Monte Carlo studies of percolation in a superconducting array

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We investigate phase transitions in a two-dimensional site-diluted superconducting array, using Monte Carlo simulations. The array is modeled via a site-diluted classical XY model on a square lattice in the regime $p_c < p < 1$, where p is the concentration of "spins" (representing the phases of the superconducting order parameters on the grains) and p_c denotes the percolation threshold. In the unfrustrated case (zero magnetic field), we find that the Kosterlitz-Thouless (KT) transition temperature $T_c(p)$ approaches zero according to the power law $T_c(p) \sim (p - p_c)^{\kappa}$ and $\kappa \approx 1.14$, as $p \to p_c$ from above. To within the accuracy of the calculation, κ equals the expected value of t, where $t \approx 1.30$ is the usual conductivity exponent. In the fully frustrated case, which in a perfect lattice ($p = 1$) is characterized by a phase transition of combined KT- and Ising-like character, we find no Ising-like character in the diluted lattice. The apparent KT behavior is broadened over a considerable temperature range, compared to the case in the perfect lattice.

I. INTRODUCTION

A two-dimensional superconducting array consists of superconducting grains arranged on the sites of an ordered two-dimensional lattice, each grain being weakly linked to its nearest neighbors via Josephson or proximity coupling. During the past decade, many workers have studied phase transitions in such arrays. Both theoretical and experimental investigations[1] have revealed that at certain temperatures, in the absence of a magnetic field, such an array will undergo a so-called Kosterlitz-Thouless[2,3] (KT) phase transition, marked by the unbinding of thermally excited vortex-antivortex pairs. The low-temperature phase of such a system is characterized by a quasi-long-range order. When a transverse magnetic field is applied to the array, the universality class of the phase transition is believed to differ from the zero-field case, and to depend sensitively on the magnitude of the so-called frustration f,[4] defined as the flux per plaquette of the lattice measured in units of a flux quantum $\Phi_0 \equiv hc/2e$. For frustrated lattices, the details of the underlying phase transitions remain incompletely understood even for perfect lattices. The case of the fully frustrated square lattice ($f = \frac{1}{2}$) has been studied more extensively than the others. It is believed, on the basis of earlier Monte Carlo simulations, that the transition to a superconducting state occurs via a phase transition with both Ising- and KT-like character at a single temperature.[5]

In recent years, a number of workers[6-16] have studied the effects of disorder on phase transitions in such arrays. In real samples, of course, various kinds of disorder are inevitable. Among the most likely types of disorder are local fluctuations in plaquette areas and grain positions. For this kind of disorder, several studies have been carried out, and a possible reentrant phase transition arising from positional disorder has been predicted.[11,15] There remains, however, a very important type of disorder—that produced by randomly diluting a two-dimensional superconducting array—which has been little explored. When this type of disorder is produced in a superconducting array, one expects a competition between classical percolation and the phase-locking superconducting transition, especially when the diluted array is near the so-called percolation threshold, where the superconducting grains just form a connected path throughout the array. A natural question to ask is, therefore, the following: Is the character of the phase transition changed by the disorder associated with such dilution?

In this article, we report the results of computer simulations on site-diluted two-dimensional XY lattices. To our knowledge, these represent the first Monte Carlo study of the question described above. Comparisons with recent measurements of Harris *et al.* [17] show excellent agreement with experiment where comparisons are possible. We also make novel predictions regarding the behavior of fully frustrated lattices, which would be interesting to verify experimentally.

II. CLASSICAL XY MODEL

In a common approximation, the static properties of an ordered superconducting array in a transverse magnetic field are described by a uniformly frustrated two-dimensional classical XY model. The Hamiltonian of this model is

$$H=-\sum_{\langle ij\rangle} J_{ij}\cos(\theta_i-\theta_j-A_{ij}) , \tag{1}$$

where θ_i is the phase of the order parameter on the ith site of the lattice, $\langle ij\rangle$ represents distinct pairs of nearest-neighbor sites, J_{ij} is the coupling strength between the ith and jth sites, which is a function of the magnetic field and of the temperature, and finally, A_{ij} is the line integral of the vector potential $\mathbf{A}$ between the ith and jth sites, i.e.,

$$A_{ij}=\frac{2\pi}{\Phi_0}\int_{\mathbf{x}_i}^{\mathbf{x}_j}\mathbf{A}\cdot\mathbf{dl} , \tag{2}$$

where $\mathbf{x}_i$ is the position of the ith site. Note that the phase difference $\theta_i-\theta_j-A_{ij}$ is gauge invariant. The frustration f is then defined by

$$\sum_p A_{ij}=2\pi f , \tag{3}$$

where the sum is over the sides of an elementary plaquette of the lattice. Thus f can be written in terms of the magnetic field B:

$$f=BA_p/\Phi_0 , \tag{4}$$

where A_p is the area of the elementary plaquette. In particular, for a square lattice with lattice constant a, the frustration is determined by $f=Ba^2/\Phi_0$. When $f=\frac{1}{2}$, the model is known as the fully frustrated XY model, first introduced by Villain.[18]

Note that several approximations have been made in writing the Hamiltonian (1). First, we have neglected quantum fluctuations associated with a finite charging energy (finite grain capacitance). Also, the magnetic field induced by the supercurrent has been neglected; this approximation corresponds to the limit of infinite London penetration depth, in which one can approximate the local magnetic field by the applied field. Finally, we have assumed "point grains" so that the phase of the order parameter within each grain is a constant and the line integral of the vector potential (2) is well defined. We also neglect any temperature dependence of the coupling constant J_{ij} and assume a constant coupling J between each pair of nearest neighbors.

Site-diluted disorder can be introduced into the array by removing grains from the various sites randomly with probability p. Thus, each pair of nearest grains has coupling either J or 0. For the frustrated lattice, we work in the London gauge $\mathbf{A}=(0,Bx,0)$ so that the line integral A_{ij} is given by

$$A_{ij}=\frac{2\pi}{\Phi_0}B\frac{x_i+x_j}{2}(y_j-y_i) , \tag{5}$$

where x_i and y_i are the x and y coordinates of the ith lattice site.

One order parameter which is expected to characterize phase transitions in these arrays is the helicity modulus tensor γ, first introduced by Fisher, Barber, and Jasnow[19] for liquid He.[4] γ measures the free-energy cost of imposing a twist in the phase at the boundaries of the array. As was shown by Ebner and Stroud,[20] the effects of the twist can be described equivalently by adding a term to the Hamiltonian (1) while still retaining periodic boundary conditions, i.e.,

$$\gamma_{ij}=\left.\frac{\partial^2 F}{\partial A_i'\partial A_j'}\right|_{\mathbf{A}'=0} , \tag{6}$$

where $\mathbf{A}'$ represents an added uniform vector potential (in addition to the vector potential $\mathbf{A}$ used to produce the applied magnetic field). One then obtains[20] expressions for all the components of the helicity modulus tensor; a typical diagonal component is

$$\gamma_{xx}=\frac{1}{N}\left[\left\langle\sum_{\langle ij\rangle}x_{ij}^2 J_{ij}\cos(\theta_i-\theta_j-A_{ij})\right\rangle - \frac{1}{k_B T}\left\langle\left[\sum_{\langle ij\rangle}x_{ij}J_{ij}\sin(\theta_i-\theta_j-A_{ij})\right]^2\right\rangle + \frac{1}{k_B T}\left\langle\sum_{\langle ij\rangle}J_{ij}x_{ij}\sin(\theta_i-\theta_j-A_{ij})\right\rangle^2\right] , \tag{7}$$

where T is the temperature, $x_{ij}=x_j-x_i$, N is the total number of grains and $\langle\ \rangle$ denotes an ensemble average. Analogous expressions hold for other components of the helicity modulus tensor.

Another quantity characterizing the phase transition is the specific heat per site (C_V), which can be estimated from fluctuations of the internal energy, i.e.,

$$C_V=\frac{1}{Nk_B T^2}(\langle H^2\rangle-\langle H\rangle^2) , \tag{8}$$

where H represents the Hamiltonian (1). By monitoring the lattice size dependence of the specific-heat peak (in the C_V-T phase diagram), one can obtain useful information regarding the universality class of the phase transition.

III. NUMERICAL RESULTS

The Monte Carlo (MC) simulations were carried out on the Cray Y-MP 8/8-64 supercomputer of the Ohio Supercomputer Center, using the standard Metropolis algorithm[21] to generate successive configurations. We studied three site-diluted lattices with site occupancy $p=70$, 80, and 90%. In order to minimize metastability problems, we cooled our system from high temperatures at constant fields, starting from a temperature 1.4 J/k_B and cooling to 0.1 J/k_B in steps $\Delta T=-0.1$ J/k_B (except for near the transition, where we used $\Delta T=-0.05$ J/k_B). We started with a random-phase configuration at $T=1.4$ J/k_B, and for subsequent temperatures always used the final (equilibrium) configuration of the previous temperature as the starting configuration to reduce the chances of being trapped in a metastable state.

In the unfrustrated case (no magnetic field), we studied a 60×60 square lattice with periodic boundary conditions. At each temperature, we made typically 20 000 passes (Monte Carlo steps per spin) through the entire lattice, of which the first 10 000 passes were discarded and the remaining 10 000 used to evaluate the expecta-

tion values of both the helicity modulus and the specific heat. Our reported results are obtained by calculating the mean $\gamma=(\gamma_{xx}+\gamma_{yy})/2$, and also averaging over five independent runs, that is, over five different realizations of the random dilution with the same p.

Figure 1 is a plot of the helicity modulus $\gamma(T,p)$ for each p. Clearly, for every concentration, the helicity modulus drops smoothly to zero at lower temperatures. In an infinitely large perfect lattice, it is well known that the helicity modulus jumps discontinuously from the value $2T_c/\pi$ to zero at the KT transition. Because the universality class of KT transition in an unfrustrated XY lattice is not altered by site dilution, we can estimate the KT transition temperature $T_c(p)$ from the intersection of the helicity modulus curve $\gamma(T,p)$ with the straight line $\gamma=(2/\pi)T$. We find that as the concentration p decreases, the transition temperature $T_c(p)$ is monotonically reduced. We have also observed that for fixed lattice size, the KT transition zone is broadened as the dilution increases. This can be understood as follows: The effect of site dilution is to increase the effective lattice constant of the lattice from a to the percolation correlation length ξ_p. Thus, *in units of* ξ_p, a lattice of fixed size is effectively becoming smaller and smaller as the percolation threshold is approached. Finite-size effects are therefore becoming more and more pronounced, leading to a KT transition which becomes broader with increasing site dilution.

Figure 2 is a log-log plot of the reduced transition temperatures $T_c(p)$ (normalized to the T_c of a perfect lattice) as a function of $p-p_c$, where $p_c=0.593$ for a square lattice at site percolation.[22] In the same figure we plot the experimental data of Harris *et al.*, [17] as obtained from dynamical measurements on a site-diluted artificial 300×300 superconducting array made by photolithographic techniques. Harris *et al.* inferred $T_c(p)$ from the measured current-voltage (I-V) characteristics. They found that voltage varied nonlinearly with current, i.e.,

$$V\sim I^{a(T,p)} . \tag{9}$$

For $f=0$ the exponent $a(T,p)$ is directly related to the helicity modulus:[23]

$$a(T,p)-1=\frac{\pi\gamma(T,p)}{T} . \tag{10}$$

It follows that, like $\gamma(T,p)$, the exponent $a(T,p)$ also exhibits a universal jump at $T=T_c(p)$. For $a(T,p)$, the jump is from 1 to 3. The experimental numbers in Fig. 2 correspond to the isotherms where $a(T,p)=3$. Agreement between the simulation and the experimental measurements is excellent. In addition, the fitted straight line in Fig. 2 suggests a power-law relation between the transition temperature $T_c(p)$ and the concentration difference $p-p_c$, namely

$$T_c(p)/T_c(1)\sim(p-p_c)^{\kappa} . \tag{11}$$

The slope of this straight line corresponds to $\kappa\approx1.14$. Ebner and Stroud[20] have speculated that κ should be identical to the exponent t describing the conductivity of a metal-insulator composite near the percolation threshold. t is approximately 1.30 for a two-dimensional lattice. A more rigorous argument for this identification has been given by Aharony.[24] The value 1.30 is to within our nu-

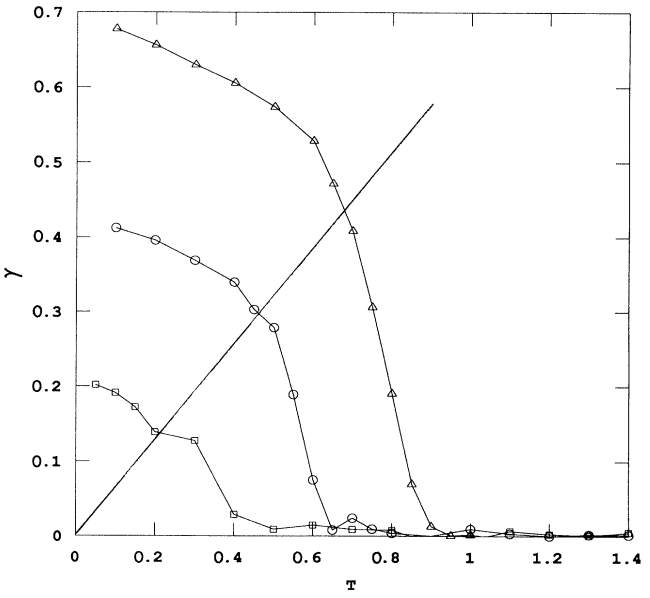

FIG. 1. Helicity modulus $\gamma(T,p)$ (in units of J) vs the temperature T (in units of J/k_B) at three different concentrations $p=70$ (squares), 80 (circles), and 90% (triangles) in zero magnetic field. The solid lines are guides to the eye. The straight line of slope $2/\pi$ represents the universal jump in helicity modulus at the Kosterlitz-Thouless transition.

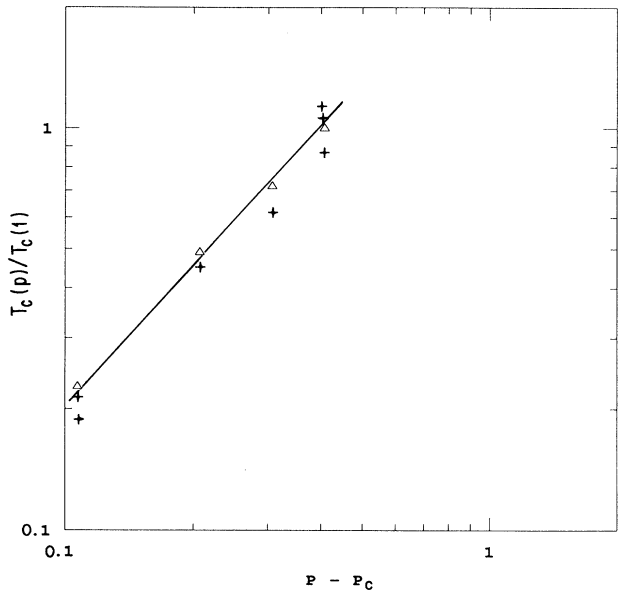

FIG. 2. Log-log plot of the reduced transition temperature $T_c(p)/T_c(1)$ as a function of $p-p_c$ [note $T_c(1)\approx0.95$ J/k_B, Ref. 5]. The line is a fit to the Monte Carlo data (triangles). The crosses are the experimental data of Ref. 17.

merical accuracy equal to the value of $\kappa \approx 1.14$ inferred from our simulation (the difference with $t=1.30$ is mainly due to the broadened transition zone, especially at lower p; see Fig. 1), and $\kappa \approx 1.16 \pm 0.13$ deduced from experiment.

To treat the fully frustrated case ($f=\frac{1}{2}$), we studied two square lattices of sizes 30×30 and 60×60 with periodic boundary condition and the Landau gauge. On the 30×30 lattice, we took 20 000 passes through the lattice, with the first 10 000 discarded, and averaged over five independent realizations of the disorder. On the 60×60 lattice, we used 50 000 passes (25 000 discarded and 25 000 for averaging) and again averaged over five independent realizations of the disorder. Results for the helicity modulus are displayed in Figs. 3 and 4 for the different lattice sizes; results for the specific heat are shown in Figs. 5 and 6.

Just as in the unfrustrated case, the helicity modulus falls smoothly to zero at lower temperatures, and the magnitude of the drop shrinks with increasing dilution. In contrast to $f=0$, no final agreement as to the universality class of the phase transition has been reached in the literature, even for a perfect XY lattice at $f=\frac{1}{2}$. The original Monte Carlo simulations of Teitel and Jayaprakash[5] showed not only a jump in the helicity modulus, indicative of a Kosterlitz-Thouless–like phase transition, but also a size-dependent peak in the specific heat, indicative of an Ising-like phase transition. More recent simulations by Berge *et al.*[25] indicated that the Ising- and Kosterlitz-Thouless–like transition may occur at the same temperature. Studies by Van Himbergen[26] suggest that while the transitions occur at the same temperature, the jump in the helicity modulus at T_c is nonuniversal. Minnhagen[27] has also predicted a Kosterlitz-Thouless–like transition with a nonuniversal jump. The nonuniversality has apparently been confirmed experimentally by Van Wees, van der Zant, and Mooij.[28]

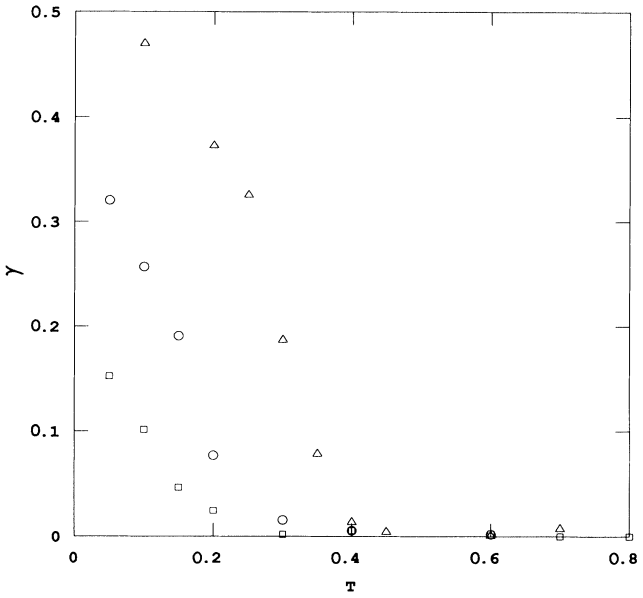

FIG. 4. Same as Fig. 3, but for 60×60 lattices.

If there is a transition characterized by a nonuniversal jump in the helicity modulus, one cannot use the geometrical construction described above to infer the transition temperature as in the unfrustrated case. Nonetheless,

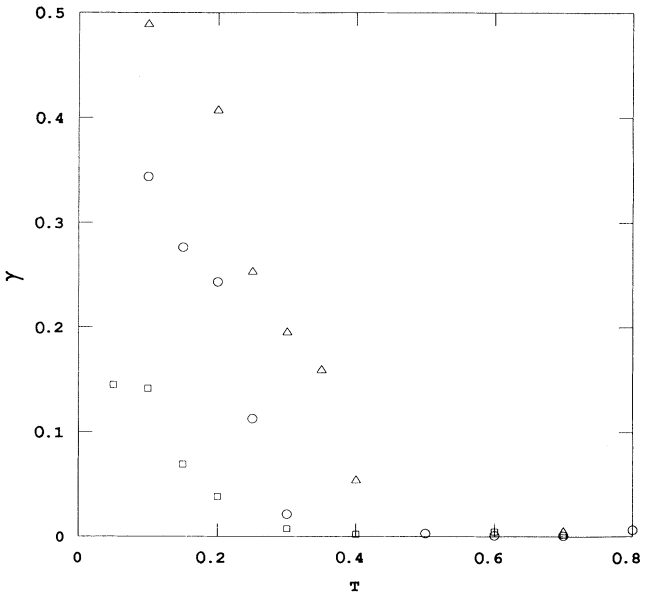

FIG. 3. Helicity modulus $\gamma(T,p)$ vs the temperature T in fully frustrated 30×30 lattices at concentrations $p=70$ (squares), 80 (circles), and 90 % (triangles).

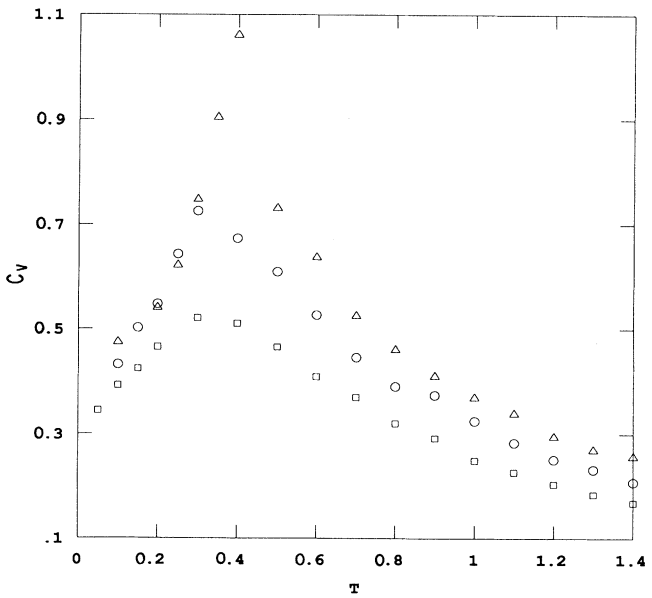

FIG. 5. Specific heat per site $C_V(T,p)$ (in units of k_B) vs the temperature T for fully frustrated 30×30 lattices at concentrations $p=70$ (squares), 80 (circles), and 90 % (triangles).

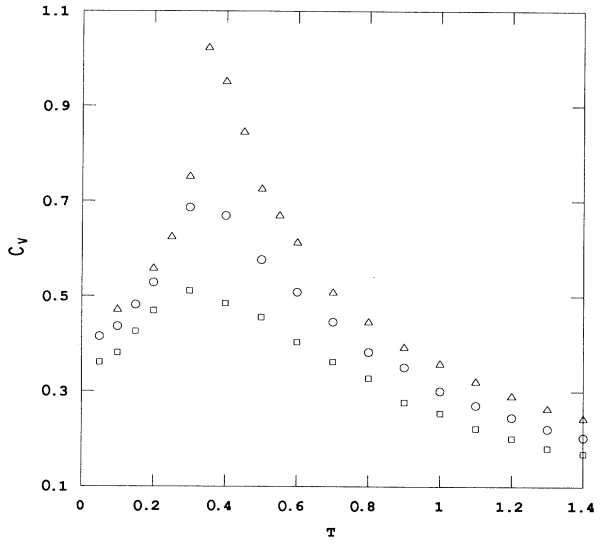

FIG. 6. Same as Fig. 5, but for 60×60 lattices.

there seems to be some evidence for a phase transition even in the diluted lattice, although it presumably would also be characterized by a nonuniversal jump. For example, at a given dilution, the helicity modulus drops to zero more sharply in the larger lattice than in the smaller one, suggesting that the apparent broadening of the jump may be a finite-size effect, which would disappear if the lattice size could be made infinite. Note also that, for fixed lattice size, as the concentration p approaches the percolation threshold p_c, the jump of the helicity modulus is more and more broadened. This suggests that the interplay between the superconducting transition and the percolative geometry is similar to that of the unfrustrated case.

Figures 5 and 6 show that the specific heat per site $C_V(T,p)$ has a pronounced peak which is more and more rounded with increasing dilution, with a maximum value which is continuously reduced as the dilution increases. There is about a 25% difference between the temperature of the specific-heat peak and the temperature of the helicity modulus jump. This difference is more pronounced than that of a perfect lattice. Most important, the maximum value of the specific-heat peak does not grow with increasing lattice size. This behavior is in sharp contrast to the case of a perfect lattice, in which the specific-heat peak grows logarithmically with lattice size, indicating an Ising-like phase transition. We conclude that, if there is a phase transition in the diluted lattice, it does not have any Ising character.

IV. DISCUSSION AND CONCLUSIONS

We have carried out Monte Carlo simulations on site-diluted unfrustrated and fully frustrated two-dimensional XY lattices. Temperature dependence of the helicity modulus and specific heat per spin have been calculated through Monte Carlo simulations in both cases. In the unfrustrated case, we find that the dilution disorder reduces the Kosterlitz-Thouless transition temperature, and as $p\rightarrow p_c$ from above, the KT transition temperature approaches zero according to the power law $T_c(p)\sim(p-p_c)^{\kappa}$, where $\kappa\approx1.14$. Furthermore, the KT transition zone is found to be broadened by dilution, in a manner which reflects a crossover from a quasihomogeneous regime to a percolative regime when the percolation coherence length approaches the lattice size of the simulations.

In the fully frustrated case at finite dilution, we also find a jump in the helicity modulus curve $\gamma(T,p)$, but only a broad peak in the specific-heat curve $C_V(T,p)$. However, the results presented here are only suggestive, not conclusive, regarding the nature of the phase transition. Even for a perfect lattice, the nature of transition at $f=\frac{1}{2}$ is still not established. Our results suggest that at this frustration the transition may be KT-like, in contrast to the KT-plus Ising-like behavior observed in the perfect lattice. Indeed, it is conceivable that there is actually *no* phase transition in the diluted, frustrated lattice. Even though our simulations are relatively long, we are dealing with a system which is both disordered and frustrated. Such systems, studied in connection with both random-field Hamiltonians[29–31] and glassy models[32–34] are typically characterized by extremely long relaxation times. If such relaxation times exist in the present model, then it is possible that our results for the helicity modulus are not fully equilibrated. Our simulations of $\gamma(T,p)$ of Figs. 3 and 4 show that $\gamma(T,p)$ tends to change from concave down to concave up when the length of the MC run is increased. This suggests that, in a sufficiently long run, $\gamma(T,p)$ might be zero for all random dilutions at any finite temperature. Such questions would need to be answered by longer computer runs, or by convincing analytical arguments.

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