

## Electrical Resistivity of Ferromagnetic Metals at Low Temperatures\*

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In a ferromagnetic metal the electrical resistance is caused by scattering of conduction electrons by phonons and by spin waves, the latter case arising from the exchange interaction between the conduction electrons and the localized magnetic electrons. Because these metals have two overlapping bands at the Fermi energy, an  $s$  band and a  $d$  band, the scattering in either case may occur within a single band or may involve  $s$ - $d$  transitions. Furthermore, both phonon and spin-wave umklapp processes can take place. The spin-wave contribution to  $\rho$ , often called the "spin-disorder resistivity," has been investigated for Fe, Co, Ni, and Gd. At the lowest temperatures (below 10°K for Fe, Co, and Ni) this varies as  $T^2$  and is reasonably well described by the single-band theory of Kasuya and others. However, it was found that at higher temperatures the main source of resistance comes from the scattering of  $s$  electrons into holes in the  $d$  band. A model consisting of spherical energy bands with Fermi momenta  $k_{F1}$  and  $k_{F2}$  has been used to study the normal processes, neglecting spin-wave umklapp processes. A consequence of the model, which is thought to be qualitatively correct, is that  $s$ - $d$  transitions require spin waves whose wave vectors exceed the radial distance between the two Fermi spheres. Thus, the  $s$ - $d$  transition mechanism is ineffective at very low temperatures. Representative calculations indicate that at higher temperatures this contribution to  $\rho$ , which has previously been overlooked, is about an order of magnitude larger than that arising from single-band scattering.

### 1. INTRODUCTION

IT is well known that in ferromagnetic metals there is a contribution to the electrical resistivity which is closely associated with the magnetic behavior of these metals. This resistivity,  $\rho_{\text{mag}}$ , sometimes called the "spin-disorder resistivity," has been the subject of a number of theoretical papers in recent years. In these theories and in the present work as well, a number of damaging approximations are introduced which make it difficult to judge the success of the final results in comparison with experiment. Nevertheless, it recently became apparent that at all but very low temperatures there was a discrepancy between theory and experiment much greater than could reasonably be attributed to the standard approximations.

In this paper a detailed investigation of  $\rho_{\text{mag}}$  in Fe, Co, Ni, and Gd is reported in which earlier theoretical work is extended to include the contribution to the electrical resistance arising from the scattering by spin waves of  $s$  electrons into holes in the  $d$  band. Illustrative calculations are presented which indicate that at temperatures above 20°K the contribution to  $\rho_{\text{mag}}$  from these  $s$ - $d$  transitions is about an order of magnitude larger than that coming from single band scattering.

White and Woods<sup>1</sup> have measured the electrical resistivities of Fe, Co, and Ni from low temperatures to room temperature, finding that below about 10°K  $\rho$  varies as  $T^2$ . Their results may be summarized by

$$\rho = \alpha T^2. \quad (1)$$

|  | Fe                  | Co                  | Ni                  |
|--|---------------------|---------------------|---------------------|
| $\alpha$ ( $\mu\Omega\text{cm deg}^{-2}$ ) | $13 \times 10^{-6}$ | $13 \times 10^{-6}$ | $16 \times 10^{-6}$ |

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White and Woods' data also show that by the time the temperature has risen to 20°K the dependence of  $\rho$  on  $T$  has increased to approximately  $T^{3.3}$ . Kondorsky, Galkina, and Tchernikova<sup>2</sup> also found for Fe and Ni that  $\rho$  is predominantly proportional to  $T^2$  below 30°K with coefficients  $\alpha$  about three times larger than the ones above. However, the data of White and Woods are probably more accurate as the residual resistivities of their samples are about one tenth of those of Kondorsky *et al.* Measurements on even purer samples of Fe and Ni than those used by White and Woods have recently been reported by Semenenko and Sudovtsov<sup>3</sup> who find in addition to the  $T^2$  term a linear term appreciable below 4°K.

The electrical resistivities of the heavy rare-earth metals Gd to Lu have been measured by Colvin, Legvold, and Spedding.<sup>4</sup> The complex magnetic structures of most of these metals, which are responsible for marked kinks and slope changes in the  $\rho$  versus  $T$  curves,<sup>5</sup> add complications which are beyond the scope of the present investigation. Accordingly, attention will be confined to Gd which is a simple ferromagnet from  $T=0^\circ\text{K}$  up to  $T_c=289^\circ\text{K}$ . Its resistivity as a function of temperature is given by the dashed curve of Fig. 1.

partially supported by the National Science Foundation, Grant G-11309.

<sup>1</sup> G. K. White and S. B. Woods, Phil. Trans. Roy. Soc. London **A251**, 273 (1958).

<sup>2</sup> E. Kondorsky, O. S. Galkina, and L. A. Tchernikova, J. Appl. Phys. **29**, 243 (1958).

<sup>3</sup> E. E. Semenenko and A. I. Sudovtsov, Zh. Eksperim. i Teor. Fiz. **42**, 1022 (1962); and E. E. Semenenko, A. I. Sudovtsov, and A. D. Shvets, *ibid.* **42**, 1488 (1962) [translations: Soviet Phys.—JETP **15**, 708 and 1033 (1962)].

<sup>4</sup> R. V. Colvin, S. Legvold, and F. H. Spedding, Phys. Rev. **120**, 741 (1960).

<sup>5</sup> A. R. Mackintosh, Phys. Rev. Letters **9**, 90 (1962); H. Miwa, Progr. Theoret. Phys. (Kyoto) **28**, 208 (1962); R. J. Elliott and F. A. Wedgwood, Proc. Phys. Soc. (London) **81**, 946 (1963).

The electrical resistivity of a ferromagnetic metal is believed to come from two main sources. One is the scattering of conduction electrons by the lattice vibrations (phonons) and the other comes from interaction with the magnetic spin system (spin waves). A further classification arises because these metals have two overlapping bands at the Fermi energy, an  $s$  band and a  $d$  band. (In Gd these are probably a  $6s$  band and a  $5d$  band.) Thus, in both the phonon case and the spin-wave case the scattering may take place within a single band or may involve  $s$ - $d$  transitions. The single-band phonon scattering is reasonably well described by the Bloch theory,<sup>6</sup> varying as  $T^5$  at low temperatures and as  $T$  above the Debye temperature  $\Theta_D$ . Less well understood is the phonon scattering involving  $s$ - $d$  transitions, a mechanism first suggested by Mott<sup>7</sup> and believed to be the main source of electrical resistance in the nonferromagnetic transition metals like Mn, Pt, and Pd. Wilson<sup>8</sup> showed that the resistivity due to this cause varies as  $T^3$  at low temperatures but, like the single-band case, varies as  $T$  above  $\Theta_D$ . It is difficult, however, to estimate the magnitude of this  $s$ - $d$  phonon resistivity, although it appears to be quite large in the nonferromagnetic transition metals.<sup>1</sup>

Another source of electrical resistance in transition metals which may be important at low temperatures comes from the collisions of  $s$  electrons with itinerant  $d$  electrons. This mechanism was investigated theoretically by Baber<sup>9</sup> who found that it leads to a contribution to  $\rho$  varying as  $T^2$  at low temperatures. However, the magnitude of this contribution also is very difficult to estimate.

As the work reported here is entirely concerned with spin-wave scattering, it would simplify the discussion considerably if the phonon contribution to the measured  $\rho$  could be estimated in some way and subtracted from the experimental curves. At temperatures above  $T_c$ , as the spin disorder reaches a maximum it is expected that  $\rho_{mag}$  will approach a constant value. Thus, the slope of  $\rho$  well above  $T_c$  can be reasonably assumed to be entirely due to phonon scattering. The value of this slope and knowledge of  $\Theta_D$  are sufficient to determine the Grüneisen function which results from the single-band Bloch theory, and this fact has been used by Anderson and Legvold<sup>10</sup> and by Weiss and Marotta<sup>11</sup> to make an approximate separation of  $\rho_{mag}$  from the experimental  $\rho$ . The result of doing this for Gd (using  $\Theta_D = 158^\circ\text{K}$ ) is shown in Fig. 1. However, it is clear that the Grüneisen function is unsuitable for describing either the phonon  $s$ - $d$  scattering or the effect of phonon

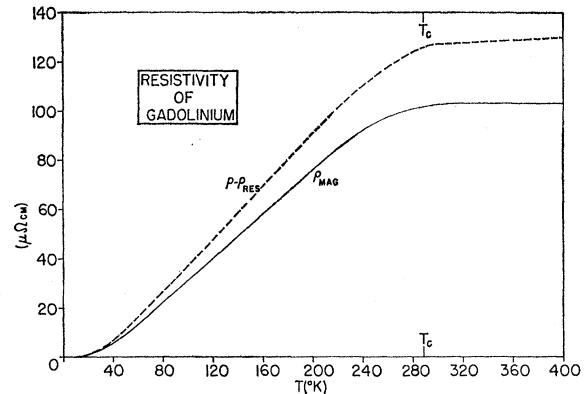


FIG. 1. Dashed curve: experimental results for Gd of Colvin, Legvold, and Spedding (see Ref. 4). Solid curve:  $\rho_{mag}$ , obtained by subtracting a very rough estimate of the phonon contribution to  $\rho$ .

umklapp processes, so that the curve labeled  $\rho_{mag}$  in Fig. 1 should not be interpreted as being anything but a very rough indication of the size and temperature dependence of  $\rho_{mag}$ .

Vonsovski<sup>12</sup> appears to have been the first person to recognize that an additional contribution to the electrical resistivity would occur in ferromagnets as a result of the exchange interaction between the conduction electrons and the localized magnetic electrons, often called the  $s$ - $d$  or  $s$ - $f$  interaction.<sup>13</sup> Subsequently, Turov<sup>14</sup> used a spin-wave treatment to show that the  $s$ - $d$  interaction leads to a contribution to  $\rho$  proportional to  $T^2$  at low temperatures, which he roughly estimated to be important below about  $10^\circ\text{K}$  in Fe.<sup>15</sup> A qualitative description of the temperature dependence of  $\rho_{mag}$  was given independently by Kasuya.<sup>16,17</sup> Representing the  $s$ - $d$  interaction by a molecular field, he obtained an expression which describes the main features of the variation of  $\rho_{mag}$  from low temperatures to temperatures above the Curie temperature. A similar approach was

<sup>12</sup> S. V. Vonsovski, Zh. Eksperim. i Teor. Fiz. **18**, 219 (1948), quoted by E. A. Turov, Ref. 14.

<sup>13</sup> In this paper the term " $s$ - $d$  interaction" will be used to refer generally to both the iron series and the rare-earth metals.

<sup>14</sup> E. A. Turov, Izv. Akad. Nauk SSSR, Ser. Fiz. **19**, 426 (1955).

<sup>15</sup> This subject has continued to receive considerable attention from Turov and his co-workers [E. A. Turov, Phys. Metals Metallog. **6**, No. 2, 13 (1958); Sh. Sh. Abel'skii and E. A. Turov, *ibid.* **10**, No. 6, 1 (1960)], but their work has been mainly concerned with attempting to explain a low-temperature term proportional to  $T$  found by Kondorsky *et al.* (cf., Ref. 2). An interaction  $\mathbf{p} \cdot \mathbf{A}$  between the momentum of a conduction electron and the dipole field of the magnetic atoms was shown to lead to a linear term, but the magnitude was estimated to be about 1000 times too small. At the present time the origin of the linear term at very low temperatures does not seem to have received a satisfactory explanation.

<sup>16</sup> T. Kasuya, Progr. Theoret. Phys. (Kyoto) **16**, 58 (1956).

<sup>17</sup> B. R. Coles [Advan. Phys. **7**, 40 (1958)] has also given a qualitative discussion of spin-disorder effects in a large number of ferromagnetic metals and transition-metal alloys. A great deal of experimental information prior to 1958 is collected together in this paper.

<sup>6</sup> See, for example, J. M. Ziman, *Electrons and Phonons* (Oxford University Press, New York, 1960), p. 357.

<sup>7</sup> N. F. Mott, Proc. Phys. Soc. (London) **47**, 571 (1935); N. F. Mott, Proc. Roy. Soc. (London) **A153**, 699 (1936).

<sup>8</sup> A. H. Wilson, Proc. Roy. Soc. (London) **A167**, 580 (1938).

<sup>9</sup> W. G. Baber, Proc. Roy. Soc. (London) **A158**, 383 (1937).

<sup>10</sup> G. S. Anderson and S. Legvold, Phys. Rev. Letters **1**, 322 (1958).

<sup>11</sup> R. J. Weiss and A. S. Marotta, J. Phys. Chem. Solids **9**, 302 (1959).

developed by de Gennes and Friedel<sup>18</sup> who examined the effects of short-range order around  $T_c$ .

In a later paper Kasuya<sup>19</sup> employed a spin-wave description of the interaction to derive a low-temperature expression for  $\rho_{\text{mag}}$ . Assuming a spin-wave dispersion law of the form  $E_q = \mathcal{D}q^2$ , he obtained

$$\rho_{\text{mag}} = \frac{\pi^3 V m G^2}{8 N e^2 \hbar E_F} (g-1)^2 j \left( \frac{kT}{k_F^2 \mathcal{D}} \right)^2. \quad (2)$$

Here  $G$  is a parameter which describes the strength of the  $s$ - $d$  interaction [denoted  $J(0)$  by Kasuya],  $g$  is the Landé  $g$  factor,  $j$  is the total angular momentum quantum number of each magnetic atom,  $E_F = \hbar^2 k_F^2 / 2m$  is the Fermi energy of the conduction electrons, and  $V$  and  $N$  are the volume and the number of atoms in the crystal. Exactly the same result was obtained by a slightly different method by Mannari<sup>20</sup> for the case of zero-orbital angular momentum ( $g=2$ ,  $j=S$ ). With estimates for Ni of  $G=0.48$  eV,  $E_F=3$  eV, and  $S=\frac{1}{2}$  Mannari obtained from (2),  $\rho_{\text{mag}} = 11 \times 10^{-6} T^2 \mu\Omega\text{cm}$ , in good agreement with the result quoted in (1).

It is evident that while the Kasuya and Mannari result may explain the behavior of  $\rho_{\text{mag}}$  at temperatures very small compared with  $T_c$ , it fails to account for the linear behavior which sets in at temperatures low enough that spin-wave theory should still be a good approximation. Furthermore, an extension of the theory to treat the hexagonal crystal structure of Gd revealed that the magnitude of  $\rho_{\text{mag}}$  in the linear region above 40°K is too small by a factor of 200 to account for the experimental results.<sup>21</sup>

In confining the conduction electrons to a single band, the spin-wave theories of Kasuya and Mannari exclude the possibility of interband transitions taking place. As mentioned at the beginning, it is the effects of such transitions caused by spin waves that are explored in this paper. A ferromagnetic metal is considered which has two bands of conduction electrons of effective masses  $m_1$  and  $m_2$ , with  $m_2$  assumed to be larger than  $m_1$ . These bands may be thought of as  $4s$  and  $3d$  bands in Fe, Co, and Ni and as  $6s$  and  $5d$  bands in Gd. They will be called simply the  $s$  band and the  $d$  band. It will be seen that the  $s$ -like or  $d$ -like character of the wave functions in the region of the atomic cores appears in the theory only through certain parameters ( $G_{11}, G_{12}, G_{22}$ ).

In order to make the problem tractable it is necessary to assume spherical energy bands with Fermi momenta  $k_{F1}$  and  $k_{F2}$ . An easily visualized consequence of this model is that  $s$ - $d$  transitions require spin waves whose wave vectors exceed the radial distance between the two Fermi spheres. By means of this greatly over-

simplified band picture, however, one can obtain a qualitative understanding of why the  $s$ - $d$  scattering mechanism is unimportant at very low temperatures where only small  $q$  spin-wave states are populated to any significant degree. This is why the one-band scattering result of Kasuya and Mannari gives a reasonable description of  $\rho_{\text{mag}}$  below about 10°K. However, it will be shown that at temperatures about 20°K, the resistivity due to  $s$ - $d$  scattering is about an order of magnitude larger than that arising from  $s$ - $s$  scattering.

The model we use implies a distinction between localized magnetic electrons and itinerant  $d$  electrons. In Gd and the other rare earths the magnetic electrons are  $4f$  electrons while the itinerant  $d$  electrons correspond to the atomic  $5d$  level. However, in the iron series ferromagnets both the localized and the itinerant electrons are  $3d$  electrons and the distinction between them is artificial. Nevertheless, it is expedient for us to suppose that, in the case of Ni, for example, 9  $d$  electrons are strongly localized, the unpaired electron being responsible for the  $s$ - $d$  interaction, and that there is in addition a fraction of a  $d$  electron per atom in a  $d$  band of itinerant electrons.

It should be mentioned that in addition to the  $s$ - $d$  exchange interaction there may also be a coupling between the conduction electron and magnetic electron spins arising from the covalent mixing mechanism of Anderson and Clogston.<sup>22</sup> This has been investigated by Kondo<sup>23</sup> in connection with the anomalous Hall effect in ferromagnets. Using a molecular-field treatment of the effective interaction Kondo estimates, roughly, that in Gd this coupling leads to a contribution to the constant  $\rho_{\text{mag}}$  above  $T_c$  about one tenth as large as that due to the  $s$ - $d$  exchange interaction. This rather complicated coupling has not been considered further in the present study.

In the sections which follow, the 2-band theory is presented in detail, the description being largely self-contained. A number of approximations in addition to those already mentioned are introduced as required and their validity is discussed. In Sec. 2 the relevant matrix elements of the scattering are obtained using a spin-wave treatment and the Boltzmann equation is derived. An approximate expression for  $\rho_{\text{mag}}$  is constructed in Sec. 3 using the variational method of Kohler and Sondheimer. This expression includes the effects of  $s$ - $s$ ,  $s$ - $d$ , and  $d$ - $d$  scattering processes and also allows for the presence of "optical" spin-wave modes in non-Bravais lattices. In Secs. 4 and 5 the general expression is simplified for cubic and hexagonal structures and the results of computations representative of Fe, Co, Ni, and Gd are presented. An examination of certain higher order scattering processes in Sec. 6 is followed by a short discussion in Sec. 7.

<sup>18</sup> P. G. de Gennes and J. Friedel, J. Phys. Chem. Solids 4, 71 (1958).

<sup>19</sup> T. Kasuya, Progr. Theoret. Phys. (Kyoto) 22, 227 (1959).

<sup>20</sup> I. Mannari, Progr. Theoret. Phys. (Kyoto) 22, 335 (1959).

<sup>21</sup> D. A. Goodings, J. Appl. Phys. 34, 1370 (1963).

<sup>22</sup> P. W. Anderson and A. M. Clogston, Bull. Am. Phys. Soc. 6, 124 (1961); P. W. Anderson, Phys. Rev. 124, 41 (1961).

<sup>23</sup> J. Kondo, Progr. Theoret. Phys. (Kyoto) 28, 846 (1962).

## 2. DERIVATION OF THE BOLTZMANN EQUATION

To begin with it is helpful to limit the description to a Bravais lattice of  $N$  magnetic spins  $\mathbf{S}_n$  at positions  $\mathbf{R}_n$ . The interaction between a single conduction electron of spin  $\mathbf{s}$  at  $\mathbf{r}$  and the magnetic spin system can be written as

$$\mathcal{H}_{sd} = -2 \sum_n G(\mathbf{r} - \mathbf{R}_n) \mathbf{s} \cdot \mathbf{S}_n, \quad (3)$$

where  $G(\mathbf{r} - \mathbf{R}_n)$  is a potential function of exchange type. The important scattering processes for the resistivity are those in which a conduction electron goes from  $\mathbf{k}$  to  $\mathbf{k}'$  with a change of spin. The corresponding matrix elements of  $\mathcal{H}_{sd}$  are

$$\begin{aligned} \langle \mathbf{k}' \pm | \mathcal{H}_{sd} | \mathbf{k} \mp \rangle \\ = -\frac{1}{N} G(\mathbf{k} - \mathbf{k}') \sum_n \exp[i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{R}_n] S_n^\mp, \end{aligned} \quad (4)$$

where

$$\begin{aligned} G(\mathbf{k} - \mathbf{k}') = \frac{1}{\Omega} \int \exp[i(\mathbf{k} - \mathbf{k}') \cdot (\mathbf{r} - \mathbf{R}_n)] \\ \times u_{\mathbf{k}'}^*(\mathbf{r} - \mathbf{R}_n) u_{\mathbf{k}}(\mathbf{r} - \mathbf{R}_n) G(\mathbf{r} - \mathbf{R}_n) d(\mathbf{r} - \mathbf{R}_n). \end{aligned} \quad (5)$$

Here  $\Omega$  is the atomic volume,  $S_n^\mp = S_n^x \mp i S_n^y$ , and  $u_{\mathbf{k}}(\mathbf{r})$  describes the Bloch character of the conduction electrons. Strictly speaking, we should write  $G(\mathbf{k}, \mathbf{k}')$  here, but if we make the common assumption that  $u_{\mathbf{k}}(\mathbf{r})$  depends only weakly on  $\mathbf{k}$ , then the integral in (5) is mainly a function of the difference  $\mathbf{k} - \mathbf{k}'$ . [ $G(\mathbf{k} - \mathbf{k}')$  is the same as the  $J(\mathbf{k} - \mathbf{k}')$  of Kasuya<sup>24</sup> and Yosida.<sup>25</sup> These authors clearly exhibit its exchange character.]

To consider the effect of the  $\mathbf{k} \mp \rightarrow \mathbf{k}' \pm$  scattering processes on the magnetic spin system we make the usual<sup>26</sup> spin-operator substitutions,  $S_n^\mp = (2S)^{1/2} a_n^\pm$ , and the transformation to spin waves,

$$a_n^\pm = (N)^{-1/2} \sum_q \exp(\mp i \mathbf{q} \cdot \mathbf{R}_n) a_q^\pm. \quad (6)$$

The matrix elements for creation and destruction of a spin wave of wave vector  $\mathbf{q}$  are

$$\begin{aligned} \langle n(\mathbf{q}) \pm 1 | S_n^\mp | n(\mathbf{q}) \rangle \\ = (2S/N)^{1/2} [n(\mathbf{q}) + \frac{1}{2} \pm \frac{1}{2}]^{1/2} \exp(\mp i \mathbf{q} \cdot \mathbf{R}_n), \end{aligned} \quad (7)$$

where  $n(\mathbf{q})$  is the number of spin waves  $\mathbf{q}$  per unit volume. From (4), the matrix elements for a conduction electron and the magnetic spin system taken together are,

$$\begin{aligned} |\langle \mathbf{k}' \pm, n(\mathbf{q}) \pm 1 | \mathcal{H}_{sd} | \mathbf{k} \mp, n(\mathbf{q}) \rangle|^2 \\ = (2S/N) [n(\mathbf{q}) + \frac{1}{2} \pm \frac{1}{2}] |G(\mathbf{k} - \mathbf{k}')|^2 \sum_{\mathbf{g}} \delta_{\mathbf{g}, \mathbf{k} - \mathbf{k}' \mp \mathbf{q}}. \end{aligned} \quad (8)$$

Here and throughout what follows the upper sign

describes the process  $\mathbf{k} - \rightarrow \mathbf{k}' +$  with creation of a spin wave  $\mathbf{q}$ , the lower sign gives  $\mathbf{k} + \rightarrow \mathbf{k}' -$  with destruction of a spin wave  $\mathbf{q}$ . The sum in (8) runs over all reciprocal lattice vectors  $\mathbf{g}$  including  $\mathbf{g} = 0$ . However, for the present we shall not consider spin-wave umklapp processes ( $\mathbf{g} \neq 0$ ) although, as will be discussed later, they are thought to be of major importance in accounting for the magnitude of  $\rho_{\text{mag}}$ .

The extension of Eq. (8) to the non-Bravais hcp lattice of Gd is straightforward and is outlined in Appendix A. Two spin-wave branches occur in this case<sup>27</sup> and, accordingly, there are matrix elements for creation and destruction of spin waves in either branch. In Appendix A it is shown that the *maximum value* of the matrix element in both cases is the same as given in Eq. (8) with  $n(\mathbf{q})$  replaced by  $n^{(i)}(\mathbf{q})$ , the number of spin waves  $\mathbf{q}$  per unit volume in the  $i$ th branch.

It is also necessary to extend our description to allow the conduction electrons to be in different bands. For the sake of clarity we shall suppose that we are dealing with a metal which has a narrow  $d$  band of itinerant electrons in addition to the main conduction band or  $s$  band. The conduction electrons are now labelled by  $\mathbf{k}$  and a band index  $\alpha$  standing for either  $s$  or  $d$ . Since the Bloch functions  $u_{\mathbf{k}}(\mathbf{r})$  are different for conduction electrons  $\mathbf{k}$  in different bands, the definition of  $G(\mathbf{k} - \mathbf{k}')$  in (5) must be extended to  $G_{\alpha\alpha'}(\mathbf{k} - \mathbf{k}')$ ; that is, we now have different quantities  $G_{ss}(\mathbf{k} - \mathbf{k}')$ ,  $G_{sd}(\mathbf{k} - \mathbf{k}')$  and  $G_{dd}(\mathbf{k} - \mathbf{k}')$ .

We can now write down a general expression corresponding to Eq. (8) which is suitable for the hcp lattice as well as for cubic lattices and allows for the possibility of conduction electrons being scattered from one band to another:

$$\begin{aligned} |\langle \mathbf{k}'\alpha' \pm, n^{(i)}(\mathbf{q}) \pm 1 | \mathcal{H}_{sd} | \mathbf{k}\alpha \mp, n^{(i)}(\mathbf{q}) \rangle|^2 \\ = (2S/N) [n^{(i)}(\mathbf{q}) + \frac{1}{2} \pm \frac{1}{2}] |G_{\alpha\alpha'}(\mathbf{k} - \mathbf{k}')|^2 \delta_{\mathbf{k}', \mathbf{k} \mp \mathbf{q}}. \end{aligned} \quad (9)$$

The corresponding transition probabilities are

$$\begin{aligned} W(\mathbf{k}\alpha \mp, n^{(i)}(\mathbf{q}) \rightarrow \mathbf{k}'\alpha' \pm, n^{(i)}(\mathbf{q}) \pm 1) \\ = (4\pi S/N\hbar) [n^{(i)}(\mathbf{q}) + \frac{1}{2} \pm \frac{1}{2}] |G_{\alpha\alpha'}(\mathbf{k} - \mathbf{k}')|^2 \\ \times \delta_{\mathbf{k}', \mathbf{k} \mp \mathbf{q}} \delta[E(\mathbf{k}\alpha \mp) - E(\mathbf{k}'\alpha' \pm) \mp E_q^{(i)}], \end{aligned} \quad (10)$$

where  $E(\mathbf{k}\alpha \pm)$  is the energy of a conduction electron  $\mathbf{k}\alpha \pm$  and  $E_q^{(i)}$  is the energy of a spin wave  $\mathbf{q}$  in the  $i$ th mode. For our purposes it is more convenient to use slightly different quantities defined by

$$\begin{aligned} W_q^{(i)}(\mathbf{k}\alpha \mp \rightarrow \mathbf{k}'\alpha' \pm) = (4\pi S/N\hbar) |G_{\alpha\alpha'}(\mathbf{k} - \mathbf{k}')|^2 \delta_{\mathbf{k}', \mathbf{k} \mp \mathbf{q}} \\ \times \delta[E(\mathbf{k}\alpha \mp) - E(\mathbf{k}'\alpha' \pm) \mp E_q^{(i)}], \end{aligned} \quad (11)$$

which have the important property,

$$W_q^{(i)}(\mathbf{k}'\alpha' \pm \rightarrow \mathbf{k}\alpha \mp) = W_q^{(i)}(\mathbf{k}\alpha \mp \rightarrow \mathbf{k}'\alpha' \pm). \quad (12)$$

These are the basic ingredients of the development which follows. Energy and momentum conservation of the spin-wave creation and destruction processes are

<sup>24</sup> T. Kasuya, Progr. Theoret. Phys. (Kyoto) **16**, 45 (1956).

<sup>25</sup> K. Yosida, Phys. Rev. **106**, 893 (1957).

<sup>26</sup> T. Holstein and H. Primakoff, Phys. Rev. **58**, 1098 (1940).

<sup>27</sup> D. A. Goodings, Phys. Rev. **127**, 1532 (1962).

clearly exhibited. Furthermore, it is to be noted that the form of the  $s$ - $d$  interaction and its strength appear in the theory entirely through the quantities  $|G_{\alpha\alpha'}(\mathbf{k}-\mathbf{k}')|^2$ .

A description of electron transport in the two-band ferromagnet under discussion involves the rate equations of four Fermi distribution functions— $f(\mathbf{k}s+)$ ,  $f(\mathbf{k}s-)$ ,  $f(\mathbf{k}d+)$ , and  $f(\mathbf{k}d-)$ . In the presence of an electric field but no thermal gradient these four equations can be written symbolically as

$$\left. \frac{\partial f}{\partial t}(\mathbf{k}\alpha\pm) \right]_{\text{field}} + \left. \frac{\partial f}{\partial t}(\mathbf{k}\alpha\pm) \right]_{\text{collisions}} = 0, \quad (13)$$

it being understood that  $\alpha$  stands for either  $s$  or  $d$ .

The collision term results from electrons entering and leaving the state  $\mathbf{k}\alpha\pm$  as a result of scattering processes in which a spin wave is created or destroyed. The situation is complicated to some extent, though not in an essential way, by the existence of spin waves in more than one mode and also by the possibility of interband transitions taking place. Allowing for these effects and making use of (12), one can write down the collision term as

$$\begin{aligned} \left. \frac{\partial f}{\partial t}(\mathbf{k}\alpha\pm) \right]_{\text{collisions}} &= \sum_{\mathbf{q}, i} \sum_{\mathbf{k}'\alpha'} \{ f(\mathbf{k}'\alpha'\mp) [1 - f(\mathbf{k}\alpha\pm)] \\ &\times [n_0^{(i)}(\mathbf{q}) + \frac{1}{2}\mp\frac{1}{2}] - f(\mathbf{k}\alpha\pm) [1 - f(\mathbf{k}'\alpha'\mp)] \\ &\times [n_0^{(i)}(\mathbf{q}) + \frac{1}{2}\mp\frac{1}{2}] \} W_{\mathbf{q}}^{(i)}(\mathbf{k}\alpha\pm \rightarrow \mathbf{k}'\alpha'\mp). \end{aligned} \quad (14)$$

If the entire system is in equilibrium at a temperature  $T$  and there is no electric field, the right side of (14) must vanish. For detailed balancing we have

$$\begin{aligned} f_0(\mathbf{k}\alpha\pm) [1 - f_0(\mathbf{k}'\alpha'\mp)] [n_0^{(i)}(\mathbf{q}) + \frac{1}{2}\mp\frac{1}{2}] \\ = f_0(\mathbf{k}'\alpha'\mp) [1 - f_0(\mathbf{k}\alpha\pm)] [n_0^{(i)}(\mathbf{q}) + \frac{1}{2}\pm\frac{1}{2}], \end{aligned} \quad (15)$$

where the equilibrium distribution functions are

$$f_0(\mathbf{k}\alpha\pm) = [\exp\{ (E(\mathbf{k}\alpha\pm) - E_F) / kT \} + 1]^{-1}, \quad (16)$$

$$n_0^{(i)}(\mathbf{q}) = [\exp(E_{\mathbf{q}}^{(i)} / kT) - 1]^{-1}. \quad (17)$$

We now consider departures from equilibrium resulting from an applied field  $\mathcal{E}$ . In the usual way we write  $f = f_0 + f_1$  and  $n = n_0 + n_1$ , and define the functions  $g(\mathbf{k}\alpha\pm)$  by

$$\begin{aligned} f_1(\mathbf{k}\alpha\pm) &= -kT [\partial f_0(\mathbf{k}\alpha\pm) / \partial E(\mathbf{k}\alpha\pm)] g(\mathbf{k}\alpha\pm) \\ &= f_0(\mathbf{k}\alpha\pm) [1 - f_0(\mathbf{k}\alpha\pm)] g(\mathbf{k}\alpha\pm). \end{aligned} \quad (18)$$

Just as the Bloch theory of phonon scattering treats the phonon system as though it were in thermal equilibrium, the magnetic spin system will be assumed here to be in thermal equilibrium, giving  $n_1^{(i)}(\mathbf{q}) = 0$ . (This must be counted as a major assumption in the present work and likewise in the theories of Kasuya, Mannari, and Turov.) The collision term (14) is now linearized in the deviations  $f_1$  and  $f_1'$  making use of

(15) and (18). If we define

$$\begin{aligned} L(\mathbf{k}\alpha\pm \rightarrow \mathbf{k}'\alpha'\mp) &= \sum_{\mathbf{q}, i} f_0(\mathbf{k}\alpha\pm) [1 - f_0(\mathbf{k}'\alpha'\mp)] \\ &\times [n_0^{(i)}(\mathbf{q}) + \frac{1}{2}\mp\frac{1}{2}] W_{\mathbf{q}}^{(i)}(\mathbf{k}\alpha\pm \rightarrow \mathbf{k}'\alpha'\mp), \end{aligned} \quad (19)$$

we can express the result as

$$\begin{aligned} \left. \frac{\partial f}{\partial t}(\mathbf{k}\alpha\pm) \right]_{\text{collisions}} \\ = \sum_{\mathbf{k}'\alpha'} L(\mathbf{k}\alpha\pm \rightarrow \mathbf{k}'\alpha'\mp) [g(\mathbf{k}'\alpha'\mp) - g(\mathbf{k}\alpha\pm)]. \end{aligned} \quad (20)$$

We also define

$$\begin{aligned} D(\mathbf{k}\alpha\pm) &= \left. \frac{\partial f}{\partial t}(\mathbf{k}\alpha\pm) \right]_{\text{field}} \\ &= -\mathbf{v}(\mathbf{k}\alpha\pm) \cdot e\mathcal{E} \frac{\partial f_0(\mathbf{k}\alpha\pm)}{\partial E(\mathbf{k}\alpha\pm)}, \end{aligned} \quad (21)$$

where  $\mathbf{v}(\mathbf{k}\alpha\pm) = \hbar^{-1} \nabla E(\mathbf{k}\alpha\pm)$  is the electron group velocity. Then our set of Boltzmann equations (13) becomes

$$\begin{aligned} D(\mathbf{k}\alpha\pm) + \sum_{\mathbf{k}'\alpha'} L(\mathbf{k}\alpha\pm \rightarrow \mathbf{k}'\alpha'\mp) \\ \times [g(\mathbf{k}'\alpha'\mp) - g(\mathbf{k}\alpha\pm)] = 0. \end{aligned} \quad (22)$$

In the next section we shall make frequent use of the fact that in these equations,

$$L(\mathbf{k}'\alpha'\pm \rightarrow \mathbf{k}\alpha\mp) = L(\mathbf{k}\alpha\mp \rightarrow \mathbf{k}'\alpha'\pm), \quad (23)$$

which follows from (12), (15), and (19).

### 3. APPLICATION OF THE VARIATIONAL PRINCIPLE

The well-known variational principle of transport theory,<sup>28</sup> first used by Kohler<sup>29</sup> and Sondheimer,<sup>30</sup> provides a suitable means of constructing an expression for  $\rho_{\text{mag}}$  in the present problem. The spin-flip feature of spin-wave scattering and the complication of having conduction electrons in two bands<sup>31</sup> make it desirable to present the theory in some detail.

Let us begin by writing down an expression for the electrical conductivity  $\sigma$ . The current density  $\mathbf{J}$  is given by

$$\begin{aligned} \mathbf{J}V &= e \sum_{\mathbf{k}\alpha} [\mathbf{v}(\mathbf{k}\alpha+) f(\mathbf{k}\alpha+) + \mathbf{v}(\mathbf{k}\alpha-) f(\mathbf{k}\alpha-)], \\ &= -ekT \sum_{\mathbf{k}\alpha} \left[ \mathbf{v}(\mathbf{k}\alpha+) \frac{\partial f_0(\mathbf{k}\alpha+)}{\partial E(\mathbf{k}\alpha+)} g(\mathbf{k}\alpha+) \right. \\ &\quad \left. + \mathbf{v}(\mathbf{k}\alpha-) \frac{\partial f_0(\mathbf{k}\alpha-)}{\partial E(\mathbf{k}\alpha-)} g(\mathbf{k}\alpha-) \right]. \end{aligned} \quad (24)$$

<sup>28</sup> See, for example, Ref. 6, p. 283.

<sup>29</sup> M. Kohler, Z. Physik **124**, 772 (1948); **125**, 679 (1949).

<sup>30</sup> E. H. Sondheimer, Proc. Roy. Soc. (London) **A203**, 75 (1950).

<sup>31</sup> The two-band situation has been treated by M. Kohler [Ann. Physik **6**, 18 (1949)], but his work is not readily adaptable to the problem at hand.

The last line is obtained by writing  $f=f_0+f_1$  as in (18) and assuming that in the equilibrium situation the Fermi surface has inversion symmetry. The conductivity is, therefore,

$$\sigma = -\frac{\mathbf{J} \cdot \boldsymbol{\varepsilon}}{\mathcal{E}^2} = \frac{kT}{V\mathcal{E}^2} \mathcal{J}_0, \quad (25)$$

where

$$\mathcal{J}_0 = \sum_{\mathbf{k}\alpha} [D(\mathbf{k}\alpha+)g(\mathbf{k}\alpha+) + D(\mathbf{k}\alpha-)g(\mathbf{k}\alpha-)]. \quad (26)$$

We now define the quantity,

$$\begin{aligned} \mathcal{J} = & 2 \sum_{\mathbf{k}\alpha} [D(\mathbf{k}\alpha+)\Phi(\mathbf{k}\alpha+) + D(\mathbf{k}\alpha-)\Phi(\mathbf{k}\alpha-)] \\ & + \sum_{\mathbf{k}\alpha\mathbf{k}'\alpha'} \Phi(\mathbf{k}\alpha+)L(\mathbf{k}\alpha+ \rightarrow \mathbf{k}'\alpha'-) \\ & \times [\Phi(\mathbf{k}'\alpha'-) - \Phi(\mathbf{k}\alpha+)] \\ & + \sum_{\mathbf{k}\alpha\mathbf{k}'\alpha'} \Phi(\mathbf{k}\alpha-)L(\mathbf{k}\alpha- \rightarrow \mathbf{k}'\alpha'+) \\ & \times [\Phi(\mathbf{k}'\alpha'+) - \Phi(\mathbf{k}\alpha-)], \quad (27) \end{aligned}$$

where for the present the  $\Phi(\mathbf{k}\alpha\pm)$  may be regarded as arbitrary functions. It is easy to see that the condition that  $\mathcal{J}$  is stationary with respect to small variations  $\delta\Phi(\mathbf{k}\alpha+)$  and  $\delta\Phi(\mathbf{k}\alpha-)$  is that  $\Phi(\mathbf{k}\alpha+)$  and  $\Phi(\mathbf{k}\alpha-)$  satisfy the Boltzmann equation (22). Therefore, we shall write our variational functions as

$$\Phi(\mathbf{k}\alpha\pm) = g(\mathbf{k}\alpha\pm) + \chi(\mathbf{k}\alpha\pm). \quad (28)$$

With a certain amount of manipulation, repeatedly using (23), one can show that

$$\begin{aligned} \mathcal{J} = & \mathcal{J}_0 - \frac{1}{2} \sum_{\mathbf{k}\alpha\mathbf{k}'\alpha'} L(\mathbf{k}\alpha+ \rightarrow \mathbf{k}'\alpha'-) [\chi(\mathbf{k}'\alpha'-) - \chi(\mathbf{k}\alpha+)]^2 \\ & - \frac{1}{2} \sum_{\mathbf{k}\alpha\mathbf{k}'\alpha'} L(\mathbf{k}\alpha- \rightarrow \mathbf{k}'\alpha'+) [\chi(\mathbf{k}'\alpha'+) - \chi(\mathbf{k}\alpha-)]^2. \quad (29) \end{aligned}$$

Consequently, since the quantities  $L(\mathbf{k}\alpha\pm \rightarrow \mathbf{k}'\alpha'\mp)$  are positive definite,  $\mathcal{J} \leq \mathcal{J}_0$ , and thus from (25),

$$\sigma \geq (kT/V\mathcal{E}^2)\mathcal{J}. \quad (30)$$

We have shown, therefore, that  $\mathcal{J}$  has its maximum value, equal to  $\mathcal{J}_0$ , when the  $\Phi(\mathbf{k}\alpha\pm)$  satisfy the Boltzmann equation. The power of the variational approach lies, however, in the fact that if the  $\Phi(\mathbf{k}\alpha\pm)$  are chosen to have a form which is approximately the same as the exact solutions of (22), then the stationary property of  $\mathcal{J}$  ensures that Eq. (30) yields a reasonable approximation for  $\sigma$ .

It is convenient to express  $\mathcal{J}$  in a slightly different form. With a little algebra, again using (23), Eq. (27) becomes

$$\begin{aligned} \mathcal{J} = & 2 \sum_{\mathbf{k}\alpha} [D(\mathbf{k}\alpha+)\Phi(\mathbf{k}\alpha+) + D(\mathbf{k}\alpha-)\Phi(\mathbf{k}\alpha-)] \\ & - \frac{1}{2} \sum_{\mathbf{k}\alpha\mathbf{k}'\alpha'} L(\mathbf{k}\alpha+ \rightarrow \mathbf{k}'\alpha'-) [\Phi(\mathbf{k}'\alpha'-) - \Phi(\mathbf{k}\alpha+)]^2 \\ & - \frac{1}{2} \sum_{\mathbf{k}\alpha\mathbf{k}'\alpha'} L(\mathbf{k}\alpha- \rightarrow \mathbf{k}'\alpha'+) [\Phi(\mathbf{k}'\alpha'+) - \Phi(\mathbf{k}\alpha-)]^2. \quad (31) \end{aligned}$$

So far we have carried through the analysis allowing  $\Phi(\mathbf{k}\alpha+)$  and  $\Phi(\mathbf{k}\alpha-)$  to be different functions. While it is not difficult to maintain this distinction in what follows, it makes the expressions cumbersome to an extent unjustified by present knowledge of the electronic structure of the ferromagnetic metals. Consequently, from this point onward we shall constrain each pair of spin-dependent functions to be represented by a single spin-independent function. (This is analogous to the constraint of the usual Hartree-Fock approximation compared with the "unrestricted Hartree-Fock" approximation.) Thus, we now have only  $\Phi(\mathbf{k}\alpha)$  and similarly  $g(\mathbf{k}\alpha)$ ,  $E(\mathbf{k}\alpha)$ ,  $\mathbf{v}(\mathbf{k}\alpha)$ , and  $f_0(\mathbf{k}\alpha)$ . With this approximation it is easy to see, using (23), that the last two terms of (31) are equal. Hence, we can write simply  $L(\mathbf{k}\alpha \rightarrow \mathbf{k}'\alpha')$  if it is understood that this quantity stands for either  $L(\mathbf{k}\alpha+ \rightarrow \mathbf{k}'\alpha'-)$  or  $L(\mathbf{k}\alpha- \rightarrow \mathbf{k}'\alpha'+)$  calculated according to (19). It is worth pointing out that if one looks at  $\mathcal{J}$  in the form (27), it is not obvious that one can do this.

We now define the quantities,

$$\mathcal{D}_\alpha = 2 \sum_{\mathbf{k}} D(\mathbf{k}\alpha)\Phi(\mathbf{k}\alpha), \quad (32)$$

$$\mathcal{L}_{\alpha\alpha} = \sum_{\mathbf{k}\mathbf{k}'} L(\mathbf{k}\alpha \rightarrow \mathbf{k}'\alpha) [\Phi(\mathbf{k}'\alpha) - \Phi(\mathbf{k}\alpha)]^2, \quad (33)$$

$$\mathfrak{N}_{11} = \sum_{\mathbf{k}\mathbf{k}'} L(\mathbf{k}1 \rightarrow \mathbf{k}'2) [\Phi(\mathbf{k}1)]^2, \quad (34)$$

$$\mathfrak{N}_{22} = 2 \sum_{\mathbf{k}\mathbf{k}'} L(\mathbf{k}1 \rightarrow \mathbf{k}'2) [\Phi(\mathbf{k}'2)]^2, \quad (35)$$

$$\mathfrak{N}_{12} = 2 \sum_{\mathbf{k}\mathbf{k}'} L(\mathbf{k}1 \rightarrow \mathbf{k}'2) \Phi(\mathbf{k}1)\Phi(\mathbf{k}'2). \quad (36)$$

Then under the spin-independent assumption introduced above, (31) becomes

$$\mathcal{J} = 2\mathcal{D}_1 + 2\mathcal{D}_2 - (\mathcal{L}_{11} + \mathfrak{N}_{11}) - (\mathcal{L}_{22} + \mathfrak{N}_{22}) + 2\mathfrak{N}_{12}. \quad (37)$$

It is useful to express  $\mathcal{J}$  in a form in which its value remains unchanged when all  $\Phi(\mathbf{k}1)$  or all  $\Phi(\mathbf{k}2)$  are multiplied by an arbitrary constant. To do this we note that if all  $\Phi(\mathbf{k}1)$  are multiplied by  $c_1$  and all  $\Phi(\mathbf{k}2)$  are multiplied by  $c_2$ ,  $\mathcal{J}$  becomes

$$\begin{aligned} \mathcal{J} = & 2c_1\mathcal{D}_1 + 2c_2\mathcal{D}_2 - c_1^2(\mathcal{L}_{11} + \mathfrak{N}_{11}) \\ & - c_2^2(\mathcal{L}_{22} + \mathfrak{N}_{22}) + 2c_1c_2\mathfrak{N}_{12}. \quad (38) \end{aligned}$$

Determining  $c_1$  and  $c_2$  from the equations  $(\partial\mathcal{J}/\partial c_1)=0$  and  $(\partial\mathcal{J}/\partial c_2)=0$  and substituting back in (38) one obtains

$$\mathcal{J} = \frac{(\mathcal{L}_{11} + \mathfrak{N}_{11})\mathcal{D}_2^2 + 2\mathfrak{N}_{12}\mathcal{D}_1\mathcal{D}_2 + (\mathcal{L}_{22} + \mathfrak{N}_{22})\mathcal{D}_1^2}{(\mathcal{L}_{11} + \mathfrak{N}_{11})(\mathcal{L}_{22} + \mathfrak{N}_{22}) - \mathfrak{N}_{12}^2}. \quad (39)$$

Thus, from (30) our expression for the resistivity is

$$\rho_{\text{mag}} \leq \frac{V \mathcal{E}^2}{kT} \times \frac{(\mathcal{L}_{11} + \mathfrak{M}_{11})(\mathcal{L}_{22} + \mathfrak{M}_{22}) - \mathfrak{M}_{12}^2}{(\mathcal{L}_{11} + \mathfrak{M}_{11})\mathfrak{D}_2^2 + 2\mathfrak{M}_{12}\mathfrak{D}_1\mathfrak{D}_2 + (\mathcal{L}_{22} + \mathfrak{M}_{22})\mathfrak{D}_1^2}. \quad (40)$$

If there is only one band of conduction electrons this reduces to the familiar expression,<sup>28</sup>

$$\rho_{\text{mag}} \leq \frac{V \mathcal{E}^2}{kT} \frac{\mathcal{L}_{11}}{\mathfrak{D}_1^2}. \quad (41)$$

We must now turn to the evaluation of  $\mathfrak{D}_\alpha$ ,  $\mathcal{L}_{\alpha\alpha}$ ,  $\mathfrak{M}_{\alpha\alpha}$ , and  $\mathfrak{M}_{12}$ . It is necessary at this point to introduce what is probably the most inaccurate approximation of the theory, namely, that the energy surfaces in each band can be adequately represented by

$$E(\mathbf{k}\alpha) = E_\alpha + \hbar^2 k^2 / (2m_\alpha), \quad (42)$$

with  $m_\alpha$  the effective mass in the  $\alpha$  band. For convenience we take  $E_s = 0$  which means that energies are measured relative to the bottom of the  $s$  band. One consequence of this assumption of spherical energy bands is that any prediction which the theory makes regarding anisotropy in  $\rho_{\text{mag}}$  cannot come from the electronic structure but only from anisotropy in the spin-wave spectrum.

The evaluation of  $\mathfrak{D}_\alpha$  is simple and illustrates ideas which are used in working out  $\mathcal{L}_{\alpha\alpha}$ ,  $\mathfrak{M}_{\alpha\alpha}$ , and  $\mathfrak{M}_{12}$ . Let the direction of the electric field  $\mathcal{E}$  be taken as axis of a polar coordinate system in which  $\mathbf{k}$  has angles  $\theta$  and  $\phi$ , and  $d\Omega = \sin\theta d\theta d\phi$ . Our assumption of spherical energy bands means that  $\mathbf{v}(\mathbf{k}\alpha)$  is in the direction of  $\mathbf{k}$  and  $\mathbf{v}(\mathbf{k}\alpha) \cdot \mathcal{E} = v_\alpha(E) \mathcal{E} \cos\theta$ . Instead of integrating over  $k = |\mathbf{k}|$  we integrate over  $E$ , introducing the density of states per unit volume (of one spin only) in the  $\alpha$  band,  $n_\alpha(E)$ . Choosing our variational function to have the usual form,

$$\Phi(\mathbf{k}\alpha) = \Phi_\alpha(E) \cos\theta, \quad (43)$$

we obtain from (32),

$$\mathfrak{D}_\alpha = -\frac{2e\mathcal{E}V}{4\pi} \int v_\alpha(E) \frac{\partial f_0}{\partial E} \Phi_\alpha(E) n_\alpha(E) \cos^2\theta dE d\Omega = \frac{2}{3} e \mathcal{E} V v_\alpha n_\alpha \Phi_\alpha, \quad (44)$$

where we have written  $v_\alpha$ ,  $n_\alpha$ , and  $\Phi_\alpha$  for  $v_\alpha(E_F)$ ,  $n_\alpha(E_F)$ , and  $\Phi_\alpha(E_F)$ . The last line of (44) is obtained from the preceding line by noting that  $v_\alpha(E)$ ,  $n_\alpha(E)$ , and  $\Phi_\alpha(E)$  are relatively slowly varying functions of energy compared with  $\partial f_0 / \partial E$  which is sharply peaked at the Fermi energy.

The calculation of  $\mathcal{L}_{\alpha\alpha}$ ,  $\mathfrak{M}_{\alpha\alpha}$ , and  $\mathfrak{M}_{12}$  is more complicated and is discussed in Appendix B. The resulting expressions involve integrals over  $\mathbf{q}$  which cannot be calculated explicitly without making some

assumption about the functions  $G_{11}(\mathbf{q})$ ,  $G_{22}(\mathbf{q})$ , and  $G_{12}(\mathbf{q})$ . Little is known about these functions except that they must approach zero for large  $\mathbf{q}$ . However, since a conduction electron experiences a strong exchange force only when it is in the region occupied by the localized  $d$  or  $f$  electrons, the range of the  $s$ - $d$  or  $s$ - $f$  potential function  $G(\mathbf{r})$  of Eq. (3) is probably not much greater than the  $d$ - or  $f$ -shell radius. As a result, it is customary<sup>24,25</sup> to represent the  $s$ - $d$  interaction by a  $\delta$  function. Thus, we shall take  $G_{11}(\mathbf{q})$ ,  $G_{22}(\mathbf{q})$ , and  $G_{12}(\mathbf{q})$  to be constants  $G_{11}$ ,  $G_{22}$ , and  $G_{12}$ , representing the various interaction strengths. [ $G_{11}$  is the  $J(0)$  of Yosida,<sup>25</sup>  $G_{22}$  is the corresponding quantity for conduction electrons in the  $d$  band and  $G_{12}$  is appropriate for the case where an  $s$  to  $d$  transition takes place as a result of spin-wave scattering.]

It should be noted here that it is not difficult to incorporate into the theory a more realistic form of  $G(\mathbf{q})$ , such as corresponds to an  $s$ - $d$  interaction of square-well shape, for example. However, the effect on the resistivity of such a sophistication is small, as is illustrated for a cubic lattice in Appendix D.

We now define the following basic integrals:

$$\mathcal{Q}_z^{(i)} = (a^4/8\pi) \int (q_z^2/q) \text{csch}(E_{\mathbf{q}}^{(i)}/2kT) d\mathbf{q}, \quad (45)$$

$$\mathcal{Q}_r^{(i)} = (a^4/8\pi) \int (q_r^2/2q) \text{csch}(E_{\mathbf{q}}^{(i)}/2kT) d\mathbf{q}, \quad (46)$$

$$\mathcal{R}_{nz}^{(i)} = (a^{4-2n}/8\pi) \int_{|k_{F1}-k_{F2}|}^{k_{F1}+k_{F2}} (q_z^2/q^{2n+1}) \times \text{csch}(E_{\mathbf{q}}^{(i)}/2kT) d\mathbf{q}, \quad (47)$$

$$\mathcal{R}_{nr}^{(i)} = (a^{4-2n}/8\pi) \int_{|k_{F1}-k_{F2}|}^{k_{F1}+k_{F2}} (q_r^2/2q^{2n+1}) \times \text{csch}(E_{\mathbf{q}}^{(i)}/2kT) d\mathbf{q}. \quad (48)$$

Here,  $q_z$  and  $q_r = (q_x^2 + q_y^2)^{1/2}$  are the components of  $\mathbf{q}$  parallel and perpendicular to  $\mathcal{E}$ , and  $a$  is the nearest-neighbor distance. In terms of these integrals the results of Appendix B, Eqs. (B10), (B11), and (B12), are

$$\mathcal{L}_{\alpha\alpha} = [(kTV^2\pi S)/(N\hbar k_{F\alpha}^4 a^4)] \Phi_\alpha^2 n_\alpha^2 G_{\alpha\alpha}^2 2 \sum_i \mathcal{Q}_z^{(i)}, \quad (49)$$

$$\begin{aligned} \mathfrak{M}_{11} = & [(kTV^2\pi S)/(N\hbar k_{F1}^3 k_{F2} a^4)] \Phi_1^2 n_1 n_2 G_{12}^2 \\ & \times \left\{ \sum_i (\mathcal{R}_{0z}^{(i)} - \mathcal{R}_{0r}^{(i)}) + 2(k_{F1}^2 a^2 - k_{F2}^2 a^2)^2 \right. \\ & \times \sum_i \mathcal{R}_{1z}^{(i)} + 2(k_{F1}^2 a^2 + k_{F2}^2 a^2) \sum_i \mathcal{R}_{1r}^{(i)} \\ & \left. + (k_{F1}^2 a^2 - k_{F2}^2 a^2)^2 \sum_i (\mathcal{R}_{2z}^{(i)} - \mathcal{R}_{2r}^{(i)}) \right\}, \quad (50) \end{aligned}$$

$$\begin{aligned} \mathfrak{M}_{12} = & [(kTV^2\pi S)/(N\hbar k_{F1}^2 k_{F2}^2 a^4)] \Phi_1 \Phi_2 n_1 n_2 G_{12}^2 \\ & \times \left\{ -\sum_i (\mathfrak{R}_{0z}^{(i)} + \mathfrak{R}_{0r}^{(i)}) + 2(k_{F1}^2 a^2 + k_{F2}^2 a^2) \mathfrak{R}_{1r}^{(i)} \right. \\ & \left. + (k_{F1}^2 a^2 - k_{F2}^2 a^2)^2 \sum_i (\mathfrak{R}_{2z}^{(i)} - \mathfrak{R}_{2r}^{(i)}) \right\}. \quad (51) \end{aligned}$$

$\mathfrak{M}_{22}$  is given by (50) with the subscripts 1 and 2 interchanged on  $k_{F\alpha}$  and  $\Phi_\alpha$ .

The range of integration of  $\mathbf{q}$  in the integrals (45)–(48) is the first Brillouin zone and the integrals  $\mathfrak{R}_{nz}^{(i)}$  and  $\mathfrak{R}_{nr}^{(i)}$ , which describe the  $s$ - $d$  scattering processes, have the additional restriction that  $q$  must be in the range  $|k_{F1} - k_{F2}| \leq q \leq k_{F1} + k_{F2}$ . This condition, which also occurs for  $s$ - $d$  phonon scattering,<sup>8</sup> arises simply because in order to conserve momentum  $s$ - $d$  transitions require spin waves whose  $q$ 's exceed the distance between the Fermi spheres of the two bands. It is evident that if  $k_{F1} = k_{F2}$  the integrals  $\mathfrak{R}_{1z}^{(i)}$ ,  $\mathfrak{R}_{1r}^{(i)}$ ,  $\mathfrak{R}_{2z}^{(i)}$ , and  $\mathfrak{R}_{2r}^{(i)}$  are infinite because each has a singularity in the integrand at  $q=0$ . However, the case  $k_{F1} = k_{F2}$  cannot arise in a ferromagnet because the bands of Eq. (42) are split at each value of  $\mathbf{k}$  by the  $s$ - $d$  interaction  $\mathfrak{H}_{sd}$ . The situation is depicted in Fig. 2. A straightforward calculation shows that the minimum value of  $|k_{F1} - k_{F2}|$  is approximately given by

$$|k_{F1} - k_{F2}| a = (m_2/m_1)^{1/2} G_{12} S (k_{F1} + k_{F2}) a / 2E_F, \quad (52)$$

which is roughly 0.6, 0.5, 0.1, and 0.7 for Fe, Co, Ni, and Gd, respectively.

Summarizing what we have obtained so far, our general expression for the electrical resistivity is Eq. (40) with  $\mathfrak{D}_\alpha$ ,  $\mathcal{L}_{\alpha\alpha}$ ,  $\mathfrak{M}_{11}$ ,  $\mathfrak{M}_{22}$ , and  $\mathfrak{M}_{12}$  given by (44) and (49)–(51). The main approximations which have been made are

- (i) neglect of spin-wave umklapp processes,
- (ii) assumption that the magnetic spin system remains in thermal equilibrium,
- (iii) assumption of spherical energy bands,
- (iv) assumption that the Bloch functions  $u_{\mathbf{k}}(\mathbf{r})$  depend only weakly on  $\mathbf{k}$ ,
- (v) representation of the  $s$ - $d$  interaction by a  $\delta$  function, [These last two assumptions lead to our taking the integral in (5) to be a constant, independent of  $\mathbf{k}$  or  $\mathbf{k}'$ .]
- (vi) constraint of certain functions, notably the density of states  $n_1$  and  $n_2$ , to be spin-independent,
- (vii) use of the variational method which provides only an upper bound to  $\rho_{\text{mag}}$  for the scattering processes considered.

It is worth mentioning that if there is only one band of conduction electrons ( $n_2=0$ ), Eq. (41) reduces to an expression reported earlier.<sup>21</sup>

#### 4. CUBIC FERROMAGNETS

For Fe, Co, and Ni there is only one spin-wave mode and the cubic symmetry leads to great simplifications. We shall first show how  $\rho_{\text{mag}}$  is computed on the basis

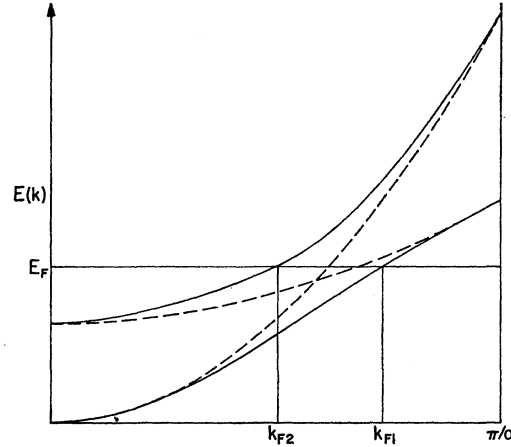


FIG. 2. Diagram illustrating how the presence of the  $s$ - $d$  interaction prevents  $k_{F1}$  and  $k_{F2}$  from being equal. Dashed curves: unperturbed parabolic bands. Solid curves: bands in the presence of the  $s$ - $d$  interaction.

of the model described in the last section, and then we shall introduce an inessential approximation for the purpose of bringing out more clearly the physical content of the theory.

At temperatures well below  $T_c$ , the spin-wave energy is adequately represented by

$$E_{\mathbf{q}} = \mathfrak{D}q^2. \quad (53)$$

The integrations over  $q_x$ ,  $q_y$ , and  $q_z$  in (45)–(48) should be confined to the first Brillouin zone so as to capture the correct number of  $\mathbf{q}$ 's. For cubic structures it is a good approximation to replace the first Brillouin zone by a Debye sphere of radius  $Q$  having the same volume in reciprocal space. Then  $\mathfrak{Q}_z = \mathfrak{Q}_r = \mathfrak{Q}$  and  $\mathfrak{R}_{nz} = \mathfrak{R}_{nr} = \mathfrak{R}_n$ , where

$$\mathfrak{Q} = (a^4/6) \int_0^Q q^3 \text{csch}(\mathfrak{D}q^2/2kT) dq, \quad (54)$$

$$\mathfrak{R}_n = (a^{4-2n}/6) \int_{|k_{F1}-k_{F2}|}^Q q^{3-2n} \text{csch}(\mathfrak{D}q^2/2kT) dq. \quad (55)$$

By means of the expansion,

$$\text{csch}x = 2 \sum_{p=0}^{\infty} e^{-(2p+1)x}, \quad (56)$$

the integrals we require are readily expressed as

$$\mathfrak{Q} = (2/3)(kTa^2/\mathfrak{D})^2 \sum_{p=0}^{\infty} (2p+1)^{-2} \times (1 - e^{-B_1} - B_1 e^{-B_1}), \quad (57)$$

$$\mathfrak{R}_0 = (2/3)(kTa^2/\mathfrak{D})^2 \sum_{p=0}^{\infty} (2p+1)^{-2} \times (e^{-B_0} - e^{-B_1} + B_0 e^{-B_0} - B_1 e^{-B_1}), \quad (58)$$

$$\mathfrak{R}_1 = (1/3)(kTa^2/\mathfrak{D}) \sum_{p=0}^{\infty} (2p+1)^{-1} (e^{-B_0} - e^{-B_1}), \quad (59)$$



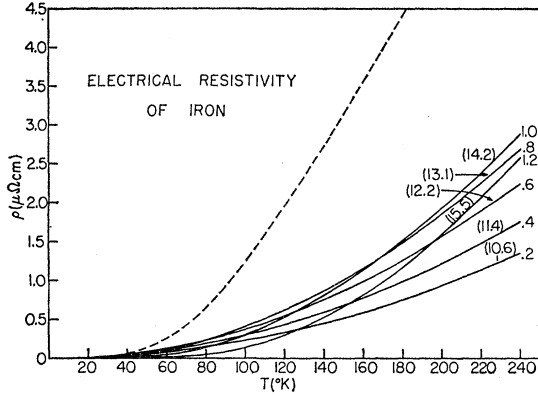


FIG. 3. Computed curves of  $\rho_{\text{mag}}$  for Fe with different values of  $(k_{F1}-k_{F2})a$ , shown at the right of each curve. The values in brackets are the corresponding effective mass ratios,  $m_2/m_1$ . The dashed curve was obtained experimentally by White and Woods.

where

$$B_0(p, T) = (2p+1)\mathfrak{D}(k_{F1}-k_{F2})^2/(2kT), \quad (60)$$

$$B_1(p, T) = (2p+1)\mathfrak{D}Q^2/(2kT). \quad (61)$$

The terms involving  $B_1$  in (57)–(59) are “zone-boundary corrections” and can be neglected here since even in the most unfavorable case ( $p=0$ ,  $T=T_c$ ),  $B_1$  has a value of 5 or more for Fe, Co, and Ni.

Equation (40) can now be reduced to a convenient form using relations such as

$$n_1/n_2 = (m_1/m_2)(k_{F1}/k_{F2}), \quad (62)$$

$$v_1/v_2 = (m_2/m_1)(k_{F1}/k_{F2}), \quad (63)$$

which hold for spherical energy bands. For compactness we define

$$A_{11} = G_{11}^2 Q + 2(m_2/m_1)(k_{F1}a)^2 G_{12}^2 \mathfrak{R}_1, \quad (64)$$

$$A_{22} = G_{22}^2 Q + 2(m_1/m_2)(k_{F2}a)^2 G_{12}^2 \mathfrak{R}_1, \quad (65)$$

$$A_{12} = G_{12}^2 [(k_{F1}^2 a^2 + k_{F2}^2 a^2) \mathfrak{R}_1 - \mathfrak{R}_0]. \quad (66)$$

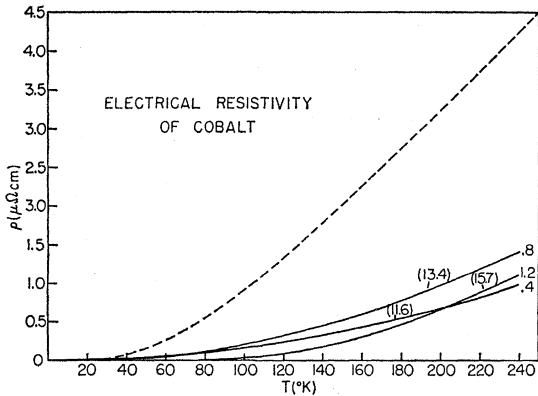


FIG. 4. Computed  $\rho_{\text{mag}}$  curves for Co shown along with the experimental results of White and Woods (dashed curve).

Then, using the relation  $\frac{1}{2}m_1v_1^2 = E_F$ , one obtains

$$\rho_{\text{mag}} = \frac{9\pi V S m_1}{4 N \hbar E_F e^2} \frac{1}{(k_{F1}a)^4} \frac{A_{11}A_{22} - A_{12}^2}{\text{Denom}}, \quad (67)$$

$$\text{Denom} = A_{22} + 2(m_1/m_2)(k_{F2}/k_{F1})^3 A_{12} + (m_1/m_2)^2 (k_{F2}/k_{F1})^6 A_{11}. \quad (68)$$

Calculations of  $\rho_{\text{mag}}$  using these expressions and (57)–(59) have been performed for Fe, Co, and Ni, and the results are displayed in Figs. 3–5. The values of the various physical parameters used in the calculations are given in Table I. There is some evidence<sup>32</sup> that metallic Fe, Co, and Ni have about one *s* electron per atom and  $k_{F1}$  and  $E_F$  were taken in each case to correspond to this number. On the supposition that only a fraction of a *d* electron per atom is itinerant, it was assumed that  $k_{F2} < k_{F1}$ . Then  $k_{F2}$  was treated as a variable parameter, the values of  $(k_{F1}-k_{F2})a$  for the different curves appearing to their right. The

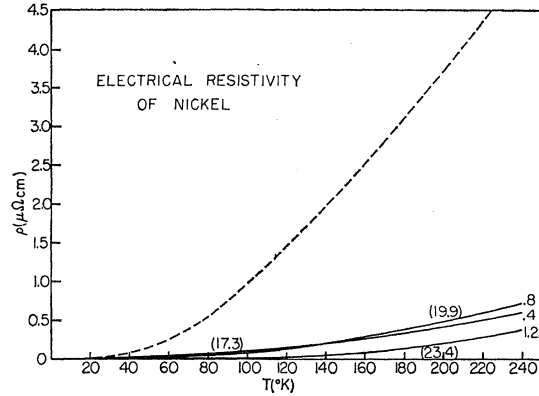


FIG. 5. Computed  $\rho_{\text{mag}}$  curves for Ni shown along with the experimental results of White and Woods (dashed curve).

effective mass, shown in brackets above each curve, was obtained by means of (62) with  $n_2/n_1$  estimated from electronic specific heat data.<sup>33</sup> The values of  $S$ , the effective spin, and  $\mathfrak{D}/k$  were deduced from low-temperature magnetization data using the standard spin-wave expression.<sup>34</sup>

The parameters  $G_{11}$ ,  $G_{12}$ , and  $G_{22}$  which occur squared in  $A_{11}$ ,  $A_{22}$ ,  $A_{12}$  and largely determine the magnitude of  $\rho_{\text{mag}}$ , are the most difficult to estimate. Tables of atomic spectra<sup>35</sup> indicate that in the free atom their value is approximately 0.2–0.4 eV with  $G_{22}$  somewhat

<sup>32</sup> L. R. Walker, G. K. Wertheim, and V. Jaccarino, Phys. Rev. Letters 6, 98 (1961).

<sup>33</sup> Reference 6, p. 127.

<sup>34</sup> F. Keffer, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, to be published).

<sup>35</sup> Charlotte E. Moore, in *Atomic Energy Levels* (National Bureau of Standards Circular No. 467, 1952), Vol. 2. For example, for Fe,  $2G_{11}S'$  is approximately the difference in energy between the  $3d^7 4s^3 F$  and  $3d^7 4s^2 F$  terms of Fe,  $S'$  being the unpaired *d*-electron spin in these terms.

larger. Also, an estimate of  $G_{11}$  in the metal can be obtained from low-temperature magnetization data assuming that the nearest neighbor  $J_{nm}$  of the Heisenberg exchange Hamiltonian is given by the indirect exchange coupling theories of Kasuya<sup>24</sup> and Yosida.<sup>25</sup> Calculations have been performed in which the  $s$ - $d$  interaction potential  $G(\mathbf{r}-\mathbf{R}_n)$  was represented by a  $\delta$ -function (which gave negative  $J_{nm}$ 's for Fe, Co, and Ni) and by square wells of radii  $3.0/k_F$  and  $5.0/k_F$ . These calculations indicate that in the metal  $G_{11} \sim 1$ - $3$  eV. While the estimates from atomic spectra are certainly too low (the free atom Hartree-Fock  $4s$  function for Fe has its main maximum at a radial distance equal to about half the  $n$ - $n$  distance in the metal), the other estimates of  $G_{11}$  are probably too high. It should be recognized that the situation regarding the origin of the coupling constants is not at all clear; for example, the Anderson-Clogston mechanism<sup>22</sup> may play a more important role than the  $s$ - $d$  interaction. The illustrated curves were computed with a value of 0.8 eV for  $G_{11}$  and  $G_{12}$  while the estimates from optical spectra were retained for  $G_{22}$ .

TABLE I. Values of physical parameters used in the calculations.

|    | $V/N$<br>( $\times 10^{-23}$<br>cm <sup>3</sup> ) | $k_{F1}a$ | $E_F$<br>(eV) | $n_2/n_1$ | $\mathcal{D}/ka^2$<br>(deg) | $S$  | $G_{11}$<br>(eV) | $G_{12}$<br>(eV) | $G_{22}$<br>(eV) |
|----|---|-----------|---------------|-----------|-----------------------------|------|------------------|------------------|------------------|
| Fe | 1.18  | 3.37      | 7.1           | 10.0      | 545                         | 1.06 | 0.8              | 0.8              | 0.6              |
| Co | 1.10  | 3.47      | 7.3           | 10.3      | 638                         | 0.77 | 0.8              | 0.8              | 0.7              |
| Ni | 1.09  | 3.46      | 7.3           | 15.3      | 761                         | 0.27 | 0.8              | 0.8              | 0.8              |
| Gd | 3.31  | 4.40      | 5.6           | ...       | ...                         | 3.5  | 0.07             | 0.12             | 0.11             |

The experimental results of White and Woods<sup>1</sup> are shown as the dashed curves in Figs. 3-5. One cannot make any very direct comparison between theory and experiment, however, because of the difficulty of separating out the phonon contribution to the total resistivity. (This must, of course, include phonon-induced  $s$ - $d$  transitions and phonon umklapp processes.) Further uncertainty arises from having neglected spin-wave umklapp processes in the calculations. Moreover, certain crucial parameters are known only very roughly. For example, the relatively low curves obtained for Ni would be greatly boosted by assuming fewer than 1.0 conduction electrons per atom in the  $s$  band and by taking  $S = \frac{1}{2}$  instead of 0.27. However, what the calculations clearly demonstrate is that a fairly large  $\rho_{\text{mag}}$  results above 10-20°K when spin-wave  $s$ - $d$  scattering is taken into account.

It is of interest to show from (67) the relative importance of  $s$ - $s$  and  $s$ - $d$  scattering. For clarity let us consider the representative case of Fe with  $(k_{F1} - k_{F2})a = 0.8$ ,  $m_2/m_1 = 13.1$ . At 20°K,  $B_0 = 8.7$  and consequently below this temperature  $\mathcal{R}_0$  and  $\mathcal{R}_1$  are completely negligible compared with  $\mathcal{Q}$ . Then to a good approximation the last factor of (67) reduces to  $G_{11}^2 \mathcal{Q}$ , and the

TABLE II. Calculated contributions to  $\rho_{\text{mag}}$  of Fe for the case  $(k_{F1} - k_{F2})a = 0.8$ ,  $m_2/m_1 = 13.1$ . Units— $\mu\Omega\text{cm}$ .

| $T$<br>(°K) | $s$ - $s$<br>term | $s$ - $d$<br>term | Third<br>term | Sum  | Eq. (67)<br>complete |
|-------------|-------------------|-------------------|---------------|------|----------------------|
| 50          | 0.002             | 0.09              | -0.02         | 0.08 | 0.06                 |
| 100         | 0.009             | 1.07              | -0.42         | 0.66 | 0.41                 |
| 150         | 0.021             | 2.95              | -1.28         | 1.70 | 1.01                 |
| 200         | 0.037             | 5.42              | -2.33         | 3.12 | 1.85                 |
| 250         | 0.058             | 8.30              | -3.48         | 4.88 | 2.92                 |
| 300         | 0.083             | 11.52             | -4.64         | 6.96 | 4.21                 |

resistivity is

$$\rho_{\text{mag}} = \frac{3\pi^3 V m_1 S G_{11}^2}{16 N e^2 \hbar E_F} \left( \frac{kT}{k_{F1}^2 \mathcal{D}} \right)^2. \quad (69)$$

This is the same as Eq. (2), the one-band result of Kasuya and Mannari, apart from a factor of  $\frac{3}{2}$  which probably is a consequence of the variational method. Thus, below about 10-20°K in Fe, Co, and Ni the spin-wave  $s$ - $d$  scattering is negligible;  $\rho_{\text{mag}}$  is almost entirely due to  $s$ - $s$  scattering and is proportional to  $T^2$ . We note that Kasuya and Mannari found their theories to be in fairly good agreement with experiment because comparison was confined to very low temperatures.

At temperatures above 10-20°K the  $s$ - $d$  scattering becomes increasingly important. In order to bring out the physical content of Eq. (67) at temperatures above 20°K, it is helpful to approximate the denominator by  $A_{22}$ , omitting the second and third terms. [While this approximation would be reasonably good for  $k_{F2} \ll k_{F1}$ , in most cases of interest the three terms of (68) are comparable in magnitude and it would probably be better to approximate the denominator by  $2A_{22}$ , say.] Then one has

$$\rho_{\text{mag}} = \frac{9\pi V m_1 S}{4 N e^2 \hbar E_F} \frac{1}{(k_{F1}a)^4} [G_{11}^2 \mathcal{Q} + 2(m_2/m_1)(k_{F1}a)^2 G_{12}^2 \mathcal{R}_1 - A_{12}^2/A_{22}]. \quad (70)$$

The first two terms of this expression arise from  $s$ - $s$  scattering and  $s$ - $d$  scattering, respectively. The meaning of the third term is not so straightforward. In Table II are shown the contributions of these terms to  $\rho_{\text{mag}}$  and their sum is compared with the result one obtains using Eq. (67) without approximations.

It is illuminating to sketch how the second term of (70) can be obtained in a simple, direct way from the terms of (20) which express the  $s$ - $d$  transitions. Suppose that an isotropic relaxation time  $\tau_{sd}$  exists which describes these scattering processes. Then from (20), neglecting  $g(\mathbf{k}d-)$  compared with  $g(\mathbf{k}s+)$ , one can write

$$\left. \frac{\partial f}{\partial t}(\mathbf{k}s+) \right]_{\text{coll}} = - \frac{f_1(\mathbf{k}s+)}{\tau_{sd}} = - \sum_{\mathbf{k}'} L(\mathbf{k}s+ \rightarrow \mathbf{k}'d-) g(\mathbf{k}s+), \quad (71)$$

with  $f_1(\mathbf{k}s+)$  given by (18). Integrating both sides over the energy  $E$  of the electron  $\mathbf{k}s+$  and using the energy-conservation  $\delta$  function to confine  $\mathbf{k}$  and  $\mathbf{k}'$  to their respective Fermi spheres, one finds

$$\frac{1}{\tau_{sd}} = -\frac{1}{2} \frac{V}{N} \frac{SG_{12}^2}{\hbar} n_2 \int \text{csch}(E_q/2kT) I(\mathbf{q}) d\mathbf{q}, \quad (72)$$

where

$$I(\mathbf{q}) = - \int \delta(\mathbf{k} - \mathbf{k}' \pm \mathbf{q}) d\Omega' \quad (73a)$$

$$= - \frac{2}{k_{F2}} \delta(k_{F1}^2 - k_{F2}^2 \pm 2k_{F1}q \cos\psi + q^2). \quad (73b)$$

The last expression for  $I(\mathbf{q})$  follows making use of the identity (B8). Here  $\psi$  is the angle between  $\mathbf{k}$  and  $\mathbf{q}$ . One can see that this  $\delta$  function restricts  $q$  to the range  $|k_{F1} - k_{F2}| \leq q \leq k_{F1} + k_{F2}$ , and, thus, the integral in (72) is  $\mathcal{R}_1$  given by (55). The equivalence of (72) with the second term of (70) is now readily established using (62) and the relation,

$$n_1 \equiv n_1(E_F) = 3N_s/(4E_F), \quad (74)$$

where  $N_s$  is the number of electrons per unit volume in the  $s$  band.

From Table II it can be seen that the third term is quite large—almost half the magnitude of the main  $s$ - $d$  scattering term in this case. As  $(k_{F1} - k_{F2})a$  is decreased, the magnitude of this term becomes an even larger proportion of that of the second term, almost cancelling the second term for the case  $(k_{F1} - k_{F2})a = 0.2$ . From the simple calculation just described it would seem that the third term of (70) can be thought of as partly due to  $d \rightarrow s$  processes which were neglected in writing down (71).

## 5. HEXAGONAL FERROMAGNETS

We now turn to the evaluation of  $\rho_{\text{mag}}$  for hexagonal structures. Because the expressions one has to work with in this case are much more cumbersome than for the cubic case, it is helpful to approximate the denomi-

nator of (40) by  $(\mathcal{L}_{22} + \mathfrak{M}_{22})\mathcal{D}_1^2$ . This is the same approximation as was introduced in writing down Eq. (70). For simplicity we also neglect the term  $-\mathfrak{M}_{12}^2/(\mathcal{L}_{22} + \mathfrak{M}_{22})\mathcal{D}_1^2$ , which corresponds to omitting the third term of (70). For a reasonably large value of  $(k_{F1} - k_{F2})a$ , we expect the effect of these two approximations will be to overestimate the magnitude of  $\rho_{\text{mag}}$  by a factor of 2–3 in the temperature region above 5°K. Making these simplifications one obtains from (40), (44), (49), and (50),

$$\begin{aligned} \rho_{\text{mag}} < [V\mathcal{E}^2/(kT)] (\mathcal{L}_{11} + \mathfrak{M}_{11})/\mathcal{D}_1^2 \\ = \frac{9\pi}{4} \frac{Vm_1}{Nc^2} \frac{S}{\hbar E_F} \frac{1}{(k_{F1}a)^4} \{ G_{11}^2 \sum_i \mathcal{Q}_z^{(i)} \\ + \frac{1}{2} (m_2/m_1) G_{12}^2 [\sum_i (\mathcal{R}_{0z}^{(i)} - \mathcal{R}_{0r}^{(i)}) \\ + 2(k_{F1}^2 + k_{F2}^2)a^2 \sum_i \mathcal{R}_{1r}^{(i)} \\ + 2(k_{F1}^2 - k_{F2}^2)a^2 \sum_i \mathcal{R}_{1z}^{(i)} \\ + (k_{F1}^2 - k_{F2}^2)^2 a^4 \sum_i (\mathcal{R}_{2z}^{(i)} - \mathcal{R}_{2r}^{(i)})] \}. \quad (75) \end{aligned}$$

The integrals  $\mathcal{Q}_z^{(i)}$ ,  $\mathcal{Q}_r^{(i)}$ ,  $\mathcal{R}_{nz}^{(i)}$ , and  $\mathcal{R}_{nr}^{(i)}$  were defined in (45)–(48) with  $q_z$  and  $q_r$  the components of  $\mathbf{q}$  parallel and perpendicular to the electric field  $\mathcal{E}$ . For  $\mathcal{E}$  along the  $c$  axis of the crystal let us denote  $\mathcal{Q}_z^{(i)}$  and  $\mathcal{Q}_r^{(i)}$  as  $\mathcal{Q}_{11}^{(i)}$  and  $\mathcal{Q}_{1z}^{(i)}$ , respectively with a similar convention for  $\mathcal{R}_{n1}^{(i)}$  and  $\mathcal{R}_{n1z}^{(i)}$ . The resistivity calculated from (75) for this case is denoted  $\rho_{11}$ . It is clear that the expression for the resistivity  $\rho_{\perp}$  corresponding to  $\mathcal{E}$  perpendicular to the  $c$  axis is obtained from the expression for  $\rho$  by merely interchanging  $\mathcal{Q}_{11}^{(i)}$  and  $\mathcal{Q}_{1z}^{(i)}$ ,  $\mathcal{R}_{n1}^{(i)}$  and  $\mathcal{R}_{n1z}^{(i)}$ . Calculations have been performed for  $\rho_{11}$  and  $\rho_{\perp}$ . It should be recognized, however, that very little significance can be attached to the calculated anisotropy because of the many approximations involved, in particular, the simple spherical band model for the electrons.

A certain amount of algebra is necessary to express

TABLE III. Temperature dependence of the integrals  $\mathcal{Q}_{11}^{(1)} + \mathcal{Q}_{11}^{(2)}$ ,  $\mathcal{Q}_{1z}^{(1)} + \mathcal{Q}_{1z}^{(2)}$ ,  $\mathcal{R}_{n1}^{(1)} + \mathcal{R}_{n1}^{(2)}$  and  $\mathcal{R}_{n1z}^{(1)} + \mathcal{R}_{n1z}^{(2)}$  for the case  $(k_{F1} - k_{F2})a = 0.9$ .

| $\theta$ | $\mathcal{Q}_{11}^{(1)} + \mathcal{Q}_{11}^{(2)}$ | $\mathcal{R}_{011}^{(1)} \pm \mathcal{R}_{011}^{(2)}$ | $\mathcal{R}_{111}^{(1)} + \mathcal{R}_{111}^{(2)}$ | $\mathcal{R}_{211}^{(1)} + \mathcal{R}_{211}^{(2)}$ | $\mathcal{Q}_{1z}^{(1)} + \mathcal{Q}_{1z}^{(2)}$ | $\mathcal{R}_{01z}^{(1)} + \mathcal{R}_{01z}^{(2)}$ | $\mathcal{R}_{11z}^{(1)} + \mathcal{R}_{11z}^{(2)}$ | $\mathcal{R}_{21z}^{(1)} + \mathcal{R}_{21z}^{(2)}$ |
|----------|---|---|---|---|---|---|---|---|
| 0.1      | 0.09  | 0.05  | 0.03  | 0.02  | 0.09  | 0.05  | 0.03  | 0.02  |
| 0.2      | 0.38  | 0.30  | 0.14  | 0.09  | 0.39  | 0.31  | 0.14  | 0.09  |
| 0.4      | 1.51  | 1.34  | 0.47  | 0.24  | 1.92  | 1.75  | 0.49  | 0.23  |
| 0.6      | 2.96  | 2.69  | 0.82  | 0.38  | 4.44  | 4.17  | 0.95  | 0.38  |
| 0.8      | 4.59  | 4.19  | 1.17  | 0.52  | 7.43  | 7.03  | 1.42  | 0.52  |
| 1.0      | 6.16  | 5.61  | 1.49  | 0.64  | 10.50   | 9.95  | 1.88  | 0.65  |
| 1.2      | 7.69  | 6.96  | 1.79  | 0.74  | 13.53   | 12.80   | 2.32  | 0.77  |
| 1.4      | 9.02  | 8.08  | 2.04  | 0.83  | 16.39   | 15.46   | 2.73  | 0.88  |
| 1.6      | 10.42   | 9.25  | 2.29  | 0.92  | 19.25   | 18.08   | 3.12  | 0.98  |
| 1.8      | 11.96   | 10.53   | 2.55  | 1.00  | 22.18   | 20.75   | 3.50  | 1.07  |
| 2.0      | 13.47   | 11.75   | 2.78  | 1.07  | 25.05   | 23.33   | 3.87  | 1.15  |

the integrals  $\mathcal{Q}_{11}^{(i)}$ ,  $\mathcal{Q}_{\perp}^{(i)}$ ,  $\mathcal{R}_{n11}^{(i)}$ , and  $\mathcal{R}_{n\perp}^{(i)}$  in a form suitable for numerical computation. The details are given in Appendix C and the values of these integrals as a function of the dimensionless parameter  $\theta = kT/12JS$  are given in Table III. In computing these integrals it was found that, in contrast with the case of cubic ferromagnets, important corrections result from confining the integrations over  $q_x$ ,  $q_y$ , and  $q_z$  to the first Brillouin zone, approximated here by a right circular cylinder. Appendix C can be briefly summarized by saying that each integral is developed as a series in increasing powers of the temperature, the leading terms varying essentially as  $T^2$  and  $T^3$  (modified by the temperature-dependent zone-boundary corrections which become increasingly important with increasing temperature). These terms have a direct mathematical correspondence with the  $T^3$  and  $T^{\frac{3}{2}}$  terms of the spin-wave expression for the magnetization.

Calculations have been performed which include the  $T^2$  and  $T^3$  contributions from the low-energy ("acoustic") spin-wave mode and from the  $T^2$  term of the

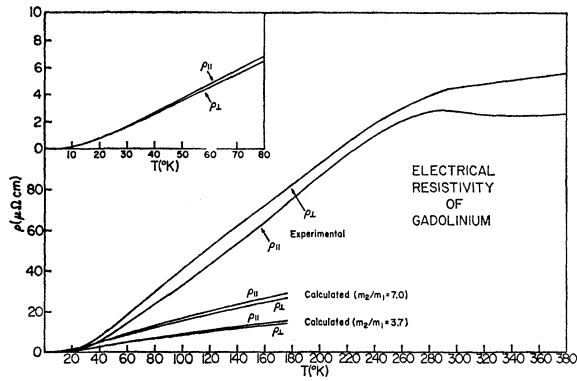


FIG. 6. Computed curves of  $\rho_{\text{mag}}$  for Gd shown with the experimental results of Nigh, Legvold, and Spedding. The inset shows in more detail at low temperatures the computed curves for the case  $m_2/m_1 = 3.7$ .

second ("optical") spin-wave mode. The results for  $\rho_{11}$  and  $\rho_{\perp}$  are given in Tables IV and V as a function of  $\theta$  and  $T$ . (For Gd the correspondence between  $\theta$  and  $T$  is made with  $J = 2.1^\circ\text{K}^{27}$ ). The values of the various physical parameters used in the calculations<sup>36</sup> are given in Table I. Somewhat arbitrarily it was assumed that band 1 has two electrons per atom while band 2 has one, giving  $(k_{F1} - k_{F2})a = 0.9$ . As the electronic specific heat of Gd is not yet known with much accuracy,<sup>37</sup> calculations were performed for two arbitrary values of the effective mass ratio,  $m_2/m_1 = 3.7$  and  $7.0$ . The results are shown in Fig. 6 along with recent single-crystal measurements of Nigh, Legvold, and Spedding.<sup>38</sup>

<sup>36</sup>  $G_{11}$ ,  $G_{12}$ , and  $G_{22}$  were estimated from the atomic energy levels of Gd obtained by H. N. Russell, J. Opt. Soc. Am. **40**, 550 (1950).

<sup>37</sup> O. V. Lounasmaa, Phys. Rev. **129**, 2460 (1963).

<sup>38</sup> H. E. Nigh, S. Legvold, and F. H. Spedding, Phys. Rev. (to be published).

TABLE IV. Contributions of the terms of Eq. (75) to  $\rho_{11}$  (in  $\mu\Omega\text{cm}$ ) for the case  $m_2/m_1 = 7.0$ .

| $\theta$ | $T$ ( $^\circ\text{K}$ ) | First term | Second term | Third term | Fourth term | Fifth term | Sum   |
|----------|--------------------------|------------|-------------|------------|-------------|------------|-------|
| 0.1      | 8.8                      | 0.001      | 0.00        | 0.21       | 0.05        | 0.00       | 0.26  |
| 0.2      | 17.6                     | 0.004      | -0.001      | 0.94       | 0.22        | 0.01       | 1.17  |
| 0.5      | 44.1                     | 0.023      | -0.09       | 4.82       | 0.98        | 0.03       | 5.76  |
| 1.0      | 88.2                     | 0.064      | -0.46       | 12.69      | 2.26        | -0.09      | 14.47 |
| 1.5      | 132.3                    | 0.101      | -0.86       | 19.73      | 3.30        | -0.28      | 21.99 |
| 2.0      | 176.4                    | 0.140      | -1.23       | 26.09      | 4.22        | -0.43      | 28.79 |

While the calculated anisotropy is of the right size, it places the curve for  $\rho_{11}$  above the curve for  $\rho_{\perp}$  in contrast with experiment. However, the author does not attach any significance to this disagreement; an examination of (75) and Tables III, IV, and V shows that a trivial adjustment of the parameters  $k_{F1}$  and  $k_{F2}$  (decreasing  $k_{F2}$ ) would yield curves ordered in the same way as the experimental curves. Because of the great inadequacies of the model, however, such an adjustment of the parameters is unlikely to have very much physical significance and consequently has not been carried out.

Tables IV and V show that, as one might expect, the main contribution to  $\rho_{\text{mag}}$  above about  $5^\circ\text{K}$  comes from the third and fourth terms of (75) which involve  $\sum \mathcal{R}_{1r}^{(i)}$  and  $\sum \mathcal{R}_{1z}^{(i)}$ . The other terms in the square brackets of (75), which are zero for a cubic ferromagnet, have a small effect on the anisotropy. The first term of (75) arises entirely from  $s$ - $s$  scattering and, as in the cubic case, is negligible except at very low temperatures.

The slopes above  $10^\circ\text{K}$  of the computed curves with  $m_2/m_1 = 7.0$  and  $3.7$  are about  $\frac{1}{3}$  and  $\frac{1}{5}$ , respectively, of the "experimental  $\rho_{\text{mag}}$ " of Fig. 1. Since the approximations introduced at the beginning of this section probably cause the calculated results to be too large by a factor of about 2 this means that our calculations account for roughly 10-15% of  $\rho_{\text{mag}}$  in the linear region. It is not unreasonable, however, to imagine that spin-wave umklapp processes can account for the remaining 85-90%.

## 6. HIGHER ORDER EFFECTS

The theory developed in Secs. 2 and 3 took into account only those scattering processes which involved a change of spin of the conduction electron with simultaneous creation or destruction of a spin wave.

TABLE V. Contribution of the terms of Eq. (75) to  $\rho_{\perp}$  (in  $\mu\Omega\text{cm}$ ) for the case  $m_2/m_1 = 7.0$ .

| $\theta$ | $T$ ( $^\circ\text{K}$ ) | First term | Second term | Third term | Fourth term | Fifth term | Sum   |
|----------|--------------------------|------------|-------------|------------|-------------|------------|-------|
| 0.1      | 8.8                      | 0.001      | 0.00        | 0.22       | 0.05        | -0.00      | 0.26  |
| 0.2      | 17.6                     | 0.004      | 0.001       | 0.96       | 0.21        | -0.01      | 1.16  |
| 0.5      | 44.1                     | 0.032      | 0.09        | 4.37       | 1.08        | -0.03      | 5.55  |
| 1.0      | 88.2                     | 0.109      | 0.46        | 10.06      | 2.86        | 0.09       | 13.58 |
| 1.5      | 132.3                    | 0.185      | 0.86        | 14.67      | 4.44        | 0.28       | 20.43 |
| 2.0      | 176.4                    | 0.260      | 1.23        | 18.75      | 5.87        | 0.43       | 26.54 |

For completeness we briefly examine here the scattering processes in which the spin of the conduction electron does not change and show that they are negligible in the low-temperature region.

The matrix elements to be considered are  $\langle \mathbf{k}' \pm | \mathcal{H}_{sd} | \mathbf{k} \pm \rangle$  which involve the spin operators  $S_n^z$ . The appropriate substitution in this case is  $S_n^z = S - a_n^+ a_n^-$  and this leads to processes involving two spin waves. Corresponding to (9) one finds for a Bravais lattice the matrix elements,

$$|\langle k' \alpha' \sigma, n(\mathbf{q} + \mathbf{k}) + 1, n(\mathbf{q} + \mathbf{k}') - 1 | \mathcal{H}_{sd} | \mathbf{k} \alpha \sigma, n(\mathbf{q} + \mathbf{k}), n(\mathbf{q} + \mathbf{k}') \rangle|^2 = N^{-2} G_{\alpha \alpha'}^2 [n(\mathbf{q} + \mathbf{k}) + 1] n(\mathbf{q} + \mathbf{k}'). \quad (76)$$

This represents the scattering of a conduction electron  $\mathbf{k} \alpha \sigma$  ( $\sigma$  is a spin index) to  $\mathbf{k}' \alpha' \sigma$ , creating a spin wave  $(\mathbf{q} + \mathbf{k})$  and destroying a spin wave  $(\mathbf{q} + \mathbf{k}')$ . Written this way, momentum conservation is automatically satisfied.

It is expected that the main contribution to  $\rho_{mag}$  from such processes will come from  $s$ - $d$  transitions. A reasonable estimate of its magnitude can be obtained by adopting the approach used in Sec. 4 of assuming than an appropriate isotropic relaxation time  $\tau_{sd}'$  exists. Starting from an equation similar to (71) one finds after a certain amount of algebra,

$$\rho_{sd}' = \frac{m_1}{N_s e^2 \tau_{sd}'} \frac{3}{16 \pi^{1/2}} \frac{m_1 V G_{12}^2 m_2}{e^2 N \hbar E_F m_1 (k_{F1} a)^2} \frac{1}{\mathcal{D}} \left( \frac{k T a^2}{\mathcal{D}} \right)^{5/2} F_{sd}, \quad (77)$$

where

$$F_{sd} = \sum_{p_1=0}^{\infty} \sum_{p_2=0}^{\infty} (2p_1+1)^{-1} (2p_2+1)^{-1} (p_1+p_2+1)^{-1/2} \times \exp \left[ - \frac{\mathcal{D}}{4kT} \frac{(2p_1+1)(2p_2+1)}{(p_1+p_2+1)} (k_{F1} - k_{F2})^2 \right]. \quad (78)$$

Here  $N_s$  is the number of conduction electrons per unit volume in the  $s$ -band. [In deriving (77) we have taken  $V/(Na^3) = 1$  which is strictly true only for a simple cubic lattice. We have also neglected a term involving a function similar to (78) with  $(k_{F1} - k_{F2})^2$  replaced by  $(k_{F1} + k_{F2})^2$ .] This expression is very similar in form to the main  $s$ - $d$  scattering contribution to  $\rho_{mag}$ , the second term of (70), which using (59) can be written as

$$\rho_{sd} = \frac{3\pi V m_1 S G_{12}^2 m_2}{2 N e^2 \hbar E_F m_1 (k_{F1} a)^2} \frac{1}{\mathcal{D}} \frac{k T a^2}{\mathcal{D}} \times \sum_{p=0}^{\infty} (2p+1)^{-1} e^{-B_0}. \quad (79)$$

At low temperatures it is a fairly good approximation to retain only the first term in each of the sums in (78) and (79). Then the ratio of these two contributions to

$\rho_{mag}$  is

$$(\rho_{sd}' / \rho_{sd}) = (8\pi^{3/2} S)^{-1} (k T a^2 / \mathcal{D})^{3/2} \times \exp[\mathcal{D}(k_{F1} - k_{F2})^2 / 4kT]. \quad (80)$$

For Fe, Co, and Ni below 300°K it is found that  $\rho_{sd}'$  is about two orders of magnitude smaller than  $\rho_{sd}$ . At higher temperatures one must include many terms in the sums in (78) and (79) and it is evident that  $\rho_{sd}'$  gradually becomes a larger fraction of  $\rho_{sd}$ . However, at temperatures less than about  $\frac{1}{2}T_c$  we do not expect the two spin-wave processes to contribute significantly to  $\rho_{mag}$ .

## 7. DISCUSSION

Since we have been preoccupied in the last few sections with a rather restricted class of scattering processes, it is fitting that the results should be briefly discussed in relation to the total resistivity of ferromagnetic metals.

As was mentioned in the Introduction, ferromagnetic metals owe a large part of their electrical resistance to  $s$ - $s$  and  $s$ - $d$  scattering by the lattice vibrations.<sup>7,8</sup> Both normal and umklapp processes can occur and it is very difficult to estimate the magnitude of either or its relative importance. It follows that the procedure used to separate  $\rho_{mag}$  from the total  $\rho$  in Fig. 1, which was based on the functional form appropriate only for single-band phonon normal processes, has little reliability and such curves have not been drawn in Figs. 3-6.

Recognizing, however, that a large part of  $\rho$  in ferromagnetic metals arises from phonon scattering, one can see, nevertheless, that the main contribution to  $\rho$  correlates strongly with the magnetic behavior. The calculations we have presented are representative of this latter contribution, but the fact that they do not take account of spin-wave umklapp processes means that their value is limited. There are also, of course, errors resulting from the other approximations listed at the end of Sec. 3, but the author believes that these are relatively unimportant. (The calculations described in Appendix D indicate that one of these approximations, the representation of the  $s$ - $d$  interaction by a  $\delta$  function, introduces only a minor error.) What the calculations show, however, is that there is a large contribution to  $\rho$  from scattering of conduction electrons by spin waves, and that, except at the lowest temperatures, this contribution arises almost entirely from the scattering of  $s$  electrons into holes in the  $d$  band.

The spin-disorder resistivity,  $\rho_{mag}$ , has often been used as a means of estimating the parameter which describes the strength of the  $s$ - $d$  interaction. It should be pointed out, however, that the parameter which appears in Kasuya's molecular field expression<sup>15</sup> for  $\rho_{mag}$  above  $T_c$  gives an effective strength for the combined effects of  $s$ - $s$  and  $s$ - $d$  scattering processes, including umklapp processes of both sorts. There is also the coupling arising from the "covalent mixing"

mechanism to be considered.<sup>23</sup> On the other hand, the parameter  $J(0)$  of Yosida's paper is the same as our  $G_{11}$ , although it may be that Yosida's theory would be appreciably modified by taking into account the presence of a band of itinerant  $d$  electrons.

Unfortunately, the present work reveals very little about the size of  $G_{11}$ ,  $G_{12}$ , and  $G_{22}$ . Since  $s$ - $d$  transitions and umklapp processes require spin-wave  $q$ 's and phonon  $q$ 's exceeding some minimum value, it might be supposed that at low enough temperatures the coefficient of  $T^2$  would provide a good estimate of the size of  $G_{11}$  alone. (This supposition depends on the Baber electron-electron interaction mechanism being unimportant at these temperatures, which may not be the case.) However, using White and Woods data and Eq. (69), assuming one conduction electron per atom, one obtains values of  $G_{11}$  of 3.2, 2.0, and 0.9 eV for Fe, Co, and Ni, respectively. These are almost certainly too large.<sup>39</sup> (The value for Ni would be larger than 0.9 if one took fewer than one conduction electron per atom.) Thus, the size of these parameters in any given problem remains uncertain within quite wide limits.

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#### APPENDIX A

In this Appendix the matrix elements of the electron scattering corresponding to Eq. (8) are calculated for the hcp lattice which has two atoms in the unit cell. The atoms are assumed to be of only one (chemical) type.

For a general crystal structure Eq. (3) is modified to

$$\mathfrak{C}_{sd} = -2 \sum_{n,i} G(\mathbf{r} - \mathbf{R}_{ni}) \mathbf{s} \cdot \mathbf{S}_{ni}, \quad (\text{A1})$$

where  $n$  labels the unit cells and  $i$  labels the atoms in the unit cell. From some origin in the unit cell the positions of the atoms are given by basis vectors  $\mathbf{b}_i$ ; thus,  $\mathbf{R}_{ni} = \mathbf{R}_n + \mathbf{b}_i$ . Equation (5) for  $G(\mathbf{k} - \mathbf{k}')$  should now be rewritten

<sup>39</sup> The large value for Fe may be a result of the relatively impure samples used by White and Woods. In fact, the recent data of Semenenko and Sudovtsov (Ref. 3) for a much purer sample of Fe give a value of 0.5 eV for  $G_{11}$  using the same procedure.

with  $\mathbf{R}_n$  replaced everywhere by  $\mathbf{R}_{ni}$ . Neglecting unimportant overlap effects we may assume that  $G(\mathbf{k} - \mathbf{k}')$  is independent of  $i$  (as well as being independent of  $n$  from translational symmetry). Therefore, we now have instead of Eq. (4),

$$\begin{aligned} \langle \mathbf{k}' \pm | \mathfrak{C}_{sd} | \mathbf{k} \mp \rangle &= -N^{-1} G(\mathbf{k} - \mathbf{k}') \\ &\times \sum_{n,i} \exp[i(\mathbf{k} - \mathbf{k}') \cdot (\mathbf{R}_n + \mathbf{b}_i)] S_{ni}^{\mp}. \end{aligned} \quad (\text{A2})$$

The spin-operator substitutions become  $S_{ni}^{\mp} = (2S)^{1/2} a_{ni}^{\pm}$  and the transformation to spin waves is

$$a_{ni}^{\pm} = \mathfrak{N}^{-1/2} \sum_{\mathbf{q}} a_{\mathbf{q}i}^{\pm} \exp(\mp i\mathbf{q} \cdot \mathbf{R}_n), \quad (\text{A3})$$

where  $\mathfrak{N}$  is the number of unit cells in the crystal.

To work out the matrix elements corresponding to Eq. (7), it is necessary to transform to operators  $c_{\mathbf{q}i}^{\pm}$  which are diagonal with respect to the spin-wave states. For the hcp structure the appropriate transformation is<sup>27</sup>

$$\begin{aligned} a_{q1}^{\pm} &= \pm (i/\sqrt{2})(c_{q1}^{\pm} \mp i c_{q2}^{\pm}), \\ a_{q2}^{\pm} &= (e^{\mp i\phi}/\sqrt{2})(c_{q1}^{\pm} \pm i c_{q2}^{\pm}), \end{aligned} \quad (\text{A4})$$

where  $\phi$  is a phase angle whose value is not of interest to us here. There are two spin-wave modes in this case; the operators  $c_{q1}^{\pm}$  create or destroy spin waves  $\mathbf{q}$  in the first ("acoustic") mode while  $c_{q2}^{\pm}$  operate on the second ("optical") mode. Thus, instead of (7) we now have matrix elements  $\langle n^{(i)}(\mathbf{q}) \pm 1 | S_{n1}^{\mp} | n^{(i)}(\mathbf{q}) \rangle$  and  $\langle n^{(i)}(\mathbf{q}) \pm 1 | S_{n2}^{\mp} | n^{(i)}(\mathbf{q}) \rangle$  with  $i=1$  or 2. Using (A3) and (A4) these are easily worked out. Combining with (A2) we obtain, after a little algebra,

$$\begin{aligned} |\langle \mathbf{k}' \pm, n^{(i)}(\mathbf{q}) \pm 1 | \mathfrak{C}_{sd} | \mathbf{k} \mp, n^{(i)}(\mathbf{q}) \rangle|^2 \\ = (2S/N) [n^{(i)}(\mathbf{q}) + \frac{1}{2} \pm \frac{1}{2}] |G(\mathbf{k} - \mathbf{k}')|^2 \\ \times f_i(\pm) \sum_{\mathbf{g}} \delta_{\mathbf{g}, \mathbf{k} - \mathbf{k}' \mp \mathbf{q}}, \end{aligned} \quad (\text{A5})$$

where

$$\begin{aligned} f_1(\pm) &= \frac{1}{2} \{1 - \sin[\phi \pm (\mathbf{k} - \mathbf{k}') \cdot (\mathbf{b}_1 - \mathbf{b}_2)]\}, \\ f_2(\pm) &= \frac{1}{2} \{1 + \sin[\phi \pm (\mathbf{k} - \mathbf{k}') \cdot (\mathbf{b}_1 - \mathbf{b}_2)]\}. \end{aligned} \quad (\text{A6})$$

When the structure factor  $f_i(\pm)$  has its maximum value, the matrix elements (A5) are the same as in Eq. (8) with  $n^{(i)}(\mathbf{q})$  replacing  $n(\mathbf{q})$ .

#### APPENDIX B

Equations (33) to (36) for  $\mathfrak{L}_{\alpha\alpha}$ ,  $\mathfrak{M}_{\alpha\alpha}$ , and  $\mathfrak{M}_{12}$  involve summations over  $\mathbf{k}$ ,  $\mathbf{k}'$ , and  $\mathbf{q}$ . We outline here how the integrations over  $\mathbf{k}$  and  $\mathbf{k}'$  may be carried out making use of the energy- and momentum-conservation conditions.

As a first step let us express  $L(\mathbf{k}\alpha \rightarrow \mathbf{k}'\alpha')$  in a convenient form. Writing  $E$ ,  $E'$  as a short notation for

$E(\mathbf{k}\alpha)$  and  $E(\mathbf{k}'\alpha')$  and  $\partial f_0/\partial E$  for  $\partial f_0(\mathbf{k}\alpha)/\partial E(\mathbf{k}\alpha)$ , it is easy to show, using (15) and (18), that

$$f_0(\mathbf{k}\alpha\pm)[1-f_0(\mathbf{k}'\alpha'\mp)][n_q^{(i)}(\mathbf{q})+\frac{1}{2}\mp\frac{1}{2}] = \frac{1}{2}F(E,E') \operatorname{csch}(E_q^{(i)}/2kT), \quad (\text{B1})$$

where

$$F(E,E') = kT \left( \frac{\partial f_0}{\partial E} \frac{\partial f_0}{\partial E'} \right)^{1/2}. \quad (\text{B2})$$

Then from (19) and (11),

$$L(\mathbf{k}\alpha \rightarrow \mathbf{k}'\alpha') = (2\pi S/N\hbar)F(E,E') \sum_{\mathbf{q},i} |G_{\alpha\alpha'}(\mathbf{q})|^2 \times \operatorname{csch}(E_q^{(i)}/2kT) \delta_{\mathbf{k}',\mathbf{k}\mp\mathbf{q}} \delta(E-E'\mp E_q^{(i)}). \quad (\text{B3})$$

In this expression, either the upper or lower sign is to be taken throughout, as noted in Sec. 2. Since a characteristic spin-wave energy  $E_q^{(i)}$  is approximately two orders of magnitude smaller than electron energies  $E$  and  $E'$ , it should be a good approximation to expand  $F(E,E')$ , taking account of energy conservation,

$$F(E,E') = F(E,E) \mp E_q^{(i)} \left. \frac{\partial F(E,E')}{\partial E'} \right]_{E'=E} + \dots, \quad (\text{B4})$$

and keep only the first term.

We are now in a position to work out  $\mathcal{L}_{\alpha\alpha}$ ,  $\mathfrak{M}_{\alpha\alpha}$ , and  $\mathfrak{M}_{12}$  along the lines which led to Eq. (44) for  $\mathfrak{D}_{\alpha}$ . Replacing  $\delta_{\mathbf{k}',\mathbf{k}\pm\mathbf{q}}$  by  $(8\pi^3/V)\delta(\mathbf{k}-\mathbf{k}'\pm\mathbf{q})$ , one finds from (33) and (B3),

$$\mathcal{L}_{\alpha\alpha} = (\pi^2 V S k T / N \hbar) \Phi_{\alpha}^2 n_{\alpha}^2 \times \sum_{\mathbf{q},i} |G_{\alpha\alpha}(\mathbf{q})|^2 \operatorname{csch}(E_q^{(i)}/2kT) l_{\alpha\alpha}(\mathbf{q}), \quad (\text{B5})$$

with

$$l_{\alpha\alpha}(\mathbf{q}) = - \int (\cos\theta' - \cos\theta)^2 \delta(\mathbf{k} - \mathbf{k}' \pm \mathbf{q}) d\Omega d\Omega'. \quad (\text{B6})$$

In (B6) it is to be understood that  $\mathbf{k}$  and  $\mathbf{k}'$  are confined to the  $\alpha$ -band Fermi sphere. The  $z$  component of the momentum-conservation condition gives

$$(\cos\theta' - \cos\theta)^2 = q_z^2 / k_{F\alpha}^2, \quad (\text{B7})$$

where  $q_z$  is the component of  $\mathbf{q}$  along the direction of the electric field and  $k_{F\alpha}$  is the radius of the Fermi sphere of the  $\alpha$  band. This quantity is constant with respect to the angular integrations in (B6) and can be brought outside the integral. The remaining integral is conveniently recast using the identity,

$$(2/k_{F\alpha}) \int_0^{\infty} k^2 \delta(k^2 - k_{F\alpha}^2) dk = 1. \quad (\text{B8})$$

Thus, we can write

$$\begin{aligned} l_{\alpha\alpha}(\mathbf{q}) &= - (4q_z^2/k_{F\alpha}^4) \int \delta(\mathbf{k} - \mathbf{k}' \pm \mathbf{q}) \\ &\quad \times \delta(k^2 - k_{F\alpha}^2) \delta(k'^2 - k_{F\alpha}^2) d\mathbf{k} d\mathbf{k}', \\ &= - (4q_z^2/k_{F\alpha}^4) \int \delta(k^2 - k_{F\alpha}^2) \\ &\quad \times \delta(k^2 \pm 2\mathbf{k} \cdot \mathbf{q} + q^2 - k_{F\alpha}^2) d\mathbf{k}, \\ &= - (4\pi q_z^2/k_{F\alpha}^3) \int \delta(\pm 2k_{F\alpha} q \cos\psi + q^2) \sin\psi d\psi, \\ &= (2\pi/k_{F\alpha}^4) (q_z^2/q). \end{aligned} \quad (\text{B9})$$

In the third step here,  $\psi$  is the angle between  $\mathbf{k}$  and  $\mathbf{q}$ . Finally, we have

$$\mathcal{L}_{\alpha\alpha} = [(kTV^2S)/(8N\hbar k_{F\alpha}^4)] \Phi_{\alpha}^2 n_{\alpha}^2 \times 2 \sum_i \int |G_{\alpha\alpha}(\mathbf{q})|^2 (q_z^2/q) \operatorname{csch}(E_q^{(i)}/2kT) d\mathbf{q}. \quad (\text{B10})$$

The evaluation of  $\mathfrak{M}_{\alpha\alpha}$  and  $\mathfrak{M}_{12}$  is carried out in a similar way, but for these cases it is expedient to perform the integrations over  $\mathbf{k}$  and  $\mathbf{k}'$  in a coordinate system with  $\mathbf{q}$  as polar axis, expressing  $\cos\theta$  and  $\cos\theta'$  in terms of angles referred to this axis. Furthermore, these quantities differ from  $\mathcal{L}_{\alpha\alpha}$  in that the states  $\mathbf{k}$  and  $\mathbf{k}'$  belong to different bands, and thus, through the energy  $\delta$  functions, become confined to different Fermi spheres. One finds

$$\begin{aligned} \mathfrak{M}_{11} &= [(kTV^2S)/(8N\hbar k_{F1}^3 k_{F2})] \Phi_1^2 n_1 n_2 \\ &\quad \times \sum_i \int_{|k_{F1}-k_{F2}|}^{k_{F1}+k_{F2}} d\mathbf{q} |G_{12}(\mathbf{q})|^2 \operatorname{csch}(E_q^{(i)}/2kT) \\ &\quad \times [(q_z^2 - \frac{1}{2}q_r^2)/q + 2(k_{F1}^2 - k_{F2}^2)q_z^2/q^3 \\ &\quad + (k_{F1}^2 + k_{F2}^2)q_r^2/q^3 + (k_{F1}^2 - k_{F2}^2)^2 \\ &\quad \times (q_z^2 - \frac{1}{2}q_r^2)/q^5], \end{aligned} \quad (\text{B11})$$

$$\begin{aligned} \mathfrak{M}_{12} &= [(kTV^2S)/(8N\hbar k_{F1}^2 k_{F2}^2)] \Phi_1 \Phi_2 n_1 n_2 \\ &\quad \times \sum_i \int_{|k_{F1}-k_{F2}|}^{k_{F1}+k_{F2}} d\mathbf{q} |G_{12}(\mathbf{q})|^2 \operatorname{csch}(E_q^{(i)}/2kT) \\ &\quad \times [-(q_z^2 + \frac{1}{2}q_r^2)/q + (k_{F1}^2 + k_{F2}^2)q_r^2/q^3 \\ &\quad + (k_{F1}^2 - k_{F2}^2)^2 (q_z^2 - \frac{1}{2}q_r^2)/q^5]. \end{aligned} \quad (\text{B12})$$

$\mathfrak{M}_{22}$  is given by (B11) with the subscripts 1 and 2 interchanged. In the derivation of these expressions one finds that the momentum-conservation  $\delta$  function limits the range of  $q$  in these integrals to  $|k_{F1} - k_{F2}| \leq q \leq k_{F1} + k_{F2}$ .

## APPENDIX C

In this Appendix we describe the method used to calculate the integrals  $\mathcal{Q}_{11}^{(i)}$ ,  $\mathcal{Q}_{\perp}^{(i)}$ ,  $\mathcal{R}_{n11}^{(i)}$ , and  $\mathcal{R}_{n\perp}^{(i)}$  defined in Sec. 5. Strictly speaking, the calculation is appropriate for Gd only as the effect of strong anisotropy fields, such as are found in the other hexagonal rare-earth metals, was not included in the spin-wave dispersion relations. The extension of the treatment to include such effects is not difficult, however.

The energies of the two spin-wave modes of a hexagonal (hcp) ferromagnet without anisotropy have been derived previously.<sup>27</sup> In terms of the dimensionless variables  $\theta = kT/(12JS)$  and

$$\lambda^2 = (q_x^2 + q_y^2)a^2 = q_r^2 a^2, \quad (C1)$$

$$\mu_1 = q_z c/2 \text{ acoustic mode,}$$

$$\mu_2 = \pi/2 - q_z c/2 \text{ optical mode } (q_z \geq 0), \quad (C2)$$

they are, to the order desired in the present work,

$$E_q^{(1)}/kT = \theta^{-1} \left( \frac{1}{3} \lambda^2 + \frac{1}{2} \mu_1^2 - \frac{5}{288} \lambda^4 - \frac{1}{24} \lambda^2 \mu_1^2 - \frac{1}{24} \mu_1^4 \right), \quad (C3)$$

$$E_q^{(2)}/kT = \theta^{-1} \left( 1 + \mu_2 + \frac{1}{4} \right). \quad (C4)$$

In calculating the magnetization of a hexagonal structure<sup>27</sup> it was found that while it is important to restrict the  $q_z$  integration to the range  $-\pi/c \leq q_z \leq \pi/c$ , negligible error is introduced if the  $q_x$  and  $q_y$  integrations are taken to infinity. In the present integrals it is also essential to cut off the  $q_z$  integration at the zone boundary. However, it was found that in order to obtain accurate results, the  $q_x$  and  $q_y$  integrations must be cut off as well, particularly for  $\mathcal{Q}_{\perp}^{(i)}$  and  $\mathcal{R}_{n\perp}^{(i)}$  which involve a higher power of  $q_x^2 + q_y^2$ . Accordingly, the integrations over  $q_x$ ,  $q_y$ , and  $q_z$  were confined to the Debye right-circular cylinder of height  $2\pi/c$  and radius  $q_0 = a^{-1}(8\pi/\sqrt{3})^{1/2}$ . For the integrals  $\mathcal{R}_{n11}^{(i)}$  and  $\mathcal{R}_{n\perp}^{(i)}$  the range of integration is further limited by the condition  $q \geq |k_{F1} - k_{F2}|$ .

Let us first consider the acoustic mode integrals  $\mathcal{R}_{n11}^{(1)}$  and  $\mathcal{R}_{n\perp}^{(1)}$ . It is useful to define the function

$$\Theta(x) = 1, \quad x \geq 0, \\ \Theta(x) = 0, \quad x < 0, \quad (C5)$$

and for convenience we shall write

$$f_p(\lambda, \mu_1) = \exp \left[ -\frac{2p+1}{6\theta} (\lambda^2 + \frac{3}{2} \mu_1^2) \right] \left\{ 1 + \left( \frac{2p+1}{2\theta} \right) \left( \frac{5}{288} \lambda^4 + \frac{1}{24} \lambda^2 \mu_1^2 + \frac{1}{24} \mu_1^4 \right) + \dots \right\}. \quad (C6)$$

Then, using Eq. (63) to write

$$\text{csch}(E_q^{(1)}/2kT) = 2 \sum_{p=0}^{\infty} f_p(\lambda, \mu_1), \quad (C7)$$

and making the substitutions (C1) and (C2), one obtains

$$\mathcal{R}_{n11}^{(1)} = \left( \frac{3}{2} \right)^{3/2} \sum_{p=0}^{\infty} \int_0^{\pi/2} d\mu_1 \mu_1^2 \int_0^{q_0 a} d\lambda \lambda [\lambda^2 + \frac{3}{2} \mu_1^2]^{-n-1/2} \\ \times f_p(\lambda, \mu_1) \Theta([\lambda^2 + \frac{3}{2} \mu_1^2]^{1/2} - |k_{F1} a - k_{F2} a|), \quad (C8)$$

$$\mathcal{R}_{n\perp}^{(1)} = \left( \frac{3}{8} \right)^{1/2} \sum_{p=0}^{\infty} \int_0^{\pi/2} d\mu_1 \int_0^{q_0 a} d\lambda \lambda^3 [\lambda^2 + \frac{3}{2} \mu_1^2]^{-n-1/2} \\ \times f_p(\lambda, \mu_1) \Theta([\lambda^2 + \frac{3}{2} \mu_1^2]^{1/2} - |k_{F1} a - k_{F2} a|). \quad (C9)$$

We now make successively for  $\lambda$  and  $\mu_1$  the substitutions,

$$u^2 = [(2p+1)/(6\theta)] [\lambda^2 + \frac{3}{2} \mu_1^2], \quad (C10)$$

$$t = \left( \frac{3}{2} \right)^{1/2} [(2p+1)/(6\theta)]^{1/2} \mu_1. \quad (C11)$$

Defining

$$\alpha(p, \theta) = [(2p+1)/(6\theta)]^{1/2} |k_{F1} a - k_{F2} a|, \quad (C12)$$

$$\delta(p, \theta) = \left( \frac{3}{2} \right)^{1/2} [(2p+1)/(6\theta)]^{1/2} \frac{1}{2} \pi, \quad (C13)$$

$$\gamma(p, \theta) = (8\pi/\sqrt{3})^{1/2} [(2p+1)/(6\theta)]^{1/2}, \quad (C14)$$

and

$$I_n^m(p, \theta) = \int_0^{\delta} dt t^{2m} \int_t^{(\gamma^2+t^2)^{1/2}} du u^{2n-2m} e^{-u^2} \Theta(u-\alpha), \quad (C15)$$

one obtains by a straightforward calculation

$$\mathcal{R}_{n11}^{(1)} = \sum_{p=0}^{\infty} [6\theta/(2p+1)]^{2-n} I_{1-n}^{-1} \\ + (1/288) \sum_{p=0}^{\infty} [6\theta/(2p+1)]^{3-n} (15I_{3-n}^{-1} - 6I_{3-n}^{-2} + 7I_{3-n}^{-3}), \quad (C16)$$

$$\mathcal{R}_{n\perp}^{(1)} = \frac{1}{2} \sum_{p=0}^{\infty} [6\theta/(2p+1)]^{2-n} (I_{1-n}^{-0} - I_{1-n}^{-1}) \\ + (1/576) \sum_{p=0}^{\infty} [6\theta/(2p+1)]^{3-n} (15I_{3-n}^{-0} - 21I_{3-n}^{-1} + 13I_{3-n}^{-2} - 7I_{3-n}^{-3}). \quad (C17)$$

The double integrals  $I_n^m(p, \theta)$  can be reduced to elementary single integrals by an integration by parts in which the integral over  $u$  is differentiated with respect to  $t$ . One finds

$$I_n^m(p, \theta) = (2m+1)^{-1} \{ b_n(\alpha) - b_n(\delta) + \delta^{2m+1} a_{n-m}(\delta) \\ - \delta^{2m+1} a_{n-m}([\gamma^2 + \delta^2]^{1/2}) - (e^{-\gamma^2}/\gamma) \int_0^{\delta} t^{2m+2} \\ \times (\gamma^2 + t^2)^{n-m} [1 + (t/\gamma)^2]^{-1/2} e^{-t^2} dt \}, \quad (C18)$$



where

$$a_l(x) = \int_x^\infty t^l e^{-t^2} dt, \tag{C19}$$

$$b_l(x) = \int_x^\infty t^{l+1} e^{-t^2} dt. \tag{C20}$$

Since  $\delta \doteq \frac{1}{2}\gamma$ , then for  $0 \leq t \leq \delta$ , an expansion of the square root in the last term of (C18) is quickly convergent. Retaining the first three terms of this expansion and defining

$$c_l(k; x) = \int_0^x t^{2k+2} (\gamma^2 + t^2)^l e^{-t^2} dt, \tag{C21}$$

one finally obtains

$$I_n^m(p, \theta) = (2m+1)^{-1} \{ b_n(\alpha) - b_n(\delta) + \delta^{2m+1} a_{n-m}(\delta) - \delta^{2m+1} a_{n-m}([\gamma^2 + \delta^2]^{1/2}) - (e^{-\gamma^2/\gamma}) [c_{n-m}(m; \delta) - (\frac{1}{2}\gamma^2) c_{n-m}(m+1; \delta) + (\frac{3}{8}\gamma^4) c_{n-m}(m+2; \delta)] \}. \tag{C22}$$

As the calculation was performed using an electronic computer, it was convenient to calculate the integrals  $a_0(x)$ ,  $a_{-1}(x)$ ,  $a_{-2}(x)$ , and  $b_{-1}(x)$  by numerical integration. The integrals  $c_{-1}(k; x)$  and  $c_{-2}(k; x)$  were expressed in terms of integrals  $c_0(k; x)$  by expanding  $[1 + (t/\gamma)^2]^{-1}$  and  $[1 + (t/\gamma)^2]^{-2}$  in power series which converge rapidly for the same reason given above. The other  $a_i$ ,  $b_i$ , and  $c_i$  integrals were then obtained from  $b_0(x) = \frac{1}{2}e^{-x^2}$  and  $c_0(k; x) = \frac{1}{2}\Gamma(k + \frac{3}{2}) - a_{k+1}(x)$  using the recursion formula:

$$a_l(x) = \frac{1}{2}x^{2l-1}e^{-x^2} + \frac{1}{2}(2l-1)a_{l-1}(x), \quad l \geq 1, \tag{C23}$$

$$b_l(x) = \frac{1}{2}x^{2l}e^{-x^2} + lb_{l-1}(x), \quad l \geq 1, \tag{C24}$$

$$c_l(k; x) = c_{l-1}(k+1; x) + \gamma^2 c_{l-1}(k; x), \quad l \geq 1. \tag{C25}$$

Once the various  $a_i$ ,  $b_i$ , and  $c_i$  integrals for some  $\theta$  and  $p$  were found, the appropriate  $I_n^m$  integrals were obtained from (C22). Then  $\mathcal{R}_{n11}^{(1)}$  and  $\mathcal{R}_{n1}^{(1)}$  for  $n=0, 1, 2$  were readily calculated from (C16) and (C17).

With regard to  $\mathcal{Q}_{11}^{(1)}$  and  $\mathcal{Q}_1^{(1)}$ , the only way in which they differ from  $\mathcal{R}_{011}^{(1)}$  and  $\mathcal{R}_{01}^{(1)}$  is that the condition  $q \geq |k_{F1} - k_{F2}|$  is not imposed. This results in  $b_n(\alpha)$  in (C22) being replaced by  $b_n(0)$ . It should be mentioned that the  $\theta^2$  terms of  $\mathcal{Q}_{11}^{(1)}$  and  $\mathcal{Q}_1^{(1)}$  were not actually calculated as they appear in (C16) and (C17) as in this form they are rather slowly convergent. Convergence is greatly improved by writing these terms as

$$\frac{3}{4}\pi^2\theta^2 + \sum_{p=0}^{\infty} [6\theta/(2p+1)]^2 (I_1^1 - \frac{1}{6}), \tag{C26}$$

$$\frac{3}{4}\pi^2\theta^2 + \sum_{p=0}^{\infty} [6\theta/(2p+1)]^2 [\frac{1}{2}(I_1^0 - I_1^1) - \frac{1}{6}]. \tag{C27}$$

In this form it was necessary to include only the first 4 terms in the summation over  $p$  to obtain an error of less than 1% at the highest temperature considered ( $\theta = 2.0$ ).

The calculation of  $\mathcal{R}_{n11}^{(2)}$ ,  $\mathcal{R}_{n1}^{(2)}$ ,  $\mathcal{Q}_{11}^{(2)}$ , and  $\mathcal{Q}_1^{(2)}$  for the optical mode follows along similar lines and will not be given in detail. The expansion (C4) shows only those terms which lead to  $\theta^{2-n}$  terms in the final result higher terms have not been considered. The expressions obtained are

$$\mathcal{R}_{n11}^{(2)} = \sum_{p=0}^{\infty} \exp[-(2p+1)/(2\theta)] \times [8\theta/(2p+1)]^{2-n} J_{1-n}^1, \tag{C28}$$

$$\mathcal{R}_{n1}^{(2)} = \frac{1}{2} \sum_{p=0}^{\infty} \exp[-(2p+1)/(2\theta)] \times [8\theta/(2p+1)]^{2-n} (J_{1-n}^0 - J_{1-n}^1), \tag{C29}$$

where

$$J_n^m(p, \theta) = \int_0^\alpha dt t^{2m} e^{t^2 + \beta(t - \delta')} \times \{ a_{n-m}(\alpha') - a_{n-m}([\gamma'^2 + t^2]^{1/2}) \} + \int_{\delta'}^{\alpha'} dt t^{2m} e^{t^2 + \beta(t - \delta')} \times \{ a_{n-m}(t) - a_{n-m}([\gamma'^2 + t^2]^{1/2}) \}, \tag{C30}$$

and  $\alpha' = (\sqrt{3}/2)\alpha$ ,  $\delta' = (\sqrt{3}/2)\delta$ ,  $\gamma' = (\sqrt{3}/2)\gamma$ , and  $\beta = 2[(2p+1)/(3\theta)]^{1/2}$ . The integrals  $J_{1-n}^0$  and  $J_{1-n}^1$  were obtained by numerical integration. As for the acoustic mode integrals,  $\mathcal{Q}_{11}^{(2)}$  and  $\mathcal{Q}_1^{(2)}$  were obtained from  $\mathcal{R}_{011}^{(2)}$  and  $\mathcal{R}_{01}^{(2)}$  by simply putting  $\alpha' = 0$  in (C30). Here also the calculation included the first four terms in the summation over  $p$ .

### APPENDIX D

It is of interest to examine the effect on the resistivity of representing the  $s$ - $d$  interaction function  $G(\mathbf{r} - \mathbf{R}_n)$  of Eq. (3) by a square well of radius  $r_0$  rather than by a  $\delta$  function. For a cubic lattice, the only effect of a square well is to introduce into the integrand of  $\mathcal{Q}$ , given by (54), the Fourier transform

$$3(\sin qr_0 - qr_0 \cos qr_0)/(qr_0)^3. \tag{D1}$$

The value of  $\mathcal{Q}$  is then changed by the factor

$$W = \frac{89}{\pi^2 2} \times \int_0^\infty \frac{[\sin(wy)^{1/2} - (wy)^{1/2} \cos(wy)^{1/2}]^2 y \operatorname{csch} y dy}{(wy)^3}, \tag{D2}$$

where the parameter  $w$  is equal to  $(2kTr_0^2/\mathcal{D})$ . This has been calculated by numerical integration as a function of  $w$ . It was found that as  $w$  varies from 0 to 1.0 (corresponding to  $T \sim T_c$ ,  $r_0 \sim 1 \text{ \AA}$ ),  $w$  decreases in an approximately linear manner from 1 to 0.73. For the integrals  $\mathcal{R}_0$  and  $\mathcal{R}_1$  which exclude small  $q$ 's, the variation will be somewhat greater.