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Static Properties of Dilute Ferri- and Antiferromagnets

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STATIC PROPERTIES OF DILUTE FERRI- AND ANTIFERROMAGNETS

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ABSTRACT

We report microscopic calculations of the static magnetic and spin-wave properties of dilute antiferromagnets (e.g. $KMn_{1-x}Zn_xF_3$) and of dilute ferrimagnetic garnets. The results are valid at low temperatures but are not restricted to low concentration of dilutents.

MACROSCOPIC THEORY

The energies of long wavelength spin waves can be expressed in terms of static quantities which can then be calculated either analytically or by Monte Carlo simulation. For ferromagnets, for example, the relation

$$\omega(q) = 2\gamma(A/M)q^2 \equiv Dq^2, \qquad (1)$$

where A is the exchange stiffness,[1] M is the magnetization per unit volume, and γ is the gyromagnetic ratio, can be derived from hydrodynamic arguments,[2] irrespective of the microscopic details of the system. The result derived for dilute ferromagnets in Ref. 3 by a microscopic calculation is a special case of Eq. (1).

The hydrodynamic[2] result for antiferromagnets is

$$\omega(q) = \gamma(2A/\chi^{\perp})^{1/2}q \equiv Cq, \qquad (2)$$

where $\chi^{\perp}$ is the susceptibility in the plane perpendicular to the staggered magnetization.

Spin excitations in ferrimagnets with oppositely oriented sublattice magnetizations, M_A and M_B, can also be treated by a classical continuum theory. The details of the calculation will be described later in a fuller paper. The main result is

$$\chi^{\perp}(\omega/\gamma)^2 + (M_A-M_B)\omega/\gamma - 2Aq^2 = 0. \qquad (3)$$

Here $\chi^{\perp}$ is a generalized perpendicular susceptibility, defined as the response, disregarding overall rotations of the magnetization, to magnetic fields, H_A and H_B, applied to the two sublattices, with the ratio of H_A to H_B such that no net torque results. Equation (3) has two roots given by

$$\omega(q) = [\omega_{opt}^2/4 + 2\gamma^2Aq^2/\chi^{\perp}]^{1/2} \pm \omega_{opt}/2, \qquad (4)$$

where

$$\omega_{opt} = \gamma|M_A - M_B|/\chi^{\perp}$$

is the frequency of the simplest optical mode at $q = 0$. When ω_{opt} is large, the smaller root reduces to the quadratic form of Eq. (1) with $M = |M_A-M_B|$. At compensation, $\omega_{opt} = 0$, and Eq. (4) reduces, as it must, to the linear antiferromagnetic result of Eq. (2). Near compensation, the dispersion relation has both quadratic and linear parts:

$$\omega(q) \approx 2\gamma(A/M)q^2 \quad \text{if } q \ll q^*, \qquad (5a)$$

$$\approx \gamma(2A/\chi^{\perp})^{1/2}q - 1/2\,\omega_{opt} \quad \text{if } q \gg q^*, \qquad (5b)$$

where $q^* = M/(2A\chi^{\perp})^{1/2}$.

MICROSCOPIC CALCULATION

The second step of the treatment is the calculation of the macroscopic quantities A and $\chi^{\perp}$ from the microscopic Hamiltonian, $\mathcal{H}$, describing the randomly diluted magnet. We take $\mathcal{H}$ to be

$$\mathcal{H} = -\sum_{ij}J_{ij}\vec{S}_i\cdot\vec{S}_j, \qquad (6)$$

where i and j are summed only over magnetically occupied sites and $\vec{S}_i$ is treated classically. We have used direct computer simulation, solving for the linear response of samples of 5000 or more spins to an applied field (for $\chi^{\perp}$) or to a weak spatial variation in the direction of magnetization (for A). Exact expressions at low dilution were obtained for all the simple lattices studied, in order to check the simulations.

To find A, we calculate the energy, E, needed to rotate the direction of magnetization through an angle θ ($\theta \ll 1$) over a distance L. Minimizing the total energy leads to the condition

$$\sum_j J_{ij}S^2(\theta_i - \theta_j) = 0 \qquad (7)$$

from which the equilibrium angle of the ith spin, θ_i, can be found. Then A is found from the relation,

$$E = 1/2\sum_{ij}J_{ij}S^2(\theta_i-\theta_j)^2 = A\theta^2\Omega L^{-2}, \qquad (8)$$

where Ω is the volume. Equation (7) is Kirchoff's law for a network of conductances in which we identify the θ_i as voltages and the $J_{ij}S^2$ as conductances. With this identification, equation (8) sums the power dissipation, IV, in each conductance. Thus, apart from units, A is the macroscopic conductivity of the equivalent disordered network.[3]

The determination of $\chi^{\perp}$ is similar. If the sublattice magnetizations are exactly equal, we may write the conditions on the equilibrium angular deflections in the presence of a perpendicular field, H, as

$$2\sum_{ij}(\theta_i+\theta_j)J_{ij}S^2 = (\gamma\hbar S)H. \qquad (9)$$

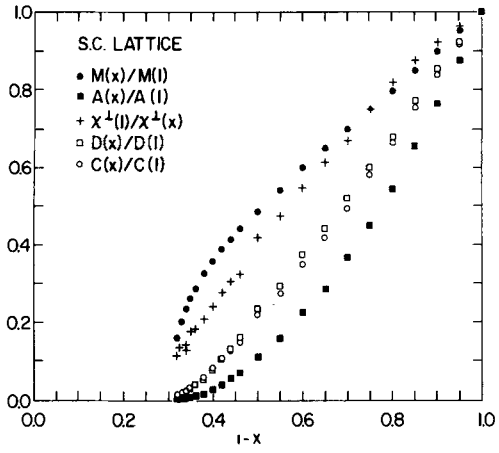
Then $\chi^{\perp}$ is determined by the analog of Eq. (8):

$$E = -1/2\gamma\hbar S\sum_i\theta_i H = -1/2\,H^2\Omega\chi^{\perp}. \qquad (10)$$

The above derivations are not limited to nearest neighbor interactions, but require only that the Neel state be a good approximation to the true ground state. Then the sublattice magnetization is proportional to the fraction of sites in the "infinite" occupied cluster. (For ferromagnetic Bravais lattices $M(x)/M(0)$ is equal to the percolation probability, $P(x)$.)

Our results for the simple cubic lattice are shown in Fig. 1. For $x \lesssim x_p$, we find $P(x) \propto (x_p-x)^{0.3\pm0.1}$, $A(x) \propto (x_p-x)^{1.6\pm0.2}$, and $\chi^{\perp}$ appears to diverge as $(x_p-x)^{-0.6}$. The divergence is cut off close to x_p in our calculations by effects of finite sample size. We attribute the divergence in $\chi^{\perp}$ to the occurrence of large regions of incompletely compensated magnetization. Fig. 1 shows that the effect of disorder on D and C is very similar. However, $D(x)/D(0)$ and $C(x)/C(0)$ have different slopes near $x = 0$, so they cannot be exactly equal.

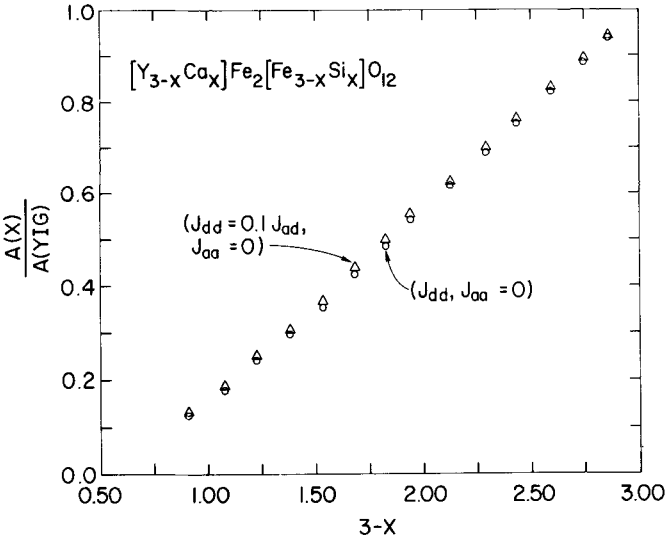
Since $T_c(x)$ is readily measured, many authors have sought to establish an empirical relation between $t \equiv T_c(x)/T_c(0)$ and either $d \equiv D(x)/D(0)$ or $a \equiv A(x)/A(0)$.



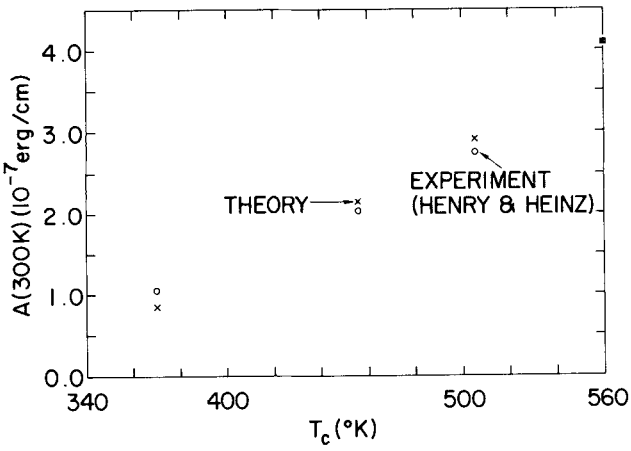
For small x the result for the sc lattice is $d(x)=1-1.53x$, $a(x)=1-2.53x$. High temperature series[4] calculations of $T_c(x)$ give $t(x)=1-1.37x$ for the sc lattice. The coefficients obtained for other 3D lattices are within .1 of these values. Clearly t and a are unrelated, while the equality between t and d is at best qualitative.

SUBSTITUTED GARNETS

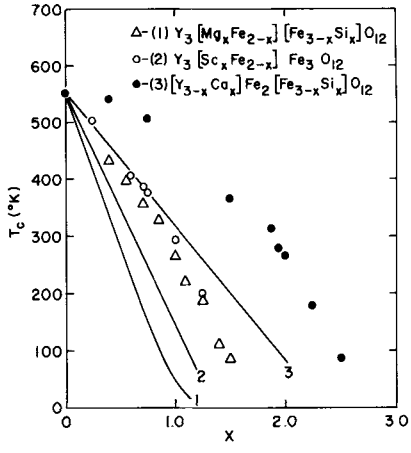
We have performed similar calculations for substituted garnets. Second neighbor interactions are small but nonnegligible in the garnets. In YIG, for example, van der Ziel et al[5] find $J_{ad}=-20cm^{-1}$, $J_{dd}=-2cm^{-1}$, and $J_{aa}=0$. However, for moderate doping or for substitution primarily into the majority sublattice, we find that the nearest neighbor approximation is accurate, as is shown by the two calculations of A in Fig. 2. Well above the percolation threshold, our results for a garnet with composition $Y_3Fe_{3(1-x)}Fe_{2(1-y)}M_{(3x+2y)}O_{12}$ may



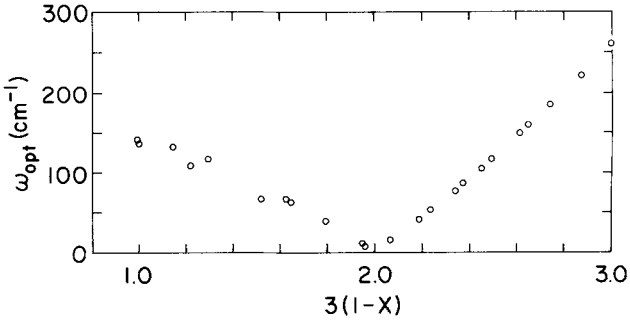
2. Calculated exchange stiffness, A, of YIG diluted on the majority sublattice only, with and without next-nearest neighbor interactions. The data (as well as those in Figs. 3-5) were obtained on Monte Carlo samples of 5x5x5 cubic unit cells, or 5000 Fe sites.



3. Comparison of calculated exchange stiffness for Ga-doped YIG with room temperature data of Ref. 6.



4. Comparison of measured (Ref. 7) T_c for three substituted YIG series and the values T_c would take (solid lines) if it were proportional to A.



5. Optical mode frequency for Si-doped YIG, calculated from Eq. (4).

be summarized by the relation

$$A(x,y)/A(0,0)=1-1.28x-1.45y+1.5xy. \qquad (11)$$

In the absence of low-temperature measurements of A on substituted garnets, we compare Eq. (11) with the recent room-temperature measurements of Henry and Heinz.[6] For this comparison we use the RPA result,

$$A(T)/A(0) = 4\langle S_a^z\rangle\langle S_d^z\rangle/25, \qquad (13)$$

where <> denotes a thermal average. To obtain the theory points in Fig. 3, we estimated the compositions not stated in Ref. 6 by comparison with the measurements of Geller et al.[7], and calculated $\langle S_a^z\rangle$ and $\langle S_d^z\rangle$ in a mean field approximation, with J_{ad} adjusted to give the observed ordering temperature, T_c. Agreement with experiment, as shown in Fig. 3, is excellent, but

due to the approximations made, it is hardly definitive.

For the dilute garnets, it is clear that $T_c(x)$ cannot be directly related to D(x). Several authors have suggested that t(x)=a(x). In Fig. 4, we test this relation by comparing the observed T_c's to the quantity a(x) for three families of diluted YIG. In no case is there qualitative agreement. In all cases, a(x) decreases more rapidly than t.

The generalized susceptibility needed to discuss the low-lying modes of Eq. (4) was calculated for Si-doped YIG. The resulting optical mode frequency, which should be experimentally observable, is plotted in Fig. 5.

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EXCITATIONS IN RANDOMLY DILUTED FERROMAGNET

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ABSTRACT

Dynamics of randomly diluted, quenched Heisenberg ferromagnet has recently been analyzed by several authors. Within an effective medium type of approach, the correct site aspect of this problem is best given by the recent work of Harris et al. Their theory, which introduces spurious degrees of freedom for the non-magnetic vacancies and then projects them out by the use of an appropriate pseudopotential, however, is applicable at low and intermediate concentrations of the nonmagnetic vacancies. For large vacancy concentrations, their results for the magnetic response leak over into the negative frequency region. Also in their theory the spin-wave stiffness becomes complex for relative vacancy concentrations of order 49%. Here we present an alternative effective medium approach to the study of this problem. We avoid the use of additional degrees of freedom for the vacancies by working directly with the equations of motion for the magnetic spins. Effective medium ansatz is introduced through the use of a generalization of the path CPA approach introduced by Brouers et al in their study of random electronic alloys. For low and intermediate vacancy concentrations, our results are found to be of comparable quality to those given by Harris et al. Moreover, the first three frequency moments of the response are preserved exactly in our work. On comparison with 'exact' results--obtained via Padé procedures making use of numerically computed frequency moments--we find that our theory continues to yield qualitatively reasonable results even when the vacancy concentration is large, e.g. 40% in a simple cubic lattice.

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