Monte Carlo study of the competition between long-range and short-range correlated disorder in a second-order phase transition

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The influence of coexisting correlated and noncorrelated impurities on the critical behavior of the three-dimensional Ising model is studied using Monte Carlo numerical simulations and finite-size scaling. The amount of correlated and noncorrelated vacancies is modified and controlled during the simulations. The long-range correlated (LRC) critical behavior is always found for any value of the concentration of correlated vacancies. The smaller the amount of correlated vacancies the larger the system size needed to detect the LRC universality class. This result explains why critical values measured in xerogel liquid-vapor experiments, where the concentration of correlated vacancies is marginal, seem to correspond to a short-range correlated disorder.

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Structural or chemical defects may change the response of many physical systems. For instance, inhomogeneities in waveguides modify the propagation of classical and quantum waves. Defects have been studied in connection with the propagation of electrons through quasi-one-dimensional wires [1] and optical fibers [2]. Phase transitions in thin films [3] may be also influenced by disorder. For example, a slight surface roughness changes electron transport through nanometric layers [4] and chemical disorder may induce a relaxor behavior in ferroelectriclike perovskites [5].

The effect produced by the disorder depends not just on the geometry but also on the kind of distribution used to the set up the randomness. When random disorder is introduced on a conducting chain, electron states can become localized, forcing the system to go through a metal-insulator transition known as Anderson localization [6]. However, if the chain has a correlated disorder, this localization may be minimized [7]. The competition between correlated and noncorrelated disorders has strong relevance in electronic transport through DNA [8], transmission through corrugated optic fibers, and classical or quantum phase transitions. In this Brief Report we will focus on the noncorrelated–long-correlated disorder competition in a second-order phase transition.

The influence of quenched disorder on second-order phase transitions is known since long time ago. Random (uncorrelated) disorder is relevant if the specific-heat critical exponent of the pure system (without disorder) is positive [9]. If the disorder is correlated, i.e., has a correlation function exhibiting an asymptotic power law with the distance, it is relevant if [10]

$$d\nu - 2 < 0 > \text{if} > a > d, \tag{1}$$

$$a\nu - 2 < 0 > \text{if} > a < d, \tag{2}$$

with d being the dimension of the system, ν being the correlation length critical exponent of the pure system, and a being the exponent of the power-law tail of the disorder correlation function. The new correlation length critical exponent of the long-range correlated (LRC) disordered system is given by $2/a$ [10].

These theoretical predictions for a long-range correlated disorder have been experimentally studied using helium ^{4}He superfluid transitions in porous gold [11], Vycor, aerogels, and xerogels [12–14]. The superfluid transition has a negative specific-heat critical exponent so it should be unaffected by uncorrelated disorder. The experimental results show that criticality was almost unchanged when using porous gold and Vycor, while it was clearly affected when using aerogel and xerogel [11,12]. First result is not surprising since porous gold and Vycor have exponentially decaying correlation functions beyond the typical size of the pore. The unexpected result comes from aerogel and xerogel experiments. Aerogels are fractals for several length scales up to a certain value that depends on the aerogel density [15] beyond this length, the structure becomes homogeneous, entering in an uncorrelated regime. This uncorrelated disorder should not affect to the superfluid phase transition at criticality. An explanation to this apparent contradiction was given using Monte Carlo simulations of the three-dimensional XY model confined in aerogel-like structures [16]. By simulating aerogels with a diffusion limited cluster-cluster aggregation algorithm [17,18] authors showed that different long-range correlated gelling clusters [16] with $a \sim 1.6$ and backbone gelling clusters with $a \sim 2.6$ were physically well defined within the whole aerogel structure, affecting to the XY model critical behavior.

There are no many studies where both kind of disorders (correlated and non correlated) coexist. Superfluid transitions are not a good scenario to study this competition, but liquid-vapor transitions, belonging to the Ising universality class with a positive specific-heat exponent, should be affected by both correlated and uncorrelated disorders. Liquid-vapor phase transitions in silica aerogel have been studied for helium and nitrogen [19,20]. The nitrogen critical exponent measured for the order parameter $\beta = 0.35 \pm 0.05$ is very close to $\beta = 0.35$ [21], corresponding to the short-range correlated (SRC) disorder. Also, for helium, the value found $\beta = 0.28 \pm 0.05$ seems to be close to the short-range correlated result.

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This competition has been also studied using numerical simulations for the Ising model in a diffusion limited cluster-cluster aggregation structure [22]. The value the authors find for the correlation length critical exponent $\nu \sim 0.65$ is close to the short-range uncorrelated expected value $\nu \sim 0.68$ [21].

From a theoretical point of view, Weinrib and Halperin studied a mixed disorder where the correlation function was a sum of power-law terms with different a exponents. They showed that the dominant term, defining criticality, was the most correlated one, i.e., the one with smallest values of a [10]. This result seems to be in contradiction with the data coming form the liquid-vapor phase transitions in aerogels, where short-range correlated disorder seems to disguise the LRC universality class.

In this Brief Report we present a possible hypothesis to explain this apparent contradiction based on the microscopic structure of the aerogel used on previous studies. Paredes *et al.* [22] determined that up to 97% of defects are due to islands (short-range correlated disorder) while only 3% are due to gelling clusters (long-range correlated disorder). If the total concentration of vacancies considered is $c=0.2$ (equal to the one used in numerical simulations [22]) then the concentration of long-range correlated vacancies is almost negligible ($c_{LRC}=0.006$). In aerogel experiments the total concentration of impurities is even smaller $c=0.05$, implying $c_{LRC}=0.0015$. It is clear from these numbers that in previous experiments and numerical simulations long-range correlated critical behavior could be hidden by the uncorrelated disorder.

In order to analyze this hypothesis we must consider systems where the amount of LRC vacancies is not negligible with respect to the SRC ones. We are going to study an Ising model with interaction coupling J, diluted in predefined structures where the amount of short-range and long-range correlated disorders is easily controlled.

Apart from diffusion limited cluster-cluster aggregation, used in [22], other methods have been used to generate long-range correlated disorder, namely, the thermal dilution [23], the Gaussian noise [24], and the dilution of the entire sets of lines [25,26]. The former diffusion limited cluster-cluster aggregation has already mixed short-range and long-range correlated disorders but not in a controlled fashion.

In this Brief Report we will study a long-range correlated disorder, with $a=2$, consisting on randomly oriented lines of vacancies embedded in a three-dimensional Ising system [25]. This kind of disorder has been experimentally observed by means of x-ray and neutron critical scattering experiments in systems (Ho and Tb) undergoing magnetic and structural phase transitions [27–29]. To establish a long-range–short-range disorder coexistence we also dilute the system randomly at single sites. By implementing this dilution method, the concentrations of correlated and uncorrelated vacancies in the Ising system are easily controlled and modified.

The three-dimensional Ising model with concentration c_{SRC} of randomly distributed vacancies and a concentration c_{LRC} of long-range correlated lines of vacancies is studied at different temperatures by Monte Carlo numerical simulations using periodic boundary conditions. Logarithmic derivatives of the moments of the magnetization M^n with respect to the coupling J are calculated through energy-magnetization co-

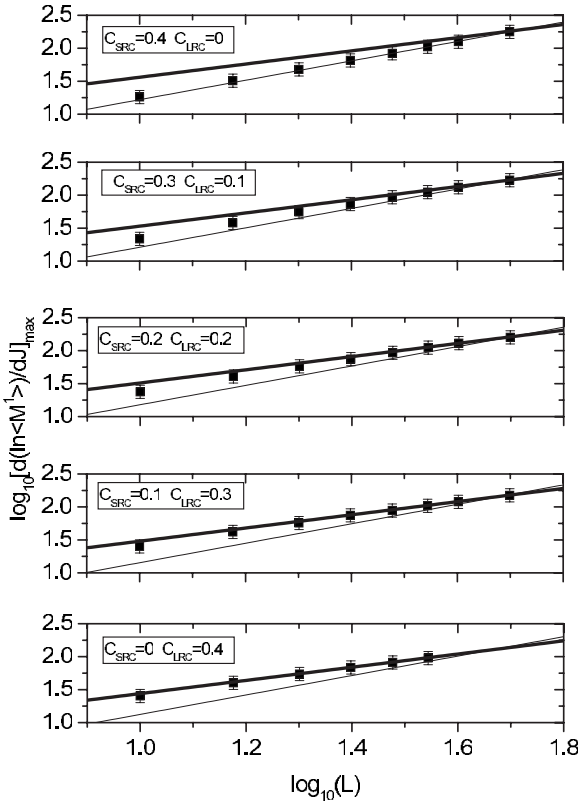

FIG. 1. Maximum of the logarithmic derivate of the first magnetization moment versus size of the system in logarithmic scale. The concentrations of SRC and LRC vacancies are ($c_{SRC}=0.4$, $c_{LRC}=0$), ($c_{SRC}=0.3$, $c_{LRC}=0.1$), ($c_{SRC}=0.2$, $c_{LRC}=0.2$), ($c_{SRC}=0.1$, $c_{LRC}=0.3$), and ($c_{SRC}=0$, $c_{LRC}=0.4$). The thin line is the expected SRC behavior [$y=(1/0.68)x+cte_S$], while the thick line is the expected LRC behavior ($y=x+cte_L$). The values cte_S and cte_L are given by the largest lateral size considered.

variance (for a detailed description see Ref. [22]). Averaging is performed over different realizations of the disorder. The correlation length critical exponent ν is calculated through finite-size scaling [30]:

$$\left[\frac{\partial \ln\langle M^n\rangle}{\partial J}\right]_{J=J_c} \sim L^{1/\nu}, \tag{3}$$

with J_c being the critical coupling.

System sizes considered range from 1000 to 125 000 spins. The first moment of the magnetization M^1 versus temperature T is determined for each lateral size L, fixing the concentration of uncorrelated c_{SRC} and correlated vacancies c_{LRC}. First we use a discrete temperature Monte Carlo calculation with $\Delta T/J=0.02$, and then, close to the maximum, we perform a continuous histogram reweighing method [31]. The calculation is repeated for 400 different realizations of the disorder.

Figure 1 shows, in logarithmic scale, the value of the maximum of logarithmic derivatives of the first magnetization moment versus the size of the system for different values of the concentration of vacancies c_{SRC} and c_{LRC}. The total amount of vacancies considered ($c_{SRC}+c_{LRC}=0.4$) is well

bellow the three-dimensional percolation value $c \sim 0.7$ [21]. Figure 1 also shows the two possible linear dependences corresponding to SRC $[y=(1/0.68)x+cte_S]$ and LRC behavior $(y=x+cte_L)$, with slope given by the finite-size scaling theory. The constants cte_S and cte_L are fixed by the value of the maxima found for the largest lateral size considered.

For $(c_{SRC}=0.4,\ c_{LRC}=0)$ the value $\nu=0.68$, corresponding to the SRC disorder, clearly fits the data for every lattice size. However, if a small amount of LRC disorder is included $(c_{SRC}=0.3,\ c_{LRC}=0.1)$ the situation changes and the expected LRC value $\nu=1$ fits our data for the largest lateral sizes considered. As the amount of LRC disorder increases $(c_{SRC}=0.2,\ c_{LRC}=0.2)$, $(c_{SRC}=0.1,\ c_{LRC}=0.3)$, and $(c_{SRC}=0,\ c_{LRC}=0.4)$ the fitting with $\nu=1$ holds for smaller sizes of the system.

Figure 1 shows how a small amount of correlated vacancies induces a LRC critical behavior. The smallest is the amount of correlated vacancies considered the largest is the correlation length needed to detect the LRC universality class. Equivalently, from the experimental point view, the smallest is the amount of correlated vacancies the closer we need to get to the critical temperature to measure LRC behavior. To analyze these results in more detail we have computed the effective correlation length critical exponent $(1/\nu_{eff})$ by considering the local (three points) slope at every data point in Fig. 1. Results are shown in Fig. 2. $(c_{SRC}=0.1,\ c_{LRC}=0.3)$ and $(c_{SRC}=0,\ c_{LRC}=0.4)$ show a LRC critical exponent, while $(c_{SRC}=0.4,\ c_{LRC}=0)$ belongs to the SRC universality class. For $(c_{SRC}=0.3,\ c_{LRC}=0.1)$ the situation is not so clear, but a logarithmic function (dotted line) with asymptotic value $1/\nu=1$ at $1/L \to 0$ fits all our data. In this particular case, where the amount of LRC disorder is small $(c_{LRC}=0.1)$, an estimated size $L=200$ is needed to obtain a value $\nu \sim 1$. The amount of LRC vacancies existing in the diffusion limited cluster-cluster algorithm $(c_{LRC}=0.006)$ or in real aerogel structures $(c_{LRC}=0.0015)$ is so small that a crossover to a LRC universality class is very difficult to detect.

To conclude, the competition between correlated and noncorrelated impurities has been studied using the Monte Carlo method in a three-dimensional Ising model where the amount of correlated and noncorrelated vacancies is controlled. Long-range correlated critical behavior if found for nonzero values of the concentration of correlated vacancies.

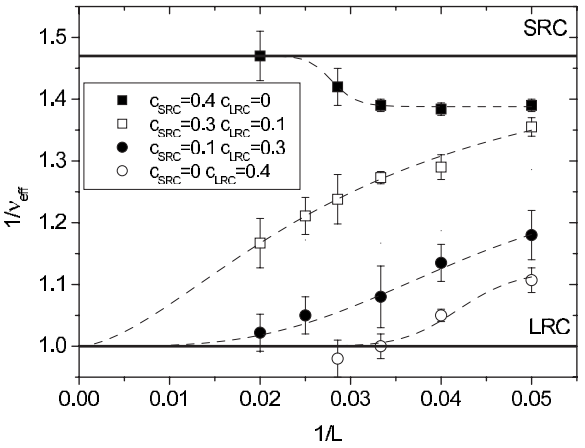

FIG. 2. Effective correlation length critical exponent $(1/\nu_{eff})$ for the different lateral sizes considered. The concentration of SRC and LRC vacancies shown are $(c_{SRC}=0.4,\ c_{LRC}=0)$, $(c_{SRC}=0.3,\ c_{LRC}=0.1)$, $(c_{SRC}=0.1,\ c_{LRC}=0.3)$, and $(c_{SRC}=0,\ c_{LRC}=0.4)$. The effective critical exponents are calculated by considering the local slope of a three points linear fit to each data point on Fig. 1. The dotted lines are logarithmic function fittings fixing $1/\nu_{eff}=1/0.68$ for $1/L \to 0$ when $(c_{SRC}=0.4,\ c_{LRC}=0)$ and $1/\nu_{eff}=1$ for $1/L \to 0$ when $(c_{SRC}=0.3,\ c_{LRC}=0.1)$, $(c_{SRC}=0.1,\ c_{LRC}=0.3)$, and $(c_{SRC}=0,\ c_{LRC}=0.4)$. The thick lines are the expected values for SRC and LRC $(a=2)$ universality classes.

If the amount of correlated vacancies considered is small the size of the system needed to detect the LRC universality class turns to be extremely large for numerical simulations. This result explains why, in contradiction with the LRC value expected from theoretical predictions, short-range correlated critical exponents are found in previous calculations based on diffusion limited cluster-cluster aggregation algorithms and in helium and nitrogen liquid-vapor experiments where the amount of LRC vacancies is negligible. Tailored experiments in disordered systems where the amount of LRC vacancies is controllable, for instance by inducing local dipole dislocations, could help us to better understand the key role played by each type of disorder.

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