INELASTIC NEUTRON SCATTERING IN FERROMAGNETIC METALS*

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The relative magnetic inelastic neutron scattering from spin waves and the continuum spin-flip band in a ferromagnetic metal is shown to depend upon the wave vector $\vec{q}$. In particular, the scattering from the continuum band vanishes as $q\rightarrow 0$, and the scattering from the spin waves vanishes as $q\rightarrow q_{max}$, the cutoff vector for spin waves.

The magnetic, inelastic neutron scattering from a ferromagnetic metal has contributions arising from both spin-wave excitations and the continuum band of spin-flip excitations. The former of these has been calculated in the long wavelength limit by Izuyama, Kim, and Kubo,[1] while the latter has been calculated by Elliott[2] in the molecular field or Stoner approximation. It is the purpose of this Letter to show that the relative contributions to the scattering depend upon the wave vector $\vec{q}$. In particular, as $q\rightarrow 0$, the magnetic scattering arises solely from spin-wave excitations with no contribution from the continuum band. On the other hand, as $q\rightarrow q_{max}$, where q_{max} is the cutoff momentum for spin waves,[3] the spin-wave scattering vanishes and we are left with only scattering due to the continuum spin-flip band. This result also means that the magnitude of the scattering from spin waves has a $\vec{q}$ dependence in addition to that arising from the form factor $F(\vec{\kappa})$ and the thermal factor $(1-e^{-\beta E})^{-1}$.

The differential cross section for magnetic, inelastic neutron scattering with the scattering vector $\vec{\kappa}$ parallel to the magnetization is given by the relationship

$$\frac{d^2\sigma}{d\Omega dE}=\frac{1}{2\pi}\left(\frac{g\gamma e^2}{2mc^2}\right)^2\frac{|F(\vec{\kappa})|^2}{1-\exp(-\beta E)}\left(\frac{k'}{k}\right)\chi_i^{-+}(\vec{q},E), \quad (1)$$

where E is the neutron energy loss, χ_i^{-+} is the imaginary part of the atomic susceptibility at the wave vector $\vec{q}$ and energy E, and $\vec{q}=\vec{\kappa}-\vec{K}$, where $\vec{K}$ is the necessary reciprocal lattice vector to bring $\vec{q}$ into the first Brillouin zone. In the random phase approximation,[1]

$$\chi^{-+}(\vec{q},E)=\chi_0^{-+}(\vec{q},E)[1-I\chi_0^{-+}(\vec{q},E)]^{-1}, \quad (2)$$

where

$$\chi_0^{-+}(\vec{q},E)=\chi_{0r}^{-+}(\vec{q},E)+i\chi_{0i}^{-+}(\vec{q},E)$$
$$=\frac{\Omega}{(2\pi)^3}\int d\vec{k}\frac{f_{\vec{k}\uparrow}-f_{\vec{k}+\vec{q}\downarrow}}{\Delta+\epsilon(\vec{k}+\vec{q})-\epsilon(\vec{k})-E} \quad (3)$$

is the susceptibility in the Stoner approximation. In this equation, Ω is the atomic volume, $\Delta=nI$ is the band splitting, n is the number of Bohr magnetons per atom, and ϵ is the one-electron band energy.

$\chi_i^{-+}(\vec{q},E)$ appearing in (1) has two contributions, $\chi_{i1}^{-+}(\vec{q},E)$ and $\chi_{i2}^{-+}(\vec{q},E)$, which arise from spin-wave and continuum-band excitations, respectively. $\chi_{i1}^{-+}(\vec{q},E)$ is singular and arises where the conditions $\chi_{0i}^{-+}(\vec{q},E)=0$ and $I\chi_{0r}^{-+}(\vec{q},E)=1$ are satisfied simultaneously. This generally restricts $\vec{q}$ to certain values[4] which in its simplest form means $q<q_{max}$. Provided these conditions are satisfied, then

$$\chi_{i1}^{-+}(\vec{q},E)=\frac{n\pi\delta(E(\vec{q})-E)}{\Delta\{(\partial/\partial E)[I\chi_{0r}^{-+}(\vec{q},E)]\}_{E=E(\vec{q})}}. \quad (4)$$

Equation (4) has been given by Izuyama, Kim, and Kubo[1] in the limit as $\vec{q}$ approaches zero for which the derivative in (4) approaches $1/\Delta$. The derivative depends on $\vec{q}$ and, in fact, becomes infinitely large as $q\rightarrow q_{max}$.[3] Hence, $\chi_{i1}^{-+}(q\rightarrow q_{max},E)\rightarrow 0$. To show this, we evaluate the derivative appearing in (4) using (3) and an effective-mass approximation. For a strong ferromagnet,

$$\chi_{i1}^{-+}(\vec{q},E)=n\pi(F^2/x^2F')\delta(E(\vec{q})-E), \quad (5)$$

where $F'=dF/dx$, $F=0.75\{2x^{-1}+(1-x^{-2})\ln[(1+x)/(1-x)]\}$, and where the auxiliary variable $x=\delta E/(\Delta'-E)$ with $\Delta'=\Delta+\hbar^2q^2/2m^*$ and $\delta E=\hbar^2qk_F/m^*$, half the width of the continuum band at q. The dispersion relation is given by $F=\delta E/\Delta$ from which we obtain $q/q_{max}=\frac{2}{3}F$. Figure 1, a plot of F^2/x^2F' vs q/q_{max}, shows the relative decrease of neutron scattering from spin waves with increasing q, arising from the susceptibility term alone.

The second contribution $\chi_{i2}^{-+}(\vec{q},E)$ is nonzero in the energy spectrum of the continuum band for which $\chi_{0i}^{-+}(\vec{q},E)$ is nonzero. Here,

$$\chi_{i2}^{-+}(\vec{q},E)=\chi_{0i}^{-+}(\vec{q},E)/D(\vec{q},E), \quad (6)$$

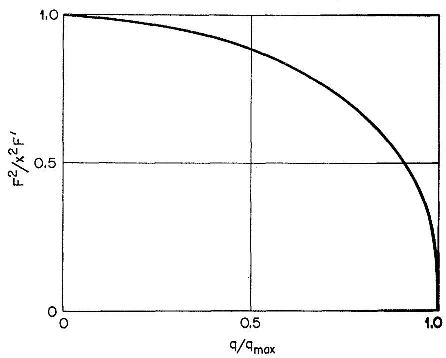

FIG. 1. Reduction factor F^2/x^2F', for scattering from spin waves as a function of wave vector $\vec{q}$ normalized to the cutoff wave vector.

with

$$\chi_{0i}^{-+}(\vec{q},E)=0, \quad |y|>1,$$

$$=\tfrac{3}{4}\pi(n/\delta E)(1-y^2), \quad |y|<1, \quad (7)$$

where $y=(\Delta'-E)/\delta E$ and where we have made the same assumptions in obtaining (7) as we have made in obtaining (5). The denominator $D(\vec{q},E)$ in (6) is given by the relation

$$D(\vec{q},E)=(1-\Delta G/\delta E)^2+(\Delta\chi_{0i}^{-+}/n)^2, \qquad (8)$$

where $G=0.75\{2y+(1-y^2)\ln[(1+y)/(1-y)]\}$. As $\vec{q}\to 0$, $D(\vec{q},E)\to\infty$ and the neutron scattering from the continuum spin-flip band vanishes. Figure 2 illustrates the effective reduction in this part of the neutron scattering compared with that calculated by Elliott.[2]

While the detailed nature of these results depends upon the model, the general nature of the results does not. For we know that

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\chi_i^{-+}(\vec{q},E)dE=\tfrac{1}{2}n, \qquad (9)$$

and hence, that

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}\chi_{i2}^{-+}(\vec{q},E)dE=\tfrac{1}{2}n(1-F^2/x^2F'). \qquad (10)$$

The limit $F^2/x^2F'\to 1$ as x and $\vec{q}\to 0$ is model independent; so χ_{i2}^{-+} must vanish identically in this limit. On the other hand, for those $\vec{q}$

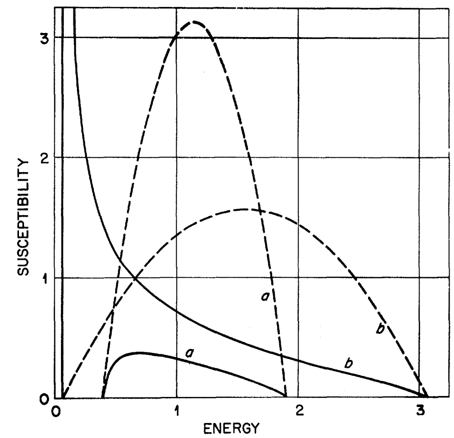

FIG. 2. The atomic susceptibility per Bohr magneton per unit of energy as a function of energy. The solid curves are calculated using Eqs. (6)-(9) of the text and the dashed curves are calculated using Eqs. (6) and (7) with $D(\vec{q},E)=1$. The dashed curves thus represent the susceptibility in the Stoner approximation and give the inelastic neutron scattering calculated by Elliott (Ref. 2). Curves a are calculated for $q/q_{max}=0.5$ and Curves b for $q/q_{max}=1.0$. The broad resonance displayed in b continues as q increases from q_{max}, the resonance moving slightly away from the bottom of the continuum band, becoming broader, and diminishing in amplitude. This resonance arises from the virtual spin-wave state lying in the continuum band. The band splitting Δ is one unit of energy and the Fermi energy is set equal to Δ for the purposes of this figure.

for which the spin-wave dispersion relation has no solution outside the continuum band, the denominator in (2) never goes to zero, χ_{i1}^{-+} vanishes, and (9) must be satisfied by $\chi_{i2}^{-+}(\vec{q},E)$. The possibility of a discontinuous change of $\chi_{i1}^{-+}(\vec{q},E)$ with $\vec{q}$ seems unlikely.

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