Three-dimensional random XY model: Application to the superfluid transition of ^{4}He in porous media

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We study a three-dimensional classical XY model with strongly fluctuating, spatially uncorrelated, bond disorder. Finite-size scaling analysis of Monte Carlo simulation data has been used to determine critical exponents. Evidence for a possible shift in exponents from the pure XY case is found. Connection to recent experiments on the superfluid phase transition of ^{4}He in porous media is discussed.

The superfluid phase transition of liquid ^{4}He in porous structures has been a topic of long-standing interest.[1-7] Much effort has been devoted to understanding the onset of superfluidity at $T=0$ as a function of increasing helium density.[2,3] Another problem has been the critical behavior at the very low transition temperatures seen in low-density thin films, which has been described in terms of a crossover to ideal-Bose-gas behavior.[2,4] At the higher transition temperatures seen in saturated pores, the nature of the superfluid transition has also been extensively studied experimentally.[1,5] In Vycor glass, a suppression of the normalized superfluid density $\rho_s(T)/\rho_s(0)$ as compared to bulk, is observed as T_c is approached from below, but the critical exponents appear to be the same as bulk.[1,5] Recent experiments in silica gels,[5] however, have reported different critical exponents for ρ_s, suggesting that the random host may shift the transition to a new universality class.

Theoretically, the superfluid transition in this higher-temperature case of saturated pores may be modeled by the classical XY model. The complex order parameter of the superfluid transition has the same symmetry as the planar spins of the XY model. Only a few attempts[6,7] have been made to model the behavior of the superfluid density in this case. Modeling the porous media as a set of interconnected one-dimensional chains, Fishman and Ziman[6] studied a regular bond-decorated spherical model. Garg *et al.*[7] carried out simulations on bond and site diluted 3D XY models, with dilutions as large as 55%. In such spin models, the helicity modulus $\Upsilon(T)$ (spin-wave stiffness constant) plays the role of the superfluid density. As $T\to T_c$ from below, Υ vanishes as $\Upsilon\sim|t|^{\nu}$, with ν equivalent to the superfluid density exponent ζ. In both the preceding models, no substantial change in $\Upsilon(T)/\Upsilon(0)$ (apart from a linear rescaling of the temperature) was observed when compared with that of a regular periodic lattice, for *all* temperatures from T_c down to $T=0$. Thus these models did not observe the suppression in $\rho_s(T)/\rho_s(0)$ near T_c characteristic of helium in porous media, nor any changes in critical behavior. The critical behavior of the 3D XY model is expected by the Harris criterion[8] to be unaffected by *weak* amounts of uncorrelated bond disorder. Weinrib and Halperin[9] introduced a model in which algebraically correlated disorder may affect critical exponents. However, no explicit model calculation was carried out for helium. In this paper we study a new random-bond-decorated 3D XY model. The disorder we introduce, motivated by a simple physical model of a porous media, is uncorrelated but very strongly fluctuating. We observe for the first time a clear suppression of the normalized helicity modulus near T_c from that of the regular periodic case, consistent with results on helium. A finite-size scaling analysis of Monte Carlo simulations is carried out to compute critical exponents, and we find results suggestive of a new universality class.

Our model is as follows. First, consider a regular 3D cubic lattice with one planar (XY) spin per node. Randomness is introduced by "decorating" each bond with a random number n of planar spins. n is taken from the probability distribution

$$p(n)=Ae^{-n/l_0}, \tag{1}$$

where l_0 sets the average number of spins on each bond and A is the normalization factor. All spins on this decorated lattice interact through nearest-neighbor couplings. The Hamiltonian of this model is given by

$$\mathcal{H}=-J\sum_{\langle ij\rangle}\left[\sum_{l_{ij}=1}^{n_{ij}-1}\boldsymbol{\sigma}_{l_{ij}}\cdot\boldsymbol{\sigma}_{l_{ij}+1}+\mathbf{s}_i\cdot\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_{n_{ij}}\cdot\mathbf{s}_j\right], \tag{2}$$

where $\mathbf{s}_i$ is the spin at node i of the lattice, and $\{\boldsymbol{\sigma}_{l_{ij}}\}$ are the n_{ij} spins on the bond-connecting nodes i and j. As usual, the sum $\sum_{\langle ij\rangle}$ is over all nearest-neighbor nodes of the cubic lattice.

The model (2) resembles some key features of superfluid ^{4}He in silica xerogel. For the xerogel in Ref. 5, the distribution of the pore diameters is sharply peaked at $d_p\approx 10$ nm which is much smaller than the coherence length of the superfluid ^{4}He in it, $\xi\sim 10^2$ nm near T_c. The spatial variation of the phase of the macroscopic

wave function may be neglected over length scales much smaller than the coherence length ξ. Therefore, one may treat the superfluid ^{4}He in one pore as a one-dimensional system and model it by a linear chain of planar spins. We simplify the very complicated topology of highly interconnected pores by modeling it as the connection of bonds on a 3D simple cubic lattice. The distribution (1) which we use, is suggested by the broad range of length scales believed appropriate for gels (Vycor in contrast, seems characterized by a narrower length distribution).[5,10]

Before numerically simulating the model (2), we first integrate over the degrees of freedom of the bond spins $\{\sigma_{l_{ij}}\}$ in the spirit of the real-space normalization group. A strict decimation over bond spins would result in an effective node-node interaction which is no longer a cosine. We simplify this by replacing the decimated bond spins by a cosine interaction with a coupling K_{ij} determined as follows: We require $\langle \mathbf{S}_0 \cdot \mathbf{S}_{n+1} \rangle_K$, the spin-spin correlation function of the chain with n intermediate spins at coupling $K = J/T$, to be equal to that of a two-spin chain with coupling K_{ij}, i.e., $\langle \mathbf{S}_0 \cdot \mathbf{S}_1 \rangle_{K_{ij}}$. These K_{ij} are given in terms of the number of bond spins n_{ij} by solving[11]

$$I_1(K_{ij})/I_0(K_{ij}) = [I_1(J/T)/I_0(J/T)]^{n_{ij}+1} . \tag{3}$$

I_n is the nth order modified Bessel function. Thus we reduce the decorated-bond problem to a random-bond XY model

$$\mathcal{H}_{\text{eff}}/T = -\sum_{\langle ij \rangle} K_{ij} \cos(\theta_i - \theta_j) , \tag{4}$$

where θ_i is the angle of the node spin $\mathbf{s}_i$. An interesting feature of the bond distribution generated by this procedure is that it is algebraic at small K. From Eqs. (1) and (3) we find at small K that the probability density to have a bond $K_{ij} = K$ is given by

$$\mathcal{P}_T(K) \sim K^{-a} ,$$
$$a = 1 + \frac{1}{l_0 \ln[I_1(J/T)/I_0(J/T)]} . \tag{5}$$

The probability distribution, and in particular the exponent a, vary with temperature. As T varies from 0 to ∞, a varies from $-\infty$ to 1. In the neighborhood of T_c, we will find $0 < a < 1$, and hence $\mathcal{P}_T(K)$ is divergent at small K.

We have carried out Monte Carlo simulations of this random XY model on simple cubic lattices of size $N = L^3$. Simulations and analysis have been carried out as in our prior work on the pure 3D XY model, and details may be found in Ref. 12. To reduce critical slowing down, we have used the over-relaxation method. For each data point, we have averaged over four different realizations of the random-bond configuration, and for each configuration we have averaged over two independent runs. Within each independent run, the system is cooled down from the disordered phase at high temperature. At each temperature, 500 passes through the lattice are discarded for equilibration, and 2000 passes used to compute averages. Each of the above "passes" consisted of eight over-relaxation steps followed by two Metropolis Monte Carlo sweeps through the lattice.

To characterize the critical behavior, we have computed the helicity modulus Υ and the "order parameter" $|M|^2$ as a function of temperature T and size L. The order parameter we chose is the magnetization squared, given by

$$|M|^2 = \frac{1}{N^2} \left\langle\!\!\left\langle \left| \sum_i \exp(i\theta_i) \right|^2 \right\rangle\!\!\right\rangle , \quad N = L^3 , \tag{6}$$

where $\langle\!\langle \cdots \rangle\!\rangle$ represents a combined thermodynamic average and average over random-bond configurations. The helicity modulus, in direction $\hat{\mu}$, is given by[13]

$$\Upsilon_{\hat{\mu}} = \frac{T}{N} \left\langle\!\!\left\langle \sum_{\langle ij \rangle} K_{ij} \cos(\theta_i - \theta_j)(\hat{\mathbf{e}}_{ij} \cdot \hat{\boldsymbol{\mu}})^2 - \left[\sum_{\langle ij \rangle} K_{ij} \sin(\theta_i - \theta_j) \hat{\mathbf{e}}_{ij} \cdot \hat{\boldsymbol{\mu}} \right]^2 \right\rangle\!\!\right\rangle , \tag{7}$$

We average Υ over $\hat{\mu} = \hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ to achieve better statistics. In Fig. 1 we show our results for normalized helicity modulus versus T/T_c, for the size $L = 10$. We show the pure XY model and our random-bond model with distributions (1) given by $l_0 = 3$, 5, and 10. We see clearly the suppression of $\Upsilon(T)/\Upsilon(0)$ near T_c for the random case as compared to the pure case.

To analyze critical behavior, the results of the helicity modulus Υ and order parameter $|M|^2$ have been fitted to second-order expansions of the finite-size scaling functions,[14]

$$\Upsilon(K,L) = L^{-v/\nu}[H_0 + H_1 L^{1/\nu}(K - K_c) + H_2 L^{2/\nu}(K - K_c)^2] , \tag{8}$$

$$|M(K,L)|^2 = L^{-2\beta/\nu}[\Phi_0 + \Phi_1 L^{1/\nu}(K - K_c) + \Phi_2 L^{2/\nu}(K - K_c)^2] , \tag{9}$$

where $K \equiv J/T$. In our fits to Υ, we have assumed the Josephson scaling relation $v = (d-2)\nu$ ($v = \nu$ in $d = 3$).[15] Our fitting procedure has been described in detail elsewhere.[12]

Simulation of the model (4) has been done for bond distributions (1) characterized by $l_0 = 3$, 5, and 10. For $l_0 = 5$, even sizes $L = 6$–14 were simulated. To test that we are in the scaling regime, we drop data from the successively lowest values of L until the fitted parameters remain unchanged. We have used only the data from $L = 10$, 12, and 14 for the final fits. For $l_0 = 3$ and 10, only sizes $L = 10$, 12, and 14 were simulated. The fitted curves for Υ and $|M|^2$, for the case $l_0 = 5$, are shown in Fig. 2. The fitted parameters are shown in Table I. Results from the helicity modulus and order parameter fittings agree within statistical error. While exponents for the case $l_0 = 3$ agree with those of the pure XY model, the exponent ν is seen to increase from the pure XY value

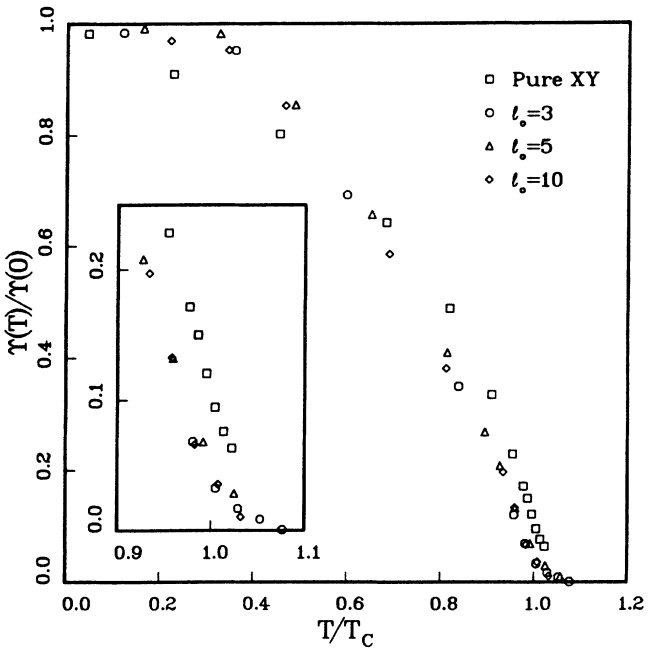

FIG. 1. Normalized helicity modulus $\Upsilon(T)/\Upsilon(0)$ vs T_c/T for the pure 3D XY model (Ref. 12) and our random model with the bond distribution (1) characterized by $l_0=3$, 5, and 10. Suppression of $\Upsilon(T)/\Upsilon(0)$ near T_c is clearly observed in the random case. Data is for a lattice of size $L=10$. Inset shows data on finer scale.

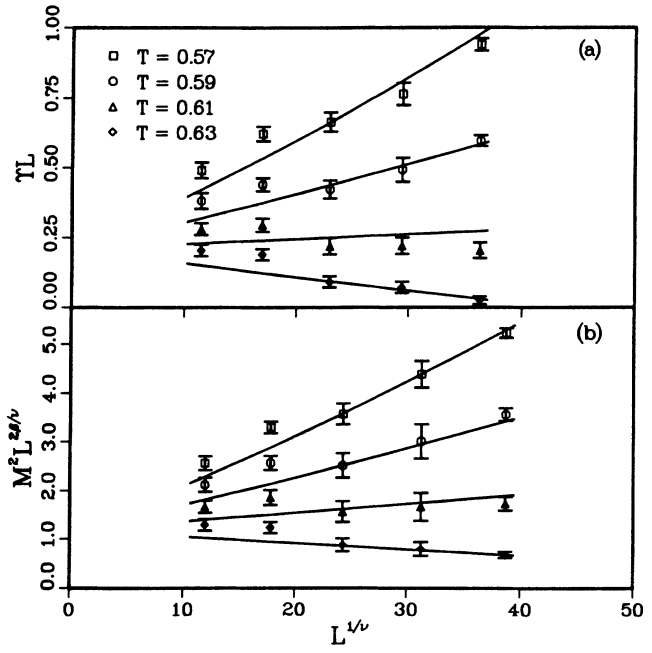

FIG. 2. The finite-size scaling behavior (a) of the helicity modulus $\Upsilon(T,L)$, and (b) of the order parameter $|\mathbf{M}(T,L)|^2$ for the bond distribution characterized by $l_0=5$. Symbols with error bars represent the Monte Carlo simulation results. The solid lines are the results of the fits to Eqs. (8) and (9) using data from sizes $L=10-14$. In (a), $\nu=0.74$ is used in making the horizontal axis of the plot. In (b), $\nu=0.72$ and $\beta=0.43$ are used in making the axes of the plot. The values of the fitted parameters are shown in Table I. $T_c\equiv 1/K_c\approx 0.613$.

as l_0 increases. Our values compare with the exponents $\zeta\sim 0.8-0.9$ found in experiments[5] on ^{4}He in silica gels ($\zeta\equiv\upsilon$, $\upsilon=\nu$ in $d=3$).

The effects of uncorrelated bond disorder on critical behavior is generally discussed in terms of the Harris criterion.[8] This argues for the irrelevance of *weak* disorder if the specific-heat exponent $\alpha<0$, as is the case for the pure 3D XY model where $\alpha=-0.007\pm 0.006$.[16] For our random bond XY model, however, disorder is *strong*. In Table I we show the value of the bond strength fluctuation, $\langle(\Delta K_{ij})^2\rangle_c/\langle K_{ij}\rangle_c^2$, at the critical temperature. We also show the value of the exponent $a(T_c)$ of the bond probability distribution (5) at small K. As one can see, the fluctuation is stronger and $\mathcal{P}_{T_c}(K)$ is more divergent at small K as l_0 gets larger. These observations suggest that the Harris criterion may not be applicable to such a strongly disordered system. A random Heisenberg model with a similar bond strength distribution diverging algebraically at $K\sim 0$ has been studied at the percolation threshold.[17] There it is found that both critical exponent t describing the vanishing of helicity modulus at the percolation threshold and the thermal-percolative crossover exponent ϕ vary with the power of the algebraic distribution.

To conclude, we have proposed a physical model for the superfluid transition of ^{4}He in porous media, which we reduce to a random-bond 3D XY model [Eq. (4)]. Disorder is strong and the Harris criterion may not apply. We have carried out Monte Carlo simulation of the model, and used finite-size scaling to find the critical exponents. We find that the normalized helicity modulus (superfluid density) is suppressed near T_c from the pure (bulk) case, as is observed experimentally. For the more

TABLE I. Table of simulation results for different bond distributions. $\nu^{(\Upsilon)}$ and $K_c^{(\Upsilon)}$ are the thermal exponent and the critical coupling as determined by fits to helicity modulus Υ, Eq. (8). $\nu^{(M^2)}$, $K_c^{(M^2)}$, and order parameter exponent β are determined by fits to $|\mathbf{M}|^2$, Eq. (9). $\nu^{(\Upsilon)},\nu^{(M^2)}$ and $K_c^{(\Upsilon)},K_c^{(M^2)}$ agree within statistical error. $\langle(\Delta K_{ij})^2\rangle_c/\langle K_{ij}\rangle_c^2$ is the fluctuation in random-bond strength at T_c. $a(T_c)$ is the exponent of the small-K bond distribution, Eq. (5), at T_c. Results for the pure XY model come from Ref. 12.

l_0	$\nu^{(\Upsilon)}$	$\nu^{(M^2)}$	$K_c^{(\Upsilon)}$	$K_c^{(M^2)}$	β	$\frac{\langle(\Delta K_{ij})^2\rangle_c}{\langle K_{ij}\rangle_c^2}$	$a(T_c)$
Pure	0.68±0.02	0.67±0.02	0.4543±0.0006	0.4533±0.0006	0.36±0.01		
3	0.70±0.05	0.65±0.04	1.199 ±0.006	1.200 ±0.006	0.37±0.04	0.86	0.50
5	0.74±0.04	0.72±0.03	1.63 ±0.01	1.61 ±0.01	0.43±0.04	1.1	0.57
10	0.85±0.06	0.92±0.08	2.46 ±0.02	2.51 ±0.02	0.42±0.05	1.4	0.64

strongly disordered cases that we studied ($l_0=5,10$), we find a helicity modulus exponent $v=\nu$ which is larger than the pure XY value. This larger exponent is consistent with the experimental trend for helium in gels. While this is suggestive of a new "random" universality class, we cannot rule out the possibility that our simulations are still in a crossover regime, and that for larger system sizes L, the pure XY values could be obtained.[18]

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