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Spin-Waves in Dilute Antiferromagnets

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Abstract

The effect of dilution on spin waves in isotropic Heisenberg antiferromagnets is studied. The model includes only nearest-neighbor interactions for a bcc lattice and spin-wave interactions are neglected, i.e. the results are correct in the limit s→∞. The dynamical susceptibility X (?,ω) and inelastic neutron cross section are obtained for arrays 8192 sites randomly occupied by a concentration c of magnetic ions. For a given array the calculation is done by inverting the dynamical matrix and thus is essentially exact. Our results are as follows. For large k we find that Ising-like resonances corresponding to different numbers of occupied neighboring sites become increasingly prominent as c is decreased. The envelope of these resonances agrees with previous results using the coherent potential approximation where fluctuations in environment are suppressed. For small k we find a single spinwave resonance broadened by the random dilution. The application of these results to $Mn_c\ Zn_{1-c}F_2$ is discussed.

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W. K. Holcomb and A. B. Harris

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SPIN-WAVES IN DILUTE ANTIFERROMAGNETS

W.K. Holcomb*, Oxford University, Oxford, England and
A.B. Harris**, University of Pennsylvania, Philadelphia, Pa. 19174

ABSTRACT

The effect of dilution on spin waves in isotropic Heisenberg antiferromagnets is studied. The model includes only nearest-neighbor interactions for a bcc lattice and spin-wave interactions are neglected, i.e. the results are correct in the limit $s\to\infty$. The dynamical susceptibility $\chi(\vec{k},\omega)$ and inelastic neutron cross section are obtained for arrays of 8192 sites randomly occupied by a concentration c of magnetic ions. For a given array the calculation is done by inverting the dynamical matrix and thus is essentially exact. Our results are as follows. For large k we find that Ising-like resonances corresponding to different numbers of occupied neighboring sites become increasingly prominent as c is decreased. The envelope of these resonances agrees with previous results using the coherent potential approximation where fluctuations in environment are suppressed. For small k we find a single spin-wave resonance broadened by the random dilution. The application of these results to $Mn_cZn_{1-c}F_2$ is discussed.

A large amount of effort has been spent studying the elementary excitations of random systems. Much of the effort has concerned itself with amorphous electronic problems, but real systems are difficult to describe in terms of models that are sufficiently simple that theoretical studies can be made. Any comparison between theory and experiment involves the difficult task of determining whether the model used is sufficiently accurate to place any real test on the theoretical approximations used. Similar comments are true for phonons in substitutional alloys. Thus much recent work has concentrated on magnetic alloys where simple models can be expected to describe the excitations accurately. The randomly diluted magnet is especially well suited for study since all the parameters in the model Hamiltonian can be determined from experiments on pure systems.

In this paper we study the randomly diluted isotropic Heisenberg antiferromagnet on a bcc lattice with lattice constant a for the purpose of clarifying the nature of the spin-wave dynamics. Explicitly, we consider the Hamiltonian

$$\mathcal{H} = s\Sigma_{ij} p_i p_j J_{ij}\left[a_i^\dagger a_i + a_j^\dagger a_j + a_i^\dagger a_j^\dagger + a_i a_j\right] \qquad (1)$$

where $J_{ij} = J$ if i and j are neighbor sites and $J_{ij} = 0$ otherwise, $p_i = 1$ or 0 depending on whether or not the site i is occupied by a magnetic atom and finally the operator a_i creates a spin deviation at the site i. In the pure case (all $p_i = 1$) many phenomena, in particular, those that do not selectively pick out long wavelength behavior are well described by the much simplier Ising model. In these cases it is the diagonal terms of (1) that are the most important. This suggests that in the dilute case one might expect to find peaks in the response function at the Ising energies corresponding to different numbers of occupied neighboring sites. Such structure has not been observed experimentally.[1,2] Previous theoretical work[1,3] has not analyzed this situation in an unbiased way. For example, the single site coherent potential approximation (CPA) for the system[3] neglects fluctuations in the number of neighbors and perforce predicts a singly peaked response. On the other hand, cluster theories[4] assume such fluctuations are the dominant effect and treat the off diagonal terms of 1 in a more approximate way and thus predict a highly structured response . In any event we expect the response at long wavelengths to have a single peak broadened and shifted from the perfect crystal value. This is because the long wavelength response samples the system in such a way that it is relatively insensative to the fluctuations.

In order to resolve the question of the existence of Ising-like structure in the dynamics we have studied the response of finite systems (8192 sites) using the technique developed by Harris[5]. We generate each system by occupying each site randomly with a nominal probability of c. The quantity of interest is the susceptibility

$$\chi(\vec{k},\omega) = \Sigma_{ij}\, e^{i\vec{k}\cdot(\vec{r}_i-\vec{r}_j)}\left[\omega\underset{\approx}{1}-\underset{\approx}{K}\right]^{-1}_{ij}, \qquad (2)$$

where $\underset{\approx}{1}$ is the unit matrix and $\underset{\approx}{K}$ is the dynamical matrix of the system using periodic boundary conditions. Here and below the indices i and j are restricted to magnetically occupied sites. The neutron scattering cross section is given essentially by

$$I(\vec{k},\omega) = \mathrm{Im}\,\chi(\vec{k},\omega - i0^+)/N, \qquad (3)$$

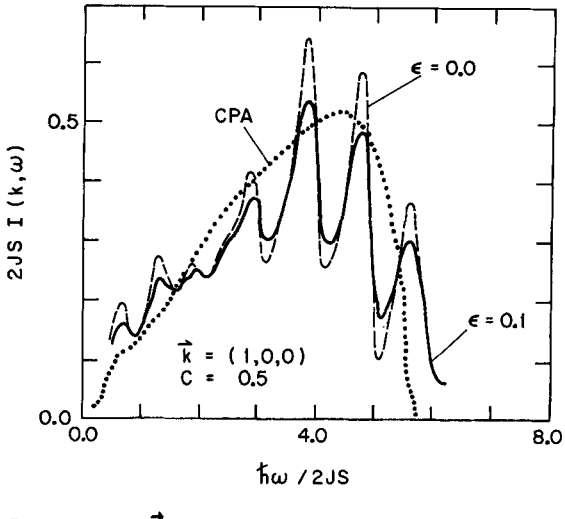
where N is the total number of sites and 0^+ is a positive infinitesimal. We find $\chi(k,\omega)=\Sigma_j x_j e^{-i\vec{k}\cdot\vec{r}_j}$ by solving the equation

$$\Sigma_j\left[(\omega - i\epsilon)\,\underset{\approx}{1} - \underset{\approx}{K}\right]_{ij} x_j = e^{i\vec{k}\cdot\vec{r}_i} \qquad (4)$$

for x_j. For each value of the parameters $\epsilon,\vec{k},\omega$ we study several samples and compute an average $\chi(\vec{k},\omega)$. To use this to represent the response on the infinite system we proceed as follows. We evaluate $\chi(\vec{k},\omega)$ only on the largest cluster and for most of the calculations ϵ was taken to be 0.1 (in units where 2Js = 1). This second step is necessary since the response for the finite system consists of a series of poles on the real axis ($\epsilon = 0$). We believe that by drawing a smooth curve through these points we have a resonable representation of the response of the infinite cluster in an infinite system. This is because besides the finite clusters which can be corrected for later, the only sharp states are the "blocked" states described by Eggarter and Kirkpatrick[6] and these are statistically rare. A plot of $I(k,\omega)$ for $\vec{k}$ at the zone boundary, $\vec{k} = (1,0,0)$, (We measure $\vec{k}$ in units of π/a.) and $\epsilon = 0.1$ is given in Fig. 1. We can extrapolate back to the real axis ($\epsilon = 0$) by taking

$$I(\vec{k},\omega) = \mathrm{Im}\left\{\chi(\vec{k},\omega - i\epsilon) + i\epsilon\, d\chi(\vec{k},\omega - i\epsilon)/d\omega\right\} \qquad (5)$$

and the second term can be estimated from our evaluation of $\mathrm{Re}\,\chi(\vec{k},\omega - i\epsilon)$. The results of such extrapolations are shown in Fig. 1. The importance of this extrapolation may be judged from the curves of Fig. 1. The



1. Response at $\vec{k}$ = (1, 0, 0) , c = 0.5 for ϵ = 0.1, solid curve; ϵ = 0.0 dashed curve; and the single site CPA also at ϵ = 0, dotted curve.

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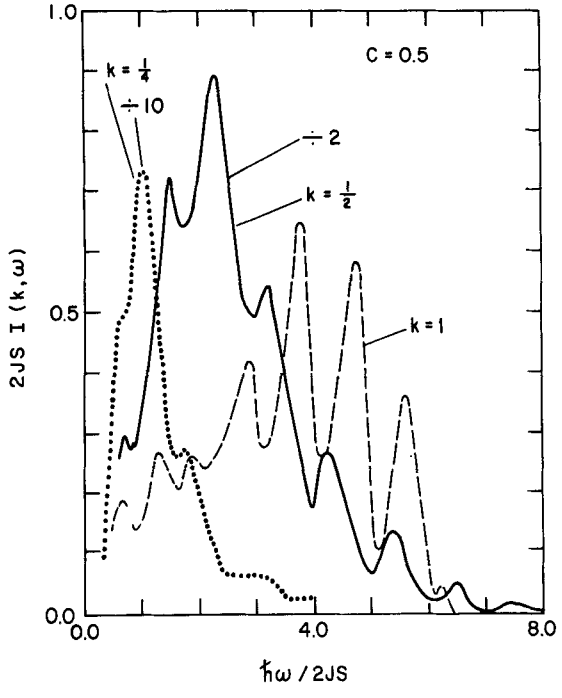
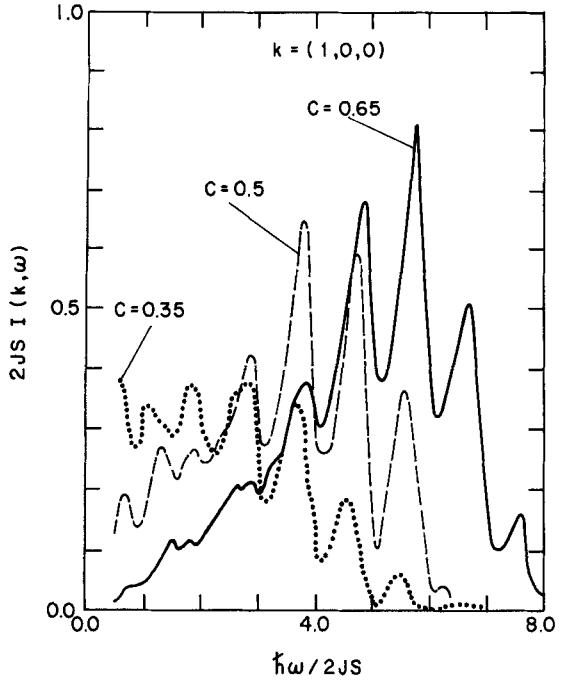
curves shown in Fig. 2 and 3 are also the results of this procedure, i.e. $I(k,\omega)$ averaged over several samples ($\epsilon = 0.1$) and then extrapolated to the real axis ($\epsilon = 0.0$). Corrections for the response due to finite clusters could be made by enumerating the smallest clusters and adding their response to that calculated above. This procedure will work except for concentrations too near the percolation concentration where large clusters become important.

The dependence on wavevector k is shown in Fig. 2 and the dependence on c is shown in Fig. 3. We see that for large k there is a sharp Ising-like structure. It is interesting to note that the peaks do not fall exactly at the Ising-energies of 1.0, 2.0, 3.0 ...(2Js). This is easy to understand as follows. If we treat the off diagonal terms of (1) as a perturbation then in second order the peak of the local density of states is shifted from the Ising-energy n (in units of 2Js) by an amount $\Delta E = -n/(n + zc)$, where z is the number of nearest neighbors. This is in agreement with our results: namely ΔE decreases as either c increases or n decreases. We also see that at small k the response goes over to a single peak as expected. This is even more pronounced in the results for k = (1/8, 0, 0) (not reproduced here) which is the smallest k we can examine for our sample sizes.

To determine if this structure is observable we must estimate the magnitude of spin-wave interactions. The Ising splitting is of order H_E/z where $H_E = 2Jsz$. Spin-wave interactions lead to a shift of order H_E/zs. If we concentrate on the case of $Mn_cZn_{1-c}F_2$ the Mn^{++} has $s = 5/2$ so this is not serious. Also in $Mn_cZn_{1-c}F_2$ we should consider the role of other neighbor interactions. If the exchange constant for the first ferromagnetic neighbor is denoted J' we have $J'/J \cong 0.2$. This could lead at worst to a splitting into peaks having relative energy shifts of 0, 0.2, and 0.4 (in units of 2Js = 1). This tends to increase the width of our peaks by 0.2 but the peaks should remain discreet. The resolution of current neutron scattering experiments[2] on $(MnZn)F_2$ is not sufficiently good to see this structure. The neutron scattering data is not inconsistent with our results. In fact the single site CPA which accurately describes the neutron scattering data[3] also accurately describes the envelope of the Ising peaks we calculate, as can be seen from the CPA curve given in Fig. 1.



2. $I(k,\omega)$ for c = 0.50 ϵ = 0,0 and $\vec{k}$ = (1,0,0) dashed; $\vec{k}$ = ($\frac{1}{2}$, 0,0) solid; k = ($\frac{1}{4}$, 0, 0) dotted.



3. $I(k,\omega)$ for $\epsilon = 0$ $\vec{k}$ = (1, 0, 0) and c = 0.65 solid; 0.5 dashed; and 0.35 dotted.

Finally we note that our technique is in principle applicable to the binary alloy. The main limitations are the time consuming nature of the calculation and the finite mesh size in space ($\Delta ak = \pi/8$).

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