

Equilibrium and out-of-equilibrium critical dynamics of the three-dimensional Heisenberg model with random cubic anisotropy

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We study the critical dynamics of the three-dimensional Heisenberg model with random cubic anisotropy in the out-of-equilibrium and equilibrium regimes. Analytical approaches based on field theory predict that the universality class of this model is that of the three-dimensional site-diluted Ising model. We have been able to estimate the dynamic critical exponent by working in the equilibrium regime and by computing the integrated autocorrelation times obtaining $z = 2.50(5)$ (without taking into account scaling corrections) and $z = 2.29(11)$ (by fixing the scaling corrections to that predicted by field theory). In the out-of-equilibrium regime we have focused on the study of the dynamic correlation length, allowing us to compute the dynamic critical exponent obtaining $z = 2.38(2)$, which is compatible with the equilibrium ones. Finally, both estimates are also compatible with the most accurate prediction $z = 2.35(2)$, from numerical simulations of the 3D site-diluted Ising model, in agreement with the predictions based on field theory.

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I. INTRODUCTION

Understanding the influence of disorder on materials is of paramount importance in both fundamental science and technology.

The effect of one of the most important kinds of disorders, the so-called quenched disorder, where the elements of disorder have characteristic times significantly longer than the typical characteristic times of the material's original components, can be studied using analytical computations [1–3], numerical simulations [4], and experiments [5,6].

Furthermore, when focusing on magnetic materials, they can be described, depending of their anisotropy, by Heisenberg, XY or even Ising models. On these models, the quenched disorder can be introduced in different ways, for example, introducing dilution (by means of non magnetic impurities) in the magnetic material or by inducing uniaxial anisotropies in the model [7].

In this paper we will focus on the dynamic critical behavior of the 3D Heisenberg model in presence of (quenched) random cubic anisotropies (the disorder is localized along the six directions of the cubic lattice) [2,8].

These studies are of special relevance in the understanding of the physical properties of structurally disordered magnetic materials. Regarding the technological applications of these materials, we can describe the possible use of rare-earth elements as refrigerants due to the presence of magnetocaloric effects [9–11].

From the analytical studies of these models, it is noteworthy that the perturbative renormalization group (RG) predictions on the critical behavior of these systems depend strongly on the characteristics of the disorder.

For the random cubic anisotropy disorder (RAM), RG shows that the system behaves at criticality like the 3D site-diluted Ising model (RSIM) [12,13] with the scaling dimension (length) of the leading irrelevant scaling field is given by $\omega_{\text{RAM}} = -\alpha_{\text{RSIM}}/\nu_{\text{RSIM}}$, being ν_{RSIM} and α_{RSIM} the thermal and specific heat critical exponent of the RSIM [12].

Surprisingly, when the disorder is isotropic, the RG finds no fixed points: hence, a first order should appear, or there may be no phase transition at all (see, for example, the discussion of Ref. [3]).

In Ref. [4] the (static) equilibrium critical phenomena of both isotropic and cubic quenched disorders was characterized by means of numerical simulations. For the cubic anisotropy disorder, a second-order phase transition in the ferromagnetic channel raised, but with critical exponents (η and ν) not near those of the RSIM but without the numerical characterization of the scaling corrections. Furthermore, in the isotropic disorder, a spin glass phase transition was found. However, the characterization of the dynamics of these models with both types of disorder is still lacking.

Given the distinct physics of cubic and isotropic disorders, we focus in this paper on the characterization of the dynamics at equilibrium and out-of-equilibrium for the cubic anisotropy disorder.

To study the equilibrium critical dynamics, the system is brought to equilibrium, and subsequently, the integrated autocorrelation time is calculated. The scaling of the integrated autocorrelation times with the lattice size (see below) allow us to compute the dynamic critical exponent.

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The constraint to be in equilibrium restricts us to simulate relatively small lattice sizes.

In the out-of-equilibrium simulations, we simulate large lattice sizes and random initial spin configurations. We then track the evolution of the spin-spin correlation function over the time. Our results consistently exhibit scaling behavior (see below), enabling us to characterize the dynamics in this regime. To remain in the out-of-equilibrium regime for large times it is compulsory to simulate large lattice sizes.

Both approaches, equilibrium and out-of-equilibrium, should provide the same dynamic critical exponent which characterizes the critical dynamics. We followed this dual approach in the computation of the dynamic critical exponent of the pure (nondisordered) 3D Heisenberg model [14].

The analytical approach to the local relaxational dynamic implemented in the numerical simulations performed in this paper is the so-called model-A dynamics [15]. The model-A dynamics of the Heisenberg model with cubic anisotropy was study in Ref. [13] using field-theoretical techniques. The outcome of this analysis is that the dynamic critical exponent is the same as in the RSIM.

The dynamic critical exponent of the RSIM was computed analytically, for example, in Refs. [16,17] and numerically in Refs. [18,19]. For future use, we report the most accurate value: $z = 2.35(2)$ [19].

The main aim of this paper is to compute the dynamic critical exponent, in equilibrium and out-of-equilibrium, to check the theoretical prediction. Therefore, this investigation will provide with the last critical exponent to fully characterize the universality class of the 3D Heisenberg model with random cubic anisotropy, where the static exponents ν and η were already computed in numerical simulations [4].

The structure of the paper is the following. In Sec. II we describe the model and the observables used in the equilibrium and out-of-equilibrium studies. Next, in Sec. III, we report details on our estimate of the dynamic critical exponent, first in equilibrium, using the integrated autocorrelation times, and then out-of-equilibrium by computing and analyzing the dynamic correlation length. In the last section we will discuss the results and report our conclusions. Finally, in an Appendix, we describe some technical details on the procedure we employed to calculate some observables in the out-of-equilibrium dynamics.

II. MODEL AND OBSERVABLES

The Hamiltonian of the three-dimensional Heisenberg model with random cubic anisotropy is

$$\mathcal{H} = -J \sum_{\langle \mathbf{x}, \mathbf{y} \rangle} \mathbf{s}_{\mathbf{x}} \cdot \mathbf{s}_{\mathbf{y}} - D \sum_{\mathbf{x}} (\hat{\mathbf{n}}_{\mathbf{x}} \cdot \mathbf{s}_{\mathbf{x}})^2. \quad (1)$$

Here, $\mathbf{s}_{\mathbf{x}}$ is a classical three-dimensional unit vector on the site $\mathbf{x}$ of a three-dimensional cubic lattice of size L and volume $V = L^3$ with periodic boundary conditions, $D > 0$ is the strength of the anisotropy, $\hat{\mathbf{n}}_{\mathbf{x}}$ is a (quenched) random unit vector pointing in the direction of the local anisotropy axis. The interaction $J > 0$ is assumed to be ferromagnetic, without loss of generality we will fix $J = 1$ hereafter. Finally, the sum $\langle \mathbf{x}, \mathbf{y} \rangle$ is over the six nearest neighbors sites $\mathbf{y}$ of the site $\mathbf{x}$. The strength of the disorder is controlled by the ratio D/J .

TABLE I. $D = 3$. Integrated correlation time of $\mathcal{M}^2$, $\tau_{\text{int}, \mathcal{M}^2}$ for $c = 10$, as a function of the lattice size, L , for the two simulated algorithms. We have also reported the number of simulated samples, n_s . We also report the length of the run at equilibrium, n_{sw} , in units of $\tau_{\text{int}, \mathcal{M}^2}$.

L	Algorithm A			Algorithm B		
	$\tau_{\text{int}, \mathcal{M}^2}$	$n_{\text{sw}}/\tau_{\text{int}, \mathcal{M}^2}$	n_s	$\tau_{\text{int}, \mathcal{M}^2}$	$n_{\text{sw}}/\tau_{\text{int}, \mathcal{M}^2}$	n_s
8	147(1)	34 013	500	44.7(2)	111 856	500
12	368(3)	13 586	500	105.3(5)	47 483	500
16	670 (6)	7462	500	197(1)	85 380	500
24	1723(17)	5803	400	490(4)	20 408	400
32	3340(41)	11 976	800	924(10)	21 640	400
48				2310(35)	12 987	400

In the cubic anisotropy disorder the vectors $\hat{\mathbf{n}}_r$ point along the six semi-axes of the cubic lattice with the same probability $1/6$:

$$p(\hat{\mathbf{n}}) = \frac{1}{6} \sum_{i=1}^3 (\delta(\hat{\mathbf{n}} - \hat{\mathbf{k}}_i) + \delta(\hat{\mathbf{n}} + \hat{\mathbf{k}}_i)), \quad (2)$$

where the $\hat{\mathbf{k}}_i$ ($i = 1, 2, 3$) are the three unit vectors pointing to the three principal directions of a cubic lattice and $\delta(\hat{\mathbf{x}}) \equiv \delta_{\hat{\mathbf{x}}, 0}$ is the Kronecker δ .

A. Equilibrium

The dynamic critical exponent, within the equilibrium regime, is computed by analyzing the integrated autocorrelation time in relation to the lattice size.

For a given observable, we compute $\mathcal{O}(t)$, the autocorrelation function [20–22] defined as

$$C_{\mathcal{O}}(t) \equiv \langle \mathcal{O}(s) \mathcal{O}(t+s) \rangle - \langle \mathcal{O}(t) \rangle^2, \quad (3)$$

and its normalized version

$$\rho_{\mathcal{O}}(t) \equiv \frac{\overline{C_{\mathcal{O}}(t)}}{\overline{C_{\mathcal{O}}(0)}}, \quad (4)$$

where $\langle (\dots) \rangle$ is the thermal average and $\overline{(\dots)}$ is the average over the disorder.

To overcome the associated bias of a finite number of measurements in a given sample (notice that we have simulated a large number of MC sweeps and the associated measurements, see Tables I and II), we have implemented the procedure described in Ref. [19].

The integrated autocorrelation time is defined as

$$\tau_{\text{int}, \mathcal{O}} = \frac{1}{2} + \sum_{t=0}^{\infty} \rho_{\mathcal{O}}(t). \quad (5)$$

In a data collection with N measurements, the number of statistically independent measurements of the observable $\mathcal{O}$ is just $N/(2\tau_{\text{int}, \mathcal{O}})$ [20–22]. If the number of measurements is limited, at large time intervals t , the noise will become more prominent than the signal in $\rho_{\mathcal{O}}(t)$. To address this issue, we employ the following self-consistent approach to calculate the

TABLE II. $D = 4$. Integrated correlation time of M^2 , τ_{int,M^2} for $c = 10$, as a function of the lattice size, L , for the two simulated algorithms. We have also reported the number of simulated samples, n_s . We also report the length of the run at equilibrium, n_{sw} , in units of τ_{int,M^2} .

L	Algorithm A			Algorithm B		
	τ_{int,M^2}	$n_{\text{sw}}/\tau_{\text{int},M^2}$	n_s	τ_{int,M^2}	$n_{\text{sw}}/\tau_{\text{int},M^2}$	n_s
8	311 (2)	16 077	500	59.1(4)	84 602	500
12	836(8)	5980	500	148(2)	33 783	500
16	1685(24)	2967	500	288(3)	17 361	500
24	4547(70)	2199	500	765(12)	13 072	400
32	9523(130)	4200	864	1579(21)	25 332	692

integrated time

$$\tau_{\text{int},\mathcal{O}} = \frac{1}{2} + \sum_{t=0}^{c\tau_{\text{int},\mathcal{O}}} \rho_{\mathcal{O}}(t), \quad (6)$$

where c is usually taken to be 6 or bigger [20–22]. In this work we have used $c = 10$.

At the critical point, the integrated autocorrelation time of a long-distance observable exhibits divergence as the system size increases [19]

$$\tau_{\text{int},\mathcal{O}} \sim L^z (1 + O(L^{-\omega})). \quad (7)$$

Here, z represents the dynamic critical exponent and ω denotes the leading correction-to-scaling exponent, which corresponds to the leading irrelevant eigenvalue of the theory.

In this paper, we will focus on the slowest mode offered by the nonlocal operator $\mathcal{O} = M^2$, where the magnetization M is defined as

$$M = \sum_x s_x, \quad (8)$$

and we will extract the z exponent by studying its integrated autocorrelation time.

B. Out-of-equilibrium

In the out-of-equilibrium regime, one of the primary observables of interest is the spin-spin correlation function, defined as

$$C(r, t) = \frac{1}{V} \sum_x \overline{\langle s_x s_{r+x} \rangle_t}, \quad (9)$$

where $\langle \dots \rangle_t$ stands for the average over different thermal histories and, as in equilibrium, the horizontal bar denotes the average over the disorder.

This correlation function satisfies, at criticality, the following scaling law [15]

$$C(r, t) = \frac{1}{r^d} f\left(\frac{r}{\xi(t)}\right), \quad (10)$$

which defines the dynamic correlation length, denoted as $\xi(t)$. As we approach the equilibrium regime, $\xi(t)$ converges to its equilibrium value.

In three dimensions, at the critical point and in equilibrium, one should expect

$$C(r, t) \sim \frac{1}{r^{d-2+\eta}} = \frac{1}{r^{1+\eta}}, \quad (11)$$

η being the anomalous dimension of the field.

The correlation length $\xi(t)$ can be estimated by calculating [23,24]

$$I_k(t) = \int_0^{L/2} dr r^k C(r, t), \quad (12)$$

by means of

$$\xi_{k,k+1}(t) \equiv \frac{I_{k+1}(t)}{I_k(t)}. \quad (13)$$

In this work, our focus lies on $\xi_{2,3}$. In spin glasses, $\xi_{1,2}$ was measured using a correlation function that decays as $1/r^{0.5}$ [23,24]. However, in our case, to reduce the influence of shorter distances, we have computed higher values of I_k . We refer the reader to Refs. [14,23–26] for a detailed description of the procedure we employed to calculate the integrals and estimate the statistical error associated with $\xi_{k,k+1}(t)$ (see the Appendix for a detailed description).

Finally, the relationship between the dynamic correlation length and time is as follows:

$$\xi_{k,k+1}(t) \sim t^{1/z} (1 + A_k t^{-\omega/z}). \quad (14)$$

III. NUMERICAL RESULTS

In this section we first report the computation of the integrated correlation time at equilibrium. After this analysis, we describe our results in the out-of-equilibrium regime.

The Metropolis algorithm was used to simulate the model's behavior in both equilibrium and nonequilibrium simulations. In addition, we have performed all the numerical simulations using the inverse critical temperatures provided by Ref. [4]: $\beta_c = 0.7083$ for $D = 4$ and $\beta_c = 0.6994$ for $D = 3$. The starting initial configuration for the out-of-equilibrium runs was a random configuration of spins.

To perform the equilibrium numerical simulations we have used two different algorithms. In the first algorithm (denoted Algorithm A) the Metropolis algorithm is implemented by modifying the original spin by adding a random vector (chosen with uniform probability on the surface of the sphere of radius δ) and normalizing the final vector to the unit sphere, the magnitude of the random vector δ is adjusted in such a way that we maintain an acceptance between 40% and 60% (see, for example, Ref. [22]).

We have also used a second algorithm (termed as algorithm B) in which the Metropolis algorithm is carried out by proposing a random spin in the unit sphere (chosen with uniform probability). Both versions of the Metropolis algorithm are supposed to belong to the same dynamic universality class [21].

The equilibrium simulations were executed on CPUs using algorithms A and B. The out-of-equilibrium simulations were run in CPUs and GPUs using algorithm A. Details on the implementation of the code in GPUs can be found in Ref. [14].

TABLE III. Values of z for the different fits assuming no correction-to-scaling terms. For all the fits reported in this paper, we have computed the minimum value of L (denoted as $L_{\min}$), so that, the p value of the least-squares fit is greater than 5%.

D	Algorithm	$L_{\min}$	z
3	A	8	2.247(8)
3	B	12	2.22(1)
4	A	8	2.46(1)
4	B	16	2.45(2)

A. Equilibrium

We have analyzed the integrated correlation times using the methodology described in the previous section. Notice, that before performing the measures we need to bring the different systems to the equilibrium. We have used in this section both versions of the Metropolis algorithm (algorithms A and B).

In Tables I and II we report the values of the integrated autocorrelation times computed for the different lattice sizes at the critical point for the two values of the disorder, $D = 3$ and 4, and for algorithms A and B. In addition we show the number of simulated samples (disorder realizations) and the number of sweeps (in units of the integrated autocorrelation time) performed at equilibrium in a given sample.

Notice that, for the same lattice size, the integrated autocorrelation times are bigger for algorithm A than for algorithm B. Moreover, the integrated autocorrelation times are bigger for $D = 4$ than for $D = 3$, reflecting that the strength of the disorder induces a slower dynamic.

To compute the statistical error of the integrated correlation time we have used the jackknife method over the samples [26].

We have analyzed the numerical data reported in Tables I and II neglecting the scaling corrections (e.g., using $\tau \propto L^z$). The results for the dynamic critical exponent are reported in Table III for the four simulated cases. Note that these z estimates are near the RSIM dynamic exponent $z = 2.35(2)$, but a bit smaller for $D = 3$ and a bit larger for $D = 4$. This results also support that both algorithms belong to the same dynamic universality class.

Moreover, assuming universality, the four cases should present the same critical behavior and to show this fact, it is compulsory to take into account the corrections to scaling (the same z exponent with the same scaling corrections) [19,27–33].

To check this scenario, we have tried a joint fit of the four cases using the same z exponent and the same field-theory result for the leading irrelevant scaling field $\omega_{\text{RAM}} = -\alpha_{\text{RSIM}}/\nu_{\text{RSIM}} = 3 - 2/\nu_{\text{RSIM}} = 0.072(6)$ [12] where we have used $\nu_{\text{RSIM}} = 0.683(2)$ [28]: this is a very small value for the ω exponent, so we are confronting strong scaling corrections.

From this fit, see Fig. 1, we obtained $z = 2.29(11)$ with $\chi^2/N_{\text{DOF}} = 18/10$ and a associated p -value=0.055.¹ To have

¹The goodness of the fit is reported via χ^2/N_{DOF} , N_{DOF} stands for the number of degrees of freedom of the fit, and the associated p -value is also denoted as Q [26].

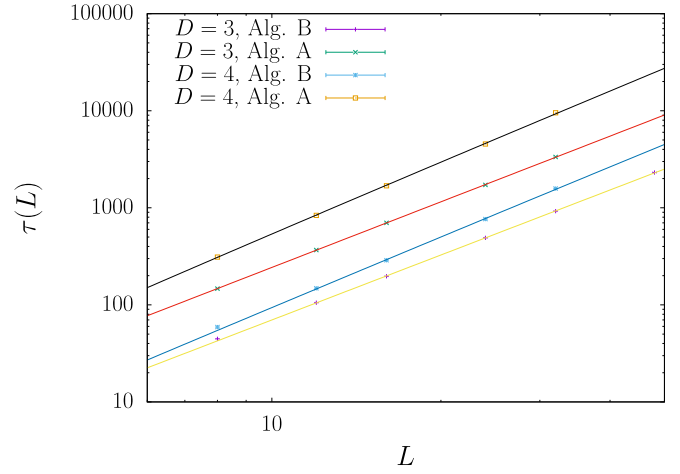


FIG. 1. Behavior of the integrated correlation time τ_{int,M^2} , as a function of the lattice size, L , for the two simulated algorithms (A and B) and for $D = 3$ and $D = 4$. We have also shown our best joint fit taking into account corrections to the scaling (see the text).

an acceptable p value we have used the $L \geq 8$ data for the Algorithm A and the $L \geq 12$ data for the algorithm B.

Taking into account the uncertainty in the value of ω provides an additional uncertainty of 5×10^{-3} in the value of z , which is negligible in confronting with the computed error (0.11). Hence, our final estimate is: $z = 2.29(11)$.

B. Out-of-equilibrium: Correlation length

In this section we compute the dynamic critical exponent using the correlation function computed in an out-of-equilibrium simulation.

First, we have studied the finite size effects of the out-of-equilibrium numerical simulations. To do that, we have computed the dynamic critical correlation length, ξ_{23} , using $L = 128$ and $L = 250$ sizes. In Fig. 2 we show the difference between the correlation length (ξ_{23}) computed simulating both lattice sizes, and we can assess that (in the statistical errors) both estimates of ξ_{23} are compatibles as far as the Monte Carlo time is less than 10^4 Monte Carlo sweeps. Hence, our out-of-equilibrium analysis will be based on the $L = 128$ lattice

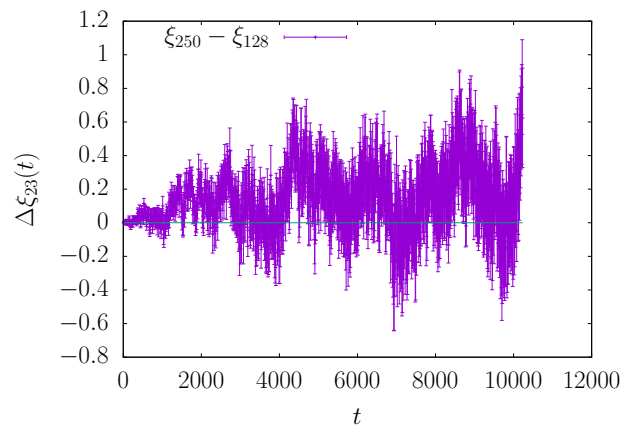


FIG. 2. Behavior of $\xi_{23}(t, L = 250) - \xi_{23}(t, L = 128)$ versus time for t and for $D = 3$. The horizontal green line marks the zero.

TABLE IV. Dynamic critical exponent from the scaling of the dynamic correlation length for $D = 3$ and $D = 4$ using $\xi_{23}(t)$.

D	L	z	n_s
3	128	2.35(3)	4000
4	128	2.44(4)	1600

for which we have simulated a larger number of samples. We report in Table IV the number of samples we have simulated in the $L = 128$ lattice for the two values of the cubic anisotropy.²

Figure 3 shows the behavior of the dynamic correlation length (ξ_{23}) as a function of time for a $L = 128$ lattice and $D = 3$ and $D = 4$. The slope of the curves (in a double logarithmic scale) provided us with the estimate of $1/z$, neglecting scaling corrections, and we report our estimates for z in Table IV. As in the equilibrium analysis, we have used the jackknife method over the samples to compute the statistical errors of the different observables, including the dynamic critical exponent [14].

Our final estimate is $z = 2.35(3)$ for $D = 3$ and a slightly higher value (but statistically compatible) $z = 2.44(4)$ for $D = 4$. The weighted average of these two values is $z = 2.38(2)$.

In the Appendix we report the detailed procedure we have followed to compute the statistical errors on the dynamic correlation length and on the z exponent.

IV. CONCLUSIONS

By computing the dynamic critical exponent z we have fully characterized the universality class of the three-dimensional Heisenberg model with cubic anisotropy by complementing the static critical exponents computed in Ref. [4].

²In the $L = 250$ simulations we have simulated 1000 samples for $D = 3$ and 1400 for $D = 4$.

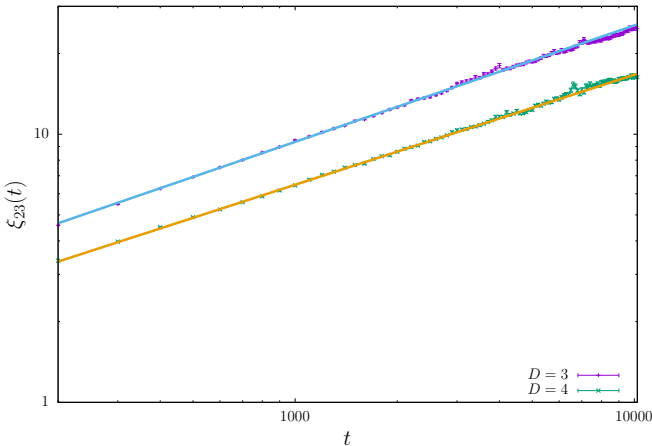


FIG. 3. Behavior of ξ_{23} versus time for $L = 128$ and for $D = 3$ and $D = 4$. The straight lines are the fit, in the interval $[1000, 6000]$ for the pure law behavior, see Eq. (14), the described in the text.

We have computed the dynamic critical exponent by using equilibrium and out-of-equilibrium approaches.

In the equilibrium simulations, we have analyzed the behavior of the integrated correlation times as a function of the lattice size. In the out-of-equilibrium simulations, we have computed the dynamic correlation length and we have studied its behavior as a function of the Monte Carlo time.

To assess universality we have analyzed, at equilibrium, the system for two values of the anisotropy coefficient D , namely, $D = 3$ and 4 , and by using two different implementations of the Metropolis algorithm.

We have obtained $z = 2.29(11)$ for the equilibrium analysis doing a joint fit of the numerical behavior of the integrated correlation time for both values of D and for both algorithms and taking into account the leading scaling correction provided by the field theoretical analysis of the model [12] [$\omega = 0.072(6)$]. The comparison of the computed value with that of the RSIM is good: $z = 2.29(11)$ versus $2.35(2)$.

Notice we have a large statistical error (a factor 6) in confronting with that of the RSIM. It is important to remark that in the equilibrium numerical studies of the Random Anisotropy model with cubic anisotropy we have simulated vector spins (instead of Ising ones) and we have not at our disposal clusters methods (to generate the equilibrated initial conditions, which will be evolved using a local Monte Carlo algorithm, the Metropolis algorithm in our case). Finally, only assuming the theoretical prediction, we can fix the scaling correction in the analysis of the equilibrium autocorrelation times.

The analysis of the out-of-equilibrium data is much more involved (mainly due to the statistical correlations of the data at different Monte Carlo times) [14], and we have not been able to take into account the scaling corrections in the fits and to perform a joint fit for both values of the anisotropy coefficient D (to check universality in the out-of-equilibrium regime). Despite these two issues, we have obtained values fully compatible with the equilibrium one, being our final value for the out-of-equilibrium analysis $z = 2.38(2)$.

The field-theoretical approach of the renormalization group shows that the universality class of the 3D Heisenberg model with cubic anisotropy is that of the RSIM for both static and dynamic. Equilibrium numerical simulations reported static critical exponents not so compatible with those of the RSIM, $\eta = 0.03(1)$ and $\nu = 0.737(8)$ [4] to be confronted with those of the RSIM: $\eta = 0.036(1)$ and $\nu = 0.683(2)$ [28]. We remark that in Ref. [4] was not possible to characterize the leading scaling corrections, and that only the exponents for the crossing point of the two larger were reported.

In summary, we have presented numerical evidences that the equilibrium dynamical behavior fit pretty well with the analytical predictions: (i) our estimate of the dynamic critical exponent is compatible with that of the diluted Ising model ($z = 2.35(2)$ [19]), and (ii) the scaling corrections could be parametrized using the results of Ref. [12]. The analysis of our out-of-equilibrium numerical simulations provides with a dynamic critical exponent compatible with that of the diluted Ising model, but, we have been unable to control the scaling corrections.

An open problem is to determine, by simulating larger lattices, whether the static exponents (for example, those obtained using the quotient method) can be described with $\omega =$

0.072 [12], and whether their extrapolation to infinite volume is compatible with the RSIM static exponents.

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APPENDIX: COMPUTATION OF THE DYNAMIC CORRELATION LENGTH AND THE z EXPONENT WITH THEIR ASSOCIATED STATISTICAL ERROR

We outline the procedure followed to compute $\xi(t)$ and its associated dynamic critical exponent z [14,23–26,34,35]. A key aspect of our approach is to avoid the use of the full covariance matrix, as it is often singular (see, e.g., Refs. [25,36]). The method proceeds as follows:

(1) The statistical error of $C(r, t)$ is estimated using the jackknife method over the set of initial conditions.

(2) To compute I_k , we introduce a cutoff to ensure reliable signal-to-noise ratios in $C(r, t)$ at large distances:

(i) The cutoff Λ is determined by the condition $\sigma[C(\Lambda, t)] = 4, C(\Lambda, t)$.

(ii) For a fixed time t , and over the range $r_{\min} < r < \Lambda$, the correlation function is fitted to the form:

$$C(r, t) = \frac{a_1}{r^{a_2}} \exp(-a_3 r^{a_4}), \quad (\text{A1})$$

where $r_{\min}$ is the minimum distance for which a good fit to Eq. (A1) is achieved, typically satisfying that the diagonal $\chi^2/\text{d.o.f.} \sim 1$.

(iii) To compute $\xi(t)$, the integral in Eq. (12) is evaluated numerically using the measured values of $C(r, t)$ for $r < \Lambda$, and the fitted values from Eq. (A1) for $\Lambda < r < L/2$.

(iv) The statistical error in $\xi(t)$ is again computed via the jackknife method over the initial conditions. The time interval used in the fit is chosen by requiring that the diagonal $\chi^2/\text{d.o.f.} \sim 1$.

(3) To compute the dynamic critical exponent, we perform the following two steps:

(i) The values of $\xi(t)$ are then used to determine z using the diagonal covariance matrix of the correlation length based on the jackknife statistical errors of the correlation length.

(ii) The associated error of z is estimated from the standard deviation across jackknife blocks of the correlation length. The extraction of z within each (jackknife) block employs the diagonal covariance matrix. Despite this simplification, the jackknife approach accurately captures correlations between different time points.

It is important to note that the diagonal $\chi^2/\text{d.o.f.}$ does not have the same statistical interpretation as the full (non-diagonal) version. As discussed in detail in Sec. B.3.3.1 of Ref. [25], this metric behaves as though there are fewer degrees of freedom, and therefore, conventional confidence intervals cannot be reliably computed.

Furthermore, Ref. [34] demonstrates that the error bars obtained via this jackknife method—ignoring interdata correlations—are essentially equivalent to those computed when such correlations are fully considered.

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