Spin Waves in Ferromagnetic Metals and the Dynamical Form of the Landau Quasi-Particle Theory

MORREL H. COHEN

Solid State Science Division
Argonne National Laboratory, Argonne, Illinois

and

Department of Physics and Institute for the Study of Metals
The University of Chicago, Chicago, Illinois

and

DAVID R. PENN

Metallurgy Division
Argonne National Laboratory, Argonne, Illinois

The measured change with temperature of spin-wave frequencies in metallic ferromagnets is proportional to $T^{5/2}$. The usual Landau quasi-particle theory would yield an incorrect $T^{3/2}$ term. Successful theories of the $T^{5/2}$ dependence have started out from hamiltonians which may be interpreted as containing dynamical quasi-particle interactions. In the present paper we supply the needed derivation of the dynamical form of the Landau quasi-particle theory for uniform systems and comment on its relation to the previous version of the theory. We show, in effect, that the derivations of the $T^{5/2}$ dependence by Izuyama and by Kawasaki are exact and thus complete the justification of Marshall's original explanations. The connection between the present form of the theory and the original Landau form and its generalizations is briefly indicated.

I. INTRODUCTION

Measurements of the temperature dependence of the spin-wave (S.W.) frequencies in ferromagnetic Ni[1,2] and Permalloy[3] have yielded $D = D_o(1 + E_{5/2}T^{5/2})$ where D is the coefficient of the quadratic term in the spin-wave dispersion relation $\omega(q) = Dq^2 + O(q^4)$. It has been known for over a decade[4] that the itinerant electron model is capable of describing spin-wave excitations as well as electron-hole excitations in ferromagnetic metals. An explicit expression for the coefficient D was derived within that framework by Izuyama, Kim, and Kubo,[5] who obtained $D = D_o(1 + E_{3/2}T^{3/2} + E_2T^2 + O(T^{7/2}))$. These authors assumed a single conduction band and a simplified electron-electron interaction (S.I.)

$$V_{INT} = U\Sigma_{kk'q\sigma\sigma'} a^+_{k+q,\sigma} a^+_{k'-q,\sigma'} a_{k'\sigma'} a_{k\sigma}$$

where $a^+_{k,\sigma}$ creates an electron in the Bloch state k with spin σ. Use of the random phase approximation (R.P.A.) then yields their expression for D. This use of the R.P.A. is completely equivalent to the use of a simple self-consistent field theory,[6] in this case Hartree-Fock, in which electrons interact only in a statistically averaged manner. It is the averaged interaction which specifically leads to the incorrect $T^{3/2}$ term in D. A Landau quasi-particle picture of a ferromagnetic metal can be

obtained directly from the usual Landau Fermi liquid theory[7] simply by making the proper distinction between the two inequivalent spin systems, as was done by Abrikosov and Dzialoshinski.[8] Nevertheless, this far more general quasiparticle theory would still yield the incorrect $T^{3/2}$ term because it, too, contains only statistically averaged interactions. However, Marshall[9] has used phenomenological arguments to develop a spin-wave hamiltonian including interactions between spin-waves which in turn give rise to a $T^{5/2}$ term in D. Izuyama and Kubo,[10] again using the S.I. obtained $D = D_o(1 + E_2T^2 + E_{5/2}T^{5/2})$ by abandoning the R.P.A. and employing instead a diagramatic form of perturbation theory. Izuyama[11] and Kawasaki[12] then showed that a more sophisticated application of the R.P.A. to the S.I. would give a S.W.-S.W. interaction of the form assumed by Marshall, thereby lending support to his phenomenological approach. To explain the fact that the T^2 term has not been observed,[1-3] it has been suggested by Kawasaki that E_2 is small.

The parameters entering the hamiltonians[5,9,10] discussed above are not well defined by the various authors, although Izuyama and Kubo[8] do remark that their interaction constant U should be viewed as a particle-particle t-matrix. If the parameters are the bare interactions and the unrenormalized single particle energies, then it is clear that all the large renormalization processes, correlation effects, etc., must be taken into account before the spin-wave theory is set

up inasmuch as the spin-wave energies are small and their interactions weak. If, on the other hand, all renormalizations are already effected, as we believe they must be, the hamiltonians describe dynamically interacting quasi-particles and have never, to our knowledge, been derived from first principles. We thus arrive at the central concern of the present paper. In order to have an adequate description of the S.W.-S.W. interactions in ferromagnetic metals, one must have a hamiltonian for Landau quasi-particles containing fully dynamical interactions among the quasi-particles in contrast to the usual formulation[7] with statistically averaged interactions. We supply here in Sec. II the lacking derivation of such a fully dynamical quasi-particle hamiltonian by making what seems to us to be the minimal required generalization of Landau's original verbal derivation.

By giving the earlier theories[5,9,10] a more rigorous basis in this way, we complete the demonstration of the essential correctness of Marshall's original explanation, as discussed in Sec. III. We also discuss there the relationship of the present theory to the standard Landau theory[7] and suggest further generalizations thereof.

II. THE DYNAMICAL HAMILTONIAN

We consider a uniform system of interacting spin-1/2 Fermions, realizations of which might be jellium or He^3. The system is supposed initially at some time T_1 in the remote past to move according to any convenient independent-particle hamiltonian, H_o, e.g., the free particle hamiltonian. H_o generates a complete set of determinantal wave functions $\Psi^{(o)}$ and energies $E^{(o)}$ which depend only on the set of occupation numbers of the single-particle plane-wave states $\{n_k\}$, the subscript k standing both for wave vector and spin,

$$H_o \Psi^{(o)}(\{n_k\}) = E^{(o)}(\{n_k\})\Psi^{(o)}(\{n_k\}). \qquad (1)$$

The states $\Psi^{(o)}(\{n_k\})$ will fall into families of states each of which is characterized by special symmetry properties, e.g., total momentum, net magnetization, etc. Each of these families of states can be labelled by a subscript α specifying such family properties, $\Psi^{(o)}(\{n_k\}_\alpha)$, α implying an appropriate restriction on the $\{n_k\}$. Within each family there will be some ground state $\Psi^{(o)}(\{n_k\}_{\alpha G})$.

We now suppose that the difference between H_o and the actual hamiltonian H is turned on adiabatically, i.e., extremely slowly, over the time interval T_2-T_1 which becomes infinite in the limit that T_1 recedes to $-\infty$. At times

within (T_1,T_2) the motion of the system is governed by the time dependent hamiltonian

$$H(t) = H_o + g(t)(H - H_o) , \tag{2}$$

where $g(t)$ varies smoothly from 0 to 1 in (T_1,T_2),

$$\begin{gathered} g(t) = 0, t<T_1;\ g(t) = 1, t>T_2, \\ 0 = g(T_1)\leq g(t)\leq 1 = g(T_2),\ T_1\leq t\leq T_2. \end{gathered} \tag{3}$$

Following the standard arguments of adiabatic perturbation theory,[13] we introduce the instantaneous eigenstates,

$$H(t)\,\phi_m(t) = E_m(t)\,\phi_m(t) , \tag{4}$$

and the adiabatic transforms of the initial eigenstates.

$$\Psi(\{n_k\}_\alpha,t) = U(t,T_1)\Psi^{(o)}(\{n_k\}_\alpha). \tag{5}$$

The latter will, in general, be distinct from the former and may be expanded in terms of them:

$$\Psi(\{n_k\}_\alpha,t) = \sum_m C_m(\{n_k\}_\alpha,t)\phi_m(t)\exp\left(\frac{-i}{\hbar}\int^t E_m(t')dt'\right). \tag{6}$$

Substituting (6) into the Schrödinger equation yields

$$\dot{C}_m(\{n_k\}_\alpha, t) = \sum_n{}' \frac{(\Phi_m, \dot{H}\Phi_n)}{E_m - E_n} C_n(\{n_k\}_\alpha, t) \qquad (7)$$

for a nondegenerate set of energies E_m. Clearly, if all of the energy levels of our macroscopic system were nondegenerate, then $\dot{C}$ would vanish since H vanishes in the adiabatic limit. The adiabatic transforms $\Psi(\{n_k\}_\alpha, t)$ of the independent-particle states $\Psi^{(o)}(\{n_k\}_\alpha)$ become identical to the instantaneous eigenfunctions $\Phi_m(t)$ at all times, including those times $t > T_2$ for which H(t) becomes identical to H. Upon neglect of degeneracy, then, the exact states of the interacting system become identical to the adiabatic transforms of the single particle states.

This neglect of degeneracy is precisely correct only for the ground state $\Psi_{\alpha G}$ of any given family Ψ_α. It is possible that the ground states of different families cross, but H has no matrix elements between them because H(t) preserves the symmetry properties on which the classification into families is based. We conclude that $\Psi(\{n_k\}_{\alpha G}, T_2)$ is an exact eigenstate of H and further it is the ground state within the family of exact eigenstates of H of symmetry type α.

We are concerned here with systems for which the actual ground state is ferromagnetic with magnetization or, more precisely, total magnetic quantum number M, the symmetry type α in this case being equivalent to M. The ferromagnetic ground state Ψ_{MG} is thus the adiabatic transform of the single

particle ground state $\Psi_{MG}^{(o)}$ of the family of single particle states having magnetization M, $\Psi_{M}^{(o)}$, despite the fact that $\Psi_{MG}^{(o)}$ need not be the absolute ground state of H_o, the initial hamiltonian.

Because Ψ_{MG} is the adiabatic transform of $\Psi_{MG}^{(o)}$, it is labelled by precisely the same set of occupation numbers as $\Psi_{MG}^{(o)}$, $\{n_k\}_{MG}$. These occupation numbers correspond to two unequally filled Fermi spheres, one for each spin. The same remains true for the exact ground state Ψ_{MG}. Whereas the occupation numbers and Fermi spheres originally related to the individual particles, they now relate to the adiabatic transforms of the individual particles, the Landau quasi-particles. Thus the complete set of excited states $\Psi_{\alpha}(\{n_k\})$ generated by the adiabatic transformation of the independent particle states provides the basis for a quasi-particle representation. This representation has the great advantage that the basis functions are in one-to-one correspondence with the free-particle states and yet include the exact ground state. Thus all matrix elements between $\Psi_{\alpha G}$ and excited states vanish; however, the excited states mix among themselves because the adiabatic theorem breaks down for them. This means that in general the quasi-particle representation of H has the property

$$\langle \{n_k\}_{\alpha} | H | \{n'_k\}_{\alpha'} \rangle = \delta_{\alpha\alpha'} f(\{n_k\}_{\alpha}, \{n'_k\}_{\alpha}), \quad (8)$$

where f does not vanish unless $\{n_k\}_\alpha$ or $\{n'_k\}_\alpha$ equals $\{n_k\}_{MG}$ and

$$|\{n_k\}_\alpha> = U(T_2,T_1)\Psi^{(o)}(\{n_k\}_\alpha). \qquad (9)$$

It is convenient at this point to forget about the classification of states by symmetry types, to drop the index α, and to eliminate the corresponding restriction on the $\{n_k\}$. The various matrix elements of H can be grouped according to the number of changes of occupation number involved, a kind of cluster expansion:

$$<\{n_k\}\ |H|\ \{n'_k\}> = \sum_{\mu=0}^{\infty} g\ (\{n_k\},\{n'_k\})\ , \qquad (10)$$

where 2μ is the number of changes of quasi-particle occupation number involved in passing from $\{n'_k\}$ to $\{n_k\}$. Thus g_o vanishes unless $\{n_k\}$ is identical to $\{n'_k\}$, g_1 vanishes unless they differ in two members, g_2 vanishes unless they differ in four members, etc. In addition, the g_μ vanish if either $\{n_k\}$ or $\{n'_k\}$ equals $\{n_k\}_G$ when $\mu > 0$. We can make this last restriction explicit by the use of projection operator $\mathcal{P}$ which vanish when acting on the ground state from either the left or the right

$$g_\mu(\{n_k\},\{n'_k\}) = \Sigma \mathcal{P}(\{n_k\},\{n''_k\})\ h_\mu(\{n''_k\},\{n'''_k\})\mathcal{P}(\{n'''_k\},\{n'_k\}), \qquad (11)$$

where the h_μ no longer are restricted in their action on the ground state and are defined for that case by continuation from low-lying excited states.

The matrix elements of ρ in (11) may be written explicitly as

$$\rho(\{n_k\},\{n'_k\}) = \delta_{\{n_k\},\{n'_k\}} - \delta_{\{n_k\},\{n_k\}_G}\,\delta_{\{n_k\}_G,\{n'_k\}}\ , \tag{12a}$$

i.e.,
$$\rho = 1 - P \tag{12b}$$

The operator P may be decomposed into the product

$$P(\{n_k\},\{n'_k\}) = \prod_k \delta_{n_k,n_k^G}\,\delta_{n_k^G,n'_k} = \prod_k P_k(n_k,n'_k) \tag{13a}$$

where n_k^G is the value of n_k in the ground state. The matrices P_k are diagonal in the n_k,n'_k representation and hence independent of one another; it is convenient to reexpress P_k as

$$P_k = 1 - p_k. \tag{13b}$$

Two equivalent expressions are readily obtained for p_k by direct examination of the matrix $\delta_{n_k,n_k^G}\delta_{n_k^G,n'_k}$:

$$p_k = \tilde{\nu}_k = \tilde{n}_k \text{ if } n_k^G = 1,$$
$$= \tilde{1} - \tilde{n}_k \text{ if } n_k^G = 0. \tag{14a}$$

$$p_k = (-1)^{\tilde{n}_k}(\tilde{n}_k - n_k^G \tilde{1}) = (-1)^{\tilde{n}_k}\tilde{\delta}_{n_k}. \tag{14b}$$

In (14) a tilde indicates an operator in second quantization, $\tilde{n}_k$ is the ordinary number operator, and $\tilde{\nu}_k$ is the number operator which switches from electron to hole character below the Fermi surface. Using (14a), for example, Φ may be written as

$$\Phi = 1 - \prod_k (1 - \tilde{\nu}_k). \tag{15}$$

One sees immediately, that any factor in (15) containing an excited quasi-particle state, $\nu_k = 1$, forces Φ to unity, whereas if no excited quasi-particles are present Φ is forced to zero. Note that Φ can be expanded in powers of the $\tilde{\nu}_k$ and truncated after the term of degree equal to the number of excited quasi-particles present.

Let us now introduce quasi-particle creation ($c^\dagger_k$) and destruction (c_k) operators as the adiabatic transforms of the particle creation ($a_k^\dagger$) and destruction (a_k) operators,

$$c^+_k = U(T_2,T_1)\ a_k^\dagger U^\dagger(T_2,T_1)$$
$$c_k = U(T_2,T_1)\ a_k\ U^\dagger(T_2,T_1) \tag{16}$$

Because of the one-to-one correspondence of the a's and C's, the C's have the same properties in the quasi-particle basis as the a's do in the independent particle basis. Thus, the operator represented by the matrix element g_o can depend only on the quasi-particle number operators $C^\dagger_k C_k$, h_1 must contain products like $C^\dagger_k C_{k'}$, $k' \neq k$, as well, and h_2 must contain products like $C^\dagger_{k_1} C^+_{k_2} C_{k_3} C_{k_4}$, with $k_1 \neq k_3, k_4$ or $k_2 \neq k_3, k_4$. Translation invariance requires that h_1 vanishes because of the restriction $k \neq k'$ and that $k_1 + k_2 = k_3 + k_4$ in h_2.

Putting all this together permits us to obtain an explicit expression for the hamiltonian in terms of the quasi-particle operators:

$$H = H_d(\{C^+_k C_k\}) + \frac{1}{2} \sum_{\substack{k,k',q \\ q\neq o, k'\neq k+q}} \frac{1}{2}[V_q(k,k', C^+C), c^+_{k+q} c^+_{k-q} c_{k'} c_k]_+ , \tag{17}$$

where we have truncated the cluster expansion by keeping only terms for which $\mu \leq 2$. In the spirit of this cluster approximation, the justification for which is that H need be accurate only for low-lying states of excitation containing few excited quasi-particles, we may expand $H_d(\{C^+_k C_k\})$ about the ground state energy in powers of the $\delta \underset{\sim}{n}_k$ and terminate the expansion after second order:

$$H_d(\{C^+_k C_k\}) = E_G + \sum_k \epsilon_k \, \delta \underset{\sim}{n}_k + \frac{1}{2} \sum'_{k\,k'} f_{k\,k'} \, \delta \underset{\sim}{n}_{k'} \, \delta \underset{\sim}{n}_k \quad , \tag{18}$$

where

$$\epsilon_k = \frac{\delta H_d(\{n_\ell\}_G)}{\delta n_k} \quad , \tag{19}$$

and

$$f_{k\,k'} = \frac{\delta^2 H_d(\{n_\ell\}_G)}{\delta n_k \, \delta n_{k'}} \quad . \tag{20}$$

The number-deviation operators $\delta\underset{\sim}{n}_k$ are defined in (14b). Eq. (18) may also be expressed in terms of the $\underset{\sim}{\nu}_k$ through a modified version of the identity implicit in (14),

$$\underset{\sim}{\nu}_k = (-1)^{n_k^G} \, \delta\underset{\sim}{n}_k \quad . \tag{14'}$$

Substituting (18) into (17) and replacing $V_q(k\,k';\{C_\ell^\dagger\, C_\ell\})$ by the extrapolation to the ground state of its eigenvalue $V_q(k,k')$ for low-lying states gives the desired hamiltonian

$$H = E_G + \sum_{k'} \epsilon_k \, \delta\underset{\sim}{n}_k + \frac{1}{2} \mathcal{P}[\sum_{k,k'}{}' f_{k\,k'} \, \delta\underset{\sim}{n}_k \, \delta\underset{\sim}{n}_{k'} +$$

$$+ \sum_{\substack{k,k' \\ q\neq o,\, k'-k}} V_q(k,k') \; C^\dagger_{k+q} \; C^\dagger_{k'-q} \; C_{k'} \; C_k] \mathcal{P} . \tag{21}$$

The projection operators may enclose the term in $\delta\underset{\sim}{n}_k \, \delta\underset{\sim}{n}_{k'}$ because it automatically annihilates the ground state.

III. DISCUSSION

Eq. (21) gives a quasi-particle hamiltonian containing dynamical interactions among the quasi-particles. It may be put into closer correspondence with the hamiltonian of the conventional form employed by Izuyama and by Kawasaki in their derivation of the $T^{5/2}$ law by writing the δn_k out explicitly as $C^+_k C_k - \frac{1}{2} n_k^G$:

$$H = U + \sum_{k'} \epsilon'_k C^+_k C_k + \frac{1}{2} \sum_{\substack{k,k' \\ q}} V_q(k,k') \rho C^+_{k+q} C^+_{k'-q} C_{k'} C_k \rho, \tag{22}$$

where

$$U = E_G + \rho \frac{1}{2} \sum'_{k,k'} f_{k\,k'}\, n_k^G n_{k'}^G \rho, \tag{23}$$

$$\epsilon'_k = \epsilon_k - \rho \sum_{k'} f_{k\,k'}\, n_{k'}^G \rho \tag{24}$$

and the restrictions in the sums over k,k' and q present in (21) have been eliminated through the reordering of $C^+_{k'} C_{k'} C^+_k C_k$ and through the identification

$$f_{k\,k'} = V_o(k,k') - V_{k'-k}(k,k'). \tag{25}$$

Thus $V_o(k,k')$ and $V_{k'-k}(k,k')$ in (22) originate in a way formally different from the origin of $V_q(k,k')$, $q \neq o$ or $k-k'$, and the derivation of (22) in no way guarantees continuity,

i.e., that

$$f_{k\,k'} = \lim_{q \to o} V_q(k,k') - \lim_{q \to k'-k} V_q(k,k') \qquad (26)$$

should hold. However, if we suppose our system to be extensive, Eq. (26) must hold. The requirement of extensiveness is equivalent to requiring that the effect of a uniform distortion of the system be the same as the effect of the limit of a slowly varying distortion. An elementary calculation done either on (21) or on (22) then shows that (26) is required.

The Hamiltonian (22) differs in form from that employed by Izuyama and by Kawasaki in the appearance of the projection operator $\mathcal{P}$. This would in no way modify the final results of their calculations because they study the equation of motion of spin-wave creation operators. This guarantees that in the course of the analysis H or a related operator is not applied directly to the ground state. The projection operators then either drop out by reducing to unity or can be incorporated into the definition of the spin-wave operators. In this way we are led to a deeper understanding of the $T^{5/2}$ term obtained by Izuyama and by Kawasaki as an essentially exact result.

The relation of our hamiltonian in the form (21) to the conventional Landau theory[7] is fairly straightforward. The ϵ_k in (21) are obviously identical to the single quasiparticle energies of Landau. On the other hand, the $f_{k\,k'}$ in

Eq. (21) are not identical to the interactions in Landau's theory,[7] nor are the $V_q(k,k')$ identical to the interactions entering generalizations of Landau's theory to nonuniform systems.[14,15] Nevertheless, one can derive the usual form of the Landau theory from (21) simply by summing virtual ladders. The justification for this is that the density of real excited quasi-particles is low and the residual interaction $V_q(k,k')$ is of finite range. The result is that the Landau interaction is the t-matrix corresponding to our $V_q(k,k')$. The derivation evidently breaks down in principle when the t-matrix has poles on the real frequency axis associated with collective modes lying outside the free particle continuum, as occurs, for instance, in ferromagnetic metals at the spin-wave frequencies. Hence the present analysis affords a starting point for going beyond the Landau theory to obtain rigorously a hamiltonian containing, for example, quasi-particle-spin-wave interactions as well as spin-wave-spin-wave interactions. In the absence of collective modes, the transformation from the dynamical form (21) to the usual Landau form changes the basis wave functions from plane-wave states for the individual quasi-particles to scattering states, and similarly for the field operators.

We note in closing that our hamiltonian for dynamically interacting quasi-particles has been derived for a uniform system whereas, of course, all real metals are nonuniform because of the electron-ion core interaction. In attempting to repeat the derivation of (21) for the nonuniform case, we

have found that the adiabatic transformation argument becomes so intricate as to lose much of its pedagogical value, and we have not yet carried it to completion.

IV. ACKNOWLEDGMENT

This paper is based on research performed in part under the auspices of the U. S. Atomic Energy Commission and supported in part by the National Aeronautics and Space Administration. It also benefitted from general support of Materials Science at the University of Chicago by the Advanced Research Projects Agency.

We are indebted to Dr. J. L. Beeby for a stimulating discussion on the relation between the present theory and the standard version of the Landau theory.

REFERENCES

1. P. E. Tannewald, J. Phys. Soc. Japan, 17, Sup. B-1, 592 (1962).

2. M. Matherly, K. Mirakawa, R. D. Lowde, J. F. Mallett, M. W. Stringellow, B. H. Torrie, J. Appl. Phys. 35, 802 (1964).

3. R. R. Weber and P. E. Tannewald, J. Phys. Chem. Solids 24, 802 (1964); Phys. Rev. 140, A498 (1965); J. Appl. Phys. 3, 937 (1966).

4. C. Herring and C. Kittel, Phys. Rev. 81, 869 (1951).

5. T. Izuyama, D. J. Kim and R. Kubo, J. Phys. Soc. Japan 18, 1025 (1963).

6. H. Ehrenreich and M. H. Cohen, Phys. Rev. 115, 786 (1959).

7. D. Landau, Sov. Phys. JETP 3, 920 (1956); 5, 101 (1957); D. Pines and P. Nozieres, The Theory of Quantum Liquids, W. A. Benjamin, Inc., New York, 1966.

8. A. A. Abrikosov and I. E. Dzialoshinski, Sov. Phys. JETP 8, 535 (1959).

9. W. Marshall, Proceedings of the Eighth International Conference on Low-Temperature Physics, Butterworths Scientific Publications, Ltd., London, 1962.

10. T. Izuyama and R. Kubo, J. Appl. Phys. 35, 1074 (1964).

11. T. Izuyama, Phys. Letters 9, 292 (1964); Phys. Rev. Letters 12, 585 (1964).

12. K. Kawasaki, Phys. Rev. 135, A1371 (1964).

13. L. Schiff, Quantum Mechanics, McGraw-Hill Book Company, Inc., New York, 1955.

14. A. M. de Graaf and R. Luzzi, Il Nuovo Cimento 38, 4864 (1964).

15. D. R. Penn and M. H. Cohen, submitted to Phys. Rev.