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Scattering of Spin Waves by Magnetic Defects*

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The scattering of spin waves by magnetic point defects is considered using a Green's function method. A partial-wave expansion for the scattering amplitude is derived. An expression for the cross section is determined which includes the effect of resonant states. Application is made to the calculation of the thermal conductivity of an insulating ferromagnet.

I. THEORY OF SCATTERING

THE scattering of spin waves by magnetic point defects is of interest in connection with the thermal conductivity of insulating ferromagnets and ferrites. It is well known that point imperfections are quite significant in the study of lattice (phonon) thermal conductivity.[1] At low temperatures, one would expect that the thermal conductivity of some ferrites and ferromagnetic insulators would be principally due to spin waves, and it is necessary then to consider the scattering of spin waves by defects. This problem has been investigated previously by Bar'yakhtar and Urushadze,[2] Douglas,[3] and Takeno.[4] Wolfram and Callaway[5] have considered the localized spin wave modes and resonant, or virtual, states which may be produced by magnetic defects.

In the calculation reported in Ref. 5, it was observed that, in analogy with the localized vibrational modes which may be produced by imperfections in crystal lattices and with the localized electronic states produced by impurities in the energy level system of a semiconductor, magnetic defects in a ferromagnet may produce localized spin-wave modes. A ferromagnet in which localized spins are coupled by a simple Heisenberg exchange interaction is considered:

$$H=-\sum_{\mathbf{R}}\sum_{\Delta} J(\mathbf{R},\,\mathbf{R}+\Delta)\mathbf{S}(\mathbf{R})\cdot\mathbf{S}(\mathbf{R}+\Delta)\,, \tag{1}$$

in which $-J$ is the effective nearest neighbor exchange interaction; $\mathbf{S}(\mathbf{R})$ is the atomic spin operator for the atom located at lattice position $\mathbf{R}$, and Δ is a vector connecting $\mathbf{R}$ with one of the Z neighboring lattice sites. A system of this type is said to contain a single magnetic defect if there is an atom at some point $\mathbf{R}'$ whose spin S' is different from those of the other atoms and which is coupled to the other atoms by an exchange interaction $\mathbf{J}'$. The problem of determining the spin-wave states is most conveniently handled by introducing a set of orthonormal functions $\varphi(\mathbf{R})$ analogous to the Wannier functions of energy band theory such that $|\varphi(\mathbf{R})|^2$ gives the probability of finding a spin deviation at the lattice site $\mathbf{R}$. It was shown in Ref. 5 that the functions $\varphi(\mathbf{R})$ satisfy a Schrodinger equation

$$E\varphi(\mathbf{R})=2\sum J(\mathbf{R},\,\mathbf{R}+\Delta)\{S(\mathbf{R}+\Delta)\varphi(\mathbf{R}) -[S(\mathbf{R})S(\mathbf{R}+\Delta)]^{1/2}\varphi(\mathbf{R}+\Delta)\} \tag{2}$$

in which $S(\mathbf{R})[S(\mathbf{R})+1]$ is the eigenvalue of $\mathbf{S}(\mathbf{R})\cdot\mathbf{S}(\mathbf{R})$.

This equation is most conveniently considered in matrix form $H\varphi=E\varphi$ where the Hamiltonian matrix H has elements

$$H(\mathbf{R}_1,\mathbf{R}_2)=2\{\delta_{\mathbf{R}_1,\mathbf{R}_2}\sum_{\Delta} J(\mathbf{R}_1,\,\mathbf{R}_1+\Delta)S(\mathbf{R}_1+\Delta) -\delta_{\mathbf{R}_1-\mathbf{R}_2,\Delta}J(\mathbf{R}_1,\,\mathbf{R}_1+\Delta)[S(\mathbf{R}_1)S(\mathbf{R}_1+\Delta)]^{1/2}\}\,. \tag{3}$$

It is desirable to separate out the magnetic defect as follows: If the defect were not present, all the spins would be equal and all the exchange integrals would be equal. Hence, we define partial Hamiltonians H_0 and H' by

$$H=H_0+H'\,, \tag{4}$$

$$H_0(\mathbf{R}_1,\mathbf{R}_2)=2JSZ\delta_{\mathbf{R}_1,\mathbf{R}_2}-2JS\delta_{\mathbf{R}_1-\mathbf{R}_2,\Delta}\,, \tag{5}$$

and

$$H'(\mathbf{R}_1,\mathbf{R}_2) =\delta_{\mathbf{R}_1,\mathbf{R}_2}[2SZ(J'-J)\delta_{\mathbf{R}_1,\mathbf{R}'}+2(J'S'-JS)\delta_{\mathbf{R}_1,\mathbf{R}'+\Delta}] -2\delta_{\mathbf{R}_1-\mathbf{R}_2,\Delta}(\delta_{\mathbf{R}_1,\mathbf{R}'}+\delta_{\mathbf{R}_2,\mathbf{R}'})[J'(S'S)^{1/2}-JS]. \tag{6}$$

Since H' may be regarded as a localized perturbation, Eq. (3) is conveniently attacked by a Green's function technique. The Green's function $G(\mathbf{R}_1,\mathbf{R}_2)$ is defined by

$$G(\mathbf{R}_1,\mathbf{R}_2)=(E-H_0)^{-1}{}_{\mathbf{R}_1,\mathbf{R}_2}. \tag{7}$$

For values of E in the region of eigenvalues of H_0, G is conveniently defined through the usual limiting procedure in which the energy is considered to have a small positive imaginary part. Let $\varphi_0(\mathbf{q},\mathbf{R})$ be a solution of

$$H_0\varphi_0(\mathbf{q},\mathbf{R})=E_0(\mathbf{q})\varphi_0(\mathbf{q},\mathbf{R})\,.$$

Then we may rewrite Eq. (2) in the form

$$\varphi(\mathbf{R})=\varphi_0(\mathbf{R})+\sum\nolimits_{\mathbf{R}_1,\mathbf{R}_2}G(\mathbf{R},\mathbf{R}_1)H'(\mathbf{R}_1,\mathbf{R}_2)\varphi(\mathbf{R}_2)\,. \tag{8}$$

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This equation, which is exactly analogous to the Lippmann-Schwinger equation of scattering theory, was studied in Ref. 5 with respect to the determination of the energies of localized states above the continuum and resonant or virtual states in the continuum. Here we will focus our attention on the problem of obtaining solutions corresponding to the scattering of spin waves by the magnetic defect. This will be done by a procedure which is the analog in solid-state physics of the partial-wave analysis of ordinary scattering theory. Equation (8) has been studied in connection with other systems, by Lax,[6] Koster,[7] Koster and Slater,[8] Lifshitz,[9] Clogston,[10] Klein,[11] Callaway,[12] and Krumhansl.[13]

The operator H' has the point symmetry of the lattice. We can form linear combinations of functions $\varphi(\mathbf{R})$ which transform according to the irreducible representations of the point group. Such functions will not be coupled by H'. This process is analogous to the customary decomposition of a plane wave into spherical partial waves.

The irreducible representations of the point group will be designated by an index ℓ, and the functions which are linear combinations of the φ will be denoted $C_\ell(\mathbf{R})$.[14] The transformation between C and φ is accomplished by a unitary operator $U(\ell,\nu)$ such that

$$C_\ell(R)=\sum_\nu U(\ell,\nu)\varphi(\mathbf{R}_\nu). \quad (9)$$

The vectors $\mathbf{R}_\nu$ which are included in the sum are those which are obtained by operating on a given one, say $\mathbf{R}'$, with all the operators in the point group.

After transformation, Eq. (8) has the form

$$C_\ell(R)=C_\ell^{(0)}(R)+\sum_{R_1,R_2}\mathcal{G}_\ell(R,R_1)\times H_\ell(R_1,R_2)C_\ell(R_2), \quad (10)$$

in which

$$\mathcal{G}_\ell(R,R_1)=\sum_{\nu,\mu}U(\ell,\nu)G(\mathbf{R}_\nu,\mathbf{R}_{1\mu})U^{-1}(\mu,\ell),$$
$$H_\ell(R,R_1)=\sum_{\nu,\mu}U(\ell,\nu)H(\mathbf{R}_\nu,\mathbf{R}_{1\mu})U^{-1}(\mu,\ell), \quad (11)$$

and $C_\ell^{(0)}$ is a symmetrized linear combination of unperturbed functions (these are plane waves)

$$C_\ell^{(0)}(R)=\sum_\nu U(\ell,\nu)\varphi_0(\mathbf{R}_\nu). \quad (12)$$

It is to be noted that Eq. (10) is diagonal in the representation index ℓ.

Up to this point, our treatment has been general. We now make use of the fact that H' is localized in the present case, extending only to first neighbors of the defect we place, for convenience, at the origin ($R'=0$). Therefore we need consider only certain representations: Γ_1, Γ_{12}, and Γ_{15} in the case of a simple cubic crystal;[15] Γ_1, Γ_{15}, $\Gamma_{25'}$, and $\Gamma_{2'}$ for body-centered cubic; and Γ_1, Γ_{15}, $\Gamma_{25'}$, Γ_{12}, and Γ_{25} for face-centered cubic structures. We can refer to functions transforming according to Γ_1 as s like, Γ_{15} as p like, Γ_{12} and $\Gamma_{25'}$ as d like, and $\Gamma_{2'}$ and Γ_{25} as f like. The rationale for this selection of representations is discussed in Ref. 5.

In addition, for all representations except Γ_1, only one term survives in the summation in Eq. (10); and for Γ_1, there are only two terms, Consider the simple cases first: we can abbreviate the matrix elements of H_ℓ as

$$H_\ell(R_1,R_2)=V_\ell\delta_{R_1,\Delta}\delta_{R_2,\Delta} \quad (\ell\neq 1). \quad (13)$$

Then Eq. (10) becomes

$$C_\ell(R)=C_\ell^{(0)}(R)+V_\ell\mathcal{G}_\ell(R,\Delta)C_\ell(\Delta). \quad (14)$$

This equation can be solved, and we find

$$C_\ell(R)=C_\ell^{(0)}(R)+[V_\ell\mathcal{G}_\ell(R,\Delta)C_\ell^{(0)}(\Delta)/(1-V_\ell\mathcal{G}_\ell(\Delta,\Delta))]. \quad (15)$$

In the case of Γ_1, H_ℓ is a 2×2 matrix. We define a quantity D_1, which is the determinant of a 2×2 matrix.

$$D_1=\det[I-\sum_{R_1}\mathcal{G}_1(R,R_1)H_1(R_1,R_2)] \quad (16)$$

in which I is a unit matrix and R and R_2 are restricted to include only 0 and Δ. We set $R=0$, Δ in (10) and solve the resulting two simultaneous equation for $C_1(0)$ and $C_1(\Delta)$. We write the solutions as follows:

$$C_1(R_1)=D_1^{-1}\sum_{R_2}Q(R_1,R_2)C_1^{(0)}(R_2). \quad (17)$$

The elements of the matrix Q are

$$Q(R_1,R_2)=(1-\delta_{R_1,R_2})\sum_{R_3}\mathcal{G}_1(R_1,R_3)H_1(R_3,R_2)+\delta_{R_1,R_2}[1-\sum_{R_3}\mathcal{G}_1(|\Delta-\mathbf{R}_1)|,R_3)\times H_1(R_3,|\Delta-\mathbf{R}_2|)] \quad (18)$$

and all the R variables are restricted to 0, Δ. Eq. (17) is substituted into (10), and we have

$$C_1(R)=C_1^{(0)}(R)+D_1^{-1}\sum P_1(R,R_1)C_1^{(0)}(R_1), \quad (19)$$

with

$$P_1(R,R_1)=\sum_{R_1,R_2}\mathcal{G}_1(R,R_2)H(R_2,R_3)Q(R_3,R_1). \quad (20)$$

We also define, for $\ell\neq 1$,

$$P_\ell(R,\Delta)=V_\ell\mathcal{G}_\ell(R,\Delta)$$
$$D_\ell=1-V_\ell\mathcal{G}_\ell(\Delta,\Delta) \quad (21)$$

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[11] M. V. Klein, Bul. Am. Phys. Soc. **8**, 207 (1963).
[12] J. Callaway, Nuovo Cimento (to be published).
[13] J. A. Krumhansl, Bul. Am. Phys. Soc. **8**, 207 (1963).
[14] If the representation is degenerate, we indicate functions transforming according to particular rows of the representation as $C_{\ell 1}$, $C_{\ell 2}$, $C_{\ell 3}$, etc., and any summation over ℓ is assumed to include the various rows where required.

[15] Representations are designated according to the notation of L. P. Bouckaert, R. Smoluchowski, and E. P. Wigner, Phys. Rev. **50**, 58 (1936).

so that Eq. (15) may be written in a form similar to (19)

$$C_\ell(R)=C_\ell^{(0)}(R)+D_\ell^{-1}\sum_{R_1}P_\ell(R,R_1)C_\ell^{(0)}(R_1). \quad (22)$$

We now have the formal solutions of the "partial-wave equations."

To interpret these equations more completely, we require the asymptotic form of the Green's function $\mathcal{G}_\ell(R_1,R_2)$ in the limit $R_1 \gg R_2$. To obtain this we require first the asymptotic form of $G(\mathbf{R}_1,\mathbf{R}_2)$. From (7), we have that

$$G(\mathbf{R}_1,\mathbf{R}_2) = \int d^3q\varphi_0^*(\mathbf{q},\mathbf{R}_1)(1/E-H_0)\varphi_0(\mathbf{q},\mathbf{R}_2)$$

$$= \int d^3q\varphi_0^*(\mathbf{q},\mathbf{R}_1)(1/E-E_0(\mathbf{q})+i\epsilon)\varphi_0(\mathbf{q},\mathbf{R}_2). \quad (23)$$

In the present case,

$$\varphi_0(\mathbf{q},\mathbf{R}_2)=(\Omega/8\pi^3)^{1/2}e^{i\mathbf{q}\cdot\mathbf{R}_2},$$

where Ω is the volume of the unit cell. Hence,

$$G(\mathbf{R}_1,\mathbf{R}_2)\equiv G(\mathbf{R}_2-\mathbf{R}_1) = (\Omega/8\pi^3)\int d^3q[e^{i\mathbf{q}_0\cdot(\mathbf{R}_1-\mathbf{R}_2)}/E-E_0(\mathbf{q})+i\epsilon] \quad (24)$$

and the integration includes the Brillouin zone. $G(\mathbf{R})$ has the full point symmetry of the crystal.

This expression is general. We are concerned with the case of large $|\mathbf{R}_2-\mathbf{R}_1|$ and in this case, (24) may be evaluated by the method of stationary phase, as has been discussed by Koster[8] and Lifshitz., If $\mathbf{q}_0$ satisfies $E(\mathbf{q}_0)=E$ and is such that the group velocity at $\mathbf{q}_0$ is parallel to $\mathbf{R}_1-\mathbf{R}_2$, then

$$G(\mathbf{R}_1,\mathbf{R}_2)\propto[e^{i\mathbf{q}_0\cdot(\mathbf{R}_1-\mathbf{R}_2)}/|\mathbf{R}_1-\mathbf{R}_2|]. \quad (25)$$

Then the second term in (22) represents an outgoing wave of the symmetry specified by the representation ℓ of the point group multiplied by a coefficient which is the scattering amplitude. We will see this result more explicitly below.

The energies of bound states and resonances are determined from the properties of the denominator D_ℓ in (22). D_ℓ can vanish only when E is outside the continuum of levels specified by $E_0(\mathbf{q})$. In such a case, there is no incident wave, and q_0 in (25) is imaginary so that the wave function decays exponentially, and a bound state exists. In the continuum, the real part of D_ℓ may vanish. Then the scattering amplitude will be large and a resonance exists. The locations and widths of resonant spin-wave states were discussed in Ref. 5.

It is now desirable to invert Eq. (9) to obtain φ.

$$\varphi(\mathbf{R}_\nu)=\sum_\ell U^{-1}(\nu,\ell)C_\ell(R) = \varphi_0(\mathbf{R}_\nu)+\sum_{\ell,R1} U^{-1}(\nu,\ell)D_\ell^{-1}P_\ell(R,R_1)C_\ell^{(0)}(R_1) \quad (26)$$

At this point, the formal theory of the scattering is complete. It remains to apply the general formula to specific cases.

As an application of the foregoing general theory, we will consider only a simple cubic system, since only in this case have the integrals involved in the Green's functions $G(0,0)$, $G(0,\Delta)$ and $G(\Delta,\Delta)$ been computed.[5] For a simple cubic lattice

$$E_0(\mathbf{q})=4JS(3-\cos q_xa-\cos q_ya-\cos q_za). \quad (27)$$

Then

$$G(\mathbf{R})=\frac{-a^3}{(2\pi)^3 4JS}\int\frac{e^{-i\mathbf{q}\cdot\mathbf{R}}d^3q}{E'-\cos q_xa-\cos q_ya-\cos q_za-i\epsilon)}$$

$$=\frac{-a^3}{(2\pi)^3 4JSi}\int\int \exp\{(-i)[\mathbf{q}\cdot\mathbf{R}+t(E^0-\cos q_xa-\cos q_ya-\cos q_za)]\}dtd^3q$$

(where $E'=3-E/4JS$). The integral is evaluated by the method of stationary phase as mentioned earlier. If $\mathbf{q}_0$ is a vector as described above (whose rectangular components are q_{0x}, etc.)

$$G(R)=(-a/8\pi JS)(e^{i\mathbf{q}_0\cdot\mathbf{R}}/R)\left[\frac{\sin^2q_{0x}a+\sin^2q_{0y}a+\sin^2q_{0z}a}{\sin^2q_{0x}a\cos q_{0y}a\cos q_{0z}a+\sin^2q_{0y}a\cos q_{0x}a\cos q_{0z}a+\sin^2q_{0z}a\cos q_{0x}a\cos q_{0y}a}\right]^{1/2}. \quad (28)$$

We require the expansion of this quantity for small q_0. We retain only the isotropic portion of the second term. We find

$$G(R)=(-a/8\pi JS)[1+(a^2q_0^2/10)](e^{iq_0R}/R). \quad (29)$$

It is necessary next to evaluate the quantities $P_\ell(R,R_1)$. This involves some rather tedious algebra. The scattering amplitude, f, is found as the coefficient of e^{iqR_ν}/R_ν in (26):

$$\varphi(R_\nu)=\varphi_0(R_\nu)+f(e^{iq_0R_\nu}/R_\nu). \quad (30)$$

For the simple cubic lattice, there are three contributions to f, which may be roughly described as s wave, p wave, and d wave. More precisely, there are the contributions from Γ_1, Γ_{15}, and Γ_{12} representations discussed previously.

$$f=f_s+f_p+f_d,$$

where

$$f_s=(-a/8\pi JSD_1)[1+(a^2q_0^2/10)] \times[F_1(0)+F_1(\Delta)C_1^{(0)}(\varkappa,\Delta)],$$

$$f_p = (-a/8\pi JSD_{15})[1+(a^2q_0^2/10)] \times \textstyle\sum_i F_{15,i}(\Delta)C_{15,i}^{(0)}(\varkappa,\Delta)\,,$$

$$f_d = (-a/8\pi JSD_{12})[1+(a^2q_0^2/10)] \times \textstyle\sum_i F_{12,i}(\Delta)C_{12,i}^{(0)}(\varkappa,\Delta)\,, \quad (31)$$

and we have used the long-wavelength approximation for the Green's functions given in (29). The sum over i includes all the rows of the irreducible representations considered and a is the lattice constant. The functions $C_{i,j}^{(i)}$ are summetrized linear combinations of plane waves belonging to the jth row or irreducible representation i as specified by (12). The incident plane wave has a wave vector $\varkappa$. The quantities F are given as follows:

$$F_1(0) = -4JS\{\epsilon(1-6c\Delta-d\rho)+6\Delta(c\epsilon+d\Delta) + (6)^{1/2}C_1^{(0)}(q_0,\Delta)[\epsilon(b\Delta+c\rho) + \Delta(1-\epsilon b-6c\Delta)]\}\,,$$

$$F_1(\Delta) = -4JS\{(6)^{1/2}[\Delta(1-6c\Delta-d\rho)+\rho(c\epsilon+d\Delta)] + C_1^{(0)}(q_0,\Delta)[6\Delta(b\Delta+c\rho) + \rho(1-\epsilon b-6c\Delta)]\}\,,$$

$$F_{15,i}(\Delta) = -4JS\rho C_{15,i}^{(0)}(q_0,\Delta)\,, \quad (32)$$

and

$$F_{12,i} = -4JS\rho C_{12,i}^{(0)}(q_0,\Delta)\,,$$

in which

$$\epsilon = 3[1-(J'/J)];\quad \Delta = \tfrac{1}{2}[(J'/J)(S'/S)^{1/2}-1]\,,$$
$$\rho = \tfrac{1}{2}[1-(J'S'/JS)]\,, \quad (33)$$
$$b = -4JSG(0)\,,\quad c = -4JSG(\Delta)\,,$$

and

$$d = -4JS[G(0)+4G(\Delta_2)+G(2\Delta)] \quad [\Delta_2 = a(1,1,0)\,;\, 2\Delta = a(2,0,0)]\,.$$

In addition, we list also explicit formulas for the quantities D_ℓ.

$$D_1 = 1-3b+(E'b-1)(2-\tfrac{1}{3}E')+J'/J \times (3b-(E'b-1)\{S'/S(1-\tfrac{1}{3}E')+1\})$$
$$D_{15} = -4JS[G(0)-G(2\Delta)] \quad (34)$$
$$D_{12} = -4JS[G(0)-2G(\Delta_2)+G(2\Delta)]\,.$$

These complicated expressions simplify considerably in the limit of small q_0, $\varkappa$. We find, after some tedious algebra, in which terms of order q_0^4 are neglected

$$f_s = (-a/4\pi D_1)q_0^2a^2(J'/J)[1-(S'/S)]\,,$$
$$f_p = (a/2\pi D_{15})q_0^2a^2[1-(J'S'/JS)]\cos\theta\,, \quad (35)$$

and

$$f_d \propto O(q^4)\,.$$

Hence to order q^2, there are contributions from f_s and f_p. It is particularly to be noted that the f_s and f_p are both of the same order in q_0a. The total scattering cross section is, to this order

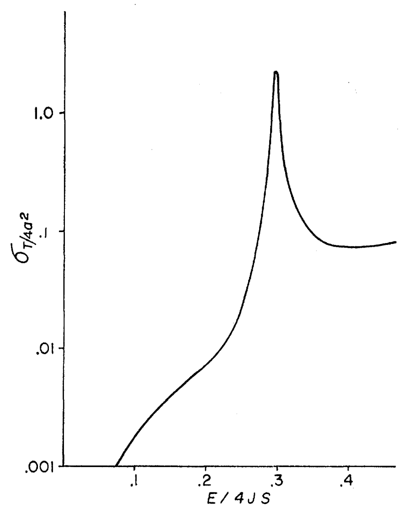

FIG. 1. A dimensionless measure of the total cross section for the scattering of spin waves by defects, $\sigma_T/4a^2$ is plotted as a function of spin-wave energy $E/4JS$ for an impurity characterized by $J'/J=.1$, $S'/S=3/7$. Note: abscissa label should be $\sigma_T/4a^2$.

$$\sigma_T = \frac{a^2}{4\pi}q_0^4a^4\left[\frac{1}{|D_1|^2}\left(\frac{J'}{J}\right)^2\left(1-\frac{S'}{S}\right)^2 + \frac{4}{3|D_{15}|^2}\left(1-\frac{J'S'}{JS}\right)^2\right]. \quad (36)$$

We have not expanded the determinants D_1 and D_{15} since these contain the possible resonant character of the cross section.

It is particularly to be noted that the contribution from s- and p-wave scattering are of the same order in q_0a, and that the scattering cross section vanishes as $(q_0a)^4$ at long wavelengths. This dependence on wave number is the same as found for phonons in a similar calculation,[12] but it is in contradiction to the predictions of the first Born approximation. A calculation of the scattering of spin waves by imperfections using the Born approximation has already been given by Douglas.[3] The expression can also be obtained from this work by formally allowing the spin-wave energy to become large so that the Green's function combinations b, c, and d go to zero. The quantities D_ℓ then approach unity. We consider only the long wavelength limit. There are two cases:

(1) The impurity has a different spin from that of the host: Then we find

$$f_s = (a/2\pi)(\epsilon+12\Delta+6\rho) = (-3a/2\pi)(J'/J) \times [(S'/S)^{1/2}-1]^2,$$
$$f_p = O(q^2)\,. \quad (37)$$

The scattering of long wavelength spin waves is then predominately s wave, and the total cross section σ_T has a constant value

$$\sigma_T = (9a^2/\pi)(J'/J)^2[(S'/S)^{1/2}-1]^4\,. \quad (38)$$

(2) The spin of the impurity is the same as that of the host, or $J'=0$. In this situation the s-wave scattering goes to zero, but the p-wave term still contributes. We have

$$f_p=(-a/2\pi)(\delta J/J)q_0^2a^2\cos\theta, \quad (39)$$

and

$$\sigma_T=(a^2/3\pi)(\delta J/J)^2q_0^4a^4, \quad (40)$$

with $\delta J=J'-J$.

It is seen that the second case agrees with the exact calculation in the appropriate limit but in the first situation a quite erroneous result for f_s is obtained. An alternate derivation of the Born approximation expressions is given in the appendix.

In Fig. 1 we show the total scattering cross section as a function of spin-wave energy for the case $(J'/J)=0.1$, $(S'/S)=3.7$. These parameters were chosen so that a low energy resonance would appear.

II. APPLICATION TO THERMAL CONDUCTIVITY

We will now apply the results of the previous discussion of spin-wave scatterings to the computation of the thermal conductivity of a spin-wave system. We will assume in this paper that the only important scattering processes are boundary scattering and defect scattering. Other processes including spin-wave phonon and spin-wave-spin-wave interactions will be considered in subsequent work. The mean free path of a spin wave is denoted by ℓ which is assumed to be a function of energy only. The thermal conductivity, $\varkappa$, is given by the expression:

$$\varkappa=(K/3(2\pi)^3)\int[e^{E/KT}/(e^{E/KT}-1)^2]\times(E/KT)^2V\ell d^3q \quad (41)$$

in which K is Boltzmann's constant, E is the spin-wave energy, and V is the group velocity,

$$V=(1/\hbar)dE/dq.$$

In the present work, we will assume that the surfaces of constant energy are spherical. Thus, we write

$$d^3q=q^2(dq/dE)dEd\Omega,$$

so that (41) becomes

$$\varkappa=(K/6\pi^2\hbar)\int_0^{E_m}[e^{E/KT}/(e^{E/KT}-1)^2]\times(E/KT)^2\ell(E)q^2(E)dE \quad (42)$$

in which E_m is the maximum energy in the spin-wave spectrum. The spin-energy is related to the wave vector q through Eq. (27) in the case of a simple cubic lattice. We do not include any external magnetic field. The generalizations required to discuss other lattices, or effects due to the internal fields are quite simple.

Equation (27) may be solved by iteration to obtain $q^2(E)$. Including second order corrections, we have

$$a^2q^2(E)=(E/2JS)[1+(E/40JS)+\cdots]. \quad (43)$$

If we substitute this expression and introduce the dimensionless variable $x=E/KT$, we have

$$\varkappa=(K^2T/3\pi^2\hbar a^2)(KT/4JS)\int_0^{x_m}[x^3e^x/(e^x-1)^2]\times[1+(xKT/40JS)]\ell(x)dx \quad (44)$$

(with $x_m=E_m/KT$).

In the presence of defect scattering and boundary scattering, we form the reciprocal mean free path for the combination by adding the reciprocal free paths for the separate processes. This procedure is based on the independence of the separate scattering processes. We characterize boundary scattering by a constant mean free path, L. The mean free path for defect scattering, ℓ_D, is determined from the differential scattering cross section, $d\sigma/d\Omega$, by[16]

$$\ell_D^{-1}=2\pi N\int(1-\cos\theta)(d\sigma/d\Omega)\sin\theta d\theta, \quad (45)$$

in which N is the concentration of defects, θ is the angle between the wave vectors of the incident and scattered waves, and

$$d\sigma/d\Omega=|f_s+f_p+f_d|^2,$$

where the scattering amplitudes are given in (31). Then

$$\ell^{-1}=L^{-1}+\ell_D^{-1}. \quad (46)$$

It is evident that if the rather complicated expressions for the scattering amplitude which were given in Eq. (31) are used, numerical integration of (44) is required. There are, however, some simple approximations which illustrate important characteristics of the results.

First, if there were no defect scattering, $N=0$, the thermal conductivity would be given at low temperatures for which we can make x_m infinite by

$$\kappa=[K(KT)^2L/2\pi^2a^2\hbar JS]\times[\zeta(3)+(KT/10JS)\zeta(4)+\cdots]. \quad (47)$$

The quantity ζ is the Reimann zeta function. This expression exhibits the familiar T^2 temperature dependence of the spin-wave thermal conductivity at low temperatures.

If we attempt to neglect the boundary scattering and consider the calculation of thermal conductivity limited by defect scattering alone, we find that the integral (44) does not converge. This problem arises since (36) implies that $\ell_D(x)$ is proportional to x^{-2} for small x. Hence, in this case the integrand of (43) is proportional

[16] J. M. Ziman, *Electrons and Phonons* (Oxford University Press, Oxford, 1960), p. 306.

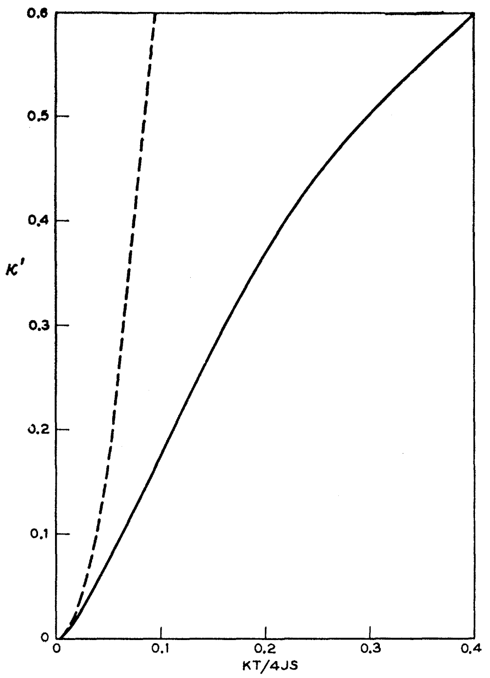

FIG. 2. A dimensionless measure of the thermal conductivity of a spin-wave system, $\kappa' = 3\pi a^4 N\hbar\kappa/4KJS$ is plotted as a function of temperature for a system of defects characterized by $J'/J=0.1$, $S'/S=3/7$, and a boundary scattering parameter. $L=10\pi/Na^2$. The dashed line shows the thermal conductivity when only boundary scattering is included.

to $1/x$ for small x, and a logarithmic divergence results. Defect scattering must, therefore, be considered in conjunction with some other scattering process, such as boundary scattering, spin-wave phonon scattering, etc. Our present considerations include only boundary scattering in addition to defect scattering.

If the defect scattering is weak compared to boundary scattering, we expand (46) as follows:

$$\ell = L[1-(L/\ell_D)+\cdots]. \tag{48}$$

To avoid numerical integration at present, we approximate ℓ_D as follows:

$$\ell_D^{-1} = NAq^4, \tag{49}$$

in which

$$A=(a^6/4\pi)\{(J'/J)^2(1-S'/S)^2+\tfrac{4}{3}[1-(J'S'/JS)] \times[1+(J'/J)-2(J'S'/JS)]\}, \tag{50}$$

and we have neglected the quantities D_1 and D_{15}, and so have ignored the possibility of resonant scattering. If Eqs. (48)–(50) are substituted into (44), the integrals can be performed in the low temperature limit, and we obtain an additional term in (47)

$$\kappa=[K(KT)^2L/2\pi^2a^2\hbar JS][\zeta(3)+(KT/10JS)\zeta(4) -20NL(KT/2JSa^2)^2A\zeta(5)+\cdots]. \tag{51}$$

The point defects give rise to a decrease in thermal conductivity which varies at T^4. Another T^4 term, which has opposite sign, arises from a higher term in the expansion (43) for $q^2(E)$.

If the contribution from defect scattering in (51) is small compared to the other terms, a thermal resistance due to the defects may be defined. The situation is analogous to that existing in the theory of lattice thermal conductivity in which it is possible to define a specific thermal resistance due to point defects only when the contribution from defects is small. To obtain the resistance, we define

$$W=1/\kappa. \tag{52}$$

Let $\kappa=\kappa_0+\Delta\kappa$, where $\Delta\kappa$ is the contribution from the defect scattering. Similarly, put $W=W_0+\Delta W$. Then

$$\Delta W=-\Delta\kappa/\kappa_0^2=10\pi^2[\zeta(5)NA\hbar/\zeta(3)JSa^2]. \tag{53}$$

The thermal resistance due to defects is, in this approximation, temperature-independent.

We now discuss the opposite situation in which the defect scattering is strong compared to boundary scattering. The criterion can be expressed in terms of a dimensionless parameter ξ, by defining

$$\xi=(NLA/a^4). \tag{54}$$

Equation (51) applies when $\xi \ll 1$. If $\xi > 1$, defect scattering will be more important than boundary scattering except for low energies. We then approximate (44) by setting $x^3e^x/(e^x-1)^2=x$ for $x<x_1$, and neglecting boundary scattering for $x>x_1$. We also let x_m go to infinity and neglect the term $xKT/40JS$. Then (44) becomes with the inclusion of (46)

$$\kappa=\frac{K^2T}{3\pi^2\hbar a^2}\left(\frac{KT}{4JS}\right)\left[L\int_0^{x_1}\frac{xdx}{1+(L/\ell_D)} +\frac{1}{N}\int_{x_1}^{\infty}\frac{x^3e^x}{(e^x-1)^2}\ell_D dx\right]. \tag{55}$$

We use the approximation (49) for ℓ_D. A reasonable choice for x_1 is unity. We then obtain for κ:

$$\kappa=\frac{KJSa^2}{6\pi^2NA\hbar}\left\{\ln\left[1+\frac{NAL}{a^4}\frac{K^2T^2}{4J^2S^2}\right]+2\sum_{n=1}^{\infty}\left(1+\frac{1}{n}\right)e^{-n}\right\}$$

$$=\frac{KJSa^2}{6\pi^2NA\hbar}\left\{\ln\left[1+\xi\left(\frac{KT}{2JS}\right)^2\right]+2.0814\right\}. \tag{56}$$

In the case of strong defect scattering, the thermal conductivity retains a logarithmic dependence on the size parameter L. The thermal conductivity as given by (56) is a slowly rising function of temperature with a much weaker dependence than the T^2 behavior predicted by (51).

It is necessary to integrate (44) numerically if resonant scattering is to be included. In this case the general temperature dependence of the conductivity is much weaker than T^2 except for $KT \ll 4JS$. The magnitude of the conductivity is much less in magnitude than predicted by (56). An example of this situation is shown in Fig. 2.

APPENDIX

In this appendix we give an alternate derivation of the formulas given in (38) and (40) as the total scattering cross section for spin waves from defects in the long wavelength limit using the Born approximation.

The Hamiltonian of Eq. (1) can be expressed as

$$H=-\sum_{R,\Delta} J(\mathbf{R},\,\mathbf{R}+\Delta)[S_z(\mathbf{R})S_z(\mathbf{R}+\Delta)+\tfrac{1}{2}S_+(\mathbf{R}+\Delta)S_-(\mathbf{R})+\tfrac{1}{2}S_+(\mathbf{R})S_-(\mathbf{R}+\Delta)]. \quad \text{(A1)}$$

We introduce spin-wave operators by the usual transformation

$$\begin{aligned} S_z(\mathbf{R})&=S(\mathbf{R})-a^\dagger(\mathbf{R})a(\mathbf{R}),\\ S_+(\mathbf{R})&=(2S(\mathbf{R}))^{1/2}a(\mathbf{R}),\\ S_-(\mathbf{R})&=(2S(\mathbf{R}))^{1/2}a^\dagger(\mathbf{R}),\\ a(\mathbf{R})&=1/(N)^{1/2}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}}a_{\mathbf{q}},\\ a^+(\mathbf{R})&=1/(N)^{1/2}\sum_{\mathbf{q}} e^{-i\mathbf{q}\cdot\mathbf{R}}a^\dagger{}_{\mathbf{q}}. \end{aligned} \quad \text{(A2)}$$

After these substitutions are made, the expression for H can be split into two parts

$$H=H_0+H',$$

in which H_0 is the spin wave Hamiltonian for the crystal with the magnetic defect replaced by a "normal" atom and H' describes the contribution of the defect. With the neglect of four-order terms, we have for H', assuming the defect is located at $\mathbf{R}'$, with exchange integral J' and spin S' (the host lattice has, as before exchange integral J and spin S).

$$H'=-2\sum_{\Delta}\bigg\{S(J'S'-JS)-\frac{1}{N}\sum_{\mathbf{q},\mathbf{q}'} a_{\mathbf{q}'}{}^+a_{\mathbf{q}}e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}}\times[(J'-J)S+(J'S'-JS)e^{i(\mathbf{q}'-\mathbf{q})\cdot\Delta}-(J'(S'S)^{1/2}-JS)(e^{i\mathbf{q}'\cdot\Delta}+e^{-i\mathbf{q}\cdot\Delta})]\bigg\}. \quad \text{(A3)}$$

The portion of H' which causes scattering can be written as

$$\frac{1}{N}\sum_{\mathbf{q},\mathbf{q}'}\gamma(q',q)a_{\mathbf{q}'}{}^+a_{\mathbf{q}}.$$

The differential scattering cross section can be computed as follows (we consider only a simple cubic lattice):

$$d\sigma/d\Omega=(a^3/V)w, \quad \text{(A4)}$$

where V is the velocity of a spin wave of wave vector q, and w is the transition probability per unit time, which can be found from the usual formula of first order time dependent perturbation theory.

$$w=(2\pi/\hbar)[a^3/(2\pi)^3]\int q'^2dq'\times\delta(E(\mathbf{q})-E(\mathbf{q}'))|\gamma(\mathbf{q}',\mathbf{q})|^2. \quad \text{(A5)}$$

We find

$$d\sigma/d\Omega=(a^2/64\pi^2J^2S^2)|\gamma(\mathbf{q}',\mathbf{q})|^2 \quad \text{(A6)}$$

in the long wavelength limit. From (A5), $|\mathbf{q}|=|\mathbf{q}'|$. Eq. (A3) yields for $|\gamma(\mathbf{q}',\mathbf{q})|^2$:

$$|\gamma(q',q)|^2=4J'^2S^2\bigg\{\Big(1-\frac{J}{J'}\Big)+\Big(\frac{S'}{S}-\frac{J}{J'}\Big)e^{i(\mathbf{q}'-\mathbf{q})\cdot\Delta}-\bigg[\Big(\frac{S'}{S}\Big)^{1/2}-\frac{J}{J'}\bigg](e^{i\mathbf{q}'\cdot\Delta}+e^{-i\mathbf{q}\cdot\Delta})\bigg\}^2. \quad \text{(A7)}$$

If $S'=S$, we obtain in the limit as $q,\,q'\to 0$,

$$|\gamma(\mathbf{q}',\mathbf{q})|^2=144J'^2S^2[1-(S'/S)^{1/2}]^2$$

so that the scattering cross section becomes

$$\sigma_T=(d\sigma/d\Omega)d\Omega=(9a^2/\pi)(J'/J)^2[1-(S'/S)^{1/2}]^4. \quad \text{(A8)}$$

This result agrees with Eq. (38).

In the case $S=S'$, we have, again in the long wavelength limit

$$|\gamma(\mathbf{q}',\mathbf{q})|^2=4S^2(J'-J)^2\{\sum_{\Delta}(\mathbf{q}'\cdot\Delta)(\mathbf{q}\cdot\Delta)\}^2=16J'^2S^2q^4a^4\cos^2\theta$$

where θ is the angle between $\mathbf{q}$ and $\mathbf{q}'$. Hence, the scattering cross section is

$$(d\sigma/d\Omega)=(a^2/4\pi)[(J'-J)^2/J^2]q^4a^4\cos^2\theta, \quad \text{(A9)}$$

$$\sigma_T=(a^2/3\pi)(\delta J/J)^2q^4a^4,$$

which agrees with Eq. (40).