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CALCULATION OF THE STATIC MAGNETISATION OF METAMAGNETIC La_2CuO_4.

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Interactions in La_2CuO_4 are predominantly antiferromagnetic. However a strong field induced transition is seen in the static magnetic susceptibility which points to the existence of a net ferromagnetic moment in the CuO layers. Here, this net ferromagnetic moment is incorporated into a description of the CuO layers by the inclusion of a modified Dzyaloshinskii-Moriya term in the Hamiltonian. The spin wave spectrum in the presence of an applied field is calculated with this Hamiltonian and the ground state is determined as a function of applied field from the free energy. A calculation of the static magnetisation as a function applied field perpendicular to the CuO layers is used to determine the parameters of the model. Comparison is made with experiment.

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Metamagnetic behavior is seen as a very rapid change in the magnetisation at some critical applied field and corresponds to a field induced transition. This behavior is seen in many compounds, some of which are characterised by local moments and others in which there is also strong itinerant character. Among the local moment compounds La_2CuO_4 has been found to exhibit metamagnetic behavior by Cheong et al.[1] and by Thio et al.[2]. at temperature below approximately 500 K where it is in the orthorhombic phase. When doped with holes this compound becomes superconducting with the holes going into the CuO plane. Doped La_2CuO_4 is the simplest of the high temperature superconducting cuprates, whose physics are thought to be dominated by CuO planes, in that it has only one CuO per unit cell and does not have the complications of chains, etc. Consequently the study of the properties of the CuO plane in La_2CuO_4 helps in the understanding of the whole class of superconducting cuprates. In this compound the metamagnetism arises because the predominantly antiferromagnetic CuO planes each have a net ferromagnetic moment and these planar moments are coupled to adjacent planar moments antiferromagnetically. The metamagnetism then follows from the competition between this coupling and the effect of an externally applied magnetic field which wants to align the planar moments ferromagnetically. The net ferromagnetic moment of the CuO planes in the orthorhombic phase may be described by an effective spin hamiltonian for spins sitting on the Cu sites which contains a Dzyaloshinskii-Moriya term[3]. The form of this term in the orthorhombic phase has recently been determined by Coffey et al.[4] from the symmetries of the CuO planes and has been shown to lead to a net ferromagnetic moment per CuO plane. Experimentally[1] the moment is found to point out of the plane and this is incorporated into an effective spin hamiltonian by introducing an anisotropy into the Heisenberg part of the hamiltonian which breaks the continuous symmetry remaining in the ground state after the inclusion of the D-M term in the hamiltonian. So one finds that the hamiltonian describing the CuO plane is

$$H_{plane} = \sum_{<i,j>} \left\{ J_1\left[S_i^x S_j^x + S_i^y S_j^y\right] + J_2 S_i^z S_j^z + \mathbf{D}_{ij} \cdot \left[\mathbf{S}_i \times \mathbf{S}_j\right] \right\} \quad (1)$$

where $\mathbf{D}_{ij}=(d_1,d_2,0)$ if the bond between sites i and j is in the x-direction, $\mathbf{D}_{ij}=(-d_2,-d_1,0)$ if the bond is in the y-direction[4], and $J_1>J_2$.

Necessary requirements for this hamiltonian to lead to a net ferromagnetic moment per CuO plane are: (i) $\mathbf{D}_{ij}$ should alternate in sign from one bond to the next and (ii) d_1 and d_2 should be of opposite sign. (i) follows from the symmetries of the CuO planes and we shall assume (ii) for present purposes. The classical ground state of the hamiltonian in Eq.(1) has spins lying in a plane perpendicular to the (1,-1,0) direction and are tilted out of the xy-plane by an angle ϕ. If d_1 and d_2 have the same sign the ground state no longer has a ferromagnetic moment. The planar moment per Cu site is

$$\mu_{Cu} = S \sin\phi \, \mathbf{k} = S \sqrt{\frac{J_{DM} - \frac{J_1+J_2}{2}}{2J_{DM}}} \, \mathbf{k} \quad (2)$$

where S is the magnitude of the sublattice magnetisation per Cu site and J_{DM} is the effective in-plane coupling. In the present calculation the interaction between the planes is modelled by an effective interplanar coupling, J_p, of a spin in one plane with the ferromagnetic moment of its nearest neighbours in the adjacent planes. In the case where the applied magnetic field is low enough the planar moments are aligned antiferromagnetically and the energy of the system does not depend on the applied field. I refer to this as case (1) and the hamiltonian is

$$H = H_{plane} - Jp\sum_i S_i \cdot \frac{\mu_{Cu}}{\mu_B} \quad (3)$$

Case (2) is where the applied magnetic field, $\mathbf{B}_{applied}=B_0\mathbf{k}$, is sufficiently strong that the planar moments are aligned ferromagnetically. The hamiltonian for this case is

$$H = H_{plane} - \sum_i S_i \cdot \left(g\mu_B B_{applied} - Jp\frac{\mu_{Cu}}{\mu_B} \right) \quad (4)$$

The difference between the two hamiltonians is in the effective magnetic field in the z-direction. The spin wave spectra are given by

$$\omega^{(i)}(q)2 = \Omega_a(q)\Omega_b(q) - \Omega_c(q)^2 \quad (5.1)$$

$$\Omega_a(q)=4S\left\{\left[J'_{DM} + \frac{g\mu_B}{4}B^{(i)}_{effective}\sin\phi + \frac{J_1+J_2}{2}f(q)\right] + \frac{(J_1-J_2)}{2}\cos\phi\,[1+f(q)]\right\} \quad (5.2)$$

$$\Omega_b(q)= 4S\left\{\frac{J_1-J_2}{2}[1+f(q)] + J'_{DM}[1-f(q)] + \frac{g\mu_B}{8}B^{(i)}_{effective}\sin\phi\right\} \quad (5.3)$$

$$\Omega_c(q)= 4Sd_b\cos\phi\left[\frac{\cos(q_x) -\cos(q_y)}{2}\right] \quad (5.4)$$

$$J'_{DM}(B_{effective})= \frac{J_1+J_2}{2}\cos(2\phi) - d_a\sin(2\phi) \quad (5.5)$$

$$d_a=\frac{d_1-d_2}{\sqrt{2}} \quad \text{and} \quad d_b=\frac{d_1+d_2}{\sqrt{2}} \quad (5.6)$$

where the angle ϕ is specifiied by the condition that the ground energy be a minimum

$$\frac{J_1+J_2}{2}\sin(2\phi) + d_a\cos(2\phi) - \frac{g\mu_B}{4}\frac{\partial}{\partial\phi}\left[B^{(i)}_{effective}\sin\phi\right] = 0 \tag{5.7}$$

and the effective magnetic fields are

$$B^{(1)}_{effective} = \frac{J_pS}{g\mu_B}\sin\phi \quad \text{and} \quad B^{(2)}_{effective} = B_0 - \frac{J_pS}{g\mu_B}\sin\phi \tag{5.8}$$

In the above equations g is taken to be 2.2[7]. Examining the two spectra one sees that there are no gapless modes due to the anisotropy in the Heisenberg term, $J_1 > J_2$, and the presence of the D-M term. The size of the gap at q=(0,0) increases with applied field. The gaps in the spectra greatly reduce the effect of fluctuations and ensure that there is magnetic order at finite temperatures even for the purely two-dimensional hamiltonian, i.e. when J_p=0.

At zero temperature the free energy of case (2) is lower than that of case (1) for magnetic fields applied in the z-direction whose strength is greater than $B_c\ J_p\mu_{Cu}/g\mu_B$. Since μ_{Cu} is S, the temperature dependence may be incorporated into the model by substituting a mean field-like expression for S as a function of temperature. From this one can see that B_c decreases as the temperature approaches the Neel temperature which is taken to be 234K[1]. The ground state energies per site for the two hamiltonians are

$$E^{(1)}_g = -2S^2\left[\frac{J_1 - J_2}{2} + J^{'}_{DM} + \frac{J_p}{2}\sin^2\phi\right]S^2 \tag{6.1}$$

$$E^{(2)}_g = -2\left[\left(\frac{J_1 - J_2}{2} + J^{'}_{DM}\right)S^2 + \frac{1}{2}\left\{g\mu_B B_0 S - J_p S^2\sin\phi\right\}\sin\phi\right] \tag{6.2}$$

Magnetisation measurements[1,2], Raman spectroscopy[6], infra absorption[7] and neutron scattering[8] provide estimates for the various parameters in the spin hamiltonian. In particular the critical field, B_c, at T=0K is estimated by Cheong et al. to be 5.7T and this agrees very well with the value found by Thio et al. of (5.3+0.3)T. The jump in the value of the magnetisation at T=0K, $M_s(0)$, is found by Cheong et al. to be $3.0\times10^{-3}\mu_B$/Cu atom and by Thio et al.[2] to be $(2.1+0.2)\times10^{-3}\mu_B$/Cu atom. Lyons et al.[6] find an average value of the in-plane coupling strength to be 1100cm^{-1} =140meV from two magnon scattering and Collins et al.[7] found a value for the spin wave gap of 1.12meV. This agrees very well with the the value of the smallest spin wave gap which Peters et al.[8] found from neutron scattering to be (1.1+0.3) meV. They also found a value of (2.5+0.5) meV for the other gap. Using the expressions found above one obtains equations for the various parameters in the hamiltonians

$$B_c = \frac{2|\mu_{Cu}|}{g\mu_B^2} J_p = 5.7 \text{ Tesla} \qquad (7.1)$$

$$M_s(0) = g\mu_B S \left\{ \sin\phi + \frac{g\mu_B B_c}{4J'_{DM}} \right\} = 2.8 \times 10^{-3}\ \mu_B \qquad (7.2)$$

There is no magnetisation for case (1) in the present model and that of case (2) contains a contribution induced by the applied field calculated from equations (5.7) and (6.2). From equations (7.1) and (7.2) one finds, using S=1/2 at T=0K, $\sin\phi = 2.15\times10^{-3}$ and J_p=340meV. In the model $\sin 2\phi = d_1/J_{DM}$ and so d_1= 0.97meV. The values of these parameters may be checked against the expressions for the gaps in the spin wave spectra calculated in the absence of an applied magnetic field which are given by

$$\omega^{(1)}(0,0) = 4S\sqrt{\left\{J_{DM}' + \frac{J_1+J_2}{2} + (J_1-J_2)\cos\phi + \frac{g\mu_B}{4}B^{(1)}_{effective}\sin\phi\right\}\left\{J_1-J_2 + \frac{g\mu_B}{8}B^{(1)}\sin\phi\right\}} \qquad (7.3)$$

$$\omega^{(1)}(\pi,\pi) = 4S\sqrt{\left\{J_{DM}' - \frac{J_1+J_2}{2} + \frac{g\mu_B}{4}B^{(1)}_{effective}\sin\phi\right\}\left\{2J_{DM}' + \frac{g\mu_B}{8}B^{(1)}_{effective}\sin\phi\right\}} \qquad (7.4)$$

Using the values of the parameters found above one finds 1.9meV for $\omega^{(1)}(\pi,\pi)$. This is in reasonable agreement with the values found by Peters et al.[8] The value of the smaller gap, (1.1+0.3)meV[7,8], gives J_1-J_2 =.002meV. These estimates are roughly the same as those of previous authors although there is a spread of values because of the experimental uncertainitities. In Figure 1 the magnetisation is plotted as a function of applied field for different temperatures where J_1= 140meV, J_1-J_2=0.002meV, d_1=-d_2=0.7meV and J_p=340meV. Experimentally there are linearly increasing contributions to the magnetisation both above and below B_c. The contribution above B_c is identified with the moment induced by the applied field. However the effect is missing below B_c in the present simple model. The calculated magnitude of the susceptibilty is = $0.27\mathrm{X}10^{-3}$ μ_BTesla^{-1}/Cu site which agrees with the experiment numbers, $0.2\mathrm{X}10^{-3}$ μ_BTesla^{-1}/Cu site[1], fairly well.

In conclusion I have calculated the spin wave spectrum of an effective spin hamiltonian which describes the metamagnetic transition. The parameters found from the hamiltonian are consistent with those found by previous authors. The spin wave spectrum has no gapless modes so that the order survives at finite temperatures, as has previously been pointed out by Collins et al.[7], and so fluctuations effects have been neglected except in as much as the sublattice magnetisation has a temperature dependence given by mean field theory.

In the above analysis I took the parameters d_1 and d_2, describing the D-M term to have the same magnitude but have opposite sign. However starting from the t-J model one may estimate the D-M term from microscopic parameters so that one may obtain information on d_1 and d_2 separately[9]. Metamagnetic behavior is also seen in itinerant systems such as the heavy-fermions[10] as well as in other compounds where microscopic models should also be derived consistent with the symmetries of these systems. The author would like to thank K. Bedell and S. Trugman for useful conversations and to acknowledge the support for this work from the U.S. D.O.E. through the Los Alamos Advanced Studies Program in High Temperature Superconductivity Theory.

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Figure Caption:

Figure 1. Magnetisation as a function of applied field for different temperatures.

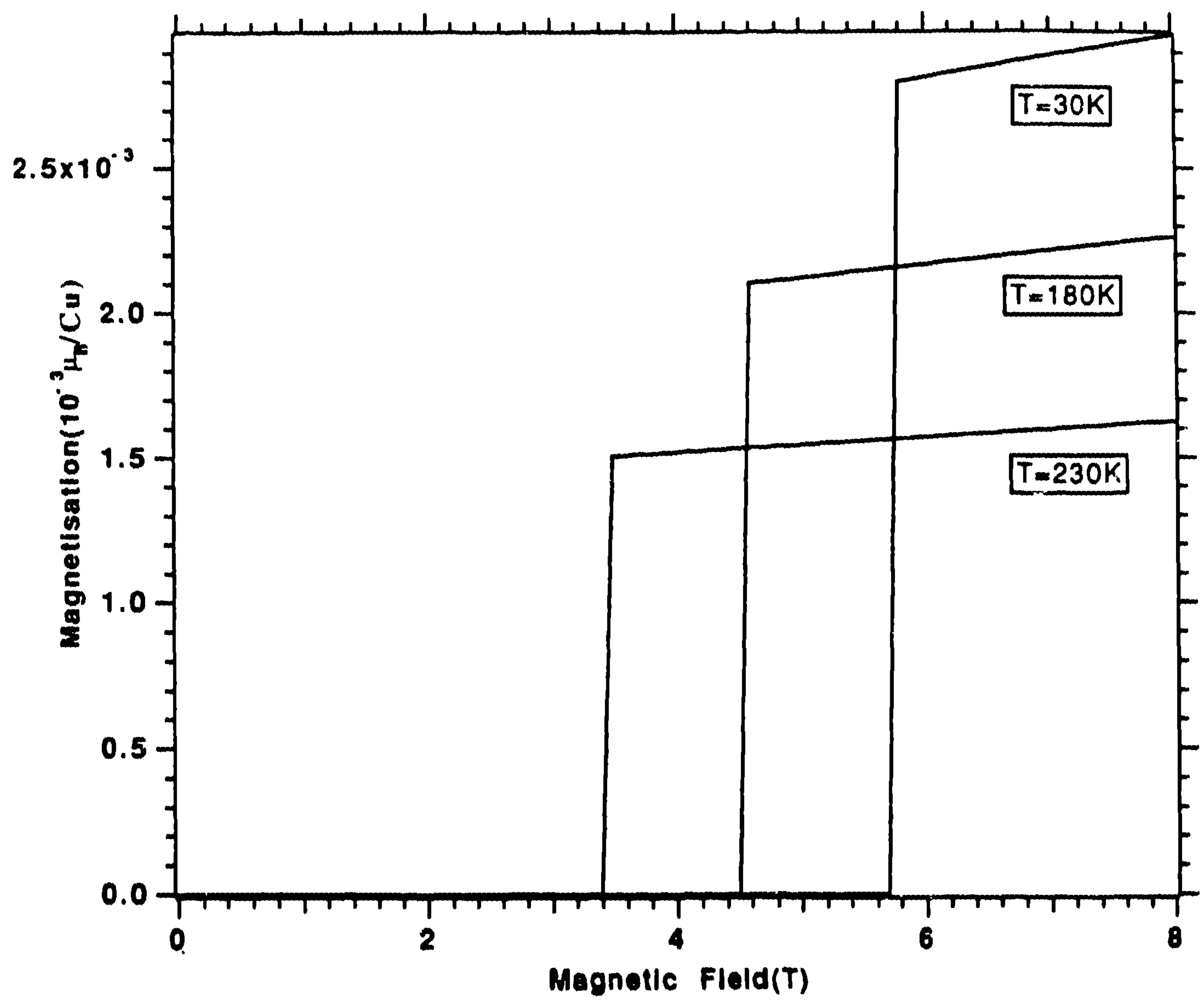
2.5x10⁻³
2.0
1.5
1.0
0.5
0.0
Magnetisation(10⁻³μB/Cu)
T=30K
T=180K
T=230K
0
2
4
6
8
Magnetic Field(T)

FIGURE 1.