

Low Temperature Static and Dynamic Behaviour of the Easy-Axis Heisenberg Antiferromagnet on the Kagome Lattice

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The antiferromagnetic Heisenberg model with easy-axis exchange anisotropy on the Kagome lattice is studied by means of Monte Carlo simulations. From equilibrium properties, we find that the values of the critical exponents associated with the magnetization at the critical temperature T_c vary with the magnitude of the anisotropy. On the other hand, the spin-spin autocorrelation functions have a stretched exponential behavior with a power law divergence of the relaxation time at a glass-like temperature $T_g \sim T_c$. From non-equilibrium dynamics at a fixed temperature below T_g , aging effects are found which obey the same scaling laws as in spin glasses and polymers.

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I. INTRODUCTION

The Kagome spin system has attracted much interest, both theoretically and experimentally. Because the geometry of the lattice consists of corner sharing triangles in a layer which surround hexagons, spin systems are highly frustrated when antiferromagnetic interactions are present¹. In the case of the nearest-neighbour antiferromagnetic spin 1/2 Ising model, the ground state is disordered and the spin-spin correlation function decays exponentially² at zero temperature. This behaviour differs from that which occurs in other periodically frustrated 2d Ising lattices such as the triangular and fully-frustrated square lattices where the correlation function decays as a power law^{3,4}. Frustration also leads to a larger macroscopic entropy⁵ in the Kagome lattice compared to the triangular lattice⁶.

The classical isotropic Heisenberg antiferromagnet on the Kagome lattice also has a ground state with macroscopic degeneracy. Various perturbations such as quantum fluctuations⁷⁻⁹, or the addition of other couplings including further neighbour interactions¹⁰, easy plane¹¹ or easy-axis anisotropy¹² and Dzyaloshinski-Moriya interactions¹³, have a strong effect on the ground state manifold. There has been a great deal of controversy about whether magnetic order^{10,14,15} exists in the ground state or if it remains disordered⁷⁻⁹. Two particular coplanar and ordered states, called the $\mathbf{q} = 0$ and the $(\sqrt{3} \times \sqrt{3})$ configurations, are favoured by entropy effects and this effect is often referred to as order by disorder. The latter ordered state¹⁶⁻¹⁸ is the one that is favoured or perhaps even a mixed disordered state of both structures¹⁹.

A chirality κ vector characterizes these ordered configurations and is defined as the pairwise vector product clockwise around a triangle:

$$\kappa = \frac{2}{(3\sqrt{3})} [\mathbf{S}_1 \times \mathbf{S}_2 + \mathbf{S}_2 \times \mathbf{S}_3 + \mathbf{S}_3 \times \mathbf{S}_1] \quad (1)$$

where 1, 2, 3 label the three sites in the unit cell and form three interpenetrating triangular sublattices. The two ordered states mentioned above are shown in figure 1 and correspond to configurations with uniform (ferromagnetic) and staggered (antiferromagnetic) chiralities respectively. The structure of these ground states allows for the formation of collective zero-energy spin rearrangements, called weathervane defects, that permit the system to explore the ground state manifold. These excitations involve the continuous rotation of the spins on two of the sublattices about the direction defined by the third. The defects may either traverse the entire lattice ("open" spin folds) as in the $\mathbf{q} = 0$ state or form localized loops ("closed" spin folds) as in the $(\sqrt{3} \times \sqrt{3})$ state^{10,11,16} (see figure 1).

It is known that most quasi-two dimensional magnetic materials exhibit some kind of spin anisotropy which may be of the easy-axis²⁰ or easy-plane²¹ type. Easy-plane 2d magnets have attracted attention due to the possibility of a topological Kosterlitz-Thouless phase transition which may exhibit glassy behavior different from that found in conventional site-disordered systems²¹. The amount of interest devoted to easy-axis magnetic systems has been considerably smaller, especially with regard to the study of dynamical properties. Kuroda and Miyashita¹² (KM) have previously studied the Ising-like Heisenberg antiferromagnet on the Kagome lattice using Monte Carlo methods. They have shown the existence of a phase transition at very low temperature with an exotic ordered phase which has no spatial long-ranged order and hence shares some similarities to spin glasses. In the present work we study both the equilibrium and dynamic properties of this model.

The paper is organized as follows: in section II we describe the model and our methods of calculation. Section III describes the equilibrium properties of the model and the critical exponents deduced from finite size scaling. Results for the spin-spin autocorrelation function are also given in this section. A good fit is obtained using a

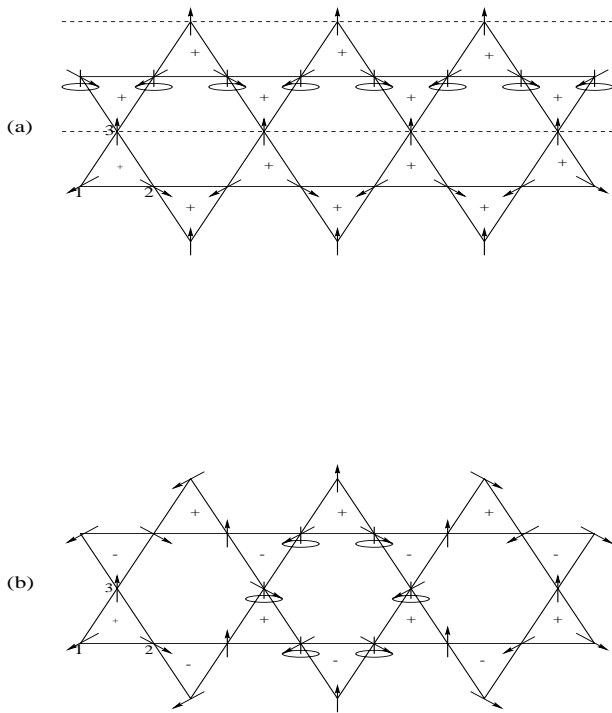


FIG. 1: Isotropic Heisenberg antiferromagnet on the Kagome lattice: (a) the $\mathbf{q}=0$ state in which the spins on each of the sublattices are parallel to each other and make an angle of 120° with the spins on the other two sublattices and (b) the $(\sqrt{3} \times \sqrt{3})$ structure has a larger unit cell. The + and - on the triangles indicate the chirality and the circles describe the open and closed spin folds in the states $\mathbf{q}=0$ and $(\sqrt{3} \times \sqrt{3})$ respectively.

functional form which has been used to describe 3d spin glasses²² and other complex systems^{23–25}. A characteristic timescale τ diverges with a power law at a temperature close to the static critical temperature. In section IV, we study the dynamical behavior below the critical temperature. The spin-spin autocorrelation function exhibits aging effects characteristic of glasses. We summarize our results in section V.

II. MODEL AND METHODS

The model is described by the following Hamiltonian

$$H = J \sum_{i < j} (S_i^x S_j^x + S_i^y S_j^y + A S_i^z S_j^z). \quad (2)$$

where $(S_i^\alpha, \alpha = x, y, z)$ represents a classical three component spin of unit magnitude located at each site i of a Kagome lattice and the exchange interactions are restricted to nearest-neighbour pairs of sites. The parameter A describes the strength of the exchange anisotropy. We restrict our attention to the case where $A > 1$ represents an easy-axis anisotropy. The limit $A \rightarrow 1$ cor-

responds to the isotropic Heisenberg model whereas the limit $A \rightarrow \infty$ corresponds to an infinite spin Ising model. The model has a macroscopic ground state degeneracy for all $A \geq 1$.

The ground state of the system for $A > 1$ corresponds to a planar configuration in which the spins on each triangle form a distorted 120° state with a net nonzero magnetization in the $\pm z$ -direction whose magnitude is related to A as $|m^z| = \frac{A-1}{A+1}$. Monte Carlo snapshots of the spin configurations at very low temperatures reveal an exotic phase for which there is no evidence of long-ranged spatial order of the individual spins. However, both the magnetization and heat capacity exhibit critical behaviour at a finite temperature T_c consistent with that of a 2d ferromagnetic Ising model¹².

We employ Monte Carlo methods using a single spin flip heat bath algorithm to study lattices containing N spins with periodic boundary conditions. The number of spins is related to the number of unit cells as $N = 3L^2$, where L is the number of up-triangles in the horizontal direction. We have calculated various thermodynamic observables such as the internal energy, the specific heat, the z -component of the magnetization as well as the associated susceptibility and Binder cumulant²⁶. Our numerical data are analyzed by using finite size scaling theory and the histogram method^{17,27,28} to extract the critical exponents of this model. A reweighting method is combined with our single spin flip algorithm in order to obtain the observables as continuous functions of temperature near T_c . We first measure the specific heat using the MC simulations on a discrete temperature grid and this step yields an estimate of the temperature T_0 at which the specific heat is maximum. Using this estimate, the histogram $\Omega_0(E)$ of the number of spin states with energy E is constructed from MC runs at the temperature T_0 over a large time interval Δt . This procedure allows us to obtain the average value of any observable Q as a continuous function of temperature T near T_0 as follows

$$\langle Q \rangle = \frac{\sum_E Q(E) \Omega_0(E) e^{-(T^{-1} - T_0^{-1})E}}{\sum_E \Omega_0(E) e^{-(T^{-1} - T_0^{-1})E}} \quad (3)$$

where $Q(E)$ is the microcanonical average of the observable. This method has been used quite successfully to extract critical exponents of both discrete²⁷ and continuous^{17,28,29} spin models.

We have also studied dynamical properties of this model by considering the double-time spin-spin autocorrelation function

$$C(t, t_w) = \frac{1}{N} \langle \sum_i S_i^z(t_w) S_i^z(t + t_w) \rangle \quad (4)$$

To measure this quantity at a given temperature T we start from a random configuration at high temperature and rapidly quench to the working temperature T . We then wait for a time t_w and measure the autocorrelation function $C(t, t_w)$ for subsequent times t . The results are averaged over many random initial states. In equilibrium

one expects $C(t, t_w)$ to be independent of t_w and it is only in equilibrium that one can define a meaningful timescale associated with relaxation. In the aging regime, $C(t, t_w)$ is waiting time dependent^{30,31}. Aging is a general phenomenon which occurs in a wide variety of off-equilibrium materials, as for example glasses. The phenomenon has been widely studied in disordered systems such as spin glasses²², frustrated systems²³ and in the phase ordering kinetics of the Ising ferromagnet²⁵, and is associated with a slow domain dynamics.

III. EQUILIBRIUM PROPERTIES

We have used our MC method to study lattice sizes $L = 6, 12, 18, 24, 36, 48, 60$ and have used $1 - 5 \times 10^5$ Monte Carlo steps (MCS) for performing our measurements after discarding the first 5×10^4 MCS to reach thermal equilibrium. In the reweighting analysis, it is important to take Δt as large as possible to have good statistics. We have used $\Delta t = 1.2 \times 10^6$ to $\Delta t = 2.6 \times 10^6$ MCS for small and large lattice sizes respectively. Also, because the energy is continuous, we have used both 10000 and 30000 bins for the histograms in order to check that the size of the bins did not affect our numerical results. In the results that follow, the magnitude of the exchange constant J is set equal to unity.

The critical temperature, T_c , can be determined by comparing the reduced Binder cumulant of the magnetization, $U_L = 1 - \langle M_z^4 \rangle / 3 \langle M_z^2 \rangle^2$, for lattices of size L with lattices of size $L' = bL$ as shown in figure 2(a) for the case of the anisotropy parameter $A = 2$. In the limit of large system sizes, the cumulants should cross at the critical temperature^{32,33} and have a common value $U_L = U^*$. However, due to finite size effects, it is necessary to extrapolate the crossing points to the limit $b \rightarrow \infty$ ³³. Our results using the Binder cumulant crossing method²⁶ to estimate the critical temperature are presented in figure 2(b). The points represent the temperatures at which the order parameter cumulant for L' crosses the cumulant for $L = 12$ or $L = 15$. There is considerable scatter in the data and care must be taken to use only results with L' sufficiently large to be in the asymptotic region where a linear extrapolation is justified ($\frac{1}{\ln b} \leq 2.2$). Using this method, the critical temperature is estimated to be $T_c = 0.077 \pm 0.001$. This value is slightly lower than the one obtained by KM from phenomenological renormalization of the magnetization but lies within their error bars. No hysteresis is observed in the order parameter nor in the energy near the critical region. In addition, no double peak structure was found in the energy histograms and the Binder energy cumulant evaluated at T_c yielded the result $U^* = 0.666665(7)$ for large L , consistent with the value $\frac{2}{3}$ expected for a continuous transition³⁴.

Finite-size scaling results for the order parameter M_z , the first temperature derivative of its Binder cumulant, the susceptibility $\chi = \frac{N}{T} (\langle M_z^2 \rangle - \langle M_z \rangle^2)$ and

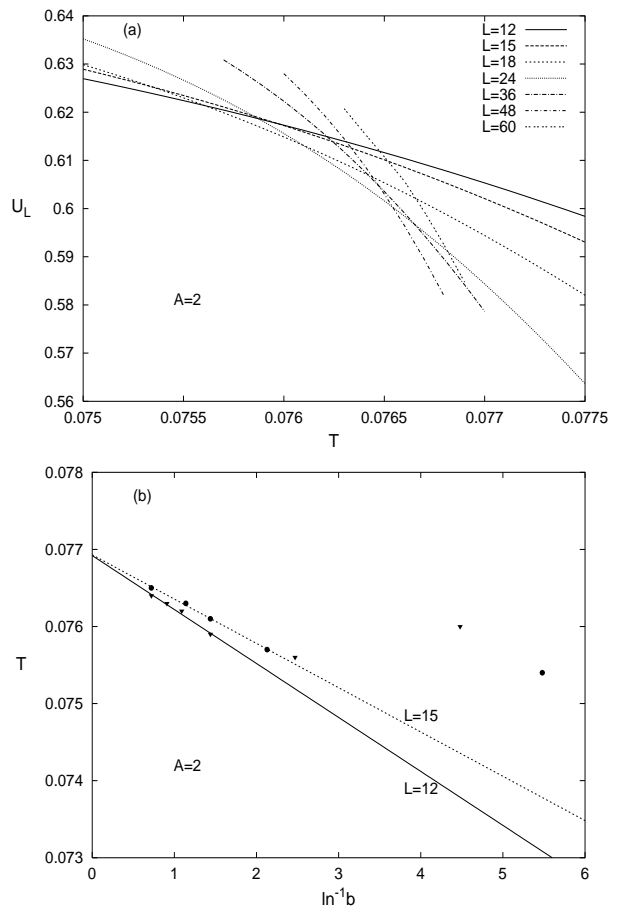


FIG. 2: (a) The order-parameter Binder cumulant U_L ($12 \leq L \leq 60$) plotted vs T obtained by optimized reweighting in the case $A=2$. (b) Estimates for T_c plotted vs inverse logarithm of the scale factor $b = L'/L$.

the specific heat are shown in figures 3 (a-d) respectively on a log-log scale. According to the standard theory of finite size scaling, the equilibrium magnetization M_z should obey the relation $M_z \sim L^{-\beta/\nu}$ for sufficiently large L . Figure 3(a) shows our results of a finite size scaling analysis for the order parameter M_z . Excluding the smallest two lattice sizes $L = 12$ and 15 from the fitting procedure, we obtained the value of the exponent ratio $\beta/\nu = 0.20 \pm 0.02$ which is significantly larger than the 2d Ising value $\beta/\nu = 1/8$.

The behavior of the reduced Binder cumulant U_L at the critical point can be used to find the value of the critical exponent ν . Finite size scaling theory predicts at T_c that $U_L = U_0(tL^{1/\nu})$ with $t = |1 - T/T_c|$ and the temperature derivative of U_L at T_c should obey the relation $U'_L(T_c) = L^{1/\nu} U'_0(0)$. In figure 3(b) we show that this prediction is obeyed quite well. The value of the static exponent ν obtained using a least-squares fit is $1/\nu = 0.98 \pm 0.02$, which is remarkably close to the two dimensional Ising value $\nu = 1$. The magnetic susceptibility χ has the scaling form $\chi \sim L^{\gamma/\nu}$ and figure 3(c) shows a least squares fit to our results using this form

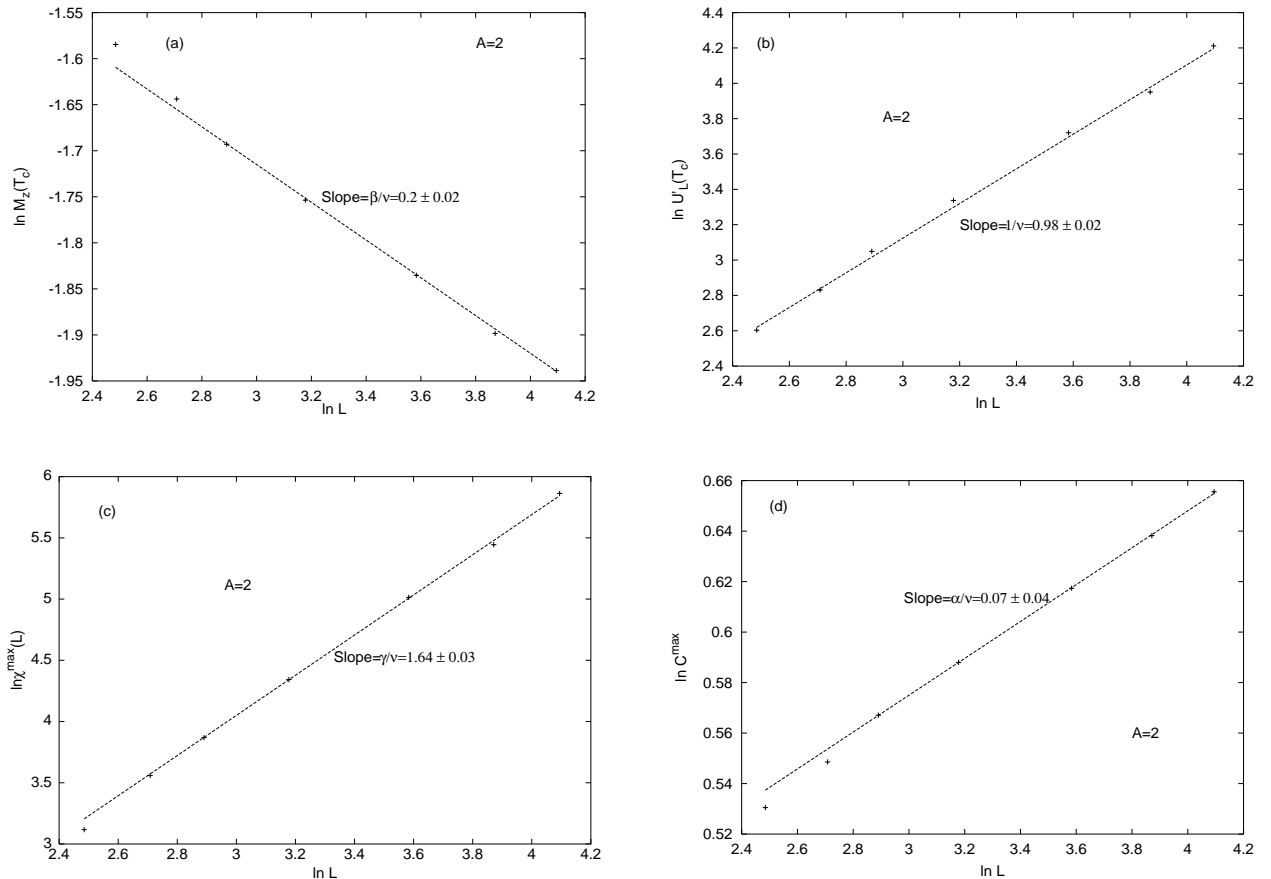


FIG. 3: Finite size scaling dependence of the critical properties for $A = 2$ (a) The order parameter M_z at T_c , (b) the temperature derivative of the Binder cumulant associated with M_z at T_c , (c) the maximum of the susceptibility χ^{max} and (d) the specific heat maximum C^{max} plotted as a function of L on a log-log scale.

and we find $\gamma/\nu = 1.64 \pm 0.03$ which is smaller than the 2d Ising value $\gamma/\nu = 7/4$ and also the value obtained by KM. The specific heat was also calculated but it is much more difficult to analyze because of the small number of points used and the scatter in the data was too large to extract a reliable estimate for α/ν . C_{max} should scale in the critical region as $C_L^{max} \simeq C_0 + aL^{\alpha/\nu}$, with C_0 representing the regular part. From our fitting procedure, $C_0 = 0$ yields the best straight line for large sizes with slope $\alpha/\nu = 0.07 \pm 0.04$.

The same analysis has been carried out for other values of the anisotropy A and the results are summarized in Table I. The critical temperature increases from zero for small deviations of A from unity, attaining a maximum near $A \sim 2$ and decreasing to very low temperatures for large A . The values of the critical exponent β/ν and γ/ν appear to depend on the value of A and approach the usual 2d Ising values only as $(A \rightarrow \infty)$. This non-universal behaviour of Ising-like exponents has also been reported for a two dimensional system of XY spins interacting via both ferromagnetic and antiferromagnetic bonds in the presence of an applied magnetic field which reduces the symmetry $O(2)$ in spin space to Z_2 ³⁵.

In order to understand the nature of this exotic struc-

ture in more detail, we have also looked at the spin-spin autocorrelation function using equilibrium dynamics at high temperatures where $C(t, t_w)$ becomes independent of t_w for $t_w > 10^4$. We fit our data with the following function²²,

$$f_0(t) = \frac{a}{t^{x(T)}} \exp(-(t/\tau)^{b(T)}) \quad (5)$$

where $a, b(T), \tau(T), x(T)$ are all fitting parameters. As shown in figure 4(a) for $A = 2$, our data are fairly well described by this functional form and we are able to extract the temperature dependent relaxation time $\tau(T)$ and the exponent $b(T)$. The behavior of these parameters is depicted in figure 4(b). The relaxation time τ appears to increase sharply as T is reduced and can be fit quite accurately by a power law divergence of the form

$$\tau \sim (T - T_g)^{-\phi} \quad (6)$$

The glass temperature, T_g , identified from the power law divergence of the relaxation time is slightly lower than the critical temperature T_c obtained from the equilibrium measurements for values of A which are not too large. For $A = 2$, it seems that there is a decoupling between

TABLE I: Results for the static critical temperature, T_c and the exponents γ/ν , β/ν and ν for various values of the anisotropy A . The last four columns are results obtained from high temperature equilibrium dynamics of the spin-spin correlation function $C(t, t_w)$: T^* is the temperature at which $C(t, t_w)$ first has a non-exponential behaviour; T_g is the critical temperature obtained from (6) where the relaxation time diverges; b_1 is the lowest value of the exponent $b(T)$ in (5) near T_g and ϕ is the relaxation time exponent in (6).

A	T_c	γ/ν	β/ν	$1/\nu$	T_g	T^*	b_1	ϕ
1.1	0.036 ± 0.006	1.44 ± 0.07	0.30 ± 0.05	0.97 ± 0.06	0.032 ± 0.001	0.05	0.76	1.5
2	0.077 ± 0.001	1.64 ± 0.03	0.2 ± 0.02	0.98 ± 0.02	0.071 ± 0.002	0.1	0.75	1.3
8	0.052 ± 0.003	1.67 ± 0.04	0.16 ± 0.01	1.09 ± 0.06	0.05 ± 0.001	0.055	0.85	0.74
30	0.022 ± 0.002	1.72 ± 0.04	0.128 ± 0.02	1.02 ± 0.04	0.022 ± 0.001	0.03	0.86	0.55

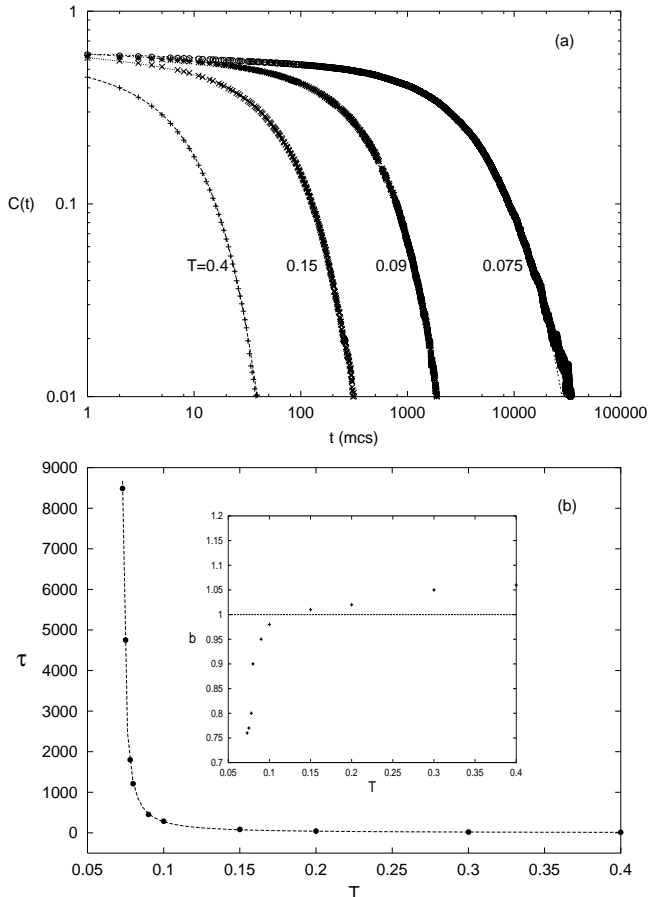


FIG. 4: (a) The spin-spin autocorrelation function for various temperatures, $T = 0.4(+)$, $T = 0.15(\times)$, $T = 0.09(*)$, $T = 0.075(\circ)$ for $A = 2$. The lines are fits to form given in (5) (b) The associated relaxation time as a function the temperature together with a fit to the power-law form (6). The inset shows the temperature dependence of the exponent $b(T)$.

the spin degrees of freedom and the net magnetization. At larger values of A the glass temperature T_g approaches the critical temperature T_c . As will be shown in the next section, T_g signifies the onset of aging phenomena and it is impossible to define a timescale below this temperature since the system is in a frozen glassy state.

The exponent $b(T)$ is plotted in the inset of figure 4(b). It is temperature dependent and lies in the range $b_1 < b < 1$ for $T_g < T < T^*$ where $b_1 = 0.75$, $T_g = 0.071$ and $T^* = 0.1$ for $A = 2$. The non-exponential behavior sets in at temperatures below T^* . The parameter $x(T)$ which characterizes the short time behaviour lies in the range $0 < x(T) < 0.1$ and decreases with temperature. A summary of our static and relaxation results for various values of A are given in Table I. The relaxation time exponent ϕ is also nonuniversal and decreases in value for larger values of A . Both non-exponential relaxation and a diverging relaxation time are features of glasses²² and this behaviour has previously been seen in frustrated systems without disorder²³.

IV. OFF-EQUILIBRIUM DYNAMICS

In order to further study the dynamics of this model, we have carried out some numerical experiments focused on revealing the presence of slow dynamics in conjunction with history-dependent phenomena which is generally referred to as 'aging'. These features are most easily found in simulations of the two-time autocorrelation function $C(t, t_w)$ which shows an explicit dependence on both times t, t_w over a wide range of time scales. Aging can be observed in real systems through different experiments. A typical example is the zero-field cooling experiments in which the sample is cooled in zero field to a subcritical temperature at time $t = 0$. After a waiting time t_w a small magnetic field is applied and subsequently the time evolution of the magnetization is recorded. It is often observed that the relaxation becomes slower as the waiting time t_w is increased.

We have measured the behavior of $C(t, t_w)$ as a function of the observation time t , for different values of t_w, A and T . We have used 1.5×10^5 MCS with a lattice size $L = 36$ and averaged the results over approximately 100 different trials. At high temperatures $T > T_g$, we found that the system does not exhibit aging since for any value of A the autocorrelation function $C(t, t_w)$ is homogeneous in time and independent of t_w .

In figures 5(a-b), the behaviour of the autocorrelation function clearly confirms the presence of aging in

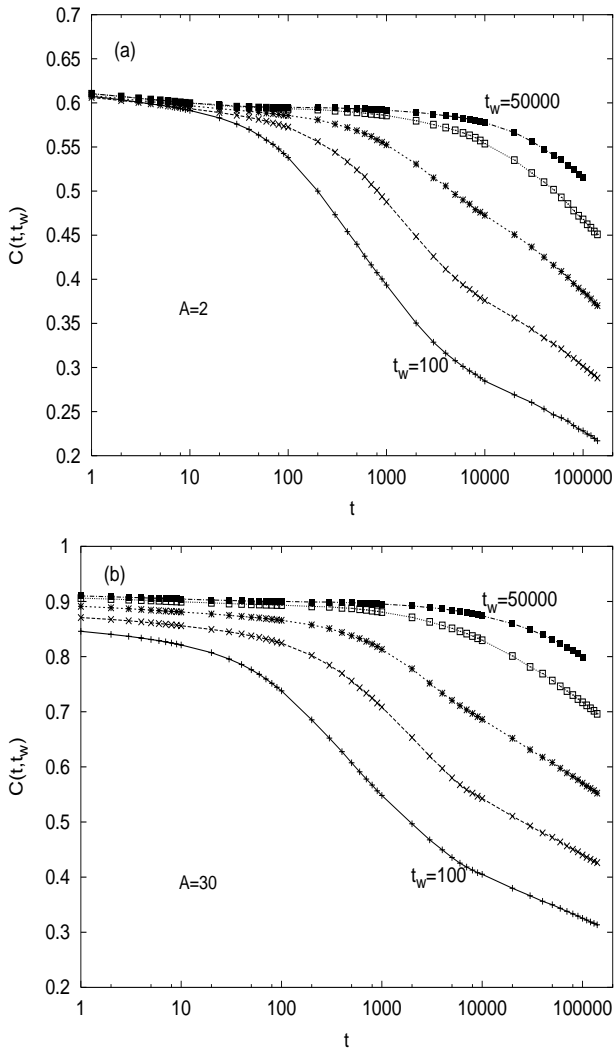


FIG. 5: Autocorrelation function $C(t, t_w)$ vs the observation time t for different waiting times t_w from bottom to top $t_w = 100, 500, 2000, 10000, 50000$ at (a) $T = 0.04$ for $A = 2$ and (b) $T = 0.01$ for $A = 30$.

this model for all values of $A > 1$ at very low temperatures $T < T_g$. For large waiting times and $t \ll t_w$, the correlations are independent of the waiting time t_w . However, for $t > t_w$, the curves show an explicit dependence on both times indicating that equilibrium has not been attained within the time of the simulation and the correlation falls to 0 for $t \rightarrow \infty$. This scenario has been called weak ergodicity breaking^{36,37}. The fluctuation dissipation theorem holds for short times but is violated at longer times.

We have attempted to find an appropriate scaling law for the aging curves. A knowledge of the scaling form could give some insight into the nature of the underlying dynamical process, even if there is no theoretical basis for determining the scaling functions. The simplest scenario

is naive aging of the form

$$C(t, t_w) = f\left(\frac{t}{t_w}\right) \quad (7)$$

in the region where both t and t_w are large.

In figure 6 we show $C(t, t_w)$ as a function of t/t_w to see if this naive form of scaling holds. Except for the largest value of $t_w = 50000$, we observe a departure from naive scaling with the function $C(t, t_w)$ increasing when $t > t_w$ and decreasing for $t < t_w$ at fixed values of t/t_w as t_w increases. A 'superaging' behaviour as observed in mean field spin glasses or the Sherrington Kirkpatrick (SK) model³⁸ could be expected for smaller waiting times but the fact that the curve for the largest waiting time, $t_w = 50000$, lies below the next smaller value, $t_w = 10000$, could be explained as follows: the system is in a 'subaging' scaling region where the relaxation of older systems becomes faster when plotted versus t/t_w although, when plotted versus t , the older the system appears to exhibit slower relaxation. Indeed, as seen in figure 7(a), a good collapse in the asymptotic region of the largest waiting times is obtained by using a variable used in glassy polymers³⁹ and recently in a topological spin glass^{21,37}, namely $[(t + t_w)^{1-\mu} - t_w^{1-\mu}]/(1-\mu)$ where in our case the value $\mu = 0.8 < 1$ is used. This subaging effect has not only been observed in glassy polymers³⁹ but also in 2d site-disordered spin glasses⁴⁰.

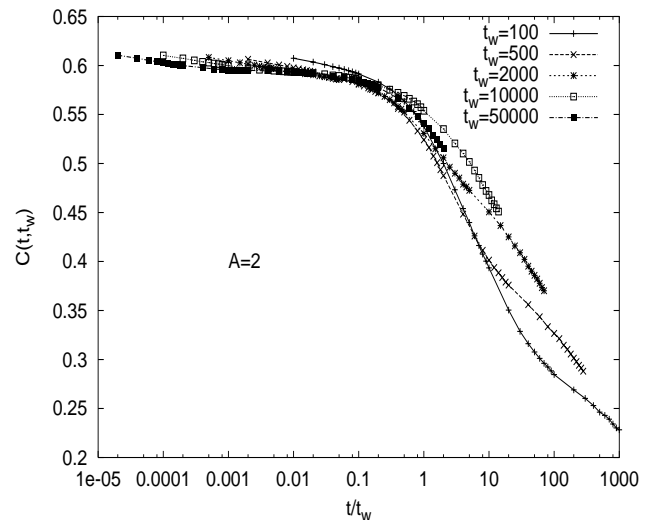


FIG. 6: Autocorrelation function $C(t, t_w)$ vs t/t_w at $T = 0.04$, for $A = 2$.

For larger values of the anisotropy, our analysis of the largest waiting times shows that simple scaling holds, compatible with the full aging scenario. Figure 7(b) shows the results for $A = 30$. This simple scaling has also been observed in the 3d Edwards-Anderson spin glass^{36,37,41}.

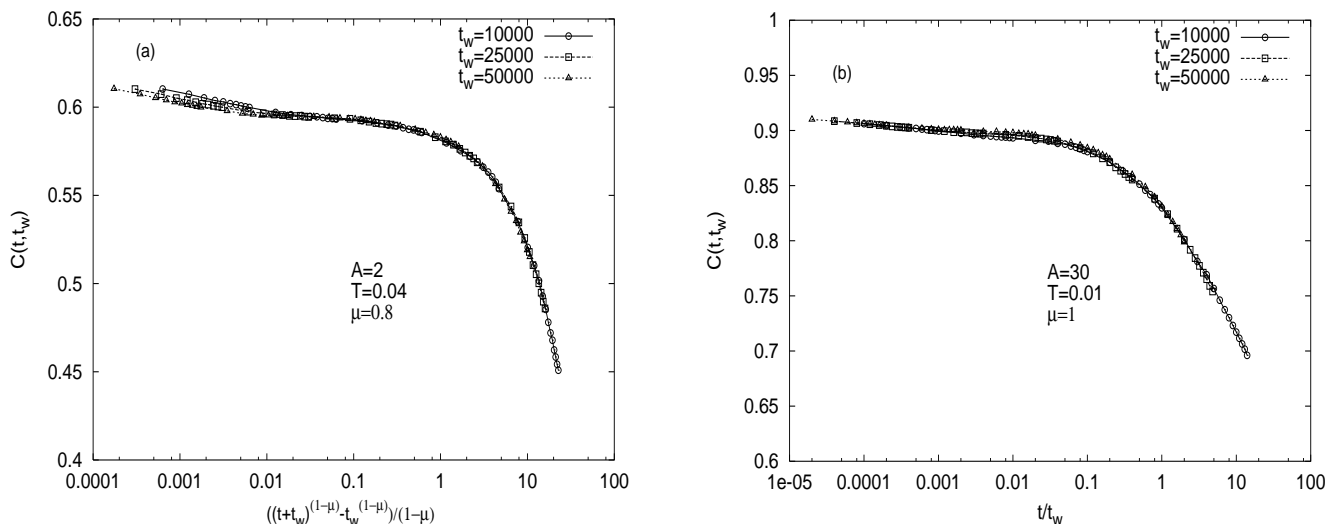


FIG. 7: Data collapse of the curves shown in figures 5(a,b) at large waiting times for (a) $T = 0.04$ and $A = 2$ as a function of the time reduced variable $[(t + t_w)^{1-\mu} - t_w^{1-\mu}]/(1-\mu)$ with $\mu = 0.8$ and (b) $T = 0.01$ and $A = 30$ as a function of t/t_w .

V. SUMMARY

In this work we have performed a numerical study of the two dimensional easy-axis Heisenberg antiferromagnet on the Kagome lattice by computing its static and dynamic properties. From the static properties, we have extracted the critical temperature and the critical exponents associated with the magnetization, the susceptibility and the correlation length respectively. Our result for the critical temperature obtained from the Binder cumulant method is in agreement with that obtained by KM¹² within statistical errors. On the other hand, our results for the critical exponents indicate that this system has a nonuniversal phase transition. Namely, the values of the exponents β and γ associated with the order parameter and the susceptibility vary with the magnitude of the easy-axis anisotropy A . However, α and ν remain unchanged and correspond within errors to the 2d Ising values. Although the magnetization indicates a finite T_c , Monte Carlo snapshots of the spins below this temperature do not indicate any long ranged spatial order. Rather, the individual spins appear to be in a frozen state similar to a glass.

We have studied the two-time spin-spin correlation function, $C(t, t_w)$, at high and low temperatures respectively. We have found that the high temperature equilibrium correlation function is described very well by the function $at^{-x} \exp(-(t/\tau)^b)$ suggested by Ogielski²² over the entire time and temperature range. The relaxation time, τ , increases according to a power law and diverges

at a temperature T_g where a transition to a glassy phase is located. Below T_g , we have found clear evidence for the presence of aging effects in the autocorrelation function from off-equilibrium dynamics. The spin-spin autocorrelation function depends on both times and the dynamics becomes slower for larger waiting times. An analysis of the autocorrelation functions from scaling forms used in polymer glasses and spin glasses has shown different behaviour. Namely, a sub-aging behavior at low values of A is seen where the relaxation time of the system grows more slowly than the waiting time t_w as observed in 2d spin glasses⁴⁰, polymer glasses³⁹ and structural glass⁴², whereas for large values of A , a full aging behavior describes the data well, where the relaxation time of the system scales with its age t_w as observed in 3d spin glasses^{36,41}. We are currently extending our investigations of this system to include the effects of a small applied magnetic field on the aging behaviour. This will enable us to check whether the fluctuation dissipation theorem is violated and to study the long-term memory of this model.

Acknowledgments

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