Magnon contribution to the magnetic specific heat of the spin-glass $Cd_{0.5}Mn_{0.5}Te$: $0.5\ K \leq T \leq 4.5\ K$

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We calculate the magnon contribution to the magnetic specific heat of the spin-glass $Cd_{0.5}Mn_{0.5}Te$. Good agreement is obtained with the measured values in the interval $0.5 \leq T \leq 4.5$ K with the interactions $J_{NN} = 10J_{NNN} = -12$ K and an anisotropy gap $\approx 2-4$ K. The theoretical results are obtained from a numerical calculation of the energies of the magnon modes in finite arrays of spins with ground-state configurations found by minimizing the energy of the corresponding classical Heisenberg Hamiltonian. The values chosen for the exchange integrals also account for the inelastic neutron scattering at $Q=(1,0,0)$, $T=1.8$ K.

I. INTRODUCTION

A number of previous studies have demonstrated that the magnetic specific heat at low temperatures of various metallic[1,2] and insulating[3] spin-glasses was dominated by the contribution from the magnon modes associated with small-amplitude spin oscillations. In this paper we show that a similar conclusion can be drawn in the case of the dilute magnetic semiconductor $Cd_{0.5}Mn_{0.5}Te$. As noted elsewhere,[4] $Cd_{1-x}Mn_xTe$ shows spin-glass behavior for $0.2 \leq x \leq 0.6$. For $0.6 \leq x \leq 0.7$ there is some evidence for an alternative type of disordered phase, while only mixed-crystal phases are obtained for $x > 0.7$. The Mn ions in $Cd_{1-x}Mn_xTe$ occupy sites on a fcc lattice, with antiferromagnetic exchange interactions between nearest and next-nearest neighbors. Estimates of the next-nearest-neighbor interaction J_{NNN} indicate that it is approximately $0.1J_{NN}$, where J_{NN} is the interaction between nearest neighbors.[5]

The magnitude of J_{NN} is a matter of some controversy. Specific-heat and susceptibility measurements[6] of pairs and triplets of Mn ions in dilute $Cd_{1-x}Mn_xTe$ indicate that $J_{NN} = -1.1$ K.[7] However, for $0.2 \leq x \leq 0.6$ one finds $J_{NN} \approx -15$ K from measurements of the paramagnetic Curie temperature.[8] Recently, inelastic-neutron-scattering data have been obtained for $Cd_{0.35}Mn_{0.65}Te$ at 1.8 K.[9] From a comparison between the measured and calculated spectra at $Q=(1,0,0)$ one infers $J_{NN} \approx -12$ K ≈ -1 meV.[9,10] As will be shown, one obtains a good fit to the magnetic specific heat in the interval $0.5 \leq T \leq 4.5$ K with this value of J_{NN}.

II. CALCULATION

The magnon contribution to the specific heat per mol of $Cd_{0.5}Mn_{0.5}Te$ is written as follows:

$$C(T) = 0.5RN^{-1}\sum_{\nu=1}^{N}\left[\frac{E_\nu}{k_BT}\right]^2 \frac{e^{E_\nu/k_BT}}{(e^{E_\nu/k_BT}-1)^2}, \quad (1)$$

where E_ν is the energy of the νth magnon mode and R is the gas constant. The calculation of E_ν in the case of $J_{NNN}=0$ is discussed in Ref. 11. Since the distribution of modes is virtually the same when $J_{NNN}=0.1J_{NN}$, we present only our results for $C(T)$.

Figure 1 shows the theoretical curves along with the experimental data from Ref. 6. The three curves are obtained using Eq. (1) and the combined data from four arrays of 250 spins. Each array was a $5\times5\times5$ fcc supercell

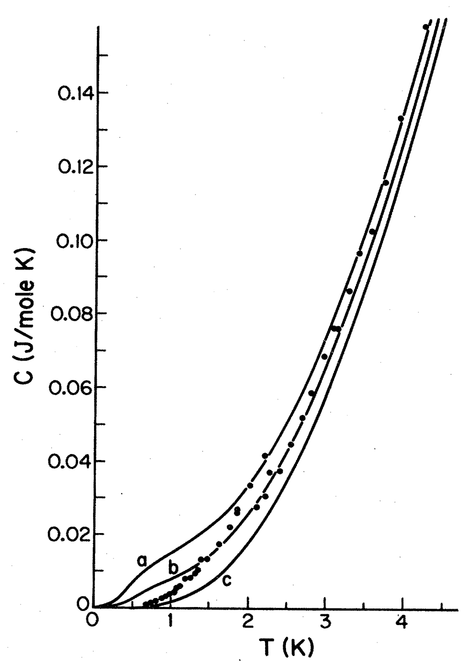

FIG. 1. Magnetic specific heat of $Cd_{0.5}Mn_{0.5}Te$. Curve a is the theoretical curve obtained with all eigenvalues. Curve b is the theoretical curve obtained omitting the lowest two eigenvalues. Curve c is the theoretical curve obtained omitting the lowest four eigenvalues. Solid circles are data points from Ref. 6.

with 500 sites, half of which were occupied at random by Mn ions. The calculations utilizied ground-state configurations obtained by minimizing the energy of the corresponding classical Heisenberg Hamiltonian. Periodic boundary conditions were assumed. The experimental data are the measured values of the specific heat from which the following have been subtracted: the nuclear contribution, $5.85\times10^{-3}T^{-2}$ J K/mol, and the lattice specific heat, 3889 $[T/\Theta_D(T)]^3$ J/(mol K), where $\Theta_D(T)$ is the effective Debye temperature. The latter is approximated by the effective Debye temperature of CdTe (Fig. 2 of Ref. 6). Curve a is obtained with the use of all of the eigenvalues. To simulate the effects of a gap in the spectrum due to dipolar anisotropy we have omitted the lowest two (out of a total of 1000) eigenvalues, $E_1=1.48$ K and $E_2=1.57$ K, in calculating curve b. Curve c was calculated by omitting the lowest four eigenvalues, $E_1,E_2,E_3=1.91$ K and $E_4=1.92$ K, with the first level counted having an energy of 4.39 K. We have limited the analysis to $T<4.5$ K since the rapid variation of the effective Debye temperature of CdTe above 4.5 K (Ref. 6) makes the approximation for the lattice specific heat somewhat doubtful at higher temperatures.

III. DISCUSSION

The results of the calculation show that the magnon excitations dominate the magnetic specific heat of $Cd_{0.5}Mn_{0.5}Te$ in the interval $0.5\leq T\leq4.5$ K. Similar to the cases of *Cu*Mn[1], *Pd*Mn,[2] and $Eu_xSr_{1-x}S$,[3] there appears to be no experimental evidence for a contribution from interconfigurational excitations, tunneling modes, etc. From a comparison between the experimental data and the theoretical curves, we infer the existence of an anisotropy gap on the order of 2–4 K. This value is somewhat below the usual estimate for antiferromagnets $2\mu_B(2H_EH_{\rm dip})^{1/2}=5.9$ K, in which μ_B is the Bohr magneton, H_E is the average exchange field $6J_{\rm NN}S/(2\mu_B)$, and $H_{\rm dip}$ is the dipolar field, $12\mu_BS/r_{\rm NN}^3$.

The results displayed in Fig. 1 depend on the choice of $J_{\rm NN}$. As noted, the value $J_{\rm NN}=-12$ K, which we use in our calculation, is consistent with the value needed to fit the inelastic-neutron-scattering data. However, it is 15–25 % less than the estimates obtained from the high-temperature susceptibility data. If we used the latter values we would obtain curves which were below the experimental data.

In conclusion, it appears that there is a good agreement between the measured and calculated values of the magnetic specific heat of $Cd_{0.5}Mn_{0.5}Te$ over the interval $0.5\leq T\leq4.5$ K. However, this conclusion is still somewhat tentative and can be made firm only with more precise values of the exchange integrals.

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