Study of an amorphous ferromagnet by the coherent-potential approximation

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An amorphous ferromagnetic system has been studied by the coherent-potential approximation method at the zero-temperature limit. Going beyond the mean-field theories the present calculation predicts the existence of a critical fluctuation of the exchange interaction beyond which ferromagnetism cannot occur. A comparison with the Green's-function theory developed by Montgomery *et al.* reveals certain important differences.

I. INTRODUCTION

Since Gubanov[1] first predicted the existence of ferromagnetism in an amorphous material, there have been several reports of evidence indicating the existence of ferromagnetism in such a material.[2] Because of the changes in exchange interactions, the magnetic properties of an amorphous ferromagnet are, in general, different from those of a crystalline ferromagnet. The changes may be due to the difference in the interatomic distances (structural disorder) or the presence of some substitutional and interstitial impurities (quantitative disorder). There are as yet no satisfactory theories which have taken into account both types of disorder simultaneously. Most of the theories have been limited to studying of the quantitative disorder only. Recently, Montgomery, Krugler, and Stubbs (MKS)[3] have studied such a system in the mean-field approximation using the Green's-function technique. They have used a "lattice model" for an amorphous ferromagnet in which the spins are fixed on the lattice points, but the magnitudes of the exchange interactions are allowed to fluctuate stochastically. They find that disorder produces a low-energy peak and a high-energy tail in the density of spin-wave states for a simple cubic geometry. Also, the ferromagnetic Curie temperature is found to decrease linearly with the mean-square fluctuation of the exchange interation in their approximation. It should, however, be pointed out that their theory is basically a mean-field theory which is expected to be valid only in the weak-scattering limit.

Recently, Foo and Wu (FW)[4] have applied the coherent-potential approximation (CPA) to a substitutionally disordered Heisenberg ferromagnetic binary alloy. The CPA, which was first introduced by Soven,[5] has been proven to be a very powerful method in studying disordered systems. It serves as an interpolating scheme between the dilute and high concentrations and between the weak- and strong-scattering limits. By using the CPA, FW were able to predict successfully the existence of a critical concentration of antiferromagnetic impurities in a ferromagnetic host system. However both MKS and FW theories have neglected the spin fluctuations at the impurity sites, the effects which become important at finite temperature especially in the strong-scattering limit. Thus the accuracy of their calculation of the disorder-dependent Curie temperature is in question, since the spin fluctuation is expected to modify the Curie temperature. However at the zero-temperature limit, the spin fluctuations are expected to be negligible and one would expect the CPA calculation to be fairly accurate even for fairly strong scattering potentials. In this paper we apply the CPA to the aforementioned "lattice model" of an amorphous Heisenberg ferromagnet at zero temperature. It should be pointed out that another drawback of the FW calculation was that they had to neglect the correlations among the adjacent exchange interactions in applying the CPA to the substitutionally disordered ferromagnetic alloys. However in the present model of an amorphous ferromagnet, there exists no such correlations since the fluctuations of the exchange interaction are supposed to be completely random.

II. THEORY

The Hamiltonian for an amorphous ferromagnet which is approximately represented by the "lattice model" is given by

$$H = \frac{1}{2}\sum_{i,j} J_{ij}\vec{S}_i \cdot \vec{S}_j , \tag{1}$$

where J_{ij} represents a randomly distributed exchange interaction between spins $\vec{S}_i$ and $\vec{S}_j$ located at the nearest-neighbor sites i and j, respectively. For the purpose of illustration, we consider a rectangular distribution for J_{ij} represented by

$$\begin{aligned} f(J) &= 1 \text{ if } |J - J_0| \leq \Delta \\ &= 0 \text{ if } |J - J_0| > \Delta , \end{aligned} \tag{2}$$

where J_0 represents the mean value of J_{ij} and Δ is the fluctuation about the mean value. This particular model is analogous to the Anderson model of cellular disorder in tight-binding band which was used in studying the electronic states.[6] We would

further assume that, even though the exchange interactions J_{ij}'s fluctuate, their effect on local magnetization at each site is more or less homogeneous. This is a reasonable approximation only at zero temperature. Thus, we can describe the actual disordered system by an effective Hamiltonian which retains the symmetry of a perfect lattice, and is characterized by a yet-to-be-determined coherent-exchange interaction J_c. In the spirit of the CPA, we consider a single actual exchange interaction J_{ij} immersed in such an effective medium. The J_c is determined self-consistently by requiring that the net scattering from the single scatterer J_{ij} must vanish on the average.

The spin-wave Green's function $\overleftrightarrow{G}$, corresponding to the Hamiltonian given by Eq. (1), is calculated by using the random-phase approximation (RPA). The equations of motion for $\overleftrightarrow{G}$ in the RPA becomes

$$\frac{\omega}{\sigma} G_{lm} - \sum_k J_{lk}(G_{km} - G_{lm}) = \delta_{lm}, \tag{3}$$

where ω and σ represent the frequency and the magnetization of the ferromagnet, respectively. Since we have assumed that the effect of the random exchange interactions on the magnetizations at each site is homogeneous, we have set $\sigma_l = \sigma$ in Eq. (3). One can also write Eq. (3) in a matrix form as

$$(E - \overleftrightarrow{H})\overleftrightarrow{G} = 1, \tag{4}$$

where

$$E = \omega/\sigma$$

and

$$\overleftrightarrow{H} = \sum_{\{i,j\}} J_{ij}[\,|i\rangle\langle i| + |j\rangle\langle j| - |i\rangle\langle j| - |j\rangle\langle i|\,]. \tag{5}$$

Here Eq. (5) is the Hamiltonian which replaces Eq. (1) after the random-phase approximation, and $|i\rangle$ represents the spin-deviation state at site i and $\{i, j\}$ represents a summation over all nearest-neighbor pairs.

Since the J_{ij}'s are uncorrelated in this amorphous model, we can treat each J_{ij} as an independent scatterer. The scattering potential corresponding to such a single scatterer is

$$\overleftrightarrow{V}_{ij} = (J_{ij} - J_c)[\,|i\rangle\langle i| + |j\rangle\langle j| - |i\rangle\langle j| - |j\rangle\langle i|\,], \tag{6}$$

immersed in an effective medium with an effective Hamiltonian

$$\overleftrightarrow{H}_c = J_c \sum_{\{i,j\}} [\,|i\rangle\langle i| + |j\rangle\langle j| - |i\rangle\langle j| - |j\rangle\langle i|\,]. \tag{7}$$

The effective Green's function $\overleftrightarrow{G}_c$ is given by

$$\overleftrightarrow{G}_c = [E - \overleftrightarrow{H}_c]^{-1}. \tag{8}$$

Then the t matrix corresponding to the scattering potential $\overleftrightarrow{V}_{ij}$ can be obtained from

$$\overleftrightarrow{T} = \overleftrightarrow{V} + \overleftrightarrow{V}\overleftrightarrow{G}_c\overleftrightarrow{T}. \tag{9}$$

Equation (9) is a 2×2 matrix. The t-matrix elements have the form,

$$T_{ii} = -T_{ij} = \frac{J_{ij} - J_c}{1 - 2(J_{ij} - J_c)(G_0 - G_1)}, \tag{10}$$

where G_0 and G_1 denote the diagonal and first off-diagonal matrix elements of $\overleftrightarrow{G}_c$. Taking the configurational average of the t matrix we have

$$\begin{aligned}\langle T_{ii}\rangle &= -\langle T_{ij}\rangle \\ &= \frac{1}{2\Delta}\int_{J_0-\Delta}^{J_0+\Delta} T_{ii}\, dJ \\ &= -\frac{\alpha}{2\Delta}\left(2\Delta + \alpha \ln\frac{J_0 - J_c - \alpha + \Delta}{J_0 - J_c - \alpha - \Delta}\right),\end{aligned} \tag{11}$$

where

$$\alpha = \tfrac{1}{2}(G_0 - G_1)^{-1}. \tag{12}$$

In the spirit of the CPA, one determines J_c by requiring

$$\langle T_{ii}\rangle = 0. \tag{13}$$

Using the relation (11), the criterion given by (13) becomes

$$J_c = J_0 - \alpha + \Delta\cot(\Delta/\alpha). \tag{14}$$

Then the spin-wave density of states can be calculated via

$$\rho(E) = -\frac{1}{\pi}\,\mathrm{Im}\, G_0(E, J_c). \tag{15}$$

For a simple cubic lattice, the Green's function has the form of

$$G_0(E, J) = \sum_{\vec{k}}\left(E - 6J + \sum_{\vec{a}} e^{i\vec{k}\cdot\vec{a}}\right)^{-1} \tag{16}$$

and

$$G_1 = \frac{1}{6J}[1 - (E - 6J)G_0], \tag{17}$$

where $\vec{a}$ represents the unit lattice vector.

For numerical computation of the spin-wave density of states, instead of the above G_0 we consider a model Green's function for the perfect lattice which has the following form:

$$G_0(E, J) = (1/18J^2)\{E - 6J - [E(E - 12J)]^{1/2}\}. \tag{18}$$

The density of states obtained from this model Green's function describes qualititively the density of states of the simple cubic lattice rather well except that it can not reproduce the Von Hove singularities. Using this Green's function and Eqs. (14) and (15) one can calculate the density of state $\rho(E)$ in the CPA. The MKS theory can be derived from Eq. (14) by letting $\Delta \to 0$, then

$$J_M = J_0 + \Delta^2/3\alpha. \tag{19}$$

The second term, $\Delta^2/3\alpha$, is the self-energy as defined in the MKS paper.

It should be noted that α in the MKS theory is obtained from Eqs. (12), (17), and (18) by taking $J=J_0$, whereas the CPA approach calls for $\alpha(E, J_c)$ in Eqs. (12), (14), (17), and (18). The $\rho(E)$ calculated via CPA has been compared with the $\rho(E)$ calculated (by using the above model Green's function) in the MKS theory by using Eq. (19), for $\Delta/J_0 = 0.5$ and 1.0 as shown in Fig. 1. The main difference between the results of these two theories is that the sharp peaks occurring at $E = 12J_0$ (which is the energy corresponding to the upper band edge for an ordered system with an exchange interaction J_0) in the MKS theory do not appear in the CPA result. We believe that this peak in the MKS calculation is a result of their perturbation approach which is proper only for certain energy regions even if the fluctuation parameter Δ/J_0 is small. The expansion parameter in their Eq. (18) which is energy dependent has a discontinuous derivative at $E = 12J_0$ and this is the cause of the appearance of the peak. We also note that in the CPA, the maximum of the density of the spin-wave states for the case of $\Delta/J_0 = 1.0$ occurs at an energy lower than obtained from the MKS theory, although this qualitative difference disappears as Δ/J_0 becomes smaller. The bandwidth in the CPA is also wider than that in the MKS theory. We have investigated several values of Δ (up to Δ_c) and

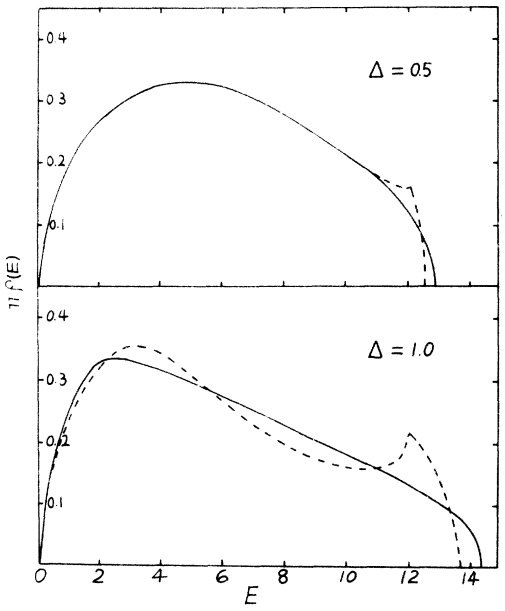

FIG. 1. Spin-wave densities of states of an amorphous ferromagnet are plotted as a function of E. E and Δ are in units of J_0. The solid line is based on the CPA and the dashed line is obtained from the MKS theory.

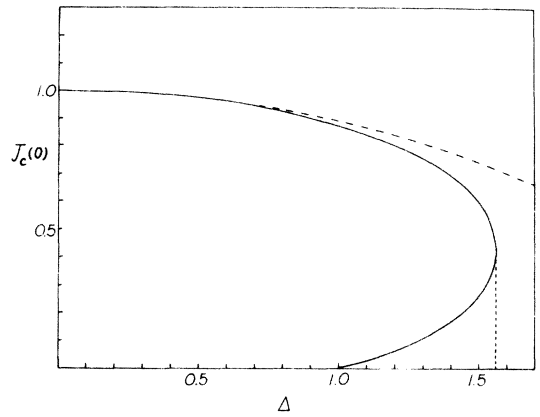

FIG. 2. Coherent exchange interaction at $E=0$, $J_c(0)$, is plotted as a function of Δ. Here both $J_c(0)$ and Δ in units of J_0. The solid line is based on the CPA and the dashed line is obtained from the MKS theory.

have found no indication of the existence of nonanalyticities in G_c off the real energy axis.[7]

In order that the ferromagnetic state be stable we require the density state $\rho(0)=0$. This stability criterion implies that $J_0(0)$ must be real. However we find that as we vary Δ, $J_c(0)$ given by

$$J_c(0) = J_0 + 3J_c(0) - \Delta \cot[\Delta/3J_c(0)] \tag{20}$$

becomes complex as Δ exceeds certain critical value Δ_c. We would like to point out that Eq. (20) is also exact for simple cubic lattice within the present approximation and is independent of the choice of (18). In Fig. 2 we have plotted the real solution for $J_c(0)$ as a function of Δ (solid line). For $\Delta > 1.56J_0$ there is no real solution for $J_c(0)$ implying that there cannot be any ferromagnetism for $\Delta > \Delta_c$. For values of Δ between J_0 and $1.56J_0$ there are two real solutions of $J_c(0)$, but we find that only the upper one gives us the physically acceptable solution. The effective J at $E=0$ in the MKS theory satisfies the following approximate equation:

$$J_M(0) \cong J_0[1 - (\Delta/3J_0)^2]. \tag{21}$$

The dashed line in Fig. 2 represents $J_c(0)$ obtained from the MKS theory. This indicates that in MKS theory no finite critical fluctuation exists. This is not surprising because the MKS theory is basically a mean-field theory and should not be expected to give reasonable results for large values of Δ.

III. DISCUSSION

We have applied the CPA to the case of an amorphous ferromagnet containing quantitative disorder for a wide range of fluctuation of the exchange in-

teraction at the zero-temperature limit. Since at this temperature the local spin fluctuation which has been neglected in our formulation is expected to be minimum, our theory should give reasonable results. Our theory predicts the existence of a critical fluctuation beyond which ferromagnetism becomes unstable—a result which cannot be reproduced by any mean-field theory. However it should be pointed out that for $\Delta > J_0$, a fraction of the exchange interactions become negative and some of the spins are expected to flip. Thus in this region our assumption of a homogeneous σ is not necessarily correct. If this spin fluctuation is taken into account, it will modify the critical fluctuation. Thus our estimate of the critical fluctuation Δ_c is only an upper bound. Both the present CPA theory and the MKS theory are "molecular" theories in which correlations between different molecular cells have been neglected. Besides the errors introduced by the "molecular" approximations which are the same for both the theories, the CPA is correct to all order in $\langle V_{ij}^n \rangle$,[8] whereas the MKS theory is correct only to second order in $\langle V_{ij}^2 \rangle$. Thus we expect the CPA theory to be more accurate than the MKS theory. Let us emphasize once again that even for small values of Δ our CPA theory produces results which are qualitatively different from the MKS results. As pointed out before, owing to the perturbative nature of the MKS theory, it gives rise to peaks in the density of states at the upper edge of the ordered lattice even for smaller values of Δ. Our CPA theory which is basically nonperturbative in nature does not produce any such peak in the density of states.

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