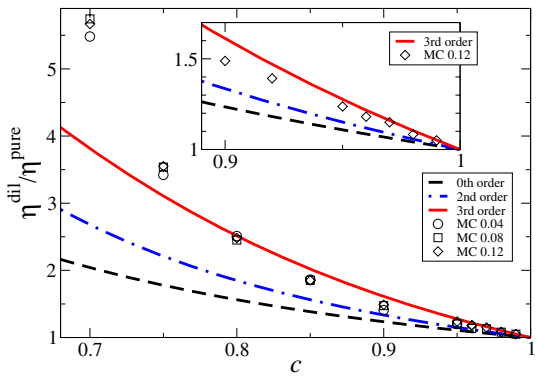

Fig. 1. The comparison between the MC data and the analytic results for the ratio $\eta^{\rm dil}/\eta^{\rm reg}$ as a function of concentration of occupied sites c obtained in different orders of the ρ-expansion. The figures written in the legend for the MC symbols refer to the value of k_BT/J. Note that close to the pure system (when $c \geq 0.96$) we used only 10^4 MCS for thermalization and the same number for measurements. The number of samples for the disorder average is still 10^3.

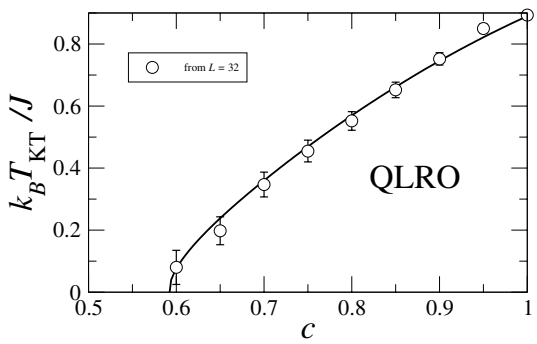

Fig. 2. Phase diagram of the disordered system (adapted from Ref. [19]).

where the last scaling relation holds in two dimensions ($L = \sqrt{N}$ is the linear size of the lattice). We implicitly assume here that universality holds in the disordered system and than the exponent measured through the size dependence $M_T \sim L^{-\frac{1}{2}\eta(T)}$ is indeed linked to that of the space decay of the correlation function, that is $G_2(R) \sim R^{-\eta(T)}$ with the same $\eta(T)$ (in 2D of course). The choice of this indirect procedure is motivated by the difficulties to get a good numerical estimate in the case of the correlation function, since it is a strongly non self-averaging quantity and numerical simulations can hardly measure average values (a too small sampling of the space of disordered configurations rather leads to most probable measurements. See e.g. [28]). *Global* quantities are less subject to fluctuations than local ones, but still the presence of non-self-averaging is an obstacle to the achievement of accurate numerical simulations. This is particularly important in the vicinity of a critical point where the correlation length diverges and we have here to face to a critical phase! The distributions of physical observables typically do not become sharper with increasing system size, rather their relative widths stay constant and a detailed analysis of this is beyond the scope of the present paper. It was nevertheless shown in many previous studies in 2 or 3 dimensions (see e.g. Refs. [29,30]) that usually a number of disorder configurations of the order of a thousand is enough in order to achieve reliable averages. In the present study, averages over disorder are performed using typically this number of 10^3 samples. There is no need of a better statistics, since we are far from the BKT point (in the vicinity of the de-confining transition, the presence of many topological defects is an obstacle to thermalization as it can be shown empirically by the analysis of autocorrelation time (see e.g. Ref. [31])).

In Figure 1, we compare the ratio $\eta^{\rm dil}/\eta^{\rm reg}$ evaluated analytically by keeping terms from the 1st to 3rd order in ρ-expansions with the MC data. One can see that up to the third order the analytic curves approach step by step the MC data: the 0th order seems to be a rough approximation, the 2nd order curve lies closer to the MC data, but still much below, and the third order curve seems to fit the MC results better, although it doesn't give perfect accordance. Of course this fact does not allow to conclude in favour of a similar agreement for higher orders, and it is possible that the expansion will not show any convergence at all. On the other hand, having more perturbation theory contributions at hand one can attempt to apply a resummation technique to improve its convergence, similarly as it is commonly done analyzing field-theoretical expansions [32].

Anyway, comparing outcomes of our analytical and MC treatments presented in Figure 1 one arrives at the conclusion about good agreement within concentrations from $c = 0.75$ to $c = 1$ at least up to the third order of the perturbation expansion. In Figure 2 we show the phase diagram of the disordered model in order to appreciate that our present study is limited to a region far from the percolation point.

Let us proceed further investigating magnetization and its distribution in a finite-size system.

3 The magnetisation probability distribution

In this section we obtain and discuss the probability distribution function of magnetisation obtained in Monte Carlo simulations of a two-dimensional XY-spin system, performed for different sizes of the lattice, temperatures and concentrations of impurities. We support the MC analysis with an analytic treatment of the magnetisation probability distribution in a model of finite size using the same approach as for the spin-spin correlation function.

3.1 The probability distribution functions

In Section 2.4 we obtained the spin-spin correlation function decay exponent by use of the finite size scaling relation (26) for the magnetisation measured in MC simulations. At the same time the probability distribution function (PDF) of magnetisation itself deserves much attention since it appears to be of non-trivial form. As we

mentioned in Introduction it is known that it is non-Gaussian in the pure 2D XY model. In the case of structural disorder we can expect also dependence on concentration of dilution.

We define instantaneous magnetisation as the scalar value of the total sum of the spins divided by the number of sites,

$$m = \frac{1}{N}\left|\sum_{\mathbf{r}} c_{\mathbf{r}}\mathbf{S}_{\mathbf{r}}\right|, \tag{27}$$

measured in a given state from the thermodynamical ensemble of states of the system with a fixed configuration of structural disorder. We should stress that with this definition, the magnetisation is normalised to c, due to the unoccupied sites. The probability to find the system in a state with magnetisation m, $P_{\mathrm{conf}}(m)$, considered as a function of m is called the probability distribution function (PDF) of magnetisation or just the magnetisation probability distribution.

The thermodynamical mean value of magnetisation defined through the usual procedure of thermodynamical averaging with the Hamiltonian of the system H:

$$\langle m\rangle = \frac{\mathrm{Tr}\left(me^{-\beta H}\right)}{\mathrm{Tr}\ e^{-\beta H}}, \tag{28}$$

can be written then in terms of the PDF as

$$\langle m\rangle = \int_0^1 mP_{\mathrm{conf}}(m)dm. \tag{29}$$

We define also the pth moment of magnetisation as

$$M_p \equiv \langle m^p\rangle = \int_0^1 m^p P_{\mathrm{conf}}(m)dm. \tag{30}$$

The PDF, $P_{\mathrm{conf}}(m)$, is a thermodynamic characteristic depending only on a macroscopic state of the system. It can be seen from the well known property of probability distribution functions that a PDF is defined uniquely by its moments [34]:

$$P_{\mathrm{conf}}(m) = \int_{-\infty}^{\infty}\frac{dx}{2\pi}e^{imx}\sum_{p=0}^{\infty}\frac{(-ix)^p}{p!}M_p. \tag{31}$$

The moments are thermodynamically averaged quantities, so it follows that the PDF of magnetization is a thermodynamic quantity too and depends on m only as on a parameter, however to find an analytic expression for the PDF is not a trivial task even for the pure model.

Thus the mean magnetisations defined by equations (28) and (29) being the same are obtained by different procedures.

Since we investigate observable quantities here we should look at the configurationally averaged values of magnetisation and its moments. In terms of the PDF it means that $P_{\mathrm{conf}}(m)$ must be averaged over the whole range of possible configurations of impurities with a fixed concentration. Then the mean magnetisation and its moments can be written as:

$$\overline{\langle m\rangle} = \int_0^1 mP(m)dm \tag{32}$$

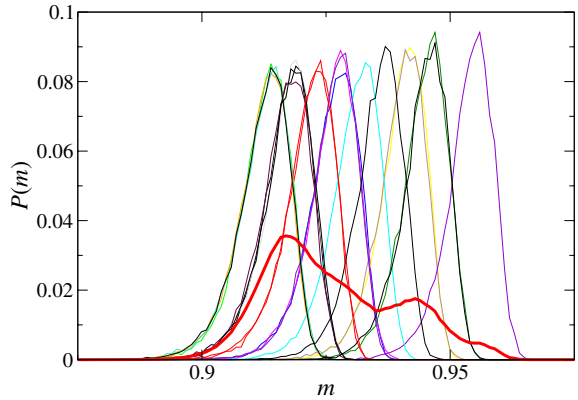

Fig. 3. The probability distributions of magnetisation for twenty different realizations for a system of size $L = 16$ at concentration $c = 0.95$ at a temperature $k_BT/J = 0.1$ (for which $T/T_{BKT}(c) \simeq 0.12$). The thick line is the average probability distribution, still very bumpy with so few configurations.

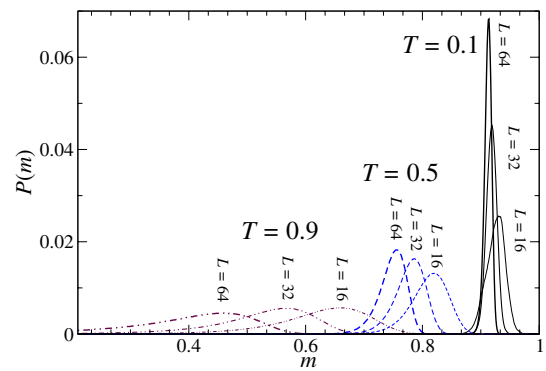

Fig. 4. The average distributions over 10^3 samples ($c = 0.95$) at temperatures $k_BT/J = 0.1$ ($T/T_{BKT}(c) \simeq 0.12$), 0.5 ($T/T_{BKT}(c) \simeq 0.60$) and 0.9 ($T/T_{BKT}(c) \simeq 1.07$) for systems of increasing sizes $L = 16$, 32, 64.

and

$$\overline{M_p} = \int_0^1 m^p P(m)dm, \tag{33}$$

where $P(m) = \overline{P_{\mathrm{conf}}(m)}$ is the configurationally averaged PDF.

The PDF of magnetization is very suitable for further analysis of results obtained in Monte Carlo simulations. In Figure 3 we illustrate the procedure of configurational averaging of MC data. From different curves of $P_{\mathrm{conf}}(m)$ obtained for different realizations of dilution we draw one averaged curve which is $P(m)$.

In the pure 2D XY model two of the main features of the PDF are that the form of the distribution at fixed temperature is universal, i.e. it does not depend on the size of the system, and it is non-Gaussian. These two statements have been derived analytically and verified by MC simulations [14,16,17].

Figure 4 illustrates the MC results for size dependence of the PDF of magnetisation in a diluted 2D XY-spin system with concentration of spins $c = 0.95$ at three different temperatures. We see that at fixed temperature the

mean magnetisation becomes smaller for bigger lattices as it should be according to equation (4) in the case of a pure system. From the curves for low temperatures it is clear that the form of the distributions is non-Gaussian like in the pure model. What is more interesting is that the form of the distributions is noticeably different for different sizes. It seems to be in contradiction with results for the pure model [14,17,16].

A suitable parameter that can characterize the form of a PDF is the variance: $\sigma = \sqrt{\overline{M_2} - \overline{M_1}^2}$. It has been proved that in the pure 2D XY model it is independent of system size. Here we see in Figure 4 a different qualitative behaviour, the variance, which is proportional to width and flatness of the distribution, grows as the size of the lattice decreases.

Since we simulated a diluted system, this must be the result of non-magnetic impurities influence. It calls for an analytic explanation of this dependence in Section 3.3.

3.2 The ring functions

Another way to display the magnetisation probability distribution observed in MC simulations is to draw a ring function obtained when one plots the successive values of the magnetisation (for each Monte Carlo step) in the plane (m_x, m_y) where m_x and m_y are the two components of the magnetisation (see Fig. 5).

Since the algorithm used here is a cluster algorithm specially dedicated to this type of spin systems, the successive spots are essentially uncorrelated. This is a very different situation with a Metropolis algorithm where the successive spots would be correlated (see Ref. [14]).

We are interested in the temperature dependence of a ring function of magnetisation in a diluted 2D XY-spin system with fixed size and concentration of impurities. For this purpose ring functions for a system of size $L = 16$ at concentration $c = 0.95$ for three different temperatures, $k_BT/J = 0.1$, 0.5 and 0.9, are shown in Figure 5. The outer ring functions (color on-line) represent the pure system of the same size and at the same temperatures.

Since we consider the magnetisation per site taking all sites into account and in a system with impurities there are missing spins, the radius of the rings of the diluted system is smaller for all temperatures than that of the corresponding "pure" ring functions. A feature of the temperature-behaviour which can be noticed in Figure 5 is that the high-density region is wider for higher temperatures and approaches to a delta-function as the temperature goes to zero. This is well known from MC and analytic investigations of the pure 2D XY model [14,16]. Both pure and diluted distributions show clear non-Gaussian character for higher temperatures which lies in the visible fact that more points are situated in the inner region of the ring functions than out of the rings of the highest density.

The discussion above concerns relatively weak dilution with $c = 0.95$. The situation appears quite different when the dilution becomes stronger. In Figure 6 we show a ring function for a system of the same size as in the previous figure at temperature $k_BT/J = 0.1$ but with much stronger

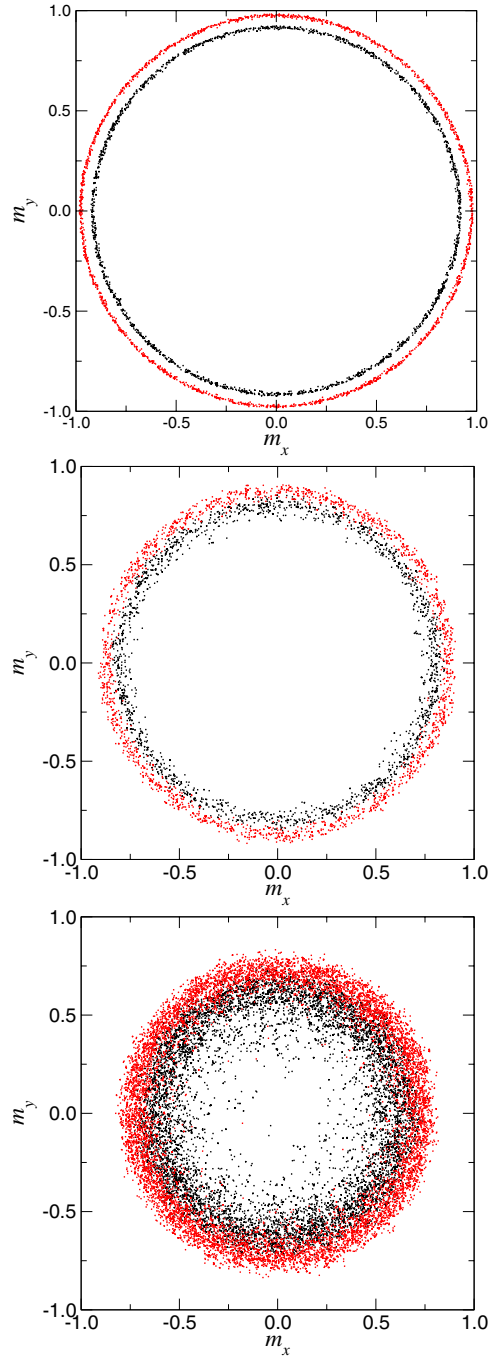

Fig. 5. Ring functions for a system of size $L = 16$ at concentration $c = 0.95$ for temperatures (from top to bottom) $k_BT/J = 0.1$, 0.5, and 0.9. The outer ring function (color on-line) represents the pure system.

dilution, $c = 0.70$. In order to make the comparison less artificial, we plot the quantity m_y/c vs. m_x/c which is normalised to unity for both diluted and pure systems. One can see now that in a system with sufficient number of non-magnetic impurities the high-density region of the ring function is much wider than in a pure system at the same temperature. We can conclude thus that the variance that characterizes the width of the distribution must be

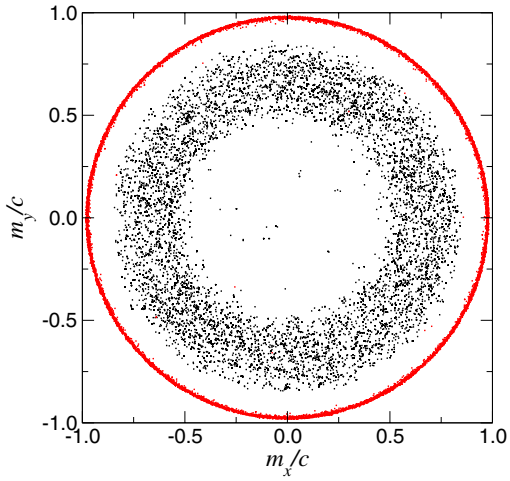

Fig. 6. A ring function for a system of size $L = 16$ at concentration $c = 0.70$ for temperature $k_BT/J = 0.1$. The outer ring function represents the pure system and the quantity shown is normalised to unity for both systems.

dependent on dilution in a 2D XY model with structural disorder. This non-trivial observation calls for an analytic support which is the point of the next subsection.

3.3 Analytic calculation of magnetisation and its moments

In this subsection we present an analytic analysis of the PDF of magnetisation in the 2D XY model in the case of structural disorder. We use here the same scheme that was presented in Section 2 to obtain the moments of magnetisation which define the magnetisation probability distribution through equation (31).

It is convenient for analytic calculation to rewrite the instantaneous magnetization (27) as

$$m = \frac{1}{N}\sum_{\mathbf{r}} c_{\mathbf{r}} \cos(\theta_{\mathbf{r}} - \overline{\theta}), \tag{34}$$

where $\overline{\theta} \equiv \frac{1}{N}\sum_{\mathbf{r}} \theta_{\mathbf{r}}$ is the algebraic mean of the angle variables.

Since we are interested in observable quantities we must consider configurationally averaged moments of magnetization:

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

where we denoted $\psi_{\mathbf{r}} = \theta_{\mathbf{r}} - \overline{\theta}$. Note here that the 1st moment of magnetisation,

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

is just the mean magnetisation $\overline{\langle m \rangle}$ by definition.

Passing from the product of cosines to a sum we write the $(n+1)$th moment as

$$\overline{M_{n+1}} = \frac{1}{2^n N^n} \sum_{\mathbf{r_1},\ldots\mathbf{r_n}} \sum_{\alpha_i=\pm 1} \overline{\langle c_0 c_{\mathbf{r_1}} \cdots \cos\left(\psi_0 + \textstyle\sum_{i=1}^n \alpha_i \psi_{\mathbf{r_i}}\right)\rangle}. \tag{35}$$

The expression that stands in the sums in (35) can be written in Fourier variables as:

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

with

$$\begin{aligned} \eta^c_{\mathbf{k}} &= 1 + \alpha_1 \cos \mathbf{k}\mathbf{r_1} + \cdots + \alpha_n \cos \mathbf{k}\mathbf{r_n}, \\ \eta^s_{\mathbf{k}} &= -\left(\alpha_1 \sin \mathbf{k}\mathbf{r_1} + \cdots + \alpha_n \sin \mathbf{k}\mathbf{r_n}\right). \end{aligned} \tag{36}$$

Substituting in (35) the result for the above expression obtained in Appendix A in the third order approximation in the ρ-expansion, equation (50), we get

$$\begin{aligned} \overline{M_{n+1}} = \frac{c^{n+1}}{2^n N^n} \sum_{\mathbf{r_1},\ldots\mathbf{r_n}} \sum_{\alpha_i=\pm 1} \langle \cos\left(\psi_0 + \textstyle\sum_{i=1}^n \alpha_i \psi_{\mathbf{r_i}}\right)\rangle_* \\ \times \Bigg[1 - \frac{1}{\beta J}\Bigg(\frac{1-c}{4c^3}\frac{1}{N^2}\sum_{\mathbf{k},\mathbf{k'}} \frac{g_{\mathbf{k},\mathbf{k'}} g_{\mathbf{k'},\mathbf{k}}}{\gamma_{\mathbf{k}}} + \frac{1-3c+2c^2}{c^4} \\ \times \Bigg(\frac{1}{2N}\sum_{\mathbf{k}} \frac{1}{\gamma_{\mathbf{k}}} - \frac{1}{4N^3} \sum_{\mathbf{k},\mathbf{k'},\mathbf{k''}} g_{\mathbf{k},\mathbf{k'}} g_{\mathbf{k'},\mathbf{k''}} g_{\mathbf{k''},\mathbf{k}} \frac{1}{\gamma_{\mathbf{k}}} \Bigg)\Bigg) \\ \times \left(n + 1 + 2\textstyle\sum_{i<j} \alpha_i\alpha_j \cos \mathbf{k}(\mathbf{r_i} - \mathbf{r_j}) \right) \Bigg] \end{aligned} \tag{37}$$

with $g_{\mathbf{k},\mathbf{k'}}$ given by equation (15). Then, using the result for a quantity of the type $\left\langle \cos \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}} + \eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle_*$ from Appendix A, equation (45), we write in the low-temperature limit

$$\begin{aligned} \langle \cos(\psi_0 + \alpha_1\psi_{\mathbf{r_1}} \cdots + \alpha_n\psi_{\mathbf{r_n}})\rangle_* &\approx 1 \\ -\frac{1}{4c^2\beta J N} \sum_{\mathbf{k}\neq 0} \frac{1}{\gamma_{\mathbf{k}}} \left(n + 1 + 2\textstyle\sum_{i<j} \alpha_i\alpha_j \cos \mathbf{k}(\mathbf{r_i} - \mathbf{r_j}) \right). \end{aligned} \tag{38}$$

Substituting this expression in (37) we are able to sum over all α_i's by help of the obvious equalities:

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

Then the $(n+1)$th moment of magnetisation reads as:

$$\begin{aligned} \overline{M_{n+1}} = c^{n+1} \Bigg[1 - \frac{n+1}{\beta J} \Bigg(\frac{1}{4c^2}\frac{1}{N}\sum_{\mathbf{k}\neq 0} \frac{1}{\gamma_{\mathbf{k}}} \\ - \frac{1-c}{4c^3}\frac{1}{N^2}\sum_{\mathbf{k},\mathbf{k'}} g_{\mathbf{k},\mathbf{k'}} g_{\mathbf{k'},\mathbf{k}} \frac{1}{\gamma_{\mathbf{k}}} + \frac{1-3c+2c^2}{2c^4} \\ \times \Bigg(\frac{1}{N}\sum_{\mathbf{k}} \frac{1}{\gamma_{\mathbf{k}}} - \frac{1}{2N^3} \sum_{\mathbf{k},\mathbf{k'},\mathbf{k''}} g_{-\mathbf{k},\mathbf{k'}} g_{\mathbf{k'},\mathbf{k''}} g_{\mathbf{k''},\mathbf{k}} \frac{1}{\gamma_{\mathbf{k}}} \Bigg)\Bigg)\Bigg]. \end{aligned} \tag{39}$$

In the limit $N \to \infty$ we find for the sums in (39) (see Appendix B):

$$\frac{1}{N}\sum_{\mathbf{k}} \tfrac{1}{\gamma_{\mathbf{k}}} \approx \text{const.} + \frac{1}{2\pi}\ln N,$$

$$\frac{1}{N^2}\sum_{\mathbf{k}}\sum_{\mathbf{k}'} g_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}',\mathbf{k}} \tfrac{1}{\gamma_{\mathbf{k}}} \approx \text{const.}' + \frac{0.73}{2\pi}\ln N,$$

$$\frac{1}{N^3}\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''} g_{-\mathbf{k},\mathbf{k}'} g_{\mathbf{k}',\mathbf{k}''} g_{\mathbf{k}'',\mathbf{k}} \tfrac{1}{\gamma_{\mathbf{k}}} \approx \text{const.}'' - \frac{0.27}{2\pi}\ln N.$$

For small enough temperatures it is now possible to write the pth moment of magnetisation in the form:

$$\overline{M_p} \approx c^p N^{-\frac{p}{4}\eta^{\text{dil}}} \tag{40}$$

with the exponent η^{dil} given by equation (25). The equality (40) can be rewritten as

$$\overline{M_p} \approx \overline{M_1}^{\,p}. \tag{41}$$

As far as all higher moments $\overline{M_p}$ can be trivially expressed in terms of $\overline{M_1}$ this relation implies absence of multifractality and it differs from that for the pure model in [16]:

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

since we neglected all the terms in the expansion containing powers of $1/(\beta J)$ higher than one. In fact the relation (41) corresponds to a delta distribution of the probability of magnetisation (when the variance is equal to zero) that is close to the truth only for very low temperatures. We stress here that the absence of multifractality *should be expected in the disordered case* [35], but our analytical analysis is not able to reproduce it, due to the approximation mentioned above.

At the same time the mean value of magnetisation which can be obtained from equation (40) in the particular case $p = 1$:

$$\overline{\langle m\rangle} \approx c N^{-\frac{1}{4}\eta^{\text{dil}}}, \tag{42}$$

recovers the finite-size scaling relation (26) and accords well with our MC simulations (see Fig. 1).

4 Conclusions

Two important modifications, quenched site-dilution and finiteness of the lattice, were brought to the usual 2D XY model in order to investigate quasi-long-range ordering, which appears in this model at low temperatures, in conditions closer to that in real many-particle systems present in nature.

We proposed a method of an analytic treatment of the 2D XY model with structural disorder based on the SWA and a sort of perturbation expansion in the parameter characterising deviation from the pure system with the renormalised coupling strength. Computing the perturbation expansion up to the third order we arrived at the result for the spin-spin correlation function decay exponent η^{dil}, equation (25), which appears to be non-universal and depends besides temperature also on concentration of non-magnetic impurities in the system. Our analytic result shows nice accordance with MC simulations for a wide range of dilution concentrations (Fig. 1). We see that up to the third order in the expansion the analytic results for the exponent converges to the MC data with every next order.

We also took into account the finiteness of the lattice which appears to be negligible for the exponent η^{dil} but brings on stage another important property of the 2D XY model: non-vanishing magnetisation that tends to zero with a power law as the size of the lattice increases. Monte Carlo simulations of diluted 2D XY-spin systems with different sizes, concentrations of dilution and temperatures, presented in terms of magnetisation probability distribution, show some interesting features that differ essentially from the case of the pure model in the same conditions. We observed that the variance of the probability distribution function of magnetisation, which serves as a characteristic of the distribution form, i.e. depends on its width and flatness, is a function of temperature, system size and concentration of dilution in contrast to the pure 2D XY model where it depends on temperature only.

We applied our analytic approach to compute the moments of magnetisation that define the probability distribution function (and its variance) but failed to explain the features present in our MC simulations because of the roughness of our approximations. At the same time the analytic calculations give a good result for the magnetisation itself in the diluted model, we found the power law decay with system size, equation (42), that accords with the finite-size scaling (26).

The convergence of the perturbation expansion applied in the analytic treatment is not undoubted but from our results we can conclude that up to the third order it gives nice accordance with the MC data. Further analysis of this question will be a subject of a separate study. Another direction of future work would be to implement the same type of perturbation expansion within the Villain model [9] and to explore the deconfining transition of the diluted model. Here the interesting part of the question does not come across the value of the exponent η, but rather in the way the vacancies couple to the unbinding mechanism.

We acknowledge the CNRS-NAS exchange programme and I.V. Stasyuk for a useful discussion. We also thank H. Chamati for interesting correspondence.

Appendix A

In this appendix we give a detailed calculation of a quantity of the type:

$$\overline{\left\langle c_{\mathbf{r_1}} \cdots c_{\mathbf{r_l}} \cos \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}} + \eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle}, \tag{43}$$

used while computing the spin-spin correlation function and the mean magnetisation of a finite-size system and its higher moments.

Expanding this quantity in the parameters $\rho_{\mathbf{q}}$'s up to the third order we have

$$\begin{aligned}
&\left\langle c_{\mathbf{r_1}} \cdots c_{\mathbf{r_l}} \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 = \\
&c^l \left\langle \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_* \Bigg[1 \\
&-\beta\left(\frac{\langle H_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_\rho\rangle_*\right) - \beta^2\left(\frac{\langle H_\rho\rangle_*\langle H_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_\rho\rangle_*^2\right) \\
&-\beta\left(\frac{\langle H_{\rho^2} \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_{\rho^2}\rangle_*\right) + \frac{\beta^2}{2}\left(\frac{\langle H^2_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H^2_\rho\rangle_*\right) \\
&+\beta^2\left(\frac{\langle H_\rho H_{\rho^2} \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_\rho H_{\rho^2}\rangle_*\right) \\
&-\beta^2\left(\frac{\langle H_{\rho^2}\rangle_*\langle H_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_{\rho^2}\rangle_*\langle H_\rho\rangle_*\right) \\
&-\beta^2\left(\frac{\langle H_\rho\rangle_*\langle H_{\rho^2} \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_\rho\rangle_*\langle H_{\rho^2}\rangle_*\right) \\
&+\frac{\beta^3}{2}\left(\frac{\langle H^2_\rho\rangle_*\langle H_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H^2_\rho\rangle_*\langle H_\rho\rangle_*\right) \\
&+\frac{\beta^3}{2}\left(\frac{\langle H_\rho\rangle_*\langle H^2_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_\rho\rangle_*\langle H^2_\rho\rangle_*\right) \\
&-\beta^3\left(\frac{\langle H_\rho\rangle_*^2\langle H_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_\rho\rangle_*^3\right) - \frac{\beta^3}{6}\left(\frac{\langle H^3_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H^3_\rho\rangle_*\right) \\
&+\frac{\beta}{c}\sum_{\mathbf{q}}\sum_{i=1}^{l} e^{i\mathbf{q}\mathbf{r}_i}\rho_{\mathbf{q}}\Bigg[\left(\frac{\langle H_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_\rho\rangle_*\right) \\
&+\left(\frac{\langle H_{\rho^2} \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_{\rho^2}\rangle_*\right) - \frac{\beta}{2}\left(\frac{\langle H^2_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H^2_\rho\rangle_*\right) \\
&+\beta\left(\frac{\langle H_\rho\rangle_*\langle H_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_\rho\rangle_*^2\right)\Bigg] \\
&-\frac{\beta}{c^2}\sum_{\mathbf{q},\mathbf{q}'}\sum_{i=1}^{l}\sum_{j=1}^{l} e^{i(\mathbf{q}\mathbf{r}_i+\mathbf{q}'\mathbf{r}_j)}\rho_{\mathbf{q}}\rho_{\mathbf{q}'}\left(\frac{\langle H_\rho \cos\rangle_*}{\langle\cos\rangle_*} - \langle H_\rho\rangle_*\right) \\
&-\frac{1}{c}\sum_{\mathbf{q}}\sum_{i=1}^{l} e^{i\mathbf{q}\mathbf{r}_i}\rho_{\mathbf{q}} + \frac{1}{c^2}\sum_{\mathbf{q}}\sum_{\mathbf{q}'}\sum_{i=1}^{l}\sum_{j=1}^{l} e^{i(\mathbf{q}\mathbf{r}_i+\mathbf{q}'\mathbf{r}_j)}\rho_{\mathbf{q}}\rho_{\mathbf{q}'} \\
&+\frac{1}{c^3}\sum_{\mathbf{q},\mathbf{q}',\mathbf{q}''}\sum_{i=1}^{l}\sum_{j=1}^{l}\sum_{k=1}^{l} e^{i(\mathbf{q}\mathbf{r}_i+\mathbf{q}'\mathbf{r}_j+\mathbf{q}''\mathbf{r}_k)}\rho_{\mathbf{q}}\rho_{\mathbf{q}'}\rho_{\mathbf{q}''}\Bigg]
\end{aligned} \tag{44}$$

where in the brackets we have noted for economy of space $\cos\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}} + \eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right) \equiv \cos$. One can easily find

$$\begin{aligned}
&\left\langle \cos \tfrac{1}{\sqrt{N}} \textstyle\sum_{\mathbf{k}} \left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}} + \eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle_* = \\
&\Re\left\langle e^{\frac{i}{\sqrt{N}}\sum_{\mathbf{k}}(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}}+\eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}})}\right\rangle_* = e^{-\frac{1}{4c^2\beta J N}\sum_{\mathbf{k}\neq 0}\frac{\eta_{\mathbf{k}}\eta_{-\mathbf{k}}}{\gamma_{\mathbf{k}}}},
\end{aligned} \tag{45}$$

where $\eta_{\mathbf{k}} \equiv \eta^c_{\mathbf{k}} + i\eta^s_{\mathbf{k}}$ and the sum runs over the whole 1st Brillouin zone except the point $k = 0$. The quantities of the form $\left\langle \theta_{\mathbf{k_1}} \cdots \theta_{\mathbf{k_n}} \cos\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}\left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}} + \eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle_*$ in (44) can be obtained using the property:

$$\begin{aligned}
&\left\langle \theta_{\mathbf{k_1}} \cdots \theta_{\mathbf{k_n}} \cos \tfrac{1}{\sqrt{N}} \textstyle\sum_{\mathbf{k}} \left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}} + \eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle = \\
&\left(\frac{\sqrt{N}}{2i}\right)^n \frac{\partial}{\partial\eta_{\mathbf{k_1}}} \cdots \frac{\partial}{\partial\eta_{\mathbf{k_n}}} \left\langle \cos \tfrac{1}{\sqrt{N}} \textstyle\sum_{\mathbf{k}} \left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}} + \eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle,
\end{aligned} \tag{46}$$

where the notation $\partial/\partial\eta_{\mathbf{k}} \equiv \partial/\partial\eta^c_{\mathbf{k}} + i\partial/\partial\eta^s_{\mathbf{k}}$ is used.

Now, taking derivatives step by step and applying the obvious equality $\partial\eta_{\mathbf{k}}/\partial\eta_{\mathbf{k}'} = 2\delta_{\mathbf{k}+\mathbf{k}',0}$, we obtain:

$$\begin{aligned}
&\left\langle \theta_{\mathbf{k}}\theta_{\mathbf{k}'} \cos \tfrac{1}{\sqrt{N}} \textstyle\sum_{\mathbf{k}} \left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}} + \eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle_* = \\
&\qquad \left\langle \cos \tfrac{1}{\sqrt{N}} \textstyle\sum_{\mathbf{k}} \left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}} + \eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle_* \\
&\qquad \times\left[-\frac{1}{(2c^2\beta J)^2 N}\frac{\eta_{\mathbf{k}}\eta_{\mathbf{k}'}}{\gamma_{\mathbf{k}}\gamma_{\mathbf{k}'}} + \frac{1}{2c^2\beta J}\frac{\delta_{\mathbf{k}+\mathbf{k}',0}}{\gamma_{\mathbf{k}}}\right],
\end{aligned} \tag{47}$$

$$\begin{aligned}
&\left\langle \theta_{\mathbf{k_1}}\theta_{\mathbf{k_2}}\theta_{\mathbf{k_3}}\theta_{\mathbf{k_4}} \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_* = \\
&\left\langle \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_* \\
&\times\Bigg[\frac{1}{(2c^2\beta J)^4 N^2}\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}}} \\
&-\frac{1}{(2c^2\beta J)^3 N}\Bigg(\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}}} \\
&\qquad + \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}}} + \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}}} \\
&\qquad + \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}}}\Bigg) \\
&+\frac{1}{(2c^2\beta 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}}} \\
&\qquad + \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)\Bigg]
\end{aligned} \tag{48}$$

and

$$\left\langle \theta_{\mathbf{k_1}}\theta_{\mathbf{k_2}}\theta_{\mathbf{k_3}}\theta_{\mathbf{k_4}}\theta_{\mathbf{k_5}}\theta_{\mathbf{k_6}} \cos\tfrac{1}{\sqrt{N}}\textstyle\sum_{\mathbf{k}}\left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}}+\eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle_* = \tag{49}$$

$$\begin{aligned}
&\left\langle \cos\tfrac{1}{\sqrt{N}}\textstyle\sum_{\mathbf{k}}\left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}}+\eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle_* \\
&\times\Bigg[-\frac{1}{(2c^2\beta J)^6 N^3}\,\frac{\eta_{\mathbf{k_1}}\eta_{\mathbf{k_2}}\eta_{\mathbf{k_3}}\eta_{\mathbf{k_4}}\eta_{\mathbf{k_5}}\eta_{\mathbf{k_6}}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_2}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_4}}\gamma_{\mathbf{k_5}}\gamma_{\mathbf{k_6}}} \\
&+\frac{1}{(2c^2\beta J)^5 N^2}\left(\frac{\delta_{\mathbf{k_1}+\mathbf{k_2},0}\eta_{\mathbf{k_3}}\eta_{\mathbf{k_4}}\eta_{\mathbf{k_5}}\eta_{\mathbf{k_6}}}{\gamma_{\mathbf{k_2}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_4}}\gamma_{\mathbf{k_5}}\gamma_{\mathbf{k_6}}}+\cdots\right) \\
&-\frac{1}{(2c^2\beta J)^4 N}\left(\frac{\delta_{\mathbf{k_1}+\mathbf{k_2},0}\delta_{\mathbf{k_3}+\mathbf{k_4},0}\eta_{\mathbf{k_5}}\eta_{\mathbf{k_6}}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_5}}\gamma_{\mathbf{k_6}}}+\cdots\right) \\
&+\frac{1}{(2c^2\beta J)^3}\left(\frac{\delta_{\mathbf{k_1}+\mathbf{k_2},0}\delta_{\mathbf{k_3}+\mathbf{k_4},0}\delta_{\mathbf{k_5}+\mathbf{k_6},0}}{\gamma_{\mathbf{k_1}}\gamma_{\mathbf{k_3}}\gamma_{\mathbf{k_5}}}+\cdots\right)\Bigg],
\end{aligned}$$

where the sums in the brackets run over all possible ways of choosing the pairs of $\mathbf{k}$'s in the delta-symbols. Averages $\langle\theta_{\mathbf{k}}\theta_{\mathbf{k}'}\rangle_*$, $\langle\theta_{\mathbf{k_1}}\theta_{\mathbf{k_2}}\theta_{\mathbf{k_3}}\theta_{\mathbf{k_4}}\rangle_*$ and $\langle\theta_{\mathbf{k_1}}\theta_{\mathbf{k_2}}\theta_{\mathbf{k_3}}\theta_{\mathbf{k_4}}\theta_{\mathbf{k_5}}\theta_{\mathbf{k_6}}\rangle_*$ can be obtained from (47)–(49) putting all the $\eta_{\mathbf{k}}$'s equal to zero.

Substituting these results in (44) and applying (20) we arrive at the expression:

$$\begin{aligned}
&\overline{\left\langle c_{\mathbf{r_1}}\cdots c_{\mathbf{r_l}}\cos\tfrac{1}{\sqrt{N}}\textstyle\sum_{\mathbf{k}}\left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}}+\eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle} = \\
&c^l\left\langle \cos\tfrac{1}{\sqrt{N}}\textstyle\sum_{\mathbf{k}}\left(\eta^c_{\mathbf{k}}\theta^c_{\mathbf{k}}+\eta^s_{\mathbf{k}}\theta^s_{\mathbf{k}}\right)\right\rangle_*\Bigg[1-\frac{1}{\beta J} \\
&\times\Bigg(\frac{1-c}{4c^3}\frac{1}{N^2}\sum_{\mathbf{k},\mathbf{k}'}g_{\mathbf{k},\mathbf{k}'}g_{\mathbf{k}',\mathbf{k}}\frac{\eta_{\mathbf{k}}\eta_{-\mathbf{k}}}{\gamma_{\mathbf{k}}}-\frac{1-3c+2c^2}{2c^4} \\
&\times\Big(\frac{1}{N}\sum_{\mathbf{k}}\frac{\eta_{\mathbf{k}}\eta_{-\mathbf{k}}}{\gamma_{\mathbf{k}}}-\frac{1}{2N^3}\sum_{\mathbf{k},\mathbf{k}',\mathbf{k}''}g_{\mathbf{k},\mathbf{k}'}g_{\mathbf{k}',\mathbf{k}''}g_{\mathbf{k}'',\mathbf{k}}\frac{\eta_{\mathbf{k}}\eta_{-\mathbf{k}}}{\gamma_{\mathbf{k}}}\Big)\Bigg)\Bigg]
\end{aligned}\tag{50}$$

with $g_{\mathbf{k},\mathbf{k}'}$ given by (15). We have neglected terms that vanish in the thermodynamic limit and terms containing higher powers of $1/(\beta J)$, since we consider low temperatures.

Appendix B

We are interested in the asymptotic behaviour of the sums:

$$S_1(R,N)\equiv\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{\sin^2\frac{\mathbf{qR}}{2}}{\gamma_{\mathbf{q}}},$$

$$S_2(R,N)\equiv\frac{1}{N^2}\sum_{\mathbf{q},\mathbf{q}'}g_{\mathbf{q},\mathbf{q}'}g_{\mathbf{q}',\mathbf{q}}\frac{\sin^2\frac{\mathbf{qR}}{2}}{\gamma_{\mathbf{q}}},$$

$$S_3(R,N)\equiv\frac{1}{N^3}\sum_{\mathbf{q},\mathbf{q}',\mathbf{q}''}g_{-\mathbf{q},\mathbf{q}'}g_{\mathbf{q}',\mathbf{q}''}g_{\mathbf{q}'',\mathbf{q}}\frac{\sin^2\frac{\mathbf{qR}}{2}}{\gamma_{\mathbf{q}}},$$

$$\tilde{S}_1(N)\equiv\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{1}{\gamma_{\mathbf{q}}},$$

$$\tilde{S}_2(N)\equiv\frac{1}{N^2}\sum_{\mathbf{q},\mathbf{q}'}g_{\mathbf{q},\mathbf{q}'}g_{\mathbf{q}',\mathbf{q}}\frac{1}{\gamma_{\mathbf{q}}},$$

$$\tilde{S}_3(N)\equiv\frac{1}{N^3}\sum_{\mathbf{q},\mathbf{q}',\mathbf{q}''}g_{-\mathbf{q},\mathbf{q}'}g_{\mathbf{q}',\mathbf{q}''}g_{\mathbf{q}'',\mathbf{q}}\frac{1}{\gamma_{\mathbf{q}}},$$

with $g_{\mathbf{q},\mathbf{q}'}$ given by equation (15), when $R\to\infty$ and $N\to\infty$.

The singularity in $1/\gamma_{\mathbf{q}}$ in the point $q=0$ defines the asymptotic behaviour of the sums. Thus we will have the same asymptotic behaviour after expanding the expressions in the sums for small $\mathbf{q}$'s:

$$S_1(R,N) = c_1 + \frac{2}{a^2}\,\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{\sin^2\frac{\mathbf{qR}}{2}}{|\mathbf{q}|},$$

$$\begin{aligned}
S_2(R,N) &= c_2+\frac{1}{2N}\sum_{\mathbf{k}\neq 0}\left(g_{\mathbf{k},\mathbf{k}}-g_{\mathbf{k},-\mathbf{k}}\right) \\
&\quad\times\frac{2}{a^2}\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{\sin^2\frac{\mathbf{qR}}{2}}{|\mathbf{q}|},
\end{aligned}$$

$$\begin{aligned}
S_3(R,N) &= c_3-\frac{1}{2N}\sum_{\mathbf{k}\neq 0}\sum_{\mathbf{k}'\neq 0}g_{\mathbf{k},\mathbf{k}'}\left(g_{\mathbf{k},\mathbf{k}'}-g_{\mathbf{k},-\mathbf{k}'}\right) \\
&\quad\times\frac{2}{a^2}\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{\sin^2\frac{\mathbf{qR}}{2}}{|\mathbf{q}|},
\end{aligned}$$

$$\tilde{S}_1(N) = \tilde{c}_1 + \frac{2}{a^2}\,\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{1}{|\mathbf{q}|},$$

$$\begin{aligned}
\tilde{S}_2(N) &= \tilde{c}_2+\frac{1}{2N}\sum_{\mathbf{k}\neq 0}\left(g_{\mathbf{k},\mathbf{k}}-g_{\mathbf{k},-\mathbf{k}}\right) \\
&\quad\times\frac{2}{a^2}\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{1}{|\mathbf{q}|},
\end{aligned}$$

$$\begin{aligned}
\tilde{S}_3(N) &= \tilde{c}_3-\frac{1}{2N}\sum_{\mathbf{k}\neq 0}\sum_{\mathbf{k}'\neq 0}g_{\mathbf{k},\mathbf{k}'}\left(g_{\mathbf{k},\mathbf{k}'}-g_{\mathbf{k},-\mathbf{k}'}\right) \\
&\quad\times\frac{2}{a^2}\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{1}{|\mathbf{q}|}.
\end{aligned}$$

c_1, c_2, c_3, $\tilde{c}_1$, $\tilde{c}_2$, $\tilde{c}_3$ are constants.

Numerical calculation gives

$$\frac{1}{2N}\sum_{\mathbf{k}\neq 0}\left(g_{\mathbf{k},\mathbf{k}}-g_{\mathbf{k},-\mathbf{k}}\right)\approx 0.73,$$

$$\frac{1}{2N}\sum_{\mathbf{k}\neq 0}\sum_{\mathbf{k}'\neq 0}g_{\mathbf{k},\mathbf{k}'}\left(g_{\mathbf{k},\mathbf{k}'}-g_{\mathbf{k},-\mathbf{k}'}\right)\approx 0.27.$$

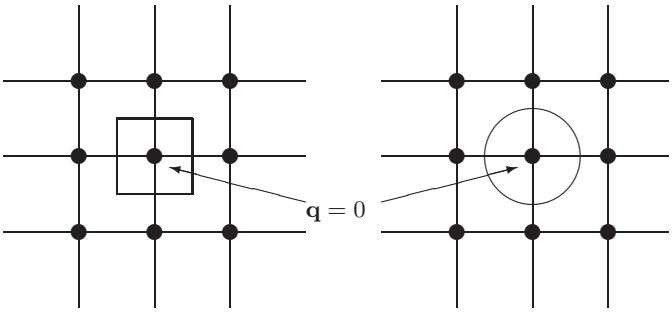

Fig. 7. The cut out of the point $\mathbf{q} = 0$.

To get the asymptotic behaviour of the sums

$$\frac{2}{a^2}\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{\sin^2\frac{\mathbf{qR}}{2}}{|\mathbf{q}|}, \frac{2}{a^2}\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{1}{|\mathbf{q}|}$$

we replace sums over the 1st Brillouin zone in the thermodynamic limit with integrals over continuous variables q_x, q_y, according to the formula

$$\sum_{\mathbf{q}} \rightarrow \frac{Na^2}{(2\pi)^2}\int dq_x \int dq_y + o(N^{-1}).$$

We take into account the absence of the terms with $q = 0$ in the sums cutting out from the continuous domains of integration spaces around the points $q = 0$ with area equal to $\frac{(2\pi)^2}{Na^2}$ (see Fig. 7):

$$\begin{cases} q_x \in \left(-\frac{\pi}{a}, -\frac{\pi}{a\sqrt{N}}\right) \cup \left(\frac{\pi}{a\sqrt{N}}, \frac{\pi}{a}\right); \\ q_y \in \left(-\frac{\pi}{a}, -\frac{\pi}{a\sqrt{N}}\right) \cup \left(\frac{\pi}{a\sqrt{N}}, \frac{\pi}{a}\right). \end{cases}$$

We should stress here that the exact value of this area is not important for the asymptotic behaviour which is the point of our interest, it only must be proportional to $1/N$.

After passing to polar coordinates $q \in \left(\frac{2\sqrt{\pi}}{a\sqrt{N}}, \frac{2\sqrt{\pi}}{a}\right)$ and $\varphi \in (0, 2\pi)$ one can write

$$\frac{2}{a^2}\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{\sin^2\frac{\mathbf{qR}}{2}}{|\mathbf{q}|} = \frac{1}{2\pi^2}\int_{\frac{2\sqrt{\pi}}{a\sqrt{N}}}^{\frac{2\sqrt{\pi}}{a}} dq \int_0^{2\pi} d\varphi \frac{\sin^2\frac{qR\cos\varphi}{2}}{q} \tag{51}$$

and

$$\frac{2}{a^2}\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{1}{|\mathbf{q}|} = \frac{1}{2\pi^2}\int_{\frac{2\sqrt{\pi}}{a\sqrt{N}}}^{\frac{2\sqrt{\pi}}{a}} \frac{dq}{q} \int_0^{2\pi} d\varphi\ . \tag{52}$$

The integral in (52) gives $\frac{1}{2\pi}\ln N$. So

$$\begin{aligned} \tilde{S}_1(N) &= \tilde{c}_1 + \frac{1}{2\pi}\ln N, \\ \tilde{S}_2(N) &= \tilde{c}_2 + 0.73\frac{1}{2\pi}\ln N, \\ \tilde{S}_3(N) &= \tilde{c}_3 - 0.27\frac{1}{2\pi}\ln N. \end{aligned}$$

Now we are interested in the behaviour of the integral in (51) in the asymptotic case: $N \rightarrow \infty$, $R \rightarrow \infty$. After change of variables, $kR/2 \rightarrow x$, we split the integrals over x in two parts:

$$\int_{\frac{R\sqrt{\pi}}{a\sqrt{N}}}^{\frac{R\sqrt{\pi}}{a}} dx \quad \rightarrow \quad \int_{\frac{R\sqrt{\pi}}{a\sqrt{N}}}^{\varepsilon} dx + \int_{\varepsilon}^{\frac{R\sqrt{\pi}}{a}} dx.$$

It is reasonable to assume that the ratio $(R/a)/\sqrt{N}$ is small in the thermodynamical limit, then we choose ε small enough to change $\sin(x\cos\varphi)$ in the limits $\left(R\sqrt{\pi}/a\sqrt{N}, \varepsilon\right)$ by its argument. In the integral over the rest of the domain, $(\varepsilon, R\sqrt{\pi}/a)$, we substitute $\sin^2$ with its mean value 1/2, this cannot change the asymptotic behaviour for a large R. Thus we have simply integrable functions now and one easily finds:

$$\begin{aligned} \frac{2}{a^2}\frac{1}{N}\sum_{\mathbf{q}\neq 0}\frac{\sin^2\frac{\mathbf{qR}}{2}}{|\mathbf{q}|} &= \frac{1}{2\pi^2}\int_{\frac{R\sqrt{\pi}}{a\sqrt{N}}}^{\varepsilon} x dx \int_0^{2\pi} d\varphi \cos^2\varphi \\ &+ \frac{1}{4\pi^2}\int_{\varepsilon}^{\frac{R\sqrt{\pi}}{a}} \frac{dx}{x}\int_0^{2\pi} d\varphi = C + \frac{1}{2\pi}\ln\frac{R}{a}. \end{aligned} \tag{53}$$

We neglected here terms containing small values $(R/a)^2/N$ and $1/N$ and collected terms with the fixed parameter ε in the constant C.

Finally we have:

$$\begin{aligned} S_1(R,N) &= c_1' + \frac{1}{2\pi}\ln\frac{R}{a}, \\ S_2(R,N) &= c_2' + 0.73\frac{1}{2\pi}\ln\frac{R}{a}\ , \\ S_3(R,N) &= c_3' - 0.27\frac{1}{2\pi}\ln\frac{R}{a}. \end{aligned}$$

Note, that the above estimates hold for finite N as well.

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