Effect of Spin Waves on the Phonon Energy Spectrum of a Heisenberg Ferromagnet

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The magnon-phonon interaction is derived via modulation of an isotropic exchange, and it is shown that the lowest-order contribution to the phonon lifetime at low temperatures comes from processes whereby the phonon emits and later reabsorbs two magnons. Interactions between the intermediate magnons can significantly influence the intermediate state, so we have retained the full magnon-magnon interaction (via the two-spin-wave t matrix) in our calculation of the phonon self-energy. We find that the phonon self-energy has singularities at the two-spin-wave bound states and resonances at the resonant two-spin-wave states. One may understand the anomalously large phonon linewidth in these regions in terms of a strong interaction (binding together) of the intermediate magnons. The rapid variation of the phonon energy shift may intuitively be explained via the large "repulsion" encountered in simple perturbation theory when two energy levels approach each other. An interesting result is that, because of the transformational properties of the bound states for $\mathbf{q}$ along the [111] direction, longitudinal phonons couple only to the singly degenerate (s-wave) bound state, and the transverse phonons couple only to the doubly degenerate (d-wave) bound state. It is pointed out that use of an external magnetic field would make experimental observation of this effect easier.

I. INTRODUCTION

It has been shown both theoretically and experimentally that the magnetic and elastic properties of magnetic solids have a mutual influence on each other. For example, a static manifestation of this magnetoelastic coupling is the phenomenon of magnetostriction, whereby a crystal may come to equilibrium in a strained configuration via the creation of an easy axis for the magnetization.[1,2] We have investigated the dynamics of the magnon-phonon system and, in particular, its effect on the phonon excitation spectrum (energy and lifetime) of a Heisenberg ferromagnet. A preliminary account of this work has previously been given.[3] The purpose of this paper is to give a more detailed account of the theory and report some more recent results.

We obtain the magnon-phonon interaction from the variation of exchange between nearest-neighbor spins with local distortions of the lattice in Sec. II. As we shall see, the analysis leads to scattering processes, whereby:

(a) One phonon is annihilated (created) and one spin wave is created (annihilated).

(b) A spin wave and a phonon are annihilated and a spin wave is created.

(c) A spin wave is annihilated and a spin wave and a phonon are created.

(d) A phonon is annihilated (created) while emitting (absorbing) *two* spin waves.

The processes described in (a) cause mixing of the excitations, and have been shown by previous authors[4–6] to give rise to magnetoelastic waves near the region of intersection of the magnon and phonon dispersion relations. The contributions of processes (b) and (c) vanish at zero temperature since both involve destruction of a spin wave. Process (d), however, does not vanish in this limit, since a phonon may emit and later reabsorb two spin waves even at zero temperature. In addition, the processes in (a) do not introduce damping, so that *the lowest-order contribution to the phonon lifetime comes from one-phonon–two-magnon processes.*

We will demonstrate below that the phonon has a finite lifetime at zero temperature even if the interactions between the intermediate magnons are neglected. Moreover, because of the attractive nature of these magnon-magnon interactions, one must consider the possibility of the intermediate magnons binding together.[7–10] Such processes will significantly affect the phonon excitation spectrum in regions of momentum space where the phonon and two-spin-wave bound state have nearly the same energy. We show how this comes about in Sec. III and present in Sec. IV numerical calculations of the phonon self-energy to lowest order in the density of spin waves (exact at zero temperature). In Sec. V, we draw some conclusions from our calculations.

II. MAGNETOELASTIC COUPLING

We treat a simple cubic Heisenberg ferromagnet described by the Hamiltonian

$$\mathcal{H}=-\frac{1}{N}\sum_{\mathbf{x}_i,\mathbf{x}_j}\sum_{\alpha\beta=x,y,z}J_{\alpha\beta}(\mathbf{x}_i-\mathbf{x}_j)S^{\alpha}(\mathbf{x}_i)S^{\beta}(\mathbf{x}_j)\,,\quad(1)$$

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[7] M. Wortis, Phys. Rev. 132, 85 (1963).
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[10] R. Silberglitt and A. B. Harris, Phys. Rev. 174, 640 (1968).

where we assume an isotropic nearest-neighbor exchange interaction, so that

$$J_{\alpha\beta}(\mathbf{x}_i-\mathbf{x}_j)=J\delta_{\alpha\beta}\,,\quad \mathbf{x}_j=\mathbf{x}_i+\boldsymbol{\delta}$$
$$=0\,,\qquad \text{otherwise} \tag{2}$$

where $\boldsymbol{\delta}$ is a vector from a lattice site to one of its nearest neighbors, in the positive or negative x, y, or z direction, but $\delta_{\alpha\beta}$ is the Kronecker δ. To obtain the coupling of magnons to lattice vibrations, we expand the exchange integral in a Taylor series about the equilibrium lattice sites:

$$J_{\alpha\beta}((\mathbf{x}_i+\Delta\mathbf{x}_i)-(\mathbf{x}_j+\Delta\mathbf{x}_j))$$
$$=J_{\alpha\beta}(\mathbf{x}_i-\mathbf{x}_j)+(\Delta\mathbf{x}_i-\Delta\mathbf{x}_j)\cdot\nabla_{\mathbf{x}_i-\mathbf{x}_j}J_{\alpha\beta}(\mathbf{x}_i-\mathbf{x}_j)\,, \tag{3}$$

where terms of order $(\Delta x)^2$ and higher are neglected. In Eq. (3), components of the gradient will determine the magnitude of the magnetoelastic coupling. This form of coupling has been discussed by Pytte,[11] who has calculated the contribution to the phonon energy spectrum from processes involving simultaneous creation and destruction of spin waves. (This contribution vanishes at zero temperature.) In our calculation, we consider simultaneous creation of *two* spin waves, a process allowed even at zero temperature.

We note that the gradient of $J_{\alpha\beta}$ is not necessarily proportional to $\delta_{\alpha\beta}$, since the lattice displacements may cause internal distortions which can lower the symmetry of the system and allow off-diagonal elements.[12] Also, since $J_{\alpha\beta}$ must be an even function of $\mathbf{x}_i-\mathbf{x}_j$, its gradient is odd. In addition, we make two assumptions concerning the behavior of ∇J. First, we assume that $\nabla J_{\alpha\beta}(\mathbf{x}_i-\mathbf{x}_j)$ vanishes except for i,j nearest neighbors. Second, we assume the following form:

$$(\partial/\partial X_\mu)[J_{\alpha\beta}(\delta_\nu)]=a_{\alpha\beta}\delta_{\mu\nu}+b_{\alpha\beta}(1-\delta_{\mu\nu})\,, \tag{4}$$

where $\mathbf{X}\equiv\mathbf{x}_i-\mathbf{x}_j$. This assumption is equivalent to the statement that the variation in exchange caused by a distortion along a given direction is different for a spin pair along that direction than for one perpendicular to it.

The lattice displacement operators may be written in terms of phonon field operators $\varphi_{\mathbf{q}\lambda}=b_{\mathbf{q}\lambda}+b_{-\mathbf{q}\lambda}^\dagger$ and polarization vectors $\hat{\epsilon}_{\mathbf{q}\lambda}$ in the usual manner[13]:

$$\delta\mathbf{x}_i=\sum_{\mathbf{q}\lambda}(2\rho\Omega_{\mathbf{q}\lambda})^{-1/2}\hat{\epsilon}_{\mathbf{q}\lambda}\varphi_{\mathbf{q}\lambda}e^{-i\mathbf{q}\cdot\mathbf{x}_i}\,, \tag{5}$$

where ρ is the density of the system and $\Omega_{\mathbf{q}\lambda}$ is the energy of a phonon of momentum $\mathbf{q}$ and polarization λ. For the spin operators in the ∇J term of Eq. (3), we use the simple spin-wave expressions,[14] since we intend to treat the magnetoelastic interaction as a perturbation which mixes the spin and phonon systems. These expressions are

$$S_i^+=(2S)^{1/2}a_i^\dagger\,,\quad S_i^-=(2S)^{1/2}a_i\,,\quad S_i^z=-S+a_i^\dagger a_i\,, \tag{6}$$

where a_i and $a_i^\dagger$ annihilate and create, respectively, bosons at site $\mathbf{x}_i$. Finally, for this isotropic system, we expect that $a_{\alpha\beta}$ and $b_{\alpha\beta}$ in Eq. (4) will have only two unique components, corresponding to $\alpha=\beta$ and $\alpha\neq\beta$.

From the above considerations and Eqs. (3)–(6), we find that the interaction terms in $\mathcal{H}$ through which a phonon may create or destroy *two* magnons are given by

$$V_{2M-P}=-\frac{1}{N}\sum_{\mathbf{kq}\lambda}g(\mathbf{kq}\lambda)\varphi_{\mathbf{q}\lambda}(a_{\mathbf{k}}^\dagger a_{\mathbf{q}-\mathbf{k}}^\dagger-a_{-\mathbf{k}}a_{\mathbf{k}-\mathbf{q}})\,, \tag{7}$$

where

$$a_{\mathbf{k}}=\frac{1}{\sqrt{N}}\sum_{\mathbf{x}_i}e^{-i\mathbf{k}\cdot\mathbf{x}_i}a_i \tag{8}$$

and

$$g(\mathbf{kq}\lambda)=\tfrac{1}{2}S\sum_{\mu,\nu=x,y,z}\{(2\rho\Omega_{\mathbf{q}\lambda})^{-1/2}\epsilon_{\mathbf{q}\lambda}{}^{\mu}\sin\tfrac{1}{2}q_\nu$$
$$\times\cos(k_\nu-\tfrac{1}{2}q_\nu)[a\delta_{\mu\nu}+b(1-\delta_{\mu\nu})]\}\,. \tag{9}$$

In Eq. (9), a and b are the values of $a_{\alpha\beta}$ and $b_{\alpha\beta}$ for $\alpha\neq\beta$, and the lattice constant has been taken to be unity. For a phonon with $\mathbf{q}$ along the [111] direction, the polarization vectors may be taken as

$$\hat{\epsilon}_l=(1/\sqrt{3})(1,1,1)\,, \tag{10a}$$

$$\hat{\epsilon}_{t_1}=(1/\sqrt{6})(1,1,-2)\,, \tag{10b}$$

$$\hat{\epsilon}_{t_2}=(1/\sqrt{2})(1,-1,0)\,, \tag{10c}$$

so that the coupling constants are given from Eq. (9) by

$$g(\mathbf{kq}l)=(C_{ql}/\sqrt{3})(a+2b)$$
$$\times(\cos K_x+\cos K_y+\cos K_z)\,, \tag{11a}$$

$$g(\mathbf{kq}t_1)=(C_{qt_1}/\sqrt{6})(a-b)$$
$$\times(\cos K_x+\cos K_y-2\cos K_z)\,, \tag{11b}$$

$$g(\mathbf{kq}t_2)=(C_{qt_2}/\sqrt{2})(a-b)(\cos K_x-\cos K_y)\,, \tag{11c}$$

where

$$C_{\mathbf{q}\lambda}=\frac{(S\sin\frac{1}{2}q)}{2(2\rho\Omega_{\mathbf{q}\lambda})^{1/2}}\,, \tag{12a}$$

$$\mathbf{K}=\mathbf{k}-\tfrac{1}{2}\mathbf{q}\,. \tag{12b}$$

Here $\mathbf{K}$ is the relative momentum of the spin-wave pair which couples to the phonon. Note that $g(\mathbf{kq}\lambda)$ is even in the components of $\mathbf{K}$ and vanishes for $\mathbf{q}=0$. Thus the coupling does not depend upon the sign of the relative momentum of the spin-wave pair and vanishes for a uniform displacement of the lattice [such a displacement does not change $J(\mathbf{x}_i-\mathbf{x}_j)$].

[11] E. Pytte, Ann. Phys. (N. Y.) 32, 377 (1965).
[12] We are grateful to Professor H. B. Callen for pointing out this fact to us.
[13] R. E. Peierls, *Quantum Theory of Solids* (Clarendon Press, Oxford, England, 1955).
[14] T. Holstein and H. Primakoff, Phys. Rev. 58, 1098 (1940).

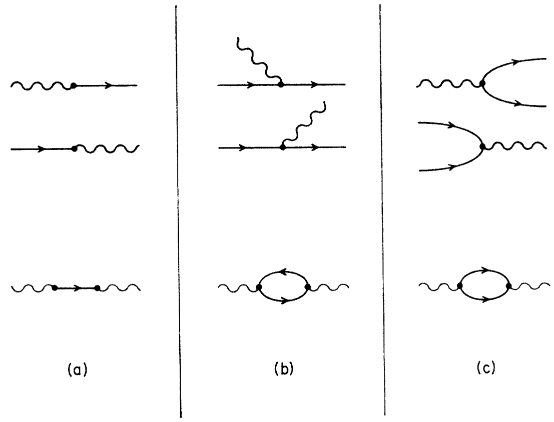

FIG. 1. Possible magnon-phonon vertices, along with a typical contribution each makes to the phonon self-energy.

III. CALCULATION OF PHONON ENERGY SPECTRUM

We assume a Hamiltonian for the magnon-phonon system given by

$$\mathcal{H}=\mathcal{H}_{\text{Heis}}+\mathcal{H}_P^{(0)}+V_{M-P}, \tag{13}$$

where $\mathcal{H}_P^{(0)}$ represents noninteracting phonons, but $\mathcal{H}_{\text{Heis}}$ allows the magnons to interact fully with each other. V_{M-P}, which causes the mixing, is the full magnetoelastic interaction [determined by the second term on the right-hand side of Eq. (3)]. However, we shall see that at low temperatures one may replace V_{M-P} with V_{2M-P} given by Eq. (7).

We will use diagrammatic Green's-function theory to calculate the phonon energy spectrum, so that we must calculate the irreducible phonon self-energy $\Sigma_{\mathbf{q}\lambda}(\omega)$.[15] As is well known, if this function is slowly varying near $\omega=\Omega_{\mathbf{q}\lambda}$, where $\Omega_{\mathbf{q}\lambda}$ is the unperturbed energy of a phonon with momentum $\mathbf{q}$ and polarization λ, its real part at $\omega=\Omega_{\mathbf{q}\lambda}$ gives the phonon energy shift, while its imaginary part gives the inverse of the phonon lifetime. $\Sigma_{\mathbf{q}\lambda}(\omega)$ is the sum of the internal parts of all irreducible diagrams[15] in which a phonon of momentum $\mathbf{q}$ and energy ω both enters and leaves, undergoing all possible intermediate (magnon-phonon) interactions allowed by V_{M-P}. Substituting the expressions for $\delta\mathbf{x}_i$ and $S^\alpha(\mathbf{x}_i)$, Eqs. (5) and (6), into Eqs. (1) and (3), we find that the intermediate magnon-phonon vertices are of three types. First, from the S^xS^z and S^yS^z terms, there are one-magnon–one-phonon vertices. Second, from the S^xS^x and S^yS^y terms, there are one-phonon–two-magnon vertices at which a spin wave is created and another is annihilated. Finally, from the S^xS^y terms, there are one-phonon–two-magnon vertices at which both spin waves are either created or annihilated. These are the terms included in V_{2M-P} given by Eq. (7). In Fig. 1, the three types of vertices are indicated, along with a typical contribution each makes to $\Sigma_{\mathbf{q}\lambda}(\omega)$.

[15] A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinskii, *Quantum Field Theoretical Methods in Statistical Physics* (Pergamon Press, Inc., New York, 1965), 2nd ed.

In our calculation, we shall neglect the mixing of magnons and phonons caused by the vertices shown in Fig. 1(a). This will be a good approximation far away from any crossover of the magnon and phonon dispersion curves. Moreover, in the neighborhood of such a crossover, these terms may be included without great difficulty.[6] Also, as we have noted earlier, these interactions introduce no damping and so by themselves make no contribution to the phonon lifetime. At low temperatures, one may utilize the diagrammatic density expansion[16–18] in which each backward magnon line gives a factor of the density of magnons. Thus, the contributions of Fig. 1(b) are of higher order in the density of spin waves than those of Fig. 1(c), since the former have one backward magnon line while the latter have none. We will include in our calculation of $\Sigma_{\mathbf{q}\lambda}(\omega)$ all diagrams having no backward magnon lines, i.e., the leading term in the magnon density expansion. Since the density of magnons vanishes at zero temperature, the calculation is exact in that limit. We will also calculate to leading order in the magnon-phonon coupling constant, which in this case is to order $|g|^2$. Then the only magnon-phonon vertices which contribute are those in Fig. 1(c), and we may use as our potential V_{2M-P} given by Eq. (7).

The contribution to $\Sigma_{\mathbf{q}\lambda}(\omega)$ shown in Fig. 1(c) would be the full contribution of order $|g|^2$ to lowest order in $\langle n\rangle_{\text{sw}}$ if the magnons did not interact. However, the Hamiltonian [Eq. (13)] includes the full magnon-magnon interaction, and there is an additional class of diagrams with spin-wave interactions which are of the same order in $|g|^2$ and $\langle n\rangle_{\text{sw}}$ as those in Fig. 1(c). In fact, the full contribution to $\Sigma_{\mathbf{q}\lambda}(\omega)$ is obtained from the diagrams shown in Fig. 2, where the box labeled t represents the sum of all magnon-magnon ladder diagrams or the two-spin-wave t matrix. The diagrams shown in Fig. 2 are all irreducible phonon self-energy diagrams with two magnon-phonon vertices and no backward magnon lines, neglecting one-magnon–one-phonon processes. One could include the one-magnon–one-phonon processes by dressing the lines in Fig. 2, but we will not do so.

The contributions of the diagrams shown in Fig. 2 may be written in terms of the following lattice sums:

$$D_{ij}(q,x)=\frac{1}{N}\sum_k\frac{\cos k_i\cos k_j}{3(x-1)+\sum_\lambda\alpha_\lambda\cos k_\lambda+i\epsilon}, \tag{14a}$$

$$D_i(q,x)=\frac{1}{N}\sum_k\frac{\cos k_i}{3(x-1)+\sum_\lambda\alpha_\lambda\cos k_\lambda+i\epsilon}, \tag{14b}$$

$$A_{ij}(q,\omega)=-(1/4S)[D_{ij}(q,\tilde{\omega})-\alpha_jD_i(q,\tilde{\omega})], \tag{14c}$$

[16] J. M. Luttinger, Phys. Rev. **121**, 942 (1961).
[17] I. E. Dzyaloshinski, Zh. Eksperim. i Teor. Fiz. **42**, 1126 (1962) [English transl.: Soviet Phys.—JETP **15**, 778 (1962)].
[18] G. Baym and A. M. Sessler, Phys. Rev. **131**, 2345 (1963).

where

$$\alpha_\lambda = \cos\tfrac{1}{2}q_\lambda\,, \tag{15a}$$

$$\tilde{\omega} = \omega/12JS\,, \tag{15b}$$

and $\epsilon \to 0^+$. In terms of the above, the two-spin-wave t matrix is given by[10]

$$t(k_1k_2q\omega) = -2J \sum_{\delta,\delta'=x,y,z} \{\cos(\mathbf{k}_1\cdot\boldsymbol{\delta}) \times[\cos(\mathbf{k}_2\cdot\boldsymbol{\delta}') - \cos(\tfrac{1}{2}\mathbf{q}\cdot\boldsymbol{\delta}')] \times[\mathbf{1}-2\mathbf{A}(q,\omega)]^{-1}{}_{\delta'\delta}\}\,, \tag{16}$$

where the label "$\delta,\delta' = x,y,z$" means that the summation is to be taken over the three nearest neighbors with positive coordinates, and where for $\mathbf{q}$ along the [111] direction we have[10]

$$(\mathbf{1}-2\mathbf{A})^{-1} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \Big/ 3(1-2A_{ii}-4A_{ij}) + \begin{bmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{bmatrix} \Big/ 3(1-2A_{ii}+2A_{ij})\,. \tag{17}$$

In Eq. (16), $\mathbf{k}_1$ and $\mathbf{k}_2$ are the relative momenta into and out of the t matrix, and $\mathbf{q}$ and ω are the total momentum and energy. The denominators in Eq. (17) vanish at the two-spin-wave bound states,[7–10] the former at the s-wave state, and the latter at the d-wave state. It is shown in Ref. 9 that the basis which diagonalizes $\mathbf{1}-2\mathbf{A}$ is $\hat{\epsilon}_l, \hat{\epsilon}_{t_1}$, and $\hat{\epsilon}_{t_2}$ of Eq. (10), where $\hat{\epsilon}_l$ corresponds to the s-wave state. Thus, we may anticipate from Eqs. (10) and (17) a longitudinal-s-wave and transverse-d-wave coupling, which we will now derive.

From Fig. 2, we find that

$$\Sigma_{\mathbf{q}\lambda}(\Omega_{\mathbf{q}\lambda}) = \Sigma_{\mathbf{q}\lambda}{}^{(0)}(\Omega_{\mathbf{q}\lambda}) + \Sigma_{\mathbf{q}\lambda}{}^{(T)}(\Omega_{\mathbf{q}\lambda})\,, \tag{18}$$

where

$$\Sigma_{\mathbf{q}\lambda}{}^{(0)}(\Omega_{\mathbf{q}\lambda}) = \left(\frac{1}{2\pi}\right)^3 \int d^3k \frac{g^2(\mathbf{kq}\lambda)}{\Omega_{\mathbf{q}\lambda} - \epsilon_{q/2+k} - \epsilon_{q/2-k} + i\delta}\,, \tag{19a}$$

$$\Sigma_{\mathbf{q}\lambda}{}^{(T)}(\Omega_{\mathbf{q}\lambda}) = \left(\frac{1}{2\pi}\right)^6 \int d^3k_1 \int d^3k_2\, g(\mathbf{k}_1\mathbf{q}\lambda) g(\mathbf{k}_2\mathbf{q}\lambda) \times t(k_1k_2q\Omega_{\mathbf{q}\lambda})(\Omega_{\mathbf{q}\lambda} - \epsilon_{\mathbf{q}/2+\mathbf{k}_1} - \epsilon_{\mathbf{q}/2-\mathbf{k}_1} + i\delta)^{-1} \times(\Omega_{\mathbf{q}\lambda} - \epsilon_{\mathbf{q}/2+\mathbf{k}_2} - \epsilon_{\mathbf{q}/2-\mathbf{k}_2} + i\delta)^{-1} \tag{19b}$$

and

$$\epsilon_k = 6JS(1 - \tfrac{1}{3}\sum_\lambda \cos k_\lambda) \tag{20}$$

is the simple spin-wave energy. Now, using Eqs. (11), (14), and (16), we obtain for a phonon with momentum along the [111] direction

$$\Sigma_{\mathbf{q}l}{}^{(0)}(\Omega_{\mathbf{q}}) = \frac{C_q{}^2(a+2b)^2}{4JS}[D_{ii}(q,\tilde{\Omega}_{\mathbf{q}}) + 2D_{ij}(q,\tilde{\Omega}_{\mathbf{q}})]\,, \tag{21a}$$

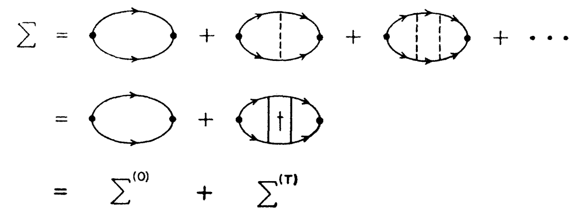

FIG. 2. Set of diagrams included in calculating the phonon self-energy. These are of lowest order in both $|g|^2$ and the density of spin waves.

$$\Sigma_{\mathbf{q}t}{}^{(0)}(\Omega_{\mathbf{q}}) = \frac{C_q{}^2(a-b)^2}{4JS}[D_{ii}(q,\tilde{\Omega}_{\mathbf{q}}) - D_{ij}(q,\tilde{\Omega}_{\mathbf{q}})]\,, \tag{21b}$$

$$\Sigma_{\mathbf{q}l}{}^{(T)}(\Omega_{\mathbf{q}}) = -\frac{C_q{}^2(a+2b)^2}{8JS^2} \sum_{ij} \mathbf{M}_{ij}{}^l(\mathbf{1}-2\mathbf{A})^{-1}{}_{ji}\,, \tag{21c}$$

$$\Sigma_{\mathbf{q}t}{}^{(T)}(\Omega_{\mathbf{q}}) = -\frac{C_q{}^2(a-b)^2}{8JS^2} \sum_{ij} \mathbf{M}_{ij}{}^t(\mathbf{1}-2\mathbf{A})^{-1}{}_{ji}\,, \tag{21d}$$

where we have assumed $\Omega_{\mathbf{q}l} = \Omega_{\mathbf{q}t}$ for convenience, C_q is given by Eq. (12), and where

$$\mathbf{M}^l = \tfrac{1}{3}(D_{ii}+2D_{ij}) \times(D_{ii}+2D_{ij}-3\alpha_jD_i) \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}\,, \tag{22a}$$

$$\mathbf{M}^{t_1} = \tfrac{1}{6}(D_{ii}-D_{ij})^2 \begin{bmatrix} 1 & 1 & -2 \\ 1 & 1 & -2 \\ -2 & -2 & 4 \end{bmatrix}\,, \tag{22b}$$

$$\mathbf{M}^{t_2} = \tfrac{1}{2}(D_{ii}-D_{ij})^2 \begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}\,. \tag{22c}$$

Note that the product of $\mathbf{M}^l$ and the d-wave part of $(\mathbf{1}-2\mathbf{A})^{-1}$ vanishes, as does the product of $\mathbf{M}^t$ and the s-wave part of $(\mathbf{1}-2\mathbf{A})^{-1}$. Thus longitudinal [111] phonons will couple only to the s-wave two-spin-wave bound state and transverse phonons only to the d-wave state.

Using the expressions for $\mathbf{M}$ and $(\mathbf{1}-2\mathbf{A})^{-1}$ given in Eqs. (17) and (22), we obtain finally

$$\Sigma_{\mathbf{q}l} = \Sigma_{\mathbf{q}l}{}^{(0)}\left(1 - \frac{D_{ii}+2D_{ij}-3\alpha_jD_i}{2S(1-2A_{ii}-4A_{ij})}\right)\,, \tag{23a}$$

$$\Sigma_{\mathbf{q}t} = \Sigma_{\mathbf{q}t}{}^{(0)}\left(1 - \frac{D_{ii}-\mathrm{D}_{ij}}{2S(1-2A_{ii}+2\mathrm{A}_{ij})}\right)\,, \tag{23b}$$

where $\Sigma_{\mathbf{q}l}{}^{(0)}$ and $\Sigma_{\mathbf{q}t}{}^{(0)}$ are given by Eq. (21), and all functions are evaluated at $(\mathbf{q},\Omega_{\mathbf{q}})$.

IV. EVALUATION OF PHONON ENERGY SPECTRUM

Comparing Eqs. (23) and (16), we see that Σ has the same singularities as the two-spin-wave t matrix. These

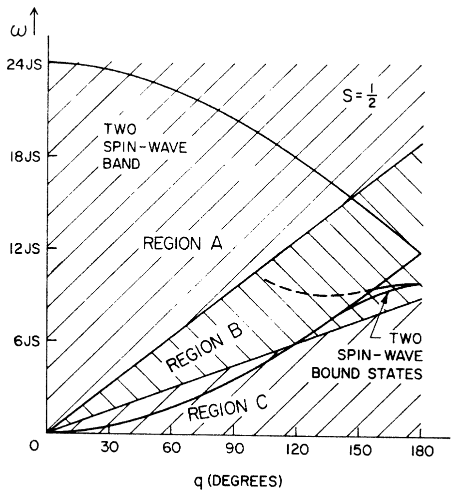

FIG. 3. Manifold of two-spin-wave states. There are bound or resonant states only in region B. See also Figs. 4, 9, and 10 of Ref. 10.

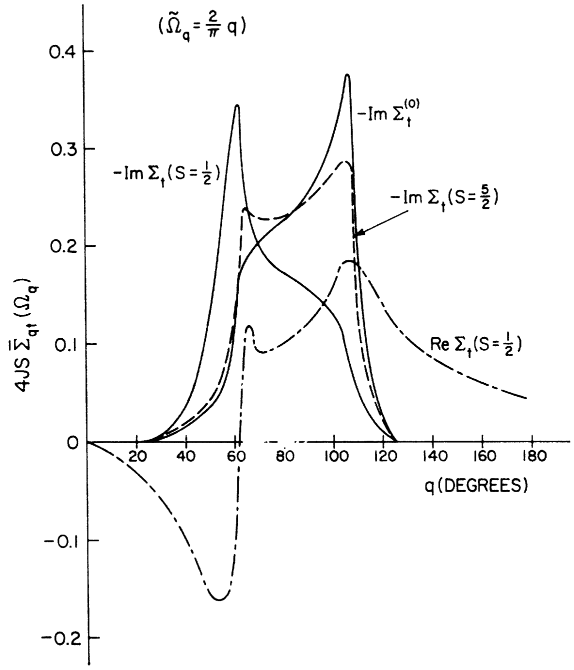

FIG. 5. Transverse phonon self-energy versus phonon momentum for a phonon in region A. $q=d$ degrees means $q_xa=q_ya=q_za=d\pi/180$ and $\bar{\Sigma}_{qt}=\Sigma_{qt}[8\rho C/S^2(a-b)^2]$.

singularities occur at the two-spin-wave bound states,[10] but, as is evident from the denominators in Eq. (23), the longitudinal self-energy is singular only at the s-wave bound state, while the transverse self-energy is singular only at the d-wave bound state. In addition, since the lattice sums given in Eq. (14) are real except within the two-spin-wave band, Σ and $\Sigma^{(0)}$ are also real outside this region. Thus, the phonon lifetime is infinite unless a spin-wave pair of total momentum $\mathbf{q}$ and energy $\Omega_\mathbf{q}$ is either within the two-spin-wave band or at one of the two-spin-wave bound states. The interpretation of this result is clear. A phonon may relax by emitting two spin waves only if there are energy states available to the spin waves, i.e., if $\mathbf{q}$ and $\Omega_\mathbf{q}$ are within the two-spin-wave band or at one of the bound states.

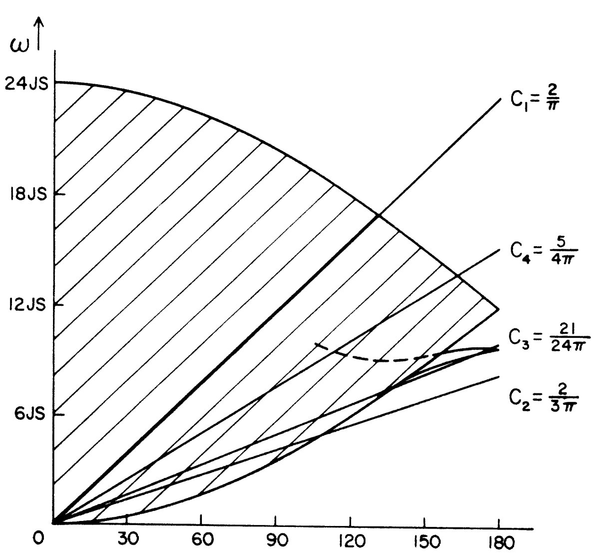

FIG. 4. Manifold of two-spin-wave states and the dispersion relations for four different phonons.

In Fig. 3, we have indicated the two-spin-wave states for total momentum $\mathbf{q}=q(1,1,1)$ and spin $\frac{1}{2}$, both the two-spin-wave band and the bound states.[19] The dashed line within the band represents the resonant d-wave state first described in Ref. 9. Since the structure of $\Sigma_{\mathbf{q}\lambda}$ will depend very much on the proximity of the phonon and two-spin-wave energies, we have divided Fig. 3 into three regions. Phonons in regions A and C will not have their dispersion curves cross any of the two-spin-wave bound or resonant states, while those in region B will. Thus, we expect to find a more dramatic, resonant-type behavior of the phonon self-energy in region B. Also, since in region C the phonon energy will rarely, if ever, be within the band, we expect smaller effects from the interactions there than in regions A or B. In order to investigate the structure of the phonon energy and lifetime, we have numerically evaluated Eq. (23) for the four phonons whose dispersion curves are shown in Fig. 4. The evaluation of the lattice sums is described in Ref. 10. Here we have taken $\tilde{\Omega}_q=cq$, where $c_1=2/\pi$, $c_2=2/3\pi$, $c_3=21/24\pi$, and $c_4=5/4\pi$. Note that $c_1\leftrightarrow$ region A, $c_2\leftrightarrow$ region C, and c_3, $c_4\leftrightarrow$ region B. Also, phonon four crosses the resonant d-wave state, while phonon three crosses the true bound states. In the following, recall that the renormalized phonon energy and phonon lifetime are obtained from $\Sigma_{\mathbf{q}\lambda}(\Omega_{\mathbf{q}\lambda})$ via the equations (valid if Σ is slowly varying near

[19] See also Figs. 4, 9, and 10 of Ref. 10.

$\omega=\Omega_{q\lambda}$),

$$\tilde{\Omega}_{q\lambda}(T)=\Omega_{q\lambda}+\mathrm{Re}\Sigma_{q\lambda}(\Omega_{q\lambda}), \tag{24a}$$

$$\Gamma_{q\lambda}(T)=-[\mathrm{Im}\Sigma_{q\lambda}(\Omega_{q\lambda})]^{-1}. \tag{24b}$$

In Fig. 5, we show $\Sigma_{qt}(\Omega_q)$ for $\tilde{\Omega}_q=c_1q$ versus q (region A). The longitudinal self-energy has similar structure. Note the peaked nature of $\mathrm{Im}\Sigma^{(0)}$, which corresponds to noninteracting magnons. This merely reflects the density of states for two free spin waves. The effect of spin-wave interactions is to shift the peak to lower q; but, as the spin increases, the effect of the interactions diminishes, as is illustrated by the spin-$\frac{5}{2}$ result. The real part of the self-energy changes sign, so that $\tilde{\Omega}_q(T)$ is smaller than Ω_q for small q and larger than Ω_q for large q. This renormalization sign change also occurs in the noninteracting case.

Figure 6 shows the behavior of $\Sigma_{q\ell}(\Omega_q)$ for $\tilde{\Omega}_q=c_2q$ (region C) and spin 1. As expected, the self-energy is small and is changed only slightly by spin-wave interactions. Contrast this behavior with that illustrated by Fig. 7, in which we have plotted $-\mathrm{Im}\Sigma_{q\ell}(\Omega_q)$ versus q for $\tilde{\Omega}_q=c_3q$ (region B). $\Sigma^{(0)}$ has very little structure, but the introduction of spin-wave interactions in the intermediate state leads to a large peak at the band edge and a δ function at $q=168°$ ($q_{\max}=180°$). The peak reflects the imminent emergence of the s-wave bound state, which causes the denominator in Eq. (23a) to become very small near the band edge. The δ function in $\mathrm{Im}\Sigma_\ell$ is due to the crossover of the phonon and s-wave two-spin-wave bound-state dispersion curves outside

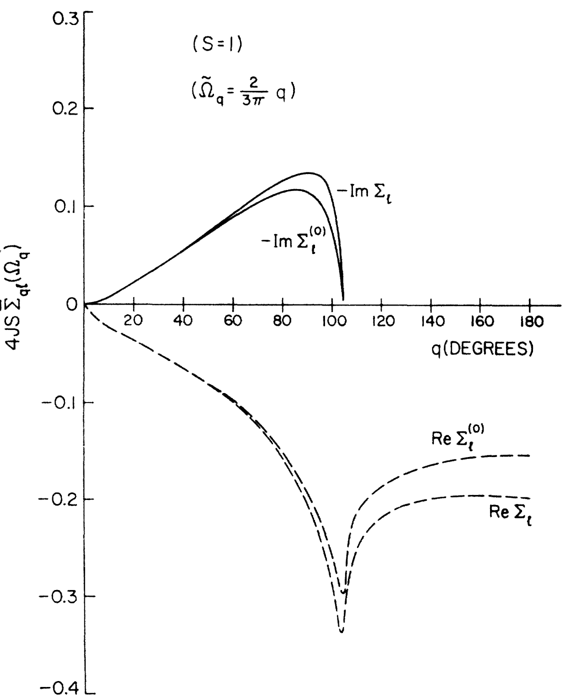

FIG. 6. Longitudinal phonon self-energy versus phonon momentum for a phonon in region C, $\bar{\Sigma}_{q\ell}=\Sigma_{q\ell}[8\rho C/S^2(a+2b)^2]$.

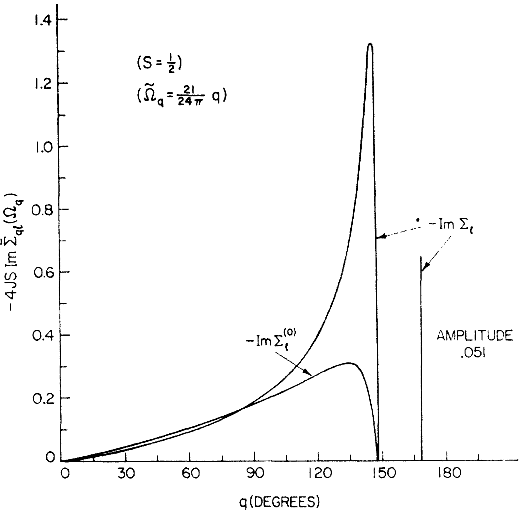

FIG. 7. Imaginary part of the longitudinal phonon self-energy versus phonon momentum for a phonon in region B.

the band and would be thermally broadened in the real system into a resonance. For the phonons discussed in Figs. 6 and 7, the transverse self-energy is quite small, although $\Sigma_{qt}(\Omega_q)$ has a pole at $q=171°$ for $\tilde{\Omega}_q=c_3q$, where the phonon and d-wave bound state cross.

The last of the four phonons that we have chosen to discuss has $\tilde{\Omega}_q=c_4q=(5/4\pi)q$. This case is particularly interesting, since Ω_q crosses the resonant d-wave state and also stays within the two-spin-wave band for extremely large q. The numerical results have some very interesting features. First, as is shown in Figs. 8 and 9, the longitudinal self-energy is not affected by a crossover with the d-wave bound state, since it couples only to the s-wave states. However, the transverse self-energy shows a resonance near the crossover ($q\approx 110°$), its imaginary part (inverse lifetime) becoming very large and its real part (energy shift) varying rapidly and

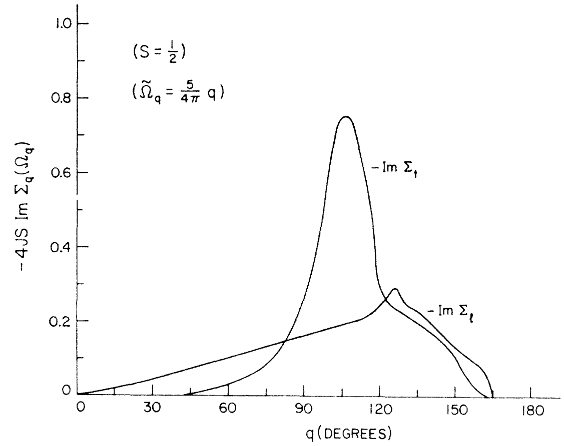

FIG. 8. Imaginary part of the phonon self-energy versus phonon momentum for a phonon in region B which intersects the resonant two-spin-wave bound state.

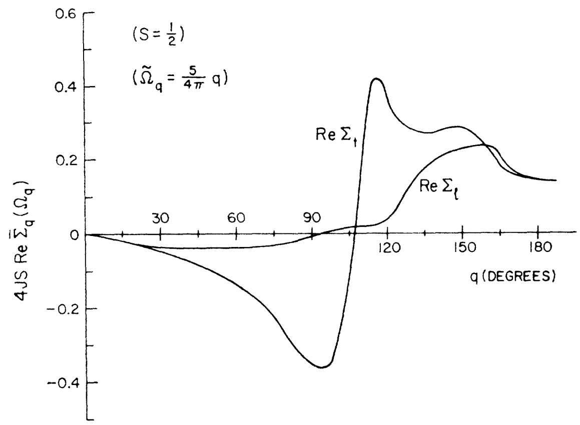

FIG. 9. Real part of the phonon self-energy versus phonon momentum for the phonon of Fig. 8.

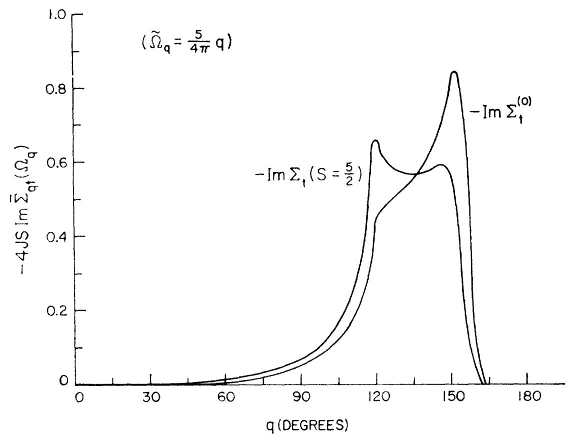

FIG. 10. Imaginary part of the transverse phonon self-energy versus momentum for the phonon of Figs. 8 and 9.

changing sign. Finally, as is shown in Fig. 10, $\Sigma_t^{(0)}$ is anomalously large in the high momentum region, even for spin $\frac{5}{2}$. This means that the full spin-wave interactions must be included in a calculation of the energy and lifetime of a phonon in this region, even for large spin.

V. SUMMARY AND CONCLUSIONS

We have shown that at low temperatures the lowest-order contribution to the phonon lifetime comes from processes whereby the phonon emits and later reabsorbs two magnons. As we have seen, the contributions of such processes are extremely sensitive to interactions between the intermediate magnons. In particular, if the energy of the phonon is near that of one of the two-spin-wave bound states, then the intermediate magnons may interact very strongly (bind together), and this causes the phonon lifetime to become extremely short. Thus a plot of linewidth versus momentum shows the resonant behavior illustrated in Fig. 8. Physically, this comes about because there is a decay mechanism for the phonon (via the two-spin-wave bound state) which is operative only in the small region of momentum space where there is close proximity between the phonon and two-spin-wave bound-state dispersion curves. The phonon energy shift in this region may also be understood intuitively via the repulsion of energy levels one encounters in simple perturbation theory. For at low q the phonon energy is below that of the bound states, while at high q it is above. Hence, one expects the energy-level repulsion to first cause a downward (negative) shift and then an upward (positive) one. This result also follows more formally from the sum rules on the phonon spectral-weight function, or the Kramers-Kronig relations for $\Sigma_{q\lambda}(\omega)$.

In the vicinity of the resonances described above, one must include all the spin-wave interaction terms displayed in Fig. 2. In addition, we have found that for large momentum and near the center of the two-spin-wave band, $\Sigma^{(0)}$ is a very bad approximation, and here, too, one must use the full two-magnon t matrix (for example, see Fig. 10). There a first Born approximation to the t matrix does not substantially alter the $\Sigma^{(0)}$ result. Finally, even far away from any resonant or nonperturbative effects, the inclusion of interactions between the intermediate spin waves can substantially alter the phonon self-energy, as shown in Fig. 5.

The variation of phonon energy and lifetime described in this paper would be most easily observable via the use of an external magnetic field. Since the field will raise the energy of the two-spin-wave states by $2g\mu_BH$ but not shift the phonon energy, it will have the effect of moving the phonon from region A to B to C in Fig. 3. Since we find resonances only in region B, moderate effects in region A, and very small effects in region C, this would make observation much easier. For example, for a phonon with $c_1 = 2/\pi$, the zero-field self-energy would be given by Fig. 5. As the field was increased, one would find a resonance, such as in Figs. 8 and 9, and then increasing the field still further would yield a behavior similar to Fig. 6. Finally, for a large enough field, one would simply find the non-interacting phonon energy and no lifetime effects from the spin waves. An added benefit of the magnetic field is that it also separates the single magnon and phonon crossover from the two-magnon bound state and phonon crossover, since the single-magnon state is raised by only $g\mu_BH$. The effects described above would most easily be observable via inelastic neutron scattering, since they occur at rather large momenta.

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