Theory of Inelastic Neutron Scattering in the Itinerant Model Antiferromagnetic Metals. I*

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The susceptibility functions $\chi^{-+}(\mathbf{K},\omega)$ and $\chi^{zz}(\mathbf{K},\omega)$ are calculated in the random-phase approximation at zero temperature for the Slater model of itinerant antiferromagnetism using the Hubbard Hamiltonian; from these susceptibility functions the neutron-scattering cross section is calculated. A pole is found in $\chi^{-+}(\mathbf{K},\omega)$ corresponding to a spin-wave model As in the Heisenberg model of spin waves, the residue of this pole approaches zero as the scattering vector $\mathbf{K}$ approaches a chemical reciprocal lattice vector τ, and becomes infinite as $\mathbf{K}$ approaches a magnetic reciprocal-lattice vector $\mathbf{Q}$. The non-spin-flip single-particle-mode scattering is found to become infinite at an energy corresponding to the magnetic splitting of the bands at the boundary of the magnetic Brillouin zone if the Fermi level lies in this gap. If the Fermi level does not lie in the gap, then there is a pole in $\chi^{zz}(\mathbf{K},\omega)$ for $\mathbf{K}$ near a magnetic reciprocal-lattice vector, at an energy equal to the gap energy when $\mathbf{K}=\mathbf{Q}$, corresponding to a collective excitation. Acoustic plasmon poles in $\chi^{zz}(\mathbf{q},\omega)$ are also discussed.

I. INTRODUCTION

RECENTLY, there has been a good deal of both experimental and theoretical interest in the electronic structure and magnetic properties of chromium and alloys of chromium with manganese.[1–3] The magnetic ordering of such metals is believed to be well described by the itinerant model of antiferromagnetism proposed by Lomer.[1,4] According to this model, the instability of the paramagnetic state towards antiferromagnetic ordering results from there being two pieces of the paramagnetic Fermi surface of nearly the same size and shape, but separated by a wave vector $\mathbf{Q}$. If these states are made to coincide by translation by $\mathbf{Q}$, there will be a tendency for states of opposite spin in these two sections of Fermi surface to mix strongly, resulting in a static spin-density-wave[5] antiferromagnetic ordering. Recent inelastic neutron-scattering experiments on these materials have led to the work that is reported in this paper.[3]

In this paper, we calculate the elementary excitation of such systems that should be observed in inelastic neutron-scattering experiments and the intensity of the scattering from these various excitations. We have also attempted to make contact with and compare the behavior of the inelastic neutron scattering expected for itinerant model of antiferromagnetism to that predicted by the itinerant model of ferromagnetism[6–8] for ferromagnets; thus we will illustrate the differences between the predictions of the two theories.

Since in this paper we are not interested in the way in which the antiferromagnetic ordering comes about, but rather in what elementary excitations an itinerant antiferromagnet should have, we will start out with a fairly simple model of the electronic structure of the system: the Hubbard model or short-range-interaction single-band model.[9] The justification for using this model rather than a more realistic model with two or more bands is that this model is both mathematically and conceptually simple and that the relevant magnetic bands resulting from this model in the antiferromagnetic state are qualitatively the same as those resulting from the two-band model.[1] Also, for simplicity, rather than use the more general spin-density-wave model, we have gone to the Slater alternant-molecular-orbital model of antiferromagnetism.[10] In this model, there are two interpenetrating sublattices with opposite spin density. The reduced translational symmetry of the lattice in the antiferromagnetic state results in a splitting of the single band of each spin into two bands for each spin. This model is easier to visualize because there exist simply two interpenetrating sublattices with a definite direction of sublattice magnetization. It is also mathematically simpler because one-electron states of different spin are not mixed. These simplifications allow us to calculate all of the susceptibility functions and to separate excitation into longitudinal and transverse excitations corresponding to spin fluctuations along and transverse to the sublattice magnetization. Our calculation of the spin-wave dispersion relation is similar to the treatment of spin waves in the same single-band Slater model by Des Cloizeaux.[11] The differences between our calculation and his are that (i) we formulate our problem in terms of double-time Green's functions, so that we can calculate the susceptibility functions, and thus the inelastic neutron-scattering cross section; and (ii) that we also consider the effect of putting the Fermi level in one of

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[3] L. D. Muhlestein, S. K. Sinha, Bull. Am. Phys. Soc. **13**, 468 (1968); S. K. Sinha (private communication); S. Liu (private communication).
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[11] J. Des Cloizeaux, J. Phys. Radium **20**, 606 (1959); **20**, 751 (1959).

the two bands rather than inside the gap between the bands. This may be important for discussing excitations in conduction bands that are polarized by magnetic ordering rather than causing the ordering. We have considered excitations in both the limits $g \ll \epsilon_F$, and $g \gg \epsilon_F$, where g is half the band splitting. The results of the first limiting case are applicable to chromium alloys. The second limiting case applies to the case of insulating antiferromagnets.

In Sec. II we formulate the problem using a canonical transformation as was done by Des Cloizeaux. In Sec. III we set up the equations of motion to calculate the transverse susceptibility and consider these equations in the narrow-band limit. In Sec. IV we calculate the susceptibility for general band widths at zero temperature and find the spin-wave dispersion relation and the scattering cross section of the spin waves. We also consider the scattering from Stoner single-particle modes. In Sec. V we calculate the longitudinal susceptibility at zero temperature. Here we find a new collective mode which exists when the Fermi level does not lie in the gap and which is found below the interband single-particle-mode continuum. When the Fermi energy does lie in the gap, this mode merges with the continuum, but near a magnetic reciprocal-lattice vector, and the single-particle-mode scattering becomes very large at energy equal to the gap energy. This is in contrast to the itinerant model of ferromagnetism.[6–8] This large inelastic single-particle-mode scattering should be observable in neutron-scattering experiments and should serve as a way of measuring the gap energy in the bulk sample to supplement the optical-reflectance measurements of this energy.[2]

II. FORMULATION OF PROBLEM

Our Hamiltonian is the well-known Hubbard Hamiltonian which can be written in the reciprocal-space representation as

$$\mathcal{H}=\sum_{\mathbf{k}\sigma} \epsilon(\mathbf{k}) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{U}{N} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}'} c_{\mathbf{k}+\mathbf{q}'\uparrow}^{\dagger} c_{\mathbf{k}'\downarrow}^{\dagger} c_{\mathbf{k}'+\mathbf{q}'\downarrow} c_{\mathbf{k}\uparrow}, \quad (1)$$

where $c_{\mathbf{k}\sigma}$ is the annihilation operator of the electron of spin σ in the Bloch function of wave vector $\mathbf{k}$.[9] We assume that the lattice has inversion symmetry [therefore, $\epsilon(\mathbf{k})=\epsilon(-\mathbf{k})$]. In our model, we consider only one band in the Hartree-Fock approximation, when the system is paramagnetic. We have not included the anisotropy energy in Eq. (1). When the system is in an antiferromagnetic state, this single band will split into two bands for each spin, one with greater charge density on sublattice A than on sublattice B, and one with more charge density on sublattice B than on sublattice A. For the opposite spin, the sublattices are interchanged (see Fig. 1). One band of each spin will lie lower in energy than the other and, therefore, will tend to contain more electrons than the other band of the same spin. For crystals with inversion symmetry, corresponding bands of opposite spin will be degenerate.[12]

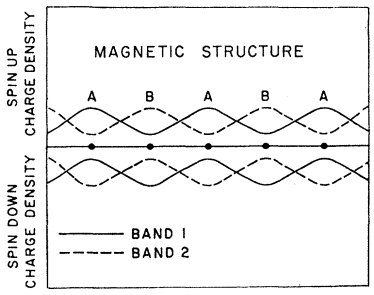

FIG. 1. Qualitative sketch of distribution of charge density of electrons of spin up and electrons of spin down in bands 1 and 2 on an alternant lattice. A and B label sites belonging to a given sublattice.

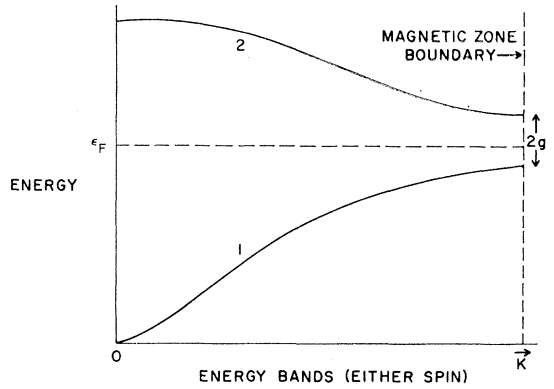

FIG. 2. Qualitative sketch of band structure: one-electron energy versus wave vector $\mathbf{k}$ for one direction of d.

Let us assume that we have such a simple lattice which can be divided into two interpenetrating sublattices A and B, such that the nearest neighbors of the A sublattice belong to the B sublattice, and let us call the lower-energy band of each spin, band 1, and the higher-energy band, band 2. Since the symmetry of the lattice is now reduced (each unit cell containing two atoms instead of one), the Brillouin zone is divided into two zones, each containing the same number of states. If $\mathbf{k}$ lies in the new first Brillouin zone, then $\mathbf{k}+\mathbf{Q}$, where $\mathbf{Q}$ is one of the magnetic reciprocal lattice vectors, is a vector in the new second Brillouin zone modulo a vector in the paramagnetic reciprocal lattice.[13] The vector $\mathbf{Q}$ has the property that $e^{i\mathbf{Q}\cdot\mathbf{R}_j}$ can be 1 on sublattice A and -1 on sublattice B. The new band structure is illustrated in Fig. 2. Because of the two-band structure shown in Fig. 2, we will get a single-particle-mode continuum for both spin-flip and non-spin-flip modes like

[12] C. Herring, in *Magnetism*, edited by George T. Rado and Harry Shul (Academic Press Inc., New York, 1966), Vol. IV, p. 312.

[13] Simple structures such as the simple cubic and bcc lattices, for which no nearest-neighbor site is a nearest neighbor of any other nearest-neighbor site, have the property that if $\mathbf{Q}$ is a magnetic reciprocal-lattice vector, all other magnetic reciprocal-lattice vectors can be written as $\mathbf{Q}+\boldsymbol{\tau}_n$, where $\boldsymbol{\tau}_n$ is a vector in the chemical reciprocal lattice.

that illustrated in Fig. 3. In Secs. III and IV we will also find collective modes in the gap $2g$ (Fig. 4).

The new one-electron wave functions, which are solutions of the problem in the Hartree-Fock approximation, are linear combinations of the two of the original paramagnetic Bloch functions, one of which is in the inner half-zone and the other of which is in the outer half-zone (as is shown on p. 312 in Ref. 12). We transform our Hamiltonian to a representation in terms of these new Bloch functions by the following canonical transformation:

$$\mathbf{d}_{\mathbf{k}1\sigma}=\mathbf{c}_{\mathbf{k}\sigma}\cos\tfrac{1}{2}\theta_{\mathbf{k}}-\sigma\mathbf{c}_{\mathbf{k}+\mathbf{Q}\,\sigma}\sin\tfrac{1}{2}\theta_{\mathbf{k}}, \tag{2a}$$

$$\mathbf{d}_{\mathbf{k}2\sigma}=\sigma\mathbf{c}_{\mathbf{k}\sigma}\sin\tfrac{1}{2}\theta_{\mathbf{k}}+\mathbf{c}_{\mathbf{k}+\mathbf{Q}\,\sigma}\cos\tfrac{1}{2}\theta_{\mathbf{k}}, \tag{2b}$$

where $d_{\mathbf{k}\lambda\sigma}$ is the annihilation operator for an electron of wave vector $\mathbf{k}$ and spin σ in the band labeled by λ, where λ takes on the values 1 and 2.

The index σ takes on values ±1 depending on whether the spin is up or down, and $\sin\frac{1}{2}\theta_{\mathbf{k}}$ and $\cos\frac{1}{2}\theta_{\mathbf{k}}$ are determined so as to make

$$i\frac{\partial}{\partial t}\mathbf{d}_{\mathbf{k}\lambda\sigma}=E_{\lambda\sigma}(\mathbf{k})\mathbf{d}_{\mathbf{k}\lambda\sigma} \tag{3}$$

in the Hartree-Fock approximation. The wave vector $\mathbf{k}$ is assumed to run over the reduced Brillouin zone. From now on all summations over $\mathbf{k}$ will be assumed to go over the reduced magnetic Brillouin zone unless otherwise specified. On making this canonical transformation, Eq. (1) becomes, in the new representation,

$$\begin{aligned}H=&\sum_{\mathbf{k}\lambda\mu\sigma}[\epsilon(\mathbf{k})R_{\lambda\mu,1}{}^{\sigma}(0,\mathbf{k})+\epsilon(\mathbf{k}+\mathbf{Q})R_{\lambda\mu,2}{}^{\sigma}(0,\mathbf{k})]\\&\times\mathbf{d}_{\mathbf{k}\lambda\sigma}{}^{\dagger}\mathbf{d}_{\mathbf{k}\mu\sigma}\\&+\sum_{\mathbf{k}\mathbf{p}\lambda\mu\xi\eta\sigma\sigma'}W(\mathbf{p}+\mathbf{q}\lambda\sigma,\,\mathbf{k}\eta\sigma';\,\mathbf{k}+\mathbf{q}\xi\sigma,\,\mathbf{p}\mu\sigma')\\&\times\mathbf{d}_{\mathbf{p}+\mathbf{q}\lambda\sigma}{}^{\dagger}\mathbf{d}_{\mathbf{k}\eta\sigma'}{}^{\dagger}\mathbf{d}_{\mathbf{p}\mu\mathbf{p}'}\mathbf{d}_{\mathbf{k}+\mathbf{q}\xi\sigma},\end{aligned} \tag{4}$$

where the matrix W is given by

$$\begin{aligned}&W(\mathbf{p}+\mathbf{q}\lambda\sigma,\,\mathbf{k}\eta\sigma';\,\mathbf{k}+\mathbf{q}\xi\sigma,\,\mathbf{p}\mu\sigma')\\&=\frac{U}{N}\sum_{j=1,3}[R_{\lambda\mu j}{}^{\sigma\sigma'}(\mathbf{q},\mathbf{p})+R_{\lambda\mu,j+1}{}^{\sigma\sigma'}(\mathbf{q},\mathbf{p})]\\&\times[R_{\xi\eta j}{}^{\sigma\sigma'}(\mathbf{q},\mathbf{k})+R_{\xi\eta,j+1}{}^{\sigma\sigma'}(\mathbf{q},\mathbf{k})].\end{aligned} \tag{5}$$

Here j is summed over the values 1 and 3 only. The matrix $R_{\xi\eta j}{}^{\sigma\sigma'}(\mathbf{q},\mathbf{k})$ is a transformation matrix defined such that

$$\mathbf{c}_{\mathbf{k}_1+\mathbf{q}\sigma}{}^{\dagger}\mathbf{c}_{\mathbf{k}_2\sigma'}=\sum_{\xi\eta}R_{\xi\eta j}{}^{\sigma\sigma'}(\mathbf{q},\mathbf{k})\mathbf{d}_{\mathbf{k}+\mathbf{q}\xi\sigma}{}^{\dagger}\mathbf{d}_{\mathbf{k}\eta\sigma'},$$

where if $j=1$, $\mathbf{k}_1=\mathbf{k}$ and $\mathbf{k}_2=\mathbf{k}$, and if $j=3$, $\mathbf{k}_1=\mathbf{k}$ and $\mathbf{k}_2=\mathbf{k}+\mathbf{Q}$. The values of $\mathbf{k}_1$ and $\mathbf{k}_2$ for $j=2$ and 4 are the above for $j=1,3$, respectively, but with $\mathbf{k}+\mathbf{Q}$ substituted for $\mathbf{k}$. Using Eq. (2), we find that

$$R_{\xi\eta j}{}^{\sigma\sigma'}(\mathbf{q},\mathbf{k})=R_{\alpha j}{}^{\sigma\sigma'}(\mathbf{q},\mathbf{k})$$

$$=\begin{bmatrix}\cos(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\cos(\frac{1}{2}\theta_{\mathbf{k}}) & \sigma\sigma'\sin(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\sin(\frac{1}{2}\theta_{\mathbf{k}}) & -\sigma'\cos(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\sin(\frac{1}{2}\theta_{\mathbf{k}}) & -\sigma\sin(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\cos(\frac{1}{2}\theta_{\mathbf{k}})\\ \sigma\sigma'\sin(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\sin(\frac{1}{2}\theta_{\mathbf{k}}) & \cos(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\cos(\frac{1}{2}\theta_{\mathbf{k}}) & \sigma\sin(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\cos(\frac{1}{2}\theta_{\mathbf{k}}) & \sigma'\cos(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\sin(\frac{1}{2}\theta_{\mathbf{k}})\\ \sigma'\cos(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\sin(\frac{1}{2}\theta_{\mathbf{k}}) & -\sigma\sin(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\cos(\frac{1}{2}\theta_{\mathbf{k}}) & \cos(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\cos(\frac{1}{2}\theta_{\mathbf{k}}) & -\sigma\sigma'\sin(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\sin(\frac{1}{2}\theta_{\mathbf{k}})\\ \sigma\sin(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\cos(\frac{1}{2}\theta_{\mathbf{k}}) & -\sigma'\cos(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\sin(\frac{1}{2}\theta_{\mathbf{k}}) & -\sigma\sigma'\sin(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\sin(\frac{1}{2}\theta_{\mathbf{k}}) & \cos(\frac{1}{2}\theta_{\mathbf{k}+\mathbf{q}})\cos(\frac{1}{2}\theta_{\mathbf{k}})\end{bmatrix}, \tag{6}$$

where $\alpha=1$ if $(\xi,\eta)=(1,1)$, $\alpha=2$ if $(\xi,\eta)=(2,2)$, $\alpha=3$ if $(\xi,\eta)=(1,2)$, and $\alpha=4$ if $(\xi,\eta)=(2,1)$. In Eq. (4), $R_{\xi\eta j}{}^{\sigma}(\mathbf{q},\mathbf{k})=R_{\xi\eta j}{}^{\sigma\sigma}(\mathbf{q},\mathbf{k})$.

We will now choose the function $\theta_{\mathbf{k}}$ so as to make $\mathbf{d}_{\mathbf{k}\lambda\sigma}$ satisfy Eq. (3) in the Hartree-Fock approximation. The equation of motion for $\mathbf{d}_{\mathbf{k}\lambda\sigma}$ in the Hartree-Fock approximation is found to be

$$\begin{aligned}&E_{\lambda\sigma}(\mathbf{k})\mathbf{d}_{\mathbf{k}\lambda\sigma}\\&=\sum_{\mu}[\epsilon(\mathbf{k})R_{\lambda\mu,1}{}^{\sigma}(0,\mathbf{k})+\epsilon(\mathbf{k}+\mathbf{Q})R_{\lambda\mu,2}{}^{\sigma}(0,\mathbf{k})]\mathbf{d}_{\mathbf{k}\mu\sigma}\\&+\sum_{\mathbf{k}'\xi\mu\sigma'}W(\mathbf{k}'\xi\sigma',\mathbf{k}\mu\sigma;\,\mathbf{k}'\xi\sigma',\mathbf{k}\lambda\sigma)n_{\mathbf{k}'\xi\sigma'}\mathbf{d}_{\mathbf{k}\mu\sigma}\\&-\sum_{\mathbf{k}'\xi}W(\mathbf{k}'\xi\sigma,\mathbf{k}\mu\sigma;\,\mathbf{k}\lambda\sigma,\mathbf{k}'\xi\sigma)n_{\mathbf{k}'\xi\sigma}\mathbf{d}_{\mathbf{k}\mu\sigma},\end{aligned} \tag{7}$$

where $n_{\mathbf{p}\lambda\sigma}=\langle d_{\mathbf{p}\lambda\sigma}{}^{\dagger}d_{p\lambda\sigma}\rangle$, in which $\langle\ \rangle$ denotes a thermal average.

Using the inverse of the transformation in Eqs. (2a) and (2b), Eq. (5), and Eq. (6), and assuming $\langle C_{k\sigma}{}^{\dagger}C_{k\sigma}\rangle$ independent of spin, we find

$$\begin{aligned}E_{1\sigma}(\mathbf{k})\mathbf{d}_{\mathbf{k}1\sigma}=&[\bar{\epsilon}(\mathbf{k})\cos^2(\tfrac{1}{2}\theta_{\mathbf{k}})+\bar{\epsilon}(\mathbf{k}+\mathbf{Q})\sin^2(\tfrac{1}{2}\theta_{\mathbf{k}})]\mathbf{d}_{\mathbf{k}1\sigma}\\&+\sigma\tfrac{1}{2}[\bar{\epsilon}(\mathbf{k})-\bar{\epsilon}(\mathbf{k}+\mathbf{Q})]\sin\theta_{\mathbf{k}}\mathbf{d}_{\mathbf{k}2\sigma}\\&-\sigma g\sin\theta_{\mathbf{k}}\mathbf{d}_{\mathbf{k}1\sigma}+g\cos\theta_{\mathbf{k}}\mathbf{d}_{\mathbf{k}2\sigma},\end{aligned} \tag{8a}$$

$$\begin{aligned}E_{2\sigma}(\mathbf{k})\mathbf{d}_{\mathbf{k}2\sigma}=&[\bar{\epsilon}(\mathbf{k})\sin^2(\tfrac{1}{2}\theta_{\mathbf{k}})+\bar{\epsilon}(\mathbf{k}+\mathbf{Q})\cos^2(\tfrac{1}{2}\theta_{\mathbf{k}})]\mathbf{d}_{\mathbf{k}2\sigma}\\&+\sigma\tfrac{1}{2}[\bar{\epsilon}(\mathbf{k})-\bar{\epsilon}(\mathbf{k}+\mathbf{Q})]\sin\theta_{\mathbf{k}}\mathbf{d}_{\mathbf{k}1\sigma}\\&+g\cos\theta_{\mathbf{k}}\mathbf{d}_{\mathbf{k}1\sigma}-\sigma g\sin\theta_{\mathbf{k}}\,\mathbf{d}_{\mathbf{k}2\sigma},\end{aligned} \tag{8b}$$

where $g=(U/N)\sum_{\mathbf{k}}(n_{\mathbf{k}1\sigma}-n_{\mathbf{k}2\sigma})\sin\theta_{\mathbf{k}}$ and $\bar{\epsilon}(\mathbf{k})=\epsilon(\mathbf{k})+U\sum_{\mathbf{k}}\langle C_{\mathbf{k}\sigma}{}^{\dagger}C_{\mathbf{k}\sigma}\rangle$. To make the right-hand side of Eqs. (8a) and (8b) proportional to $\mathbf{d}_{\mathbf{k}1\sigma}$ and $\mathbf{d}_{\mathbf{k}2\sigma}$, respectively, we take

$$\tan\theta_{\mathbf{k}}=2g/[\bar{\epsilon}(\mathbf{k}+\mathbf{Q})-\bar{\epsilon}(\mathbf{k})]. \tag{9}$$

The angle $\theta_{\mathbf{k}}$ takes on values from 0 to $\pi/2$.

After some manipulation, we find from Eqs. (8) and (9) that

$$\begin{pmatrix} E_{1\sigma}(\mathbf{k}) \\ E_{2\sigma}(\mathbf{k}) \end{pmatrix} = \tfrac{1}{2}[\tilde{\epsilon}(\mathbf{k}+\mathbf{Q})+\tilde{\epsilon}(\mathbf{k})] \mp [g^2+\{\tfrac{1}{2}[\tilde{\epsilon}(\mathbf{k})-\tilde{\epsilon}(\mathbf{k}+\mathbf{Q})]\}^2]^{1/2}. \quad (10)$$

We see from Eq. (10) that the parameter g can be interpreted as half the minimum energy gap between bands 1 and 2. The one-electron term in Eq. (4) may be rewritten as

$$\sum_{\mathbf{k}\lambda\sigma} E_{\lambda\sigma}(\mathbf{k}) d_{\mathbf{k}\lambda\sigma}^{\dagger} d_{\mathbf{k}\lambda\sigma} - V_{\mathrm{HF}}, \quad (11)$$

where

$$V_{\mathrm{HF}} = \sum_{\mathbf{k}\lambda\sigma} (-1)^{\lambda}[\tfrac{1}{4}(\tilde{\epsilon}(\mathbf{k}+\mathbf{Q})-\tilde{\epsilon}(\mathbf{k}))^2+g^2]^{1/2} \times \sin^2(\tfrac{1}{2}\theta_{\mathbf{k}}) \mathbf{d}_{\mathbf{k}\lambda\sigma}^{\dagger} d_{\mathbf{k}\lambda\sigma} + \sum_{\mathbf{k}\sigma} \sigma \tfrac{1}{2}[\tilde{\epsilon}(\mathbf{k}+\mathbf{Q})-\tilde{\epsilon}(\mathbf{k})] \times \sin\theta_{\mathbf{k}}[\mathbf{d}_{\mathbf{k}1\sigma}^{\dagger}\mathbf{d}_{\mathbf{k}2\sigma}+\mathbf{d}_{\mathbf{k}2\sigma}^{\dagger}\mathbf{d}_{\mathbf{k}1\sigma}].$$

The Hamiltonian is now in the same form as the Hamiltonian in Yamada and Shimizu's paper.[6] The term V_{HF} is an effective field term like the one that Yamada and Shimizu add to their Hamiltonian to make the band indices correspond to the band indices of the Hartree-Fock approximation one-electron states. The basic differences between the antiferromagnetic problem and the multiband ferromagnetic problem are that the wave functions of the various one-electron states in the antiferromagnetic state must depend on spin in such a way as to give the interpenetrating sublattice structure and the bands of opposite spin in the antiferromagnet do not have a net spin splitting. If we do not require that $\langle C_{\mathbf{k}\sigma}^{\dagger} C_{\mathbf{k}\sigma}\rangle$ be independent of σ but allow there to be a net magnetization, we could treat an itinerant ferrimagnet. Had we made $\mathbf{c}_{\mathbf{k}\sigma}$ and $\mathbf{c}_{\mathbf{k}+\mathbf{Q}\,\sigma}$ in Eq. (2) be of opposite spin, let $\mathbf{Q}$ take on any value in the first Brillouin zone, and let $\mathbf{k}$ go over the whole zone, we would have treated a general spiral spin-density-wave state. In this paper we will for simplicity restrict ourselves to the simple two-sublattice antiferromagnetic state. Many of the results for the simple antiferromagnet should carry over to the more general spin-density wave state. For the simple antiferromagnet, the problem is simplified because, since there is a definite direction of sublattice magnetization, the equations of motion for spin-correlation functions along and transverse to the direction of sublattice magnetization are not coupled.

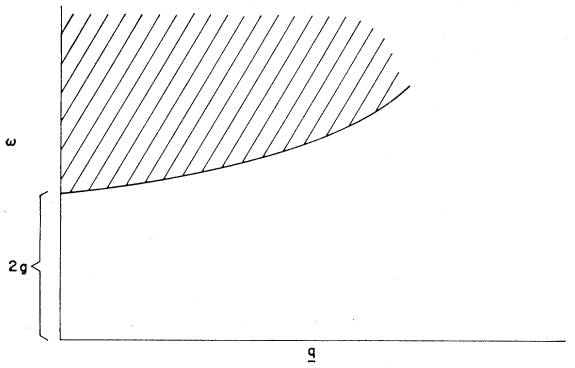

FIG. 3. Qualitative sketch of single-particle excitation continuum corresponding to the electronic structure of Fig. 2: excitation energy versus total wave vector of electron-hole pair making up excitation.

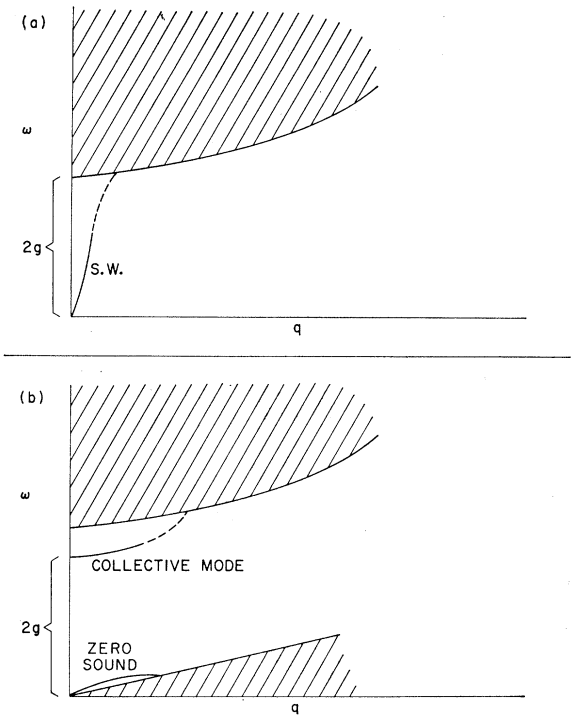

FIG. 4. Qualitative sketch of complete excitation spectrum: (a) the transverse spin excitations; (b) the longitudinal excitations for ϵ_F not in the gap. Dashed lines denote part of collective-mode spectrum not calculated.

Besides making contact with Yamada and Shimizu's treatment of ferromagnetic spin waves, another advantage in transforming the single-band antiferromagnetic problem to a multiband problem is that this formulation makes contact with other simplified multiband models of antiferromagnetism, such as Lidiard's model.[14] We obtain this model by neglecting the $\mathbf{k}$ and $\mathbf{p}$ dependence of the matrix elements W and by keeping only intraband and interband exchange interactions. Lidiard's model does not allow the bands to overlap onto both sublattices and hence misrepresents the behavior of the magnetized bands. More will be said of this model in the next section.

Had we used a two-band Hamiltonian but neglected the wave-vector and band-index dependence of the interaction, the development would essentially follow the same path, but in that case the index j on the matrix (6) would label transitions between two bands—one evaluated with wave vector $\mathbf{k}$ and one with wave vec-

[14] A. B. Lidiard, Proc. Roy. Soc. (London) A224, 161 (1954).

tor $\mathbf{k}+\mathbf{Q}$ —instead of one band at these points in the Brillouin zone. The transformed Hamiltonian [Eq. (4)], however, would have essentially the same form as it does for the single-band model.

III. THE TRANSVERSE SUSCEPTIBILITY

In this section we will obtain the equations necessary to calculate the transverse susceptibility function $\chi^{-+}(\mathbf{q},\omega)$, which is given by the well-known expression

$$\chi^{-+}(\mathbf{q},\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dt\, e^{i(\omega-i\delta)t}\langle\langle S^{-}(\mathbf{q});S^{+}(-\mathbf{q})\rangle\rangle, \quad (12)$$

where $\langle\langle\ \rangle\rangle$ signify a double-time, retarded thermal Green's function of time argument t, and the spin operator $S^{\pm}(\mathbf{q})=S^{x}(\mathbf{q})\pm iS^{y}(\mathbf{q})$.[6] By definition, the poles of this susceptibility function give the spin-wave energies. The inelastic neutron-scattering cross section of magnetic excitations is given by the well-known formula

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega}=\left(\frac{2\gamma e^2}{mc^2}\right)^2\frac{k'}{k}\sum_{\alpha\beta}(\delta_{\alpha\beta}-\hat{k}_\alpha\hat{k}_\beta)|F(\mathbf{K})|^2 \times\frac{2\hbar}{1-\exp(-\hbar\omega/k_B t)}\frac{1}{\pi}\mathrm{Im}\chi^{\alpha\beta}(\mathbf{K},\omega), \quad (13)$$

where γ is the gyromagnetic ratio of the neutron, m is the electronic mass, $\mathbf{k}$ and $\mathbf{k}'$ are the incident and final wave vectors of the neutron, $\mathbf{K}=\mathbf{k}-\mathbf{k}'$, and $F(\mathbf{K})$ is the atomic form factor.[15,16]

In order to find the transverse susceptibility, we consider the Green's function

$$G_{\lambda\mu j'}(\mathbf{q},\mathbf{p})=\frac{1}{2\pi}\int_{-\infty}^{\infty}dt\, e^{i(\omega-i\delta)t}\langle\langle \mathbf{d}_{\mathbf{p}+\mathbf{q}\lambda\downarrow}{}^{\dagger}\mathbf{d}_{\mathbf{p}\mu\uparrow};S_{j'}{}^{+}(-\mathbf{q})\rangle\rangle, \quad (14)$$

where $S_{j'}{}^{+}(-\mathbf{q})=S^{+}(-\mathbf{q})$ if $j'=1$, and $S^{+}(-\mathbf{q}+\mathbf{Q})$ if $j'=3$. Making use of the relationship

$$S_j{}^{-}(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}(\mathbf{c}_{\mathbf{p}+\mathbf{q}\downarrow}{}^{\dagger}\mathbf{c}_{\mathbf{p}\uparrow}+\mathbf{c}_{\mathbf{p}+\mathbf{Q}+\mathbf{q}\downarrow}{}^{\dagger}\mathbf{c}_{\mathbf{p}+\mathbf{Q}\uparrow}) =\frac{1}{N}\sum_{\mathbf{p}\lambda\mu}[R_{\lambda\mu j}{}^{\downarrow\uparrow}(\mathbf{q},\mathbf{p})+R_{\lambda\mu\, j+1}{}^{\downarrow\uparrow}(\mathbf{q},\mathbf{p})]\mathbf{d}_{\mathbf{p}+\mathbf{q}\lambda\downarrow}{}^{\dagger}\mathbf{d}_{\mathbf{p}\mu\uparrow},$$

which follows from Eqs. (2) and (6), we find that

$$\langle\langle S_j{}^{-}(\mathbf{q});S_{j'}{}^{+}(-\mathbf{q})\rangle\rangle =\frac{1}{N}\sum_{\mathbf{p}\lambda\mu}[R_{\lambda\mu j}{}^{\downarrow\uparrow}(\mathbf{q},\mathbf{p})+R_{\lambda\mu\, j+1}{}^{\downarrow\uparrow}(\mathbf{q},\mathbf{p})] \times\langle\langle \mathbf{d}_{\mathbf{p}+\mathbf{q}\lambda\downarrow}{}^{\dagger}\mathbf{d}_{\mathbf{p}\mu\uparrow};S_{j'}{}^{+}(\mathbf{q})\rangle\rangle, \quad (15)$$

using Eqs. (2) and (6). It will be assumed from now on that

$$R_{\lambda\mu j}(\mathbf{q},\mathbf{p})=R_{\lambda\mu j}{}^{\downarrow\uparrow}(\mathbf{q},\mathbf{p}).$$

[15] T. Izuyama, D. J. Kim, and R. Kubo, J. Phys. Soc. Japan 18, 1025 (1963).
[16] L. Van Hove, Phys. Rev. 95, 1374 (1954).

In Eq. (15), when $j=1$, $\mathbf{q}$ is measured from a chemical reciprocal-lattice vector, and when $j=3$, it is measured from a magnetic reciprocal-lattice vector.

Taking the commutator of $\mathbf{d}_{\mathbf{p}+\mathbf{q}\,\lambda\downarrow}{}^{\dagger}\mathbf{d}_{\mathbf{p}\mu\uparrow}$ with Eq. (4), writing out $S_j{}^{+}(-\mathbf{q})$ in terms of the d operators, and decoupling in the random-phase approximation, we find

$$[E_{\lambda\downarrow}(\mathbf{p}+\mathbf{q})-E_{\mu\uparrow}(\mathbf{p})-\omega]G_{\lambda\mu j'}(\mathbf{q},\mathbf{p})-(n_{\mathbf{p}\mu\uparrow}-n_{\mathbf{p}+\mathbf{q}\lambda\downarrow}) \times\sum_{\mathbf{k}\xi\eta}W(\mathbf{p}+\mathbf{q}\,\lambda\downarrow,\mathbf{k}\eta\uparrow;\mathbf{k}+\mathbf{q}\xi\downarrow,\mathbf{p}\mu\uparrow)G_{\xi\eta j'}(\mathbf{q},\mathbf{k}) =-(n_{\mathbf{p}\mu\uparrow}-n_{\mathbf{p}+\mathbf{q}\lambda\downarrow})[R_{\lambda\mu j'}(\mathbf{q},\mathbf{p})+R_{\lambda\mu\, j+1}(\mathbf{q},\mathbf{p})]. \quad (16)$$

For the case of the simple antiferromagnet, we have $n_{p\lambda\sigma}$ independent of σ, and hence from now on we will drop the spin indices on the average occupation numbers and one-electron energies. The interaction matrix W now has a complicated $\mathbf{k}$ and $\mathbf{p}$ dependence because of the complicated behavior of the Bloch functions as a function of $\mathbf{k}$, which leads to the correct two-sublattice magnetization structure. In Lidiard's model we approximate W, neglecting its complicated wave-vector dependence. We do this by confining each of the two bands of each spin to its own sublattice.

One way of accomplishing this is to make the Coulomb interaction U very large compared to the bandwidth. We find from Eq. (9) that in this limit $\theta_{\mathbf{k}}$ is identically equal to $\frac{1}{2}\pi$. We see from Eqs. (5) and (6) that, in this strong interaction limit, bands localized on different sublattices do not interact. In our notation we see that, for example, electrons in band 1 of spin up interact only with electrons in band 2 of spin down, since bands 1 and 2 of opposite spin are localized on the same sublattice. Hence, in this limit, our model reduces to Lidiard's model without interband exchange.

In the rest of this section, we will calculate the transverse susceptibility in this limit and compare the results to the results obtained when an interatomic exchange interaction is included. Since $\theta_{\mathbf{k}}$ is now a constant, we know from Eq. (6) that $R_{\lambda\mu}(\mathbf{q},\mathbf{k})=R_{\lambda\mu}$, independent of $\mathbf{k}$ and $\mathbf{q}$. From Eqs. (5) and (6), we find that W is independent of $\mathbf{k}$ and $\mathbf{p}$, and

$$W(1\downarrow,1\uparrow;1\downarrow,1\uparrow)=W(1\downarrow2\uparrow;2\downarrow,1\uparrow) =W(2\downarrow,2\uparrow;2\downarrow,2\uparrow)=0,$$
$$W(1\downarrow,1\uparrow;2\downarrow,1\uparrow)=W(2\downarrow,1\uparrow;2\downarrow2\uparrow) =W(1\downarrow,1\uparrow;2\downarrow,2\uparrow)=0,$$

and

$$W(1\downarrow,2\uparrow;1\downarrow,2\uparrow)=W(2\downarrow,1\uparrow;2\downarrow,1\uparrow)=2U/N.$$

Hence Eq. (16) reduces to

$$[E_{\lambda}(\mathbf{p}+\mathbf{q})-E_{\mu}(\mathbf{p})-\omega]G_{\lambda\mu j'}(\mathbf{q},\mathbf{p}) =2U/N(n_{\mathbf{p}\mu}-n_{\mathbf{p}+\mathbf{q}\lambda})\sum_{\mathbf{k}}G_{\lambda\mu j'}(\mathbf{q},\mathbf{k}) -(n_{\mathbf{p}\mu}-n_{\mathbf{p}+\mathbf{q}\lambda})(R_{\lambda\mu j'}+R_{\lambda\mu j'+1}) \quad (17)$$

when $\lambda\neq\mu$, and when $\lambda=\mu$ the right-hand side of Eq. (17) becomes zero. Solving Eq. (17) for $(1/N)\sum_{\mathbf{p}}G_{\lambda\mu j'}$

$\times(\mathbf{q},\mathbf{p})$ and using Eqs. (12) and (15), we find that

$$\chi_{jj}^{-+}(\mathbf{q},\omega)=-\sum_{\substack{\lambda\mu\\ \lambda\neq\mu}}(R_{\lambda\mu j}+R_{\lambda\mu\, j+1})^2\frac{L_{\lambda\mu}^0(\mathbf{q})}{1-2UL_{\lambda\mu}^0(\mathbf{q})}, \quad (18)$$

where

$$L_{\lambda\mu}^0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\frac{n_{\mathbf{p}\mu}-n_{\mathbf{p}+\mathbf{q}\lambda}}{E_\lambda(\mathbf{p}+\mathbf{q})-E_\mu(\mathbf{p})-\omega}.$$

Now, $1-2UL_{21}^0(\mathbf{q})$ has a zero at $\omega=0$, $\mathbf{q}=0$, which goes into a spin wave for nonzero $\mathbf{q}$, since in the large-U limit $E_\lambda(\mathbf{p})$ reduces to $\frac{1}{2}[\tilde{\epsilon}(\mathbf{p}+\mathbf{Q})+\tilde{\epsilon}(\mathbf{p})]\pm g$, and hence at $\mathbf{q}=0$ we have

$$L_{21}^0(\mathbf{q}=0)=\frac{1}{2g}\frac{1}{N}\sum_{\mathbf{p}}(n_{\mathbf{p}1}-n_{\mathbf{p}2}).$$

Since by definition $g=(U/N)\sum_{\mathbf{p}}(n_{\mathbf{p}1}-n_{\mathbf{p}2})\sin\theta_{\mathbf{p}}$, in the large-$U$ limit we get zero at $\omega=0$, $\mathbf{q}=0$, for $1-2UL_{21}^0(\mathbf{q})$. Since $(R_{21j}+R_{21j+1})^2$ has the same value in the large-U limit for $j=1$ and $j=3$, the scattering is the same on both magnetic and chemical reciprocal lattice points. This is in contradiction to the Heisenberg-model results.[17] The reason for this contradiction is that here the bands become restricted completely to separate sublattices in the large-U limit, and, since in our model electrons must be on the same lattice site to interact, electrons on different sublattices are no longer coupled. Essentially, we are getting ferromagnetic spin waves on a single sublattice, as normally occurs in the Heisenberg model antiferromagnet at the zone boundary. We must include an interatomic exchange in order to get correct ground-state spin fluctuations,[18] as was done by the treatment of this model by Rajagopol and Brooks.[19] In the Appendix we consider the zero bandwidth limit when an interatomic exchange is included in Eq. (1), as was done by Antonoff and Englert in their paper; as expected, we recover the Heisenberg-model results. In particular, we find that on chemical reciprocal-lattice vectors the spin-wave scattering goes as KT/J, and near magnetic reciprocal-lattice vectors the scattering goes as $KTJ/(Cq)^2$, where C is the spin-wave velocity, as expected.[17] Also, the spin-wave energy is given by

$$\omega=m\{(J(\mathbf{q})-J(\mathbf{Q}))[J(\mathbf{Q}+\mathbf{q})-J(\mathbf{Q})]\}^{1/2},$$

which agrees with the Heisenberg model.[20]

IV. INELASTIC NEUTRON SCATTERING FROM SPIN-WAVE AND STONER SINGLE-PARTICLE MODES

In this section, we will calculate the susceptibility when U is finite and bands are allowed to overlap onto both sublattices. We will not include interatomic exchange in this section.

Dividing Eq. (16) by $E_\lambda(\mathbf{p}+\mathbf{q})-E_\mu(\mathbf{p})-\omega$, multiplying by $1/N[R_{\lambda\mu j}(\mathbf{q},\mathbf{p})+R_{\lambda\mu\, j+1}(\mathbf{q},\mathbf{p})]$, and summing over $\mathbf{p}$, λ, and μ, we obtain

$$G_{jj'}(\mathbf{q})=U\sum_{l=1,3}G_{jl}^0(\mathbf{q})G_{lj'}(\mathbf{q})-G_{jj'}^0(\mathbf{q}), \quad (19)$$

where all indices run over the values 1 and 3 only, and where

$$G_{jj'}^0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}\lambda\mu}M_{\lambda\mu j}(\mathbf{q},\mathbf{p})\times\frac{n_{\mathbf{p}\mu}-n_{\mathbf{p}+\mathbf{q}\lambda}}{E_\lambda(\mathbf{p}+\mathbf{q})-E_\mu(\mathbf{p})-\omega}M_{\lambda\mu j'}(\mathbf{q},\mathbf{p}) \quad (20)$$

and

$$G_{jj'}(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}\lambda\mu}M_{\lambda\mu j}(\mathbf{q},\mathbf{p})G_{\lambda\mu j'}^0(\mathbf{q},\mathbf{p}),$$

with

$$M_{\lambda\mu j}(\mathbf{q},\mathbf{p})=R_{\lambda\mu j}(\mathbf{q},\mathbf{p})+R_{\lambda\mu\, j+1}(\mathbf{q},\mathbf{p}).$$

For simplicity, let us first consider the zero-temperature case with $n_{\mathbf{p}2}\equiv 0$ and $n_{\mathbf{p}1}\equiv 1$ in the Hartree-Fock ground state. Then, using Eq. (6), Eq. (20) becomes

$$G_{11}^0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\sin^2\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}+\theta_{\mathbf{p}})\times[T_{21}^0(\mathbf{q},\mathbf{p},\omega)+T_{21}^0(\mathbf{q},\mathbf{p},-\omega)], \quad (21a)$$

$$G_{33}^0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\cos^2\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}-\theta_{\mathbf{p}})\times[T_{21}^0(\mathbf{q},\mathbf{p},\omega)+T_{21}^0(\mathbf{q},\mathbf{p},-\omega)], \quad (21b)$$

$$G_{13}^0(\mathbf{q})=G_{32}^0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\sin\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}+\theta_{\mathbf{p}})\cos\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}-\theta_{\mathbf{p}})\times[T_{21}^0(\mathbf{q},\mathbf{p},\omega)-T_{21}^0(\mathbf{q},\mathbf{p},-\omega)], \quad (21c)$$

where

$$T_{\lambda\mu}^0(\mathbf{q},\mathbf{p},\omega)=\frac{n_{\mathbf{p}\mu}-n_{\mathbf{p}+\mathbf{q}\lambda}}{E_\lambda(\mathbf{p}+\mathbf{q})-E_\mu(\mathbf{p})-\omega}.$$

We have made use of $\epsilon(\mathbf{k})=\epsilon(-\mathbf{k})$ in obtaining Eqs. (21) from (20). Expanding Eqs. (21a), (12b), and (21c) to lowest order in $\mathbf{q}$ and ω, with the help of Eq. (9) and the definition of q, we find

$$G_{11}^0(\mathbf{q})\approx 2(2g)^2D+O(\omega^2)+O(\mathbf{q}^2), \quad (22a)$$

$$G_{33}^0(\mathbf{q})\approx(1/U)+2D(\omega^2-v_2^2q^2), \quad (22b)$$

$$G_{13}^0(\mathbf{q})\approx 4g\omega D, \quad (22c)$$

where

$$D=\left(\frac{1}{2g}\right)^3\frac{1}{N}\sum_{\mathbf{p}}(n_{\mathbf{p}1}-n_{\mathbf{p}2})\sin^3\theta_{\mathbf{p}} \quad (23)$$

and

$$Dv_2^2=\left(\frac{1}{2g}\right)^3\frac{1}{N}\sum_{\mathbf{p}}(n_{\mathbf{p}1}-n_{\mathbf{p}2})\times\sin^2\theta_{\mathbf{p}}[g(\hat{q}\cdot\nabla_{\mathbf{p}})^2E_2(\mathbf{p})-\sin\theta_{\mathbf{p}}|\hat{q}\cdot\nabla_{\mathbf{p}}E_2(\mathbf{p})|^2]. \quad (24)$$

[17] R. J. Elliott and R. D. Lowde, Proc. Roy. Soc. (London) **A230**, 46 (1955).
[18] P. W. Anderson, *Concepts in Solids* (W. A. Benjamin, Inc., New York, 1964), p. 175.
[19] A. K. Rajagopol and H. Brooks, Phys. Rev. **158**, 552 (1967).
[20] J. M. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, London, 1964), p. 320.

In deriving Eq. (22b) we have made use of the definition of g:

$$g=\frac{U}{N}\sum_{\mathbf{p}}(n_{\mathrm{p}1}-n_{\mathrm{p}2})\sin\theta_{\mathbf{p}}.$$

When written out, Eq. (19) becomes

$$\begin{pmatrix}1-(2g)_2{}^2UD & -4gUD\omega\\ -4gUD\omega & -2UD(\omega^2-v_2{}^2q^2)\end{pmatrix}\begin{pmatrix}G_{11}(\mathbf{q}) & G_{13}(\mathbf{q})\\ G_{31}(\mathbf{q}) & G_{33}(\mathbf{q})\end{pmatrix}=\begin{pmatrix}-(2g)^2D & -2gD\omega\\ -2gD\omega & -(1/2U)-2D(\omega^2-v_2{}^2q^2)\end{pmatrix}. \quad (25)$$

This equation has a solution

$$G_{11}(\mathbf{q})=\frac{1}{U}+\frac{1}{U}\frac{D(\omega^2-v_2{}^2q^2)}{D\omega^2-D[1-(2g)_2{}^2UD]v_2{}^2q^2}, \quad (26a)$$

$$G_{33}(\mathbf{q})=\frac{1}{U}-\frac{1}{U}\frac{1-2g^2UD}{UD\omega^2-UD[1-(2g)_2{}^2UD]v_2{}^2q^2}, \quad (26b)$$

which has a pole at

$$\omega=[1-2(2g)^2UD]^{1/2}v_2q. \quad (27)$$

From Eqs. (12), (14), (15), and (27), for the residues at chemical and magnetic reciprocal lattice points we have

$$\mathrm{Res}\chi^{-+}(\mathbf{q},\omega)\,|_{\text{chemical point}}=\mathrm{Res}G_{11}(\mathbf{q})=\frac{(2g)^2Dv_2q}{2[1-2(2g)^2UD]^{1/2}}, \quad (28a)$$

$$\mathrm{Res}\chi^{-+}(\mathbf{q},\omega)\,|_{\text{magnetic point}}=\mathrm{Res}G_{33}(\mathbf{q})=\frac{[1-2(2g)^2UD]^{1/2}}{2U^2Dv_2q}. \quad (28b)$$

From Eq. (23) and the definition of q, we know that $(2g)^2UD$ is of the order of but smaller than 1. Hence, we have the same q-dependent behavior of the residue of $\chi^{-+}(\mathbf{q},\omega)$ at spin-wave poles near chemical and magnetic reciprocal lattice points as in the Heisenberg model.[7] When we include the Bose factor in Eq. (13), we find that we have a cross section near chemical reciprocal-lattice points which becomes small at low temperatures, and one near magnetic points which becomes very large as the wave vector of $\chi^{-+}(q,\omega)$ approaches the magnetic reciprocal-lattice point.

Now let us examine the expression for the spin-wave energy in some detail. From Eq. (27), it is seen that we must know the parameter $v_2{}^2$ in order to calculate ω. In order to get some quantitative feel for the behavior of the spin-wave energy as a function of the parameters U and the Fermi energy, let us consider the following simplified model of the band structure of the system. If we approximate our energies by nearest-neighbor tight-binding functions, the energy is given by

$$\epsilon(\mathbf{k})=B\sum_{\mathbf{a}}e^{i\mathbf{k}\cdot\mathbf{a}}, \quad (29)$$

where $\mathbf{a}$ is summed over nearest-neighbor lattice sites and B is a constant. By the definition of the magnetic reciprocal lattice vector $\mathbf{Q}$,

$$\epsilon(\mathbf{k}+\mathbf{Q})=-\epsilon(\mathbf{k}). \quad (30)$$

Let us approximate $\epsilon(\mathbf{k})$ as linear in $k=|\mathbf{k}|$ and, hence, the Fermi surface as a sphere. Then we may write

$$\epsilon(\mathbf{k})=v(k-k_c), \quad (31a)$$

$$\epsilon(\mathbf{k}+\mathbf{Q})=-v(k-k_c), \quad (31b)$$

where the Fermi energy is chosen to be zero, where v is the Fermi velocity, and where k_c is the magnitude of the vector $\frac{1}{2}\mathbf{Q}$. These one-electron energies are mathematically of the same form as those in Fedders and Martin's work.[1] From Eqs. (23), (24), and (10), we obtain the following integrals:

$$Dv_2{}^2=\left(\frac{1}{2g}\right)^3\frac{\Omega}{(2\pi)^3}\int d^3p(n_{\mathrm{p}1}-n_{\mathrm{p}2})\times\left[\sin^3\theta_{\mathbf{p}}v^2x^2(\sin^2\theta_{\mathbf{p}}-\cos^2\theta_{\mathbf{p}})+g\cos\theta_{\mathbf{p}}\sin^2\theta_{\mathbf{p}}\frac{v}{p}(1-x^2)\right], \quad (32a)$$

$$D=\left(\frac{1}{2g}\right)^3\frac{\Omega}{(2\pi)^3}\int d^3p(n_{\mathrm{p}1}-n_{\mathrm{p}2})\sin^3\theta_{\mathbf{p}}, \quad (32b)$$

where Ω is the volume of the magnetic unit cell, x is $\hat{p}\cdot\hat{q}$, and the integral is taken over the magnetic Brillouin zone, which, in the model of Eq. (31), will be spherical (of course, $n_{p1}-n_{p2}\equiv 1$ in this zone). In the limit $2g\ll vk_c=\epsilon_F$, by integrating Eqs. (31a) and (31b) and using the definition of $\theta_{\mathbf{p}}$ in Eq. (9), we obtain

$$Dv_2{}^2=\frac{1}{8}\frac{1}{2\pi^2}\frac{1}{9}v^2\frac{\gamma}{v^3k_c{}^3}\left(\frac{vk_c}{g}\right)^2, \quad (33a)$$

$$D=\frac{1}{8}\frac{1}{2\pi^2}\frac{\gamma}{v^3k_c{}^3}\left(\frac{vk_c}{g}\right)^2, \quad (33b)$$

where γ is a numerical factor chosen so that $\gamma/k_c{}^3=\Omega$. From Eq. (27) we have

$$\omega^2=\tfrac{1}{9}v^2q^2\left[1-\frac{1}{8}\frac{1}{2\pi^2}\gamma\left(\frac{2g}{vk_c}\right)^2\frac{U}{vk_c}\ln\left(\frac{2vk_c}{g}\right)\right]\approx\tfrac{1}{9}v^2q^2 \quad (34)$$

when $g\ll vk_c$. Just as Fedders and Martin get a large velocity spin wave in a spin-density wave state, we also get a collective spin-wave mode with large velocity. This is consistent with the neutron diffraction results of Muhlestein and Sinha,[3] who observe a mode with velocity at least as high as 10^6 cm/sec.

The occurrence of a real spin-wave energy and, hence, a stable antiferromagnetic state for $\epsilon_F\gg g$, is purely a consequence of the form that we took in Eqs. (31a) and (31b) for the one-electron energies. Had we chosen the one-electron energies in a more realistic manner for

a single-band model, we might get a positive imaginary spin-wave energy at some value of g/ϵ_F because there is no *a priori* reason to believe that the single-band model will lead to a stable antiferromagnetic state.

Now let us consider the case where the Fermi energy lies below the top of band 1. In that case there will appear extra terms in Eq. (21) due to intraband transition. There will probably be no new spin-wave poles due to intraband excitation since the interaction in Eq. (16) tends to pull collective states out of the bottom intraband continuum rather than push them out of the top, and the intraband continuum starts at $\omega=0$. We will now show that the main effect of intraband excitations on the spin waves will be to modify the spin-wave velocity. From Eqs. (6) and (20), we find that the intraband terms to be added to Eqs. (21) are given by

$$\Delta G_{11}{}^0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\cos^2\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}+\theta_{\mathbf{p}})\times[T_{11}{}^0(\mathbf{q},\mathbf{p},\omega)+T_{22}{}^0(\mathbf{q},\mathbf{p},\omega)], \quad (35a)$$

$$\Delta G_{33}{}^0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\sin^2\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}-\theta_{\mathbf{p}})\times[T_{11}{}^0(\mathbf{q},\mathbf{p},\omega)+T_{22}{}^0(\mathbf{q},\mathbf{p},\omega)], \quad (35b)$$

$$\Delta G_{13}{}^0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\sin\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}-\theta_{\mathbf{p}})\cos\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}+\theta_{\mathbf{p}})\times[T_{11}{}^0(\mathbf{q},\mathbf{p},\omega)-T_{22}{}^0(\mathbf{q},\mathbf{p},\omega)]. \quad (35c)$$

Let us assume that $n_{\mathbf{p}2}\equiv 0$ and band 1 is nearly completely filled. Then $T_{22}{}^0(\mathbf{q},\mathbf{p},\omega)$ is zero. For small $\mathbf{q}\propto\omega$, we may expand $T_{11}{}^0$ to lowest order in q and ω. Proceeding in this way, we find that Eqs. (35) at $T=0$ become

$$\Delta G_{11}{}^0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\cos^2\theta_{\mathbf{p}}\left(\frac{\mathbf{q}\cdot\nabla_{\mathbf{p}}E_1(\mathbf{p})}{\mathbf{q}\cdot\nabla_{\mathbf{p}}E_1(\mathbf{p})-\omega}\right)\times\delta(E_1(\mathbf{p})-E_F), \quad (36a)$$

$$\Delta G_{33}{}^0(\mathbf{q})=\frac{1}{16}\frac{1}{N}\sum_{\mathbf{p}}[\cot(\tfrac{1}{2}\theta_{\mathbf{p}})+\tan(\tfrac{1}{2}\theta_{\mathbf{p}})]\times(\mathbf{q}\cdot\nabla_{\mathbf{p}}\cos\theta_{\mathbf{p}})^2\left(\frac{\mathbf{q}\cdot\nabla_{\mathbf{p}}E_1(\mathbf{p})}{\mathbf{q}\cdot\nabla_{\mathbf{p}}E_1(\mathbf{p})-\omega}\right)\times\delta(E_1(\mathbf{p})-E_F), \quad (36b)$$

$$\Delta G_{13}{}^0(\mathbf{q})=-\frac{\omega}{4}\frac{1}{N}\sum_{\mathbf{p}}\cos\theta_{\mathbf{p}}[\cot(\tfrac{1}{2}\theta_{\mathbf{p}})+\tan(\tfrac{1}{2}\theta_{\mathbf{p}})]\times\frac{\mathbf{q}\cdot\nabla_{\mathbf{p}}\cos\theta_{\mathbf{p}}}{\omega}\left(\frac{\mathbf{q}\cdot\nabla_{\mathbf{p}}E_1(\mathbf{p})}{\mathbf{q}\cdot\nabla_{\mathbf{p}}E_1(\mathbf{p})-\omega}\right)\delta(E_1(\mathbf{p})-E_F). \quad (36c)$$

If we examine Eq. (36) we see that, as q and ω approach zero such that $\omega=cq$, where c is some finite constant, G_{11} is of zeroth order in q, $G_{22}{}^0$ is of second order in q, and $G_{12}{}^0$ is of first order in q. Hence, the Green's functions in Eq. (22) are still the same order in q and ω. Therefore, the form of Eq. (25) does not change, but the various constants $v_2{}^2$ and D appearing in it do change; they are dependent on the ratio ω/q, but not on q or ω independently. Thus, we find that the spin-wave dispersion relation will still be linear in q for small q, and the residues calculated in Eqs. (28) will still have the same dependence on q. Of course, it is entirely possible that when ϵ_F lies in band 1, the ground state is not stable, and hence the spin-wave energy could turn out to be positive imaginary, signaling this instability. The stability of the state with ϵ_F in band 1 is not considered in this paper.

Let us now consider neutron scattering from Stoner excitations (spin-flip single-particle excitations) between bands 1 and 2. The intraband single-particle excitations are of low energy, and the neutron scattering from them is qualitatively not much different from the scattering from a paramagnet. To calculate neutron scattering from the interband Stoner excitations near the bottom of the continuum for small $q(\omega\sim 2g)$, we need only consider the interband contributions to the Green's functions given by Eq. (21), since the intraband contributions of Eq. (35) are small for small q and nonzero $\omega\sim 2g$. Now in Eq. (21), for $\omega\approx 2g$, only $T_{21}{}^0(\mathbf{q},\mathbf{p},\omega)$ contributes significantly, and most of the contribution to G^0 in the summation comes from values of $\mathbf{p}$ of the order of k_c, where $\sin\theta_{\mathbf{p}}\approx 1$. Therefore, all three Green's functions $G_{11}{}^0$, $G_{33}{}^0$, and $G_{13}{}^0$ are approximately equal to the function G^0, which is given by

$$G^0(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}T_{21}{}^0(\mathbf{q},\mathbf{p},\omega). \quad (37)$$

Using the simplified band structure of Eq. (35), we get

$$\mathrm{Im}G^0(\mathbf{q}=0)\propto\pi\int_{-k_c}^{0}(k+k_c)^2dk\,\delta[2(v^2k^2+g^2)^{1/2}-\omega]\cong\frac{\pi k_c{}^2}{2v}\left(\frac{g}{\omega-2g}\right)^{1/2}. \quad (38)$$

The real part of G^0 remains finite as $\omega\to 2g$, and we find from Eq. (24) that

$$G_{11}(\mathbf{q})=G_{33}=-G^0/(1-2UG^0). \quad (39)$$

Therefore when $\omega\to 2g$, $G_{11}(q)$ and $G_{22}(\mathbf{q})\to 1/2U$, a real number. Hence, the single-interband Stoner-mode scattering becomes zero when ω is of the order of the gap energy. In the case of single-particle excitations without spin flip, however, we will find in the next section that there is very strong single-particle-mode neutron scattering near $\omega=2g$. [Fig. 4(a) illustrates the results of this section.]

V. LONGITUDINAL SUSCEPTIBILITY: ZERO SOUND AND LONGITUDINAL SPIN WAVES

We now wish to calculate the longitudinal susceptibility (susceptibility for magnetic field along the sub-

lattice magnetization) which is given by

$$\chi_{jj'}{}^{zz}(\mathbf{q},\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dt e^{i(\omega-i\delta)t}\langle\langle S_j{}^z(\mathbf{q});S_{j'}{}^z(-\mathbf{q})\rangle\rangle, \quad (40)$$

where j and j' can take on the values 1 and 3. Using the relation

$$S_j{}^z(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}\sigma}\frac{\sigma}{2}\mathbf{c}_{\mathbf{p}+\mathbf{q}\sigma}{}^\dagger\mathbf{c}_{\mathbf{p}\sigma}$$

$$=\frac{1}{N}\sum_{\mathbf{p}\sigma\lambda\mu}\sum_{l=j}^{j+1}\frac{\sigma}{2}R_{\lambda\mu l}{}^\sigma(\mathbf{q},\mathbf{p})\mathbf{d}_{\mathbf{p}+\mathbf{q}\lambda\sigma}{}^\dagger\mathbf{d}_{\mathbf{p}\mu\sigma}, \quad (41)$$

which follows from Eqs. (2) and (6), we find that

$$\chi_{jj'}{}^{zz}(\mathbf{q},\omega)=\frac{1}{N}\sum_{\mathbf{p}\mu\lambda\sigma}\sum_{l=j}^{j+1}\frac{\sigma}{2}R_{\lambda\mu l}{}^\sigma(\mathbf{q},\mathbf{p})G_{\lambda\mu j'}{}^\sigma(\mathbf{q},\mathbf{p}), \quad (42)$$

where

$$G_{\lambda\mu j'}{}^\sigma(\mathbf{q},\mathbf{p})$$

$$=\frac{1}{2\pi}\int_{-\infty}^{\infty}dt e^{i(\omega-i\delta)t}\langle\langle\mathbf{d}_{\mathbf{p}+\mathbf{q}\lambda\sigma}{}^\dagger\mathbf{d}_{\mathbf{p}\mu\sigma};S_{j'}{}^z(\mathbf{q})\rangle\rangle. \quad (43)$$

Proceeding in the same way as we proceeded to get Eq. (16), we find

$$[\omega-E_\lambda(\mathbf{p}+\mathbf{q})+E_\mu(\mathbf{p})]G_{\lambda\mu j'}{}^\sigma(\mathbf{q},\mathbf{p})$$

$$+\sum_{\mathbf{k}\xi\eta}W(\mathbf{p}+\mathbf{q}\lambda\sigma,\mathbf{k}\eta-\sigma;\mathbf{p}\mu\sigma,\mathbf{k}+\mathbf{q}\xi-\sigma)$$

$$\times(n_{\mathbf{p}\mu}-n_{\mathbf{p}+\mathbf{q}\lambda})G_{\xi\eta j'}{}^{-\sigma}(\mathbf{q},\mathbf{k})$$

$$=-\frac{\sigma}{2}(n_{\mathbf{p}\mu}-n_{\mathbf{p}+\mathbf{q}\lambda})[R_{\lambda\mu j'}{}^\sigma(\mathbf{q},\mathbf{p})+R_{\lambda\mu j'+1}{}^\sigma(\mathbf{q},\mathbf{p})], \quad (44)$$

where W is given by Eq. (5), but can be rewritten in the following more illuminating form:

$$W(\mathbf{p}+\mathbf{q}\lambda\sigma,\mathbf{k}\eta\sigma';\mathbf{p}\mu\sigma,\mathbf{k}+\mathbf{q}\xi_l\sigma')$$

$$=\frac{U}{N}\sum_{j=1,3}[R_{\lambda\mu j}{}^\sigma(\mathbf{q},\mathbf{p})+R_{\lambda\mu j+1}{}^\sigma(\mathbf{q},\mathbf{p})]$$

$$\times[R_{\xi\eta j}{}^{\sigma'}(\mathbf{q},\mathbf{k})+R_{\xi\eta j+1}{}^{\sigma'}(\mathbf{q},\mathbf{k})]. \quad (45)$$

Taking the large-U limit, as was done in Sec. II, we find from Eqs. (6) and (45) that W is zero unless $\lambda=\mu$ and $\xi=\eta$. Hence, in this limit only intraband collective excitations are possible—as is expected, since electrons of the same spin can only interact if they are both on the same site; since each band is confined to a different sublattice, they must be in the same band to interact. Hence, in the large-U limit, there will be no poles in the longitudinal susceptibility corresponding to interband collective modes.

Let us now consider the more general case of U and the bandwidth being comparable and look for possible collective modes. To do this we calculate the Green's function of Eq. (43) by solving Eq. (44). To solve Eq. (44), divide it by $E_{\lambda\sigma}(\mathbf{p}+\mathbf{q})-E_{\mu\sigma}(\mathbf{p})-\omega$, multiply by $R_{\lambda\mu j}{}^\sigma(q,p)+R_{\lambda\mu,j+1}{}^\sigma(\mathbf{q},\mathbf{p})$, and sum over $\mathbf{p}$ to obtain

$$G_{jj'}{}^\sigma(\mathbf{q})+U\sum_l G_{jl}{}^{0\sigma}(\mathbf{q})G_{lj'}{}^{-\sigma}(\mathbf{q})=-\frac{\sigma}{2}G_{jj'}{}^{0\sigma}(\mathbf{q}), \quad (46)$$

where

$$G_{jj'}{}^{0\sigma}(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}\lambda\mu}[R_{\lambda\mu j}{}^\sigma(\mathbf{q},\mathbf{p})+R_{\lambda\mu j+1}{}^\sigma(\mathbf{q},\mathbf{p})]$$

$$\times\frac{n_{\mathbf{p}\mu}-n_{\mathbf{p}+\mathbf{q}\lambda}}{E_\lambda(\mathbf{p}+\mathbf{q})-E_\mu(\mathbf{p})-\omega}[R_{\lambda\mu j'}{}^\sigma(\mathbf{q},\mathbf{p})+R_{\lambda\mu j'}{}^\sigma(\mathbf{q},\mathbf{p})], \quad (47)$$

and where

$$G_{jj'}{}^\sigma(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}\lambda\mu}\sum_{l=j}^{j+1}R_{\lambda\mu l}{}^\sigma(\mathbf{q},\mathbf{p})G_{\lambda\mu j'}{}^\sigma(\mathbf{q},\mathbf{p}). \quad (48)$$

We solve the matrix equation (46); and using Eq. (42), we find

$$\chi_{11}{}^{zz}(\mathbf{q})=\frac{1}{2U}-\frac{1}{2U}\frac{[1+UG_{11}{}^{0\sigma}(\mathbf{q})][1-U^2\Gamma_{33}{}^\sigma(\mathbf{q})]+U^3G_{31}{}^{0\sigma}(\mathbf{q})\Gamma_{13}{}^\sigma(\mathbf{q})}{[1-U^2\Gamma_{11}{}^\sigma(\mathbf{q})][1-U^2\Gamma_{33}{}^\sigma(\mathbf{q})]-U^4\Gamma_{31}{}^\sigma(\mathbf{q})\Gamma_{13}{}^\sigma(\mathbf{q})}, \quad (49a)$$

$$\chi_{33}{}^{zz}(\mathbf{q})=\frac{1}{2U}-\frac{1}{2U}\frac{[1+UG_{33}{}^{0\sigma}(\mathbf{q})][1-U^2\Gamma_{11}{}^\sigma(\mathbf{q})]-U^3G_{13}{}^{0\sigma}(\mathbf{q})\Gamma_{31}{}^\sigma(\mathbf{q})}{[1-U^2\Gamma_{11}{}^\sigma(\mathbf{q})][1-U^2\Gamma_{33}{}^\sigma(\mathbf{q})]-U^4\Gamma_{31}{}^\sigma(\mathbf{q})\Gamma_{31}{}^\sigma(\mathbf{q})}, \quad (49b)$$

where

$$\Gamma_{jj'}{}^\sigma(\mathbf{q})=\sum_{l=1,3}G_{jl}{}^{0\sigma}(\mathbf{q})G_{lj'}{}^{0-\sigma}(\mathbf{q}). \quad (50)$$

From Eqs. (6) and (47) at zero temperature when $n_{\mathbf{p}1}\equiv1$ and $n_{\mathbf{p}2}=0$, we have

$$G_{11}{}^{0\sigma}(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\sin^2\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}-\theta_{\mathbf{p}})$$

$$\times[T_{21}{}^0(\mathbf{q},\mathbf{p},\omega)+T_{21}{}^0(\mathbf{q},\mathbf{p},-\omega)], \quad (51a)$$

$$G_{33}{}^{0\sigma}(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}\cos^2\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}+\theta_{\mathbf{p}})$$

$$\times[T_{21}{}^0(\mathbf{q},\mathbf{p},\omega)+T_{21}{}^0(\mathbf{q},\mathbf{p},-\omega)], \quad (51b)$$

$$G_{13}{}^{0\sigma}(\mathbf{q})=-\sigma\frac{1}{N}\sum_{\mathbf{p}}\sin\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}-\theta_{\mathbf{p}})\cos\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}+\theta_{\mathbf{q}})$$

$$\times[T_{21}{}^0(\mathbf{q},\mathbf{p},\omega)-T_{21}{}^0(\mathbf{q},\mathbf{p},-\omega)], \quad (51c)$$

using the notation of Eq. (21). Let us examine Eqs.

(52a) and (52b) for poles corresponding to collective modes, when $\mathbf{q}=0$. When $\mathbf{q}=0$, we see from Eq. (51) that only $G_{33}{}^{0\sigma}(\mathbf{q})$ is nonzero. Hence, in this limit, Eq. (49) reduces to

$$\chi^{zz}(\mathbf{q}=0)\,|_{\text{chemical point}}=0, \tag{52a}$$

$$\chi^{zz}(\mathbf{q}=0)\,|_{\text{magnetic point}}=\frac{1}{2U}-\frac{1}{2U}\frac{1}{1-UG_{33}{}^{0}(\mathbf{q})}, \tag{52b}$$

using Eq. (50). The result in Eq. (51a) is well known for the Heinsenberg-model insulating antiferromagnets. In our model, it is a consequence of having the Fermi energy fall in the gap. Had the Fermi energy not been in the gap, this result would be correct only for $\omega\neq 0$.

From Eqs. (9) and (51b), we have

$$G_{33}{}^{0\sigma}(0)=-\frac{4}{N}\sum_{\mathbf{p}}\frac{D(\mathbf{p})^2}{[D(\mathbf{p})^2+g^2]^{1/2}}\frac{n_{\mathbf{p}1}-n_{\mathbf{p}2}}{4D(\mathbf{p})^2+4g^2-\omega^2}, \tag{53}$$

where

$$D(\mathbf{p})=\tfrac{1}{2}[\epsilon(\mathbf{p}+\mathbf{Q})-\epsilon(\mathbf{p})].$$

From the definition of g in Eq. (25) and from Eq. (9), we find from Eq. (53) that when $\omega^2=4g^2$, $G_{33}{}^{0\sigma}(0)$ is 1 and hence (52b) has a pole. This result is true at all temperatures below the Néel temperature. The pole occurs at the bottom of the continuum ($\omega=2g$), and therefore it appears to be a type of resonant state (i.e., a collective mode that does not get completely pulled out of the continuum). It is a spin-fluctuation state associated with oscillations in the z component of the magnetization. When the Fermi energy does not lie in the continuum but instead lies in band 1, we see from Fig. 2 that the interband single-particle continuum will begin at a higher energy. We must include intraband terms in Eq. (51) in this case, but, when $q=0$ and $\omega\neq 0$, these terms are zero; hence the analyses leading to Eqs. (52) and (53) are identical. We see from Eq. (53) that this new mode will still be found at $\omega=2g$, and hence it will be a real collective mode pulled out of the single-particle excitation continuum.

Let us calculate the dispersion relation of this mode for small q. To do this, we must consider Eqs. (51) to lowest order in q and $2g-\omega$. Letting

$$\alpha(\mathbf{p},\mathbf{q})=E_2(\mathbf{p}+\mathbf{q})-E_2(\mathbf{p}), \tag{54a}$$

$$\beta(\mathbf{p},\mathbf{q})=\cos^2\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}+\theta_{\mathbf{p}})-\cos^2\theta_{\mathbf{p}}, \tag{54b}$$

$$\mu^2=(2g)^2-\omega^2, \tag{54c}$$

we write Eq. (51b) to lowest order in q and u as

$$G_{33}{}^{0}(\mathbf{q})\approx\frac{1}{U}+\frac{1}{N}\sum_{\mathbf{p}}\frac{4\beta(\mathbf{p},\mathbf{q})(D(\mathbf{p})^2+g^2)^{1/2}-4\alpha(\mathbf{p},\mathbf{q})-u^2(D(\mathbf{p})^2+g^2)^{-1/2}}{4D(\mathbf{p})^2+u^2+4\alpha(\mathbf{p},\mathbf{q})[D(\mathbf{p})^2+g^2]^{1/2}}. \tag{55}$$

Using the simplified band structure of Eq. (30), the summation in Eq. (55) can be written as

$$\frac{\Omega}{(2\pi)^2}\int_{-1}^{1}dx\int_{-k_c}^{k_F-k_c}(k+k_c)^2dk\times\frac{4\beta(\mathbf{k},\mathbf{q})(v^2k^2+g^2)^{1/2}-4\alpha(\mathbf{k},\mathbf{q})-u^2(v^2k^2+g^2)^{1/2}}{4v^2k^2+u^2+4\alpha(\mathbf{k},\mathbf{q})(v^2k^2+g^2)^{1/2}}, \tag{56}$$

where x is the cosine of the angle between $\mathbf{k}$ and $\mathbf{q}$ and where $k=p-k_c$. We can break up the integral over k into an integral from $-k_c$ to $-k_1-k_c$, where $u^2\ll v(k_c-k_1)\ll g$, and an integral from k_1-k_c to k_F-k_c. The integral from $-k_c$ to k_1-k_c can be shown to contribute to order q^2 and u^2, whereas the integral from k_1-k_c to k_F-k_c contributes a term of first order in q and u, if $v(k_c-k_F)$ and u are of the same order of magnitude. Hence, to lowest order we integrate from k_1-k_c to k_F-k_c to obtain

$$\frac{\Omega}{(2\pi)^2}\frac{k_c^2}{2v}\int_{-1}^{1}dx\frac{(u^2+2v^2q^2x^2)^{1/2}}{g}\times\left\{\frac{\pi}{2}-\arctan\left[\frac{-2v(k_c-k_F)}{(u^2+2v^2q^2x)^{1/2}}\right]\right\} \tag{57}$$

for $u^2>0$. If we place the Fermi energy in the gap (i.e., set $k_F=k_c$), we integrate (57) to get

$$\frac{\Omega}{(2\pi)^2}\frac{k_c^2}{2v}\frac{\pi}{2g}\left[\sqrt{2}vq(u^2+2v^2q^2)^{1/2}+u^2\ln\left|\frac{\sqrt{2}vq+(u^2+2v^2q^2)^{1/2}}{\sqrt{2}vq-(u^2+2v^2q^2)^{1/2}}\right|\right]. \tag{58}$$

Since this factor does not become zero for $q\neq 0$ for any $u^2\geq 0$, we see that if the Fermi energy falls in the gap, the collective mode will not pull out of the continuum as q increases. Let us now integrate the second term in Eq. (55) for $\omega>2g$ but $\omega-2g<v(k_c-k_F)$.

To accomplish this, we substitute $\bar{u}^2=-u^2=\omega^2-(2g)^2$. Proceeding as previously, we obtain, to lowest order in $v(k_c-k_F)/g$,

$$\frac{\Omega}{(2\pi)^2}\frac{k_c^2}{2v}\int_{-1}^{1}dx\frac{(2v^2q^2x^2+g^2)^{1/2}}{2g}\times\ln\left|\frac{2v(k_c-k_F)+(2v^2q^2x^2-\bar{u}^2)^{1/2}}{2v(k_c-k_F)-(2v^2q^2x^2-\bar{u}^2)^{1/2}}\right|, \tag{59}$$

which, to lowest order in $(2v^2q^2x-\bar{u}^2)^{1/2}/v(k_c-k_F)$, is

given by

$$\frac{\Omega}{(2\pi)^2}\frac{k_c^2}{2v}\frac{1}{2g}\int_{-1}^{1}dx\frac{2v^2q^2x^2-\tilde{u}^2}{v(k_c-k_F)}$$
$$=\frac{\Omega}{(2\pi)^2}\frac{k_c^2}{2v}\frac{1}{gv(k_c-k_F)}(\tfrac{2}{3}v^2q^2-\tilde{u}^2). \quad (60)$$

This expression is set equal to zero to give a collective-mode dispersion relation of the form

$$\omega=[(2g)^2+\tfrac{2}{3}v^2q^2]^{1/2}\approx 2g+\tfrac{1}{3}(v^2q^2/2g). \quad (61)$$

Hence, a collective mode does pull out of the continuum if the Fermi energy lies outside of the gap.

Experimental data is consistent with having the Fermi energy within the gap.[2,21] Therefore, we will investigate the intensity of the neutron scattering for ϵ_F in the gap for ω of the order of and slightly greater than the minimum energy of the single-particle continuum ($2g$ in this case). From Eq. (52b), we find

$$\mathrm{Im}\chi_{33}(\mathbf{q})$$
$$=-\frac{1}{2}\frac{\mathrm{Im}G_{33}{}^{0\sigma}(\mathbf{q})}{[1-U\,\mathrm{Re}G_{33}{}^{0\sigma}(\mathbf{q})]^2+[U\,\mathrm{Im}G_{33}{}^{0\sigma}(\mathbf{q})]^2}. \quad (62)$$

We integrate the second term in Eq. (56) by dividing up the region of integration into one in which $D(\mathbf{p})\ll g$ and one in which $D(\mathbf{p})\gg u^2$, as is done in integrating Eq. (56), where $u^2=\omega^2-(2g)^2$ in this integration, and approximate the integrand in each case. We thus obtain

$$\frac{1}{U}-\mathrm{Re}G_{33}{}^0=\frac{2\Omega}{(2\pi)^2}\frac{k_c^2}{4v}\frac{u^2}{g^2}, \quad (63a)$$

$$\mathrm{Im}G_{33}{}^0=\frac{2\Omega}{(2\pi)^2}\frac{k_c^2}{v}2\pi\frac{u}{g}. \quad (63b)$$

Substituting in Eq. (62), we obtain

$$\mathrm{Im}\chi_{33}(\mathbf{q})\approx\tfrac{1}{4}(1/U^2)(\pi v k_c/\Omega k_c{}^2)(g/\omega-2g)^{1/2}, \quad (64)$$

for ω close to $2g$.

Therefore, we see that if the Fermi energy lies in the gap, there should be strong inelastic scattering at an energy equal to the gap energy. This strong scattering is not simply a result of there being a high density of states near the gap, but it is a result of electronic interaction since it does not exist in the Hartreee-Fock approximation. It should be observable in a neutron-scattering experiment since the gap energy is known from optical data to be of the order of 0.15 eV.[2] Such energies have been reached at Oak Ridge in neutron scattering from ferromagnets.[22] A measurement of the gap in this way by inelastic neutron scattering would serve as a check on measurements of the gap by optical reflectance.[2] Whereas light measures closer to the surface of the sample, neutrons measure bulk properties. Thus, we would perhaps get some idea of the amount by which optical reflectance measurements are affected by differences of electronic structure in the surface of a metal from that in the bulk metal. Of course, this strong neutron scattering may get smeared out at temperatures near T_N.[2]

For completeness, let us consider neutron scattering from zero-sound oscillation in the itinerant antiferromagnet. In our short-range model, the plasma mode will be zero-sound mode, a collective excitation whose energy goes to zero at $q=0$. The possible existence of such a mode in a real metal can be justified as follows: If some part of the Fermi surface were to lie in band 1 near the top of the band or in band 2 near the bottom, instead of being in the gap, then there could be intraband excitations involving charge carriers at this point in the band. These carriers have high effective mass because of the flatness of the bands. If there were other bands whose effective masses at the Fermi surface were smaller, the carriers in these bands could screen the interaction of the carriers in bands 1 or 2, resulting in an acoustic plasmon.[23] This is not inconsistent with existing band calculations.[24] (In addition to the main gap which results in the truncation of part of the Fermi surface, there could be gaps lying in other bands near, but not at, the Fermi surface for some alloys of chromium.) This zero-sound mode, which is an oscillation of charge density, will also cause the spin density to oscillate when the system is magnetic and the Fermi energy is near the gap; thus it should scatter neutrons.

To calculate the zero-sound mode, we assume that the Fermi energy lies in band 1 and calculate the Green's functions of Eq. (51) for small q and ω, including the intraband terms. Using Eqs. (6) and (47), we obtain

$$G_{11}{}^{0\sigma}(\mathbf{q})\approx\frac{1}{N}\sum_{\mathbf{p}}\cos^2\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}-\theta_{\mathbf{p}})$$
$$\times[T_{11}{}^0(\mathbf{q},\mathbf{p},\omega)+T_{22}{}^0(\mathbf{q},\mathbf{p},+\omega)], \quad (65a)$$

$$G_{33}{}^{0\sigma}(\mathbf{q})\approx\frac{1}{N}\sum_{\mathbf{p}}\sin^2\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}+\theta_{\mathbf{p}})$$
$$\times[T_{11}{}^0(\mathbf{q},\mathbf{p},\omega)+T_{22}{}^0(\mathbf{q},\mathbf{p},+\omega)]$$
$$+\frac{1}{2g}\frac{1}{N}\sum_{\mathbf{p}}\cos^2\theta_{\mathbf{p}}\sin\theta_{\mathbf{p}}(n_{\mathbf{p}1}-n_{\mathbf{p}2}), \quad (65b)$$

$$G_{13}{}^{0\sigma}(\mathbf{q})\approx-\sigma\frac{1}{N}\sum_{\mathbf{p}}\cos\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}-\theta_{\mathbf{p}})\sin\tfrac{1}{2}(\theta_{\mathbf{p}+\mathbf{q}}+\theta_{\mathbf{p}})$$
$$\times[T_{11}{}^0(\mathbf{q},\mathbf{p},\omega)-T_{22}{}^0(\mathbf{q},\mathbf{p},\omega)]. \quad (65c)$$

In our model, when the Fermi energy is much larger than the gap energy, we may neglect the second summation in Eq. (65b) compared to the first; hence only intraband excitations contribute to the zero-sound mode. The net result is that we may write Eq. (65) for

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small $\mathbf{q}$ as

$$G_{11}{}^{0\sigma}(\mathbf{q})=\alpha(\mathbf{q}), \tag{66}$$

$$G_{33}{}^{0\sigma}(\mathbf{q})=\alpha(\mathbf{q})\sin^2\theta_{pF}, \tag{67}$$

$$G_{13}{}^{0\sigma}(\mathbf{q})=-\sigma\alpha(\mathbf{q})\sin\theta_{pF}, \tag{68}$$

where

$$\alpha(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}} T_{11}{}^{0}(\mathbf{q},\mathbf{p},\omega),$$

for small $\mathbf{q}$ and ω. Using Eqs. (49) and (50), we obtain

$$\chi_{11}(\mathbf{q},\omega)=\frac{1}{2U}-\frac{1}{2U}\frac{2U^3\alpha^3(\mathbf{q})\sin^2\theta_{pF}\cos^2\theta_{pF}+U\alpha(\mathbf{q})+[1+U^2\alpha^2(\mathbf{q})\sin^2\theta_{pF}\cos^2\theta_{pF}]}{1-U^2\alpha^2(\mathbf{q})\cos^3\theta_{pF}}, \tag{69a}$$

$$\chi_{33}(\mathbf{q},\omega)=\frac{1}{2U}-\frac{1}{2U}\frac{-2U^3\alpha^3(\mathbf{q})\cos^2\theta_{pF}\sin^2\theta_{pF}+U\alpha(\mathbf{q})\sin^2\theta_{pF}+[1-U^2\alpha^2(\mathbf{q})\cos^2\theta_{pF}]}{1-U^2\alpha^2(\mathbf{q})\cos^4\theta_{pF}}. \tag{69b}$$

Equations (69a) and (69b) both have a pole corresponding to a zero-sound mode when

$$1+U\alpha(\mathbf{q})\cos^2\theta_{pF}=0. \tag{70}$$

By the definition of $\alpha(\mathbf{q})$ and $T_{11}(\mathbf{q},\mathbf{p},\omega)$ below Eq. (21), the zero-sound-mode dispersion relation can be found for small $\mathbf{q}$ in much the same way as for a paramagnetic system,[25] except that for the antiferromagnet the Fermi velocity and density of states of the paramagnetic system are replaced by those for the antiferromagnetic system. According to Eq. (70), when the Fermi energy is close to the gap, since $\cos\theta_{pF}$ is small, we are in the weak coupling region,[25] and therefore the zero-sound velocity is close to the Fermi velocity and, hence, very small. If we calculate the residue of Eq. (69), we find that, since it is multiplied by a factor of $1/\cos\theta_{pF}$, the residue can be quite large. In general, since the residue must be multiplied by the Bose factor, the cross section will be of order KT/U on both magnetic and chemical points. When the Fermi energy is far away from the gap, we see from Eq. (69) and (70) that, since $\cos\theta_{pF}=1$ and $\sin\theta_{pF}\cong 0$, there will be no zero-sound pole in the susceptibility. This is true because the zero-sound oscillations, which correspond to Fermi surface oscillations, will not affect the spin density if the Fermi surface is not near a gap in the band. Of course, if it happened that the Fermi surface did fall right below the gap in a real system, the acoustic plasmon or zero-sound mode would still probably be strongly damped by mixing of the bands, but it could still lead to strong single-particle-mode scattering at low energies for small q. [Fig. 4(b) illustrates the main results of this section].

VI. CONCLUSION

By canonically transforming the Hubbard Hamiltonian[9] to a representation in terms of the one-electron wave functions of the Slater alternant-molecular-orbital model of antiferromagnetism,[10] we have calculated the longitudinal and transverse susceptibility functions at zero temperature in the random-phase approximation. We find a pole in the transverse susceptibility as expected, corresponding to a spin-wave mode. The energy of the mode is linear in the wave vector, and the expression for the spin-wave velocity is like that found by Des Cloizeaux[11] for this same model. The velocity, calculated using one-electron energies like the ones Fedders and Martin used, is of the same order of magnitude as theirs. The q dependence of the residue of the spin-wave pole near magnetic and chemical reciprocal-lattice vectors is found to be similar to the behavior in the Heisenberg model.[17] When intraband contributions to the spin-wave energy are considered, we find that the dispersion relation does not change qualitatively; it is still linear in q.

We have also calculated the longitudinal susceptibility $\chi^{zz}(q,\omega)$ at zero temperature. Near a magnetic reciprocal-lattice vector, if the Fermi energy does not fall in the gap, χ^{zz} is found to have a pole corresponding to a collective mode at $\omega=2g$ when $q=0$, with a dispersion relation quadratic in q. When the Fermi energy lies in the gap, this mode merges with the continuum, but there is still intense single-particle-mode scattering near the gap energy $2g$. This should be observable in inelastic neutron-scattering experiments, and it would serve as a measure of the gap energy $2g$ in the bulk sample to be compared with optical reflectance experiments.[2]

We plan to follow this paper with another in which our results will be calculated explicitly at temperatures close to the Néel temperature. We also plan to consider some of the effects of band structure on the spin-wave energy.

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APPENDIX: INCLUSION OF INTERATOMIC EXCHANGE IN THE NARROW-BAND LIMIT

In order to make contact with the Heisenberg model, let us include a $\mathbf{q}$-dependent interatomic exchange and let the effective mass go to infinity. If we include an exchange interaction between Wannier functions on neighboring sites, as was done by Englert and Antonoff[26] in their treatment of ferromagnetic spin waves, we must add to the expression for W in Eq. (5) a term of the form

$$J(\mathbf{p}+\mathbf{q}\sigma,\ \mathbf{k}n\sigma';\ \mathbf{k}+\mathbf{q}\xi\sigma,\ \mathbf{p}\mu\sigma')$$
$$=\frac{1}{N}\sum_{j=1,3}[R_{\lambda\mu j}(\mathbf{q},\mathbf{p})+R_{\lambda\mu j+1}(\mathbf{q},\mathbf{p})]J_j(\mathbf{q})$$
$$\times[R_{\xi\eta j}(\mathbf{q},\mathbf{k})+R_{\xi\eta j+1}(\mathbf{q},\mathbf{k})], \quad \text{(A1)}$$

where

$$J_j(\mathbf{q})=J(\mathbf{q}) \quad \text{if} \quad j=1$$
$$=J(\mathbf{q}+\mathbf{Q}) \quad \text{if} \quad j=3,$$

and where $J(\mathbf{q})$ is the interatomic exchange as defined in Ref. 26.

An effect of adding this term is that now $W(1,1;2,2)$ is no longer zero in the zero bandwidth limit; hence an excitation in which an electron is taken from band 1 and placed in band 2 is coupled to one in which an electron is taken from band 2 and placed in band 1. This means that even if band 2 were completely empty in the Hartree-Fock ground state, in the real ground state it would be occupied part of the time. Therefore, this model now allows for ground-state spin fluctuations even in the large-U limit because the two sublattices are still coupled in this limit. Eq. (17) now becomes

$$[E_\lambda(\mathbf{p}+\mathbf{q})-E_\mu(\mathbf{p})-\omega]G_{\lambda\mu j'}(\mathbf{q},\mathbf{p})$$
$$=[2U+J(\mathbf{q})+J(\mathbf{q}+\mathbf{Q})](n_{\mathbf{p}\mu}-n_{\mathbf{p}+\mathbf{q}\lambda})\frac{1}{N}\sum_{\mathbf{k}}G_{\lambda\mu j'}(\mathbf{q},\mathbf{k})$$
$$+[J(\mathbf{q})-J(\mathbf{q}+\mathbf{Q})](n_{\mathbf{p}\mu}-n_{\mathbf{p}+\mathbf{q}\lambda})\frac{1}{N}\sum_{\mathbf{k}}G_{\mu\lambda j'}(\mathbf{q},\mathbf{k})$$
$$-(n_{\mathbf{p}\mu}-n_{\mathbf{p}+\mathbf{q}\lambda})[R_{\lambda\mu j'}+R_{\lambda\mu j'+1}] \quad \text{(A2)}$$

for $\lambda\neq\mu$. Again, the right-hand side is zero for $\lambda=\mu$. We take the limit as the paramagnetic effective mass goes to infinity and sum over $\mathbf{p}$ to obtain

$$(2g\mp\omega)G_{\lambda\mu j'}(\mathbf{q})$$
$$=\{U+\tfrac{1}{2}[J(\mathbf{q})+J(\mathbf{q}+\mathbf{Q})]\}mG_{\lambda\mu j'}(\mathbf{q})$$
$$+\{\tfrac{1}{2}[J(\mathbf{q})-J(\mathbf{q}+\mathbf{Q})]\}mG_{\mu\lambda j'}(\mathbf{q})$$
$$+m[R_{\lambda\mu j'}+R_{\lambda\mu\, j'+1}], \quad \text{(A3)}$$

where

$$G_{\lambda\mu j'}(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{p}}G_{\lambda\mu j'}(\mathbf{q},\mathbf{p}),$$

and m is the sublattice magnetization per lattice site. We take the upper signs in Eq. (A2) when $\lambda=2$ and $\mu=1$ and the lower signs when $\lambda=1$ and $\mu=2$. Using Eq. (6), the solution of the pair of equations expressed by Eq. (A3) is found to be

$$\chi^{-+}(\mathbf{q},\omega)$$
$$=m^2\left[\frac{J(\mathbf{Q})-J(\mathbf{Q}+\mathbf{q})}{\omega^2-m^2[J(\mathbf{q})-J(\mathbf{Q})][J(\mathbf{q}+\mathbf{Q})-J(\mathbf{Q})]}\right], \quad \text{(A4)}$$

if $\mathbf{q}$ is measured from a chemical reciprocal lattice point. If $\mathbf{q}$ is measured from a magnetic reciprocal lattice point, we make the substitution $\mathbf{q}\rightarrow\mathbf{q}\pm\mathbf{Q}$ in (A4), which changes the numerator to $J(\mathbf{Q})-J(\mathbf{q})$. Equation (A4) has a pole at

$$\omega=m\{[J(\mathbf{Q})-J(\mathbf{q})][J(\mathbf{Q})-J(\mathbf{Q}+\mathbf{q})]\}^{1/2}, \quad \text{(A5)}$$

which agrees with the Heisenberg-model results[20] as the anisotropy energy goes to zero.

The residues of (A4) at the spin-wave pole are

$$\mathrm{Res}\chi^{-+}(\mathbf{q},\omega)\,|_{\text{chemcial point}}$$
$$=\frac{m}{2}\left[\frac{J(\mathbf{Q})-J(\mathbf{q}+\mathbf{Q})}{J(\mathbf{Q})-J(\mathbf{q})}\right]^{1/2}, \quad \text{(A6a)}$$

$$\mathrm{Res}\chi^{-+}(\mathbf{q},\omega)\,|_{\text{magnetic point}}$$
$$=\frac{m}{2}\left[\frac{J(\mathbf{Q})-J(\mathbf{q})}{J(\mathbf{Q})-J(\mathbf{q}+\mathbf{Q})}\right]^{1/2}. \quad \text{(A6b)}$$

We find, using Eq. (13), that for small $\mathbf{q}$ in (A6) the total scattering cross section for the spin wave on chemical peaks becomes proportional, to

$$\tfrac{1}{2}m[kT/(J(\mathbf{Q})-J(0))],$$

which for $T\ll T_c$ is very small. On magnetic peaks, it becomes very large, being proportional to

$$\tfrac{1}{2}m[kT/(J(\mathbf{Q})-J(\mathbf{Q}+\mathbf{q}))],$$

i.e., to $1/q^2$, as it should be.[17] Thus we have made contact with the Heisenberg-model theory of antiferromagnetic spin waves.

[26] F. Englert and M. M. Antonoff, Physica 30, 429 (1964).