Three-dimensional Ising model confined in low-porosity aerogels: a Monte Carlo study

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The influence of correlated impurities on the critical behaviour of the 3D Ising model is studied using Monte Carlo simulations. Spins are confined into the pores of simulated aerogels (diffusion limited cluster-cluster aggregation) in order to study the effect of quenched disorder on the critical behaviour of this magnetic system. Finite size scaling is used to estimate critical couplings and exponents. Long-range correlated disorder does not affect critical behavior. Asymptotic exponents differ from those of the pure 3D Ising model (3DIS), but it is impossible, with our precision, to distinguish them from the randomly diluted Ising model (RDIS).

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I. INTRODUCTION

The influence of quenched disorder on phase transitions has been studied since long time ago now. In 1974, Harris established this famous criterion: uncorrelated disorder is not relevant, for a second order phase transition, if the specific heat exponent is negative (α < 0). The criterion was generalized by Weinrib and Halperin (WH) for any disorder distribution whose correlation function exhibits a power-law tail, i.e., \( g(r) \sim r^{-a} \) as \( r \rightarrow \infty \). Disorder is shown to be relevant in these cases:

\[
\begin{align*}
\alpha - 2 &< 0 \quad \text{if} \quad a \geq d, \\
\alpha - 2 &> 0 \quad \text{if} \quad a < d,
\end{align*}
\]

being \( d \) the dimension, and \( \nu \) the correlation length exponent of the pure system. After Josephson hyperscaling \((2 - \alpha)\) Harris criterion is recovered in the short-range correlated (SRC) regime. In contrast, the long-range correlated (LRC) regime extends the criterion to systems satisfying condition, even if \( \alpha < 0 \). This generalization explains why critical exponents for the superfluid (SF) transition of \( ^4\text{He} \) change when the fluid is confined in very light aerogels, and not when confined in, for example, porous gold. Aerogels are fractal for several length scales, while porous gold has exponentially decaying correlations beyond the size of a typical pore. Nevertheless, authors argued that the critical behaviour of SF \( ^4\text{He} \) in aerogels yet poses intriguing questions to be solved.

For instance, light aerogels are fractal for several length scales, up to a certain value \( \Lambda \) that depends on aerogel density. Beyond this length, the disordered structure becomes homogeneous, entering an uncorrelated regime. After Harris criterion, as the SF correlation length \( \xi \) gets larger than \( \Lambda \), disorder should become irrelevant, because \( \alpha \approx -0.011 \) is negative for this system. Yoon et al. estimated that this crossover should appear at \( t = |T - T_c|/T_c \approx 10^{-4} \) but, although they approached \( T_c \) as close as \( t \approx 10^{-3} \), no crossover to bulk exponents was observed. A different universality class was evident for the SF transition of \( ^4\text{He} \), when confined in aerogels. An explanation to these changes was given using Monte Carlo (MC) simulations of the three-dimensional XY (3DXY) model, confined in aerogel-like structures. The SF transition belongs to the 3DXY universality class, and correlated disorder could be relevant provided that the WH condition at \( r \rightarrow \infty \) is fulfilled. Vásquez et al. showed that changes occur because of hidden LRC, inherent to the process of aerogel formation. Using simulated aerogels, made by diffusion limited cluster-cluster aggregation (DLCA), authors showed that different LRC subsets are physically well defined within the whole aerogel structure. Specifically, gelling clusters (to be defined later in this paper) are shown to be the relevant structures defining the critical behaviour of the 3DXY model in DLCA aerogels.

In this paper, we study the three-dimensional Ising model (3DIS), in presence of such aerogel-like structures. The pure 3DIS has a positive specific heat exponent (\( \alpha \approx 0.11 \)), so any type of disorder, correlated or not, will be relevant. If Ising spins are collocated in the pores of aerogels, criticality will be affected by LRC as well as by SRC disorder. Our main purpose is to elucidate which among these effects dominates the critical behaviour of the 3DIS model in this case. Along this paper, we report the results of extensive MC simulations of the 3DIS in the pores of DLCA aerogels at fixed porosity \( \varphi = 80\% \), in order to clarify this point.

The rest of this paper is organized as follows: Section II is a brief review about diluted Ising systems studied in the past. Section III is due to explain the model first, then the simulation procedure in detail, with a preamble on self-averaging, in order to validate our procedure; two methods to obtain accurate values of the critical coupling are presented at the end. Thermal and magnetic effective exponents are presented, and their asymptotic behaviours are discussed in Section IV. Finally, section V is due to present some concluding remarks.
II. ANTECEDENTS ON THE DILUTED 3DIS

Many experimental, theoretical, and computational works have been done to date, in order to study the critical behaviour of the 3DIS model in presence of quenched disorder. Most of numerical and theoretical works address the random-diluted 3DIS (RDIS), i.e., the Ising model in presence non-correlated distributions of impurities. Appart, concerning disordered LRC structures, Ballesteros and Parisi simulated the 3DIS, with dislocations represented by lines of impurities generated at random. Correlations for this type of disorder decay with an exponent $\alpha = 2$. They obtain a correlation length exponent $\nu_{\text{LRC}} \approx 1$ for the impure system, thus confirming the result of WH, that this exponent should be $2/\alpha$. Marqués et al. also simulated a diluted 3DIS, but with spins located on LRC sites. These sites were provided by a previous simulation of the pure 3DIS model; taking all sites from the cluster of dominating spin orientation at $T_c$, these are then occupied by the interacting Ising spins to simulate. Clusters for this thermally diluted Ising system have anomalous dimension $\eta_{\text{pure}} \approx 0.03$, which gives $a = 2 - \eta_{\text{pure}} \approx 1.97$. They obtain an exponent $\nu_{\text{LRC}} \approx 1$, also in agreement with the WH expression. In both cases, LRC disorder is relevant for criticality. Nevertheless, this particular result from WH has proven recently not to be correct at more accurate approximations. Using two-loop expansions, Prudnikov et al. showed that the exponent $\nu_{\text{LRC}}$ depends on both, the internal dimension of the order parameter $m$ and the exponent $a$, not the case in WH’s conjecture, independent of $m$. For both systems, Prudnikov’s prediction yields $\nu_{\text{LRC}} \approx 0.72 \neq 1$.

Experiments about the critical point of the liquid-vapour (LV) transition of $^4\text{He}$ and $\text{N}_2$, confined in 95% porous aerogels, concern directly the problem we are addressing in this paper. Bulk $^4\text{He}$ near its LV critical point belongs to the 3DIS universality class, and aerogel-like disorder has proven to contain both, LRC and SRC influences. The 3DXY model in pores of DLCA aerogels, for instance, presents new exponents due only to the presence of gelling clusters, which are LRC, while the SRC components are irrelevant to the transition. However, for the Ising model under the same kind of confinement, two different effects may be present. Simulations under strictly LRC types of disorder, give exponents consistent with the result of Weinrib and Halperin. On the other hand, experimental results about the critical point of LV transitions in aerogels, point to the relevance of the uncorrelated part of disorder.

III. THE MODEL AND SIMULATION PROCEDURE

The 3DIS in the presence of impurities, on a simple cubic lattice with nearest-neighbor interaction, is described by the Hamiltonian:

$$\beta H = -\frac{J}{k_B T} \sum_{\langle ij \rangle} \epsilon_i \epsilon_j s_i s_j,$$

where $s = \pm 1$ are the spin variables, $k_B$ is the Boltzmann constant, and $J$ is the coupling. In what follows, $k_B = 1$ and $T = 1$. The sets $\{\epsilon_i\}$ represent quenched variables chosen to be 0 if the site is an impurity and 1 if the site is occupied by a spin. These sets of impurities are taken randomly (RDIS) or from DLCA aerogels (AEIS).
A. Disorder generation and MC simulations

At the beginning, sites are occupied by a uniform random distribution of \( N \) particles, so their volume fraction is \( c = N/L^3 \). To simulate the RDIS, this initial distribution of disorder is held through the rest of the MC simulation.

Instead, for AEIS simulations to take place, aerogels are generated through the on-lattice DLCA algorithm\(^{5,10}\) with periodic boundary conditions (PBC). Monomers and clusters diffuse randomly with diffusivity constants \( D \) which depend on their mass \( n \) through \( D \sim n^{-1/d_f} \). The fractal dimension \( d_f \) has been taken equal to its value in three dimensions, \( d_f \approx 1.8 \). They stick irreversibly when they come in contact, and then the process follows up until a single cluster is obtained. This model is known to reproduce well the geometric features of real aerogels\(^{36}\).

At a given stage in this DLCA process, the first aggregate to reach opposite sides of the simulation box in any direction is called the gelling cluster (GC). It has been shown\(^{44,45}\) that the correlation function for this GC is algebraic up to a cutoff, which diverges as \( L \to \infty \). In other words, these objects are fractal (LRC). Right after the GC is built, many other smaller clusters (islands) continue to diffuse, and finally attach themselves to the GC at random sites. The resulting DLCA cluster (GC with islands) becomes homogeneous at a very small cutoff, in spite of the existence of a physically well-defined fractal structure, the GC. This cutoff increases as the concentration decreases, a feature already observed for real silica aerogels\(^{47}\). At the volume fraction employed in the present work, \( c = 0.2 \), the cutoff is so small (a few lattice constants) that DLCA clusters must be considered as non-fractals. Thus, the presence of islands, which represent the SRC subset within the whole DLCA cluster, actually hide the LRC behaviour of gelling clusters. It is in this sense that aerogel-like structures must be considered as a mixture of LRC and SRC disorder distributions.

Disordered samples are generated by the procedures described above. A MC simulation is performed for each sample of interacting 3DIS spins, placed at empty sites left by impurities. Physical observables, denoted by calligraphs \( \mathcal{O} \), are calculated at each independent MC step, and then corresponding ensemble (thermal) averages \( \langle \mathcal{O} \rangle \) are taken over the MC time-series. Wolff algorithm\(^{48,49}\) is used to update spins. In disordered systems, this algorithm tends to prevent some regions from being visited by growing Wolff clusters. If the concentration of impurities is small, this problem can be solved by adding some Metropolis updates along the simulation process\(^{49}\). We chose this method and include some Metropolis sweeps to shake all spins, after a fixed number of Wolff steps. An independent step is taken after one correlation time \( \tau \), which has been estimated from preliminary simulations. After enough steps for thermalization, a fixed number (\( N_T = 1000 \)) of independent MC steps are performed to calculate thermal averages. Equivalent simulations take place for \( N_S = 2000 \) different samples and, finally, averages over disorder are taken \( \mathcal{O} = [\langle \mathcal{O} \rangle] \) (denoted by square brackets). System sizes are \( L = 8, 12, 16, 24, 32, 48, 64, 96 \) for the RDIS, and \( L = 8, 12, 16, 24, 28, 32, 40, 48, 56, 64, 80, 96 \) for the AEIS.

B. Measured observables.

The magnetization (order parameter) is calculated by

\[
\mathcal{M} = \frac{1}{N} \sum_i \epsilon_i s_i, \tag{4}
\]

where \( N = cL^3 \) is the total number of spins. Thermal averages \( \langle \mathcal{M} \rangle \) are taken, and averages over disorder \( M(J) = [\langle \mathcal{M} \rangle] (J) \), are then calculated after the former have been extrapolated by reweighting\(^{50}\). The procedure is described below in detail. In terms of the magnetization, we define the susceptibility as:

\[
\chi = JL^3 \left[ \langle \mathcal{M}^2 \rangle - \langle \mathcal{M} \rangle^2 \right]. \tag{5}
\]

The energy is correspondingly defined by

\[
\mathcal{E} = -J \sum_{\langle ij \rangle} \epsilon_i \epsilon_j s_i s_j, \quad E = [\langle \mathcal{E} \rangle] \tag{6}
\]

and then the specific heat is obtained from fluctuations of the energy:

\[
c_h = L^{-3} \left[ \langle \mathcal{E}^2 \rangle - \langle \mathcal{E} \rangle^2 \right]. \tag{7}
\]

Logarithmic derivatives of \( n^{th} \) moments \( M^n \) of the magnetization \( (n = 1, 2, 4) \), respect to the coupling, are calculated through the energy-magnetization covariance:

\[
\left[ \frac{\partial \ln \langle M^n \rangle}{\partial J} \right] = - \left[ \frac{\langle M^n \mathcal{E} \rangle - \langle \mathcal{E} \rangle \langle M^n \rangle}{\langle M^n \rangle} \right] \tag{8}
\]

C. Simulation temperatures and reweighting.

Vásquez et al.\(^{51}\) found the phase diagram for the 3DXY model in the pores of DLCA aerogels. They obtained \( T_c(c)/T_c(0) = J_c(0)/J_c(c) \) as a function of the concentration of impurities \( c \), being \( J_c(0) \) the 3DXY critical coupling at volume fraction \( c \) of the aerogel. The shape of this phase diagram comes basically from the porous structure of disorder, specially at low concentrations. Using this information and the critical coupling \( J_c(0) = 0.2216595(26) \) for the pure 3DIS\(^{38}\), Vásquez made a rough estimate for the critical coupling for the 3DIS in the pores of DLCA aerogels at \( c = 0.2 \). Making simulations at this rough estimate, and using lattice sizes \( L = 10 - 80 \) and finite size scaling, the value \( J_c(0.2) = 0.25855(3) \) is obtained for the critical coupling.
Although for those simulations the number of disorder realizations is low ($N_S = 30$), they obtain critical exponents close enough to those reported for the RDIS.

In the present work, all simulations were done at $c = 0.2$, using simulation temperatures $\tilde{J}_c = 0.285745$ for the RDIS (following Calabrese et al.\cite{15}), and at the above estimate $\tilde{J}_c = 0.25855$ for the AEIS. Physical quantities at $J \approx \tilde{J}_c$, are obtained by the reweighting method introduced by Ferrenberg and Swendsen\cite{16}. This procedure was used for each disorder realization at each system size $L$. Each thermodynamic quantity was then averaged over disorder for each $J$ within the extrapolation interval. Finally, maxima of $[\chi(J,L)]$, $[c(J,L)]$ and $[\partial \ln \langle M^n \rangle / \partial J(J,L)]$ were obtained from averaged curves, with their corresponding pseudocritical couplings $J^*_c(L)$.

### D. Disorder sampling and self-averaging.

This part is dedicated to determine a suitable number $N_S$ of disorder realizations to obtain critical exponents for the AEIS at enough accuracy. A complete study on probability distributions for different thermodynamic quantities is performed, and results compared with the corresponding ones for the RDIS to decide $N_S$. As an example, in Fig. 1 we depict critical susceptibility points, obtained for corresponding disorder samples in the RDIS (left) and AEIS (right) cases (both at $c = 0.2$). Points come from simulations at the couplings $\tilde{J}_c$ estimated above, using the largest lattice sizes ($L = 96$). This distribution looks sharper in the AEIS case, and notably more symmetrical with respect to the average than in the RDIS case. Top of Fig. 2 shows the probability distribution for the susceptibility in both cases.

As remarked, the distribution for AEIS (filled circles) is sharper and more symmetric than that for the RDIS (data taken from Fig. 1). (Bot.) Distributions at different lattice sizes for simulations of the AEIS. The distribution width appears independent on the lattice size.

![FIG. 2: (Color online) Probability distribution of the normalized susceptibility $x = \chi_i/\langle \chi \rangle$. (Top) Distribution for the susceptibility in both cases.](image)

Self-averaging can be quantitatively checked by the normalized squared width,\cite{41} $R_A$:

$$R_A(L) = \frac{\langle A^2(L) \rangle - \langle A(L) \rangle^2}{\langle A(L) \rangle^2},$$

being $A$ any given thermodynamic quantity. In this paper, $R_A(L)$ was estimated for the RDIS to compare with previously reported values. We obtain, as $L \to \infty$, $R_M \to 0.054$ for the magnetization, and $R_X \to 0.016$ for the susceptibility, both in agreement with previous results.\cite{42} The ratio here obtained $R_M/R_X \approx 3.4$ disagrees with RG predictions: Aharony and Harris\cite{43} obtained, using $\epsilon = 4 - d$ expansions, that the leading term is $R_M/R_X = 1/4$. The discrepancy may come from higher order terms in the expansion, and not from the definition of the susceptibility as
was suggested by Berche et al.\cite{Berche}. Note also that, in
the present work, the definition for the susceptibility,
\[ \chi = J L^3 \left[ \langle M^2 \rangle - \langle M \rangle^2 \right], \]
differs from that used by Wiseman and Domany,\cite{Wiseman} \[ \chi = J L^3 \langle M^2 \rangle. \]

Results for \( R_A(L) \), plotted versus \( L^{-1} \), in the AEIS
case, are shown on Fig. 3, being the order parameter \( M \), the
magnetization \( (M) \), the susceptibility \( (\chi) \), and the specific heat
\( (c_h) \), evidence the lack of self-averaging in these quantities.
The power-law behaviour \( R_E \sim L^{-x} \), with a fi-
ting exponent \( x \approx 2.58 < d \), indicates that the energy \((E)\) is
weakly self-averaged.

FIG. 3: (Color online) Normalized squared widths \( R_A \) ver-
sus inverse system size \( L^{-1} \) for the AEIS at criticality. (Top)
Asymptotic non-zero values for \( R_A \) as \( L \to \infty \), for the mag-
etization \( (M) \), the susceptibility \( (\chi) \), and the specific heat
\( (c_h) \), respectively. As observed for \( M, \chi \) and \( c_h \) (top),
\( R_A \) tends to non-zero values as \( L \to \infty \), though asymptot-
tic limits for \( R_A \) are smaller for the AEIS than for the
RDIS, as expected (\( R_M \to 0.020 \) and \( R_\chi \to 0.0028 \), as
\( L \to \infty \)). The power-law behaviour \( R_E \sim L^{-x} \) has been
depicted for the energy (bottom), being the fitting exponent
\( x \approx 2.58 \). Thus, the energy is weakly self-averaged \( (x < d) \).
The same type of behaviour is obtained, in this work, for the energy in the RDIS case, in agree-
ment with previously reported results\cite{Wiseman}. According to
these analyses, the number \( N_S \) of disorder realizations, suitable to estimate critical exponents, is larger for the
RDIS than for the AEIS. In next section, we report some
values for effective critical exponents for both models. Our results for the RDIS agree well with previously published results,\cite{Wiseman} thus, the same number of realizations for the AEIS
will be enough to estimate critical exponents, as the values of the normalized squared widths \( R_A \) are
substantially lower than those obtained for the RDIS.

E. Critical couplings

We use two methods to estimate the critical coupling out of our present simulations. Binder magnetization fourth cumulant

\[
U_4 = 1 - \frac{\langle M \rangle^4}{3\langle M^2 \rangle^2}
\]

is universal, i.e., independent on the system size\cite{Binder} at the critical point. Thus, the critical coupling \( J_c \) can be
obtained with high accuracy at the point where \( U_4 - J \) plots coincide for all system sizes \( L \). Fig. 4 shows
these plots for the largest system sizes, for the RDIS (top) and the AEIS (bottom). In both cases, the cou-
ping used in simulations has been marked by a vertical dashed line. For the RDIS case, taking the curves for the two largest sizes \((L = 64, 96)\), we obtain an estimate (circle) \( J_{cRDIS} = 0.285747(11) \) for the critical coupling, which agrees well with that of Calabrese et al.\cite{Calabrese},
\( J_{cRDIS} = 0.285747(24) \). In the AEIS case, we depict
the same plots for lattice sizes \( L = 56 - 96 \). The intersection for \( L = 80, 96 \) (circle) gives the critical coupling
\( J_{cAEIS} = 0.258575(10) \), close to the value used in simu-
lations, \( J_{cAEIS} = 0.25855 \) (\( \Delta J_c/J_c \approx 10^{-4} \)).

On the other hand, following the FSS theory\cite{Calabrese}, deviations of pseudocritical couplings \( J_{c}^*(L) \) from the critical coupling \( J_c \) scale as:

\[
J_{c}^*(L) - J_c \sim L^{-1/\nu},
\]

where \( J_{c}^*(L) \) is defined as the positions of maxima for a
given critical quantity, being \( J_c \equiv J_{c}^*(L \to \infty) \). For in-
stance, values \( J_{c}^*(L) \) for the susceptibility \( \chi \) and loga-
rithmic derivatives \( \chi' \), obtained from reweighted curves,
have been depicted in Fig. 5 as functions of \( L^{-1/\nu} \), where
the rough value \( 1/\nu \approx 1.4 \) has been estimated through
non-linear fits of points corresponding to \( L = 56 - 96 \).
As expected, the linear behaviour\cite{Berche} is observed, and
the lines cross the \( L \to \infty \) axis at an average point
\( J_c = 0.258570(13) \), quite close to the value estimated
above, using the intersection of Binder fourth cumulants.

IV. EFFECTIVE EXPONENTS

A. Correlation length exponent

Finite size scaling (FSS)\cite{Binder} has been used to estimate
effective critical exponents for the RDIS and the AEIS. This method allows us estimate critical exponents \( \beta/\nu, \gamma/\nu, \alpha/\nu \), and the correlation length inverse exponent \( 1/\nu \). The latter has already been roughly estimated above, using the scaling law for the position of the
maxima of logarithmic derivatives of the magnetization moments $\langle M^n \rangle$ ($n = 1, 2, 4$), and the susceptibility. More accurate estimations are made directly taking averages over disorder on quantities obtained at $J_c = 0.25855$, used in our extensive simulations, which is close to the previously estimated $J_c$:

$$\frac{\partial \ln \langle M^n \rangle}{\partial J} \bigg|_{J=J_c} \sim L^{1/\nu}. \quad (12)$$

We look first to this exponent in order to determine the effect of disorder on the critical behaviour of the 3DIS. Previous works\textsuperscript{14} report that exponents $\beta/\nu$ and $\gamma/\nu$ for the RDIS are almost the same as those for the pure 3DIS, and as shown later, this is the case for the AEIS.

Logarithmic derivatives of moments $n = 1, 2, 4$ of the magnetization are plotted, versus system size $L$, in Fig. 4 for the AEIS case. Points were obtained from averages over disorder at the simulation coupling $\tilde{J}_c = 0.25855$ which is quite close to $J_c$, as estimated above. Dashed lines are power-law fits to the equation (12) using the four largest system sizes ($L = 56 – 96$), and give a FSS exponent $1/\nu = 1.501 \pm 0.007$ for the AEIS. We recall that exponents determined by this method are effective exponents, and only their asymptotic behaviour would give a hint to what the universal critical exponent tends to. This study is addressed in next paragraphs.

Effective exponents $(1/\nu)_{\text{eff}}$ have been depicted in Fig. 7 as calculated from FSS of logarithmic derivatives in both cases, RDIS and AEIS. As in Fig. 5, values were obtained from averages over disorder at the simulated couplings $\tilde{J}_c \approx J_c$, being $\tilde{J}_c = 0.285745$ for the former, and $J_c = 0.25855$ for the latter, as stated above. Each value $(1/\nu)_{\text{eff}}$ is then obtained from power-law fits to the FSS expression (12), taking four consecutive points whose maximum size is $L = L_{\text{max}}$. Results for the RDIS (empty circles) yield $(1/\nu)_{\text{eff}} = 1.478(5)$ at $L_{\text{max}} = 96$. A rough estimate of the asymptote $1/\nu$ is obtained by
extrapolating these points to the $L^{-1}_{\text{max}} \to 0$ axis, as seen in Fig. 7 (dotted line). The extrapolation yields $1/\nu \approx 1.464$, well in agreement with previously reported results for the RDIS\cite{18}. Results for the AEIS (filled squares) give $(1/\nu)^{\text{eff}} \approx 1.501(7)$ at $L_{\text{max}} = 96$. Effective exponents in this case clearly depart from values corresponding to the LRC fixed point\cite{18}, through a region close but above the SRC fixed point at $L_{\text{max}} \approx 48$. However, at larger lattice sizes, greater values suggest that another fixed point may rule the critical behaviour at the thermodynamic limit.

For the stable uncorrelated (SRC) disorder fixed point, the theory\cite{13} predicts that the exponent $1/\nu$ should be smaller than $3/2$. Additionally, the WH condition\cite{13} is well satisfied for this AEIS, where $\nu$ is the pure 3DIS exponent, and $a = 2(d - d_f)$ comes from LRC of gelling clusters (GC) within DLCA aerogels\cite{17}. In effect, the fractal dimension for the GC within aerogels at $c = 0.2$ is $d_f \approx 2.2$, as reported elsewhere\cite{17}. This condition, together with theoretical predictions reported by Prudnikov et al.\cite{18}, would give $1/\nu \approx 1.4$ for the 3DIS with LRC defects, at the corresponding $a \approx 1.6$. From Fig. 7 it is clear that $(1/\nu)^{\text{eff}}$ is far above this value. Thus, it is not the LRC subset of disorder (the GC) which rules the critical behaviour of the AEIS, in the way it certainly does for 3DXY universality class in aerogels\cite{17}.

The exponent $(1/\nu)^{\text{eff}}$ at $L_{\text{max}} = 96$ was also obtained taking averages of logarithmic derivatives from average reweighted curves, at the critical coupling estimated above (Section III E), $J_c = 0.258570$. For $L = 56 - 96$ we obtain $(1/\nu)^{\text{eff}} \approx 1.497$ (triangle, Fig. 7). In addition, less extensive additional realizations of the AEIS also for $L = 56 - 96$ (600 for each size), were made at this more accurate value $J_c = 0.258570$, and averages over disorder were taken directly from simulations. The power-law fit for these points gives an estimate $(1/\nu)^{\text{eff}} \approx 1.493$ (diamond). Although these effective exponents are lower than $3/2$, there exists yet not enough evidence in this work that the RDIS fixed point would be reached at $L_{\text{max}} \to \infty$.

### B. Specific heat and energy exponents

To check our results about the correlation length exponent for the AEIS, we study the FSS of the specific heat and the energy, at the simulation coupling $J_c$. [Diagram]

![Diagram showing specific heat and energy exponents](image)

**FIG. 8.** (Top) Specific heat $c_h$ versus $L$ for the AEIS in a linear-log scale. A logarithmic singularity ($\alpha = 0$) for the specific heat at $J_c$ follows from the fit (dashed line). This result reinforces the estimated $1/\nu \approx 1.5$ (Fig. 7). (Bottom) Energy plotted against $L^{(\alpha - 1)/\nu}$, taking $\alpha = 0$ and $1/\nu = 3/2$, and the corresponding linear fit is shown (dashed line).

Top of Fig. 8 shows the specific heat $c_h$ plotted versus $L$ using a linear-log scale. The dashed line is a logarith-
mic fit using the four largest lattice sizes, 56 – 96. This results indicates that the singularity of the specific heat could be logarithmic, consistent with our result $1/\nu \approx 1.5$ for $L_{\text{max}} = 96$. After Josephson hyperscaling relation $(\alpha = 2 - dv)$ a specific heat exponent $\alpha \approx 0$ would be expected. Bottom of Fig.9 shows the linear dependence of the energy $E$ on $L^{(\alpha-1)/\nu}$, taking $\nu = 2/3$ and $\alpha = 0$, which confirms the results stated above. We made additional analyses to specific heat data, and the energy as well, using the scaling of both quantities in these experiments on the critical point of the LV transition of $T_\text{LV}$. Non-linear fits to these expressions, using the six largest lattice sizes, 40 – 96, give self-consistent results $\alpha/\nu \approx -0.022$ and $(\alpha - 1)/\nu \approx -1.512$, in agreement with our correlation length exponent $1/\nu \approx 1.49$. This result agrees with the tendency shown by the effective values in Fig.4. Experiments on the critical point of the LV transition of $^4\text{He}$ in aerogels, report a cusplike peak in the specific heat, but authors do not report an estimate for the exponent $\alpha$. Our results point for the largest lattice sizes to a logarithmic singularity, which may also be consistent with these experimental results.

FIG. 9: Order parameter (left) and susceptibility (right), at the simulated critical point, versus $L$ for the AEIS. The magnetization $M$ (circles) scales as $L^{-\beta/\nu}$, and the averaged Wolff cluster size $\langle n_w \rangle$ (squares) scale with $L^{-2\gamma/\nu}$. The FSS power-law fit for the susceptibility gives $\gamma/\nu = 2.044(4)$. All power-law fits have been made for $L = 56 – 96$.

C. Magnetic exponents

According to the FSS theory, the magnetization and the susceptibility scale as $M \sim L^{-\beta/\nu}$ and $\chi \sim L^{\gamma/\nu}$, respectively. In Fig.9 we plot the order parameter $M$ (left) and the susceptibility (right) as a function of $L$ for the AEIS. Magnetization data (circles) have been fit to the preceding power-law FSS expression (continuous line), giving $\beta/\nu = 0.523(3)$. Average sizes of Wolff clusters divided by $L^3$, $\langle n_w \rangle$ (squares), scale with the same exponent as the squared magnetization. This is confirmed by the power-law fit (dashed line) which yields $2\beta/\nu = 1.019(6)$. These results give an average estimate of $\beta/\nu = 1.032(6)$. Together with $1/\nu \approx 1.5$ this gives $\beta = 0.34(4)$, close to the pure 3DIS exponent and to the RDIS exponent. On the right side of Fig.9 points for the susceptibility obtained from simulations near the critical point fit to the FSS power-law expression with the exponent $\gamma/\nu = 2.044(4)$. All fits have been made for $L = 56 – 96$.

![Graphs showing order parameter and susceptibility](image)

FIG. 10: (Color online) (a) Effective exponents for the susceptibility give $(\gamma/\nu)_{\text{eff}} = 2 - \eta_{\text{eff}} > 2$. Extrapolation using $L_{\text{max}} \geq 48$ suggests that $\gamma/\nu < 2$ in the thermodynamic limit. (b) Effective exponents $(\beta/\nu)_{\text{eff}}$ for the magnetic magnetization (circles) and for the average mass of Wolff clusters (squares). At $L_{\text{max}} = 96$ both approach the pure 3DIS theoretical estimate of $(\beta/\nu)_{\text{eff}} \approx 0.517$. (c) The hyperscaling relation $\gamma/\nu + 2\beta/\nu = d = 3$, not satisfied for effective exponents, tends to hold for larger lattice sizes.

Results for magnetic effective FSS exponents, obtained by fitting four consecutive points from Fig.9 ending at $L_{\text{max}}$, have been depicted in Fig.10. Fig.10(a), shows the effective exponent for the susceptibility, $(\gamma/\nu)_{\text{eff}}$, plotted versus $L_{\text{max}}^{-1}$. This exponent tends to increase for $L_{\text{max}} < 48$, but beyond this size the tendency is to stabilize at a value close to that of percolation, $(\gamma/\nu)_{\text{eff}} = 2 - \eta \approx 2.05$. For larger $L_{\text{max}}$, it turns to approach a value lower than 2.00 (positive $\eta$). The asymptotic ex-
trapolated value seems to be the pure 3DIS exponent \( \gamma/\nu = 1.966(3) \), or the RDIS exponent \( \gamma/\nu = 1.963(5) \). Berche and collaborators\(^{22}\) estimated effective values \( \gamma/\nu > 2 \) for smaller concentrations in the RDIS case. Using the result for \( L_{\text{max}} = 96 \), \( \gamma/\nu = 2.044(4) \), and our estimate \( \nu = 2/3 \), the exponent \( \gamma \) found in the present work is 1.363(9), slightly above the value \( \gamma = 1.344(9) \) found in our MC simulations for the RDIS, and \( \gamma = 1.342 \) obtained by Calabrese et al.\(^{33}\) for the same system. The tendency for larger \( L \) is to be closer to RDIS results.

We must remind at this point, that theoretical most accurate results, by Prudnikov et al.\(^{34}\), predict a magnetic exponent \( \eta < 0 \) for the 3DIS in LRC disordered structures with an algebraic decay similar to that of the gelling clusters within DLCA aerogels at \( c = 0.2 \).

On Fig. 10(b) and (c), squares represent effective exponents \( (\beta/\nu)_{\text{eff}} \) obtained from \( \left\{ n_m \right\} \), and circles, those obtained directly from \( M \). There is a strong variation of these results with \( L_{\text{max}} \). As stated above, the exponent obtained averaging both results with \( L_{\text{max}} = 96 \) is \( \beta/\nu = 0.516(6) \), close to that of the pure 3DIS \( \beta/\nu = 0.517(3) \). In addition, our results agree well with those reported for the RDIS case by Ballesteros et al.\(^{36}\), \( \beta/\nu = 0.519(3) \). In this work, we obtain \( \beta/\nu = 0.516(5) \) for the RDIS. The last effective value \( (\beta/\nu)_{\text{eff}} \) (\( L_{\text{max}} = 96 \)), together with \( 1/\nu \approx 1.5 \) gives an exponent \( \beta = 0.343(9) \) for the order parameter. This result agrees well with experiments about the critical point of the LV transition of \( N_2 \) in 95% porous aerogels \( c = 0.05 \), reported by Wong et al.\(^{37}\), which yield \( \beta = 0.35(5) \).

Care must be taken with this agreement because, our results were obtained using DLCA at concentrations \( c = 0.2 \), and these structures are quite different from those at \( c = 0.05 \). For the latter, most of impurities belong to the LRC gelling clusters, giving the DLCA aerogels a less random overall structure.

As stated above, a possible explanation for these magnetic exponents is the influence of the LRC disorder fixed point. The fractal dimension of the aerogel gelling cluster is \( d_f \approx 2.2 \), giving an exponent \( a \approx 1.6 \) associated to this structure. Following Table IV from Prudnikov et al.\(^{37}\), a value \( \gamma/\nu > 2.0205 \) \( (\eta < -0.0205) \) is expected. The effective value found in this work is close to this prediction, but it follows from Fig. 10(b) that a tendency exists to approach a value closer to the corresponding RDIS fixed point. Finally, using effective values the hyperscaling relation \( \gamma/\nu + 2\beta/\nu = 3 \) seems not to hold, as seen in Fig. 10(c). The violation of this hyperscaling relation suggest that our results do not yet reach asymptotic values. Extensive simulations rest still to be performed at the more accurate value \( J_c = 0.2588570 \).

V. CONCLUDING REMARKS

Extensive Monte Carlo simulations of the 3D Ising model (3DIS) with impurities have been reported in this paper. Using finite size scaling, critical couplings and exponents have been estimated for the 3DIS, in presence of randomly distributed impurities (RDIS), and confined in aerogel-like structures (AEIS). For the latter we have collocated Ising spins in the pores of simulated DLCA aerogels at \( c = 0.2 \). At this concentration, these objects are known to be non-fractal. However, the presence of hidden LRC could affect criticality, as predicted by the theory.\(^{38}\) It has been concluded elsewhere that these LRC structures, the gelling clusters, modify the critical behaviour of the 3DXY model, when confined in the same kind of aerogel-like structures. In the 3DIS case, however, our results for thermal exponents \( 1/\nu \lesssim 1.5 \) and \( \alpha/\nu \lesssim 0 \) rest far above those for the LRC fixed point predicted by the theory.\(^{38}\) Complementary simulations at a more accurate value of the critical coupling, \( J_c = 0.2588570(13) \), give an exponent \( 1/\nu \approx 1.49 \). Although similar thermal exponents have been reported by Pakhnin and Sokolov\(^{38}\) for the RDIS universality class, the asymptotic critical regime could have not been reached in our simulations, and more extensive simulations are yet to be performed at this more accurate \( J_c \) value.

Effective critical exponents observed here for the AEIS change from a fixed point (LRC) at box sizes \( L \leq 48 \), to another (SRC) at box sizes \( L > 48 \) (Figs. 7 and 10), probably indicating an oscillating approach to the stable fixed point. Theoretical predictions based on the Weinrib and Halperin model\(^{38}\), able to explain changes on the critical behaviour of the 3DXY model in the pores of DLCA aerogels, may also explain the influence of this type of disorder on the 3DIS. In this case, two competing effects are present: the random SRC subset of the disorder (defined in Section III A), which already affects the critical behaviour of the 3DIS, and the LRC subset which, after the extended criterion \(^{2}\), may be relevant as well. This is certainly not the case for the 3DXY model, where Harris criterion prevents the SRC subset of impurities (islands) to be relevant: only the weak LRC distribution of impurities (GC) is relevant\(^{38}\) for the 3DXY. For the 3DIS, theory predicts that both, LRC and SRC subsets may be relevant. Which one finally dominates the critical behaviour?

Results presented in this paper suggest that, in the AEIS case, the critical behaviour is ruled by the SRC fixed point. A plausible explanation to these dominating SRC effect is provided by theoretical works\(^{38}\) for the 3DIS, RG flows converge to a more stable SRC fixed point, because at \( m = 1 \) the LRC fixed point is less stable (marginal). However, it has been mentioned before, without a proof\(^{38}\), that amplitudes of disorder may in some cases affect criticality. Added in proof, we have to mention that in preliminary simulations of the 3DIS in presence of mixed kinds (LRC and SRC) of disorder\(^{49}\), evidence of a continuous flow from the LRC fixed point to the SRC one has been observed, when relative strengths are tuned from a pure LRC distribution of defects to a 1 : 1 proportion. In the AEIS case, we have analyzed relative amplitudes (strengths) of the LRC and the SRC subsets of disorder, for \( L = 128 \), to determine that up to
97% of defects are due to islands (SRC), while only 3% are due to the GC (LRC).

To conclude, it has to be stated that the influence of aerogel-like distributions of impurities on the critical behaviour of the 3DIS is yet far from being completely understood. The problem is similar to that of phase transitions in Ising systems with non-integer dimension or in fractal structures. It becomes clear that the fractal dimension, related to the exponent $a$ of subjacent long-range correlations, may not be the only parameter to determine the universality class of the impure system.

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