Band-Model Approach to Magnetic Excitations in a Disordered Ferromagnet: One-Dimensional Case

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A disordered ferromagnet is studied with use of the Hubbard model. A systematic method of finding the spin transverse susceptibility for any random configuration is developed. The computer results for a one-dimensional case reveal gapless magnetic excitations centered around a wave vector corresponding to the first maximum of the structure factor in qualitative accordance with recent experimental data.

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As a contribution to the discussion concerning the nature of short-wavelength magnetic excitations observed in amorphous ferromagnets I present a new theoretical approach based on the itinerant-electron model. The experiments[1-3] show, apart from distinct spin-wave excitations around the wave vector $q=0$, some extra magnetic excitations around the first peak of the structure factor. There is still some controversy about these excitations and the basic question is whether they are gapless or not. The measurements by Mook *et al.*[1,2] have suggested a considerable gap and relatively sharp spectrum while recent experiments[3-4] suggest no gap at all.

The present aim is to calculate the spin transverse susceptibility with use of the single-band Hubbard Hamiltonian

$$H=\sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U\sum_i c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}. \qquad (1)$$

where the standard notation is used and the sums go over sites distributed at random. The organization of the calculations is as follows. First we generate a random configuration of lattice sites and then solve an electronic problem by means of a one-body Green function

$$g_{ij\sigma}(t) = -i\theta(t)\langle [c_{i\sigma}(t), c_{j\sigma}^{\dagger}]_{+}\rangle.$$

This Green function is calculated within the Hartree-Fock (HF) approximation from its equation of motion. In terms of eigenvalues λ_α^σ and eigenfunctions $u_{\alpha i}^\sigma$ of the Hamiltonian (1) it reads

$$g_{ij\sigma}(\omega) = \sum_\alpha u_{i\alpha} u_{\alpha j}/(\omega - \lambda_\alpha^\sigma),$$

where α is a normal-mode label.

Next we construct a two-body Green function

$$\chi_{ij}(t) = -i\theta(t)\langle [c_{i\uparrow}^{\dagger}(t) c_{i\downarrow}(t), c_{j\downarrow}^{\dagger} c_{j\uparrow}]_{-}\rangle$$

and calculate it within the random-phase approximation (RPA). The HF approximation for a one-body problem combined with the RPA for a two-body problem gives the well-known "ladder" approximation leading to the following matrix equation for the susceptibility:

$$[\underline{1} - U\underline{\chi}^0(E)]\,\underline{\chi}(E) = \underline{\chi}^0(E), \qquad (2)$$

where

$$\chi_{ij}^0(E) = \sum_{\alpha\beta}\{[f(\lambda_\alpha^{\uparrow}) - f(\lambda_\beta^{\downarrow})]/(\lambda_\beta^{\downarrow} - \lambda_\alpha^{\uparrow} - E)\} \times u_{\alpha 1}^{\uparrow} u_{\alpha n}^{\uparrow} u_{\beta 1}^{\downarrow} u_{\beta n}^{\downarrow}$$

is the energy Fourier component of

$$\chi_{ij}^0(t) = -\langle c_{i\uparrow}^{\dagger}(t) c_{j\uparrow}\rangle g_{ij\downarrow}(t) - \langle c_{j\downarrow}^{\dagger} c_{i\downarrow}(t)\rangle g_{ij\uparrow}(t)$$

with

$$\langle c_{j\sigma}^{\dagger} c_{i\sigma}(t)\rangle = -\pi^{-1}\int_{-\infty}^{\infty} d\omega \exp(-i\omega t) f(\omega)\,\mathrm{Im}\, g_{ij\sigma}(\omega)$$

and f the Fermi-Dirac distribution function. The zeros of the determinant of the expression in the brackets in (2) determine the energies of the magnetic excitations while the imaginary part of χ gives the scattering law (spectral density function):

$$S(q,E) = -\frac{1}{\pi}\frac{1}{N}\sum_{ln} \exp[iq(R_l - R_n)]\,\mathrm{Im}\,\chi_{ln}(E).$$

The calculations have to be repeated for various configurations and finally averaged.

So far I have solved a one-dimensional problem. I have considered a chain of randomly distributed rigid nonoverlapping linear segments of length a and imposed the Born-Karman boundary conditions. The hopping integral is taken in the following form (cf., Hall and Faulkner[5]):

$$t_{i,i+1} = \begin{cases} -|t|\exp[1-(R_{i+1}-R_i)\eta/a], & i<N; \\ -|t|\exp[1-N+(R_N-R_1)\eta/a], & i=N, \end{cases}$$

with η being the order parameter varying from $\eta=1$ for an ordered system to $\eta=0$ when the amount of disorder increases. The order parameter η is equal to Na/L, where L is the length of the system, equal to Na for $\eta=1$ and tending to infinity for $\eta\to 0$. For $\eta=1$ the segments are close packed and there is perfect order, whereas for $\eta<1$ the structure gets looser and some disorder is allowed. It is worth noting that a/η is the average distance between the segments and therefore the ratio $(R_{i+1}-R_i)\eta/a$ remains finite (and fluctuates about 1) even for very small η.

Computer results have been obtained for 20 different configurations of a chain consisting of $N=20$ atoms. Strong ferromagnetism has been assumed with up (down) spin electrons per site $n_\uparrow=1$ ($n_\downarrow=0.4$), $U=15|t|$, $\eta=0.75$, and $T=0$ K. I have chosen the parameters so that the ordered-system RPA spin-wave stiffness constant is positive (which implies $U>7.64|t|$). The proper order of magnitude of the stiffness constant (see Shirane *et al.*[3]) is then achieved for roughly 0.1 eV $<|t|<0.3$ eV. The energy spectrum of magnetic excitations in an ordered system corresponding to this choice of parameters (with $\eta=1$) is plotted in Fig. 1. There is no intersection of the magnon branch with the Stoner (high-energy) excitations. Figure 2 shows the magnon density-of-states histogram for a disordered system. It reveals the two maxima, located just at energies where the ordered system has sharp peaks, and some rather substantial broadening of the magnon bandwidth. Figure 3 shows the scattering law for a few energy values (averaged over the intervals marked on the E axis). For $E=0$ there is a sharp magnon peak at $q=0$ and a broad one about $q=Q_0=1.6\pi/a$. For $E=0.5|t|$ there are two high-q peaks distributed symmetrically about Q_0. The distance of these peaks from Q_0 is equal to the distance of the first (magnon) peak from the E axis. This means that at least for small E the magnon and the high-q branch have the same slope (as reported in Refs. 1 and 2). The features mentioned above seem to hold for $E=|t|$ too, although this case has to be treated with caution since it corresponds to a rather low value of the density of states (see Fig. 2) and the statistics involved here is poorer than in other cases. As E increases the distance between the high-q peaks increases as well, and the left-hand peak and the

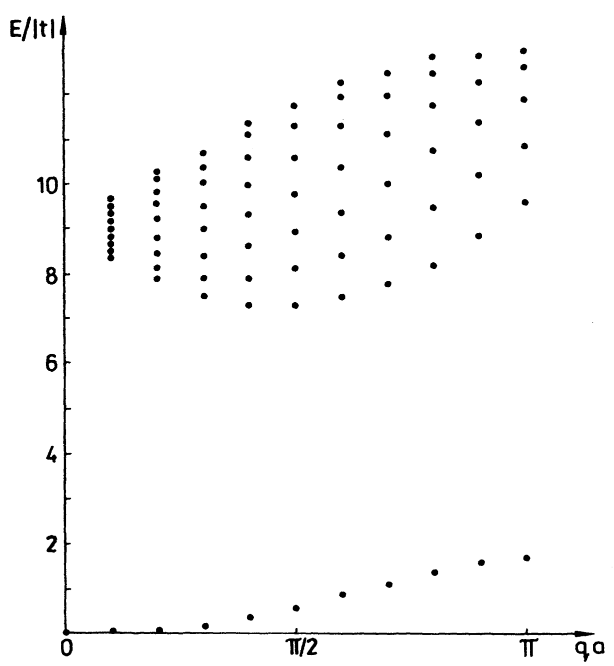

FIG. 1. Ordered-system energy spectrum of magnetic excitations.

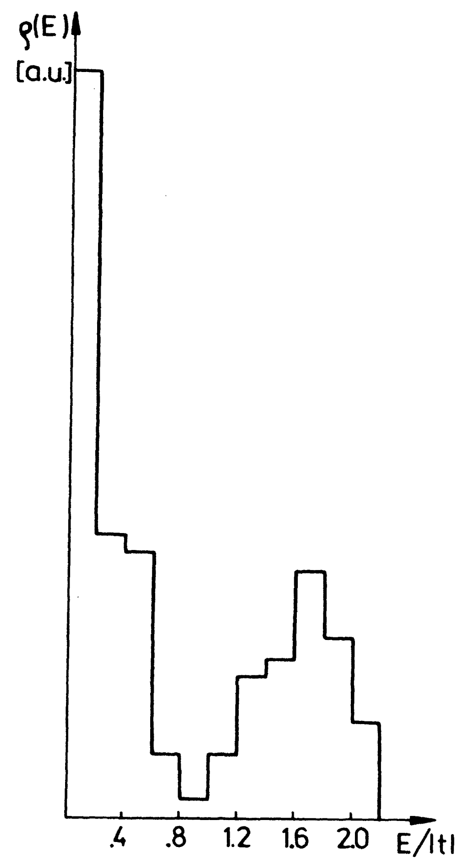

FIG. 2. Magnon density of states for the disordered system.

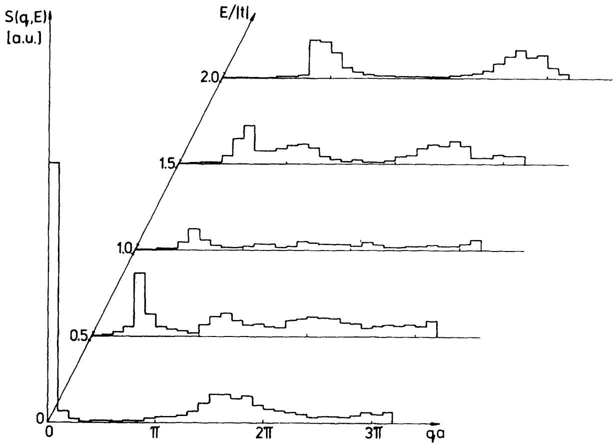

FIG. 3. Scattering law as a function of energy.

magnon one get closer and closer and eventually merge into each other (for E exceeding the bandwidth of the ordered system). For each of the 20 configurations I have computed a radial distribution function and then by Fourier transformation, a structure factor. The configurationally averaged structure factor is presented in Fig. 4; it clearly shows a maximum just at $q = Q_0$.

It seems to be instructive to compare our Fig. 3 with its counterparts from other papers based on other models (localized spin models and tight-binding models). It turns out that the overall behavior of $S(q, E)$ is always quite similar and the existence of the short-wave excitations of various types appears to be the universal, model-independent feature of disordered systems regardless of whether they are amorphous,[5-8] polycrystalline,[7] or liquid.[9,10] In some cases, however, the short-wavelength peak appears only for energy exceeding some critical value, i.e., there is a gap. From this point of view, for instance, the magnon spectrum in the amorphous system studied by Alben[7] as well as the magnon and vibrational spectra of Hall and Faulkner[5] and the phonon spectrum of Axe[8] can be classified as gapless.

In conclusion, this Letter offers the first theoretical evidence, to my knowledge, for the appearance of short-wavelength magnetic excitations around the first peak of the structure factor in a disordered system described by the Hubbard Hamiltonian. The fact that there is a peak in the scattering law at $(Q_0, 0)$ means that the excitations of this type are gapless which is consistent with recent measurements.[3,4] More studies are required to verify whether these one-dimensional results really do carry over to three dimensions.

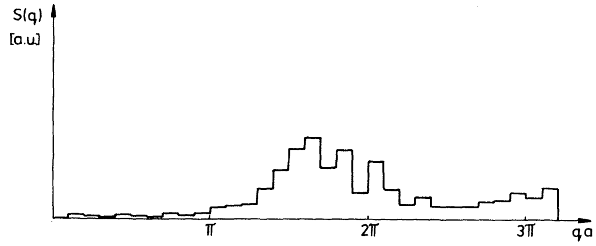

FIG. 4. Configurationally averaged structure factor.

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