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# Neutron Scattering from Itinerant-Electron Ferromagnets*

J. F. Cooke

*Solid State Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee* 37830

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An improved formalism is proposed for calculating the cross section for the magnetic scattering of neutrons by itinerant ferromagnets. This procedure is based on a simple extension of the random-phase approximation of the relevant Green's-function equation and an interpolation formalism for treating wave functions and matrix elements. In contrast to previous work, this formalism incorporates momentum-dependent splitting of the electronic energy bands as proposed by Hodges, Ehrenreich, and Lang as well as multiband effects. The scattering cross section is found to depend only on parameters which are determined directly from a self-consistent treatment of the ferromagnetic-band-structure calculation. The results obtained from this formalism were found to be too complicated to treat analytically for realistic band-structure models, and therefore meaningful numerical results must be obtained from computer calculations.

## I. INTRODUCTION

Over the past ten years there has been a considerable amount of theoretical work on the problem of obtaining a proper description of the neutron-scattering cross section associated with itinerant magnetic systems.[1-4] The major difficulty encountered in any approach to this problem is that the neutron couples to the magnetic system through its interaction with the "unpaired" itinerant electrons. Therefore, an adequate description of the electronic properties of itinerant systems is needed in order to proceed. This difficult problem has been under investigation for some 35 years, but as yet there does not exist a good theory based on first principles. There are, however, some parametric band-structure models that have been proposed which seem to do a rather good job of explaining the "single-particle" properties of itinerant systems.[5,6]

Another important aspect to be considered in connection with this problem is that even if an adequate description of the electronic system could be found, the expressions obtained for the scattering cross section are sufficiently complicated that analytic solutions for realistic models are impossible. Therefore, extensive computer calculations are a necessity. Until recently such calculations would have required large amounts of computer time to get rather crude results. However, within the past few years computer programs have been developed which are capable of providing fast and relatively accurate numerical results for many of the neutron-scattering expressions which have been proposed.[7] That is, a relatively complicated expression for the neutron-scattering intensity should no longer be treated necessarily as a useless academic result.

A case in point is the recent work of Lowde and Windsor (LW) on neutron scattering in ferromagnetic nickel[4] which is based on the random-phase approximation (RPA). They used a generalized form of the enhanced-susceptibility expression to calculate the scattering intensity. The electronic energy bands were rigidly spin split and $s$-$d$ hybridization and the "$s$-band" electrons were ignored. With these basic approximations they were able to obtain a good over-all fit to the scattering intensity. There were, however, several important discrepancies which occurred with respect to the spin-wave peak in the scattering cross section. First the position of the peak (the spin-wave energy) was found to shift much more slowly with momentum than the experimental results indicated. They were able to compensate for this by introducing into the scattering expression a momentum-dependent term $I(\vec{q})$ which was adjusted to provide a good fit to the spin-wave energy. Such a momentum-dependent term can be obtained in the theory provided certain assumptions are made with regard to a particular Coulomb matrix element (see Sec. IV), but the magnitude of this term cannot be determined *a priori*. Lowde and Windsor found that $I(\vec{q})$ must change by about 25% as $\vec{q}$ is allowed to vary from zero to one-fourth of the distance to the Brillouin-zone boundary in the [100] direction. The second problem associated with the theoretically calculated spin-wave peak was its relatively large width at about 40 meV. This could possibly be the result of statistical noise in the calculation. In any event the experimental results of Mook *et al.*[8] indicate that no appreciable broadening occurs below about 100 meV in the [100] direction at room temperature.

In addition to these points, one further problem exists with respect to the band structure which was used in the calculations. The approximations which have to be made in order to obtain an en-

hanced-susceptibility expression such as that used by LW also require that the "$d$ bands" be rigidly spin split. That is, all bands are spin split by a single splitting parameter. If one takes any of the paramagnetic potentials suggested in the literature for nickel and adjusts the spin-splitting parameter to give the correct spin-only moment, then one always finds a set of hole pockets associated with the $X_2$ energy level. This is also found to be true for the "first-principles" calculations of Connolly[9] and Wakoh and Yamashita.[10] Experimental de Haas–van Alphen measurements[11,12] indicate that this set of hole pockets does not exist. Thus we are faced with the problem that the approximation which leads to the enhanced-susceptibility expression also leads to an incorrect prediction of the ferromagnetic band structure.

The work of LW does represent a significant contribution to our understanding of the neutron-scattering results in an itinerant system like nickel. It could be argued that their results might be improved if a "more realistic" rigid spin-split band structure were used. However, because of the argument presented in the previous paragraph it seems clear that one must go beyond the approximations which lead to the enhanced-susceptibility expression based on a rigid spin-splitting model. One obvious approach is to extend the results of LW beyond the RPA. However, a rather casual inspection of the RPA theory indicates that it is a Coulomb matrix approximation and not the RPA itself which leads to rigid spin splitting and the enhanced-susceptibility expression. It is the purpose of this paper to show that a more realistic approximation of these particular Coulomb matrix elements leads to an improved result for the neutron-scattering intensity within the tractable limits of a simple extension of the RPA which is based on a more general momentum-dependent spin-splitting model of the electronic energy bands. Furthermore, it will be shown that all of the terms which appear in the theory are determined directly from a self-consistent solution of the energy-band equations.

Section II of this paper presents some background material which is necessary for the development of the theory. The equation of motion and the RPA theory are discussed in Sec. III. Matrix-element approximations which allow the equation of motion to be solved in closed form are discussed in Sec. IV. The results of the calculation are obtained in Sec. V and Sec. VI contains a summary of conclusions.

## II. NEUTRON-SCATTERING FORMALISM

The magnetic scattering of unpolarized neutrons by an electronic system contains both spin and orbital terms. The spin-only part of the cross section is given by the expression[1]

$$\frac{d^2\sigma}{d\Omega\, d\omega}=\left(\frac{e^2\gamma}{mc^2}\right)^2\frac{k_0'}{k_0}\sum_{\alpha\beta}(\delta_{\alpha,\beta}-e_\alpha e_\beta)\times\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}e^{-i\omega t}\langle S_{\vec{q}}^{\alpha}(0)S_{-\vec{q}}^{\beta}(t)\rangle\,dt, \quad (1)$$

where $\vec{k}_0$ and $\vec{k}_0'$ are the incident and scattered neutron wave vectors, respectively, $\vec{q}=\vec{k}_0-\vec{k}_0'$, $\vec{e}=\vec{q}/|\vec{q}|$, $\hbar\omega=\hbar^2k_0^2/2m_N-\hbar^2k_0'^2/2m_N$ is the neutron energy loss, $m$ and $m_N$ are the electron and neutron masses, respectively, and $\gamma$ is the gyromagnetic ratio of the neutron. The Fourier transform of the spin operator $\vec{S}$ is given by

$$S_{\vec{q}}^{\alpha}=\int e^{-i\vec{q}\cdot\vec{r}}\Psi^{\dagger}(\vec{r})S^{\alpha}\Psi(\vec{r})\,d^3r, \quad \alpha=x,y,z \quad (2)$$

where $\Psi^{\dagger}(\vec{r})$ is the two-component electron-creation operator in the second quantization formalism.

The spin-wave scattering terms are contained in the transverse part of (1), that is the $xx$ and the $yy$ terms. The remainder of this paper will be devoted to a calculation of this transverse-scattering intensity within a Green's-function formalism. The other terms in (1) can be calculated in a straightforward manner within the framework of the theory presented below, but the results will not be given here.

The Green's function appropriate for this calculation is defined by

$$G_{\alpha\beta}(\vec{q},t)=-i\,\langle TS_{\vec{q}}^{\alpha}(0)S_{-\vec{q}}^{\beta}(t)\rangle\,, \quad (3)$$

where $T$ is the time-ordering operator and $\langle A\rangle$ represents the thermal average of the operator $A$. Let

$$G_{\alpha\beta}^{>}(\vec{q},t)=\langle S_{\vec{q}}^{\alpha}(t)S_{-\vec{q}}^{\beta}(0)\rangle\,, \quad (4)$$

then

$$\int_{-\infty}^{\infty}e^{-i\omega t}\langle S_{\vec{q}}^{\alpha}(0)S_{-\vec{q}}^{\beta}(t)\rangle\,dt=\int_{-\infty}^{\infty}e^{i\omega t}\langle S_{\vec{q}}^{\alpha}(t)S_{-\vec{q}}^{\beta}(0)\rangle\,dt \equiv G_{\alpha\beta}^{>}(\vec{q},\omega)\,. \quad (5)$$

The Fourier transform of $G_{\alpha\beta}^{>}$ is related to $G_{\alpha\beta}$ by

$$G_{\alpha\beta}^{>}(\vec{q},\omega)=[1+f(\omega)]A_{\alpha\beta}(\vec{q},\omega)\,, \quad (6)$$

$$f(\omega)=(e^{\beta_0\omega}-1)^{-1}, \quad \beta_0=1/k_BT\,, \quad (7)$$

$$A_{\alpha\beta}(\vec{q},\omega)=i\lim_{\epsilon\to 0}[G_{\alpha\beta}(\vec{q},\omega+i\epsilon)-G_{\alpha\beta}(\vec{q},\omega-i\epsilon)]. \quad (8)$$

As a result of Eqs. (5) and (6) the transverse part of the scattering cross section given in (1) can be shown to reduce to

$$\left.\frac{d^2\sigma}{d\Omega\, d\omega}\right|_T=\left(\frac{e^2\gamma}{mc^2}\right)^2\frac{k_0'}{k_0}(1+e_z^2)(1+f(\omega))\times\frac{1}{4\pi\hbar}[A_{-+}(\vec{q},\omega)+A_{-+}(-\vec{q},-\omega)]\,, \quad (9)$$

where $A_{-+}(\vec{q},\omega)$ is the spectral function for the Green's function

$$G_{-+}(\vec{q},t) = -i\langle TS^{-}_{\vec{q}}(t)S^{+}_{-\vec{q}}(0)\rangle , \tag{10}$$

with

$$S^{\pm}_{\vec{q}} = S^{x}_{\vec{q}} \pm iS^{y}_{\vec{q}} . \tag{11}$$

Let $\{B_{n\vec{k}\sigma}(\vec{r})\}$ represent a complete set of single-particle states with band index $n$, wave vector $\vec{k}$, and spin $\sigma$ defined in terms of a scalar position-dependent set $\{\psi_{n\vec{k}\sigma}(\vec{r})\}$ and the spinor $\chi_\sigma$ by

$$B_{n\vec{k}\sigma}(\vec{r}) = \psi_{n\vec{k}\sigma}(\vec{r})\,\chi_\sigma . \tag{12}$$

The components of the spinor $\Psi(\vec{r})$ can then be written

$$\Psi_\sigma(\vec{r}) = \sum_{n\vec{k}} B_{n\vec{k}\sigma}(\vec{r})\,C_{n\vec{k}\sigma} . \tag{13}$$

The operators $C^{\dagger}_{n\vec{k}\sigma}$ and $C_{n\vec{k}\sigma}$ create and destroy, respectively, a particle in band $n$ with wave vector $\vec{k}$ and spin $\sigma$.

Substitution of (13) into (2) gives

$$S^{-}_{\vec{q}} = \sum_{\vec{k},n,m} (n\vec{k}\downarrow|e^{-i\vec{q}\cdot\vec{r}}|m\vec{k}+\vec{q}\uparrow)\,C^{\dagger}_{n\vec{k}\downarrow}C_{m\vec{k}+\vec{q}\uparrow} , \tag{14}$$

$$S^{+}_{-\vec{q}} = (S^{-}_{\vec{q}})^{\dagger} . \tag{15}$$

It will be assumed throughout this paper that whenever matrix elements are calculated, the spin dependence of the functions $\psi_{n\vec{k}\sigma}(\vec{r})$ can be neglected. Thus,

$$(n\vec{k}\downarrow|e^{-i\vec{q}\cdot\vec{r}}|m\vec{k}+\vec{q}\uparrow) \simeq (n\vec{k}|e^{i\vec{q}\cdot\vec{r}}|m\vec{k}+\vec{q}) = \int \psi^{*}_{n\vec{k}}(\vec{r})\,e^{-i\vec{q}\cdot\vec{r}}\psi_{m\vec{k}+\vec{q}}(\vec{r})\,d^3r . \tag{16}$$

Thus the Green's function $G_{-+}(\vec{q},t)$ can be written in the form

$$G_{-+}(\vec{q},t) = \sum_{\vec{k},n,m} (n\vec{k}|e^{-i\vec{q}\cdot\vec{r}}|m\vec{k}+\vec{q})\,\hat{G}(n\vec{k},m\vec{k}+\vec{q};t), \tag{17}$$

$$\hat{G}(n\vec{k},m\vec{k}+\vec{q};t) = -i\langle TC^{\dagger}_{n\vec{k}\uparrow}(t)\,C_{m\vec{k}+\vec{q}\uparrow}(t)S^{+}_{-\vec{q}}(0)\rangle . \tag{18}$$

The object now is to calculate the Green's function $\hat{G}$.

## III. EQUATION OF MOTION FOR $\hat{G}$

The equation of motion for $\hat{G}$ is given by

$$i\hbar\frac{\partial}{\partial t}\hat{G}(n\vec{k},m\vec{k}+\vec{q};t) = \hbar\delta(t)\langle[C^{\dagger}_{n\vec{k}\uparrow}C_{m\vec{k}+\vec{q}\uparrow},S^{+}_{-\vec{q}}]\rangle - i\langle P[\mathcal{H},C^{\dagger}_{n\vec{k}\uparrow}(t)\,C_{m\vec{k}+\vec{q}\uparrow}(t)]\,S^{+}_{-\vec{q}}(0)\rangle , \tag{19}$$

where $\mathcal{H}$ is the Hamiltonian which describes the electronic system. Let

$$\mathcal{H} = \mathcal{H}_0 + U , \tag{20}$$

$$\mathcal{H}_0 = T_0 + V_{\text{ion}} . \tag{21}$$

The operator $\mathcal{H}_0$ is composed of a kinetic energy part $T_0$ and the ionic potential $V_{\text{ion}}$. The electrons interact with each other through the Coulomb potential $U$. The second quantization form of (20) is given by

$$\mathcal{H} = \sum_{n,m;\vec{k},\sigma} (n\vec{k}|\mathcal{H}_0|m\vec{k})\,C^{\dagger}_{n\vec{k}\sigma}C_{m\vec{k}\sigma} + \tfrac{1}{2}\sum_{i,j;n,m}\sum_{\vec{k},\vec{p},\vec{K};\alpha,\beta}(i\vec{k},j\vec{p}+\vec{K}|U|n\vec{p},m\vec{k}+\vec{K}) \times C^{\dagger}_{i\vec{k}\alpha}\,C^{\dagger}_{j\vec{p}+\vec{K}\beta}\,C_{n\vec{p}\beta}\,C_{m\vec{k}+\vec{K}\alpha} , \tag{22}$$

$$(n\vec{k}|\mathcal{H}_0|m\vec{k}) = \int \psi^{*}_{n\vec{k}}(\vec{r})\,\mathcal{H}_0\,\psi_{m\vec{k}}(\vec{r})\,d^3r , \tag{23}$$

$$(i\vec{k},j\vec{l}|U|n\vec{p},m\vec{q}) = \int \psi^{*}_{i\vec{k}}(\vec{r})\psi^{*}_{j\vec{l}}(\vec{r}\,')\,U(|r-r'|) \times \psi_{n\vec{p}}(\vec{r}\,')\psi_{m\vec{q}}(\vec{r})\,d^3r\,d^3r' . \tag{24}$$

Starting with Eq. (19), an infinite set of equations can be generated which must be solved in order to obtain $\hat{G}$.[13] The simplest approximation is to terminate the series by using a generalized RPA given by[14]

$$C^{\dagger}_1C^{\dagger}_2C_3C_4 = f_1(\delta_{1,4}\,C^{\dagger}_2C_3 - \delta_{1,3}\,C^{\dagger}_2C_4) + f_2(\delta_{2,3}\,C^{\dagger}_1C_4 - \delta_{2,4}\,C^{\dagger}_1C_3) , \tag{25}$$

where "1" represents $n_1\vec{k}_1\sigma_1$, etc., and

$$f_1 = \langle C^{\dagger}_1C_1\rangle \tag{26}$$

is the fermion occupation number. The thermal average implied in (26) is to be calculated with respect to the single-particle Hamiltonian which generates the set $\{\psi_{n\vec{k}\sigma}(\vec{r})\}$. Therefore,

$$\langle C^{\dagger}_{n\vec{k}\alpha}\,C_{m\vec{p}\beta}\rangle = f_{n\vec{k}\alpha}\,\delta_{n,m}\,\delta_{\vec{k},\vec{p}}\,\delta_{\alpha,\beta} , \tag{27}$$

$$f_{n\vec{k}\sigma} = (e^{\beta_0[E(n\vec{k}\sigma)-E_F]}-1)^{-1} , \tag{28}$$

where $E(n\vec{k}\sigma)$ is the electronic energy and $E_F$ is the Fermi energy.

In order to further simplify the equation for $\hat{G}$ it is convenient to require that the $\{\psi_{n\vec{k}\sigma}\}$ satisfy Hartree–Fock equations. However, energy bands obtained from the solution of the Hartree–Fock equations would be unsatisfactory for the transition metals because, for example, screening effects are ignored. One method of going beyond the RPA is based on a functional-derivative method which can be used to establish an iteration procedure based on an effective screened interaction $U_{\text{eff}}(\vec{r},\vec{r}\,')$, rather than the bare interaction $U$.[13] The equation for $U_{\text{eff}}$ is coupled to the one-particle (electron) Green's function and the equations for these two functions must be solved simultaneously. For example, it can be shown that if vertex corrections can be ignored the Hartree–Fock equations are valid provided that $U$ is replaced by $U_{\text{eff}}$ in the exchange term. A generalization of these arguments indicates that such a replacement is required in all Coulomb matrix-element terms in the RPA equation for $\hat{G}$ except those terms which ultimately lead to the direct Coulomb term in the electronic energy. If this substitution is made, the equation for $\hat{G}$ becomes

$$i\hbar\frac{\partial}{\partial t}\hat{G}(n\vec{k},m\vec{k}+\vec{q};t)=\hbar\delta(t)(m\vec{k}+\vec{q}|e^{i\vec{q}\cdot\vec{r}}|n\vec{k})(f_{n\vec{k}\uparrow}-f_{m\vec{k}+\vec{q}\uparrow})+\sum_i\Big((m\vec{k}+\vec{q}|\mathcal{H}_0|i\vec{k}+\vec{q})$$
$$+\sum_{j,\vec{p},\beta}(m\vec{k}+\vec{q},j\vec{p}|U|j\vec{p},i\vec{k}+\vec{q})f_{j\vec{p}\beta}-\sum_{j,\vec{p}}(m\vec{k}+\vec{q},j\vec{p}|U_{eff}|i\vec{k}+\vec{q},j\vec{p})f_{j\vec{p}\uparrow}\Big)\hat{G}(n\vec{k},i\vec{k}+\vec{q};t)$$
$$-\sum_i\Big((i\vec{k}|\mathcal{H}_0|n\vec{k})+\sum_{j,\vec{p};\beta}(j\vec{p},i\vec{k}|U|n\vec{k},j\vec{p})f_{j\vec{p}\beta}-\sum_{j,\vec{p}}(i\vec{k},j\vec{p}|U_{eff}|n\vec{k},j\vec{p})f_{j\vec{p}\uparrow}\Big)\hat{G}(i\vec{k},m\vec{k}+\vec{q};t)$$
$$-(f_{n\vec{k}\uparrow}-f_{m\vec{k}+\vec{q}\uparrow})\sum_{i,j;\vec{p}}(m\vec{k}+\vec{q},i\vec{p}|U_{eff}|n\vec{k},j\vec{p}+\vec{q})\hat{G}(i\vec{p},j\vec{p}+\vec{q};t)\,. \quad (29)$$

In order to simplify this equation, the states $\{\psi_{n\vec{k}\sigma}\}$ are now required to satisfy the Hartree–Fock-like equation

$$\mathcal{H}_0\psi_{n\vec{k}\alpha}(\vec{r})+\sum_{m,\vec{p};\beta}f_{m\vec{p}\beta}\psi_{n\vec{k}\alpha}(\vec{r})$$
$$\times\int\psi^*_{m\vec{p}\beta}(\vec{r}')\,U(|r-r'|)\psi_{m\vec{p}\beta}(\vec{r}')\,d^3r'$$
$$-\sum_{m,\vec{p}}f_{m\vec{p}\alpha}\psi_{m\vec{p}\alpha}(\vec{r})\int\psi^*_{m\vec{p}\alpha}(\vec{r}')U_{eff}(\vec{r},\vec{r}')\psi_{n\vec{k}\alpha}(\vec{r}')\,d^3r'$$
$$=E(n\vec{k}\alpha)\psi_{n\vec{k}\alpha}(\vec{r}). \quad (30)$$

Then

$$E(n\vec{k}\sigma)\delta_{n,m}=(m\vec{k}|\mathcal{H}_0|n\vec{k})+\sum_{i,\vec{p};\alpha}f_{i\vec{p}\alpha}(m\vec{k},i\vec{p}|U|i\vec{p},n\vec{k})$$
$$-\sum_{i,\vec{p}}f_{i\vec{p}\sigma}(m\vec{k},i\vec{p}|U_{eff}|n\vec{k},i\vec{p})$$
$$\equiv\epsilon_p(n\vec{k})+\sum_{i,\vec{p}}[f_{i\vec{p}-\sigma}-(f_{i\vec{p}-\sigma})^{\rm para}](m\vec{k},i\vec{p}|U_{eff}|n\vec{k},i\vec{p}),$$
$$\text{if } n=m \quad (31)$$

where $\epsilon_p(n\vec{k})$ is the paramagnetic energy and $f$ and $f^{\rm para}$ are, respectively, the ferromagnetic and paramagnetic occupation numbers.[5] Equations (29) and (30) together with the equation for $U_{eff}$ and the one-particle Green's function could form the basis of a "first-principles" calculation of the electronic band structure and the neutron-scattering intensity which, at present, would be impossible to carry out. As a means of circumventing this problem, we could simply treat $U_{eff}$ as an adjustable term to be fixed by experimental data. Equations (29) and (30) then provide us with a method of parametrizing the problem. This does not seem inappropriate since, at present, we must rely on parametrized band structures to provide a reliable description of itinerant systems. It should also be pointed out here that we are tacitly assuming that Eq. (30) is general enough to provide an adequate "first-principles" description of the electronic band structure for some appropriate choice of $U_{eff}$.

If the complex transform of $\hat{G}$ is defined by[13]

$$\hat{G}(t)=\frac{1}{-i\beta_0}\sum_\nu e^{-iz_\nu t}G(Z_\nu)\,,$$
$$Z_\nu=\pi\nu/(-i\beta_0),\quad \nu=\text{odd integer} \quad (32)$$

then substitution of (31) and (32) into (29) gives

$$[\hbar Z-E(m\vec{k}+\vec{q}\uparrow)+E(n\vec{k}\downarrow)]\hat{G}(n\vec{k},m\vec{k}+\vec{q};Z)$$
$$=\hbar(m\vec{k}+\vec{q}|e^{i\vec{q}\cdot\vec{r}}|n\vec{k})\,(f_{n\vec{k}\downarrow}-f_{m\vec{k}+\vec{q}\uparrow})-(f_{n\vec{k}\downarrow}-f_{m\vec{k}+\vec{q}\uparrow})$$
$$\times\sum_{i,j;\vec{p}}(m\vec{k}+\vec{q},i\vec{p}|U_{eff}|n\vec{k},j\vec{p}+\vec{q})\hat{G}(i\vec{p},j\vec{p}+\vec{q};Z)\,, \quad (33)$$

where $\hat{G}(Z)$ is the analytic continuation of $\hat{G}(Z_\nu)$.

Equation (33) represents an approximation of (19) which can be solved exactly provided certain assumptions are made concerning the matrix elements. There is, however, one special case corresponding to $\vec{q}=0$, where (19) itself can be solved exactly. It is straightforward to prove from (17), (19), and (22) that

$$G_{-+}(\vec{q}=0,Z)=(n_\downarrow-n_\uparrow)/Z\,, \quad (34)$$

$$n_\sigma=\sum_{n\vec{k}}f_{n\vec{k}\sigma}\,. \quad (35)$$

Thus, from (8),

$$A_{-+}(\vec{q}=0,\omega)=2\pi\delta(\omega)\,. \quad (36)$$

This is nothing more than a statement that it costs no energy to turn over-all spins in the system at the same time in zero field or, put another way, the spin-wave energy must go to zero as $\vec{q}\to 0$.

Equation (33) can also be solved exactly at $\vec{q}=0$ provided one uses

$$\sum_{i\vec{p}}(f_{i\vec{p}\uparrow}-f_{i\vec{p}\downarrow})(m\vec{k},i\vec{p}|U_{eff}|n\vec{k},i\vec{p})=0\,,\quad n\neq m \quad (37)$$

which follows from (31). The ultimate result for $G_{-+}$ is exactly the same as that given in (34) with the modification that $n_\sigma$ is to be calculated with respect to the single-particle Hamiltonian which generates the $\{\psi_{n\vec{k}\sigma}\}$ instead of the one given in (22). This result is important since it guarantees that the solution of (33) has built into it the feature that the spin-wave energy, which is obtained from the position of the spin-wave peak in the scattering intensity, must go to zero as $\vec{q}\to 0$. It should also be noted that the above argument is independent of the choice of the paramagnetic energy $\epsilon_p(n\vec{k})$ defined in (31).

## IV. MATRIX-ELEMENT APPROXIMATIONS

Equation (33) cannot be solved without an explicit knowledge of the band and momentum dependence

of the matrix elements of $U_{eff}$ and $e^{i\vec{q}\cdot\vec{r}}$. This type of calculation would be very difficult since it would require a detailed knowledge of the band wave functions which are not readily available at the present time.

An alternative approach is to try to extract the band and momentum dependence in some realistic fashion. The usual approach to this problem is to expand the Bloch functions in terms of Wannier functions which can in turn be used to obtain a multicenter integral expansion of the matrix elements. On the basis of this type of expansion, Englert and Antonoff[15] suggest that

$$(n_1\vec{k}_1, n_2\vec{k}_2 | U_{eff} | n_3\vec{k}_3, n_4\vec{k}_1+\vec{k}_2-\vec{k}_3) \simeq A_0(n_1,n_2,n_3,n_4) + A_1(\vec{k}_3-\vec{k}_1; n_1,n_2,n_3,n_4) , \quad (38)$$

where $A_0$ and $A_1$ can be used as adjustable parameters. Then the $U_{eff}$ matrix element in (33) becomes

$$(m\vec{k}+\vec{q}, i\vec{p} | U_{eff} | n\vec{k}, j\vec{p}+\vec{q}) \simeq A_0(m,i,n,j) + A_1(-\vec{q}; m,i,n,j) . \quad (39)$$

Since this approximation removes the $\vec{k}$ and $\vec{p}$ dependence of the matrix element, (33) can be converted into an $N_B \times N_B$ matrix equation, where $N_B$ is the number of bands considered. This is essentially the path followed by Yamada and Shimizu[14] in their paper on spin waves in ferromagnetic metals.

The approximation given in (38) also has consequences as far as the ferromagnetic band structure is concerned. If the $U_{eff}$ matrix element which contributes to the spin-dependent part of the expression for $E(n\vec{k}\sigma)$, given in (31), is calculated using (38), it is found to have no momentum dependence at all. Thus each band is rigidly spin split but the splitting depends on the band index. This represents a generalization of the rigid-splitting model to include multiband effects. Unfortunately, in a realistic multiband calculation the number of parameters $\{A_0\}$ and $\{A_1\}$ could be large and they cannot be calculated *a priori*.

If the $e^{i\vec{q}\cdot\vec{r}}$ matrix element in (33) is expanded in terms of Wannier functions, and the overlap of these functions on different sites is neglected, then[1]

$$(m\vec{k}+\vec{q} | e^{i\vec{q}\cdot\vec{r}} | n\vec{k}) \simeq F_{mn}(\vec{q}) \quad (40)$$

and the $\vec{k}$ dependence is removed.

One way to further simplify the calculation is to consider only a single-band system, in which case all band indices can be dropped. If (39) and (40) are substituted into (33), the equation can easily be solved to give

$$G_{-+}(\vec{q},Z) = \hbar |F(\vec{q})|^2 \frac{\chi_0(\vec{q},Z)}{1+I(\vec{q})\chi_0(\vec{q},Z)} , \quad (41)$$

$$\chi_0(\vec{q},Z) = \sum_{\vec{k}} \frac{f_{\vec{k}\downarrow} - f_{\vec{k}+\vec{q}\uparrow}}{\hbar Z - E(\vec{k}+\vec{q}\uparrow) + E(\vec{k}\downarrow)} , \quad (42)$$

$$I(\vec{q}) = A_0 + A_1(-\vec{q}) . \quad (43)$$

This result was proposed and examined by Thompson[16] and it reduces to the Izuyama *et al.*[1] result if $A_1$ is ignored. Since $\chi_0$ is the susceptibility for a noninteracting system of electrons $[I(\vec{q})=0]$, Eq. (41) is usually called the enhanced-susceptibility result.

A slight generalization of (41) was made by LW[4] in order to extend the result to the multiband case. Since it is known for a multiband system that

$$\chi_{0\,MB}(\vec{q},Z) = \sum_{\vec{k};n,m} |(m\vec{k}+\vec{q}|e^{i\vec{q}\cdot\vec{r}}|n\vec{k})|^2 \times \frac{f_{n\vec{k}\downarrow} - f_{m\vec{k}+\vec{q}\uparrow}}{\hbar Z - E(m\vec{k}+\vec{q}\uparrow) + E(n\vec{k}\downarrow)} , \quad (44)$$

LW assumed

$$G_{-+}(\vec{q},Z) = \hbar \frac{\chi_{0\,MB}(\vec{q},Z)}{1+I(\vec{q})|F(\vec{q})|^{-2}\chi_{0\,MB}(\vec{q},Z)} , \quad (45)$$

where $F(\vec{q})$ is the magnetic form factor. The $e^{i\vec{q}\cdot\vec{r}}$ matrix element was calculated using an interpolation approach which will be reproduced later on in this paper. This result is consistent with (33) provided all band indices and the $\vec{k}$ and $\vec{p}$ dependence of the $U_{eff}$ matrix element are ignored. This assumption also requires that all paramagnetic energy bands must be rigidly spin split by the same amount. As has been pointed out before, they found that the $\vec{q}$ dependence of $I$, represented here by $A_1(-\vec{q})$, could not be ignored in their calculation.

The major difference between the theory presented by LW and the theory presented here is that the interpolation formalism is to be applied to the $U_{eff}$ matrix element as well as the $e^{i\vec{q}\cdot\vec{r}}$ matrix element. The use of the interpolation formalism enables us to include the $\vec{k}$ and $\vec{p}$ dependences of the $U_{eff}$ matrix element and, therefore, it represents a step beyond the approximation given by (39).

The interpolation formalism[5] is based on an expansion of the Bloch functions given by

$$\psi_{n\vec{k}\sigma}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{l,\mu} a_{n\mu\sigma}(\vec{k}) e^{i\vec{k}\cdot\vec{R}_l} \phi^{\sigma}_{\mu}(\vec{r}-\vec{R}_l) , \quad (46)$$

where the $\{a_{n\mu\sigma}(\vec{k})\}$ are expansion coefficients with $n$ representing the band index and $\mu$ the symmetry orbital index. The $\{\phi^{\sigma}_{\mu}\}$ are atomiclike symmetry orbitals and $\vec{R}_l$ is a lattice vector. The first five orbitals are chosen to be $d$-like symmetry orbitals and the remaining orbitals could be related to orthogonalized plane waves.[5] Three of the $d$-like orbitals have $t_{2g}$ symmetry and the remaining two have $e_g$ symmetry. It is further assumed that the $d$-like $\phi^{\sigma}_{\mu}$ located on separate sites do not overlap, that is, $\phi^{\sigma}_{\mu}(\vec{r})\phi^{\sigma}_{\nu}(\vec{r}-\vec{R}_l)=0$ for $\mu,\nu=1,5$ unless $\vec{R}_l$

$=0$. This particular approximation allows for the overlap of predominantly $d$-like Wannier functions on separate sites since, in this case,

$$w^*_{n\sigma}(\vec{r})w_{m\sigma}(\vec{r}-\vec{R}_p)\simeq\frac{1}{N^2}\sum_{\mu,l,\vec{k};\nu,\vec{k}'}e^{i(\vec{k}'-\vec{k})\cdot\vec{R}_l}e^{i\vec{k}'\cdot\vec{R}_p}\times a^*_{n\mu\sigma}(\vec{k})\,a_{m\nu\sigma}(\vec{k}')\,\phi^{\sigma*}_\mu(\vec{r}-\vec{R}_l)\,\phi^\sigma_\nu(\vec{r}-\vec{R}_l)\ , \quad (47)$$

where

$$w_{n\sigma}(\vec{r}-\vec{R}_l)\equiv\frac{1}{\sqrt{N}}\sum_{\vec{k}}e^{i\vec{k}\cdot\vec{R}_l}\psi_{n\vec{k}\sigma}(\vec{r}) \quad (48)$$

is the Wannier function associated with the $l$th site. Clearly, if the momentum dependence of the $\{a_{n\mu\sigma}\}$ could be neglected in (47), the momentum sums would yield $\delta_{\vec{R}_p,0}$ and the Wannier functions would not overlap.

If we calculate the $U_{eff}$ matrix element within the interpolation formalism as outlined above, the result is (neglecting spin dependence)

$$(n\vec{k}_1,m\vec{k}_2|\,U_{eff}\,|i\vec{k}_3,j\vec{k}_1+\vec{k}_2-\vec{k}_3)\simeq\sum_{\mu\nu\eta\xi}a^*_{n\mu}(\vec{k}_1)\,a^*_{m\nu}(\vec{k}_2)\times a_{i\eta}(\vec{k}_3)\,a_{j\xi}(\vec{k}_1+\vec{k}_2-\vec{k}_3)\,U_{eff}(\mu,\nu,\eta,\xi)\ , \quad (49)$$

$$U_{eff}(\mu,\nu,\eta,\xi)=\frac{1}{N}\sum_l\int\phi^*_\mu(\vec{r}-\vec{R}_l)\phi^*_\nu(\vec{r}'-\vec{R}_l)\,U_{eff}(\vec{r},\vec{r}')\times\phi_\eta(\vec{r}'-\vec{R}_l)\,\phi_\xi(\vec{r}-\vec{R}_l)\,d^3r\,d^3r'\ . \quad (50)$$

Since $U_{eff}$ is undetermined, the matrix element in (50) cannot be evaluated and thus the following simplifying assumption is made:

$$U_{eff}(\mu,\nu,\eta,\xi)=NU^{d-d}_{eff}\,\delta_{\mu,\nu}\delta_{\mu,\eta}\delta_{\mu,\xi},\quad \mu=1,\ldots,5$$
$$=0,\qquad\qquad\text{otherwise.} \quad (51)$$

This approximation takes into account only an averaged "diagonal" interaction between "$d$ electrons" and ignores the $s$-$d$ and $s$-$s$ effects which also contribute to the matrix element. This does not mean, however, that $s$-$d$ hybridization has been neglected, since such mixing terms are present in $\mathcal{H}_0$. It does mean that exchange splitting of the $s$-like Bloch states has been ignored. Such terms could be carried along in the analysis but there is some doubt as to what form the $s$-$d$ spin coupling should actually have.[5]

As a result of (51) the $U_{eff}$ matrix element takes the form

$$(n\vec{k}_1,m\vec{k}_2|\,U_{eff}\,|i\vec{k}_3,j\vec{k}_1+\vec{k}_2-\vec{k}_3)\simeq U^{d-d}_{eff}\sum_{\mu=1}^{5}a^*_{n\mu}(\vec{k}_1)\times a^*_{m\mu}(\vec{k}_2)\,a_{i\mu}(\vec{k}_3)\,a_{j\mu}(\vec{k}_1+\vec{k}_2-\vec{k}_3)\ , \quad (52)$$

and in particular

$$(m\vec{k}+\vec{q},i\vec{p}\,|\,U_{eff}\,|n\vec{k},j\vec{p}+\vec{q})\simeq U^{d-d}_{eff}\sum_{\mu=1}^{5}a^*_{m\mu}(\vec{k}+\vec{q})\,a_{n\mu}(\vec{k})\,a^*_{i\mu}(\vec{p})\,a_{j\mu}(\vec{p}+\vec{q})\ , \quad (53)$$

$$(n\vec{k},i\vec{p}\,|\,U_{eff}\,|i\vec{p},n\vec{k})\simeq(n\vec{k},i\vec{p}\,|\,U_{eff}\,|n\vec{k},i\vec{p})\simeq U^{d-d}_{eff}\sum_{\mu=1}^{5}|\,a_{n\mu}(\vec{k})\,|^2|\,a_{i\mu}(\vec{p})\,|^2\ . \quad (54)$$

The matrix-element approximations above represent a step beyond previous work in that they retain the $\vec{k}$ and $\vec{p}$ dependence.

The $e^{i\vec{q}\cdot\vec{r}}$ matrix element can also be calculated within the interpolation formalism. The result is

$$(m\vec{k}+\vec{q}\,|\,e^{i\vec{q}\cdot\vec{r}}\,|\,n\vec{k})\simeq\sum_{\mu\nu}a^*_{m\mu}(\vec{k}+\vec{q})\,a_{n\nu}(\vec{k})\,F_{\mu\nu}(\vec{q}), \quad (55)$$

$$F_{\mu\nu}(\vec{q})=\int\phi^*_\mu(\vec{r})\,e^{i\vec{q}\cdot\vec{r}}\,\phi_\nu(\vec{r})\,d^3r\ . \quad (56)$$

Following LW,[4] we assume

$$F_{\mu\nu}(\vec{q})\simeq F(\vec{q})\delta_{\mu,\nu} \quad (57)$$

with $F(\vec{q})$ as the magnetic form factor. Thus,

$$(m\vec{k}+\vec{q}\,|\,e^{i\vec{q}\cdot\vec{r}}\,|\,n\vec{k})\simeq F(\vec{q})\sum_\mu a^*_{m\mu}(\vec{k}+\vec{q})\,a_{n\mu}(\vec{k})\ . \quad (58)$$

Note that there are two types of sums that appear in (58) and (52). The one in (58) is over all symmetry orbital indices $\mu$, while the one in (52) is only over the $d$ orbitals ($\mu=1,5$). In order to avoid confusion and to simplify notation, the following convention will be adopted:

$$\sum_\mu{}'\ \rightarrow\ \sum_{\mu=1}^{5}\ , \quad (59)$$

$\sum_\mu\rightarrow$ sum over all $\mu$.

## V. SOLUTION FOR $G_{-+}(\vec{q},Z)$

If the matrix-element approximations developed from the interpolation formalism in Sec. IV are substituted in the expression for $\hat{G}$ given by (33), the result is

$$[\hbar Z-E(m\vec{k}+\vec{q}\uparrow)+E(n\vec{k}\downarrow)]\,\hat{G}(n\vec{k},m\vec{k}+\vec{q};Z)=\hbar F(\vec{q})\sum_\mu a^*_{m\mu}(\vec{k}+\vec{q})\,a_{n\mu}(\vec{k})\,(f_{n\vec{k}\downarrow}-f_{m\vec{k}+\vec{q}\uparrow})-U^{d-d}_{eff}(f_{n\vec{k}\downarrow}-f_{m\vec{k}+\vec{q}\uparrow})\sum_{ij;\vec{p}}\sum_\mu{}'a^*_{m\mu}(\vec{k}+\vec{q})\,a_{n\mu}(\vec{k})\times a^*_{i\mu}(\vec{p})\,a_{j\mu}(\vec{p}+\vec{q})\,\hat{G}(i\vec{p},j\vec{p}+\vec{q};\,Z)\ , \quad (60)$$

where from (31),

$$E(n\vec{k}\sigma)=\epsilon_p(n\vec{k})+U^{dd}_{eff}\sum_\mu{}'|\,a_{n\mu}(\vec{k})\,|^2[f_{\mu,-\sigma}-(f_{\mu,-\sigma})^{\text{para}}]\ , \quad (61)$$

$$f_{\mu,\sigma}=\sum_{n,\vec{p}}|\,a_{n\mu}(\vec{p})\,|^2f_{n\vec{p}\sigma}\ , \quad (62)$$

$$(f_{\mu,\sigma})^{\text{para}}=(f_{\mu,-\sigma})^{\text{para}}=\sum_{n,\vec{p}}|\,[a_{n\mu}(\vec{p})]^{\text{para}}\,|^2\,(f_{n\vec{p}\sigma})^{\text{para}}\ .$$

The function $f_{\mu,\sigma}$ represents the "number of electrons" with symmetry orbital index $\mu$ and spin $\sigma$. It follows from (62) and some group theory that

$$f_{1,\sigma}=f_{2,\sigma}=f_{3,\sigma}\ , \quad (63)$$

$$f_{4,\sigma}=f_{5,\sigma}\ , \tag{64}$$

where $3f_{1\sigma}$ is the number of "$t_{2g}$ electrons" and $2f_{4\sigma}$ is the number of "$e_g$ electrons" with spin $\sigma$. These relations also hold for $f^{\text{para}}$.

The electronic energy-band model which has emerged from the theory is precisely the one suggested by Hodges *et al.*[5] (HEL). The most important feature of this model is that the spin-dependent part of the energy given in (61) is, in general, momentum dependent. For example, HEL found that in their energy-band calculation for nickel the $t_{2g}$ and $e_g$ splittings were roughly 400 and 100 meV, respectively. At an arbitrary point in the Brillouin zone where the Bloch function is a mixture of $e_g$ and $t_{2g}$ symmetry, the splitting will be somewhere in between these limits depending on how much $e_g$ or $t_{2g}$ character the wave function contains. This is an important feature since $\hat{G}$, and therefore $G_{-+}$, depends on energy differences. Thus we should expect to get a different answer for $\hat{G}$ calculated on the basis of the momentum-dependent spin-splitting model than we would from the rigid-splitting model. Another important feature of this model is that it is in general very easy to eliminate the $X_2$ hole pockets in nickel and the particular band structure proposed by HEL was chosen so that this was the case.

It should be emphasized that it is the band-structure model proposed originally by HEL which has emerged here and not any particular band structure. The interpolation scheme suggested by HEL to treat this model can be used to obtain an appropriate band structure for any particular system and also to provide an efficient means of generating the electronic energies and the expansion coefficients $a_{n\mu}(\vec{k})$, which will ultimately be required to calculate $\hat{G}$ (or $G$). This method also requires that $U_{\text{eff}}^{d\text{-}d}$ be fixed to give the correct spin-only moment for the ferromagnetic system under consideration and, therefore, there are no adjustable parameters in this theory once an appropriate band structure has been determined.

Another important aspect of the $U_{\text{eff}}$ matrix-element approximation is that it has separated the $\vec{k}$ and $\vec{p}$ dependences so that (60) can be solved to obtain an answer in closed form. In order to simplify the solution of (60), define

$$X_\mu(\vec{q},Z)=\frac{1}{\hbar F(\vec{q})}\sum_{n,m;\vec{k}} a_{n\mu}^*(\vec{k})\,a_{m\mu}(\vec{k}+\vec{q}) \times\hat{G}(n\vec{k},m\vec{k}+\vec{q};Z)\ . \tag{65}$$

Then from (58) and (17),

$$G_{-+}(\vec{q},Z)=\hbar\left|F(\vec{q})\right|^2\sum_\mu X_\mu(\vec{q},Z)\ , \tag{66}$$

and from (60),

$$\sum_\nu{}'\left[\delta_{\mu,\nu}+U_{\text{eff}}^{d\text{-}d}\,\Gamma_{\mu\nu}(\vec{q},Z)\right]X_\nu(\vec{q},Z)=\sum_\nu\Gamma_{\mu\nu}(\vec{q},Z)\ , \qquad \mu=1,5 \tag{67}$$

$$X_\mu(\vec{q},Z)=\sum_\nu\Gamma_{\mu\nu}(\vec{q},Z)-U_{\text{eff}}^{d\text{-}d}\sum_\nu{}'\Gamma_{\mu\nu}(\vec{q},Z)X_\nu(\vec{q},Z)\ , \qquad \mu>5 \tag{68}$$

$$\Gamma_{\mu\nu}(\vec{q},Z)=\sum_{n,m;\vec{k}}\frac{a_{n\mu}^*(\vec{k})a_{m\mu}(\vec{k}+\vec{q})\,a_{m\nu}^*(\vec{k}+\vec{q})\,a_{n\nu}(\vec{k})(f_{n\vec{k}\downarrow}-f_{m\vec{k}+\vec{q}\uparrow})}{\hbar Z-E(m\vec{k}+\vec{q}\uparrow)+E(n\vec{k}\downarrow)}\ . \tag{69}$$

The sum in (69) runs over all bands and over the entire first Brillouin zone. Thus in order to obtain $G_{-+}$ we must first solve the set of five equation given in (67) for $X_\mu$, $\mu=1,5$, and then substitute this result into Eq. (68) to obtain $X_\mu$, $\mu>5$.

The solution of (67) can be obtained quite simply by first defining

$$\Lambda_{\mu\nu}(\vec{q},Z)=\Gamma_{\mu\nu}(\vec{q},Z),\quad \mu=1,5\ ,\quad \nu=1,5\ . \tag{70}$$

Then from (67),

$$X_\mu(\vec{q},Z)=\sum_\nu\sum_{\nu'}{}'\left[I+U_{\text{eff}}^{d\text{-}d}\,\Lambda(\vec{q},Z)\right]^{-1}_{\mu\nu'}\Gamma_{\nu',\nu}(\vec{q},Z)\ , \qquad \mu=1,5 \tag{71}$$

where $I$ is the $5\times5$ unit matrix. This result can be simplified further by noting that

$$\sum_{\nu'}{}'\left[I+U_{\text{eff}}^{d\text{-}d}\,\Lambda(\vec{q},Z)\right]^{-1}_{\mu\nu'}\Gamma_{\nu',\nu}(\vec{q},Z) =\left[I+U_{\text{eff}}^{d\text{-}d}\,\Lambda(\vec{q},Z)\right]^{-1}_{\mu\nu}-\delta_{\mu,\nu}\ , \tag{72}$$

and therefore

$$X_\mu(\vec{q},Z)=-1+\sum_\nu{}'\left[I+U_{\text{eff}}^{d\text{-}d}\,\Lambda(\vec{q},Z)\right]^{-1}_{\mu\nu} +\sum_{\nu>5}\sum_{\nu'}{}'\left[I+U_{\text{eff}}^{d\text{-}d}\Lambda(\vec{q},Z)\right]^{-1}_{\mu\nu'}\Gamma_{\nu',\nu}(\vec{q},Z)\ , \qquad \mu=1,5\ . \tag{73}$$

Since the scattering intensity is proportional to the imaginary part of $\hat{G}$, and thus $X_\mu$, the $-1$ term in (73) is of no consequence.

With $X_\mu$ ($\mu=1,5$) determined by (73) and $X_\mu$ ($\mu>5$) determined by (68), the transverse neutron-scattering cross section is given by

$$\frac{d^2\sigma}{d\Omega\,d\omega}\bigg|_T=\left(\frac{e^2\gamma}{mc^2}\right)^2\frac{k_0'}{k_0}\,(1+e_Z^2)\,[1+f(\omega)]\left|F(\vec{\tau}+\vec{q})\right|^2 \times\frac{1}{2\pi}\sum_\mu\left[\operatorname{Im}X_\mu(\vec{q},\omega-i\epsilon)+\operatorname{Im}X_\mu(-\vec{q},-\omega-i\epsilon)\right]\ , \tag{74}$$

which follows from (66), (9), and (8). In order to put this result in standard form, the replacement $\vec{q}\to\vec{\tau}+\vec{q}$ has been made where $\vec{\tau}$ is a reciprocal-lattice vector and $\vec{q}$ is restricted to the first Brillouin zone. The identity

$$X_\mu(\vec{\tau}+\vec{q},Z)=X_\mu(\vec{q},Z) \tag{75}$$

has also been used.

## VI. DISCUSSION AND CONCLUSIONS

In Secs. I–V a result for the transverse neutron-scattering cross section has been derived within the framework of a simple extension of the RPA and an interpolation formalism. The latter approximation allowed us to solve the equation for the scattering intensity without having to ignore the $\vec{k}$, $\vec{p}$, or $\vec{q}$ dependence of the $U_{eff}$ matrix element, given in Eq. (33), as has been done in previous theoretical treatments. This theory also leads us directly to the ferromagnetic-band-structure model proposed by Hodges *et al.*[5] which involves a momentum-dependent spin splitting of the electronic energy bands. Thus Eqs. (74), (73), and (68) represent a generalization of the scattering theory which incorporates momentum-dependent exchange effects as well as multiband effects. This result reduces to the expression used by Lowde and Windsor in the limit that all paramagnetic energy bands are rigidly spin split by the same amount. In this limit the results also reproduce the single-band theory of Thompson[16] and Izuyama *et al.*[1]

Since a "first-principles" calculation based on a properly screened Coulomb interaction is beyond our capabilities at the present time, it appears that we must rely on a parametric description of the scattering intensity based on model band-structure Hamiltonians such as the one proposed by HEL. In their treatment, the paramagnetic Hamiltonian which gives the $\epsilon_p(n\vec{k})$ in (61) is parametrized and the parameters are chosen to give agreement with known single-particle paramagnetic properties of the itinerant system under investigation. Once this has been accomplished, the ferromagnetic band structure is generated self-consistently with $U_{\rm eff}^{d\text{-}d}$ being chosen to give the correct spin-only moment. One advantage of this model over the rigid spin-splitting model is that it is relatively easy to produce a reasonable ferromagnetic band structure for nickel which does not predict $X_2$ hole pockets.[5] Their theory also provides us with the expansion coefficients $a_{n\mu}(\vec{k})$. Looking back at the result for $X_\mu$ given in Sec. V, it is clear that there are no other undetermined parameters in the theory. Thus, once the ferromagnetic band structure is determined the scattering intensity follows automatically.

The momentum-dependent effects of the $U_{eff}$ matrix element are carried by the interpolation coefficients $a_{n\mu}(\vec{k})$. They occur in both the numerator and the denominator of the function $\Gamma_{\mu\nu}$ and thus their ultimate effect on the final result for $X_\mu$ is difficult to determine *a priori*. It is clear, however, that as a result of the momentum dependence they impart to the spin-dependent term in the electronic energy expression, there will be a larger number of low-lying spin-flip excitations (Stoner excitations) than that predicted by the rigid spin-splitting model, which in turn should produce noticeable changes in the spin-wave energy and lifetime. In fact, it could be argued that the effects of the $I(\vec{q})$ which Lowde and Windsor used have been incorporated in this theory in a self-consistent way.

The scattering cross section given by Eq. (74) is dominated at low $\vec{q}$ by spin-wave scattering which will contribute a large peak at the spin-wave energy corresponding to that $\vec{q}$. The spin-wave energy at low $\vec{q}$ is therefore equal to the lowest energy at which the real part of the determinant of the matrix $[I + U_{\rm eff}^{d\text{-}d}\Lambda(\vec{q}, \omega - i\epsilon)]$ vanishes [see Eq. (71)]. The lifetime of the spin-wave state is related to the inverse of the width of the spin-wave peak, which in this theory is a very complicated expression. Thus we can no longer rely on the enhanced-susceptibility result that the lifetime of the spin-wave state is simply related to the Stoner band density of states.

Because of the termination of the Green's-function equation, the results presented in this paper should be restricted to low temperatures. If the scattering cross section can be described reasonably well at low temperatures by Eq. (74), it is tempting to investigate the temperature dependence suggested by this theory as was done with the LW result. The first problem which must be considered in order to do this, however, is connected with the temperature dependence of the electronic band energies. For example, should the paramagnetic band structure be considered as temperature independent, should $U_{\rm eff}^{d\text{-}d}$ have a temperature dependence, etc. A temperature analysis of Eq. (74) and comparison with experimental results may help to answer some of these questions within the context of this particular theory.

The expression derived for the scattering cross section is clearly of such a complicated nature that analytic results for a system such as nickel are apparently not possible, even at very small $\vec{q}$. The result is not, however, purely academic since computer programs do exist which can treat the HEL ferromagnetic-band-structure model and which can also calculate the function $\Gamma_{\mu\nu}(\vec{q}, \omega - i\epsilon)$ and, therefore, the scattering cross section. Extensive computer calculations based on this model are now under way for the case of nickel. Preliminary results indicate that the spin-wave dispersion curve as obtained from the calculated scattering intensity agrees extremely well with experimental data. The results of this calculation will be reported in a later paper.[17]

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# Theory of $s$-$d$ Exchange Interaction in Dilute Magnetic Alloys: Formalism*

Anupam Madhukar
*W. M. Keck Laboratory of Engineering Materials, California Institute of Technology, Pasadena, California 91109*
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Formal methods of field-theoretic scattering theory are employed to present a simple formalism for the problem of $s$-$d$ exchange scattering in dilute magnetic alloys. The single-particle scattering equations obtained include all multiparticle intermediate states and are exact in the thermodynamic limit. The effect of the multiparticle intermediate states leads to a natural redecomposition of the Hamiltonian and is easily realized as the familiar renormalization process common to scattering phenomena in field theory. Boundary conditions to be satisfied by the scattering amplitudes in the thermodynamic limit are invoked to obtain determining equations which fix the essential nature of renormalization. Although we have not been able to obtain exact solutions to these equations, it is shown that if the conduction-electron exchange-correlation energy is considered a slowly varying function of the momenta in the narrow region of interest around the Fermi surface, an approximation which may be expected to hold fairly well for narrow conduction bands, then the two determining equations reduce to a simple set of transcendental equations which may be easily solved numerically. Finally, we check our results against previously obtained results in the appropriate limits.

## I. INTRODUCTION

The theory of $s$-$d$ exchange interaction in dilute magnetic alloys has been the subject of intensive investigation since Kondo's[1] explanation of the phenomenon of resistivity minimum. Fairly complete and extensive review articles[2] now exist and provide a very good idea of the theoretical as well as experimental status of the field. The methods of double-time Green's function and $S$-matrix theory, pioneered by Nagaoka[2] and Suhl,[2] respectively, have been used by many workers in the last few years and it appears that one has reached the limit of their practical utility. Thus the tendency in the more recent past has been to go over to functional integration methods.[3]

The present paper deals with another formulation of the problem which we find to be straightforward, physically intuitive, and immensely less complicated mathematically than the previous formulations. We employ the concepts of formal theory of scattering, developed in the context of field theory, to provide a formulation of the theory of $s$-$d$ exchange interaction in dilute magnetic alloys. It is significantly different conceptually, as well as in its mathematical content from the $S$-matrix formulation, although there are many points of contact with it and with the formalism of Green's functions. Thus many results of these well-established formalisms can be used to our advantage.

Before we present our formalism, a few words on some conceptual points seem in order. As is usually done in describing physical systems, we also start by characterizing the nonmagnetic host plus the magnetic impurity system by the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_{s\text{-}d} ,$$

where $\hat{H}_0$ and $\hat{H}_{s\text{-}d}$ are the usual free-electron and $s$-$d$-exchange Hamiltonians.[2] In the usual consid-