Intermediate-Coupling Theory for Itinerant Ferromagnetism

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(Received 24 March 1972)

Electron-magnon interaction processes afford a basis for understanding the large many-body effects in itinerant ferromagnets. Careful observance of the requirements of rotational invariance leads to important corrections to the electron-magnon vertex function. The result is a self-consistent intermediate-coupling theory expected to be applicable to Ni.

This Letter describes an attempt to fill the gap between weak- (Stoner) and strong- (Hubbard) coupling theories of itinerant ferromagnetism, taking the random-phase approximation (RPA) theory as a starting point. We will talk in terms of the conventional single-band model with zero-range interactions.[1] The interaction is assumed to include at the outset the electron-electron correlation effects discussed by Kanamoir.[2] We discuss here the case of strong ferromagnetism, where one of the spin bands is either full or empty. Nickel and cobalt are commonly held to fall under this classification. To be specific, assume that in the ground state, all the electrons have spin up (partially filling the up band). The bottom of the down spin band then lies above the Fermi level.

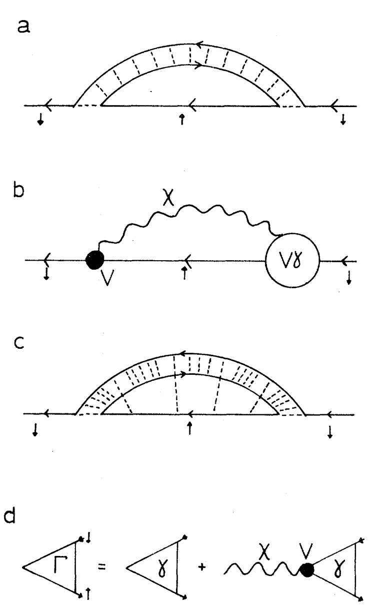

FIG. 1. Self-energy and vertex diagrams: (a) the lowest-order class of self-energy corrections; (b) the (formally exact) self-energy; (c) dominant corrections to (a). The ladders and vertices should, of course, be replaced by their renormalized values. (d) The structure of the full vertex Γ.

The up electrons are then inert, since any contribution to their self-energy requires the creation of an electron-hole pair in the empty down spin band. Spin-up electron-hole pairs can be created, though, leading to large and important contributions to the self-energy of the down electrons. Our initial approximation is motivated by a consideration of the possible final-state interactions, given the picture of a spin-down electron and an excited spin-up electron-hole pair. The Pauli principle forbids interaction between the up electron and hole because the force is zero range, and the repeated scattering of the two electrons is included in the interaction implicitly. We are left with the strong resonant scattering of down electron and up hole, which is responsible for the ferromagnetic instability in the first place. The electron-hole triplet "bound state" is the magnon.

We are then led to a magnon-dominance sort of theory, with the simplest sort of self-energy diagram that shown in Fig. 1(a).[3] At $T=0$,

$$\Sigma_0(\vec{k},E)=V^2\sum_{k'}\int\frac{dE'}{2\pi i}\times G_\uparrow(\vec{k}',E')\chi^{+-}(\vec{k}-\vec{k}',E-E'), \qquad (1)$$

where V is the interaction strength. The transverse susceptibility χ^{+-} includes both a magnon pole and the Stoner continuum of spin-flip excitations. For a strong ferromagnet, the Stoner excitations lie at high energies and have little spectral weight, so on both counts their contribution to Σ is small. Furthermore, even when the spin-wave mode merges with the Stoner continuum, there will still be a strong resonance near the magnon energy, so it makes good sense to approximate χ by a simple magnon pole form

$$\chi^{+-}(\vec{q},\omega)=\sigma/(\omega_q-\omega-i\delta). \tag{2}$$

(This form is exact as $\vec{q}\to 0$, where the Stoner excitations have vanishing spectral weight.) In that case, (1) is simply

$$\Sigma_0(\vec{k},E)=V^2\sigma\sum_{k'}\frac{1-f_{k'\uparrow}}{E-\epsilon_{k'}-\omega_{k-k'}+i\delta}, \tag{3}$$

where σ is the magnetization ($=\langle n\uparrow\rangle$ here). An important point is that with or without the spin-wave pole approximation, Σ_0 only has spectral weight above a sharp threshold which is always at or above the Fermi energy.[4]

This level of theory has two serious drawbacks. First, in attempts to apply it to real metals, it leads to energy shifts which are unrealistically large.[5] And more alarmingly, it leads to the following vexing self-consistency problem. In order to make the theory self-consistent, dressed spin-down electron propagators should be used in the ladder of Fig. 1. But the resulting susceptibility is unacceptable because the magnon pole now appears at a negative energy (for sufficiently small q and certainly for $q=0$). This behavior violates the Goldstone theorem (an expression of rotational invariance), which demands that the pole in χ occur at $\omega=0$ for $q=0$ and positive ω for finite q. This inconsistency was also discussed by Brandt.[6]

We now show how to construct a theory which gives a reasonable description of many-body effects and at the same time maintains rotational invariance. As we will see, it has several interesting features. The idea is to keep a generalized magnon dominance picture, but with a renormalized electron-magnon vertex function [Fig. 1(b)] and to use the requirement of spin conservation to dictate the renormalized vertex. The formal tool for imposing this condition is a Ward identity.

The identity is straightforward to derive, following the Takahashi procedure.[7] To summarize it, one considers the coupling of the system to an external four-vector field F_μ. The time component F_0 couples to the spin density $\vec{S}(z)$; we take it to be, say, the component $H^+=H_x+iH_y$ of a magnetic field. [It then couples to $S^-(z)$.] The spatial components F_i couple to the spin current density $J_i^-(z)$. Perturbation theory then gives the first-order response of the spin-flip electron propagator $G_{\uparrow\downarrow}(x,y)$ as $\langle T[J_\mu^-(z)\psi_\uparrow(x)\psi_\downarrow^+(y)]\rangle$. In this notation, x means $(\vec{x},t)$ and $J_0^-(z)$ is the spin density $S^-(z)$. One defines the vertex function $\Gamma_\mu(x,y,z)$ by setting this response equal to $\int d^4x' \times d^4y'\, G_\uparrow(x,x')\Gamma_\mu(x',y',z)G_\downarrow(y',y)$. Taking the four-divergence of both these expressions, using the spin conservation condition $(\partial/\partial z_\mu)J_\mu(z)=0$, and Fourier transforming, we arrive at the conventional form

$$q^\mu\Gamma_\mu(p,p-q)\equiv q_0\Gamma_0(p,p-q)-\vec{q}\cdot\vec{\Gamma}(p,p-q)$$
$$=G_\downarrow^{-1}(p)-G_\uparrow^{-1}(p-q). \tag{4}$$

An important point here is that in the ferromagnetic state, (4) cannot be reduced to the usual differential form $\Gamma_\mu(p,p)=\partial G^{-1}(p)/\partial p_\mu$ because the right-hand side is finite at $q=0$.

Consider now $\gamma(p,p-q)$, the irreducible part of $\Gamma_0(p,p-q)$. By "irreducible," we mean that a diagram for it cannot be divided into two disconnected pieces by removing an interaction vertex. Figure 1(d) shows the relationship between Γ and γ. If we divide any reducible diagram for Γ at its rightmost point of reducibility, everything to the left of that point is a contribution to the full $\chi(q)$ and everything to the left a contribution to $\gamma(p,p-q)$:

$$\Gamma_0(p,p-q)=\gamma(p,p-q)+V\chi(q)\gamma(p,p-q). \tag{5}$$

The irreducible vertex is important because a separation exactly like (5) may be made in the structure of all the diagrams which replace the RPA ladder of Fig. 1(a) in diagrams for the self-energy, resulting in the identification of $V\gamma(\boldsymbol{k},\boldsymbol{k}')$ as the electron-magnon vertex function in Fig. 1(b).

To generate our estimate of γ, we first take the limit $\vec{q}\to 0$ in (4) to get rid of $\vec{\Gamma}$. [Actually, one must check that $\vec{\Gamma}$ does not contain any singular ($\sim 1/|\vec{q}|$) terms in this limit. In fact it does, but they cancel at $\vec{q}=0$.] Conbining this with (5) and using the magnon propagator (2) (exact in this limit), we obtain at $q_0=0$

$$\gamma(p,p)=[\Sigma(p)+\Delta]/\Delta, \tag{6}$$

where $\Delta=V\sigma$ is the Hartree-Fock band splitting and Σ is the rest of the self-energy (all the many-body effects). Then approximating $\gamma(\boldsymbol{k},\boldsymbol{k}')$ by $\gamma(\boldsymbol{k},\boldsymbol{k})$, it is simple to solve for

$$\Sigma(\vec{k},E)=\gamma(\vec{k},E;\vec{k},E)\Sigma_0(\vec{k},E)$$
$$=\Sigma_0(\vec{k},E)/[1-\Sigma_0(\vec{k},E)/\Delta], \tag{7}$$

where Σ_0 is given by (1) with the full $\chi(\boldsymbol{k}-\boldsymbol{k}')$ in place of the RPA expression. It is also illuminating to exhibit the form of the total self-energy, including the Hartree term:

$$\Sigma_{tot}(\vec{k},E)=\Delta+\Sigma(\vec{k},E)$$
$$=\Delta/[1-\Sigma_0(\vec{k},E)/\Delta]. \quad (8)$$

That is, all the many-body effects are concisely expressible in terms of a $\vec{k}$- and E-dependent renormalization of the band splitting.

Furthermore, it is easy to check that using $V\gamma$ in place of V in calculating χ leads to the proper long-wavelength, low-frequency behavior required by the Goldstone theorem. We have (exactly)

$$\chi(q)=\varphi(q)/[1-V\varphi(q)], \quad (9)$$

where

$$\varphi(q)=(2\pi)^{-4}i\int d^4k\,\gamma(k,k-q)G_\downarrow(k)G_\uparrow(k-q), \quad (10)$$

and at $q=0$, the choice (6) makes the denominator of (9) vanish.

Diagrammatically speaking, the source of the vertex corrections lies in processes where the spin-down electron in the χ ladder can scatter off the up electron as well as the up hole, as shown in Fig. 1(c). One can isolate an effective bare vertex Λ for direct electron-magnon scattering; at zero momentum and energy for the spin wave, we find

$$\Lambda=-i(2\pi)^{-4}V^3\int d^4k\,\gamma^2(k,k)G_\downarrow^2(k)G_\uparrow(k)$$
$$=V/\sigma. \quad (11)$$

Summing up all the processes of Fig. 1, we are again led to (7). Edwards[8] summed diagrams of this class for the special case of a nearly half-filled band, finding a result like (8).

Figure 2 shows typical spectral weight functions obtained in this approximation for down electrons in a parabolic band model. We have chosen a bandwidth W such that the "band" contains half an electron state per atom. The Hartree-Fock band splitting is $1.18W$ and the net magnetization σ is 0.417. We calculated Σ_0 from (3), assuming a quadratic spin-wave dispersion relation $\omega_q=Dq^2$, with $2mD=0.3$ (m is the electron effective mass). This estimate of D was obtained from the analysis of Edwards.[8] One sees the possibility of extra quasiparticle peaks well below the Hartree-Fock energies, for small k. The lower peak corresponds to the magnetic polaron discussed, for example, by Izyumov, Kassan-Ogly, and Medvedev.[9]

Several consequences are manifest. First, it is evident that the measured band splitting will be considerably less than the Hartree-Fock Δ, and this fact should be kept in mind in attempts to infer the value of Δ or V from optical or photoemission data. Furthermore, the minority spin density of states should be distorted into a two-humped structure, and this effect should also be reflected in such experiments. (Recall that in real transition metals, the d-band holes play the role analogous to that of the electrons here. Therefore, the states whose structure is so affected will be the majority electron states below the Fermi energy.)

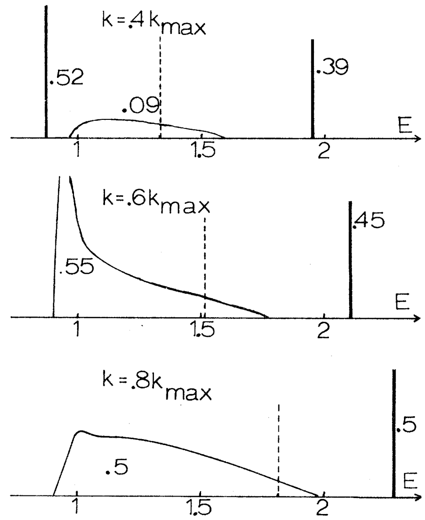

FIG. 2. Spectral weight functions for down electrons. Energy is measured in units of the bandwidth, and k_{max} is the largest wave vector in the band. The numbers next to the different parts of the functions give the relative spectral weights in each region. The Hartree-Fock energy is marked by the dotted line. (The Hartree-Fock spectral weight function is just a spike of unit weight at this energy.)

Also of interest is the pole in Σ when $\Sigma_0=\Delta$, at which energy $G_\downarrow$ can have no spectral weight. If the position of this pole is relatively independent of $\vec{k}$ (as happens in the heavy-magnon limit, $D\to 0$), the minority band is likely to split.

We used the $q=0$ limit of γ partly because of the tremendous analytic simplification it led to. However, we should point out that it is not a completely satisfactory procedure. For example, it is easy to check that it is necessary to retain the q_0 dependence of various quantities in the steps leading to (6) in order that (10) reduce to the correct limit (2) as $q\to 0$. Furthermore, we need the q dependence of γ to get the correct magnon mass out of (10). We have developed a technique, based on the finite-q Ward identity (4), which allows one to extract the correct long-wavelength limit of the spin-wave stiffness constant. We do not have space to discuss that here, so we simply note that this trick permits a sort of approximation wherein one computes Σ_0 from (3) with this self-consistently corrected magnon dispersion relation. Despite these objections, the present theory is useful because of its analytic simplicity and as a starting point for more sophisticated approaches.

It is also straightforward to generalize to a weak ferromagnet, where both $\Sigma_\uparrow$ and $\Sigma_\downarrow$ are nonvanishing, although then (3) is no longer a good approximation to $\Sigma_{0\downarrow}$.

We believe that this theory is highly relevant to an understanding of real transition-metal magnetism, in the context of a more realistic band structure. A detailed application to Ni is in progress, together with treatments of the finite-q Ward identity and the weakly ferromagnetic case. They will be published elsewhere.

We are indebted to Professor P. W. Anderson, Professor S. Doniach, Professor J. R. Schrieffer, and Professor E. P. Wohlfarth for many enlightening discussions of these ideas.

*Work supported by the U.K. Science Research Council and the U. S. Air Force Office of Scientific Research under Grant No. 1052-69. Part of this work was begun while this author was at the University of Pennsylvania, supported by the U. S. National Science Foundation.

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Upper Limit on the X-Ray Flux Associated with Gravitational Radiation*

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(Received 23 March 1972)

An upper limit in the x-ray flux accompanying pulses of gravitational radiation has been determined with relatively simple balloon-borne apparatus. The minimum detectable flux in space, approximately 2×10^{-5} erg/cm^2 event, is about 9 orders of magnitude below the energy flux which produces the gravitational signals observed by Weber. Furthermore, it is lower than that attainable with the much more elaborate and difficult ground-based methods which have been suggested so far.

Following Weber's reports[1-3] of evidence for the discovery of pulses of gravitational radiation, attempts to detect associated electromagnetic radiation have been made in the vhf (151 MHz)[4] and microwave (19 GHz)[5] radio frequency bands. Field, Rees, and Sciama[6] pointed out that it might be fruitful to scan the records of orbiting γ-ray detectors for pulses of photons, into which it seems plausible to suppose that an appreciable fraction of the energy of a collapsing object would go. Jelley[7] has recently called attention to the sensitivities that might be attained by utilizing the ground-based upper-air x-ray fluorescence technique for detecting such emissions in the x-ray band, while Baird and Francey[8] have suggested that it may be possible to detect the ionospheric effects of such x rays.

In this Letter, we point out that long-duration