Interplay of topological and structural defects in the 2D XY model

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Abstract.

The present work is devoted to the investigation of the interaction between vortices (topological defects) and site-impurities (structural defects) in the 2D XY model and its influence on the well-known properties of the pure system. The main goal is a theoretical description of the Berezinskii-Kosterlitz-Thouless (BKT) temperature reduction by quenched non-magnetic impurities, based on the vacancy-vortex interactions and the vortex-pair dissociation mechanism of the transition. The non-magnetic impurity interaction with a system of vortices can be found either from the phenomenological theory of topological defects or from the Villain model. We take both paths and compare the results obtained. Our prediction for the BKT temperature reduction is confirmed by the available Monte Carlo data.

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1. Introduction

An object of our interest is the two-dimensional $XY$ model, described by the Hamiltonian:

$$H = -J \sum_{\langle r, r' \rangle} \left( S^x_r S^x_{r'} + S^y_r S^y_{r'} \right).$$

Here, $S_r$ are unit spins placed on the sites of the square lattice with the nearest neighbour interaction $J$. This model is well known for its extraordinary properties connected with the presence of topological defects (vortices). It can also be considered as the limiting case of the 2D easy-plane Heisenberg model: $H_{e.p.} = -J \sum_{<r, r'>} (S^x_r S^x_{r'} + S^y_r S^y_{r'} + \lambda S^z_r S^z_{r'})$, when $\lambda = 0$. It has been argued that quasi-two-dimensional types of real magnetic materials, like layered magnets or ultrathin magnetic films can be satisfactory described within the 2D easy-plane Heisenberg model \cite{1}, and since the behaviour of this model has been found qualitatively similar to that of the 2D $XY$ model in a rather wide range of anisotropy parameter \cite{2, 3}, it seems natural to use the 2D $XY$ model as a suitable device for the study of real quasi-2D magnets. Thus the question of the influence of impurities, always present in the lattice structure of real materials, should be and has been posed in recent years \cite{4, 5, 6}.

We define here the 2D $XY$ model without the non-interacting (and thus unimportant) component $S^z_r$ in the trace of the system, as is often done in literature. This case is also referred to by some authors as the planar rotator model (see, for example, \cite{7}). This should not confuse the reader, since the non-interacting component would not change the qualitative picture anyway.

The Hamiltonian (1) can be written in a more convenient form for calculation in terms of the angle variables $-\pi < \theta_r \leq \pi$:

$$H = -J \sum_r \sum_{\alpha=x,y} \cos(\theta_{r+a_\alpha} - \theta_r)$$

where $a_x = (a, 0)$ and $a_y = (0, a)$ form an elementary basis of the lattice, and $J$ is the ferromagnetic coupling. Then, since we want to study a system with non-magnetic impurities (vacancies) in the lattice we introduce the “occupation numbers”:

$$c_r = \begin{cases} 1, & \text{if there is a spin;} \\ 0, & \text{if the site is empty.} \end{cases}$$

and construct the Hamiltonian:

$$H = -J \sum_r \sum_{\alpha=x,y} \cos(\theta_{r+a_\alpha} - \theta_r)c_r c_{r'}.$$
being in thermodynamical equilibrium with the spin degrees of freedom, so the averaging over the occupation numbers \( \langle \rangle \) should be taken already in the partition function \([9]\).

In the quenched dilution case, the impurities are frozen at their positions with some fixed probability and one should average the observable quantities (like the spin-spin correlation function or the free energy of the system) over different configurations, and not the partition function itself. The latter statement, formulated in \([9]\), was subsequently rigorously proven in \([10]\).

The random (quenched) dilution means that probability to remove a spin from a site is fixed and independent on the other sites state. So the averaging for all the possible configurations of vacancies can be written as

\[
\langle \ldots \rangle = \sum_{\{c_r\} = 0,1} P(\{c_r\}) \langle \ldots \rangle ,
\]

(5)

with the probability function

\[
P(\{c_r\}) = \prod_r [c \delta_{c_r,1} + (1-c) \delta_{c_r,0}] .
\]

(6)

This distribution is set in such a way that we obtain in average a system with concentration of magnetic sites \( c \) (or fraction of impurities \( 1-c \)).

Although the case of annealed impurities seems to be well studied and clear enough \([11, 12, 13]\), the influence of quenched dilution is a problem for which there are still unsolved questions and which deserves attention. For example, up to our knowledge, so far there are only Monte Carlo results for the phase diagram \( (T_{BKT}, c) \) \([5, 6]\), showing the reduction of \( T_{BKT} \) with decreasing concentration \( c \) of the magnetic component, and no theoretical constructions trying to explain this reduction. Also an approach to investigate the diluted model in the spin-wave approximation has been proposed in \([14]\).

It is well known that the Berezinskii-Kosterlitz-Thouless transition is driven by the topological defects and is in some sense equivalent to the neutral 2d Coulomb gas transition to conducting state \([15, 16]\). In the present paper we describe the critical temperature reduction by an analysis based on the vacancy-vortex interactions (Section 3). The form of this interaction can be found either from the phenomenological theory of topological defects \([17, 18]\) or directly from the Villain model \([19]\) which can be regarded as a low temperature approximation of the 2d XY model \([20]\) (Sections 2 and 4 respectively).

2. The vacancy interaction in a system with vortices

An efficient way to study vortices in the 2D XY model is a continuous elastic medium approximation where the spin-wave excitations are forgotten and the topological defects are obtained from the “elastic” energy minimization under some special topological constraints. The spin variables \( \theta_r \), defined on the sites of the initial lattice are promoted
to a continuous field $\theta(\mathbf{r})$, and the continuous limit of the spin-wave (harmonic) approximation of the Hamiltonian $[2]$ is taken as the “elastic” energy of the system:

$$E_{el} = \frac{1}{2}J \sum_\mathbf{r} \sum_\alpha \Delta_\alpha \theta(\mathbf{r})^2 \approx \frac{1}{2}J \int d\mathbf{r} (\nabla \theta(\mathbf{r}))^2 . \quad (7)$$

The configuration of the field $\theta(\mathbf{r})$ that satisfies the topological condition $\oint d\theta = 2\pi q$ (definition of a vortex with winding number $q$), where the integral is over an arbitrary path enclosing the point defined as the vortex center, and has the minimal elastic energy $[7]$, can be written in a polar coordinates system (centered at the center of the vortex) as:

$$\theta = q\varphi + \text{const} , \quad (8)$$

and its gradient, $\nabla \theta = \frac{q}{r}(-\sin \varphi, \cos \varphi)$, can be found easily. This gradient is always perpendicular to the radius-vector of the point drawn from the origin. The configuration obtained is called a vortex with the charge (winding number) $q$. The vortex is completely set by its charge, the constant in $[5]$ is absolutely arbitrary, since one can switch from a configuration with one constant to a configuration with another constant without changing the energy (although the field configuration visually depends on the value of the constant).

Actually, the total energy of such a configuration can not be correctly expressed by $[7]$, since in the continuous limit we have a singularity in the center of the vortex. Due to this, one has to specify the core energy of the vortex which is always finite and the elastic energy becomes:

$$E_{el}^{\text{pure}} = q^2 J \pi \int_{\frac{L}{A}} d\mathbf{r} = q^2 J \pi \ln(\frac{L}{A}) .$$

It is divergent with the system size $L$ and $A$ is the radius of the core. We do not touch here the nontrivial question about the size of this core region and its energy estimation $[18]$.

The elastic energy of a vortex with a non-magnetic vacancy at some sufficient distance $r$ from the center can be found as the energy that corresponds to the four bonds removed (square lattice) subtracted from the energy of the pure system:

$$E_{el}^{\text{dil}} = E_{el}^{\text{pure}} - E_{\text{vac}} = E_{el}^{\text{pure}} - \frac{1}{2}J \sum_{\alpha=x,y} [(\nabla \theta \cdot \mathbf{a}_\alpha)^2 + (-\nabla \theta \cdot \mathbf{a}_\alpha)^2] \quad (9)$$

$$= E_{el}^{\text{pure}} - \frac{1}{2}J^2 \frac{a^2}{r^2} \left\{ 2\sin^2 \varphi + 2 \cos^2 \varphi \right\} = E_{el}^{\text{pure}} - Jq^2 \left( \frac{a}{r} \right)^2 .$$

Thus, a non-magnetic vacancy has an attractive interaction with either a positive or a negative vortex charge. This is in good agreement with references $[4, 21]$. Of course, this result is obtained via the assumption that the vacancy does not disturb the vortex configuration, an hypothesis which was reliably argued in $[4]$. Our result is almost
equivalent to that found in the paper mentioned, but seems to be a bit more definite since in [4] the coefficient in the interaction depends on the way of cutting out an area of the continuous field around the vacancy, and in our case it is only a matter of the lattice structure.

We go further and consider a vortex pair (winding numbers \( q, q' \)) containing an impurity. The spin configuration of the pair is simply the superposition of the single-vortex fields: \( \theta(r) + \theta'(r) \) and thus the gradient is \( \nabla \theta + \nabla \theta' \). For the pure system the simple integration gives the elastic energy of such a pair:

\[
E_{\text{el}}^\text{pure} = -2\pi Jqq' \ln(R/A) + \pi J(q + q')^2 \ln(L/A),
\]

where \( R \) is the distance between the two vortices. Note that the second term, which is divergent, vanishes for a neutral pair \( (q' = -q) \).

Let the polar coordinates of the impurity be \((r, \varphi)\) in the coordinate system centered on the vortex \( q \) and \((r', \varphi')\) in the system centered on the second vortex \( q' \). We write down the result for the energy associated with this vacancy:

\[
E_{\text{vac}} = Ja^2 ((q/r)^2 + (q'/r')^2 + 2(q/r)(q'/r') \cos(\varphi - \varphi')).
\]

For a system with an arbitrary number of vortices and a vacancy at the point \( r \) we can generalize the elastic energy as:

\[
E_{\text{el}}^\text{dil} = E_{\text{el}}^\text{pure} - E_{\text{vac}}(r)
\]

\[
= E_{\text{el}}^\text{pure} - J \sum_{\mathbf{R}} \sum_{\mathbf{R}'} q(\mathbf{R})q(\mathbf{R}')a^2 \frac{(\mathbf{R} - \mathbf{r})(\mathbf{R}' - \mathbf{r})}{|\mathbf{R} - \mathbf{r}||\mathbf{R}' - \mathbf{r}|},
\]

where the sums span all the topological defects present in the system.

So far we have been considering only one impurity in the system. Of course, a single vacancy does not have any influence on an infinite system, but, having formula (11) for the vortex-pair-vacancy interaction, we can pass to the case of a finite fraction of empty sites and make some conclusions about the critical temperature behaviour with the concentration \( c \). This will be the subject of the following section.

3. The critical temperature reduction by quenched dilution

In the previous section we obtained the form of the spinless site interaction with a system of topological defects. Instead of this, one considers now a single vortex pair in a system with some fraction of spins removed. The elastic energy can be written as

\[
E_{\text{el}}^\text{dil} = E_{\text{el}}^\text{pure} - \sum_{r_{\text{vac}}} E_{\text{vac}}(r),
\]

where \( E_{\text{el}}^\text{pure} \) is the pure system energy, \( E_{\text{vac}}(r) \) is the energy associated with a vacancy at the point \( r \), given by (11), and the sum is over all the vacancies in the system.

Obviously (13) is not exact because there are certainly some impurities which occupy neighbouring sites and thus destroy smaller numbers of links per vacancy. Their
Interplay of topological and structural defects in the 2D XY model

contribution to the energy will be different, but (13) can be considered as a reasonable approximation when the concentration of dilution is weak enough. Eq. (13) can be equally written in the continuous approximation:

\[
E_{\text{dil}} = E_{\text{pure}} - \int d\mathbf{r} \rho_{\text{vac}}(\mathbf{r}) E_{\text{vac}}(\mathbf{r}),
\]

with the impurity density introduced as

\[
\rho_{\text{vac}}(\mathbf{r}) = \sum_{\mathbf{r}'} \delta(\mathbf{r} - \mathbf{r}') (1 - c_\mathbf{r}),
\]

here \(\delta\) is for a delta-function and \(c_\mathbf{r}\)-s are the occupation numbers (3).

The energy (14) can serve to estimate the transition temperature, \(T_{\text{BKT}}\). Consider an ideal system that is constituted of a single neutral pair of vortices with winding numbers of modulus 1, thus one has only one degree of freedom, the separation \(R\) between the vortices. One can define \(T_{\text{BKT}}\) as the temperature when this pair dissociates [22], i.e. the thermodynamical average

\[
\langle R^2 \rangle = \frac{\int_0^\infty R^3 e^{-\beta E_{\text{el}}(R)} dR}{\int_0^\infty R e^{-\beta E_{\text{el}}(R)} dR}
\]

(16)
goesto infinity. With the undiluted system it happens at \(kT_{\text{BKT}}/J \approx \pi/2\), since \(E_{\text{pure}}(R) = 2\pi J \ln(R/a)\) and one easily finds \(\langle R^2 \rangle = a^2 (\pi \beta J - 1)/(\pi \beta J - 2)\). Using the best present estimate of the BKT temperature, \(kT_{\text{BKT}}/J \approx 0.893\) [23], it is obvious that this calculation gives quite a rough result. Nevertheless, in spite of a quantitative vagueness, this approach is qualitatively correctly based on the BKT transition mechanism. We choose to use it due to its simplicity and expect it to be satisfactory to examine the influence of non-magnetic dilution on the critical temperature.

Now, with the energy (14) of a vortex-antivortex system with spin dilution, we can search the BKT point as the temperature where (16) diverges. With \(\rho_{\text{vac}}\) defined for an arbitrary configuration of impurities as (15) it is quite complicated, however one can use some approximate form of the density, reflecting its essential features. Here the quenched and annealed dilutions should be discriminated. In the frozen case the spins are removed randomly with the same probability for each site, so there is no preference for any part of the lattice to be more or less diluted than the rest of the system. Of course, fluctuations of random nature rather than thermal origin exist. The probability for these fluctuations goes to zero as the size of the lattice increases to infinity. Based on these arguments, a perturbation expansion has been proposed [14] where the 0th order can be considered as a “perfectly homogeneous” dilution. Here we get the corresponding approximation replacing (15) with a “smeared” density:

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

which is simply the number of empty sites divided by the total volume. Now the integral in (14) can be simply calculated and gives \(E_{\text{el}}(R) = [1 - 2(1 - c)] 2\pi J \ln(R/a)\). It follows
that the BKT temperature is just $kT_{\text{BKT}}^{\text{dil}}/J = [1 - 2(1 - c)]\pi/2$, or, normalizing to the pure model critical temperature,

$$T_{\text{BKT}}^{\text{dil}}/T_{\text{BKT}}^{\text{pure}} = 1 - 2(1 - c) .$$

(17)

The critical temperature decreases with the dilution concentration, as one naturally expects due to the decrease of the average coordination number. Moreover, although our derivation was based on the assumption of a weak dilution, formula (17) predicts a vanishing of the $T_{\text{BKT}}$ at $c = 0.5$. Being qualitatively correct, the last estimate differs from the known site percolation threshold concentration on a square lattice $c \simeq 0.59$ [24].

![Figure 1](image.png)

**Figure 1.** The phase diagram of the 2D XY model with the quenched dilution of concentration $p = 1 - c$ ($c$ is the concentration of magnetic sites). The Monte Carlo simulation results of [6] are compared with our theoretical prediction (17). The insert shows the vicinity of the percolation threshold.

While the influence of quenched dilution in particular spin models, for example in the 2D and 3D Ising model [25, 26], is well studied in numerous Monte Carlo simulations, for the model under consideration the computer experiment results are rather poor. We compare our result (17) with the available Monte Carlo data for the diluted two-dimensional XY model [6] (Fig.1). The simulations were performed for the XY and planar rotator models with quenched dilution in two dimensions. Note that in terms of the paper [6] our model (4) is the planar rotator model (PRM). Results of [6] for the PRM critical temperature estimated from two different methods, by the helicity modulus jump (PRM-Y) and by the spin correlation function exponent $\eta$ behaviour
Interplay of topological and structural defects in the 2D XY model

(PRM-η), differ essentially in the region of weak dilution. The XY model points are again different. Although all three MC results go eventually to the correct percolation threshold (see the insert in Fig.1) there are few low concentration points and they do not seem to be reliable enough to make some strong conclusion about our result. However, at least the linear character of equation (17) seems to be present in all three MC sets in the weak dilution range, and this observation is also supported by [5].

4. The Villain model with nonmagnetic impurities

According to [20] the Villain model can be derived in the low temperature limit from the Hamiltonian

\[ H = -J \sum_{\langle r, r' \rangle} \left[ \cos(\theta_r - \theta_{r'}) - 1 \right] \]  

which is equivalent to that of the 2D XY model (2). We apply here the scheme of this derivation to the case of a diluted model, starting with the Hamiltonian

\[ H = -J \sum_{\langle r, r' \rangle} \left[ \cos(\theta_r - \theta_{r'}) - 1 \right] c_r c_{r'} , \]  

with \( c_r \)-s being the occupation numbers [3]. The partition function of the model is then written:

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

with \( V(\theta) = K \left[ \cos \theta - 1 \right] \) and \( K = J/k_BT \).

The goal of the derivation is to find an approximate form of the expression under the integral in (20), which preserves its initial symmetry and is easier to integrate. Namely it will be a superposition of exponents with quadratic arguments like in the SWA, but some new discrete variables will appear which subsequently can be associated with the vortex excitations in the system. Going through this procedure with the impurity variables \( c_r \)-s one can expect to find the influence of dilution on the vortex energy contribution.

As the first step one has to decompose the Boltzmann factor in (20) in Fourier series:

\[ \exp \left[ \sum_{\langle r, r' \rangle} V(\theta_r - \theta_{r'}) c_r c_{r'} \right] = \prod_{\langle r, r' \rangle} \sum_{s=-\infty}^{+\infty} \Theta(s) e^{is(\theta_r - \theta_{r'})} e^{\tilde{V}(s)c_r c_{r'}} , \]  

where \( \Theta(s) = c_r c_{r'} + (1 - c_r c_{r'}) \delta_{s,0} \) naturally appears to ensure the equality when \( c_r c_{r'} = 0 \). The Fourier variable \( s \) depends on two real space variables: \( s = s(\mathbf{r}, \mathbf{r'}) \).

Now, applying the Poisson summation formula [27]:

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

usually used to improve the convergence of the series, to each of the sums in (21), one can rewrite the partition function as:

\[ Z = \left( \prod_r \int_{-\pi}^{\pi} \frac{d\theta_r}{2\pi} \right) \sum_{m_{r,r'}=-\infty}^{+\infty} \Theta(m_{r,r'}) e^{\sum_{(r,r')} V_0(\theta_r - \theta_{r'} - 2\pi m_{r,r'}) c_r c_{r'}}, \] (23)

with \(e^{V_0(\theta)} = \int_{-\infty}^{\infty} d\phi \, e^{\tilde{V}(\phi)} \, e^{i\phi\theta}.\) So far, no special assumption have been made and the result above is exact.

Now let us consider the low temperature limit. In this approximation it is not difficult to find that \(e^{\tilde{V}(s)} = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\theta \, e^{-i\theta} \, e^{K(\cos \theta - 1)} \approx \frac{1}{\sqrt{2\pi K}} \, e^{-s^2/(2K)}.\) One obtains the partition function

\[ Z = \sum_{m_{r,r'}=-\infty}^{+\infty} \Theta(m_{r,r'}) \left( \prod_r \int_{-\pi}^{\pi} \frac{d\theta_r}{2\pi} \right) e^{-K \sum_{(r,r')} (\theta_r - \theta_{r'} - 2\pi m_{r,r'})^2 c_r c_{r'}}, \] (24)

of the desirable form, but as far as the limits of integration remain \((-\pi, \pi)\) all terms with \(m \neq 0\) give vanishing contribution (as \(K \to \infty\)) and (24) is equivalent to the SWA. To repair this, extending the limits of integration, one can use the equality:

\[ \int_{-\pi}^{\pi} d\varphi f(\varphi) = \lim_{\varepsilon \to 0} 2\sqrt{\beta \pi \varepsilon} \int_{-\infty}^{\infty} d\varphi \, e^{-\beta \varepsilon \varphi^2} f(\varphi), \] (25)

true for any periodic function \(f(\varphi) = f(\varphi + 2\pi).\) Eq. (25) can be easily checked by passing to the Fourier transform: \(f(\varphi) = \sum_{s=-\infty}^{\infty} e^{is\varphi} F(s).\) The left part of (25) is just \(2\pi F(0).\) Integrating term by term the right part of (25) and taking the limit \(\varepsilon \to 0\) one finds again \(2\pi F(0).\)

Finally, one has the partition function that describes the Villain model with non-magnetic impurities:

\[ Z = \sum_{m_{r,r'}=-\infty}^{+\infty} \Theta(m_{r,r'}) \left( \prod_r \int_{-\infty}^{\infty} \frac{d\theta_r}{2\pi} \right) e^{-\beta H^{\text{dil}}_{\text{Vill}}}, \] (26)

with the Hamiltonian

\[ H^{\text{dil}}_{\text{Vill}} = J \sum_{(r,r')} (\theta_r - \theta_{r'} - 2\pi m_{r,r'})^2 c_r c_{r'} + \varepsilon \sum_r \theta_r^2. \] (27)

When all the \(c_r\)-s are taken equal 1 it turns to the Hamiltonian of the regular Villain model [19].

It is known that the pure Villain model Hamiltonian can be divided into two parts: one corresponding to the spin-wave excitations and another one that corresponds to the vortex contribution. It is achieved by the Fourier transformation of the spin variables,

\[ \theta_r = \frac{1}{\sqrt{N}} \sum_k e^{-ikr} \theta_k, \quad \theta_k = \frac{1}{\sqrt{N}} \sum_r e^{ikr} \theta_r, \]

Fourier transformation of the discrete variables \(m_{r,r'},\)
Interplay of topological and structural defects in the 2D XY model

\[ m_{r,r+a_\alpha} = \frac{1}{\sqrt{N}} \sum_q e^{-i q (r + a_\alpha/2)} m_q^\alpha, \quad \alpha = x, y \]

\[ m_q^\alpha = \frac{1}{\sqrt{N}} \sum_r e^{i q (r + a_\alpha/2)} m_{r,r+a_\alpha}, \quad \alpha = x, y \]

and the shift of the Fourier transform of the spin variable:

\[ \theta_k = \varphi_k - 2\pi i \frac{\sum_\alpha K_\alpha(k) m_k^\alpha}{\sum_\gamma K_\gamma^2(k)} \]

with \( K_\alpha(k) \equiv 2 \sin \frac{k_\alpha a_\alpha}{2} \).

Applying this scheme to the diluted Hamiltonian (27) we find that again, as in the pure case, the two parts - the spin-wave and the vortex one - can be distinguished but now a third term appears which depends both on the spin and vortex degrees of freedom. Thus the Hamiltonian is made of three terms as:

\[ H_{\text{Vill}}^{\text{dil}} = H_{\text{SW}}^{\text{dil}} + H_{\text{Vort}}^{\text{dil}} + H_{\text{SW,Vort}}^{\text{dil}}. \]  

(28)

Of course, the cross-term, \( H_{\text{SW,Vort}}^{\text{dil}} \), vanishes in the pure model limit: \( c_r = 1, r = 1, ..., N \). It has the form:

\[ H_{\text{SW,Vort}}^{\text{dil}} = 4\pi J \sum_{k,k'} \rho(k + k') \left( L_x(k + k') K_x(k) K_y(k') \right. 
- L_y(k + k') K_y(k) K_x(k') \right) \left( K_x^2(k') + K_y^2(k') \right)^{-1} \varphi_k \varphi_{k'} , \]  

(29)

where \( q_k = i(K_y(k) m_k^x - K_x(k) m_k^y) \) are the Fourier transforms of the vortex charges, \( L_\alpha(k) = \cos \frac{k_\alpha a_\alpha}{2}, K_\alpha(k) \) was defined before, and

\[ \rho(q) = \frac{1}{N} \sum_r e^{iqr} (1 - c_r) . \]  

(30)

The parameter (30) characterizes the strength of dilution [5]. When there are no impurities in the system one gets \( \rho(k + k') = 0 \) and thus \( H_{\text{SW,Vort}}^{\text{dil}} = 0 \). The spin-wave and vortex parts of the Hamiltonian also contain terms which depend on \( \rho \) and which turn to zero in the pure case as well.

The spin-wave term:

\[ H_{\text{SW}}^{\text{dil}} = \frac{J}{2} \sum_k \sum_\alpha \frac{K_\alpha^2(k) \varphi_k \varphi_{-k}}{2} \]

\[ + J \sum_{k,k'} \rho(k + k') \left( \sum_\alpha L_\alpha(k + k') K_\alpha(k) K_\alpha(k') \right) \varphi_k \varphi_{k'} , \]  

(31)
contains the “pure” spin-wave Hamiltonian (first term) and a contribution of the dilution that vanishes when $\rho(k + k') = 0$. The dilution contribution naturally has exactly the same form as was found in [5].

The new result here is the form of the vortex energy in the presence of non-magnetic dilution:

$$H_{\text{dil}}^\text{Vort} = 2\pi J \sum_{k \neq 0} \frac{q_k q_{-k}}{\sum_\gamma K_\gamma^2(k)} + 4\pi J \sum_{k, k'} \rho(k + k')$$

$$\times \left( \frac{L_x(k + k')K_y(k)K_y(k') + L_y(k + k')K_x(k)K_x(k')}{(K_x^2(k) + K_y^2(k))(K_x^2(k') + K_y^2(k'))} \right) q_k q_{k'}.$$

Again one has the vortex interactions similar to those of the pure Villain model (first term) while the dilution effect is represented by the second term. It is known for the “pure” Villain term that:

$$H_{\text{pure}}^\text{Vort} = 2\pi^2 J \sum_{k \neq 0} \frac{q_k q_{-k}}{\sum_\gamma K_\gamma^2(k)}$$

$$\simeq -2\pi \sum_{R, R'} q(R) q(R') \ln(|R - R'|/a) + \pi^2 J \sum_R (q(R))^2,$$

where $R, R'$ span the sites of the dual lattice and $q(R)$-s are the vortex charges or winding numbers [19].

Note, that in order to present the dilution contributions of the Hamiltonian (28) in an easily readable form we have not included into Eq. (29), (31) and (32) the terms quadratic in $\rho$. Anyway, one can neglect them in the approximation of a weak dilution (see [5]) which is the case here.

The expression presented in (29) and especially the form of the impurity contribution to the vortex part of the Hamiltonian, Eq. (32), can further serve to analyze the impact of dilution on the peculiarities of the BKT transition. Let us first find an approximation that would correspond to the “smeared” impurity density approximation of Section 3.

Imagine that the fraction $1 - c$ of sites is removed in such a way that the vacancies form some regular structure, then

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

Of course, with random dilution this is not the case, but, as was argued in [14], (34) can be considered as the zero approximation when one neglects the random fluctuations (homogeneous dilution). Moreover, (34) is the disorder averaged value of $\rho$. We will see that this replacement with its average value corresponds to the “smeared” impurity density approximation of Section 3. In this case we obtain the vortex energy:

$$H_{\text{Vort}}^\text{dil} = 2\pi [1 - 2(1 - c)] J \sum_{k \neq 0} \frac{q_k q_{-k}}{\sum_\gamma K_\gamma^2(k)}.$$
As a consequence the energy of a neutral vortex pair is \( E_{\text{int}}(R) = [1 - 2(1 - c)]2\pi J \ln(R/a) \), exactly the same result as what was found from the topological defect theory approach under the assumption of the “smeared” density of vacancies. This leads of course to the same estimate of the critical temperature as well.

5. Conclusions

We have exploited two different approaches to account for the influence of quenched impurities on the vortices in the two-dimensional \( XY \) model: in the frame of the topological defects phenomenological theory and from the Villain model Hamiltonian. The interaction of a vacancy with vortices in the theory of topological defects was found to be attractive, in good accordance with other works on this subject [4, 21]. In order to estimate the critical temperature change we used an approach based on the vortex-pair dissociation mechanism of the BKT transition. The “smeared” impurity density approximation leads to the same predictions for the critical temperature within the two approaches (topological defects theory and the Villain model). The dependence of the transition temperature on the magnetic sites concentration, \( T_{\text{dil}}^{\text{BKT}}(c) \), obtained under the assumption of a weak dilution, however gives a percolation threshold which differs from the known real site percolation threshold for a 2D square lattice. Comparing with the currently available Monte Carlo results [6] which unfortunately are not accurate enough to make reliable conclusion about the weak dilution range, we recover the linear character of the critical temperature decrease close to \( c = 1 \).

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Interplay of topological and structural defects in the 2D XY model

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