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Computer simulation of the low-frequency spin dynamics in $Eu_xSr_{1-x}S$

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We report the results of a computer simulation of the low-frequency harmonic magnon modes in $Eu_xSr_{1-x}S$ for $x=0.8$ and 0.4. No evidence of hydrodynamic spin-wave modes is found in the spin-glass phase ($x=0.4$) for wave vectors $q \gtrsim \pi a/6$ (where a is the lattice constant), in contrast to the ferromagnetic phase ($x=0.8$) where ferromagnetic spin waves are present. Comparisons are made with experimental results for the reentrant spin-glass $Fe_{0.26}Cr_{0.74}$.

I. INTRODUCTION

Magnon excitations in Heisenberg spin-glasses are believed to make significant contributions to the magnetic specific heat and dynamic spin susceptibility in the low-temperature regime.[1] Despite the important role they play little is known about the nature of the excitations at very low frequencies. Hydrodynamic models[2] as well as equation-of-motion calculations[3] have suggested that the low-frequency magnons are weakly damped, propagating modes with a linear relation between frequency and wave vector. However, neither experiment nor a variety of computer simulations have given any evidence for such modes. Instead it was found that the structure in the imaginary part of the dynamic susceptibility, $\chi''(\vec{q},\omega)$, collapses to an apparent central peak in the limit as the wave vector $\vec{q}$ approaches zero.

The computer simulations have involved numerical studies of the dynamics of the Edwards-Anderson model[4] (a periodic array of spins with a Gaussian distribution of nearest-neighbor interactions) and the dilute fcc antiferromagnet with nearest-neighbor interactions.[5] In this paper we extend the numerical studies to a realistic model of the dilute fcc magnet $Eu_xSr_{1-x}S$ which in the low-temperature regime shows spin-glass behavior for $0.13 \lesssim x \lesssim 0.65$ and ferromagnetic ordering for $x > 0.65$.[6] Simulations of the spin dynamics of this system have been reported in several earlier publications.[7,8] In Ref. 7 the density of spin-wave modes was calculated along with the corresponding specific heat while in Ref. 8 $\chi''(\vec{q},\omega)$ was obtained from a continued fraction expansion. However as discussed in Ref. 4 due to finite "instrumental resolution" it is difficult to distinguish between a central peak and a very-low-frequency propagating mode. It was found that this problem could be largely circumvented by considering the sine transform of $\chi''(\vec{q},\omega)$ which is proportional to the correlation function $F(\vec{q},t)$ defined by

$$F(\vec{q},t)=(i/\pi)\sum_\alpha \langle [S_\alpha(\vec{q},t),S_\alpha(-\vec{q},0)]\rangle \ , \quad (1)$$

where $S_\alpha(\vec{q},t)$ ($\alpha=x,y,z$) denotes the spatial Fourier transform of the local spin operator:

$$S_\alpha(\vec{q},t)=\sum_{j-1}^{N} S_{\alpha j}(t)e^{i\vec{q}\cdot\vec{r}_j} \ , \quad (2)$$

$\vec{r}_j$ being the position of the jth spin. Were the susceptibility to be dominated by the contribution from a single, weakly damped propagating mode, $F(\vec{q},t)$ would vary as

$$\sin[\omega(\vec{q})t]\exp[-\lambda_{\vec{q}}t] \ ,$$

where $\lambda_{\vec{q}}$ is a measure of the width of the corresponding peak in $\omega^{-1}\chi''(\vec{q},\omega)$.

In Sec. II we display results for $F(\vec{q},t)$, $x=0.8$ and 0.4, for a variety of wave vectors. In the spin-glass phase ($x=0.4$) we find no evidence of weakly damped hydrodynamic spin-wave modes. Rather, it appears that the modes become overdamped as $q \rightarrow 0$. These results are in contrast to the behavior in the ferromagnetic regime, $x=0.8$, where there are hydrodynamic spin waves.

II. RESULTS

In this section we display our results for $F(\vec{q},t)$ for various values of $\vec{q}$ and x. The calculations were carried out for a dilute fcc (magnetic) lattice using experimentally determined values for the nearest- and next-nearest-neighbor exchange interactions which appear as parameters in the Heisenberg Hamiltonian

$$H=-2\sum_{(i,j)} J_{ij}\vec{S}_i\cdot\vec{S}_j \ . \quad (3)$$

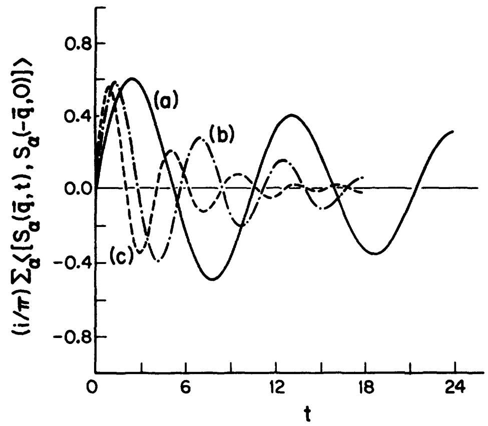

FIG. 1. $(i/\pi)\sum_\alpha \langle [S_\alpha(\vec{q},t),S_\alpha(-\vec{q},0)]\rangle$ $(\alpha=x,y,z)$ vs t for $x=0.80$. Time is measured in units of $\hbar$/K (7.64×10^{-12} s). Results from a single configuration of an array of 4×12^3 sites occupied by a fraction x of Eu ions. (a) $\vec{q}=(\pi/6)(2,0,0)$; (b) $\vec{q}=(\pi/6)(2,2,0)$; (c) $\vec{q}=(\pi/6)(2,2,2)$.

We took[9]

$$J_{\rm NN}=0.221 \text{ K} , \qquad (4)$$

$$J_{\rm NNN}=-0.100 \text{ K} . \qquad (5)$$

Since the procedures followed were identical to those outlined in our analysis of the Edwards-Anderson model we will not discuss them in any detail. All calculations were carried out on arrays of $4\times12^3=6912$ sites with a fraction x of them occupied at random by Eu^{2+} ($S=\frac{7}{2}$) ions. We assumed periodic boundary conditions so that the range of wave vectors was limited to $(2\pi/12)$ (n_1,n_2,n_3) (n_i integers). Thus the smallest wave vector corresponded to $(\pi/6)$ (1,0,0) in units of the reciprocal of the lattice constant $a=5.97$ Å.

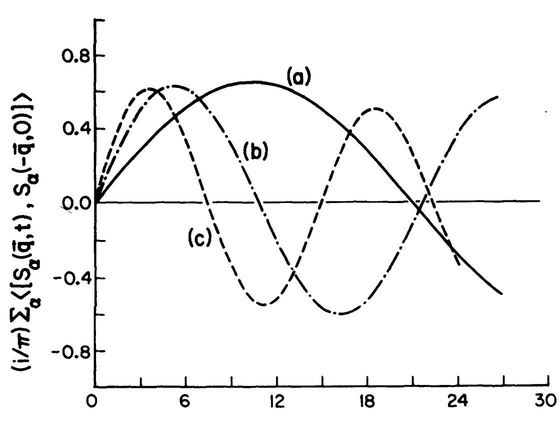

FIG. 2. Same as Fig. 1. (a) $\vec{q}=(\pi/6)(1,0,0)$; (b) $\vec{q}=(\pi/6)(1,1,0)$; (c) $\vec{q}=(\pi/6)(1,1,1)$.

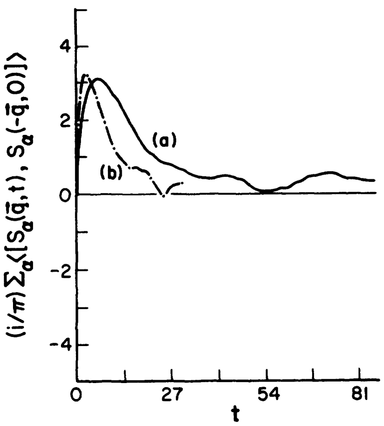

FIG. 3. Same as Fig. 1 except $x=0.4$. (a) $\vec{q}=(\pi/6)(2,0,0)$; (b) $\vec{q}=(\pi/6)(2,2,0)$. Note the contraction of the time scale relative to Figs. 1 and 2.

We calculated $F(\vec{q},t)$ for wave vectors $\vec{q}=(\pi/6)$ $(n,0,0)$ $(\pi/6)$ $(n,n,0)$, and $(\pi/6)$ (n,n,n) with $n=1,2$ and $x=0.8$ and 0.4. The results are shown in Figs. 1–4 where the correlation functions are plotted against time measured in units of $\hbar$/K ($\hbar$/K $=7.64\times10^{-12}$ s). Particularly noticeable is the qualitative change in the behavior between $x=0.8$ and $x=0.4$. The well-defined oscillations characteristic of the ferromagnetic phase become overdamped in the spin-glass regime. Calculations of the dynamic structure factor for $x=0.8$ indicate that the oscillations are associated with a spin-wave mode having a quadratic dispersion relation

$$\hbar\omega_q=Dq^2 , \qquad (6)$$

with $D=18\pm2$ K Å^2. This value is to be compared with the result for $x=1$ (EuS) $D=30$ K Å^2. The

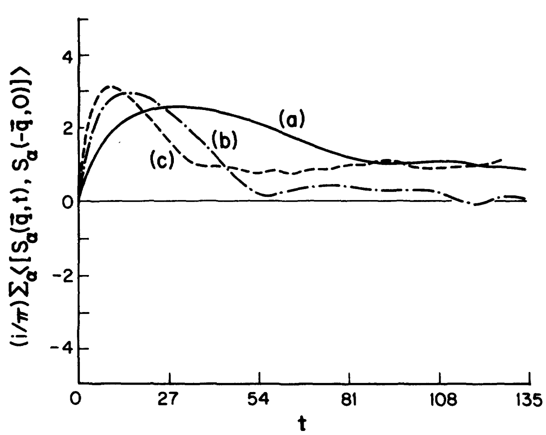

FIG. 4. Same as Fig. 1 except $x=0.4$. (a) $\vec{q}=(\pi/6)(1,0,0)$; (b) $\vec{q}=(\pi/6)(1,1,0)$; (c) $\vec{q}=(\pi/6)(1,1,1)$. Note the contraction of the time scale relative to Figs. 1 and 2.

behavior displayed in Figs. 1–4 is analogous to that found in inelastic neutron scattering studies of the reentrant spin-glass $Fe_{0.26}Cr_{0.74}$, where there are spin waves in the ferromagnetic phase which become overdamped as the temperature is lowered to the point where the system becomes a spin-glass.[10]

III. DISCUSSION

The low-frequency harmonic excitations in the spin-glass phase of $Eu_xSr_{1-x}S$ resemble those in the other spin-glass systems which we have studied in comparable detail. As in the Edwards-Anderson model and the dilute fcc antiferromagnet the modes are overdamped at small $\vec{q}$. We find no evidence for weakly damped spin-wave modes down to wave vectors

$$q \approx (\pi/6)(8.8\times 10^{-2}\text{Å}^{-1}) \;.$$

Two points must be kept in mind. First, the absence of hydrodynamic spin-wave modes in the spin-glass phase does not preclude the existence of high-q oscillatory modes mirroring the short-range order in the system.[5,8] Second, it must be emphasized that the term "damping" is being used in connection with the *zero-temperature* dynamic susceptibility. Since we are working within the harmonic approximation the excitations have an infinite lifetime. The decay of $F(\vec{q},t)$ reflects the dephasing of the various modes which contribute to the response at a particular wave vector. In contrast, in a translationally invariant system where $\vec{q}$ is a good quantum number only a single mode contributes so that $F(\vec{q},t)$ is an undamped sine wave.

It is apparent that there continues to be a significant gap in our knowledge of the magnon modes in spin-glasses. While the computer simulations have given quantitative information about the excitations they do not lead to a detailed understanding comparable to that provided by analytic theories of magnons in translationally invariant systems.

ACKNOWLEDGMENT

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