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On the topological phase transition of the two-dimensional XY-model on the Voronoi–Delaunay lattice

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Abstract
We numerically investigate the static properties of the two-dimensional (2D) XY-model on the Voronoi–Delaunay lattice, with average connectivity $\bar{k} \sim 6$. The critical temperature, magnetization and vortex density are obtained. For instance, in this lattice the critical temperature, above which free vortices take place, reads $T_{cr}^{VD} \approx 1.22$ (in units of J, the exchange constant), higher than their counterparts for regular square, $T_{cr}^{SL} \approx 0.79$, and triangular lattices $T_{cr}^{TL} \approx 1.156$, with constant connectivity given by 4 and 6, respectively. Such results lead us to argue that not only the connectivity number but also how the sites are distributed and linked among themselves is also important for determining these physical quantities.

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1. Introduction and motivation

The XY-model and its version with only two spin components, i.e. the planar rotator model (PRM; which is $S0(2)$ rotationally invariant), are two of the most important and well-studied models in statistical mechanics and condensed matter physics [1–3]. They find applications in several areas of physics such as superconductivity, superfluidity, magnetism, etc. In two spatial dimensions (2D) these systems exhibit a topological phase transition based on the

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mechanism of unbinding of vortices [1, 2]. At low temperature, only pairs of bounded vortex–antivortex are observed while at the critical temperature T_{cr}^{BKT} (the Berezinskii–Kosterlitz–Thouless temperature), the system exhibits a landscape characterized by the presence of free vortices and, as a consequence, it becomes considerably disordered. In the past few years, the interest in magnetic vortex-like excitations has been renewed, once they have been often observed in micro and submicro samples with several sizes and geometries. In turn, such observations were possible by virtue of remarkable advances in material science fabrication and characterization. In addition, there is a considerable appeal and realist proposals for using their magnetic properties, namely vortex-type magnetization, in new mechanisms and devices for data storage, logical operations, ultra-precise sensors and so on [4]. As a byproduct, the study of magnetic models defined on other 2D geometrical supports, besides the usual planar one, has received considerable attention. Therefore, a number of variants of the Heisenberg exchange model (including XY, easy-plane, PRM, etc) have recently been studied in discrete lattice and continuum 2D spaces with curvature and/or non-trivial topology. Among them, we quote cylindrical [5–7], spherical [8], toroidal [9, 10], conical [11–13] and pseudospherical supports [14–16].

Another related topic of importance is the effect of structural or artificial defects such as nonmagnetic impurities or bond dilutions introduced in regular 2D lattices [17–21]. Besides, there is an increasing interest in the investigation of the physical properties of magnetic systems on complex networks, such as lattices with unusual distributions of sites [22–24]. Such problems have motivated us to consider the XY-ferromagnetic model on the Voronoi–Delaunay lattice, where the number of connections between the sites follow a Poisson distribution. In physics, besides its several applications, the Voronoi cells may serve as a tool for analyzing theoretical models whenever comparing their results with those well established for regular lattices. For instance, Voronoi construction is the natural way to define ‘neighborhood’ relations between randomly located spatial sites in a lattice. Indeed, in a dense configuration of real particles, these cells define lattice defects, somewhat similar to those observed in diluted systems. In these circumstances, it should be important to know how these rather distinct defects affect some static and dynamic properties of topological excitations. In this paper, we shall focus on the question whether the XY-model on the Voronoi–Delaunay lattice presents a BKT-type phase transition and what are the quantitative and qualitative changes in the physical properties of the system and their relations with vortices.

2. Model and method

To build the Voronoi–Delaunay (VD) network we consider a bounded domain Γ in a d-dimensional space where a set of N nodes is randomly placed with uniform distribution. The Voronoi diagram of this set is a sub-division of the domain into regions V_i ($i = 1, 2, \ldots, N$), such that any point in V_i is closer to the node i than any other node j in the set. In figure 1(*a*) we show a Voronoi diagram obtained on a square region of size $L = 20$ with L^2 nodes. All cells sharing a face are considered neighbors and the network obtained by linking the neighbor sites is the VD lattice of the diagram. Figure 1(*b*) shows the dual lattice obtained using the Voronoi diagram presented in figure 1(*a*). In this work we closely follow the technique described in [25] to build the lattice, and we have used periodic boundary conditions (PBC) whenever calculating thermodynamic quantities in order to minimize finite size effects, in such a way that the obtained results rapidly converge to their thermodynamic limit counterparts. An important ingredient to generate the VD lattices is that the number of connections (links) for each site is chosen randomly and follows a Poisson distribution, as shown in figure 2 for the normalized frequency $P(k)$ (in logarithmic scale) as a function of the number of connections

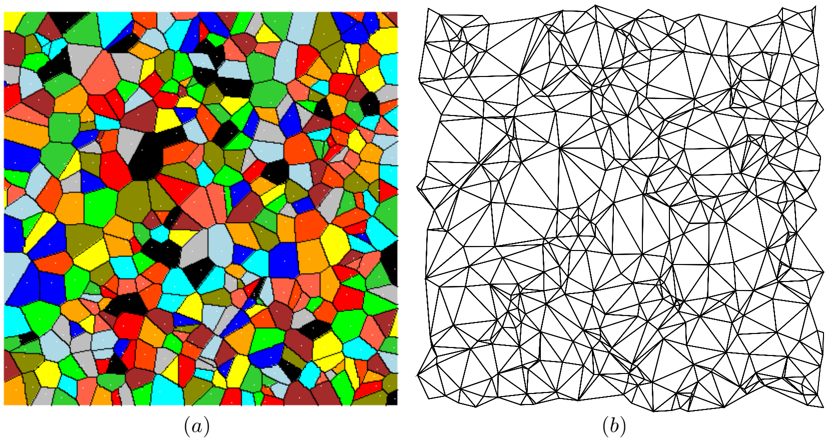

Figure 1. (*a*) An example of the VD network with 400 sites distributed on a square region of size $L = 20$. (*b*) The corresponding VD lattice for the diagram shown in (*a*). Clearly, the number of connections of site i is not necessarily equal to that of site j.

(This figure is in colour only in the electronic version)

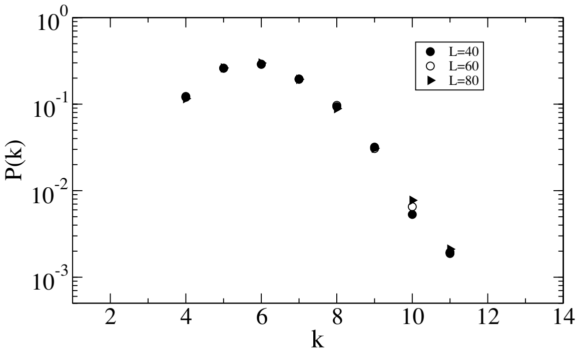

Figure 2. The normalized frequency $P(k)$ (in the logarithmic scale) versus the number of nearest neighbor, k, in the VD lattice. For the sizes L above the connectivity reads around $\overline{k} = 6$.

k for the Voronoi–Delaunay lattice. The connectivity, i.e. the mean number of connections per site, $\overline{k} = \frac{1}{L^2}\sum_{i=1}^{L^2} k_i = 6$, where k_i is the number of links of site i (more precisely, our values range in the interval [5.999, 6.003] in obtaining all results throughout this paper). Let us recall that for regular square (SL), triangular (TL) and hexagonal (HL) lattices we have 4, 6 and 3, respectively. Distinct from a regular lattice, where the number of connections is constant throughout the system, in the VD framework it varies randomly, averaging to 6, at the thermodynamic limit, $L \to \infty$. This paper is devoted to investigate how the variation in the number, and mainly the geometrical distribution of links in the lattice may affect some statistical quantities, namely those concerned with the (topological) phase transition, such as the critical temperature and the vortex saturation density, at high temperatures. As randomly diluted systems with XY-symmetry in square lattices (thus, with $\overline{k} < 4$) have attracted considerable attention in the past few years [17–21], it would be interesting to know how things change as connectivity is varied and randomly distributed, now for $\overline{k} > 4$.

Now, we consider the XY-model described by the Hamiltonian below:

$$H = -J \sum_{\langle i,j\rangle} \left(S_i^x S_j^x + S_i^y S_j^y\right), \tag{1}$$

where $\sum_{\langle i,j\rangle}$ indicates a summation over all 'nearest-neighbor' site pairs and $J > 0$ is the ferromagnetic coupling constant, assumed to have the same value for all pairs of spins. In the XY-model the classical spin vectors $\vec{S}_i$ have three components $\vec{S}_i = \left(S_i^x\right)\hat{i} + \left(S_i^y\right)\hat{j} + \left(S_i^z\right)\hat{k}$. At this point, we should stress that the Hamiltonian above also describes the $SO(2)$ rotationally invariant planar rotator model (PRM). The main difference between XY and PRM lies in the fact that while in the first, S^z acquires non-trivial values through true dynamics (coming about from the non-vanishing quantum-mechanical commutator $[S^z, H] = i\hbar(d/dt)S^z$), in the latter S^z identically vanishes, making PRM a rigid model whose 'dynamics' is strictly confined to the plane. We also remark that in our calculations we have used a hybrid Monte Carlo algorithm which includes cluster and single spin updates to calculate some thermodynamic quantities for the model defined by the Hamiltonian (1). Each Monte Carlo step (MCS) in our scheme consists of four Metropolis [26] updates, say, $4 \times L^2$ spin updates, followed by one Wolff [27, 28] update of the planar components of the spins. This hybrid algorithm was used to prevent critical slowing down and correlations between different configurations. The simulations were performed considering different number of spins, $N = L^2$, and we have mainly used $L = 32, 40, 52, 60$ and 80 (note that the number of spins is the same of a regular square lattice of size L). We start from a completely random configuration in the highest temperature, running 10^5 MCS for equilibration at each temperature and 6×10^5 MCS to obtain thermal averages, which have been obtained by taking 20 samples into account. After obtaining such averages, at a given temperature, we take the last configuration to be the initial one for the next step, and so forth. For a fixed size L we have performed an average over two different VD lattices, say, two distinct random distributions of the L^2 sites. In the figures, the error bars are not shown when the statistical errors are smaller than the symbols themselves and, for convenience, the temperature is measured in units of J, the exchange constant, introduced in Hamiltonian (1).

3. Results and discussions

The lack of significant sharp peaks in the thermodynamic quantities as functions of temperature for this model, especially for finite lattice systems, means that the determination of the critical temperature, T_{cr}, is not a so easy task. As discussed in [18, 29–31], an interesting method to determine T_{cr} for the XY-model is the size dependence of Binder's fourth-order cumulant, as below. This quantity is usually considered for Berezinskii–Kosterlitz–Thouless-type phase transitions. Binder's fourth-order cumulant [29, 30], U, is formally defined as

$$U = 1 - \frac{\left\langle \left(M_x^2 + M_y^2\right)^2 \right\rangle}{2\left\langle M_x^2 + M_y^2 \right\rangle^2}, \tag{2}$$

where M_x and M_y are the in-plane magnetization components. For every analyzed lattice the asymptotic values of U are $U(T \ll T_{cr}) = 0.5$ and $U(T \gg T_{cr}) = 0$. At the critical temperature, U is practically independent of L and, hence, T_{cr} is obtained from the crossing point of curves of U for several lattice sizes, L. Figure 3 shows how U behaves for different L's, and our estimate for the phase transition temperature for the Voronoi–Delaunay (left figure) and regular triangular (at the right) lattices, $T_{cr}^{VD} = 1.221 \pm 0.007$ J and $T_{cr}^{TL} = 1.156 \pm 0.002$, respectively.

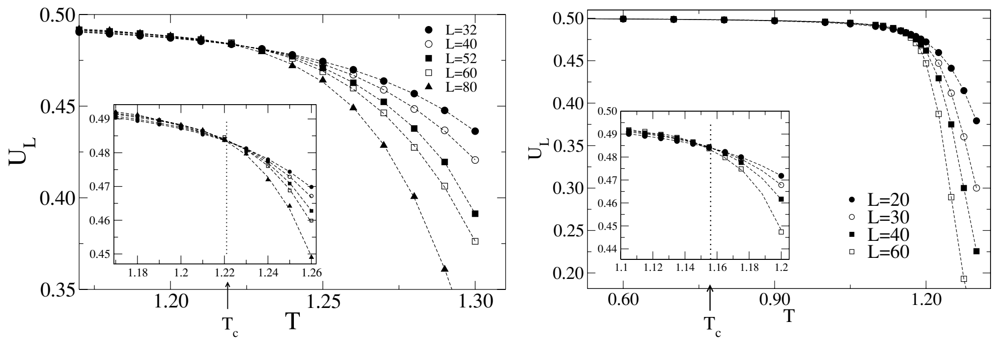

Figure 3. Binder's cumulant, U_L, versus temperature, T, for different values of L. The inset shows a view around the estimated transition temperature for each lattice. On the left, for the VD network, while for the regular triangular lattice on the right. Their respective critical temperatures read $T_{\rm cr}^{\rm VD} = 1.221 \pm 0.007$ J and $T_{\rm cr}^{\rm TL} = 1.156 \pm 0.002$, indicated by the vertical dotted line. The lines linking the symbols are just to guide the reader.

It is noteworthy to remark that while they share the same connectivity number, their $T_{\rm cr}$ are distinct to each other by about 5–6%. Such a difference may be attributed to the different topologies and/or geometries of the spins interaction in these two lattices. Our results indicate that keeping the connectivity but distorting the structure of the lattice, an extra amount of energy is demanded for vortex-pair unbinding take place. This appears to be an interesting interplay between the connectivity number, $\overline{k}$, and the (topological) phase transition: the critical temperature is raised as long as $\overline{k}$ increases, as exemplified above. Such an interplay also holds if $\overline{k}$ is diminished; for instance, whenever dilution (spin vacancies, etc) is incorporated to the system the critical temperature is observed to get lower as long as more and more vacancies are introduced, in such a way that as dilution approaches the percolation threshold, ∼41%, then $T_{\rm cr}$ vanishes (extinction of the BKT-like transition) [17–21]. However, a given variation in $\overline{k}$ does not yield a linear change in $T_{\rm cr}$, as clearly shown by comparing the respective results for VD and triangular lattices. The deviation from a linear dependence may be credited to how spins are linked in the network, as pointed out above. In this respect, it would be desirable to carry out further studies adopting networks which could have their connectivity varied, but keeping the structure of sites distribution, in order to shed some extra light on this issue. Such an investigation has additional relevance once it could be related to a number of actual disordered lattices, like in amorphic materials.

Figure 4 shows the behavior of the in-plane magnetization $\langle m_{xy}\rangle = \sqrt{M_x^2 + M_y^2}$, as a function of the temperature, for $L = 40$, 60 and 80, whose behavior is qualitatively similar to that verified in usual lattices.

As is well known, for the XY-model the thermodynamic quantities have a fundamental dependence on the topological excitations, namely on vortex-like objects. Therefore, it should be important to look for vortices in this disordered model and analyze their proliferation. To do this, we have measured the vortex density, ρ_v, defined as

$$\rho_v(L) \equiv \frac{1}{L^2} \sum_l \delta_{2\pi, \sum_{ij}(\phi_i^l - \phi_j^l)}, \tag{3}$$

where δ is the Kronecker delta, the summation $\sum_l$ is performed over the set of spins that share the same 'neighbors', and $\phi_i^l - \phi_j^l$ is the difference among the angles of adjacent spins, with ϕ being the angle that the spin vector makes with some fixed direction in the plane. Note that

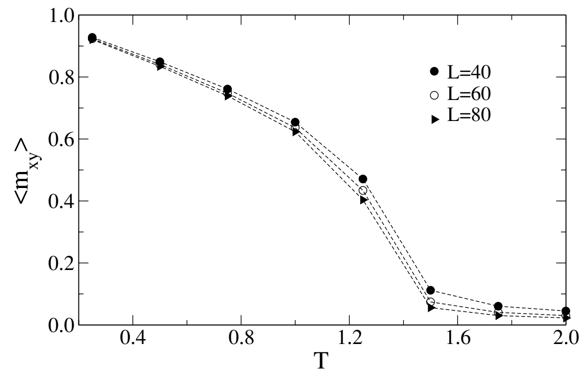

Figure 4. The in-plane magnetization, $\langle m_{xy} \rangle$, versus the temperature T for some lattice sizes. Its behavior is similar to its counterpart from regular lattices. The lines linking the symbols are just to guide the reader.

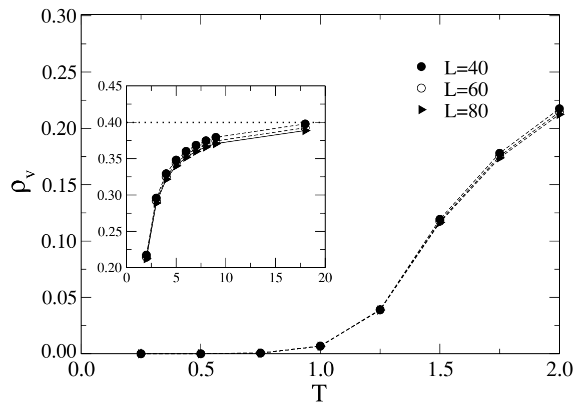

Figure 5. The vortex density ρ_v as a function of the temperature T for some L-values. Note that ρ_v increases considerably around the critical temperature, $T_{\text{cr}}^{\text{VD}} \approx 1.22$ J, indicating that the transition may be understood as a Berezinskii–Kosterlitz–Thouless-type (BKT) phase transition caused by the unbinding of vortex pairs. The inset shows the vortex density saturation $\rho_{\text{sat}} = 0.399\,756 \pm 0.000\,004$ (horizontal dotted line), obtained for $L = 80$, at high temperature. To obtain that we have performed an average over five different samples. The lines linking the symbols are just to guide the reader.

only the set of spins, indexed by l, whose summation $\sum_{ij} \phi_i^l - \phi_j^l$ is 2π (in fact, very close to 2π, due numerical errors) contributes to ρ_v [32]. Here, it is also important to distinguish L^2 from the plaquette number: in a square lattice both quantities acquire the same meaning and value, but in a VD network they are quite different. We have kept L^2 in the denominator of expression (3) for the sake of later comparison. In addition, we consider only excitations with topological charge $Q = +1$ (the number of antivortices, with $Q = -1$, exactly equals the number of vortices, due to topological charge conservation). The vortex density, ρ_v, slowly rises until the transition temperature $T_{\text{cr}}^{\text{VD}} \approx 1.22$ J, where a pronounced increase is observed. Therefore, it is reasonable to associate this transition with the mechanism of vortex–antivortex unbinding, in analogy with what happens in the BKT phenomenology. To understand more deeply the intrinsic relation between vortices and the BKT transition, it should be instructive to compare the total vortex densities (including also the antivortices) in regular square (SL) and VD lattices (these total densities will be referred to as $\rho_{\rm SL}$ and $\rho_{\rm VD} = 2\rho_v$, respectively). Results from [32, 33] dictate that $\rho_{\rm SL}$ is much larger than $\rho_{\rm VD}$ for a wide range of temperatures, say, for $T < T_0$, with a certain $T_0 > T_c^{\rm VD}$. Such greater proliferation of vortices at relatively low temperatures justifies the lower critical temperature observed in the square lattice. On the other hand, for $T > T_0$, $\rho_{\rm VD}$ overcomes $\rho_{\rm SL}$. Indeed, the inset of figure 5 shows the behavior of ρ_v (and consequently $\rho_{\rm VD}$), for a larger range of T. Note that it increases monotonically up to a maximum value saturating to $\rho_{\rm VD}^{\rm sat} \approx 0.798$ as $T \to \infty$ (in a SL one has $\rho_{\rm SL}^{\rm sat} \approx 0.333$ [32, 33]). This fact can be explained as follows: although we are considering the same number of sites for SL and VD lattices, the number of plaquettes in the VD lattice is much larger than that in the SL. For example, for $L = 40$, there are 1600 plaquettes in SL and 5044 in the VD lattice, say, there is 'more space' to put in much more vortices in the VD framework. Therefore, at high temperature, the study of the XY-model in a VD lattice may be also useful to generate insights about the properties of systems in the regime of high density of topological objects.

4. Concluding remarks

We have performed Monte Carlo simulations for studying the 2D XY-model and the BKT transition in a Voronoi–Delaunay lattice. Since this system is constructed by randomly distributing L^2 sites on a square region of linear length L, the number of connections between the spins varies from site to site, while the mean number of connections per site reads $\bar{k} \approx 6$. Essentially, the different topology of the interactions in the VD lattice changes the thermodynamical properties of the model, increasing the critical temperature and modifying the vortex density when compared to the regular lattices. In addition, we recall that in diluted systems (e.g., with spin vacancies randomly incorporated) the decrease in $\bar{k}$ is inevitably accompanied by a decrease in the critical temperature, which vanishes if vacancies get beyond the square lattice percolation threshold, $\varrho \approx 0.41$ [17, 18, 20, 21]. Thus, an interesting interplay between $\bar{k}$ and $T_{\rm cr}$ can be realized: as long as one of these quantities is raised, the same occurs to the other, and vice versa. However, such a relation is not a linear function, this is illustrated by considering the triangular and VD lattices, which have the same connectivity, but distinct $T_{\rm cr}$, by about 5%. Such a difference is then associated with the structure of the lattice itself, say, how the sites are distributed. A similar analogy concerns vortex densities. Actually, we have seen that $\rho_{\rm SL} > \rho_{\rm VD}$ for temperatures $T < T_0$, while the converse takes place for $T > T_0$, which is a reference temperature satisfying $T_0 > T_c^{\rm VD}$ (see figure 5 and the related text). Additionally, at low temperature, $T < T_{\rm cr}$, the vortex density in regular lattices is smaller than that in diluted systems (smaller connectivity), while the situation is inverted at high temperatures [34]. Thus, the vortex proliferation and the mean number of connections per site are somewhat related, at low temperature, since as long as $\bar{k}$ decreases, the vortex density appears to increase. Moreover, in diluted materials, even excitations with much higher energies such as vortices with double topological charge ($Q = 2$) are easier to observe in the simulations [34, 35]. How the structure and topology of the links in a given lattice may affect the appearance of higher-charged vortices is under investigation and concerning results will be published elsewhere.

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