Journal of Magnetism and Magnetic Materials 140–144 (1995) 1493–1494

ELSEVIER

Journal of magnetism and magnetic materials

Simulation of spin dynamics on kagomé and square lattices

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Abstract

The spin–spin correlation function $\langle S(t)S(0)\rangle$ of classical Heisenberg spins on the kagomé lattice is numerically evaluated for varying concentrations of non-magnetic impurities. This function is also used to obtain the correlation time τ as a function of temperature for the kagomé and square lattices.

It has been shown that the Heisenberg model with an antiferromagnetic interaction between near neighbors on the frustrated kagomé lattice has some very unusual thermodynamical properties [1–4]. This suggests that the dynamical properties of the kagomé lattice are equally compelling, and we therefore simulate the time evolution of spins in this system and evaluate the spin–spin correlation function (SSCF). Since most of the experimental work on the kagomé lattice has been done on systems with non-magnetic impurities, we evaluate the SSCF for lattices with varying degrees of vacancy concentration. Using the SSCF, we also obtain the correlation time as a function of temperature $\tau(T)$. As a test case we compute the correlation time on the non-frustrated square lattice, as it is also 4-fold coordinated.

Our algorithm is designed to perform the following three tasks: (i) to solve the equations of motion $\dot{S}_i = -S_i \times \sum_{i:j} S_j$, where S_i is a three-component unit vector and the sum is taken over the nearest neighbors of the ith spin (employing periodic boundary conditions); (ii) to estimate $\langle S(0)S(t)\rangle = \sum_{IC}(\exp(-E/T)/Z)[S(0)S(t)]_{IC}$, where the sum is taken over initial conditions (IC), E is the total energy of the system, T is the temperature, [ ] denotes the sample average, and Z is the partition function; and (iii) to obtain the correlation time $\tau = \int_0^\infty \langle S(0)S(t)\rangle \, dt$. This algorithm is fully described in Ref. [5].

In Fig. 1 we show the SSCF for the kagomé lattice at $T = 0.01$ for several values of the non-magnetic impurity concentration (x). It is clear that the initial relaxation rate of the SSCF is nearly independent of the impurity concentration, even for values of x larger than the percolation threshold ($1 - p_c = 0.3473$) [3]. This result indicates that the dynamic on the kagomé lattice is mostly governed by local excitations and does not involve a collective motion of spins on the lattice.

We also see that the terminal value of the SSCF ($\langle S(4000)S(0)\rangle$) increases as x increases. This behavior is expected since as x increases, more and more spins become isolated and stay correlated at all times. In the inset of Fig. 1 we show the terminal value of the SSCF as a function of x. This value is determined by fitting the SSCF at greater time values to an exponentially relaxing function, as demonstrated by the broken line for the $x = 40\%$ case. At an impurity concentration smaller than the percolation threshold, the terminal value of the SSCF is consistent with zero, but as we cross the threshold this value goes up dramatically. It should also be pointed out that the SSCF has a zero derivative at $t = 0$, as predicted by several authors [6].

In Fig. 2 we show τ (normalized by $\tau(10)$) as a function of temperature for three different sizes of kagomé

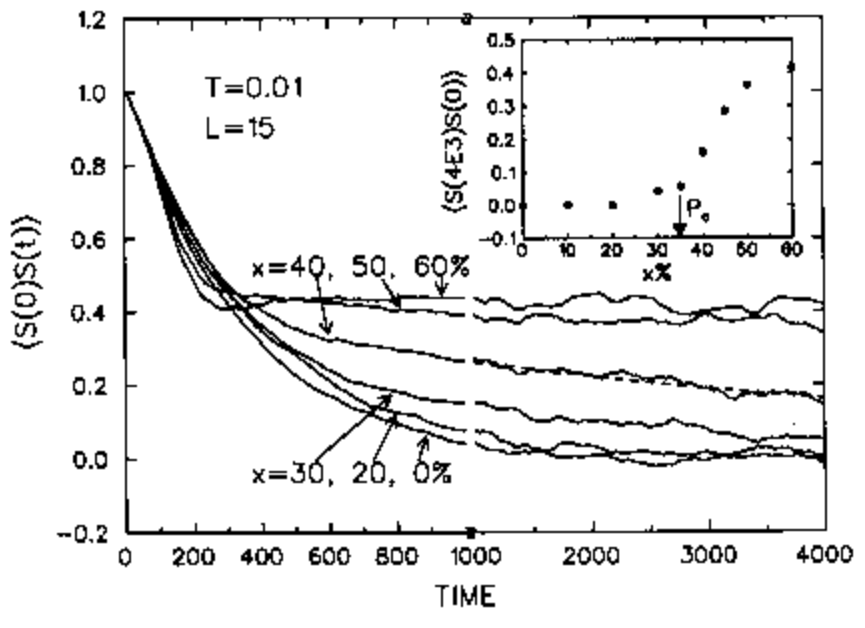

Fig. 1. Spin–spin correlation function for various values of the non-magnetic impurity concentration x. The broken line demonstrates a fit to an exponential at greater time values with which we obtain the terminal value of this function. The inset shows the terminal value as a function of x.

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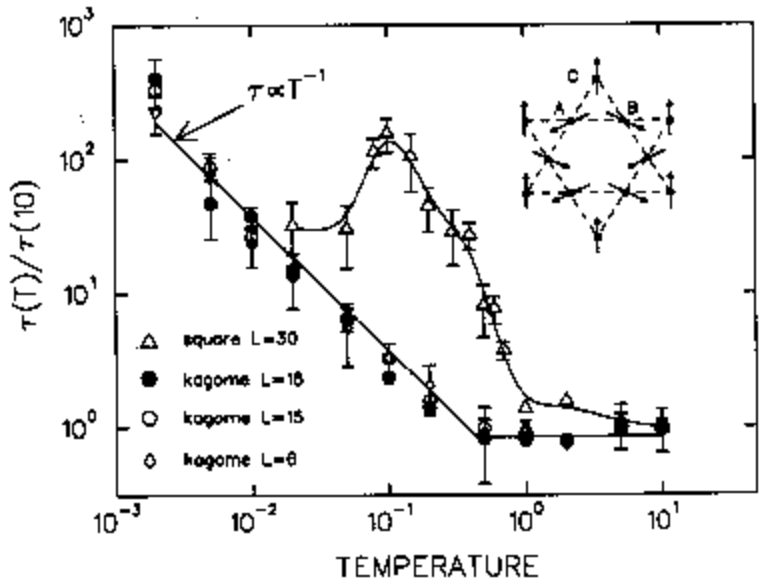

Fig. 2. Correlation time τ, normalized by $\tau(10)$, plotted against temperature. The normalization factors are: 1.12 in the square with $L = 30$ spins; 2.40 in the kagomé with $L = 18$ spins; 2.36 in the kagomé with $L = 15$ spins; and 1.17 in the kagomé with $L = 6$ spins. The solid lines and the inset are discussed in the text.

lattice, as well as for one square lattice. The solid lines are, in principle, guides for the eye. In the square lattice we see a maximum in τ at $T = 0.1$, while in the kagomé lattice τ is monotonically increasing with decreasing temperature. In addition, we see a very weak lattice-size dependence in the kagomé case.

The peak of τ in the square case is not surprising, since at $T \sim 0.5$ the correlation length reaches the lattice size and the system is effectively ordered [7]. However, the continuous increase in τ in the kagomé case, even for a small system, is not trivial. This is especially surprising in light of the increase, below $T = 0.01$, in the order parameter corresponding to the $\sqrt{3} \times \sqrt{3}$ state ($m_{\sqrt{3}}$) [4]. The spin arrangement in the $\sqrt{3} \times \sqrt{3}$ configuration is shown in the inset of Fig. 2 [4]. The order parameter $m_{\sqrt{3}}$ also increases with decreasing lattice size at $T \to 0$ [4]. These results, again, suggest that the difference between the square and kagomé lattices is due to a local motion of spins in the kagomé system.

The data shown in Fig. 2 are too noisy to be accurately fitted to a specific model of critical dynamics. Nevertheless, the diagonal line in the kagomé case below $T = 0.5$ is plotted using $\tau \propto T^{-\nu z}$, where $\nu z = 1$. As can be seen, this line is in agreement with the simulation results and also with the critical exponents $\nu = 1/2$ and $z = 2$. These exponents arise in several models of critical dynamics where the correlation length diverges near the critical temperature [8]. However, the simulation results indicate that $\tau(T)$ in the case of the kagomé lattice should be more appropriately described by a model which emphasizes the local modes.

References

[1] For a review, see E.F. Shender and P.C.W. Holdsworth, in: Fluctuations and Order: The new Synthesis, ed. M. Milonas (Springer-Verlag, Berlin, 1994).
[2] E.F. Shender, V.B. Cherepanov, P.C.W. Holdsworth and A.J. Berlinsky, Phys. Rev. Lett. 70 (1993) 3812; A.B. Harris, C. Kallin and J. Berlinsky, Phys. Rev. B 45 (1992) 2899; J.T. Chalker, P.C.W. Holdsworth and E.F. Shender, Phys. Rev. Lett. 68 (1992) 855; C. Zeng and V. Elser, Phys. Rev. B 42 (1990) 8436.
[3] A.F. Ramirez, G.P. Espinosa and A.S. Cooper, Phys. Rev. B 45 (1992) 2505.
[4] Jan N. Reimers and A.J. Berlinsky, Phys. Rev. B 48 (1993) 9539.
[5] A. Keren, Phys. Rev. Lett. 72 (1994) 3254.
[6] E.B. Brown, Phys. Rev. B 45, 10809 (1992); M.H. Lee, Phys. Rev. B 47 (1993) 8293.
[7] H. Shenker and J. Tobochnik, Phys. Rev. B 22 (1980) 4462.
[8] S. Ma, Modern Theory of Critical Phenomena (Addison-Wesley, Reading, MA, 1976).