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Local-band theory of itinerant ferromagnetism. I. Fermi-liquid theory*

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Itinerant ferromagnetism, particularly in iron, nickel, and cobalt, is described by a fluctuating-local-band theory, a new concept which generalizes the old band theory. In this description, the old unexplained localized-itinerant complementarity is resolved. It is noted that band structure itself is determined locally, on the scale of a few neighbors, and that the main coordinate which changes in space and time is $\hat{M}$, the collective variable representing the magnetization direction. Because these changes are relatively slow, their effects on band structure can be calculated in a perturbation theory. It is stressed that the classical variable $\hat{M}$ is appropriate, even though quantization is in some cases eventually necessary. In this paper a ferromagnetic-Fermi-liquid theory is set up and compared with previous versions which it generalizes. The range of validity of the theory is shown to extend well above T_C, the Curie temperature. Some estimates of T_C on the basis of the new theory are obtained, which are encouraging. Agreement with a range of experiments is found. Papers II and III discuss nonlinear magnetization-fluctuation interactions, and their bearing on experiment.

I. INTRODUCTION

Theorists have never been able to present a satisfying picture of itinerant ferromagnetism capable of explaining the major phenomena which are observed. It is the purpose of this series of papers to present such a picture and to outline the main new results, some of which have been briefly announced previously.[1,2] It is to be emphasized, however, that one of the most significant virtues of this idea, which we call the "fluctuating-local-band theory" of itinerant ferromagnetism, or "local-band theory" for short, is that it incorporates and generalizes in a natural manner many previous theoretical efforts which have been extremely successful in explaining this or that experimental result.

The results may be summarized as follows:

(i) We develop a new concept giving explicit meaning to spin-split ferromagnetic bands which continue to be spin split even above T_C. This result immediately and naturally explains the photo-[3] and field-emission data,[4] as well as work-function,[5] thermodynamic,[6] and neutron data.[7,8]

(ii) Ferromagnetic-Fermi-liquid theory, like band theory, can also be reformulated and extended above T_C. We have estimated the parameters of this theory, in the band approximation.

(iii) It is feasible to do serious calculations of the influence of local magnetic order on the spin-wave damping and softening as a function of temperature. We have found new terms which are likely to be the dominant contributions to these effects. A model calculation gives results in encouraging agreement with experiment. This calculation is made in Paper II of this series.[9]

(iv) The theory has been found to apply numerically to pure iron, Fe(Si), and nickel, the cases for which the best data are available. We make no fundamental distinction between these materials, in contrast to many other authors. We expect the theory to apply to cobalt and the weak ferromagnets, such as $ZrZn_2$, as well. With some modifications the theory should also work for magnetic alloys of transition metals. We obtain estimates of T_C which are encouraging, and estimates which show the theory is valid even well above T_C.

The concept of "local-band theory" is of much wider application than to magnetism. In most of our development it is not necessary to make a commitment to any special form of band theory, or even to a single-particle scheme. Doing so, however, allows one to find results of considerable intuitive appeal.

The "local-band theory" is a generalization of the ordinary band theory, or perhaps one should say of ordinary band theories, since there are so many schemes for carrying out band calculations that one must be a specialist to appreciate the finer points of this art. Band theory (at zero temperature) has, overall, been a resounding success, for the itinerant ferromagnets as well as for other transition metals (not to speak of the simple metals and semiconductors). It is, however, numerically rather complex and a number of apparent failures of band theory, for example, the results of experiments on photo- or field-emission or polarized electrons, may well be attributed to approximations made in applying the theory, rather than to a fundamental breakdown of the theory itself.[10,11]

However, for a decade or more it was fashion-able to argue that the strong correlations which are a concomitant of narrow energy bands changed things in a fundamental way in the direction of producing localized electronic states, or at any rate states which had a local character not consistent with the usual band theory, even though these states must evidently retain a delocalized itinerant character in order to be in agreement with experiment.[12] The success of Mott in describing the metal-insulator transitions in certain antiferromagnets,[13] as well as the relative success of the Heisenberg model in describing the magnetic phase transitions of the itinerant magnets lent credence to the view that there are somehow local atomic-like magnetic d electrons which are more or less free to have their magnetic moment point in any direction relative to neighboring spins.

At the same time, the finite-temperature band theory, which we know under the name "Stoner theory," fails rather dismally to predict the magnetization or susceptibility as a function of temperature, although the literature is not without papers claiming success for the Stoner theory, particularly for nickel. However, Stoner theory, if done on the basis of realistic bands, gives far too high a transition temperature[14] T_S and in any case gives detailed magnetization curves which are strongly band-structure dependent, in contrast to the experimental fact that the reduced magnetization curves of iron, nickel, and cobalt are very similar. On the other hand, certain modern experiments (photoemission,[3] work function,[5] de Haas–Van Alphen[15]) indicate that the bands do not change rapidly with temperature. These results are in numerical agreement with Stoner theory, (as we reinterpret it), since $T_S \gg T_C$.

The beginning of an answer to all these problems is, and has been, rather obvious. Spin waves, magnons, and spin fluctuations (terms we shall use more or less interchangeably) must be included. This has been carried out by a kind of perturbation theory in the case where the deviation of the spin from perfect alignment is small. The random-phase approximation (RPA) is an obvious choice to study the magnon dispersion. A careful numerical treatment of the RPA seems capable of giving reasonable numerical agreement with magnon dispersions as measured by neutron scattering.[16] A theory of interacting electrons and magnons, analogous to that of electrons and phonons, can then be built up.

One of two courses has been followed. One may make a formal graphical perturbation theory, in which special account is taken of the pole in the electron-hole-of-opposite-spin ladder graphs, i.e., the RPA magnon. An immediate difficulty arises, since unlike the electron-phonon coupling, the magnon-electron coupling is found to be large and approximately independent of magnon momentum.[17] [In the short-range, one-band "Hubbard" model (SROB model) the coupling is just U, the intra-atomic Coulomb potential.]

Suppose one considers the energy shift of an electron due to the existence of long-wavelength magnons of wave number q. It is clear that this shift must be proportional to q^2N_q where N_q is the number of magnons present. That the shift vanishes with q follows from the consideration that a spin wave of long wavelength is nearly equivalent to a rigid rotation of spin, which cannot affect the electron energy.[18] That it is proportional to q^2N_q (for small N_q) follows from Fermi-liquid theory (see below).

On the other hand, in the presence of these magnons, there is a spin rotation proportional to N_q and the electron wave function is modified to order N_q, not q^2N_q. For this reason, the electron-magnon vertex must be large,[17] as noted. Elementary graphs are, as a result, individually large, but careful calculation produces the necessary cancellation, at least in lowest order in N_q.[19] Higher-order graphs must also maintain this cancellation due to spin rotational invariance, but a systematic approach is difficult.

The other approach is Fermi-liquid theory which concentrates on energetics and thus avoids this problem. However, it should not be naively interpreted, as we shall show. One may give an intuitive derivation of Fermi-liquid theory, following Landau,[20] by assuming that the energy $\mathcal{E}$ is a function of N_q and $n_{k,s}$, the quasiparticle occupation number for crystal momentum k and spin s. The magnon and quasiparticle energies are, respectively, with $\hbar = 1$,

$$Dq^2 = \omega_q = \delta\mathcal{E}/\delta N_q, \tag{I.1}$$

$$E_{ks} = \delta\mathcal{E}/\delta n_{ks}. \tag{I.2}$$

The electron energy depends on magnon occupation by

$$\frac{\delta E_{k,s}}{\delta N_q} = \frac{\delta\omega_q}{\delta n_{ks}} = q^2\frac{\delta D}{\delta n_{ks}} = q^2 g_{ks}, \tag{I.3}$$

thus showing the correct q^2 dependence (for small q).

As an aside, we make several remarks in order not to mislead the reader. First, we note that the form of the theory in which magnon variables do not explicitly appear but in which the magnon is derived is wrong, as shown in Herring.[12] Connected with this, we remark that spin labels s corresponding to a definite direction must be used, rather than the matrix notation of Landau. This is because the transverse spin fluctuations are counted in the magnons. A more formal derivation, again following Landau, studies the singularity structure (for long wavelength and low frequency) of certain vertex functions,[21] and distinguishes between the transverse and longitudinal (with respect to the total magnetization) cases.

Both Fermi-liquid theory and band theory plus RPA are successful at low temperatures. Both fail near or above T_C.

The advantage of Fermi-liquid theory over band theory is its presumed exactitude in certain limits. Our theory shares with Fermi-liquid theory this advantage. It reinterprets and extends the Fermi-liquid theory far beyond its original range of validity, in fact to above the Curie temperature. We do not, of course, pretend that Fermi-liquid theory is *exact* at such elevated temperatures since lifetimes of electron and magnon states will be finite. In fact, our theory allows a study and reinterpretation of these lifetimes. The renormalizations which distinguish Fermi-liquid theory from band theory can, however, be included in principle.

On the other hand, band theory, even if not exact, is very valuable in interpreting optical, photoemission, and other experiments. Our picture provides a generalization of *either* band theory *or* Fermi-liquid theory.

The basic idea of the local-band theory is hardly novel. It is to set up a hierarchy of the length and time scales of the important physical processes. One then works out the effects of the fastest and most local processes first, and describes these effects by a renormalized, or effective, Hamiltonian governing the remaining degrees of freedom. It thus proceeds systematically from fast to slow, from local to extended. If we are concerned with an experiment which probes a relatively fast and local process, we may find the effects of slower disturbances by calculating the fast process in the presence of a typical slow disturbance and then performing an appropriate average over the degrees of freedom of the slow disturbance.

We illustrate this by an example from nuclear physics.[22] In a deformed nucleus, the slow processes may be taken to be the rotation of the nucleus, and the fast processes the establishment of single-particle states. (Even faster processes involving meson exchange, or quarks and gluons, are eliminated in favor of an effective Hamiltonian.) Single-particle states in a self-consistently deformed potential are first worked out. If we wish to study only the rotation, we may "integrate out" the single-particle states and their self-consistent potential replacing this complex by a simpler Hamiltonian described by a moment of inertia, whose value is computed via the single-particle-state wave functions. If the single-particle levels are to be studied experimentally, an appropriate average over orientations must be made, which is in this case determined by the principles of quantum mechanics.

We note that in this case the deformation is collective, thus involving some questions of principle in the counting of degrees of freedom, although this counting problem is not significant in practice. Further, we note that although the collective motion must be quantized, so that in the ground state no net direction of orientation remains, it would be a mistake to average the orientation direction before finding the single-particle levels.

Our picture of itinerant ferromagnetism is closely analogous. The single-particle states of band theory (or other self-consistent field theories) are known to be established very quickly and remarkably locally. There may be certain energetically important correlations which also are established rapidly and which are taken into account by a renormalization of the band parameters or by resort to Fermi-liquid phenomenology. Such, for example, are the screening of the Coulomb interaction, and the corrections to the effective value of the intra-atomic Coulomb repulsion.[12]

The collective degrees of freedom are described by a classical variable which we take to be the direction of the local magnetization $\hat{M}(\vec{r})$. This is assumed to be relatively slowly varying in space and time. (We integrate out if necessary, the fast, short-wavelength fluctuations in this quantity.) Only later, does one average over the motion of $\hat{M}(\vec{r})$. It is only at this stage, if at all, that it may be necessary to quantize the motion of $\hat{M}$. In fact, this quantization is only possible at low temperatures when $\hat{M}(\vec{r})$ deviates little from constancy. If $\hat{M}(\vec{r})$ deviates significantly from its average direction, quantization necessarily involves large magnon numbers and nonlinear magnon effects, so the quantization scheme must be changed, although the classical description retains and indeed improves its validity.

The natural coordinate system in which to discuss the single-particle states, given $\hat{M}(\vec{r})$, is one in which the z axis of spin is locally rotated to be in the direction $\hat{M}(\vec{r})$. The Hamiltonian in this system of coordinates acquires perturbing terms proportional to the gradient of $\hat{M}$. Hence, the appropriate measure of spin excitation is not the deviation of $\hat{M}$ from some standard direction, but rather $\nabla\hat{M}$, or in scalar form $\sum_{\alpha,\beta}(\nabla_\alpha M_\beta)^2 \equiv (\nabla\hat{M})^2$.

The coupling of single-electron variables to the collective variables, in this theory, is found to be proportional to the wave number of the collective disturbance. We must underscore the fact that this result is obtained only by using locally rotated spin states.

Again, the novelty of this result should not be overestimated. Already in the case of the electron-phonon interaction, it is, strictly speaking, necessary to use locally translated electron states in order to have an electron-phonon interaction vanishing with phonon wave number. A small uniform displacement of the lattice results in a small uniform displacement of the electronic states. If the displaced states are described in terms of undisplaced states, contributions from higher bands are necessary. These contributions are proportional to the displacement. This change of coordinate system is not usually made explicit, because the unstrained original coordinate system is not observable. The "deformation potential" approach[23] is rather analogous to ours and makes clear the use of locally displaced states.

In the case of the ferromagnet, an external axis is fixed, for example, by application of an external field, so it is not possible to forget entirely about the original coordinate system. However, using the locally spin rotated system avoids the calculationally difficult but physically trivial problem of describing rotated spins in terms of unrotated ones. It thus much improves the perturbation theory.

We therefore take as the fundamental variables of the system $\hat{M}(\vec{r})$ and the single-particle variables characteristic of a band structure whose spin quantization direction is $\hat{M}(\vec{r})$ and whose states are correct to order $\nabla\hat{M}(\vec{r})$.

Correspondingly, in Fermi-liquid theory, we abandon N_q as a variable in favor of $(\nabla\hat{M})^2$. At the same time, the quasiparticle states are regarded as having spin quantization in direction $\hat{M}$.

Insofar as the perturbations due to $\nabla\hat{M}$ are small, the spin fluctuations have little influence on the energy bands. We present evidence that in fact these perturbations are small up to and above T_C, so that the persistence of spin splitting, for example, is immediately understood. The Curie temperature T_C is characterized only by the disappearance of *long-range* spin order. If $\nabla\hat{M}$ is small at T_C, we may conclude that there is sufficient *short-range* magnetic order to permit a well-defined local band structure. The Stoner temperature T_S gives the temperature region below which the local bands acquire a spin splitting.

To complete the picture we need to know how to compute averages over $\hat{M}$. In most cases, this may be done by averaging over all other variables to obtain $\mathcal{F}[\hat{M}]$, the free energy for given $\hat{M}(\vec{r})$. (At low temperatures one must quantize $\hat{M}$.) The thermodynamic weight of $\hat{M}$ will be $e^{-\mathcal{F}[\hat{M}]/T}$ as usual. The step of carrying out the averages over $\hat{M}$ is unfortunately unsolved numerically, although much is known in principle, and approximate methods are available.

The time dependence of $\hat{M}$ is given by the Landau-Lifshitz equation. We shall not dwell on this interesting question at great length, but shall usually make the adiabatic approximation of neglecting the time dependence.

Relatively few components of this paper are distinctly new. It is the picture as a whole which is new. We are perhaps the first to suggest using stochastic (rather than quantum) fluctuations in the collective variable of a "band" theory. We are among the first to stress the fact that the itinerant magnets have sufficient short-range order even above T_C to make our theory applicable there.[1,2,24] Our form of Fermi-liquid theory is also an innovation. We have also obtained a few important new results on specific details of the elementary excitations.

In this paper we shall present results on a new formulation of Fermi-liquid theory, and on thermodynamics. In paper II we obtain results on the nonlinear interaction of magnetization fluctuations which give new interpretations of the observed spin-wave broadening and dispersion.

II. LOCAL SPIN COORDINATE SYSTEM

A. Coordinate transformation

In this subsection we make a straightforward transformation which rotates the spin coordinate system locally, so that the new z direction is in the direction $\theta(\vec{r}), \phi(\vec{r})$ with respect to the laboratory z direction, where θ, ϕ are the polar and azimuthal angles in the laboratory spherical coordinate system. A further arbitrary Euler angle $b(\vec{r})$ is necessary to specify completely the orientation of the spin coordinate system. The arbitrariness of this angle is a gauge invariance which will not concern us deeply in this paper. The direction $\theta(\vec{r}), \phi(\vec{r})$ is taken to be the direction of the local magnetization.

Let $\phi_\alpha(\vec{r})$ be the annihilation operator for an electron in the laboratory frame, with $\alpha = \pm$ referring to spin quantization along the laboratory z axis. Let $\psi_\gamma(\vec{r})$ be the corresponding operator with quantization along the local (θ, ϕ) z axis. Then

$$\phi_\alpha = \sum_\gamma R(\vec{r})_{\alpha\gamma}\psi_\gamma, \qquad \text{(II.1)}$$

with

$$R(\vec{r})_{\alpha\gamma} = \begin{pmatrix} \exp[-\tfrac{1}{2}i(\phi + b)]\cos\tfrac{1}{2}\theta, & -\exp[-\tfrac{1}{2}i(\phi - b)]\sin\tfrac{1}{2}\theta \\ \exp[\tfrac{1}{2}i(\phi - b)]\sin\tfrac{1}{2}\theta, & \exp[\tfrac{1}{2}i(\phi + b)]\cos\tfrac{1}{2}\theta \end{pmatrix}. \qquad \text{(II.2)}$$

The next step is to express the Hamiltonian in the new coordinate system, which is done by substituting ψ in place of ϕ using Eq. (II.1). The Hamiltonian used depends on what further approximations are to be made. We shall adopt a very general Hamiltonian at this stage, and make, for purposes of illustration, some drastic approximations later. One could equally well start with an approximate Hamiltonian, at the cost of having somewhat more complicated expressions in the locally rotated frame. Accordingly, we assume that

$$\mathcal{H}_0 = (2m)^{-1} \int d^3r \sum_{\alpha} \nabla\phi^\dagger_\alpha \cdot \nabla\phi_\alpha + \mathcal{H}_{e\text{-}l} + \mathcal{H}_{e\text{-}e}. \tag{II.3}$$

Here $\mathcal{H}_{e\text{-}l}$ is the electron-lattice potential and $\mathcal{H}_{e\text{-}e}$ is the electron-electron (Coulomb) interaction. These two terms are local and invariant to local spin rotations, if we neglect spin-orbit interactions as we do. In the locally rotated system we find for the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0[\psi_\mu] + \sum_{\mu\nu} \left(\int A_{\mu\nu}\rho_{\mu\nu} + \int \vec{\mathrm{B}}_{\mu\nu} \circ \vec{\mathrm{j}}_{\mu\nu} \right) = \mathcal{H}_0 + \mathcal{H}_1. \tag{II.4}$$

Here $\mathcal{H}_0$ has the same form as (II.3) with ψ substituted for ϕ. The operators ρ and $\vec{\mathrm{j}}$ are defined as

$$\rho_{\mu\nu} = \psi^\dagger_\mu(\vec{\mathrm{r}})\psi_\nu(\vec{\mathrm{r}}), \tag{II.5}$$

$$\vec{\mathrm{j}}_{\mu\nu} = [\psi^\dagger_\mu \vec{\nabla}\psi_\nu - (\vec{\nabla}\psi^\dagger_\mu)\psi_\nu]/2mi. \tag{II.6}$$

The coefficient matrices are

$$A_{\mu\nu} = \sum_{\alpha} \vec{\nabla} R^{-1}_{\mu\alpha} \circ \vec{\nabla} R_{\alpha\nu}/2m, \tag{II.7}$$

$$\vec{\mathrm{B}}_{\mu\nu} = i \sum_{\alpha} \vec{\nabla} R^{-1}_{\mu\alpha} R_{\alpha\nu} = -i \sum_{\alpha} R^{-1}_{\mu\alpha} \vec{\nabla} R_{\alpha\nu}. \tag{II.8}$$

The matrix A may easily be seen to commute with the rotation matrix R, using (II.8) and it is found to be proportional to the unit matrix. Thus,

$$A_{\mu\nu} = \delta_{\mu\nu}[\,|\vec{\mathrm{a}}(\vec{\mathrm{r}})|^2 + |\vec{\mathrm{g}}(\vec{\mathrm{r}})|^2]/2m, \tag{II.9}$$

$$\vec{\mathrm{B}}_{\mu\nu} = \vec{\mathrm{a}}^*(\sigma^+)_{\mu\nu} + \vec{\mathrm{a}}(\sigma^-)_{\mu\nu} - \vec{\mathrm{g}}(\vec{\mathrm{r}})(\sigma^z)_{\mu\nu}, \tag{II.10}$$

with

$$\vec{\mathrm{a}}(\vec{\mathrm{r}}) = \tfrac{1}{2}[\sin\theta(\vec{\mathrm{r}})\vec{\nabla}\phi(\vec{\mathrm{r}}) - i\vec{\nabla}\theta(\vec{\mathrm{r}})]e^{-ib(r)}, \tag{II.11}$$

and

$$\vec{\mathrm{g}}(\vec{\mathrm{r}}) = \tfrac{1}{2}[\vec{\nabla}b(\vec{\mathrm{r}}) + \cos\theta(\vec{\mathrm{r}})\vec{\nabla}\phi(\vec{\mathrm{r}})]. \tag{II.12}$$

We have employed the Pauli spin matrices σ^z and $\sigma^\pm = \frac{1}{2}(\sigma^x \pm i\sigma^y)$.

B. Time dependence and $\vec{g}$ terms

We now take up the consequences of a time dependence of $\hat{M}$, i.e., of θ and ϕ. Since the annihilation operator obeys ($\partial/\partial t$ is represented by a dot)

$$i\dot{\phi}_\alpha = [\phi_\alpha, \mathcal{H}_0] \tag{II.13}$$

in the laboratory frame, we have

$$i\frac{\partial}{\partial t}\sum_{\gamma}(R_{\alpha\gamma}\psi_\gamma) = \sum_{\gamma} R_{\alpha\gamma}[\psi_\gamma, \mathcal{H}], \tag{II.14}$$

from which it follows that

$$i\dot{\psi}_\gamma = [\psi_\gamma, \mathcal{H}] - i\sum_{\alpha\delta} R^{-1}_{\gamma\alpha}(\mathring{R}_{\alpha\delta})\psi_\delta. \tag{II.15}$$

This acts for many purposes like an additional term in $\mathcal{H}$ given by

$$\mathcal{H}_t = \sum_{\gamma\delta} \int \psi^\dagger_\gamma C_{\gamma\delta}\psi_\delta \tag{II.16}$$

with

$$\begin{aligned} C_{\gamma\delta} &= -i\sum_{\alpha} R^{-1}_{\gamma\alpha}\dot{R}_{\alpha\delta} \\ &= -\tfrac{1}{2}(\sigma^z)_{\gamma\delta}(\dot{b} + \cos\theta\,\dot{\phi}) \\ &\quad + \tfrac{1}{2}(\sigma^+)_{\gamma\delta}[(\sin\theta\,\dot{\phi} + i\dot{\theta})e^{ib}] + \mathrm{H.c.} \end{aligned} \tag{II.17}$$

The perturbing term $\mathcal{H}_t$ will be small, if we choose θ, ϕ to correspond to $\hat{M}$ and the time evolution of this quantity to be given by the Landau-Lifshitz equation. In this case, a time derivative is, in order of magnitude, proportional to the square of a spatial derivative.

We wish to discuss the energy to order $(\nabla\hat{M})^2$. In this case we need to consider only the lowest-order effects of $\mathcal{H}_t$, and then only its diagonal part. Let

$$G_{\alpha\beta} = \langle\langle \phi_\alpha(\vec{\mathrm{r}}t); \phi^\dagger_\beta(\vec{\mathrm{r}}'t')\rangle\rangle \tag{II.18}$$

be the Green's function, and let

$$\tilde{G}_{\gamma\delta} = \langle\langle \psi_\gamma; \psi^\dagger_\delta\rangle\rangle \tag{II.19}$$

be the Green's function of the operators appropriate to the rotated frame. Clearly

$$G = R\tilde{G}R^{-1}. \tag{II.20}$$

Then G satisfies $i\dot{G} = 1 + \mathcal{H}_I G + G^{(2)}$ where $\mathcal{H}_I$ is the single-particle part of $\mathcal{H}_0$ (expressed in Schrödinger form) and $G^{(2)}$ is a two-particle Green's function. Correspondingly

$$i\dot{\tilde{G}} = 1 + (\mathcal{H}_I + \mathcal{H}_1 + \mathcal{H}_t)\tilde{G} + \tilde{G}^{(2)}. \tag{II.21}$$

The energy, however, is given by

$$\langle\mathcal{H}_0\rangle = \tfrac{1}{2}\mathrm{Tr}\int d^3r \left(i\frac{\partial}{\partial t} + \mathcal{H}_I\right) G\,|_{t'=t}, \tag{II.22}$$

where t' is set equal to t and $\vec{\mathrm{r}}'$ to $\vec{\mathrm{r}}$ in an appropriate fashion. Thus,

$$\begin{aligned} \langle\mathcal{H}_0\rangle &= \tfrac{1}{2}\mathrm{Tr}\int d^3r\, R^{-1}\left(i\frac{\partial}{\partial t} + \mathcal{H}_I\right) R\tilde{G} \\ &= \tfrac{1}{2}\mathrm{Tr}\int d^3r \left(i\frac{\partial}{\partial t} + \mathcal{H}_I + \mathcal{H}_1 - \mathcal{H}_t\right)\tilde{G}. \end{aligned} \tag{II.23}$$

Because of the negative sign of $\mathcal{H}_t$ appearing in this expression, neglect of $\mathcal{H}_t$ creates no error in lowest order. We shall accordingly neglect $\mathcal{H}_t$ in the rest of this paper.

The term in $\vec{g}$ can be represented as the vector potential corresponding to a magnetic field, depending on spin, but acting on the orbits, given by

$$\vec{h}=(\hbar c/2e)\sigma_z(\vec{\nabla}\cos\theta\times\vec{\nabla}\phi). \qquad \text{(II.24)}$$

The time-dependent effects can be regarded as arising from an electric field

$$\vec{e}=\frac{\hbar}{2e}\,\sigma_z\left(\vec{\nabla}\cos\theta\,\frac{\partial\phi}{\partial t}-\frac{\partial\cos\theta}{\partial t}\,\vec{\nabla}\phi\right). \qquad \text{(II.25)}$$

Clearly, $\vec{h}$ is of second order, $\vec{e}$ of third, in the spatial gradients. The vector $\vec{g}$ can also have no important effect on the energetics. The argument here is that, as in Landau diamagnetism, the change of the total energy is proportional to $|\vec{h}|^2$, which is here of fourth order in gradients. In discussing spin-wave–spin-wave interactions $\vec{g}$ is of importance and we shall discuss it in papers II and III of this series. We shall ignore it in most of the remainder of this paper, however. This is an important simplification as it reduces the two variables θ, ϕ to the single variable $\vec{a}$.

For the effective electric and magnetic fields not to vanish, the spin fluctuations have to be of some complexity. From Eqs. (II.24) and (II.25) it is clear that there must be more than one wave number involved. The main physical effect of these fields is the real scattering, without spin flip, of the electrons by the spin fluctuation. In magnon language this requires the absorption and emission of magnons of different wave number, which is another way of seeing why the spatial structure of the spin fluctuation must be complex to be effective.

III. BAND THEORY IN THE ROTATED FRAME

A. Single-electron states

In this section, keeping only the terms in $\vec{a}$, we calculate the single-electron states, in the sense of band theory. These states are calculated to first order in $\vec{a}$. (The effect of $\vec{g}$ on the wave function is to contribute a phase factor, since it is the vector potential of an effective field, and can be treated in the quasiclassical approximation.) If the Bloch states of $\mathcal{H}_0$ are given by $\phi_{k+}(\vec{r})\binom{1}{0}$, $\phi_{k-}(\vec{r})\binom{0}{1}$,

$$\psi_{k+}=\mathfrak{C}\begin{pmatrix}\phi_{k+}\\ -\phi_{k-}\vec{v}(\vec{k})\cdot\vec{a}(\vec{r})/\Delta\end{pmatrix}, \qquad \psi_{k-}=\mathfrak{C}\begin{pmatrix}\phi_{k+}\vec{v}(\vec{k})\cdot\vec{a}^*(\vec{r})/\Delta\\ \phi_{k-}\end{pmatrix}. \qquad \text{(III.1)}$$

We have simplified the writing by assuming the spatial variation of $\vec{a}$ is slow compared with that given by k. More exactly, neighboring $\vec{k}$ values are mixed into the wave function labeled by $\vec{k}$. We also have written $\epsilon_{k-}-\epsilon_{k+}=\Delta$ as a constant. Here $\epsilon_{k\alpha}$ is the energy of the unperturbed Bloch state. We have not written out interband matrix elements, which can be approximately included by introducing the velocity $\vec{v}(\vec{k})$ instead of $\vec{k}/m$. $\mathfrak{C}$ is the normalization $(1+|\vec{v}\cdot\vec{a}|_{\text{av}}^2/\Delta^2)^{-1/2}$, where av indicates the volume average.

We shall continue to write results in the approximation equivalent to using the SROB model, occasionally also assuming parabolic bands. The purpose of so doing is to arrive at expressions transparent enough to be understood, while not losing really essential features of the theory, even though numerical results will be untrustworthy.

The states of Eq. (III. 1) are not aligned perfectly parallel to $\hat{M}(\vec{r})$, but rather are tilted away from it. Classically, the electron spin precesses about the mean direction. As the electron passes into a new region with a different $\hat{M}$, the exchange gives a torque which causes the precession. Because the precession is fast, (frequency ~$\Delta/\hbar$) the average spin of the electron points in the direction $\hat{M}$, but the contribution of that spin to the magnetization is somewhat reduced.

The energies to second order are given by

$$E_{k\pm}=\epsilon_k+\tfrac{1}{2}|\vec{a}|_{\text{av}}^2/m\mp|\vec{v}\cdot\vec{a}|_{\text{av}}^2/\Delta\mp\tfrac{1}{2}U\langle\sigma_z\rangle. \qquad \text{(III.2)}$$

We have introduced the intra-atomic exchange U of the SROB model. $\langle\sigma_z\rangle$ is given by

$$\langle\sigma_z\rangle=\int(dk)\,[f_+(\vec{k})-f_-(\vec{k})]\mathfrak{C}^2(1-|\vec{v}\circ\vec{a}|_{\text{av}}^2/\Delta^2), \qquad \text{(III.3)}$$

where $f_\pm(\vec{k})$ gives the actual occupation, including any repopulation because of the existence of $\vec{a}$. We abbreviate $d^3k/(2\pi)^3$ by (dk). Thus,

$$U\langle\sigma_z\rangle=\Delta-2U\int(dk)\,[f_+(\vec{k})-f_-(\vec{k})]\,|\vec{v}\cdot\vec{a}|_{\text{av}}^2/\Delta^2, \qquad \text{(III.4)}$$

where $\Delta=U(N_+-N_-)$ includes possible repopulation. It need not be distinguished from the Δ appearing in energy denominators to the order of approximation we are using. Denoting

$$\langle A(\vec{k})\rangle=\frac{U}{\Delta}\int(dk)\,(f_+-f_-)A(\vec{k}) \qquad \text{(III.5)}$$

as the average over singly occupied states, we find

$$E_{k\pm}=\epsilon_k+\tfrac{1}{2}|\vec{a}|_{\text{av}}^2/m\mp\tfrac{1}{2}\Delta\mp(|\vec{v}\cdot\vec{a}|_{\text{av}}^2-\langle|\vec{v}\cdot\vec{a}|_{\text{av}}^2\rangle)/\Delta. \qquad \text{(III.6)}$$

Thus, corrections to $E_{k-}-E_{k+}\equiv\Delta_k$ are proportional to $(\nabla\hat{M})^2$, not M_z as in Stoner theory. Clearly $\langle\Delta_k\rangle=\Delta$. Note also, $\langle\sigma_z\rangle$ is not given by the population difference, but is reduced from that by tilting of individual spins away from their mean direction. This Δ does not vanish at T_C, explaining the photoemission and other results.[1,5]

We remark that properties of single-particle states at the Fermi surface are observed at low temperatures, e.g., by the de Haas–van Alphen effect. The shifts of Eq. (III.6), being of order $|\vec{a}|^2$ are much smaller than that predicted by Stoner theory. This is in accord with the experiments of Lonzarich and Gold.[15]

B. Free energy

We have calculated the total energy in the presence of a nonvanishing $\vec{a}$ by two methods. The first, direct, formal perturbation theory, is interesting, since if $\vec{a}$ represents a single spin-density wave, of very long wavelength, the expression gives an exact formula for D, the spin-wave constant. This formula has been obtained previously,[25] so we do not reproduce it here.

The band-theory approximation to the energy is interesting as well. If applied to find the spin-wave constant, it gives the RPA expression. If it is used to find the total free energy, it gives approximations to the Landau-theory parameters. It is the most direct way to discuss repopulation of single-particle states.

We seek to find the difference between free energies per unit volume keeping the single-particle occupation fixed. We thus want $\delta\mathcal{F} = \mathcal{F}[T, n_{k\alpha}, \vec{a}] - \mathcal{F}[T, n_{k\alpha}, 0]$. This, however, is also equal to the difference in energies, since if the $n_{k\alpha}$ are fixed, there is no change in entropy. The energy, in band theory, is obtained by adding, for all occupied states, the kinetic part of the single-particle energies to half the potential part. Since H_1 is all kinetic, $\langle \psi_{k\alpha} | H_1 | \psi_{k\alpha} \rangle = |\vec{a}|^2_{\text{av}}/2m - 2|\vec{v}\cdot\vec{a}|^2_{\text{av}}/\Delta$ is the kinetic energy part of E_k. Straightforward calculation yields

$$\delta\mathcal{F} = \int (dk)\,[f_+(\vec{k}) + f_-(\vec{k})]\,|\vec{a}|^2_{\text{av}}/2m - [f_+(\vec{k}) - f_-(\vec{k})]\,|\vec{v}_k\cdot\vec{a}|^2_{\text{av}}/\Delta\,. \tag{III.7}$$

The most common case will be that the occupations are sufficiently isotropic to allow the replacement of $|\vec{v}_k\cdot\vec{a}|^2_{\text{av}}$ by $\frac{1}{3}|\vec{v}_k|^2|\vec{a}|^2_{\text{av}}$. Noting $|\vec{a}|^2_{\text{av}} = V^{-1}\int d^3r \times\frac{1}{4}(\nabla\hat{M})^2$, we have $\mathcal{F} = V^{-1}\int d^3r\, A(\nabla\hat{M})^2$ with the RPA formula for A,

$$A = \frac{1}{4}\int (dk)\; \frac{f_+ + f_-}{2m} - \frac{f_+ - f_-}{3\Delta}\,|\vec{v}|^2\;. \tag{III.8}$$

The usual relation between A and D, the spin-wave constant, holds at low temperature and is $D = 2A/M$, where $2M = N_+ - N_-$.

C. Repopulation

In the presence of a magnetization fluctuation $\vec{a}$, the single-particle energies will shift and in consequence, there may be a change in occupation number. This repopulation can be taken into account by using the appropriate single-particle energies in the Fermi functions giving the occupations. Alternatively, the free energy whose shift was just calculated can be minimized with respect to occupation number.

To proceed by the latter method, we need to know properties of $\mathcal{F}[T, n_{k\alpha}, 0]$. This quantity, however, if calculated in the band approximation, is just that given by the usual Stoner theory. The result is exactly as in Fermi-liquid theory, to which the band theory provides an approximation.

If we are interested only in the gross features of the repopulation, we may eliminate the individual $n_{k\alpha}$ as variables and use only $N_\alpha = \sum n_{k\alpha}$. In fact, for simplicity, we assume $N = N_+ + N_-$ is fixed. [If N includes all the electrons, this is guaranteed by the long-range Coulomb force. If it is to represent just the d electrons, it is still likely to be a good approximation.] Then we may write

$$\mathcal{F}[T, N, \tfrac{1}{2}(N_+ - N_-), 0] = \mathcal{F}[T, N, M_S, 0] + \tfrac{1}{2}\chi_S^{-1}[\tfrac{1}{2}(N_+ - N_-) - M_S]^2\,. \tag{III.9}$$

In (III.9) M_S is the Stoner saturation magnetization and χ_S is the band susceptibility, given in the present model by

$$\chi_S^{-1} = \mathcal{N}_+^{-1} + \mathcal{N}_-^{-1} - 2\langle \mathcal{N}^{-1}\rangle\,. \tag{III.10}$$

We define

$$A_\alpha = \int d\epsilon\, A(\epsilon)\,\frac{-\partial f_\alpha}{\partial\epsilon} \tag{III.11}$$

as the (in principle, temperature-dependent) value of a function at the α-spin Fermi surface. $\mathcal{N}_\alpha$ is given by (III.11) with $A(\epsilon) = \mathcal{N}(\epsilon)$ the density of states, and $\langle \mathcal{N}^{-1}\rangle$ by (III.5) with $A = \mathcal{N}^{-1}$. In the SROB approximation $\langle \mathcal{N}^{-1}\rangle = U$. For simplicity, we have assumed a rigid exchange shift, as predicted by this model.

To find the repopulation, $\mathcal{F}[T, N, \frac{1}{2}(N_+ - N_-), |\vec{a}|^2_{\text{av}}]$ is minimized with respect to $N_+ - N_-$. For this purpose it is necessary to compute $\delta A/\delta(N_+ - N_-)$. Only the second term (proportional to $|\vec{v}\cdot\vec{a}|^2_{\text{av}}$) contributes, as $f_+ - f_-$ and Δ depend on this quantity. We obtain the result

$$N_+ - N_- - 2M_S = 2\chi_S(\mathcal{M}_+/\mathcal{N}_+ + \mathcal{M}_-/\mathcal{N}_- - 2\langle\mathcal{M}\rangle/\langle\mathcal{N}^{-1}\rangle)\,. \tag{III.12}$$

Here $\mathcal{M}(\epsilon) = \int (dk)\,\delta(\epsilon_k - \epsilon)\,|\vec{v}\cdot\vec{a}|^2_{\text{av}}/\Delta$, and Eqs. (III.5) and (III.11) define the quantities appearing in (III.12). Note that, at zero temperature, strong ferromagnetism (with a completely full or completely empty band) gives no repopulation, as $\mathfrak{N}_+$, $\mathfrak{M}_+$, (or $\mathfrak{N}_-$, $\mathfrak{M}_-$) will vanish, together with the susceptibility, χ_S. In fact χ_S is rather small as a general rule, and repopulation is not an important effect even at higher temperatures.

We have here assumed that there are no entropic contributions to $\mathfrak{F}$ from fluctuations in $\vec{a}$ which are of importance. More generally (see Eq. IV.1) $\mathfrak{F}[n_{k\alpha}] = -T \ln \sum_{\vec{a}} \exp[-\mathfrak{F}(n_{k\alpha}, \vec{a})/T]$. At high temperatures $\sum_{\vec{a}}$ is given by a functional integral over $\theta(r)$, $\phi(r)$. Then it is easily seen that the preceding formulas hold.

At low temperature, one must quantize $\vec{a}$, in which case somewhat different results are obtained (see Sec. IV C). In this case $\vec{a}$, in effect, depends on the variables $n_{k\alpha}$ and the repopulation is given by adding the quantity $4D|\vec{a}|^2_{\text{av}}$ to the right side of Eq. (III.12) which for parabolic bands causes a slight increase in majority over minority spin. At high temperatures, this term does not appear and the repopulation is small and negative.

We conclude by making some remarks about whether repopulation can actually take place. It might seem at first sight that thermodynamic formulas for repopulation would only be valid if the single-particle states come into thermal equilibrium in a time short compared with the time over which $\vec{a}$ changes. This would require an investigation of scattering rates. However, it should be noted that even for an arbitrary, fixed $\vec{a}$ what appears in the perturbation formulas for the single-particle energy is $|\vec{a}|^2_{\text{av}}$ and $|\vec{a}\cdot\vec{\nabla}|^2_{\text{av}}$, in other words, the spatial averages. This happens because the matrix elements are between delocalized, itinerant states. Now, unless $\vec{a}$ refers to a magnetization fluctuation which is not thermal, we know that even though $\vec{a}$ may have a significant time dependence on the scale of electron relaxation times, $|\vec{a}|^2_{\text{av}}$ will be constant in time. Hence the repopulation has time to take place as discussed above. A case where this does not happen is in ferromagnetic resonance, where $\vec{a}$ is driven by an external electromagnetic wave. For this case there is a "normal" regime in which the electrons are locally in equilibrium, and an "anomalous" one where they are not. Such effects are discussed in Ref. 26–28.

IV. FERMI LIQUID THEORY

A. Band approximation

In Sec. III we found a formula for the free-energy difference,

$$\mathfrak{F}[T, n_{k\alpha}, \vec{a}] - \mathfrak{F}[T, n_{k\alpha}, 0],$$

which is also equal to the energy difference. We first say a word about the entropic contribution to $\mathfrak{F}$. Clearly, the single-particle entropy is given by the usual formula, so if there is no change in occupation, there is no change in single-particle entropy.

The entropy for any fixed value of $\vec{a}(\vec{r})$ is the same as it is for the special value $\vec{a} = 0$. However, there are many different values of $\vec{a}$ with the same $|\vec{a}|^2_{\text{av}}$, and this will contribute to the entropy. These entropic considerations can be taken care of automatically by defining

$$e^{-\mathfrak{F}/T} = \sum_{\vec{a}} e^{-\mathfrak{F}[n_{n\alpha}, \vec{a}]/T} \tag{IV.1}$$

where the sum is over possible values of $\vec{a}$ [keeping some variable, such as $|\vec{a}|^2_{av}$ fixed if desired]. Exactly how this sum is performed will depend on several factors, among them whether it is necessary to quantize $\vec{a}$. For most purposes, it is only here, if at all, that $\vec{a}$ need be quantized. Previous versions of Fermi-liquid theory have insisted upon quantization, unnecessarily, in our opinion, and consequently have had to restrict considerations to very low temperatures.

We therefore avoid committing ourselves to specifying how (IV.1) is to be carried out until the very end. This leaves our version of Fermi-liquid theory somewhat incomplete. In compensation, the range of validity of the theory is enormously improved, and much can be learned without specification of an exact form for (IV.1).

With this understanding, we consider the energy, rather than the free energy. After Landau, an expansion of the energy functional is made,

$$\begin{aligned}\mathcal{E}[n_{k\alpha}, \vec{a}] = {} & \mathcal{E}[n^0_{k\alpha}, 0] + \sum_{\alpha} \int E^0_{k\alpha}\, \delta n_{k\alpha}\, (dk) + 4A\, |\vec{a}|^2_{\text{av}} + \frac{1}{2} \sum_{\alpha,\alpha'} \int (dk) \int (dk')\, f_{k\alpha, k'\alpha'}\, \delta n_{k\alpha}\, \delta n_{k'\alpha'} \\ & + \sum_{\alpha} \int (dk)\, g'_{k\alpha}\, |\vec{a}|^2_{\text{av}}\, \delta n_{k\alpha}\,.\end{aligned} \tag{IV.2}$$

We have here dropped terms of order a^4 which should, strictly speaking, be kept, as they are formally of the same order. This term will be discussed in the following paper.

In the SROB model, treated in band theory, $f_{k\alpha, k'\alpha'}$ is just U, for $\alpha \neq \alpha'$.

Eq. (III.6) gives for $g'_{k\alpha}$ the band approximation result

$$g'_{k\alpha}=1/2m-\tfrac{1}{3}\alpha(|\vec{v}|^2-\langle|\vec{v}|^2\rangle)/\Delta. \qquad \text{(IV.3)}$$

Equation (IV.2) gives the form of a new version of Fermi-liquid theory in which the variables are $n_{k\alpha}$, quasiparticles with spin parallel and antiparallel to the local magnetization, and a variable $\vec{a}$ describing the gradient of magnetization direction.

B. Rapidly established correlations

As a rule, band theory naively applied is not completely adequate numerically. There are certain correlation effects which are not properly described by the mean-field approximation. Such fast correlations are, for example, the screening of the long-range Coulomb force, and the adjustments to the effective value of U as reviewed by Herring.[12] From a practical point of view, probably the best approach is to reduce the Hamiltonian to an effective one in which these effects are taken into account by renormalizations of the parameters.

We may, however, follow the technique of Landau to make plausible the idea that these fast correlations will do no more than renormalize the parameters E_k, A, f, and g' of (IV.2). In this approach one studies various vertex functions, or Green's functions, and makes it plausible that the leading poles at low freqency and long wavelength have appropriate properties.

To be more specific, one can study the single-particle Green's function, to order $|\vec{a}|^2$, not in band theory, but to higher orders in the electron-electron interactions. In the customary case, the Green's function to every order of perturbation in this interaction has the appropriate singular properties at long wavelength and low frequency. This is a "proof" or plausibility argument for the validity of Fermi-liquid theory.[29]

Naive calculation would give the same results in the rotated frame. On the one hand, however, it is known the $\mathcal{H}_0$ describes a system whose low-lying excitations include spin waves, and on the other hand, it is clear that, in the rotated frame we should exclude these excitations, since they are taken into account by the local rotation itself. Thus, some means must be found to exclude from the space of states available to the system those states which are described by the local rotation itself. We have not yet succeeded in divising a completely satisfactory formal theory which projects out these states, so we content ourselves with a couple of remarks. First, for given finite $\vec{a}$ there will be electron lifetime corrections, since $\vec{a}$ represents a disordered scatterer. The corrections will be of order a^4, which may be formally negligible. Second, it seems plausible that the single-electron Green's function will continue to have only quasiparticle poles near the Fermi surface, since the spin-wave states projected out are the ones which could have been troublesome.

In summary, we argue that the form of Fermi-liquid theory is preserved in approximations going beyond the band approximation. The band approximation with an appropriate starting Hamiltonian is probably sufficiently accurate for practical purposes, however.

C. Comparison of old and new theories

All previous ferromagnetic Fermi-liquid theories have regarded the magnon number as the appropriate variable to describe the spin fluctuations. A seeming inconsistency then arises as follows:

The pure magnon contribution to the energy, which we have written

$$\mathcal{E}_m=4A|\vec{a}|^2_{\text{av}} \qquad \text{(IV.4)}$$

is written in the old theory as $\int(dq)Dq^2N_q$.

Thus

$$|\vec{a}|^2_{\text{av}}=\int(dq)\,q^2N_q/2M, \qquad \text{(IV.5)}$$

where we have assumed a temperature so low that higher powers of N_q/M are negligible. The single-electron energies are given by

$$E_{k\gamma}=E^0_{k\gamma}+\delta\mathcal{E}_m/\delta n_{k\gamma}\big|_{\vec{a}}=E^0_{k\gamma}+g'_{k\gamma}|\vec{a}|^2_{\text{av}} \qquad \text{(IV.6)}$$

in the new theory.

In the old version,[20] the energy is given by

$$\hat{E}_{k\alpha}=E^0_{k\alpha}+\delta n_{k\alpha}/\delta\mathcal{E}_m\big|_{N_q}$$
$$=E^0_{k\alpha}+\int(dq)\,g_{k\alpha}q^2N_q. \qquad \text{(IV.7)}$$

The state α must correspond to quantization in the lab frame, since for fixed N_q no local frame is well defined.

Paradoxically, it would seem, $E_{k\alpha}\neq\hat{E}_{k\alpha}$. This happens because according to Eq. (IV.5), the relation between $|\vec{a}|^2_{\text{av}}$ and N_q contains a factor M which depends on single-particle occupation. In the band approximation, using Eq. (IV.4), we have

$$\hat{E}_{k\alpha}=E_{k\alpha}-\alpha\int(dq)\,N_qDq^2/2M. \qquad \text{(IV.8)}$$

We thus find that although the total energy is the same in either representation, the energy associated with an electron quasiparticle in the presence of a spin fluctuation (or the energy associated with a spin fluctuation in the presence of an electron fluctuation) differs in the two descriptions.

Which is correct? The answer, we believe, is that both are correct. It is just a matter of using different coordinate systems.

To clarify this point, let us consider the single-particle Green's function in the band approximation for the special case in which the spin fluctuation is a spin-density wave. We choose θ to be a small constant, and $\phi = \vec{q}\cdot\vec{r} - \Omega_q t$ with $\Omega_q = Dq^2\cos\theta$. The number of magnons, all of wave number q, required to produce such a wave is $N_q = 2M\sin^2\frac{1}{2}\theta$. We find $|\vec{a}|^2_{av} = \frac{1}{4}q^2\sin^2\theta = (N_q/2M)(1 - N_q/2M)q^2 \approx (N_q/2M)q^2$, agreeing with Eq. (IV.4). This Green's function we calculate in the locally rotated frame. We find (again in the SROB case), using the definition of Eq. (II.19)

$$\tilde{G}(\vec{r}t, \vec{r}', t') = \int (dk)\; e^{i\vec{k}\cdot(\vec{r}-\vec{r}')} \times \left[e^{-iE_{k+}(t-t')} \begin{pmatrix} \mathfrak{C}^2, & \mathfrak{C}\mathfrak{D}^* e^{ib'} \\ \mathfrak{C}\mathfrak{D}e^{-ib}, & |\mathfrak{D}|^2 e^{i(b'-b)} \end{pmatrix} + e^{-iE_{k-}(t-t')} \begin{pmatrix} |\mathfrak{D}|^2 e^{i(b-b')}, & -\mathfrak{C}\mathfrak{D}^* e^{ib} \\ -\mathfrak{C}\mathfrak{D}e^{-ib'}, & \mathfrak{C}^2 \end{pmatrix} \right]. \tag{IV.9}$$

Here $E_{k\gamma}$ is given by Eq. (III.2), $\mathfrak{C}$ is the normalization defined in Eq. (III.1), and $\mathfrak{D} = -\mathfrak{C}\vec{v}(k)\cdot\vec{a}e^{ib}/\Delta$. In this case, we may choose $b = -\phi(\vec{r}t)\cos\theta$, $b' = -\phi(\vec{r}', t')\cos\theta$, so that $\vec{g}(\vec{r}, t)$ vanishes. Note also $\mathfrak{C}^2 + |\mathfrak{D}|^2 = 1$ and $\mathfrak{D}$ may be chosen real. As we discussed earlier, the fact that $\mathfrak{D} \neq 0$ is interpreted as a rapid precession of the individual electron spin about the mean spin.

We next work out the Green's function in the laboratory system, which can be accomplished by use of Eqs. (II.20) and (II.2). The result is

$$G(\vec{r}t, \vec{r}'t') = \int (dk) \exp[i\vec{k}\cdot(\vec{r} - \vec{r}')] \times \sum_\alpha \exp[-i\hat{E}_{k\alpha}(t - t')]M_\alpha, \tag{IV.10}$$

where M_α has a large constant component in the (α, α) position, with small off-diagonal and $(-\alpha, -\alpha)$ components. Here $\hat{E}_{k\alpha}$ is given by

$$\hat{E}_{k\alpha} = E_{k\alpha} - \alpha N_q Dq^2/2MV + \alpha\vec{q}\cdot\vec{v}_k N_q/2MV. \tag{IV.11}$$

This is consistent with (IV.8) where the last term does not appear because it has been assumed that the average over directions of $\vec{q}$ is isotropic. The reason $\hat{E}$ differs from E, according to this point of view, is that the transformation R is time dependent. In other words, the spin-density wave is moving, and we have taken into account the Doppler shift in changing the frames of reference.

It may seem strange that the energy relation Eq. (IV.8) is a consequence of either the Doppler shift or a change of variable from $\vec{a}$ to N_q. However, the fact that the free energy is preserved, as discussed in Sec. III B, guarantees this nice result.

Fermi-liquid theory is derived by a procedure whereby the pole in the Green's function with large residue is renormalized to have unit residue, and the other parts of the spectrum are accounted for by renormalization, or in this case, by introduction of a new kind of excitation. Where both theories are valid, they are equivalent, at least insofar as the nature of the wave functions does not come into question, but only the energies.

Do the sundry Fermi-surface experiments measure properties of the states in the lab frame or the locally rotated frame? From a practical point of view, there is no difference, as the shift is very small, proportional to $\int q^2 N_q(dq)$, not $\int N_q(dq)$, in either case. Further, insofar as the geometry of the Fermi surface is the measured quantity, both forms give the same result, since they both result from a minimization of the same free energy.

We have mentioned this point at the end of Sec. III. In this context, it means that to find the free energy which is to be minimized with respect to $n_{k\alpha}$ and $\vec{a}$, we must subtract the entropy term TS from the energy of Eq. (IV.2). The standard boson expression for the entropy will be $-V^{-1}\sum_q[N_q\ln N_q - (1 + N_q)\ln(1 + N_q)]$. If one uses this expression and Eq. (IV.5), specialized to Fourier components of $\vec{a}$, it is found that the energies $\hat{E}_{k\alpha}$ are those which determine the occupations; at elevated temperatures, the standard boson expression will not give the correct entropy and one expects $\sum_{\vec{a}}$ in Eq. (IV.1) to be given by a functional integral over $\theta(r), \psi(r)$. In this case $E_{k\alpha}$ determines the occupations. We have not attempted to map out the crossover in detail since we expect repopulation to be of minor importance in any case.

It is interesting to note that the residue of the dominant pole of the laboratory-frame Green's function is reduced by a factor $[1 - \langle(\vec{q}\cdot\vec{v})^2\rangle]/\Delta^2$, thus giving a $T^{5/2}$ term in the magnetization. This is just the same as our reduction of $\langle\sigma_z\rangle$ due to tilting of individual electron spins away from their mean direction. Fermi-liquid theory renormalizes this residue and is correct only to order T^2 in the magnetization. The difference between the old and new versions thus first appears in going to higher order in $\int (dq)N_q/M$, or in subtler questions, such as that of the quasiparticle lifetimes, as well as in the question of the range of validity of the two theories.

V. VALIDITY OF THE FLUCTUATING-LOCAL-BAND THEORY

We here treat briefly the fundamental question of the range of validity of the new form of band theory (or Fermi-liquid theory). Clearly the old form cannot be valid in any situation in which the magnetization is reduced appreciably from its zero-temperature value.

There are two questions to be studied in this section. The first is: What is the range of validity of the new theory? The second is: Why is the range what it is? The second question is much more difficult than the first and we can make only some remarks. The first can be treated semiphenomenologically.

A. Phenomenological range of validity

We regard the foregoing theory as valid if the quantity $\vec{a}$ is small enough so that corrections to single-particle energies, etc. are adequately given by the perturbation developed in the previous sections. If this is so, then the energy bands in most respects will look rather similar to those at zero temperature.

Because of electron lifetime effects, details of energy bands cannot be measured very accurately except at the very lowest temperature. Nevertheless, what evidence is available indicates that bands continue to exist above T_C much like those below. We have cited photoemission,[3] work function,[5] and other data[4,6,7] which show no anomalies at T_C in support of this contention. An analysis of thermodynamic data also leads to this conclusion.[6]

We can also attempt to find, phenomenologically, the size of $|\vec{a}|^2_{\text{av}}$ as a function of temperature. To do this, we can take the expression for the magnetic energy Eq. (IV.4) and compare it with that extracted from specific-heat measurements. For nickel, from the analysis of Pawel and Stansbury,[30] we find that the *total* magnetic energy (for $T \gg T_C$) is 1.2×10^{-2}eV/atom. This gives $|\vec{a}|^2_{\text{av}} \simeq 5 \times 10^{-2}$ Å^{-2} as the maximum. With $\Delta \sim 0.8$ eV according to Wang and Calloway,[31] and $v \sim 10^7$ cm/sec, we have $|\vec{a}\cdot\vec{v}|/\Delta \sim 0.18$. The value of $\vec{v}$ is not well known. It should be an average over the singly occupied states. In nickel the bands are extremely flat near the point X where the pockets of holes in the minority band are believed to exist. Direct estimates of the magnetic energies based on spin-wave extrapolation give values of $|\vec{a}|^2_{\text{av}}$ somewhat smaller than this.

A corollary of this is that $|\vec{a}|^2_{\text{av}}$, according to the specific-heat data, varies slowly except relatively close to T_C. It rises from small values below T_C and saturates shortly above, which has a bearing on observations[7,8] to be discussed in paper II of this series. Its critical behavior at T_C is inconspicuous, since measured and theoretical values of the specific-heat critical exponent α indicate a small negative value for this quantity.

Another argument is as follows. $\vec{a}$ can be small for two reasons. The gradients can be small, or the angle of tilt can be small, or we can imagine the local rotation to be compounded of two rotations, a first through a large angle but with small gradients, followed by a second through a small angle, but with larger gradients. This will also give a small value of $\vec{a}$. Since the larger-gradient, i.e., shorter-wavelength, disturbances of the magnetization correspond to higher-energy spin waves, it is clear that the amplitude of these disturbances will be small. These short-wavelength disturbances are ripples on the longer wavelength and slower "ground swell," which is of large amplitude above T_C. To predict their amplitude, these ripples must be quantized. They should be observable by neutron scattering and in fact are the famous spin waves observed above the transition temperature.

Since spin waves with considerable width, but nevertheless distinctly defined have been observed for $q > Q_0 \sim 0.25$ Å^{-1} in nickel[7] and iron,[8] we can draw the conclusion that there is short-range magnetic order on this scale. Superimposed on this local order are the small amplitude, relatively fast, and short-wavelength spin fluctuations, which must be quantized, as well as the even faster and/or shorter-wavelength fluctuations of the single-particle states.

The spin fluctuation for $q > Q_0$ are weak enough in amplitude to be treated by perturbation theory, i.e., RPA. The spin fluctuations for $q < Q_0$ clearly have a maximum contribution to $\vec{a}$ of order Q_0, which corresponds to a wavelength of order 25 Å. The shorter-wavelength waves can be estimated by spin-wave theory to make a somewhat smaller contribution to $|\vec{a}|^2_{\text{av}}$.

This consideration also affords an escape from the difficulties posed by the fact that the spin-wave spectrum is known not to be purely quadratic in crystal momentum, as our theory apparently predicts. In fact for shorter wavelengths we do not have to rely on the smallness of the gradient, and our results go over to the RPA approximation, which is believed to be substantially valid numerically. (One must not neglect the time dependence of the magnetization wave in this case. Several of the approximations made in Sec. III in the interests of simplicity have to be improved for a short-wavelength spin fluctuation. The following paper discusses this case at greater length.)

The conclusion of this section is that $|\vec{a}|^2_{\text{av}}$ is small enough, even well above T_C, so that the pertrubation theory of Secs. II and III is approximately valid.

B. Theoretical consideration

In this section we consider briefly the question: Why is $|\vec{a}|^2_{\rm av}$ so small? Why, in other words, does short-range magnetic order persist? How general is this result?

Part of the answer to this question may be due to the circumstance that the spin-wave constant D is much larger here than in, say, a nearest-neighbor Heisenberg model. In the latter case $DG^2 \sim T_C$ where G is a zone-boundary wave vector, whereas in the itinerant case $DG^2 \gg T_C$. At T_C, then, a nearest-neighbor Heisenberg model has a rather large mean angle between neighboring spins.

That D is large relates to the effective range of exchange forces, as well as to the oscillating nature of this exchange. A local magnetization disturbance is carried in an oscillatory fashion by the Ruderman-Kittel-Kasuya-Yosida (RKKY) mechanism to affect electrons at a considerable distance. This RKKY mechanism is microscopically just the propagation of virtual particle-hole pairs, the same mechanism really as appears in the RPA, or in our considerations of Sec. III. The length scale of the RKKY has been shown by Stearns[32] to play a role in the theory.

However, why does the magnetic energy saturate so relatively close to T_C? Again the RKKY argument may play a role. Because the spins on further neighbors may have an antiferromagnetic exchange, the exchange forces on nearest neighbors has to be very strongly ferromagnetic. If the nearest-neighbor exchange alone were kept, the value of T_C would be much greater. According to our estimate of the maximum $|\vec{a}|^2_{\rm av}$, one might say that the magnetic energy saturates when the spins on neighboring atoms begin to be seriously misaligned. This of course is a quasisaturation: there will certainly be a gradual further increase in magnetic energy at higher temperatures which cannot be disentangled from other types of energy in the data analysis.

How literally one can take these RKKY considerations remains to be seen. There certainly are differences between the itinerant magnets and the rare earths where RKKY exchange forces clearly dominate. It remains an interesting aim of future work to understand completely the questions raised in this section.

VI. THERMODYNAMICS OF THE FLUCTUATING-LOCAL-BAND THEORY

A. Low temperature

In the low-temperature case the prediction of our theory is identical to that of the old form of Fermi-liquid theory. For the magnetization there is a $T^{3/2}$ contribution from magnons and a T^2 term from single-particle excitation (except in the case of "strong" ferromagnets). The theories start to differ in the terms of order $T^{5/2}$ where several higher-order effects come in, among them the tilting of the electron moments away from the local average spin direction.

B. Phase transition

Finally in this section we must come to grips with the question of integrating over possible values of $\vec{a}$, first raised in Eq. (IV.1). At low temperatures $\vec{a}$ must be quantized. At higher temperatures the long-wavelength parts of $\vec{a}$ cannot be quantized, since the angles of spin deviation are large, but a classical treatment will be valid.

The shorter-wavelength ripples will still have to be quantized, however. There is no definite wave number giving a demarcation between these two regimes, which in fact merge smoothly. The most that can be hoped for is a region which can be treated with equal validity by the quantum or classical method. On the basis of neutron evidence,[7,8] we see that for $q \geq Q_0 \sim 0.25$ Å^{-1} spin waves are pretty well defined, but since the quantum energy is still rather less than T_C in this wave-number region, the classical treatment will also be valid.

Before turning to the difficulties posed by this quantum-classical transition region, let us examine what an even simpler approximation gives. In this case we treat the entire spin-fluctuation spectrum classically, which may not be too bad if thermodynamics alone is being studied. Then we have for the free energy of Eq. (IV.1) the equivalent functional integral form[33]

$$e^{-\mathfrak{F}/T} \simeq \int \mathfrak{D}\hat{M}(\vec{r}) \exp\left(-\int d^3r\, A(\nabla\hat{M})^2/T\right). \qquad \text{(VI.1)}$$

Not too much is known about functional integrals of this type. Recently, however, renormalization-group studies based on expansions about dimension 2 are for arbitrary n (the vector character of the order parameter, 3 in this case), have been made.[34] The prediction is made

$$A/T_C = (K^{d-2}/4\pi)(n-2)/(d-2), \qquad \text{(VI.2)}$$

where K is a cutoff wave number. Five things are uncertain about this formula: first, the coefficient of K^{d-2} (known only for $d-2 \ll 1$), second, the value of A, third, the value of K, and fourth, the degree to which quantum effects are important. In addition, there is the problem that the spin-wave spectrum is not accurately parabolic, as it tacitly assumed in adopting the form (VI.1).

TABLE I. Values of the exchange stiffness, zone-boundary vector, and the ratio of T_C as predicted by Eq. (VI.2) to the observed value. The exchange stiffness values are from neutron data.

Element	A (meV Å^{-1})	G(Å^{-1})	$4\pi A/GT_C$
Fe	14.2 [a]	1.55	1.28
Co (hcp)	17.5 [b]	1.44	1.27
Ni	6.9 [c]	1.54	1.04

[a] Reference 8.

[b] G. Shirane, V. J. Minkiewicz, and R. Nathans, J. Appl. Phys. 39, 383 (1960).

[c] Reference 7.

There is some indication that the coefficient is not too bad. At least an alternative derivation (below) gives a similar result.

The value of A clearly depends on the value of K. In fact, for small enough K, A/K must be constant (we take $d=3, n=3$ from now on) because we expect if the cutoff is made very small, formula (VI.1) must become exact, and the result follows on dimensional grounds. This dependence of A on K is just an example of the renormalization of parameters as shorter-wavelength fluctuations are integrated out in the renormalization-group scheme.[33]

Let us take K large enough to include all magnetization fluctuations. We adopt the zone boundary $K=G$ as a cutoff value, although it is difficult to justify this choice in detail. In this case, it is natural to choose A according to a formula like (III.8) or better yet, from experiment, using the fact that such band-structure-dependent quantities are nearly independent of temperature. We use the low-temperature neutron value for A, which derives from a parabolic fit to the magnon dispersion over a wide wave-number range. Table I gives the results, which are rather remarkable. (In cobalt, the crystallographic phase change gives further uncertainty.) Although the uncertainties just discussed make the agreement rather fortuitous, for any one element, the correlations between A/K and T_C are probably not chance.

We next discuss the behavior of Eq. (VI.1), [or Eq. (IV.1)] as the cutoff K is reduced, i.e., as the short-wavelength fluctuations are integrated out. If (VI.1) indeed holds, one has the option of renormalizing A, as just discussed. Alternatively, it can be recognized that reducing the cutoff wave number is equivalent to averaging $\vec{M}(\vec{r})$ over larger and larger regions. This of course makes $\vec{M}$ depend on K, in such a way that it eventually vanishes (for $T \geq T_C$). In this case, one can hope to express $\mathfrak{F}$ as an expansion in the components M_k, which is of course nothing but the Ginzburg-Landau type of expansion.

A formal expression for this expansion can be given by means of the Stratonovich-Hubbard transformation.[35,36] A discussion of this transformation has recently been given by Gomes and Lederer.[37] In practice, however, the method must rely on rather drastic approximations which, except perhaps for the weak ferromagnets,[36] cannot really be expected to give numerically accurate results for "nonuniversal" quantities.

In particular, this type of theory transforms away single-particle properties in favor of time-dependent magnetization fluctuations. This is not a natural description, and so there is no reason to believe in the numerical accuracy of the approximations made.

According to the discussion above, a natural type of free-energy functional to use for large K is that given in Eq. (VI.1) in which fluctuations in the magnitude of M are neglected, whereas for very small K, we can use a Ginzburg-Landau type of free-energy expression, which allows for fluctuations in the magnitude of the magnetization. [Alternatively, as mentioned, the magnitude fluctuations can be integrated out to maintain the form (VI.1)]. In order to pass smoothly from one form to the other, we rewrite, approximately, the free energy in (VI.1) as

$$e^{-\mathfrak{F}[\vec{M}]/T} = \exp\left(-\int A(\nabla\hat{M})^2 d^3r/T\right)\delta(M-M_0)/M_0^2$$
$$\approx \exp\left(-\frac{1}{2}\int [CM^2(\nabla\hat{M})^2+\chi^{-1}(M-M_0)^2]/T\right). \tag{VI.1$'$}$$

Here

$$CM^2=2A, \tag{VI.3}$$

M_0 is the magnitude of magnetization, and χ is a susceptibility against magnitude fluctuations.

As the cutoff K is lowered by integrating out the short-wavelength fluctuations, M_0 and χ will change their values. M_0 will become smaller, representing the mean magnitude of the magnetization-averaged-over-a-region-of-size-$1/K$, and χ will become larger, as the stiffness against magnetization magnitude fluctuations decreases (we restrict consideration to the case $T \geq T_C$). The constant C, however, is appropriately regarded as independent of K, as is well known in renormalization-group theory.[33] It is therefore nearly independent of temperature as well, since it may be calculated from (VI.3) for large cutoff, where we know that A is nearly temperature independent, for $T \ll T_S$. [The value of A as often quoted is one appropriate to a theory with a small cutoff K, and does depend on temperature through M. It is clearly C that appears in the Landau-Lifshitz equation and in the Ornstein-Zernike expression for the static susceptibility above T_C.] This discussion explains, for the first time, the observed constancy of C as a function of temperature.[38]

The form (VI.1′) still does not pass over to the Ginzburg-Landau form. First, the gradients of the magnetization magnitude must be included. In principle, this might be done by allowing χ to be wave-number dependent, and making a low-wave-number expansion. There are, however, some unsolved difficulties connected with the use of a sharp cutoff K which prevent numerically accurate calculations.[39]

To deal with this case, we make the following fairly extreme approximations. (a) We suppose that we may choose the cutoff K so small that the gradients are given as they would be in the Ginzburg-Landau limit, i.e., $CM^2(\nabla\hat{M})^2 \stackrel{\prime}{\rightarrow} C(\nabla\vec{\mathrm{M}})^2$. (b) We can replace $\frac{1}{2}\chi^{-1}(M-M_0)^2$ by $\frac{1}{8}(M_0^2\chi)^{-1}(M^2-M_0^2)^2$ if χ is not too large. (c) In the short-wavelength region, small-fluctuation theory (spin-wave theory) should be valid, and (d) in the remaining region the classical approximation should be valid. By choosing $K=Q_0\approx 0.25$ Å^{-1} conditions (c) and (d) are satisfied. Whether conditions (a) and (b) can be simultaneously satisfied we do not know, but later present evidence suggesting that these approximations are not very accurate.

The next step is to estimate the parameters of the theory; M_0, C, and χ. C, being constant, we may take from experiment. M_0 is the mean magnetization magnitude, reduced from the low-temperature value by short-wavelength fluctuations, (and assuming no long-wavelength fluctuation). We try spin-wave approximation

$$M_0(T)=M_s-\int(dq)/(e^{\omega_q/T}-1), \tag{VI.4}$$

with $\omega_q=Dq^2$. Here we have neglected thermal single-particle repopulation. We also must cutoff the spin-wave momentum below K.

In a similar way, we may use the spin-wave susceptibility

$$\chi=T^{-1}\int(dq)/(e^{\omega_q/T}-1)^2. \tag{VI.5}$$

We have used formulas for the reduction of M_z and for the χ_{zz} susceptibility. Here we have taken the local z direction to be, say, in the direction of

$$\vec{\mathrm{M}}(\vec{\mathrm{r}})=\int(dq)\,\vec{\mathrm{M}}_q e^{i\vec{\mathrm{q}}\cdot\vec{\mathrm{r}}}, \quad q<K. \tag{VI.6}$$

Therefore these forms are reasonable enough for $q\gg K$, but break down for $q\sim K$. In fact, because of the nonlinear relation between the components of $\vec{\mathrm{M}}$ and the angles of $\hat{M}$, the simple cutoff procedure specified in (VI.6) will lead to inaccuracies near the cutoff. Nevertheless, we simply exclude the region $q<K$ in the integrations of (VI.4) and (VI.5) as a first approximation.

We may then evaluate (VI.4) as (approximately)

$$M_0=M_s(1-C_{3/2}T^{3/2})+\alpha TK/D2\pi^2, \tag{VI.7}$$

where $C_{3/2}$ is a well-known constant function of D, which can alternatively be taken semiphenomenologically from experiment. We have introduced a factor α for later convenience.

In the same way,

$$\chi\sim(T/2\pi^2D^2)(K^{-1}-K_D^{-1}), \tag{VI.8}$$

where K_D is an upper cutoff given approximately by $K_D\sim(T/D)^{1/2}$. This expression for χ has the attractive feature of becoming large for small K.

By this sequence of approximations, we have achieved a Ginzburg-Landau form for the free energy,

$$\mathfrak{F}[\vec{\mathrm{M}}]=\int d^3x\,[\tfrac{1}{2}C(\nabla\vec{\mathrm{M}})^2-\tfrac{1}{2}a|\vec{\mathrm{M}}|^2+\tfrac{1}{4}b|\vec{\mathrm{M}}|^4] + \text{constant} \tag{VI.9}$$

with $a=(2\chi)^{-1}, b=(2\chi M_0^2)^{-1}$. The constant term has absorbed the quantity $M_0^2/8\chi$.

We restrict our discussion of the thermodynamics of this $\mathfrak{F}$ to an estimate of the transition temperature. This we estimate in the Hartree approximation, i.e., we replace the $|\vec{\mathrm{M}}|^4$ term by the best possible quadratic.[36,40] Then we find T_C is given by the relation $\xi^{-2}=0$, where

$$\xi^{-2}=(5/3M_0^2C\chi)\int_{q<K}(dq)\,\langle\vec{\mathrm{M}}(q)\cdot\vec{\mathrm{M}}(-q)\rangle-1/C\chi, \tag{VI.10}$$

and

$$\langle\vec{\mathrm{M}}(q)\cdot\vec{\mathrm{M}}(-q)\rangle=3T/C(q^2+\xi^{-2})\,. \tag{VI.11}$$

The value of T_C is then

$$T_C=2\pi^2CM_0^2/5K. \tag{VI.12}$$

If T_C is to be independent of K, we must have

$$\frac{d\ln T_C}{dK}=0=\left(\frac{2}{M_0}\right)\frac{dM_0}{dK}-\frac{1}{K}\,. \tag{VI.13}$$

By use of (VI.7) we find

$$\frac{d\ln T_C}{dK}=\frac{\alpha T_C}{\pi^2DM_0}-\frac{1}{K} \tag{VI.14}$$

which vanishes according to (VI.12) if $D=\frac{2}{5}\alpha CM_0$. Thus, we may choose α to satisfy this condition. The degree to which it differs from unity is a measure of the inadequacy of the sharp cutoff approximation in (VI.7) and (VI.8).

We next examine (VI.12) numerically. It is

TABLE II. Values of Ornstein-Zernike parameter C and M_0/M_s as defined in the text. The values of C are ferromagnetic resonance determinations by S. M. Bhagat and P. Lubitz, Phys. Rev. B 10, 179–185 (1974).

Element	C (eV Å^5)	$(M_0/M_s)_1$
Fe	3.2	0.49
Ni	15	0.61

clearly closely related to (VI.2). A difference is that C appears, and the cutoff K is quite small. The measured spin-wave dispersion at $T=0$ is distinctly nonparabolic. Therefore it is probably better to take a value of C appropriate to long wavelengths rather than the larger value corresponding to the choice of A in Table I. For K we take 0.25 Å^{-1}. Equation (VI.12) then predicts a value of M_0/M_s, denoted in Table II as $(M_0/M_s)_1$.

The expression (VI.7), however, does not agree very well with this. Using the low-temperature values for $C_{3/2}$ gives $C^0_{3/2}T_C^{3/2}=0.12$ for both Fe and Ni. Making the crude fit to the data that the measured spin-wave spectrum for $q>0.25$ Å^{-1} is given by Dq^2 with $D_{T_C}\sim 0.55D_0$, and setting $C_{3/2}=C^0_{3/2}(D_0/D_{T_C})^{3/2}$ gives a value for M_0/M_s, due to this term alone, of 0.71. Using Eq. (VI.4) gives an unrealistically large value of the final term of Eq. (VI.7). Even with $\alpha=1$, this contribution is of order $0.1M_s$. Thus the theory is unsatisfactory in that (VI.12) suggests a lower value of M_0 than that predicted by (VI.7). Further, this cannot be rectified by use of the correction factor α. However, we found it necessary to resort to rather drastic approximations. Furthermore, as we shall see in paper II (hereafter referred to as II) the spin-wave spectrum at high temperature does not have the quadratic form we attributed to it in the above analysis. However, our results in II cannot be readily carried over at this stage, since it is in precisely the cutoff region that significant uncertainties appear. Some progress has been made in this region in the context of the nonlinear Landau-Lifshitz equation. We continue however, to be encouraged by the fact that iron, nickel, and probably cobalt all show quite similar discrepancies between theory and experiment.

We finally remark that, by use of (VI.8), an estimate can be made of the fluctuations in the magnitude of the magnetization. Using (VI.13), we find $\langle (M-M_0)^2\rangle \approx \beta M_0^2$ where the numerical factor β depends on details of the averaging process.

However, $\beta \approx 1-K/K_D$ which is a plausible behavior, as for K very small, large-magnitude fluctuations are expected. Our derivation of (VI.9) was based on the assumption of small-magnitude fluctuations, so this is a source of error. Probably, therefore, the errors listed as (a) and (b) before Eq. (VI.8) are not insignificant.

VII. SUMMARY

We have presented a theory of itinerant magnetism based on a classical treatment of the collective variable $\hat{M}$. In zeroth approximation, the state of the system is that given by band theory, or by Fermi-liquid theory with the spin quantization in the direction of $\hat{M}$.

Much can be learned without specifying how $\hat{M}(\vec{r})$ is to be calculated. These results serve to give a qualitative understanding of many hitherto puzzling observations. To compute the actual thermodynamics of the phase transition requires averages over $\hat{M}(\vec{r})$. The machinery encountered is that used in renormalization-group studies of the phase transition. This machinery is not, however, sufficiently developed to give reliable numerical results for the nonuniversal quantities. However, the theory applies equally to iron, nickel, and cobalt, and probably to the weak ferromagnets as well. The numerical results are consistent with this.

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