Local-band theory of itinerant ferromagnetism. II. Spin waves*

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The short-wavelength magnons which are observed by neutron scattering above as well as below the Curie temperature T_c are studied by the methods of the local-band theory, described in the preceding paper. We find a temperature shift of the spin-wave constant D, of a type previously proposed, but which we estimate to be numerically small. A novel downward shift mechanism gives a lowering $-2D|\vec{a}|^2_{av}$, where $|\vec{a}|^2_{av}$ is proportional to the magnetic energy. $|\vec{a}|^2_{av}$ saturates shortly above T_c at about $5 \times 10^{-2} \text{ Å}^{-2}$ in both iron and nickel. The form of this term is strictly correct only for $q^2 > |\vec{a}|^2_{av}$. However, it accounts for the greater part of the observed magnon energy shift, both in temperature dependence and shape of the dispersion curve. Finally, we find a new magnon-width mechanism Γ_q proportional to $|\vec{a}|^2_{av}q$ which seems capable of accounting for the observed width.

I. INTRODUCTION

In this paper we treat the short-wavelength magnons which are riding on the long-wavelength magnetization fluctuations which exist at and above the Curie point T_C .^{1,2} These are the famous spin waves observed by neutron scattering above T_C .^{3,4}

We find a broadening of the magnons and a downward shift in their energy. This downward shift is a new mechanism, never before proposed. The broadening mechanism we find, which is also new, apparently accounts for a substantial part of the broadening seen above T_c . It does not change significantly with temperature above T_c , in agreement with experiment. We propose that the energy shift coming from the nonlinearity accounts for most of the observed softening of high-q magnons. Again, this saturates shortly above T_c , as is observed. The remaining three- and four-magnon interaction terms seem to have a smaller effect.

In the first paper⁵ of this series, it was argued that the collective magnetization fluctuations were best treated as a classical variable, $\hat{M}(\vec{r})$. Quantization of this variable may in some cases follow, but only to determine the amplitude of the fluctuation. In fact, the collective motion fluctuates, either thermally or quantally, and the two types of fluctuation have similar effects, for the most part.

In I, we pointed out that although the magnetization fluctuations have a large effect on the original single-particle states at zero temperature, the great bulk of this effect is relatively trivial, namely, the spin-quantization direction is twisted into the direction $\hat{M}(\vec{r})$. The residual effect is proportional to $\nabla \hat{M}$, and even in this case, the major physical effect is proportional to that part of \hat{M} represented by $\vec{a}(\vec{r}) \equiv \frac{1}{2}(\sin\theta \, \vec{\nabla} \phi - i \vec{\nabla} \theta)$ where θ, ϕ are the polar directions of \hat{M} . [I: Eq. (II. 11)] The wave functions are modified in order \vec{a} and the energies in order \bar{a}^2 . A local spin rotation making the local spin z axis parallel to \hat{M} makes this result clear. Thus the smallness of \bar{a} is crucial, rather than the smallness of the deviation of \hat{M} from its mean direction.

It was noted in I that \mathbf{a} can be small for two reasons; the angle of tilt θ can be small, or the gradients can be small. In paper I we concentrated on the novel case, never before treated, of small gradients. In that case we could neglect the time dependence of $\hat{M}(\mathbf{r})$, for the most part, as well as making further approximations connected with the smallness of the gradient. The case of small tilt angle, if treated in band theory, is equivalent to the random-phase approximation (RPA), which is believed to be numerically reasonable where it applies.⁶

In this paper we treat the compounded case, in which there is a short-wavelength ripple (to be treated in RPA) superimposed on a long-wavelength large-amplitude thermal spin fluctuation, treated by the methods of I.

These shorter-wavelength excitations are observed by neutron scattering as spin waves, even above T_c .^{3,4} That they exist is obvious from our point of view. Any method which does not neglect the local spin ordering will, if correctly applied, gives such excitations, as is physically clear, but it is not always easy to produce this result in a given formalism. Indeed, the methods previously applied are not very transparent, and in particular, do not focus on the magnetization gradients or on local spin order, but rely on Green's-function truncations⁷ (in the Heisenberg model)^{8,9} or diagramatic approximations.¹⁰ In fact, only in Ref. 9 is any mention even made of "clusters of correlated spins."

Our method is straightforward, although the actual computations are tedious. We calculate the

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susceptibility in the RPA, and use as single-particle states those we found in I for the locally rotated frame. (One could also have calculated a susceptibility in the rotated frame and then transform it to the laboratory frame, if desired.) In this paper we concentrate on the predicted magnon dispersion relation and find it correct to order $Q^2 |\vec{a}|^2$ where Q is the magnon wave number. We also assume $Q \gg a$.

In fact it is, strictly speaking, numerically inconsistent to assume Q small enough to justify a small-Q expansion and at the same time to make it larger than \vec{a} , at least if we want the theory to apply at or above T_c . We could, in principle, find the dispersion numerically to order $|\vec{a}|^2$ for large Q in RPA. Our justification for the procedure we use is that we wish to obtain results which are simple enough that they can be understood and interpreted. There is no fundamental reason why the Q^2 term we find should not still be dominant for Q > a. We have indeed made further important approximations which include the use of the shortrange one-band (SROB) model, and even, upon occasion, parabolic bands. However, although the final numerical results are hardly to be accorded quantitative significance, we believe that they are qualitatively indicative of the kind of result that would be produced by a full-fledged RPA calculation, correct to order $|\vec{a}|^2$.

There are three terms in the result: a term $h'Q^2 |\vec{a}|_{av}^2$, a damping term, Γ_Q , proportional to $Q |\vec{a}|_{av}^2$, and a term $-2D |\vec{a}|_{av}^2$. Of these, only the first has been studied previously.¹¹

The first term is expected on the basis of Fermiliquid theory. It was dropped in the development of I, because there we kept the energy functional to order $|\vec{a}|^2$ only. The Fermi-liquid theory allows us to identify h' as $(\delta D/\delta |\vec{a}|^2)_{\vec{a}=0}^*$ where D is the spin-wave constant. The only previous estimate of this term was made by Izuyama.¹¹ We estimate, like him, that h' > 0, but think it is probably quite small. Strictly speaking, our estimates are not comparable, as we have assumed $Q \gg |\vec{a}|$, but for this term this restriction is probably not too significant.

The origin of the damping term is also clear. The Hamiltonian in the locally rotated frame, according to I: Eq. (II.4) has in it terms proportional to a which flip the spin of electrons. These same terms, which act like a spatially random spin-flipping potential will clearly allow magnons to decay into quasiparticles. It is in a crude sense equivalent to the finite-cluster-size effect of Liu.⁹ We, however, have a rather different picture than the "clusters" he proposes. The temperature dependence in our picture is interpreted differently also. In our model, the temperature dependence of the damping is that of $|\vec{a}|_{av}^2$, which is proportional to the magnetic energy. This quantity, therefore, on experimental grounds, increases rather rapidly somewhat below T_c and effectively saturates shortly above. This is very close to the observed behavior. A further discussion is to be found in I.

The origin of the final term, $-2D|\vec{a}|_{av}^2$, is less clear. It is of course no surprise that spin-dependent terms which, at least locally, break the isotropy of the original Hamiltonian \mathcal{K}_0 , should give rise to a shift of the spin wave energy, just as an external field does. Clearly, since $Q^2 > |\vec{a}|_{av}^2$, we are dealing with a local property and there is no question of a breakdown of overall spin rotational invariance.

Nevertheless, since this term has never been found before, and since it seems to be of substantial numerical importance, we have investigated it carefully. The most instructive analysis is that carried out on the Landau-Lifshitz equation in paper III (hereafter referred to as III)¹² of this series. There it is seen to be a new, although in a sense trivial, type of nonlinear spin-wave effect.

This term is, by our estimates, quite significant numerically, and has qualitative features which agree with observation. In addition to the saturation of the observed shift above T_C mentioned earlier, the shift is relatively constant in Q, for $Q > |\vec{a}|$, as we predict.

A major further problem is to extend this work to the case $Q \sim |\vec{a}|$, and then to $Q < |\vec{a}|$. Some progress has already been made in this direction in the framework of the nonlinear Landau-Lifshitz equation.¹²

Considerable information is already available in the limit $Q \ll a$. The results depend on the temperature region. Restricting our remarks to the case $T \ge T_c$, we know that at long enough wavelength, the spin motion is diffusive. The criterion for the boundary region between diffusion and propagation is $\Gamma_Q \sim \Omega_Q^0$ or alternatively $\Omega_Q \sim \Omega_Q^0 - 2D |\vec{a}|_{av}^2 \approx 0$. Both criteria give the same result, in order of magnitude, namely, $Q \sim (|\vec{a}|_{av}^2)^{1/2} \sim 0.2 \text{ Å}^{-1}$, for Fe and Ni. This is in agreement with experiment. However, since both Γ_Q and $-2D|\vec{a}|_{av}^2$ must necessarily be quite different for $Q < |\vec{a}|$, we can expect that the expressions we have found will be modified appreciably as Q approaches this region from above.¹³ Some of the difficulties in doing a calculation in the region $Q \sim |\vec{a}|$ were discussed in I.

In Sec. II we write down the equation for the susceptibility, using the rotated-frame wave functions of I. In Sec. III, we expand these equations to order $|\vec{a}|_{av}^2$, and to order Q^2 , with $Q^2 \gg |\vec{a}|_{av}^2$. The results are solved, after a number of further approximations, for the dispersion and damping. A numerical study of these results follows in Sec. IV. We conclude in Sec. V with several remarks about the calculation. Some of the more tedious calculations are presented in the Appendix.

II. RPA EQUATION FOR SUSCEPTIBILITY

The susceptibility $\chi^{ij}(x, x')$ is the response of the magnetization density $\langle M^i(x) \rangle$ to a perturbing magnetic field. It may be written in terms of the single-particle Green's function as $(x \equiv \mathbf{r}, t)$

$$\chi^{ij}(x, x') = \operatorname{Tr}\sigma^{i}\delta G(x, x) / \delta H_{j}(x') . \tag{1}$$

Here σ^i is the Pauli matrix and G is the matrix Green's function, I: Eq. (II.18). Now because of the thermal magnetization excitation, the Green's function G is not diagonal, and the equation for χ will couple it to the excitations in charge density. These however are suppressed, as discussed in I. We accordingly project out these charge fluctuations, and then write χ in terms of a vertex function Γ . Using a summation convention, we write

$$\chi^{ij}(x, x') = -i \int K^{i\,i}(x, \overline{x}) \Gamma^{I\,j}(\overline{x}, x') \, d^4 \overline{x}, \qquad (2)$$

where Γ satisfies (in the SROB model)

$$\Gamma^{ij}(x, x') = -\frac{1}{2} \delta^{ij} \delta(x - x') + \frac{1}{2} \int U K^{i}(x, \overline{x}) \Gamma^{ij}(\overline{x}, x') d^{4} \overline{x}, \qquad (3)$$

and the kernel K is

$$K^{ij}(x, x') \equiv i \operatorname{Tr} \sigma^{i} G(x, x') \sigma^{j} G(x', x) .$$
(4)

(It should be noted that ignoring the projection above gives only a small change in the coefficients of our final results. It corresponds to allowing sums over σ matrices to include σ^0 , the unit matrix.)

The kernel contains all the information about the dynamics and statistical state of the system. For a state with a definite magnetization configuration, we write G in terms of rotated-frame states as

$$G(x, x') = R(x)\tilde{G}(x, x')R^{-1}(x'), \qquad (5)$$

where R(x) is defined in [I: Eq. (II.2)]. The retarded function in the rotated frame is

$$\tilde{G}(x, x') = \int \frac{d\omega}{2\pi} \frac{\psi_{\mu}(\tilde{\mathbf{r}}'t)\psi_{\mu}^{*}(\tilde{\mathbf{r}}'t')}{\omega - E_{\mu} + i\eta} e^{-i\omega(t-t')}.$$
(6)

Here ψ_{μ} is the single-particle state in the locally rotated frame, E_{μ} its energy given by [I: Eq. (III.6)] and μ is the pair $\mathbf{k}\alpha$. The implied summation over μ means $\int (dk) \sum_{\alpha} \tilde{G}$ is written out in I: Eq. (IV.9).

We take, as discussed in I, the quasiparticle occupations, f_{μ} , to be those appropriate to E_{μ} at

the given temperature. Putting Eqs. (5) and (6) into Eq. (4), doing the sums over imaginary frequency and continuing to the real axis, we find the kernel

$$K^{ij}(x, x') = -\int \frac{d\Omega}{2\pi} e^{-i\Omega(t-t')} \frac{f_{\nu} - f_{\mu}}{\Omega - E_{\mu} + E_{\nu} + i\eta} \times \hat{\sigma}^{i}_{\nu\mu}(x) \hat{\sigma}^{j}_{\mu\nu}(x'), \qquad (7)$$

where

$$\hat{\sigma}^{i}_{\mu\nu}(x) = \left[\psi^{*}_{\mu}(x)R^{-1}(x)\sigma^{i}R(x)\psi_{\nu}(x)\right].$$

It is convenient now to define

$$A_{\mu\nu}(\Omega) = \int d^{4}\overline{x} \ \frac{e^{i\Omega \,\overline{t}} \hat{\sigma}_{\mu\nu}^{i}(\overline{x}) \Gamma^{ij}(\overline{x}, x')}{\Omega - E_{\mu} + E_{\nu} + i\eta}$$

where we have suppressed the dependence on j and x'. In terms of A, the equation of motion (3) reads

$$(\Omega - E_{\mu} + E_{\nu})A_{\mu\nu}(\Omega)$$

= $-\frac{1}{2}e^{i\Omega t'}\hat{\sigma}^{j}_{\mu\nu}(x')$
 $-U\int \frac{d\overline{\Omega}}{(2\pi)}\Lambda_{\mu\nu,\overline{\mu}}\overline{\nu}(\Omega - \overline{\Omega})(f_{\overline{\nu}} - f_{\overline{\mu}})A_{\overline{\mu}}\overline{\nu}(\overline{\Omega}),$ (8)

with

$$\Lambda_{\mu\nu,\overline{\mu}}\overline{\nu}(\Omega) \equiv \frac{1}{2} \int d^4x \, e^{i\Omega t} \hat{\sigma}^i_{\mu\nu}(x) \hat{\sigma}^{i}_{\overline{\mu}}\overline{\nu}(x) \,. \tag{9}$$

The susceptibility is then

$$\chi^{ij}(x, x') = i (2\pi)^{-1} \int d\Omega \, e^{-i\Omega t} (f_{\nu} - f_{\mu})$$
$$\times A_{\mu\nu}(\Omega) \hat{\sigma}^{i}_{\nu\mu}(x) \,. \tag{10}$$

Using the properties of σ matrices, we rewrite the time Fourier transform of Eq. (9) as

$$\Lambda_{\mu\nu\,\overline{\mu}\,\overline{\nu}\,}(t) = \int d^{3}\boldsymbol{r} \left[(\psi_{\mu}^{*}\psi_{\overline{\mu}})(\psi_{\overline{\nu}}^{*}\psi_{\nu}) - \frac{1}{2}(\psi_{\mu}^{*}\psi_{\nu})(\psi_{\overline{\nu}}^{*}\psi_{\overline{\mu}}) \right],$$
(11)

and note that $\Lambda(t)$ is Hermitian, $\Lambda_{\mu\nu,\overline{\mu}\ \overline{\nu}} = \Lambda_{\overline{\mu}\ \overline{\nu},\mu\nu}^*$. Finally, we return to the original momentum and spin labels $k\alpha$ and write

$$\begin{split} \left[\Omega - E_{\alpha}(k) + E_{\beta}(k')\right] A_{\alpha\beta}(kk', \Omega) \\ &= I - U\Lambda_{\alpha\beta,\overline{\alpha}} \overline{\beta}(kk', \overline{k} \overline{k}', \Omega - \overline{\Omega}) \\ &\times \left[f_{\overline{\beta}}(\overline{k}') - f_{\overline{\alpha}}(\overline{k})\right] A_{\overline{\alpha}} \overline{\beta}(\overline{k}, \overline{k}', \overline{\Omega}), \quad (12) \end{split}$$

where integrations over $\overline{k}, \overline{k'}$, and $\overline{\Omega}$ are understood and where we have written I for the inhomogenous term. This last will be dropped in this paper since we shall only be looking for the excitation energy, which is given by the solution of the homogeneous equation. A further discussion of it will be given in III.

In what follows we will define $Q \equiv k - k'$, $\overline{Q} = \overline{k} - \overline{k'}$, and $A(kk'\Omega) = A(k, Q, \Omega)$. We shall also use $k^{\pm} \equiv k$ $\pm \frac{1}{2}Q$, where the Q involved will be clear from context.

III. MAGNON DISPERSION

In this section we obtain the magnon dispersion correct to order $Q^2 |\vec{a}|^2$. The susceptibility equation (12) differs from its zero-temperature, ordinary RPA counterpart in three ways: the eigenenergies $E_{k\alpha}$ depend on \vec{a} , the occupations $f_{k\alpha}$ may therefore differ, and the kernel Λ will be modified. The latter effect happens because the electron spins in the local frame are tilted somewhat away from the local direction of magnetization.

In the magnetic ground state, the single-particle states are

$$\phi_{k+}^{0}(\mathbf{\ddot{r}}) = e^{i\,\mathbf{\vec{k}}\cdot\mathbf{r}} \begin{pmatrix} 1\\ 0 \end{pmatrix}, \quad \phi_{k-}^{0}(\mathbf{\ddot{r}}) = e^{i\,\mathbf{\vec{k}}\cdot\mathbf{r}} \begin{pmatrix} 0\\ 1 \end{pmatrix},$$

so that

$$\Lambda^{0}_{\alpha\beta,\overline{\alpha}}_{\beta,\overline{\alpha}} \overline{\beta}(kk', \overline{k}\,\overline{k}', t)$$

$$= (\delta_{\alpha\overline{\alpha}}\delta_{\beta\overline{\beta}} - \frac{1}{2}\delta_{\alpha\beta}\delta_{\overline{\alpha}}\overline{\beta})(2\pi)^{3}\delta(\overline{\mathbf{Q}} - \overline{\mathbf{Q}}').$$
(13)

Calling A^{0} the solution of Eq. (12) with Λ^{0} , the magnon creation part of A^{0} satisfies

$$[\Omega - E_{-}(k^{+}) + E_{+}(k^{-})]A^{0}_{-+}(kQ\Omega)$$

= + U $\int [f_{-}(\overline{k}^{+}) - f_{+}(\overline{k}^{-})]A^{0}_{-+}(\overline{k}Q\Omega)(d\overline{k})$ (14)

with similar equations for the z and + components. Now Eq. (14) is a familiar equation for the spinwave energy and wave function in the RPA. The interpretation here is that it predicts an eigenexcitation which is a tipping of the magnetization vector from its local mean direction. The value for Ω_Q found from it differs from the RPA result D_0Q^2 only through the perturbed energies E(k) and the resultant perturbed occupations f(E(k)). We shall proceed by first solving Eq. (14) to order Q^2 and $|\mathbf{\dot{a}}|^2$. The change in kernel $\delta \Lambda = \Lambda - \Lambda^0$ modifies the character of the state by mixing in some excitation of the σ_z type, in the local frame. We shall treat it as the perturbing potential in a Schrödinger equation, and find the resulting shift in the energy Ω in second-order perturbation theory. The shift will include an imaginary part, which will give the magnon decay rate, coming from the continuum of σ_z -type states with which the excitation is degenerate. The energies to be used in Eq. (14) are given by [I: Eq. (III.6)]

$$E_{\pm}(\vec{\mathbf{k}}) = \epsilon(\vec{\mathbf{k}}) \mp \frac{1}{2} \Delta \mp \frac{1}{2} \delta(\vec{\mathbf{k}}) + |\vec{\mathbf{a}}|_{av}^2 / 2m, \qquad (15a)$$

$$\Delta = U(N_+ - N_-) = \Delta_0 + \Delta', \qquad (15b)$$

and

$$\delta(\vec{\mathbf{k}}) = 2(|\vec{\mathbf{a}} \cdot \vec{\mathbf{v}}|_{\mathbf{av}}^2 - \langle |\vec{\mathbf{a}} \cdot \vec{\mathbf{v}}|_{\mathbf{av}}^2 \rangle) / \Delta.$$
(15c)

Here Δ' is the shift in Δ due to repopulation, proportional to $\|\vec{a}\|_{\omega}^2$. Using these, Eq. (14) is

$$1 = U \int (dk) \left[f_+(k_-) - f_-(k_+) \right] / \left[\Delta - \Omega + \vec{\mathbf{Q}} \cdot \vec{\mathbf{v}} + \delta + \frac{1}{8} (\vec{\mathbf{Q}} \cdot \vec{\nabla}_k)^2 \delta \right].$$
(16)

Expanding the denominator to include all terms of order Q^2 and $Q^2 |\bar{\mathbf{a}}|_{sv}^2$, expanding f_{\pm} in powers of Q and occasionally integrating by parts we find $\Omega = \Omega_0 + \Omega_1 + \Omega_2$, with

$$\Omega_0 = D_0 Q^2 = \rho U Q^2 / 2 m \Delta - \langle (\vec{\mathbf{Q}} \cdot \vec{\mathbf{v}})^2 \rangle / \Delta , \qquad (17a)$$

$$\Omega_{1} = \langle (\vec{\mathbf{Q}} \cdot \vec{\nabla}_{k})^{2} | \vec{\mathbf{a}} \cdot \vec{\nabla} |_{\mathbf{a}v}^{2} \rangle / 2\Delta + 4D_{0}Q^{2} \langle | \vec{\mathbf{a}} \cdot \vec{\nabla} |_{\mathbf{a}v}^{2} \rangle / \Delta^{2} - 2 \langle | \vec{\mathbf{a}} \cdot \vec{\nabla} |_{\mathbf{a}v}^{2} \rangle \langle (\vec{\mathbf{Q}} \cdot \vec{\nabla}_{k})^{2} \rangle / \Delta^{3} + [6\langle I \rangle - 2(I_{+} + I_{-})] / \Delta^{3}, \quad (17b)$$

$$\Omega_2 = (U/\Delta) \int (dk) \left\{ Q^2 (\delta f_+ + \delta f_-)/2m - (\vec{\mathbf{Q}} \cdot \vec{\mathbf{v}})^2 (\delta f_+ - \delta f_-)/\Delta - [D_0 Q^2 - \langle \vec{\mathbf{Q}} \cdot \vec{\mathbf{v}})^2 \rangle /\Delta \right] (\Delta'/\Delta).$$
(17c)

In Eq. (17a) m^{-1} is the average inverse mass over occupied states of both spins. We have identified D_0 , the RPA ground-state magnon stiffness constant, and defined the expressions

$$\langle I \rangle \equiv \langle \vec{\mathbf{Q}} \cdot \vec{\mathbf{v}} \, \rangle^2 \, \left| \vec{\mathbf{a}} \cdot \vec{\mathbf{v}} \, \right|_{av}^2 \rangle, \qquad (18a)$$

$$I_{\alpha} \equiv -U \int (dk) \frac{\partial f_{\alpha}}{\partial \epsilon} \left(\vec{\mathbf{Q}} \cdot \vec{\mathbf{v}} \right)^2 |\vec{\mathbf{a}} \cdot \vec{\mathbf{v}} \rangle|_{av}^2 , \qquad (18b)$$

using the notation $\langle \rangle$ of I: [Eq. (III.5)] for the aver-

age over singly occupied states. In Eq. (17c) there are no terms involving $|\vec{a}|_{a}^{2}$ explicitly, since Δ' and δf are already of this order. Now

$$\delta f_{\alpha} = \frac{\partial f_{\alpha}}{\partial \epsilon} \left[\left| \vec{\mathbf{a}} \right|_{\mathbf{A}}^2 / 2m - \delta \mu \mp \frac{1}{2} \left(\Delta' + \delta \right) \right], \tag{19}$$

where $\delta\mu$ and Δ' are found by self-consistently solving Eqs. (19) and (15b) while conserving the total particle number. Using Eq. (19), simplifying Ω_1 by replacing $\nabla_k v$ by a constant 1/m, and dropping the first term in Ω_2 we find for Eq. (17)

$$\Omega_{1} + \Omega_{2} = |\vec{\mathbf{Q}} \cdot \vec{\mathbf{a}}|_{av}^{2} / m^{2} \Delta + 6D_{0}Q^{2} \langle |\vec{\mathbf{a}} \cdot \vec{\nabla}|_{av}^{2} \rangle$$
$$+ 3(2\langle I \rangle - I_{+} - I_{-}) / \Delta^{3}$$
$$- (\delta \mu)Q^{2} / m \Delta - 2\Delta' D_{0}Q^{2} / \Delta.$$
(20)

The simplifications introduced here are tantamount to the parabolic band approximation. Here and below they are introduced to allow economy of expression of results. To treat the effect of $\delta \Lambda$, we concentrate on the solution of Eq. (14) characterized by a definite value of Q, and the eigenvalue $\Omega = \Omega_0 + \Omega_1 + \Omega_2$. Then $A_{1,-}^0 = A_{1,+}^0 = A_{2,-}^0 = 0$ and

$$A^{0}_{-+}(k,Q') \propto \delta(Q-Q') [\Omega - E_{-}(k^{+}) + E_{+}(k^{-})]^{-1}.$$
 (21)

Now we will find that $\Lambda_{-+,++} = \delta \Lambda_{-+,++}$ is of order \overline{a} while $\delta \Lambda_{-+,-+}$ is of order $|\overline{a}|^2$. From the homogeneous part of Eq. (12), the first-order change of the wave function is

$$A_{\pm\pm}^{1}(\overline{k},\overline{Q},\overline{\Omega}) = U\Lambda_{\pm\pm,-+}(\overline{k},\overline{Q},k'Q';\overline{\Omega}-\Omega')[f_{-}(k'^{+})-f_{+}(k'^{-})]A_{-+}(k',Q',\Omega')/[\overline{\Omega}-E_{\pm}(\overline{k}^{-})+E_{\pm}(\overline{k}^{+})],$$
(22)

where integration over k', Q', Ω' is understood. The term in $\Lambda_{\pm\pm,\pm\pm}A_{\pm\pm}$ has no effect and has been dropped. Putting Eq. (22) back into the homogeneous part of Eq. (12) we find

$$\left[\Omega - E_{-}(k^{+}) + E_{+}(k^{-})\right]A_{-+}(kQ\Omega) + U\left[f_{+}(\overline{k}^{-}) - f_{-}(\overline{k}^{+})\right]A_{-+}(\overline{k}Q\Omega)$$

$$= -U\delta\Lambda_{\rm eff} \left(kQ, \overline{k}\,\overline{Q}, \Omega - \overline{\Omega}\right) \left[f_+(\overline{k}^-) - f_-(\overline{k}^+)\right] A_{-+}(\overline{k}\,\overline{Q}\,\overline{\Omega})\,, \quad (23)$$

where

$$\delta\Lambda_{\rm eff}(kQ, \overline{k} \overline{Q}, \Omega - \overline{\Omega}) = \delta\Lambda_{-+,-+}(kQ, \overline{k} \overline{Q}, \Omega - \overline{\Omega}) - U \left\{ \Lambda_{-+,++}(kQ, k'Q', \Omega - \Omega') [f_+(k'^-) - f_+(k'^+)] \right. \\ \left. \times \Lambda_{++,-+}(k'Q', \overline{k} \overline{Q}, \Omega' - \overline{\Omega}) [\Omega' - E_+(k'^+) + E_+(k'^-)]^{-1} \right. \\ \left. + \operatorname{term with}(++) - (--) \right\}$$
(24)

again with integrations over k', Q', and Ω' understood. This yields an energy shift to order $|\vec{a}|^2$

$$\Omega_{3}(Q) = -\frac{U\int (dk) (dk') A_{-+}^{0}(kQ) [f_{+}(k^{-}) - f_{-}(k^{+})] \delta_{\Lambda_{\text{eff}}}(kQ, \bar{k}\bar{Q}, 0) [f_{+}(\bar{k}^{-}) - f_{-}(\bar{k}^{+})] A_{-+}^{0}(\bar{k}Q)}{\int (dk) A_{-+}^{0}(kQ) [f_{+}(k^{-}) - f_{-}(k^{+})] A_{-+}^{0}(kQ)}.$$
(25)

This is just the expectation value of the perturbing potential in the unperturbed state. The denominator normalizes the unperturbed wave function, and shows the form of the scalar product needed to make the original Schrödinger equation Hermitian. Similar arguments have been used by Korenman and Prange.¹⁴ The remainder of the calculation is relatively straightforward, though tedious. We therefore give at once the resultant contribution to the dispersion, Ω_3 , and relegate the actual calculation to the Appendix. This Ω_3 is to be added to $\Omega_1 + \Omega_2$ of Eq. (20) to obtain the total excitation energy correct to order $Q^2 |\tilde{a}|^2$. We find

$$\Omega_{3} = -2D |\vec{a}|_{av}^{2} + 2D |\vec{a}|_{av}^{2} \langle (\vec{Q} \cdot \vec{v})^{2} \rangle / \Delta^{2} + 2DQ^{2} \langle |\vec{a} \cdot \vec{v}|_{av}^{2} \rangle / \Delta^{2} + 2[\overline{I} - \frac{1}{2}(I_{+} + I_{-})] / \Delta^{3} + D^{2}Q^{2} |\vec{a}|_{av}^{2} U(\mathfrak{N}_{+} + \mathfrak{N}_{-}) / \Delta + |\vec{Q} \cdot \vec{a}|_{av}^{2} [1 - 2m^{2}D^{2} - U(\mathfrak{N}_{+} + \mathfrak{N}_{-})(\frac{1}{4} + D^{2}m^{2})] / \Delta m^{2} - i\pi DU(\mathfrak{N}_{+} v_{+} + \mathfrak{N}_{-} v_{-})(Q^{2} |\vec{a}|_{av}^{2} - |\vec{Q} \cdot \vec{a}|_{av}^{2}) / 4Q\Delta.$$
(26)

Although these expressions are still far from transparent, the general form of the excitation energy is clear. The terms in $Q^2 |\bar{a}|_{av}^2$ represent a change in stiffness constant D due to thermal magnetization fluctuations. In the presence of these fluctuations the excitation, dominantly of spin-flip type in the locally rotated frame, mixes with the continuum of particle-hole states with the same spin. The imaginary part of Eq. (26) is the resultant damping. Finally, there is the term $-2Da^2$, which is a Q-independent softening of the magnetic excitation. This term is surprising, as it seems to violate rotation invariance. However, this anomalous term is not an error. It appears already in the classical Landau-Lifshitz equation when nonlinear effects are included to lowest order. There is no violation of rotational invariance since the limit $Q \rightarrow 0$ cannot be taken, because Q has to be large compared to |a| for our analysis to be correct. We believe the softening found in Eq. (26) to be a real effect, and will return to discuss it below.

IV. NUMERICAL ESTIMATES

To allow crude numerical estimates, we express our perturbed energy directly in terms of the parameters of a parabolic band model. It is simplest to take the "strong" limit, appropriate for nickel, where the minority spin subband lies entirely above the Fermi energy and is empty.

In terms of the "majority" (i.e., minority hole) spin Fermi momentum p, some of the quantities we have defined are:

$$\begin{aligned} \Delta &= Up^{3}/6\pi^{2}, \quad \Delta' = 0, \\ D_{0} &= (1 - 2p^{2}/5m\Delta)/2m, \\ \delta\mu &= -2 \left|\vec{a}\right|_{av}^{2} p^{2}/15m^{2}\Delta, \\ \left[\langle I \rangle - \frac{1}{2} (I_{+} + I_{-})\right] &= -\Delta (\frac{1}{2}p^{2} - \frac{1}{7}p^{4}/m\Delta) \\ &\times \left[\left|\vec{a}\right|_{av}^{2} Q^{2} + 2\left|(\vec{a} \cdot \vec{Q})\right|_{av}^{2}\right]/5m^{3}, \end{aligned}$$
(27)

giving

$$\Omega_{1} + \Omega_{2} = (1 - 6p^{2}/5m\Delta + 12p^{4}/35m^{2}\Delta^{2})$$

$$\times |(\vec{Q} \cdot \vec{a})|_{av}^{2}/m^{2}\Delta$$

$$+ (2p^{2}/15m\Delta - 12p^{4}/175m^{2}\Delta^{2})$$

$$\times Q^{2} |\vec{a}|_{av}^{2}/m^{2}\Delta. \qquad (28)$$

Here it is convenient to define a parameter

$$y \equiv p^2 / 2m\Delta, \tag{29}$$

where $y \le 1$ defines the strong limit. In terms of y we write

$$\begin{split} \Omega_{1} + \Omega_{2} + \Omega_{3} + 2D \left| \vec{a} \right|_{av}^{2} \\ &= \left(-\frac{3}{2} + \frac{21}{5}y - \frac{132}{25}y^{2} + \frac{528}{175}y^{3} \right) \left| \vec{Q} \cdot \vec{a} \right|_{av}^{2} / m p^{2} \\ &+ \left(\frac{3}{4} - \frac{6}{5}y + \frac{136}{75}y^{2} - \frac{48}{35}y^{3} \right) Q^{2} \left| \vec{a} \right|_{av}^{2} / m p^{2} \\ &- \left(\frac{3}{4} i \pi \right) D_{0} Q^{2} \left[1 - \left| \left(\vec{Q} \cdot \vec{a} \right) \right|_{av}^{2} / Q^{2} \left| \vec{a} \right|_{av}^{2} \right] \left| \vec{a} \right|_{av}^{2} / p Q. \end{split}$$

$$\end{split}$$

$$(30)$$

Although the parabolic band model is an extremely crude representation of a real transition metal, lacking a better calculation we use it for estimates of the temperature dependence of magnon properties.

The model we use for nickel puts 0.56 spin-down holes per atom into six spherical pockets, at X, giving $p \approx 0.8$ Å⁻¹. (Band calculations¹⁵ give six pockets although only three have been observed.) Using $m^* \sim 5.5 m_e$,¹⁶ and $\Delta \sim 0.8$ eV,¹⁵ makes y = 0.55, $v_F = 1.6 \times 10^7$ cm/sec.

To extract a temperature dependence from Eq. (30) we must perform a thermodynamic average over configurations of \vec{a} . In any such average $|\vec{Q} \cdot \vec{a}|_{av}^2$ will be replaced by $\frac{1}{3}Q^2|\vec{a}|_{av}^2$. Combining terms yields

$$\Omega_{1} + \Omega_{2} + \Omega_{3} + 2D \left| \vec{a} \right|_{av}^{2}$$
$$= \left(\frac{1}{4} + \frac{1}{5}y + \frac{4}{75}y^{2} - \frac{64}{175}y^{3} \right) Q^{2} \left| \vec{a} \right|_{av}^{2} / m p^{2} - i\Gamma_{Q} \quad (31)$$

with

$$\Gamma_{Q} = \pi \Omega_{0} |\vec{\mathbf{a}}|_{\mathrm{av}}^{2} / 2pQ. \qquad (32)$$

The term in parentheses, $\equiv B$, is easily shown to be positive for $y \leq 1$. It ranges from 0.14 for y = 1to a broad maximum of 0.32 at y = 0.48, and falls to 0.25 at y = 0.

As discussed in I, for low temperatures $|\vec{a}|_{*}^{2}$ can be approximated as $\sum q^2 N_q / 2M$. This gives rise to a positive $T^{5/2}$ term in the effective stiffness constant *D*. Using the values $D_0 \approx 0.56$ eV Å², $2M_0 \approx 0.05$ spins/Å³, we find

$$\vec{a}|_{av}^2 \approx 4.5 \times 10^{-10} T^{5/2} \text{ Å}^{-2}$$
. (33)

Letting $m \approx 5 m_e$, we find the relative energy shift

$$\delta D/D = B \|\vec{\mathbf{a}}\|_{av}^2 / m \, p^2 D \approx 3 \times 10^{-10} T^{5/2} \tag{34}$$

(T in degrees K). At $T = T_c = 627$ K, $\delta D/D \approx 0.003$, a very small effect.

Now this expression for $|\vec{a}|_{w}^{2}$ is clearly not good near T_{C} , since the spin-wave approximation does not reproduce the critical energetics. We use the approximation discussed in I, expressing $|\vec{a}|_{w}^{2}$ in terms of the total magnetic energy above T_{C} , $|\vec{a}|_{w}^{2} \approx 5 \times 10^{-2} \text{ Å}^{-2}$. This is a factor of 10 larger than the estimate of Eq. (33). We conclude that these terms give a change of D, which is probably small and positive, but hard to predict in detail.

The only previous determination of this quantity of which we are aware, that of Izuyama,¹¹ is also positive, though somewhat different than ours. [Corresponding to Eq. (31), he has the square bracket as $\frac{16}{15}y^2 - \frac{64}{175}y^3$, which is 0.7 at y=1 and 0.22 at y=0.5]. The only available experimental data also suggest a positive sign for this term, but they are not very reliable.

For the magnon damping, we have $\Gamma_Q/\Omega_0 \approx \pi (6 \times 10^{-2} \text{ Å}^{-1})/2Q$ which is unity for $Q \sim 0.1 \text{ Å}^{-1}$ for $T > T_C$. This is about half the observed value of the magnon width. However, there are sources of damping we have not considered, as well as inhomogeneous broadening¹² which also depends on $\langle |\vec{a}|_{av}^2 \rangle$. In addition, we will argue that the observed magnon energy is smaller than DQ^2 . Both these effects suggest that the damping mechanism we have found is a major damping effect, and explains the value of the lower magnon cutoff and its insensitivity to temperature above T_C , as well as the general temperature dependence of the magnon damping for all wave vectors above this lower cutoff.

The term $-2D|\vec{a}|_{av}^2$ is discussed in detail in the accompanying paper,¹² which is an analysis of the nonlinear Landau-Lifshitz equation. We here discuss the numerical importance of this term.

The form $-2D|\vec{a}|^2_{av}$ represents a limit when $Q \gg |\vec{a}|$. It is expected to become smaller for Q near $|\vec{a}|$. Using the preceding estimate for $|\vec{a}|^2_{av}$ of 5×10^{-2} Å⁻² and using D = 0.5 eV Å² gives a lowering of 50 meV in nickel. As this is in accord

with observation,³ it suggests that the apparent lowering of the short-wavelength magnon energies with temperature as observed by neutron scattering is largely due to this effect, and that the value of the short-wavelength D is relatively constant with temperature as we found above.

The data for iron and Fe(Si) appear to confirm this result quite well.⁴ Taking $|\mathbf{\vec{a}}|_{\mathbf{k}}^2$ to have the same value,⁴ and estimating the zero-temperature $D_{\mathbf{F} \bullet (\mathbf{S} \mathbf{i})}$ to be about 270 meV Å² we predict the shift to be about 27 meV. The room-temperature shift is estimated to be 6 meV, leaving a shift between room temperature and high temperature of 21 meV. This can be compared with the data of Fig. 1. The good agreement implies that the temperature dependence of D is weak. Since iron is a weak ferromagnet for which a parabolic band approximation is not even remotely appropriate, we can not easily calculate how big the possibly positive term in $Q^2 |\mathbf{\vec{a}}|_{av}^2$ is. There will also be a T^2 term from single-particle excitations, which in principle can be estimated from the Fermi-liquid consideration of I. However, the above analysis would suggest that these shifts in D are small.

We stress that D is a quantity appearing in our formulas, nearly equal to the low-temperature spin-wave constant for short-wavelength magnons. It is not equal to the finite-temperature, long-wave-



FIG. 1. Spin-wave dispersion in Fe(Si). From Ref. 4.

length-limit spin-wave constant, which is proportional to the total, not local, magnetization, nor is it the coefficient of a parabolic fit to the observed high-temperature short-wavelength spectrum, a number which is sometimes quoted.

V. DISCUSSION

We have, up to now, glossed over several interesting points. These points are most clearly illustrated in our study of the Landau-Lifshitz equation in III.

We recall that in the method developed in I, the Hamiltonian was simplified by going to the locally rotated frame. In this frame, in addition to the correction terms proportional to \bar{a} , there are terms in the form of a vector and scalar potential, i.e., $\nabla + \nabla + i\sigma_z \bar{g}$, $\partial/\partial t + \partial/\partial t + i\sigma_z \tilde{g}$. Here $2\bar{g} = \nabla b$ $+\cos\theta \ \nabla \phi$ and $2\bar{g} = b + \cos\theta \phi$. The arbitrariness of the third Euler angle, b, is the expression of gauge invariance for these fields.

In the rotated frame, the only physical effects are those proportional to the fields. The magnetic "field" is

$$\tilde{h} = -\sigma_z \nabla \times \tilde{\mathbf{g}} = \frac{1}{2} \nabla \theta \times \sin \theta \nabla \phi \sigma_z = \frac{1}{2i} \tilde{\mathbf{a}}^* \times \tilde{\mathbf{a}} \sigma_z.$$

The electric field is $\tilde{e} = \frac{1}{2}\sin\theta(\nabla\phi\dot{\theta} - \dot{\phi}\nabla\theta)\sigma_z$; it can also be written in terms of \tilde{a} if use is made of the Landau-Lifshitz equation to express the time derivatives of the angles. The result is $\tilde{e} = -\vec{\nabla} \cdot \vec{\phi}\sigma_z$ with the dyadic $\vec{\phi}$ given by $\vec{\phi} = \vec{a}\vec{a}^* + \vec{a}^*\vec{a} - \vec{1}\vec{a}\cdot\vec{a}^*$.

Clearly, both \tilde{e} and \tilde{h} are of order $|\tilde{a}|^2$. Being vectors with random directions, they cannot come into the quasiparticle energies in first-order (if they do not split a degeneracy). There will be some scattering effects, corresponding to absorption and remission of magnons without spin flip. However, as the \tilde{e} and \tilde{h} fields are slowly varying this scattering will be nearly forward.

The effect of all this on the susceptibility can be taken into account by quasiclassical methods made familiar to condensed-matter physicists by Gor'kov in his derivation of the Ginzburg-Landau theory of superconductivity.¹⁷ The same kind of development can and has been followed through in the calculation of χ . We have, in order to simplify an already cumbersome calculation, totally ignored these effects in writing out the preceding calculation, however.

The results of including the potentials is most easily stated in terms of the equation of motion for χ in the locally rotated frame.¹² One simply replaces $\partial/\partial t$ by $\partial/\partial t + 2i\tilde{g}$ and ∇ by $\nabla + 2i\tilde{g}$. The doubling of the field is familiar from the superconductivity case, were the pair susceptibility depends on the propagation of a pair with charge 2*e*. Here, the propagation is of a particle and hole, but as they are of opposite spin and the fields change sign with spin, the fields again add constructively.

At this stage, it may be argued that if the electric and magnetic fields are small enough to be negligible in the single-electron problem, twice these fields will still be negligible in the susceptibility. Remarkably, this is not always true, and even more remarkable, it is not true that the potentials can be neglected even in the case that the fields vanish identically.

As this point is illustrated in III, we do no more than state the result here. Although in most cases the spectrum of the susceptibility in the rotated frame is negligibly affected by the existence of the potentials, just because the fields are small, the susceptibility $\chi(rt, r't')$ in the lab frame acquires additional phase factors, linearly dependent on the potentials. These phase factors are written down in III. They are of course gauge invariant. Since the phase factors are space and time dependent, they affect the relationship between energy and wave number in the lab and the locally rotated frame. (Actually, even in I we have seen an example of this.)

The shift $-2D|\vec{a}|_{av}^2$ is in the locally rotated frame. At least for the case near and above T_c , we show in III that the transcription back to the lab frame preserves this shift. It introduces a Doppler or inhomogeneous broadening of the same order of magnitude as the shift, which along with the direct decay term Γ_{φ} would seem to account for most of the observed short-wavelength magnon broadening.

We do not yet know the effects of the transcription from locally rotated frame to lab frame at intermediate temperatures. There is some indication that this transcription will introduce shifts in addition to inhomogeneous broadening. In fact the shift, $-2D|a|_{av}^2$, is somewhat smaller than that observed at temperatures of the order of $\frac{1}{2}T_c$.

The numerical results of this paper are therefore restricted in their validity to the temperature region near and above T_c . Accordingly, following the discussion of I, we have used the single-particle energies $E_{k\alpha}$ to determine the quasiparticle populations. However, the repopulation effect is small in any case and it is not numerically significant to distinguish between the energies $E_{k\alpha}$ and $\hat{E}_{k\alpha}$ defined in I.

A final point is that the susceptibility, at very long wavelength, involves zero-order frequencies $\omega < D |\vec{a}|^2$. In this regime, the magnetic field $2\hbar$ is not a small perturbation. This long-wavelength case can be studied by renormalization-group techniques, but the transition region $\omega \sim D |\vec{a}|^2$ remains a difficult case to study.

VI. CONCLUSION

We have estimated the shift of the short-wavelength magnon energy in the local-band model. One term, $h'Q^2 |\vec{a}|_{av}^2$, representing a shift of the spinwave constant, is likely to be small and positive. A damping term Γ_Q , proportional to $|\vec{a}|_{av}^2 Q$ may account for a substantial part of the observed linewidth. A novel term $-2D|\vec{a}|_{av}^2$ seems capable of accounting for the bulk of the observed shift.

This term is probably not band-structure sensitive as are the other two, as it appears in the nonlinear Landau Lifshitz equation. It will be interesting to see if such a term can be identified in the case of Heisenberg ferromagnets as well as the itinerant ones.

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APPENDIX

We here finish the calculation of the contribution of $\delta\Lambda$ to the dispersion. We first evaluate $\delta\Lambda$, using Eq. (11) and the wave functions found in I: Eq. III.1) rewritten

$$\begin{split} \psi_{k+}(\vec{\mathbf{r}}) &= e^{i\vec{k}\cdot\vec{\mathbf{r}}} \begin{pmatrix} 1+\alpha_{+}(k)\\ \beta_{+}(k) \end{pmatrix} , \\ \psi_{k-}(\vec{\mathbf{r}}) &= e^{i\vec{k}\cdot\vec{\mathbf{r}}} \begin{pmatrix} \beta_{-}(k)\\ 1+\alpha_{-}(k) \end{pmatrix} , \end{split}$$

where

$$\beta_{+}(k) = -\vec{\mathbf{v}}(k) \cdot \vec{\mathbf{a}}(r) / \Delta,$$

$$\beta_{-}(k) = +\vec{\mathbf{v}}(k) \cdot \vec{\mathbf{a}}^{*}(r) / \Delta,$$
 (A1)
and $\int dr (1 + \alpha + \alpha^{*} + |\beta|^{2}) = V.$

Noting that only the real part of $\delta \Lambda_{-+},{}_{-+}$ is important we find

$$\delta\Lambda_{-+,-+}(kQ,\bar{k}Q) = -\frac{1}{2} \int dr \left\{ |\beta_{-}(k^{+}) - \beta_{-}(\bar{k}^{+})|^{2} + |\beta_{+}(k^{-}) - \beta_{+}(\bar{k}^{-})|^{2} + [\beta_{-}^{*}(k^{+}) + \beta_{+}(k^{-})][\beta_{+}^{*}(\bar{k}^{-}) + \beta_{-}(\bar{k}^{+})] \right\}.$$

For simplicity, we again effectively assume parabolic bands by writing

$$\beta_{-}(k^{+}) - \beta_{-}(\overline{k}^{+}) = \overline{a}^{*}(r) \cdot \left[\overline{v}(k^{+}) - \overline{v}(\overline{k}^{+})\right] / \Delta - \overline{a}^{*}(r) \cdot \left[\overline{v}(k) - \overline{v}(\overline{k})\right] / \Delta$$

and

$$\beta^{\star}(k^{+}) + \beta_{\star}(k^{-}) = \overline{a}(r) \cdot [\overline{v}(k^{+}) - \overline{v}(k^{-})] / \Delta - \overline{a} \cdot \overline{Q} / m \Delta,$$

to find

$$\delta\Lambda_{-+,-+}(kQ,\bar{k}Q) = -\int dr \left\{ \left| \left[\vec{v}(k) - \vec{v}(\bar{k})\right] \cdot \vec{a}(r) \right|^2 + \frac{1}{2} \left| \vec{Q} \cdot \vec{a} \right|^2 / m^2 \right\} / \Delta^2 \right\}.$$
(A2)

Similarly

$$\Lambda_{-+,++}(kQ,\bar{k}\bar{Q},\Omega') = \int dr \, dt \exp\{i[(\bar{\bar{Q}}-\bar{Q})\cdot\bar{r}+\Omega't]\}\bar{a}(\bar{r})\cdot[\bar{v}(k^+)+\bar{v}(k^-)-2\bar{v}(\bar{k}^+)]/2\Delta,$$

which we rewrite, doing the Fourier transform, as

$$\Lambda_{-+,++}(kQ, \overline{k} \overline{Q}, \Omega') = \vec{a}(Q - \overline{Q}, \Omega') \cdot [\vec{v}(k) - \vec{v}(\overline{k} + \frac{1}{2}\overline{Q})]/\Delta,$$

$$\Lambda_{-+,--}(kQ, \overline{k} \overline{Q}, \Omega') = \vec{a}(Q - \overline{Q}, \Omega') \cdot [\vec{v}(\overline{k} - \frac{1}{2}\overline{Q}) - \vec{v}(k)]/\Delta,$$

$$\Lambda_{++,-+}(\overline{k} \overline{Q}, k'Q, -\Omega') = \vec{a}^*(Q - \overline{Q}, \Omega') \cdot [\vec{v}(k') - \vec{v}(\overline{k} + \frac{1}{2}\overline{Q})]/\Delta,$$

$$\Lambda_{--,-+}(\overline{k} \overline{Q}, k'Q, -\Omega') = \vec{a}^*(Q - \overline{Q}, \Omega') \cdot [\vec{v}(\overline{k} - \frac{1}{2}\overline{Q}) - \vec{v}(k')]/\Delta.$$
(A3)

We next find $\delta \Lambda^{\text{eff}}$ by using Eqs. (A2) and (A3) in Eq. (24). Here we may use the $\vec{a} = 0$ values for E(k) and n(k) since $\delta \Lambda^{\text{eff}}$ is already explicitly of order $|\vec{a}|^2$. We also note that $q\vec{a}(q, \Omega')$ and $\Omega'\vec{a}(q, \Omega')$ involve second and higher gradients of the magnetization distribution, and so are of order a^2 and higher. We drop these terms for consistency. Grouping together the terms of various types we find

$$\delta \Lambda^{\text{eff}}(kQ, k'Q, 0) = -\Delta^{-2} \int (dq) \left\{ |\vec{\nabla}(k) \cdot \vec{a}|^2 + |\vec{\nabla}(k') \cdot \vec{a}|^2 - [2 - U(A_+ + A_-)] \vec{\nabla}(k) \cdot \vec{a}^* \vec{U}(k') \cdot \vec{a} - U[(\vec{\nabla}(k) \cdot \vec{a})(\vec{a}^* \cdot \vec{Q}/m) + (\vec{\nabla}(k') \cdot \vec{a}^*)(\vec{a} \cdot \vec{Q}/m)] [C_+ + C_- + \frac{1}{2}(A_+ - A_-)] + U(B_+ + B_-) + [1 + 2U(C_+ - C_-) + \frac{1}{2}U(A_+ + A_-)] |\vec{Q} \cdot \vec{a}|^2 / 2m^2 \right\},$$
(A4)

where \vec{a} means $\vec{a}(q)$ and we have defined the Fermi-surface integrals

$$A_{\alpha}(Q, \Omega) \equiv \int \frac{(dk) \left[f_{\alpha}(k^{-}) - f_{\alpha}(k^{+}) \right]}{\left[\Omega - E_{\alpha}(k^{+}) + E_{\alpha}(k^{-}) \right]},$$

$$B_{\alpha}(Q, \Omega) \equiv \int \frac{(dk) \left[f_{\alpha}(k^{-}) - f_{\alpha}(k^{+}) \right] \left| \vec{\nabla} \cdot \vec{a}(q) \right|^{2}}{\left[\Omega - E_{\alpha}(k^{+}) + E_{\alpha}(k^{-}) \right]},$$

$$\vec{Q} \cdot \vec{a}(q) C_{\alpha}(Q, \Omega) / m \equiv \int \frac{(dk) \left[f_{\alpha}(k^{-}) - f_{\alpha}(k^{+}) \right] \left(\vec{\nabla} \cdot \vec{a} \right)}{\left[\Omega - E_{\alpha}(k^{+}) + E_{\alpha}(k^{-}) \right]}.$$
(A5)

Finally, we put $\delta \Lambda^{eff}$ into Eq. (25). We note that the \vec{k} and \vec{k} integrals separate. Using Eq. (20) for A[°], we find

$$\Omega_{3} = (U/\Delta^{2}) \{ 2Y_{2}Y_{0} - Y_{1}Y_{1}^{*}[2 - U(A_{+} + A_{-})] - 2Y_{0}Y_{1}(\vec{a}^{*} \cdot \vec{Q}/m)U[C_{+} + C_{-} + \frac{1}{2}(A_{+} - A_{-})] + Y_{0}^{2}[U(B_{+} + B_{-}) + [1 + 2U(C_{+} - C_{-}) + \frac{1}{2}U(A_{+} + A_{-})] |\vec{Q} \cdot \vec{a}|^{2}/2m^{2}] \} / Y,$$
(A6)

where we have defined new integrals

$$Y \equiv \int (dk) \frac{f_{+}(k^{-}) - f_{-}(k^{+})}{\left[\Omega - E_{-}(k^{+}) + E_{+}(k^{-})\right]^{2}}, \qquad (A7)$$

$$Y_{\nu} \equiv \int (dk) \frac{\left[f_{+}(k^{-}) - f_{-}(k^{+})\right] |\vec{\nabla} \cdot \vec{a}|^{\nu}}{\Omega - E_{-}(k^{+}) + E_{+}(k^{-})}.$$
 (A8)

These may be evaluated as

$$UY = \left[1 + \langle (\vec{\mathbf{Q}} \cdot \vec{\mathbf{v}})^2 \rangle / \Delta^2 \right] / \Delta, \qquad (A9)$$

$$UY_0 = -1$$
, (A10)

$$UY_1 = -D(\bar{\mathbf{Q}} \cdot \bar{\mathbf{z}}), \tag{A11}$$

$$UY_{2} = -\langle |\vec{\nabla} \cdot \vec{a}|^{2} \rangle (1 + DQ^{2}/\Delta) -[\langle I \rangle - \frac{1}{2} (I_{+} + I_{-})]/\Delta^{2} - |\vec{Q} \cdot \vec{a}|^{2}/4m^{2}.$$
(A12)

$$A_{\alpha} = -\int (dk) \frac{(\vec{\mathbf{v}} \cdot \vec{\mathbf{Q}})(\partial f / \partial \epsilon)}{\Omega - \vec{\mathbf{v}} \cdot \vec{\mathbf{Q}} + i/\tau}, \qquad (A13)$$

$$A_{\alpha} = -\Re_{\alpha} + (\Omega + i/\tau) I_0^{\alpha},$$

$$C_{\alpha} = m(\Omega + i/\tau) A_{\alpha}/Q^2, \qquad (A14)$$

$$B_{\alpha} = -\int (dk) \frac{-\partial n_{\alpha}}{\partial \epsilon} |\vec{\nabla} \cdot \vec{a}|^{2} + \frac{1}{2} \left(\Omega + \frac{i}{\tau} \right) \left[|\vec{a}|^{2} v_{\alpha}^{2} I_{0}^{\alpha} - \left(\Omega + \frac{i}{\tau} \right) |\vec{a}|^{2} \frac{A_{\alpha}}{Q^{2}} \right] - \frac{1}{2} \left(\Omega + \frac{i}{\tau} \right) \left[|\vec{Q} \cdot \vec{a}|_{av}^{2} v_{\alpha}^{2} I_{0}^{\alpha} - 3 \left(\Omega + \frac{i}{\tau} \right) |\vec{Q} \cdot \vec{a}|_{av}^{2} A_{\alpha}/Q^{2} \right] / Q^{2}$$

$$(A15)$$

where \mathfrak{N}_{α} is the density of states at the α Fermi

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- †Based in part on a thesis presented to the Faculty of the Graduate School of the University of Maryland in partial fulfillment of the requirements for the Ph.D. degree.
- Present address: National Bureau of Standards, Washington, D. C. 20234.
- ¹A preliminary account of this work was given in R. E. Prange and V. Korenman, AIP Conf. Proc. <u>24</u>, 325 (1975).
- ²V. Korenman, J. L. Murray, and R. E. Prange, AIP Conf. Proc. 29, 321 (1976).
- ³H. A. Mook, J. W. Lynn, and R. M. Nicklow, Phys. Rev. Lett. 30, 556 (1973).
- ⁴J. W. Lynn, Phys. Rev. B 11, 2624-2637 (1975).
- ⁵V. Korenman, J. L. Murray, and R. E. Prange (preceding paper). This paper is referred to as I. Equations from it are quoted with prefix I: The notation of I is followed in this paper.
- ⁶J. F. Cooke, J. W. Lynn, and H. L. Davis, Solid State Commun. 20, 799 (1976); J. F. Cooke, Phys. Rev. B <u>7</u>,

level, v_{α} the α th Fermi velocity, and

$$I_0^{\alpha} = + \int (dk) \frac{(-\partial n_{\alpha}/\partial \epsilon)}{(\Omega - \vec{\nabla} \cdot \vec{Q} + i/\tau)}.$$
 (A16)

For definiteness (considering the rather large Q values of interest) we evaluate I_0^{α} in the limit $\Omega \tau \ll 1 \ll Q v \tau$,

$$I_0^{\alpha} = \mathfrak{N}_{\alpha}(\Omega/Q^2 v_{\alpha}^2 - i\pi/2 Q v_{\alpha}), \qquad (A17)$$

and, inserting Eqs. (A9) through (A17) into Eq. (A6), find Eq. (26) of the text.

- 1108 (1973).
- ⁷J. B. Sokoloff, Phys. Rev. Lett. <u>31</u>, 1417 (1973).
- ⁸H. S. Bennett and P. C. Martin, Phys. Rev. <u>138</u>, A608 (1963).
- ⁹S. H. Liu, Phys. Rev. B <u>13</u>, 2979 (1976).
- ¹⁰T. Moriya, J. Phys. Soc. (Jpn.) 10, 933-946 (1976).
- ¹¹T. Izuyama, Phys. Lett. 9, 203 (1964).
- ¹²V. Korenman, J. L. Murray, and R. E. Prange (following paper). This paper is denoted as III.
- ¹³As an aside, we remark that one should not confuse the length scale given by $|\mathbf{\tilde{a}}|$ to that given by the coherence length ξ . The latter, for example, becomes infinite at T_C whereas the former is finite there. As discussed in I, $|\mathbf{\tilde{a}}|$ is related to the cutoff used in Ginzburg-Landau-Wilson theories of critical behavior.
- ¹⁴V. Korenman and R. E. Prange, Phys. Rev. B <u>6</u>, 2769 (1972).
- ¹⁵C. S. Wang and J. Callaway, Phys. Rev. B <u>9</u>, 4897 (1974).
- ¹⁶D. M. Edwards and D. Fisher, J. Phys. (Paris) <u>32</u>, C1-697 (1971).
- ¹⁷L. P. Gor'kov, Sov. Phys.-JETP 9, 1364 (1959).