A Cluster-Bethe-Lattice Approach To Spin-Waves In Dilute Ferromagnets.

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Abstract

We study the spin-wave spectra of a dilute ferromagnet within the cluster-Bethe-lattice approximation. Short range order effects for the alloy are included. A study of finite size clusters connected at their edges to Bethe lattices of the same coordination number allows us to determine: (i) the stability condition for the magnetic system; (ii) the continuum spin-wave local density of states; and (iii) the existence of localized states below and above the continuum states.

Resumée

Nous étudions le spectre d'ondes de spin d'un ferromagnet dilué dans l'approximation d'un groupe d'atomes liés à des réseaux de Bethe. Nous avons considéré les effets de courte portée dans l'alliage. Une étude des groupes finis d'atomes entourés de réseaux de Bethe avec le même nombre de coordination nous a permis de déterminer: (i) la condition de stabilité du systéme magnétique; (ii) la partie continue de la densité locale d'états des ondes de spin; (iii) l'éxistence d'états localisés a des énergies plus grandes e plus faibles que celle du continu.

The study of spin-wave spectra in dilute ferromagnets is one of the classical problems in alloy theory[1-7]. Its solution involves a detailed study of percolation theory[8,9] and the determination of a critical concentration of magnetic atoms below which the ferromagnetic state of the system is no longer stable. It is the purpose of this communication to apply the cluster-Bethe-lattice method, which has been successfully employed to determine electronic density-of-states curves in various systems[10-12] and alloys,[13,14] to this problem. It is our conclusion that the method is ideally suited for the purpose, and that the results are very encouraging. It provides a complementary approach to the usual CPA methods[7], specially since, unlike the CPA, it allows for a straightforward investigation of localized modes.

Our system consists of N atoms in a constitutionally disordered two-component alloy of coordination number z. Of these, $x_M N$ atoms are magnetic and the rest $(1-x_M)N$ are non-magnetic. The magnetic atoms have a spin S and the non-magnetic ones a spin zero. The hamiltonian of the system consists of a nearest-neighbor Heisenberg interaction between magnetic atoms only. It can be written

$$H = -J \sum_{n,\Delta} \left\{ S^z(n) S^z(n+\Delta) + S^+(n) S^-(n+\Delta) \right\} \tag{1}$$

where n indicates lattice sites and Δ is an index which runs over the z nearest neighbors. The operators S^z, $S^\pm$ are either the normal spin S operators in the case of magnetic atoms, or zero for non-magnetic ones[15].

The one-spin-wave[7,15] Green's function $G_{mn}(\omega)$ satisfies the equation of motion

$$\left[\omega - E(m)\right] G_{mn} = \delta_{mn} - \sum_{\Delta} U(m,m+\Delta)\, G_{(m+\Delta)n}, \tag{2}$$

where

$$E(m) = 2J \sum_{\Delta} S(m+\Delta), \tag{3}$$

$$U(m, m+\Delta) = 2J \left[S(m) S(m+\Delta) \right]^{1/2} \tag{4}$$

where $S(m) = S$ or zero depending on whether the ion is magnetic or not. The local density of states for spin-wave excitations is given by the usual formula

$$D_n(\omega) = -\frac{1}{\pi}\, \mathrm{Im}\, G_{nn}(\omega) \tag{5}$$

In order to solve the equations (2)-(5) for a dilute ferromagnet we first define a probability parameter p ($0 < p \leq 1$) which gives the probability that a given nearest neighbor of a given magnetic atom is also a magnetic atom. In other words the average number of magnetic nearest neighbors of an arbitrary magnetic atom is (zp).

Following the treatment developed previously for alloys,[13,14] we select a given cluster of (N_s+1) sites, with a magnetic central atom 0. For the atoms in the periphery of the cluster we saturate their coordination number with Bethe lattices of coordination number z and probability p. We then solve Dyson's equation (2) by a transfer-matrix method and determine the density of spin-wave states by averaging over the various clusters ν of different composition

$$D_0(\omega) = -\frac{1}{\pi} \sum_{\nu} p_\nu \, \mathrm{Im} \; G_{00}(\omega;\nu) \tag{6}$$

with a weight factor P_ν.

The simplest case is the one-atom cluster, for which the equations reduce to

$$\begin{cases} (\omega - E_0) \; G_{00} = 1 - pz \; U \; G_{10}, \\ (\omega - E_1) \; G_{n0} = -U \; G_{(n-1)0} - p(z-1) \; U \; G_{(n+1)0} \, , \quad n \geq 1 \end{cases} \tag{7}$$

where

$$U = 2JS$$
$$E_0 = pzU \qquad E_1 = U + p(z-1)U \tag{8}$$

Equations (7) - (8) can be solved by assuming[11]

$$G_{n0} = T \, G_{(n-1)0}, \quad n \geq 1, \tag{9}$$

which inserted in (7) yields

$$G_{00} = \frac{2(z-1)}{(z-2)\omega - [2(z-1)E_0 - zE_1] \mp z[(\omega - E_1)^2 - 4p(z-1)\,U^2]^{1/2}} \tag{10}$$

An analysis of (10) produces the following results:

(a) Spin waves exist in this model in the energy range

$$U[1 - \sqrt{(z-1)p}]^2 \leq \omega \leq U[1 + \sqrt{(z-1)p}]^2 \tag{11}$$

where the square root in the denominator of (10) is negative.

(b) No other modes of the system appear for $p > p_c = (z-1)^{-1}$.

(c) For $p < p_c$ there is a discrete mode at $\omega = 0$ which has a total strength

$$D_{00}(\omega \simeq 0) = \frac{1 - p(z-1)}{1+p} \delta(\omega) \tag{12}$$

Such a mode, with zero energy, indicates an instability of the ferromagnetic state at any finite temperature. It is interesting to note that the instability disappears at $p = p_c$, which is the classical percolation limit,[8,9] for which a linked ferromagnetic chain can exist across the macroscopic sample. The density of states corresponding to this model and various values of p, for $z = 8$ are shown in Figure 1.

We have calculated a more realistic case of a cluster of 9 atoms for $z = 8$ (body-centered cubic lattice) for values of p equal to 0.25, 0.50, 0.75 and 1.0. In each case we have considered all nine clusters with $(\nu + 1)$ magnetic atoms ($\nu = 0$ trough 8) and, in computing the average (6) we have taken the binomial probability

$$P_\nu = \frac{8!}{\nu!(8-\nu)!} p^\nu (1-p)^{8-\nu} \tag{13}$$

The results are shown in Figure 2. The following points are worth remarking:

(1) For $p < p_c$ the instability of the system is indicated by a contribution to the density of states of the form (12).

(2) Localized low frequency modes are split off below the lower edge of the band at frequencies

$$\omega_\nu = \nu\left(1 + \frac{1}{\nu - p(z-1)}\right) U$$

for $0 \leq \nu < p(z-1) - \sqrt{p(z-1)}$. (14)

The mode for $\omega = 0$ corresponds to the isolated magnetic atoms. Their contribution, according to (13) gives a delta function of strength $(1-p)^8$.

(3) Localized high frequency modes can also be split off the top of the band. The frequencies at which these modes occur is given by the expression (14) for $\nu > p(z-1) + \sqrt{p(z-1)}$. Such modes arise thus from configurations with a large number of magnetic neighbors.

(4) The peak structure in the continuum is a consequence of these localized modes, which, for a given p, are "almost" ready to be split off the continuum.

The structure features observed in the density-of-states curves for these spin wave modes are all based on sensible physical causes and point out to the suitability of the cluster-Bethe-lattice model. Larger clusters, with more involved topological features which include closed rings are presently being studied and will be reported elsewhere.

References

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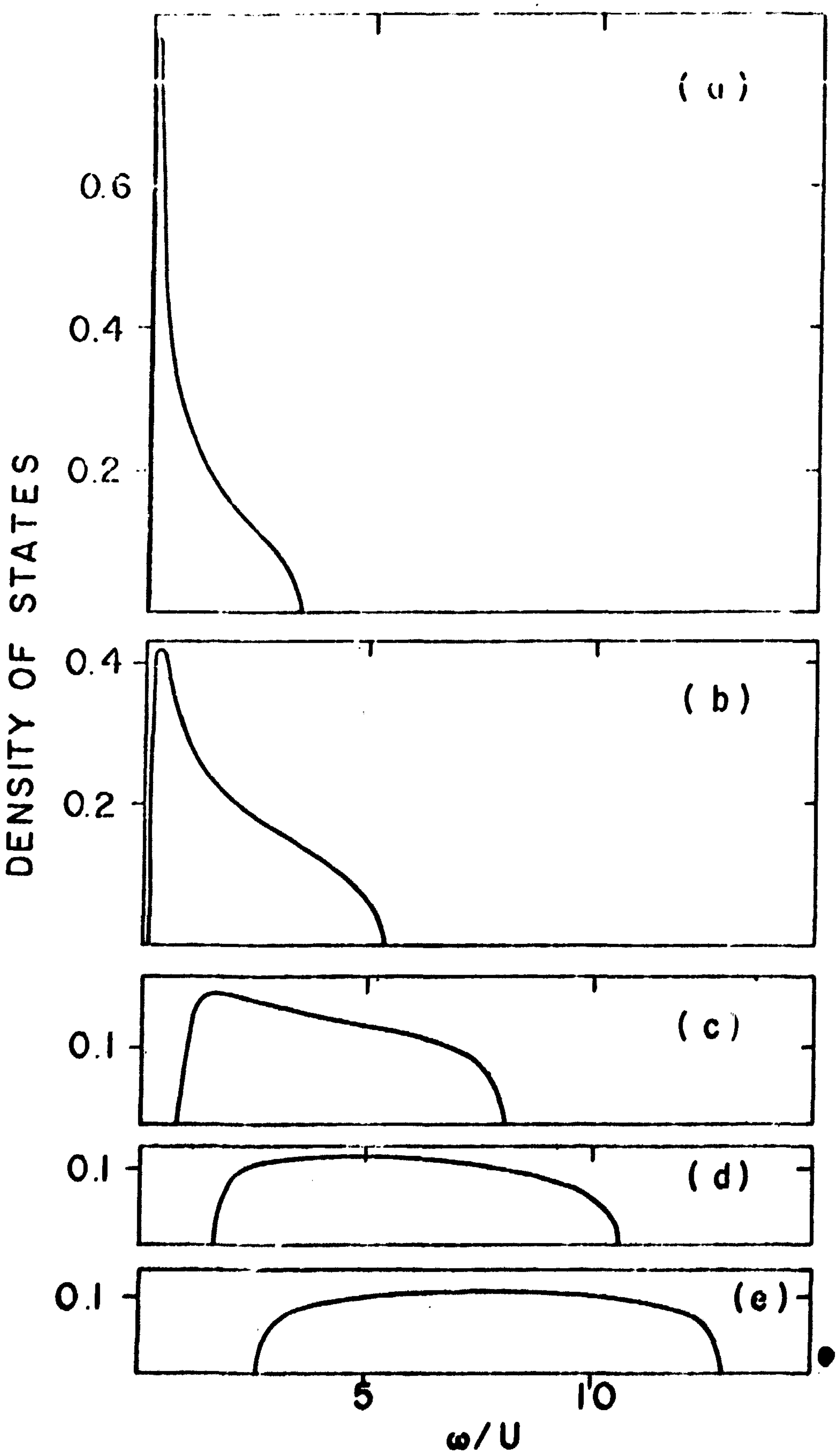
Figure Captions

Figure 1. - Bethe-lattice local density of states at a magnetic ion for $z = 8$, for a) $p = 0.1$, b) $p = 0.25$, c) $p = 0.50$, d) $p = 0.75$ and e) $p = 1.00$. For $p = 0.1$ the delta function at $\omega = 0$ indicates the instability of the system ($p_c = 0.143$). The density of states is normalized to 1 and not to the concentration x_M.

Figure 2. Cluster-Bethe-lattice local density of states at central magnetic atom for cluster of nine atoms, for a) $p = 0.25$, b) $p = 0.50$, c) $p = 0.75$ and d) $p = 1.00$. Localized states are indicated by shaded area under broadened delta functions. The density of states is normalized to 1.


DENSITY OF STATES
0.6
0.4
0.2
(a)
0.4
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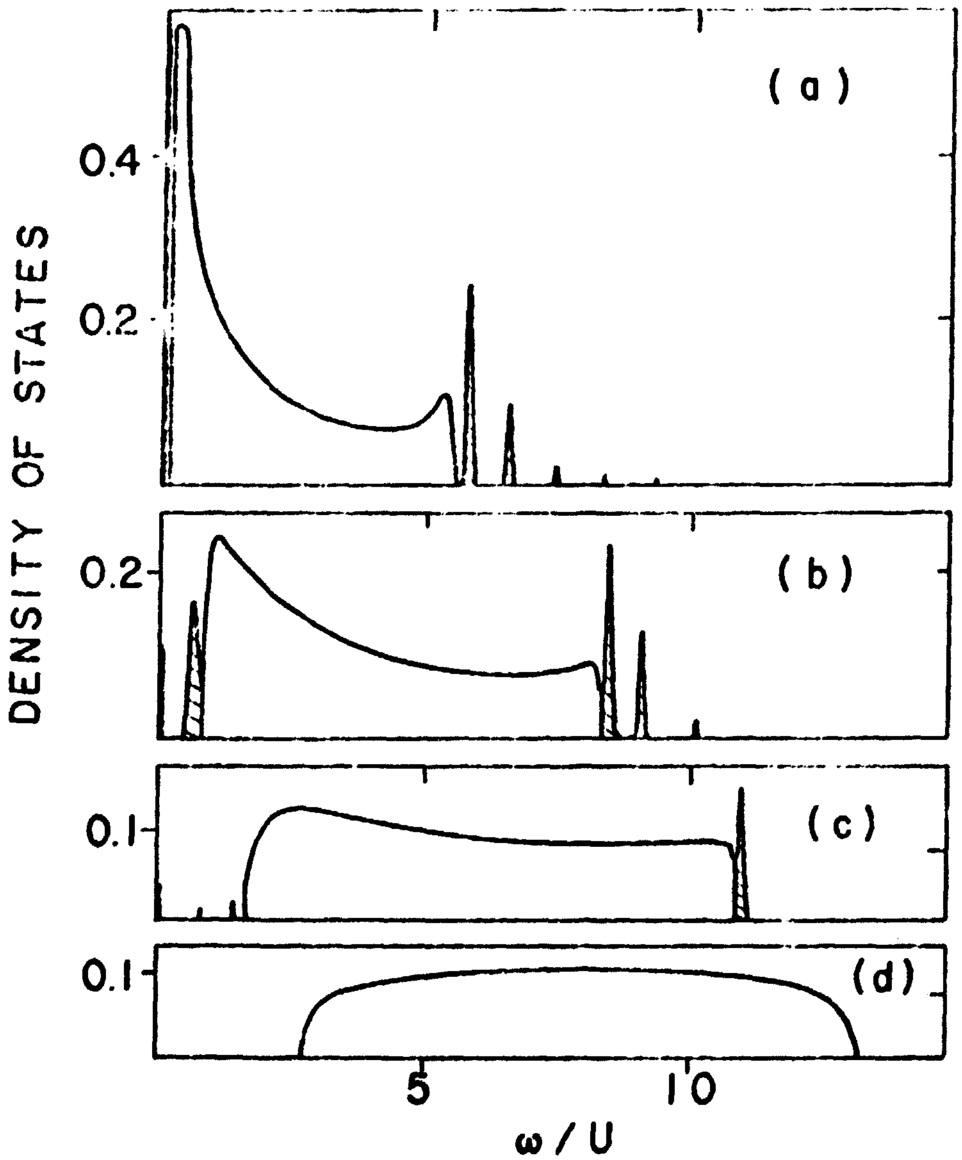

DENSITY OF STATES
0.4
0.2
(a)
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ω / U