Generalized Langevin equation formulation for anomalous diffusion in the Ising model at the critical temperature

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We consider the two- (2D) and three-dimensional (3D) Ising models on a square lattice at the critical temperature T_c, under Monte Carlo spin flip dynamics. The bulk magnetization and the magnetization of a tagged line in the 2D Ising model, and the bulk magnetization and the magnetization of a tagged plane in the 3D Ising model, exhibit anomalous diffusion. Specifically, their mean-square displacements increase as power laws in time, collectively denoted as $\sim t^c$, where c is the anomalous exponent. We argue that the anomalous diffusion in all these quantities for the Ising model stems from time-dependent restoring forces, decaying as power laws in time—also with exponent c —in striking similarity to anomalous diffusion in polymeric systems. Prompted by our previous work that has established a memory-kernel based generalized Langevin equation (GLE) formulation for polymeric systems, we show that a closely analogous GLE formulation holds for the Ising model as well. We obtain the memory kernels from spin-spin correlation functions, and the formulation allows us to consistently explain anomalous diffusion as well as anomalous response of the Ising model to an externally applied magnetic field in a consistent manner.

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I. INTRODUCTION

In the case of normal diffusion the mean-square displacement (msd) of a particle $\langle \Delta r^2(t) \rangle$ increases linearly in time. The term anomalous diffusion is used to denote a particle's mean-square displacement $\langle \Delta r^2(t) \rangle$ deviating from (its normal behavior of) increasing linearly in time t, and commonly refers to the power-law behavior $\langle \Delta r^2(t) \rangle \sim t^c$ for some $c \neq 1$. Although the term "anomalous" diffusion was originally coined to denote an anomaly—in this case, a deviation from normal diffusion—anomalous diffusion has increasingly become the norm [1]. Observed in many materials and systems, such as in fractal systems and disordered media [2,3], financial markets [4], transport in (crowded) cellular interiors [5], migration of cells [6] and bacteria [7], and animal foraging [8], anomalous diffusion has naturally received intense attention in the last decade. Interest in the topic revolves largely around the following questions. What causes the exponent to differ from unity? Can one predict the exponent from the underlying dynamics of the system? Are there universality classes for systems exhibiting anomalous diffusion?

A number of distinct classes of stochastic processes have been developed/identified for anomalous diffusion in recent years. The three most prominent theoretical (stochastic) models of anomalous diffusion are the following:

(1) Transport on fractals: a popular model used for percolating and disordered materials [3,9–11], wherein the moving particle encounters obstacles on its path.

(2) Continuous-time random walk (CTRW): a model where particles move from trap to trap [12–15], where times of waiting at the traps as well as the trap-to-trap distance is power-law distributed, and

(3) Gaussian models like fractional Brownian motion (fBm), which describes a Gaussian process with power-law memory [16,17], attributed to the "material medium" that surrounds the particle that undergoes anomalous diffusion.

An overview of the available theoretical models, including a summary of their distinctive features and stochastic properties can be found in a recent perspective article [18].

Despite the above progress achieved, which model best describes an instance of (experimentally) observed anomalous diffusion is often the subject of fierce debate, as evidenced by the recent case of anomalous diffusion observed for tracer particles in cell cytoplasms [19–24], where all three of the above stochastic models have been fitted to the experimental data [20–27]. For physical systems where the dynamical rules for particles movement are known (in contrast to a complicated medium like cell cytoplasm), one would expect to have a much easier task to model anomalous diffusion, yet it can still remain quite a challenge. For polymeric systems, where anomalous diffusion is commonplace, it is only recently that one of us has established that the anomalous diffusion for tagged monomers is explained by "restoring forces" that decay as a power law in time with the anomalous exponent of diffusion [28,29]. From these characteristics it has been shown that anomalous diffusion in polymeric systems can be modeled by a generalized Langevin equation (GLE) with a memory kernel, and it belongs to the class of fBm [30]. The fBm characteristics of anomalous diffusion have been verified for flexible [31,32] and semiflexible polymers [33] and for polymer membranes [34–36]. Importantly, they have been used to successfully explain the dynamics of translocation of polymers across membranes [37–40]. The fBm model framework has been generalized/extended to the linear transport regime for flexible

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polymers [29], and has similarly been used to explain field-driven polymer translocation [41] and polymer adsorption [42] for weak fields and adsorption energies. It has also found applications in strong nonlinear regimes for flexible polymers [43].

In this paper, we take on characterizing anomalous diffusion in magnetization space for the Ising model on a square lattice at the critical temperature, undergoing Monte Carlo spin-flip dynamics. That the total magnetization for this model exhibits anomalous diffusion was reported by one of us in Ref. [44]. Additionally, we report that the magnetization of a tagged line in the two-dimensional (2D) Ising model, and the magnetization of a tagged plane in the three-dimensional (3D) Ising model, also exhibit anomalous diffusion. We argue that the anomalous diffusion for all these quantities for the Ising model stems from time-dependent restoring forces, decaying as power laws in time—with the anomalous exponent of diffusion—in striking similarity to polymeric systems, and show that a closely analogous GLE formulation holds for the Ising model as well. We obtain the memory kernel from spin-spin correlation functions, and the formulation allows us to consistently explain anomalous diffusion as well as anomalous response of the Ising model to an externally applied magnetic field in a consistent manner.

The organization of this paper is as follows. In Sec. II we introduced the Ising model and report the anomalous exponents of magnetization. In Sec. III we explain how restoring forces—that hold the key to anomalous diffusion—develop and work. In Sec. IV we develop the GLE formulation for anomalous diffusion in the Ising model. The paper is concluded with a discussion in Sec. V.

II. THE ANOMALOUS DIFFUSION IN THE ISING MODEL AT THE CRITICAL TEMPERATURE

A. The model and dynamics

We consider the Ising model on a square lattice. The Hamiltonian, at zero external magnetic field, is given by

$$\mathcal{H}_0 = -J \sum_{\langle ij \rangle} s_i s_j, \tag{1}$$

where $s_i = \pm 1$ is the spin at site i, and J is the coupling constant of interaction among the spins. The summation runs over all the nearest-neighbor spins. The linear size of the system is L; i.e., $0 \leqslant (i,j) < L$. Our samples satisfy periodic boundary conditions at all times, and all properties we report here are studied (or measured) at the critical temperature T_c.

The key quantity of focus in this paper is the mean-square displacement (MSD) for magnetization $M(t)$ at time t as

$$\langle \Delta M^2(t) \rangle = \langle [M(t) - M(0)]^2 \rangle, \tag{2}$$

where $M(t)$ can take several forms. All angular brackets in this paper, including those in Eq. (2), denote ensemble average. In the two-dimensional (2D) Ising model, we consider the respective cases where it is the bulk magnetization $M_{2\mathrm{D},b}$ or the "line magnetization" $M_{2\mathrm{D},l}$, the magnetization of a tagged line of spins in the y direction. Similarly, in the three dimensions, we consider the bulk magnetization $M_{3\mathrm{D},b}$ and the magnetization $M_{3\mathrm{D},p}$ of a tagged xz plane.

We simulate the dynamics of the system using Monte Carlo moves, following the Metropolis algorithm. At any time step a spin is randomly selected to flip, and the resulting change ΔE, where E is the energy of the system, is measured. The move is accepted with unit probability if $\Delta E \leqslant 0$; if not, then the move is accepted with the usual Metropolis probability $e^{-\Delta E/(k_\mathrm{B} T_c)}$, where k_B is the Boltzmann constant.

All simulation results reported here use $k_B = J = 1$.

B. Anomalous diffusion in the Ising model

Let us denote by D the spatial dimension *of the support* of the tagged magnetization given by M, meaning $D = 1$ for a tagged line and $D = 2$ for bulk in the 2D Ising model, while for the 3D Ising model $D = 2$ for a tagged plane and $D = 3$ for bulk. At short times $t \lesssim 1$, the individual spin flips in the model are uncorrelated, and, since there are L^D spins altogether in these entities spatial dimensions,

$$\langle \Delta M^2(t) \rangle \simeq L^D t. \tag{3}$$

At long times, $t \gg L^{z_c}$, where z_c is the dynamic exponent for the Ising model at T_c, we expect $\langle M(t)M(0) \rangle = 0$. This means that

$$\langle \Delta M^2(t) \rangle \equiv \langle [M(t) - M(0)]^2 \rangle \underset{t \gg L^{z_c}}{=} 2\langle M^2 \rangle, \tag{4}$$

which is a purely equilibrium quantity which we can calculate from the equilibrium spin-spin correlations. We then have

$$\langle M^2 \rangle = \sum_{i \in L^D} \sum_{j \in L^D} \langle s_i s_j \rangle = \sum_{i \in L^D} \sum_{j \in L^D} r_{ij}^{2-d-\eta}$$
$$\approx \int_1^L \frac{d^D r}{r^{d-2+\eta}} \sim L^{2D-d+2-\eta}, \tag{5}$$

where r_{ij} is the Euclidean distance between the two spins i and j, d is the spatial dimension of the model (i.e., $d = 2$ and 3 for two- and three-dimensional Ising models respectively), and the critical exponent η is related to γ and ν via the scaling relation $2 - \eta = \gamma/\nu$. (Note this result requires an integral $\int_1^L \frac{d^D r}{r^{d-2+\eta}}$ to be dominated by large r, which is why we have excluded line magnetization $D = 1$ in three dimensions, $d = 3$, from our paper.)

We now make the scaling assumption of an intervening power law with time,

$$\langle \Delta M^2(t) \rangle \propto t^c, \tag{6}$$

connecting across intermediate times from Eq. (3) at $t \simeq 1$ to Eqs. (4) and (5) at $t \simeq L^{z_c}$. The match at $t \simeq 1$ forces $\langle \Delta M^2(t) \rangle \simeq L^D t^c$, and the match at large time L^{z_c} then requires $L^{D+cz_c} \simeq L^{2D-d+\gamma/\nu}$, leading to

$$c = \frac{D - d + \gamma/\nu}{z_c}. \tag{7}$$

The full scaling prediction valid for all $t \gg 1$ is then

$$\langle \Delta M^2(t) \rangle / L^{2D-d+\gamma/\nu} = f(t/L^{z_c}), \tag{8}$$

where $f(x) \simeq x^c$ for $x \ll 1$. Using the values of the critical exponents corresponding to $k_B = J = 1$, as presented in Table I,

TABLE I. The relevant critical exponents and the critical temperature in the Ising model [45–47], using $k_B = J = 1$ for the critical temperature T_c.

Ising model dimension d	γ	ν	z_c	T_c
2	7/4	1	2.1665(12)	$\frac{2}{\ln(1+\sqrt{2})}$
3	1.237075(10)	0.629971(4)	2.03(4)	4.5116174(2)

the explicit power laws for $1 \lesssim t \lesssim L^{z_c}$ become

$$\begin{aligned}\left\langle \Delta M^2_{\mathrm{2D},l}(t)\right\rangle &\sim L t^{(\gamma/\nu-1)/z_c} \approx L t^{0.35},\\ \left\langle \Delta M^2_{\mathrm{2D},b}(t)\right\rangle &\sim L^2 t^{\gamma/(\nu z_c)} \approx L^2 t^{0.81},\\ \left\langle \Delta M^2_{\mathrm{3D},p}(t)\right\rangle &\sim L^2 t^{(\gamma/\nu-1)/z_c} \approx L^2 t^{0.48},\\ \left\langle \Delta M^2_{\mathrm{3D},b}(t)\right\rangle &\sim L^3 t^{\gamma/(\nu z_c)} \approx L^3 t^{0.97},\end{aligned} \tag{9}$$

indicating that anomalous diffusion in the Ising model is ubiquitous at the critical temperature. As pointed out earlier, the results of the bulk magnetizations were first obtained by one of us in Ref. [44].

The power laws in Eq. (9) are verified in Fig. 1. To obtain these data, we first thermalized the system. We then produced a number of independent time series of $M(t)$, from which we measured $\langle \Delta M^2(t)\rangle$. In some of the plots in Fig. 1 we notice a small deviation from the power laws at late times: we have verified that this is caused by periodic boundary conditions—they are different when free boundary conditions are employed. Two examples of this can be found in Appendix A.

III. RESTORING FORCES: THE PHYSICS OF ANOMALOUS DIFFUSION IN THE ISING MODEL

In this section we focus on the physics of anomalous diffusion. We argue that anomalous diffusion in the Ising model stems from restoring forces, in close parallel to polymeric systems.

A. Restoring forces

Imagine that the value of the tagged magnetization M changes by an amount δM due to thermal spin flips on the tagged line at $t = 0$. Due to the interactions dictated by the Hamiltonian, the spins within and surrounding the tagged region, in the ensuing times, will react to this change. This reaction will be manifest in the two following ways: (a) the surrounding spins will to some extent adjust to the change over time, and (b) during this time the value of M will also readjust to the persisting values of the surrounding spins, undoing at least a part of δM. It is the latter that we interpret as the result of "inertia" of the surrounding spins that resists changes in M, and the resistance itself acts as the restoring force to the changes in the tagged magnetization.

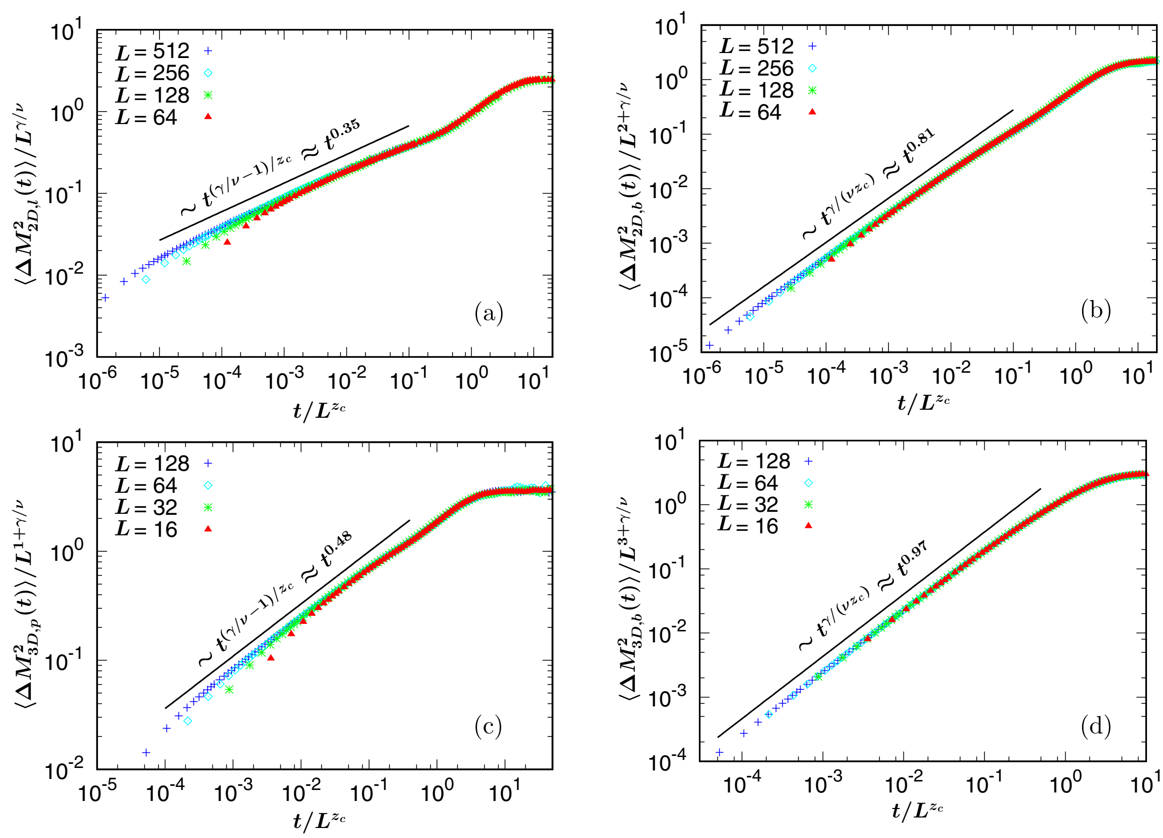

FIG. 1. The mean-square displacement (MSD) of the magnetizations $\langle \Delta M^2(t)\rangle$ in the Ising model at T_c: (a) tagged line magnetization for 2D Ising model, (b) bulk magnetization for 2D Ising model, (c) tagged plane magnetization for 3D Ising model, and (d) bulk magnetization for 3D Ising model. The x and y axes are scaled according to Eq. (8), leading to excellent data collapse over different L. The black solid lines denote the power laws shown in Eq. (6).

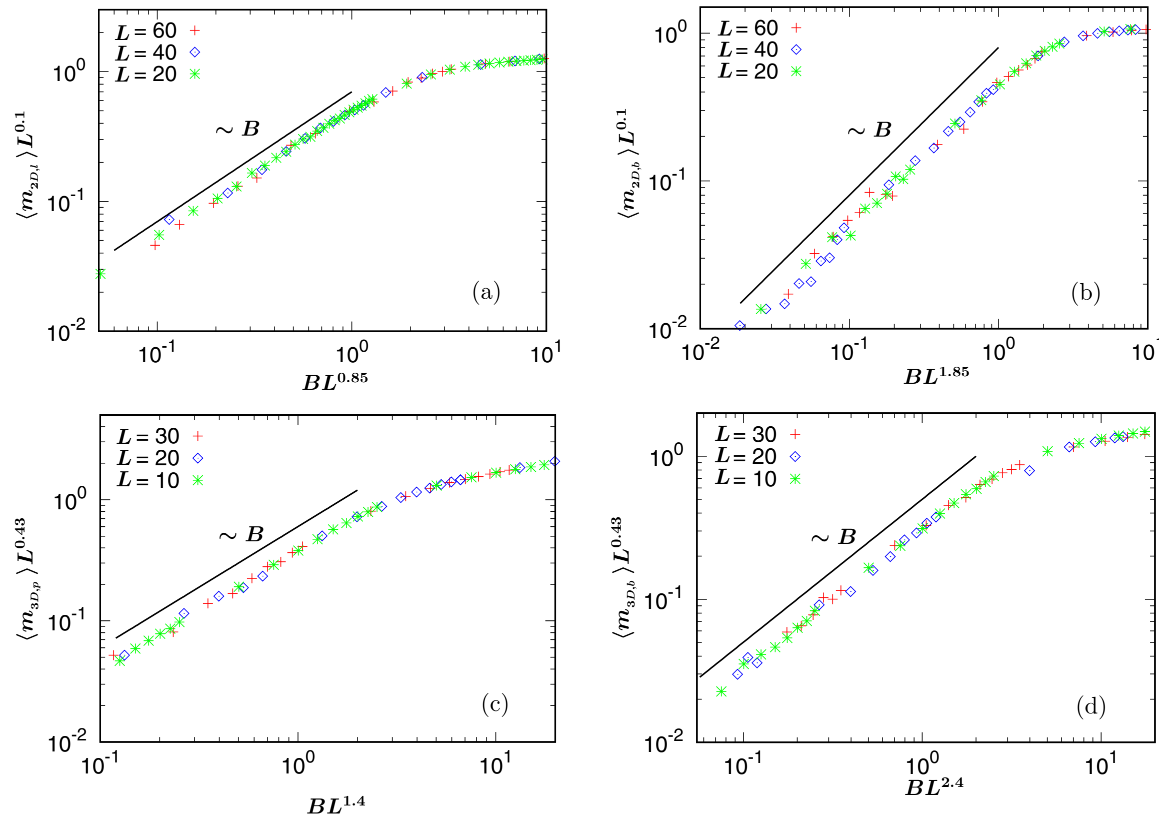

FIG. 2. Plots showing the scaling form $\langle m\rangle L^{\kappa} \sim f(BL^{\lambda})$ with $\kappa-\lambda = D-d+\gamma/\nu$, confirming Eq. (11). The (numerically found) values of λ is 0.1 in 2D and 0.43 in 3D: (a) $\langle m_{2\mathrm{D},l}\rangle$ (b) $\langle m_{2\mathrm{D},b}\rangle$, (c) $\langle m_{3\mathrm{D},p}\rangle$ and (d) $\langle m_{3\mathrm{D},b}\rangle$ (note: $\gamma/\nu \approx 1.75$ in 2D and $\approx$1.97 in 3D).

Since the part of the imposed change δM will be partially undone for $t>0$, we can expect the "velocity" autocorrelation function $\langle \dot M(0)\dot M(t)\rangle$ to be negative, an ingredient that we will use to establish the connection between the restoring forces and anomalous diffusion in Sec. III C.

B. The time-decay behavior of restoring forces

The main ingredient to connect the restoring forces and anomalous diffusion lies in how the former decays in time. To this end, we first consider the following thought-experiment, along the line described above in Sec. III A. On an equilibrated set of samples of the two-dimensional Ising model we create a small excess tagged magnetization δM at $t=0$ with the constraint that we do not allow this excess to be subsequently undone; this corresponds to an imposed evolution of the tagged magnetization $dM(t)/dt = (\delta M)\,\delta(t)$, where $\delta(t)$ is the Kronecker delta function. The resulting restoring force at later time t we will then write as

$$f(t) = -k(t)\,\delta M, \qquad (10)$$

where we interpret $k(t)$ as the magnetic analog of a spring constant: in conventional magnetic language this is related to the susceptibility of the tagged magnetization through $k^{-1} = L^D\chi$.

For long times $t \gg L^{z_c}$ our spring constant will be the equilibrium one, which is given by the equilibrium fluctuation theorem as

$$k^{-1} = \beta\langle M^2\rangle \sim L^{2D-d+\gamma/\nu}. \qquad (11)$$

Equation (11) can be confirmed by equilibrating samples under the magnetic analog of an externally applied force, which is an external field applied to the tagged magnetization (i.e., the field is applied on the domain of support of the magnetization), such that the Hamiltonian becomes $\mathcal{H} = \mathcal{H}_0 - MB$. We then expect a mean tagged magnetization density $\langle m\rangle = ML^{-D} = k^{-1}BL^{-D} \simeq BL^{D-d+\gamma/\nu}$ at small values of B, which is the manifestation of linear response of the system under weak external forcing. More generally, we can expect a full scaling form $\langle m\rangle L^{\kappa} \sim f(BL^{\lambda})$ for some κ and λ, where the scaling function $f(x)$ has the property that $f(x\to\infty)\to$ constant, and $f(x\to 0)\sim x$ due to the linear dependence of $\langle m\rangle$ on B as $B\to 0$. The latter condition implies that $\kappa-\lambda = D-d+\gamma/\nu$.

The scaling form $\langle m\rangle = ML^{-D} = k^{-1}BL^{-D} \simeq BL^{D-d+\gamma/\nu}$ with $\kappa-\lambda = D-d+\gamma/\nu$ is confirmed in Fig. 2. The quantity λ is numerically found to be 0.1 and 0.43 for Ising models in two and in three dimensions respectively.

For intermediate times we expect equilibrium response to be achieved only locally across a length scale $\ell(t)\sim t^{1/z_c}$ within and around the tagged zone (see Fig. 3). Within a region of the tagged zone of side $\ell(t)$ we then expect a contribution of tagged magnetization $\langle\Delta M\rangle_{\ell(t)} \sim B\ell(t)^{2D-d+\gamma/\nu}$. Adding the response from $(L/\ell(t))^D$ such regions then leads to

$$\langle M(t)\rangle = k(t)^{-1}B \sim BL^D\ell(t)^{D-d+\gamma/\nu} \sim BL^Dt^c, \qquad (12)$$

where the exponent c is as already given in Eq. (7). The various cases of this result are verified in Fig. 4.

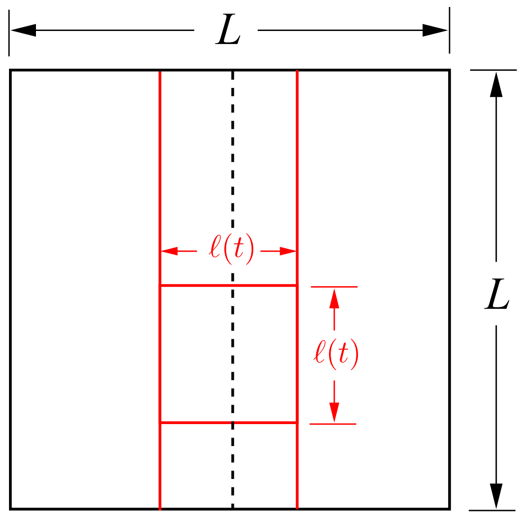

FIG. 3. The thought experiment performed on the tagged line magnetization for the two-dimensional Ising model. A small excess (line) magnetization $\delta M_{2\mathrm{D},l}$ is created on the tagged line of spins, denoted by the dashed line, with the constraint that we do not allow the excess magnetization to be undone. Up to time t, this action creates a rectangular zone of width $\ell(t) \sim t^{1/z_c}$ around the tagged line, shown by the red solid lines, which we can consider equilibrated to the new situation, in the following sense. If we consider the red square of size $\ell(t) \times \ell(t)$, then after time t the spins therein will all have equilibrated to the segment of the tagged line within that square, and vice versa.

To summarize, the key result of this section is that if we create an excess tagged magnetization δM at $t = 0$ and do not allow it to relax away, then a time-dependent restoring force $f(t)$ acts in such a way that would reverse it, where

tagged line magnetization in two dimensions:

$$f_{\mathrm{rest}}(t) = -L^{-1}\, t^{-(\gamma/\nu-1)/z_c}\, \delta M_{2\mathrm{D},l};$$

bulk magnetization in two dimensions:

$$f_{\mathrm{rest}}(t) = -L^{-2}\, t^{-\gamma/(\nu z_c)}\, \delta M_{2\mathrm{D},b};$$

tagged plane magnetization in three dimensions: (13)

$$f_{\mathrm{rest}}(t) = -L^{-2}\, t^{-(\gamma/\nu-1)/z_c}\, \delta M_{3\mathrm{D},p}; \text{ and}$$

bulk magnetization in three dimensions:

$$f_{\mathrm{rest}}(t) = -L^{-3}\, t^{-\gamma/(\nu z_c)}\, \delta M_{3\mathrm{D},b}.$$

C. Anomalous diffusion stems from these restoring forces

The main result of Sec. III B, for which $\dot{M}(t) \propto \delta(t)$, can be represented as the following formal time-dependent "impedance-admittance relation" [37–39]:

$$f_{\mathrm{rest}}(t) = -\int_0^t dt'\, \mu(t-t')\dot{M}(t'), \qquad (14)$$

with a causal memory function given by $\mu(t) = k(t) \sim L^{-D} t^{-c}$ as in Eq. (13) for $t > 0$, and $\mu(t) = 0$ for $t < 0$. Equation (14) is obtained from Eq. (13) using the superposition

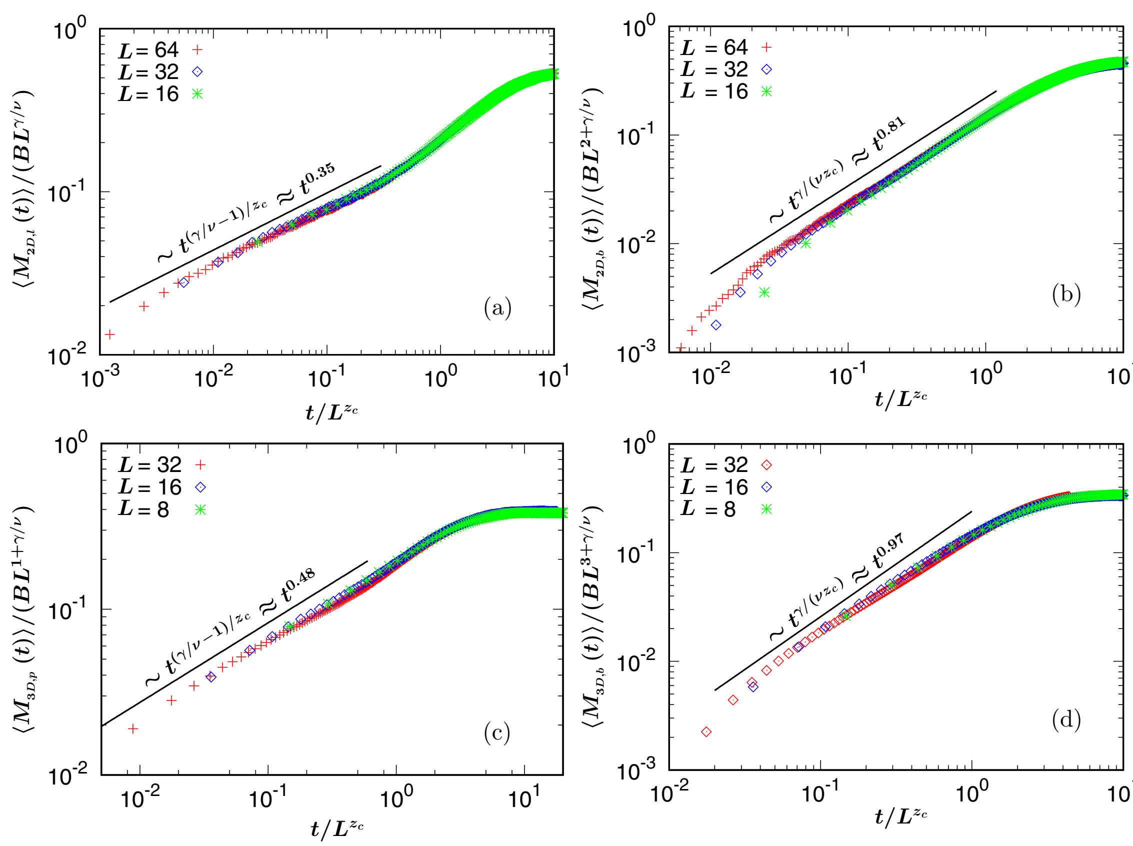

FIG. 4. Average magnetizations as a function of time when the magnetic field is switched on the equilibrated samples at $t = 0$: (a) tagged line magnetization $\langle M_{2D,l}(t)\rangle$ and (b) bulk magnetization $\langle M_{2D,b}(t)\rangle$ for the 2D Ising model, and (c) the tagged plane magnetization $\langle M_{3D,p}(t)\rangle$ and (d) bulk magnetization $\langle M_{3D,b}(t)\rangle$ for the 3D Ising model.

TABLE II. Memory functions and anomalous diffusion of magnetization in the Ising model. The anomalous diffusion applies only until the terminal relaxation time scaling $\sim L^{z_c}$.

Magnetization of	$\mu(t)$	$\langle\Delta M(t)\rangle^2$
tagged line in 2D	$L^{-1}t^{-(\gamma/\nu-1)/z_c}$	$Lt^{(\gamma/\nu-1)/z_c}$
bulk in 2D	$L^{-2}t^{-\gamma/(\nu z_c)}$	$L^2t^{\gamma/(\nu z_c)}$
tagged plane in 3D	$L^{-2}t^{-(\gamma/\nu-1)/z_c}$	$L^2t^{(\gamma/\nu-1)/z_c}$
bulk in 3D	$L^{-3}t^{-\gamma/(\nu z_c)}$	$L^3t^{\gamma/(\nu z_c)}$

principle: the total restoring force at time t is a sum of all preceding δM values weighted by the (power-law) memory kernel μ. In this formulation, $\dot{M}(t)$ plays the role of current through a circuit, with $f_{\text{rest}}(t)$ playing the role of the voltage, and $\mu(t)$ is the time-dependent impedance. On the one hand, this formulation means that $\langle f_{\text{rest}}(t) f_{\text{rest}}(t')\rangle_{\dot{M}=0} = \mu(|t-t'|)$, while on the other, we can invert Eq. (14) to express $\dot{M}(t)$ as a function of $f_{\text{rest}}(t)$ involving the time-dependent admittance $a(t)$ as

$$\dot{M}(t) = -\int_0^t dt'\, a(t-t') f_{\text{rest}}(t'), \tag{15}$$

and correspondingly $\langle \dot{M}(t)\dot{M}(t')\rangle_{f_{\text{rest}=0}} = a(t-t')$, with the impedance and the admittance following the relation $\tilde{a}(s)\tilde{\mu}(s) = 1$ in the Laplace space s. These imply that $a(t) = \langle \dot{M}(t)\dot{M}(0)\rangle_{f_{\text{rest}=0}} \sim -L^D t^{c-2}$. Integrating this quantity twice in time using the Green-Kubo relation we obtain

$$\langle \Delta M(t)\rangle^2 \simeq L^D t^c \tag{16}$$

(we will return to this calculation more formally in Sec. IV), leading us not only to the anomalous exponents of Eq. (6), but also the correct L-dependent prefactors for the data collapse in Fig. 1. The results are summarized in Table II.

D. Restoring forces and anomalous diffusion: a similar story for polymer dynamics

Although slightly off topic, we now briefly point out that the dynamics of the restoring forces and anomalous diffusion for magnetization in the Ising model is practically identical to those in polymer dynamics [28,29,31,37–39,41,42]. This subsection forms the basis of Sec. IV, where we discuss the generalized Langevin equation formulation of anomalous diffusion in the Ising model.

Even though anomalous diffusion in polymeric systems is the norm rather than an anomaly, we specifically pick the Rouse polymer to demonstrate the similarity; for instance, the anomalous diffusion of a tagged monomer in the Rouse model, which scales as $t^{2\nu/(1+2\nu)}$ until the terminal Rouse time $\tau_R \sim N^{1+2\nu}$ (and diffusively thereafter). Here, ν is the Flory exponent (=3/4 in two and ≈0.588 in three dimensions), and N is the polymer length.

Imagine that we move a tagged monomer by a small distance $\delta\vec{r}$ at $t=0$ and hold it at its new position $\forall t>0$ (just like in our thought experiment of Sec. III B, where we created an excess magnetization δM at $t=0$ and did not allow it to be undone). For more details, we refer the reader to Ref. [31], where we analyzed this thought experiment. In the ensuing time, all the monomers within a backbone distance $n_t \sim t^{1/(1+2\nu)}$, counting away from the tagged monomer will equilibrate to the new position of the tagged monomer. However, the end-to-end distance of these equilibrated set of monomers is no longer their natural spatial extent ($\sim n_t^\nu$), but is instead stretched by an amount $\propto \delta\vec{r}$. With the (entropic) spring constant of these n_t equilibrated monomers scaling as $\sim n_t^{-2\nu}$, the mean force the tagged monomer experiences at its new position is then given by $\vec{f}_{\text{rest}}(t) \sim -n_t^{-2\nu}(\delta\vec{r}) \sim -t^{-2\nu/(1+2\nu)}(\delta\vec{r})$ [i.e., force = (spring constant) × stretching distance]. This relation is identical in formulation to Eqs. (13), and the rest of the emulated analysis (14)–(16) leads one to the result that the mean-square displacement of the tagged monomer increase as $t^{2\nu/(1+2\nu)}$. Of course this result only holds till the polymer's terminal Rouse time $\tau_R \sim N^{1+2\nu}$, just like the anomalous diffusion in the Ising model survives until the terminal relaxation time scaling $\sim L^{z_c}$.

The reader may find a comparison of Table I in Ref. [29] and Table II of this paper interesting. Note that at the critical temperature the system size L corresponds to the polymer length N: both systems reach criticality when these parameters reach infinity.

IV. GENERALIZED LANGEVIN EQUATION FORMULATION FOR ANOMALOUS DIFFUSION IN THE ISING MODEL

In the previous section we focused on the physics of the anomalous diffusion in the Ising model. Using a thought experiment we argued that the time-decay behavior of the restoring forces is the key ingredient to describe the relation between the restoring forces and anomalous diffusion in terms of the memory function $\mu(t)$. Equation (14) and its inverse formulation led us not only to the anomalous exponents for the mean-square displacements, but also to the correct L-dependent prefactors to obtain the data collapse in Fig. 1. These results pose now an interesting question: Could we formulate a stochastic differential equation for the anomalous diffusion in the Ising model?

A comparison to the corresponding relations between the restoring forces and anomalous diffusion for polymeric systems—taken up in the elaborate paper [29] by one of us—offers a clue to a possible answer to the above question. Therein the (anomalous) dynamics of a tagged monomer is shown to be described by the two following stochastic differential equations involving the monomeric velocity $v(t)$, the respective internal and external forces $f(t)$ and f_{ext} that it experiences, and the memory function $\mu(t)$:

$$\begin{aligned} \gamma v(t) &= f(t) + q_1(t), \\ f(t) &= -\int_0^t dt'\mu(t-t')\, v(t') + f_{\text{ext}} + q_2(t). \end{aligned} \tag{17}$$

Here γ is the viscous drag on the monomer by the surrounding (effective) medium, $q_1(t)$ and $q_2(t)$ are two noise terms satisfying $\langle q_1(t)\rangle = \langle q_2(t)\rangle = 0$, and the fluctuation-dissipation theorems (FDTs) $\langle q_1(t)\, q_1(t')\rangle \propto \gamma\delta(t-t')$ and $\langle q_2(t)\, q_2(t')\rangle \propto \mu(t-t')$ respectively. (Note that factors of $k_B T$ terms have been suppressed from these equations.) The idea behind Eq. (17) is that while the internal restoring force builds on the history of the monomeric velocity, the latter simply responds instantaneously to the force it experiences.

Similarity between the second of Eqs. (17) and Eq. (14) prompts us to propose the total force as

$$f(t) = -\int_0^t dt'\,\mu(t-t')\dot{M}(t') + f_{\rm ext} + g(t) \quad (18)$$

for the Ising model, where $f_{\rm ext}$ is simply the externally applied force, such as a magnetic field. The noise term $g(t)$ satisfies the condition that $\langle g(t)\rangle = 0$ and the corresponding FDT $\langle g(t)g(t')\rangle = \mu(|t-t'|)$. As we have done before, Eq. (18) can be inverted, in terms of the admittance $a(t)$, to write

$$\dot{M}(t) = -\int_0^t dt'\,a(t-t')f(t') + \omega(t). \quad (19)$$

The noise term $\omega(t)$ similarly satisfies $\langle\omega(t)\rangle = 0$, and the FDT $\langle\omega(t)\omega(t')\rangle = a(|t-t'|)$. The impedance and the admittance are related to each other in the Laplace space as $\tilde{a}(s)\tilde{\mu}(s) = 1$.

Additionally, we propose that, in the Monte-Carlo dynamics, magnetization in the Ising model instantaneously responds to the internal force as

$$\zeta\dot{M} = f(t) + q(t), \quad (20)$$

with a damping coefficient ζ and a corresponding white noise term $q(t)$. Thereafter, having combined Eqs. (18) and (20) we obtain

$$\zeta\dot{M} = -\int_0^t dt'\,\mu(t-t')\dot{M}(t') + f_{\rm ext} + g(t) + q(t) \quad (21)$$

or

$$\dot{M} = \int_0^t dt'\,\theta(t-t')[f_{\rm ext} + g(t') + q(t')], \quad (22)$$

where in the Laplace space $\tilde{\theta}(s)[\zeta + \tilde{\mu}(s)] = 1$. Here, without the ζ term $\theta(t)$ is identical to $a(t)$, introduced in Eq. (15).

At zero external magnetic field the dynamics of M simplifies to

$$\dot{M} = \int_0^t dt'\,\theta(t-t')[g(t') + q(t')], \quad (23)$$

similar to Eq. (17) for polymeric systems. Without further ado, we then simply follow Ref. [29] to conclude, with $\mu(t) \sim L^{-D}t^{-c}$, that

$$\langle\dot{M}(t)\dot{M}(t')\rangle = -\theta(t-t') \sim -L^D(t-t')^{c-2}. \quad (24)$$

Note that in Eq. (24) we have ignored the ζ term, which essentially means that we are ingoring the (uninteresting) timescale $\lesssim\zeta^{-1}$. Subsequently, by integrating Eq. (24) twice in time using the Green-Kubo relation, the MSD of the magnetization can be obtained as

$$\langle\Delta M^2(t)\rangle \sim L^D t^c, \quad (25)$$

which are the same results obtained in Eq. (16). An example verification for the velocity autocorrelation function (24) can be found in Appendix B.

This GLE formulation demonstrates that the anomalous diffusion in the Ising model at the critical temperature is non-Markovian, with a power-law memory function $\mu(t)$. Quite simply, if $\mu(t) \sim t^{-c}$, then the anomalous diffusion exponent is c.

A. Numerical confirmation of the GLE formulation (and determination of the damping coefficient ζ)

It is now imperative that we numerically test our proposed GLE formulation for anomalous diffusion for the Ising model. Our key test is to check the FDT $\langle f_{\rm rest}(t)f_{\rm rest}(t')\rangle_{\dot{M}=0} = \mu(t-t')$, for which we describe our approach below, followed by presentation of the numerical results.

Conceptually, the task is simple. At a fixed value of M, i.e., $\dot{M} = 0$ at all times, we need to numerically measure $\langle f_{\rm rest}(t)f_{\rm rest}(t')\rangle$. However, we cannot measure forces in the Monte Carlo dynamics of the model since by definition one does not have forces in discrete lattice models. In order to circumvent this difficulty, we use Eq. (20) as a proxy for $f(t)$ by choosing $\zeta = 1$ and use the value $\overline{\dot{M}}_{\rm free}$ (see below), which would have applied to the tagged magnetization if the fixed M constraint were to be lifted at that time.

We start with a thermalized system at $t = 0$. For $t > 0$ we fix the value of M (this does not mean that all tagged spins are frozen), which we achieve by performing nonlocal spin-exchange moves. Specifically, for the magnetization of a tagged line in 2D and tagged plane in 3D, we avoid extreme values of M by choosing to fix it in the interval $-0.2 < m = ML^{-D} < 0.2$ (note that in the scaling limit all values of m belong to this range). We then keep taking snapshots of the system at regular intervals, and compute, at every snapshot (denoted by t), the expectation value $\overline{\dot{M}}_{\rm free}(t)$ conditional on the current configuration, which for our Metropolis–Monte Carlo dynamics is given by

$$\overline{\dot{M}}_{\rm free}(t) = \sum_{i\in\text{tagged}}(-2s_i)\,\text{Min}(1,e^{-\Delta E_i/(k_BT_c)}) = f(t). \quad (26)$$

This means that, for every snapshot we take, we consider an attempt to flip each spin in turn and find the expected change in M which would have occurred if this move had been implemented, totalled over all the spins.

Finally, we note that since simulations are performed for finite systems with M fixed at its $t = 0$ value, in any particular run we need a nonzero value of $f_{\rm ext} = -\langle f(t)\rangle$ acting to sustain the initial value of M. Further, given that that in our proxy measurement for $f(t)$ using Eq. (20) we can only access $f_{\rm rest}(t) + f_{\rm ext}$, but not $f_{\rm rest}(t)$ directly, it is the quantity

$$\begin{aligned}\Gamma(\dot{M}_{2{\rm D},l}(t)) &= \langle\dot{M}(t)\dot{M}(t')\rangle - \langle\dot{M}(t)\rangle\langle\dot{M}(t')\rangle\\ &= L^{2D}(\langle f(t)f(t')\rangle - \langle f(t)\rangle\langle f(t')\rangle)\end{aligned} \quad (27)$$

that should correctly proxy $\langle g(t)g(t')\rangle_{\dot{M}=0} = \mu(t-t')$, and we expect the following results:

$$\begin{aligned}\Gamma(\dot{M}_{2{\rm D},l}(t)) &\sim Lt^{-(\gamma/\nu-1)/z_c} \approx Lt^{-0.35},\\ \Gamma(\dot{M}_{2{\rm D},b}(t)) &\sim L^2t^{-\gamma/(\nu z_c)} \approx L^2t^{-0.81},\\ \Gamma(\dot{M}_{3{\rm D},p}(t)) &\sim L^2t^{-(\gamma/\nu-1)/z_c} \approx L^2t^{-0.48},\\ \Gamma(\dot{M}_{3{\rm D},b}(t)) &\sim L^3t^{-\gamma/(\nu z_c)} \approx L^3t^{-0.97}.\end{aligned} \quad (28)$$

These results are verified in Fig. 5, along with the effective exponents as numerically obtained derivative $d(\ln\Gamma)/d(\ln t)$ as insets.

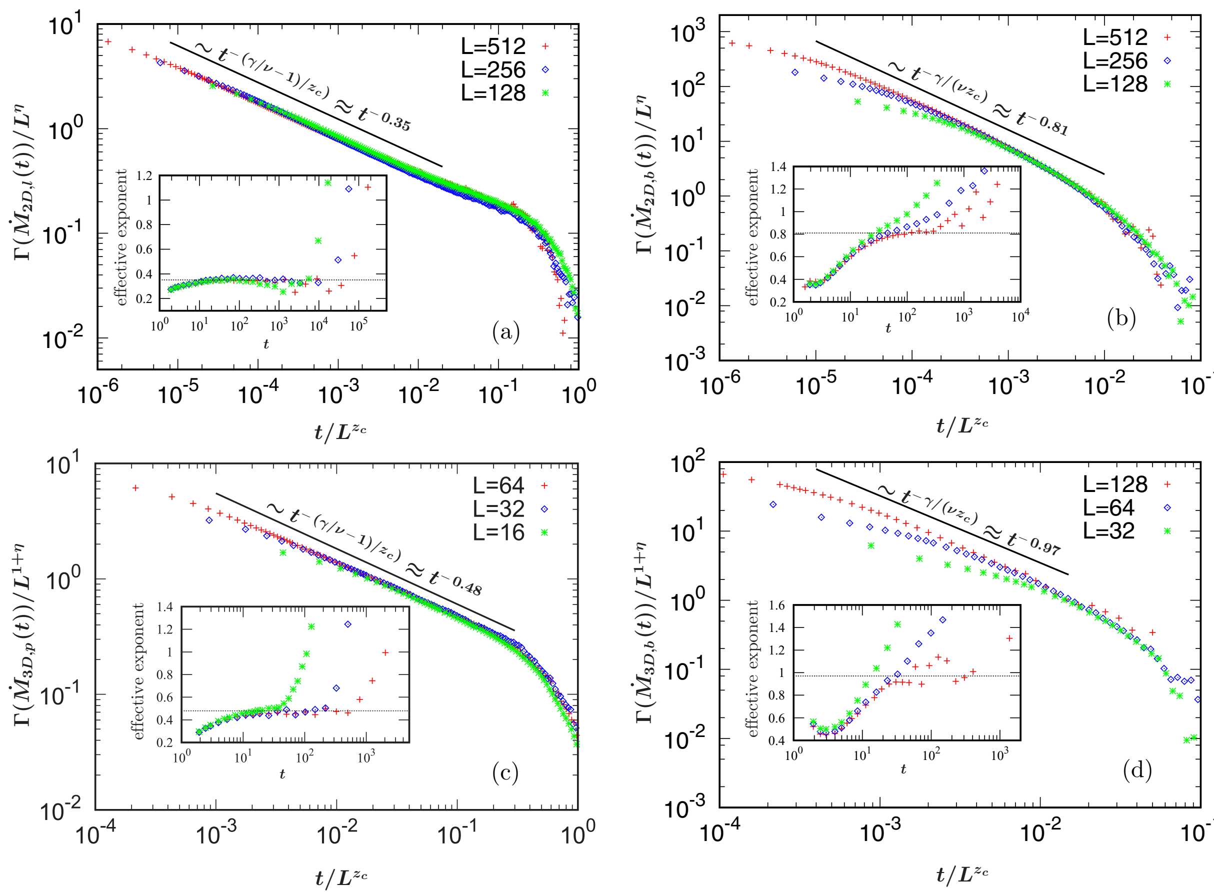

FIG. 5. Plots showing the scaling of (a) $\Gamma(\dot{M}_{2D,l}(t))$, (b) $\Gamma(\dot{M}_{2D,b}(t))$, (c) $\Gamma(\dot{M}_{3D,p}(t))$ and (d) $\Gamma(\dot{M}_{3D,b}(t))$ as a function of t/L^{z_c}. Insets show the effective exponent, numerically obtained derivative $-d(\ln\Gamma)/d(\ln t)$, with the dotted lines denoting the expected values of the slope. Note that the critical exponent η is related to γ and ν via the scaling relation $\eta = 2 - \gamma/\nu$.

In Fig. 5, the data quality for 3D bulk at long times suffers from the difficulty of collecting statistically independent datasets at long times. There are also small deviations from the power laws at late times for line magnetization in 2D and plane magnetization in 3D; we suspect that these relate to similar deviations observed in Fig. 1.

Additionally, we have followed the procedure described in Ref. [48] to obtain the power-law exponents from data in Fig. 5; these values, together with the error bars, for the respective largest system sizes, can be found in Table III. We have chosen the largest system sizes for this purpose since they contain the least amount of finite size effects.

TABLE III. Power-law exponents from data in Fig. 5, together with error bars, for the respective largest system sizes. Evidently, the data compare well with the expected exponents.

System	Estimated exponent from Fig. 5	Expected value
tagged line in 2D, $L = 512$	-0.35 ± 0.02	-0.35
bulk in 2D, $L = 512$	-0.81 ± 0.03	-0.81
tagged plane in 3D, $L = 64$	-0.47 ± 0.02	-0.48
bulk in 3D, $L = 128$	-0.97 ± 0.04	-0.97

B. The GLE formulation for driven Ising systems

The GLE formulation (19)–(20) also describes the anomalous response of the model to external magnetic fields. Starting from Eq. (22) and focusing on the response to an external field $f_{\rm ext} = B$ switched on at $t = 0$, we readily obtain the results of Eq. (12) for the tagged magnetization induced for times $1 \lesssim t \lesssim L^{z_c}$ by taking an ensemble average that reduces the noise terms $g(t)$ and $q(t)$ to zero; specifically,

$$\begin{aligned} \langle M_{2D,l}(t)\rangle &\sim BLt^{(\gamma/\nu-1)/z_c} \approx BLt^{0.35},\\ \langle M_{2D,b}(t)\rangle &\sim BL^2t^{\gamma/(\nu z_c)} \approx BL^2t^{0.81},\\ \langle M_{3D,p}(t)\rangle &\sim BL^2t^{(\gamma/\nu-1)/z_c} \approx BL^2t^{0.48},\\ \langle M_{3D,b}(t)\rangle &\sim BL^3t^{\gamma/(\nu z_c)} \approx BL^3t^{0.97}, \end{aligned} \tag{29}$$

which have been verified already in Fig. 4.

V. DISCUSSION

In summary, in this paper we report that the Ising models in two and three dimensions exhibit ubiquitous anomalous diffusion behavior at the critical temperature. We have performed four case studies for this: the bulk magnetizations in 2D and 3D and magnetization of a tagged line in 2D and that of a tagged plane in 3D. We have argued that the anomalous diffusion

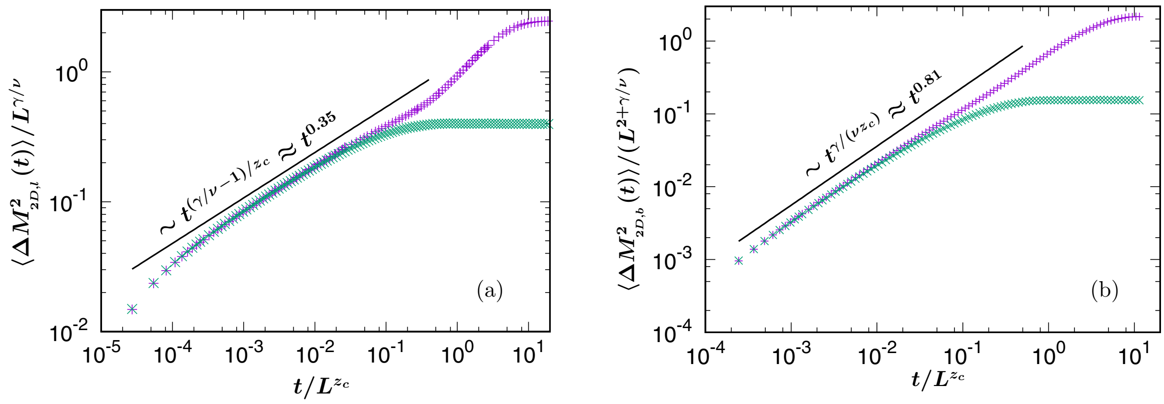

FIG. 6. Comparison of the mean-square displacement for the line [Fig. (a), system size $L = 128$], and bulk [Fig. (b), system size $L = 64$] magnetizations for the Ising model in 2D, with periodic boundary conditions (magenta pluses) and free boundary conditions (green crosses). The data for the two different boundary conditions are on top of each other in the scaling regime, differing only at late times.

stems from a time-dependent restoring force that involves a power-law memory kernel. We have derived these power laws as well as the corresponding L-dependent prefactors.

Further, we have shown that the physics of anomalous diffusion in the Ising model bears strong similarities to that in polymeric systems, allowing us to propose a GLE description for anomalous diffusion in the Ising model. We have also numerically verified that the anomalous diffusion for the tagged magnetizations in the Ising model belongs to the fractional Brownian motion (fBm) class, although we do not explicitly report it in this paper. We have numerically tested the specific aspects of the GLE (such as the FDTs), and the GLE description is also consistent with the observed anomalous response of magnetizations to externally applied magnetic fields. In a future paper, work on which is already in progress, we will expand the GLE formulation to the Ising model around the critical temperature.

Having said the above, we have not mathematically proved the GLE or the fBm, for the Ising model. Some other kinds of models may also be consistent with the anomalous diffusion behavior observed by us in this paper. They should, however, feature restoring forces, transient response to an external magnetic field, and a negative velocity autocorrelation function (observed in Fig. 7), in a consistent manner as presented here. In particular, we note that the Ising model we study here is at equilibrium at T_c, and therefore time reversible, so anomalous diffusion models that are developed for time-irreversible aging-type systems will not be applicable here.

Finally, we believe that the anomalous diffusion of the order parameter at the critical temperature can be found in other Ising-like systems, and, if so, the GLE formulation introduced in this paper can be employed to describe those anomalous behavior as well. In particular, if we know the critical temperature T_c and the critical exponents γ and ν for a specific Ising-like system, then this method can be used to obtain the critical dynamical exponent z_c from the power laws as well as the scaling of the terminal time $\sim L^{z_c}$ (in other words, anomalous diffusion can be effectively used to measure the critical dynamic exponent z_c). We will test these ideas in future work.

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APPENDIX A

In this appendix we demonstrate, in Fig. 6, using two examples, that the deviations from the power-law behavior at late times, as seen in Fig. 1, are indeed caused by the periodic boundaries.

APPENDIX B

In this appendix, in Fig. 7 we present a verification for the Green-Kubo relation used to convert the vecolity autocorrelation function (24) to anomalous diffusion (25): i.e., for an anomalous diffusion exponent c the velocity autocorrelation function anomalous exponent must be $c - 2$, as well as having an overall negative sign in front.

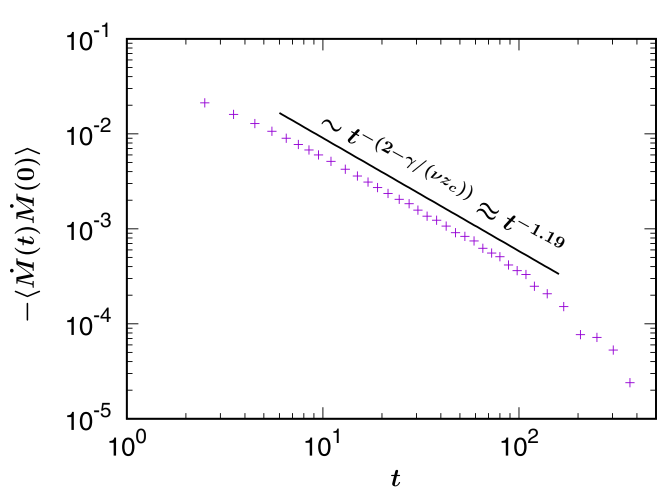

FIG. 7. Velocity autocorrelation function $\langle \dot{M}(t)\dot{M}(0)\rangle$ of the 2D bulk magnetization as a function of t. This quantity is negative, and behaves $\sim -t^{-2-\gamma/(\nu z)} \approx -t^{-1.19}$. The system size used in the simulation is $L = 30$.

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