

ON THE THEORY OF FERROMAGNETISM

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Synopsis

An attempt is made to specify the conditions under which Heisenberg's model of ferromagnetism is correct. It is found that in addition to the exchange term there are other terms in the hamiltonian, describing the effects of the band width and of polar states. The new hamiltonian, which has a simple form, is naturally represented in terms of Fermi creation and absorption operators. The molecular field approximation applied to this new formulation leads essentially to the results of Stoner's collective theory. A better treatment in the low temperature region gives the familiar $T^{3/2}$ -law. A new type of spin wave is found, which should not be difficult to detect experimentally.

1. *Introduction.* In a recent article¹⁾ Löwdin reviewed the present status of the theory of magnetism. In broad outline he came to the following conclusions.

The band theory of electrons in metals, which serves as a basis for the collective electron theory of magnetism, has two main shortcomings. First of all it neglects all correlation effects and secondly it does not treat the parallel and antiparallel spins on the same footing, since only for the former the exclusion principle is active. In the Heitler-London-Heisenberg theory some correlation is taken into account, but it is assumed that the basic orbitals are orthogonal. This is certainly incorrect. For a better treatment one should either avoid this orthogonality assumption or, what amounts to the same, consider also polar states.

The main purpose of the present paper will be to work with strictly orthogonal (Wannier) states and to show how the inclusion of polar states manifests itself in the hamiltonian. In the next two sections we will derive this hamiltonian and show how it can be brought into a simple form. Section 4 is devoted to the molecular field approximation. In section 5 a truncated form of the original hamiltonian is studied and some new features are discussed.

2. *The hamiltonian.* We consider a rigid Bravais lattice with the unit cell defined by the fundamental translation vectors ($\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$) and we take $N = (2G + 1)^3$ lattice points \mathbf{R}_l defined by

$$\mathbf{R}_l = \sum_{i=1}^3 l_i \mathbf{a}_i (l_i = 0, \pm 1, \dots, \pm G)$$

in the volume Ω . The vectors $(\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3)$ are given by

$$(\mathbf{a}_i \cdot \mathbf{b}_j) = \delta_{ij}$$

and the wave vectors in the reciprocal lattice are

$$\mathbf{k} = \frac{2\pi}{2G+1} \sum_{i=1}^3 n_i \mathbf{b}_i \quad (n_i = 0, \pm 1, \dots, \pm G).$$

They satisfy

$$(\mathbf{k} \cdot \mathbf{L}_i) = 2\pi n_i,$$

where each of the three vectors

$$\mathbf{L}_i = (2G+1) \mathbf{a}_i$$

connects two corresponding points on opposite faces of the crystal. Periodic boundary conditions are therefore automatically fulfilled. The vectors \mathbf{Q}_m are defined by

$$\mathbf{Q}_m = 2\pi \sum_{i=1}^3 m_i \mathbf{b}_i \quad (m_i = 0, \pm 1, \dots, \pm \infty)$$

so that

$$\exp[i\mathbf{Q}_m \cdot \mathbf{R}_l] = 1. \quad (2.1)$$

We now consider the system consisting of N ions of positive charge Ze , each of them being fixed on a lattice site, and $N' = NZ$ electrons. The hamiltonian for this system is $H = H_0 + H_1 + H_2$ with

$$\begin{aligned} H_0 &= \sum_{\mu} H(\mathbf{r}_{\mu}); \quad H(\mathbf{r}_{\mu}) = -\frac{\hbar^2}{2m} \Delta_{\mu} + \sum_{l=1}^N V_0(\mathbf{r}_{\mu} - \mathbf{R}_l); \\ H_1 &= \sum_{\lambda < \mu} V_1(\mathbf{r}_{\lambda} - \mathbf{r}_{\mu}); \quad V_1(\mathbf{r}) = \frac{e^2}{r}; \quad H_2 = \sum_{\mu} V_2(\mathbf{r}_{\mu}, \sigma_{\mu}) \end{aligned} \quad (2.2)$$

Greek indices run from 1 to N' . The constant and divergent self energy of the ionic lattice is not written down. Together with the divergent part of the electron-electron interaction it will be cancelled by the divergent part of the ion-electron interaction.

$V_0(\mathbf{r}_{\mu} - \mathbf{R}_l)$ is the interaction of an electron at \mathbf{r}_{μ} with the l 'th ion and is supposed to be independent of the spin of the electron.

$V_1(\mathbf{r}_{\lambda} - \mathbf{r}_{\mu})$ is the Coulomb interaction between two electrons and $V_2(\mathbf{r}_{\mu}, \sigma_{\mu})$ is the energy of an electron in an external field. This energy may depend on the spin σ_{μ} of the electron.

We now assume that the one-electron problem in the periodic potential of the ions has been solved. The eigenstates and energies are indicated by $|\mathbf{k}, \sigma, \gamma\rangle$ and $E_{\gamma}(\mathbf{k})$. \mathbf{k} takes the values given before, $\sigma = \sigma_z$ is $+$ or $-$ for up or down spin and γ denotes the band (and other quantum numbers if

degeneracy occurs). In the coordinate representation the one-electron states are

$$\langle \mathbf{r}, \sigma', | \mathbf{k}, \sigma, \gamma \rangle = \psi_{\mathbf{k},\gamma}(\mathbf{r}) \delta_{\sigma'\sigma}, \tag{2.3}$$

where

$\psi_{\mathbf{k},\gamma}(\mathbf{r})$ are Bloch waves, normalized as follows

$$\int_{\Omega} d\mathbf{r} \psi_{\mathbf{k},\gamma}^*(\mathbf{r}) \psi_{\mathbf{k}',\gamma'}(\mathbf{r}) = \delta_{\mathbf{k},\mathbf{k}'} \delta_{\gamma\gamma'}.$$

They are, as usual, written in the form

$$\psi_{\mathbf{k},\gamma}(\mathbf{r}) = \frac{1}{\sqrt{N}} e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k},\gamma}(\mathbf{r}),$$

where $u_{\mathbf{k},\gamma}(\mathbf{r})$ is invariant for a translation

$$u_{\mathbf{k},\gamma}(\mathbf{r} + \mathbf{R}_l) = u_{\mathbf{k},\gamma}(\mathbf{r})$$

and satisfies the normalization condition

$$\int_{v_0} d\mathbf{r} u_{\mathbf{k},\gamma}^*(\mathbf{r}) u_{\mathbf{k},\gamma'}(\mathbf{r}) = \delta_{\gamma\gamma'} \tag{2.4}$$

$v_0 = \Omega/N$ is the volume of a unit cell.

We now introduce the creation and absorption operators for electrons in Bloch states. They obey the usual anticommutation relations

$$\{b_{\sigma\gamma}(\mathbf{k}), b_{\sigma'\gamma'}(\mathbf{k}')\} = \{b_{\sigma\gamma}^*(\mathbf{k}), b_{\sigma'\gamma'}^*(\mathbf{k}')\} = 0; \{b_{\sigma\gamma}(\mathbf{k}), b_{\sigma'\gamma'}^*(\mathbf{k}')\} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'} \delta_{\gamma\gamma'}.$$

Using these operators the hamiltonian can be written in second quantized form and the result is the following:

$$H_0 = \sum_{\mathbf{k}\sigma\gamma} E_{\gamma}(\mathbf{k}) b_{\sigma\gamma}^*(\mathbf{k}) b_{\sigma\gamma}(\mathbf{k}) \tag{2.5}$$

$$H_2 = g\beta_0 \mathcal{H} \sum_{\mathbf{k}\sigma\gamma} S_{\sigma}^z b_{\sigma\gamma}^*(\mathbf{k}) b_{\sigma\gamma}(\mathbf{k}), (S_{\sigma}^z = \pm \frac{1}{2} \text{ for } \sigma = \pm) \tag{2.6}$$

if a homogeneous external magnetic field \mathcal{H} is applied in the z -direction. g is the Landé-factor and β_0 is the Bohr magneton $\beta_0 = e\hbar/2mc$ ($e > 0$).

$$H_1 = - \frac{1}{2N} \sum V_{\gamma_1\gamma_2}(\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4) \Delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) b_{\sigma_1\gamma_1}^*(\mathbf{k}_1) b_{\sigma_2\gamma_2}^*(\mathbf{k}_2) \cdot b_{\sigma_3\gamma_3}(\mathbf{k}_3) b_{\sigma_4\gamma_4}(\mathbf{k}_4) \tag{2.7}$$

where the summation extends over $(\sigma_1\sigma_2\gamma_1\gamma_2\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4)$ and where the following abbreviations are used

$$V_{\gamma_1\gamma_2}(\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4) = \int_{v_0} d\mathbf{r}_1 \int_{\Omega} d\mathbf{r}_2 \exp -i[(\mathbf{k}_1 - \mathbf{k}_3) \cdot \mathbf{r}_1 + (\mathbf{k}_2 - \mathbf{k}_4) \cdot \mathbf{r}_2] \cdot u_{\mathbf{k}_1\gamma_1}^*(\mathbf{r}_1) u_{\mathbf{k}_2\gamma_2}^*(\mathbf{r}_2) \cdot V_1(\mathbf{r}_1 - \mathbf{r}_2) u_{\mathbf{k}_3\gamma_3}(\mathbf{r}_1) u_{\mathbf{k}_4\gamma_4}(\mathbf{r}_2).$$

$\Delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) = 1$ when $\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4 = \mathbf{Q}_m$ and zero otherwise.

In order to keep the formulae as simple as possible, but not as an inevitable approximation, it is assumed in the derivation of (2.7) that there are *no inter band transitions*.

A simpler discussion of all the terms occurring in the hamiltonian can be given if the creation operators for electrons in Wannier states are used:

$$b_{\sigma\gamma}^*(\mathbf{R}_l) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_l} b_{\sigma\gamma}^*(\mathbf{k}) \tag{2.8}$$

These operators are again Fermi-operators. In the coordinate representation the Wannier states are

$$F_{\gamma}(\mathbf{r} - \mathbf{R}_l) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}_l} \psi_{\mathbf{k}\gamma}(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{R}_l)} u_{\mathbf{k}\gamma}(\mathbf{r}). \tag{2.9}$$

These functions of \mathbf{r} extend over at most a few neighbours of \mathbf{R}_l . They are properly *normalized* since

$$\int_{\Omega} d\mathbf{r} F_{\gamma}^*(\mathbf{r} - \mathbf{R}_l) F_{\gamma'}(\mathbf{r} - \mathbf{R}_m) = \delta_{lm} \delta_{\gamma\gamma'}. \tag{2.10}$$

If the $\psi_{\mathbf{k}\gamma}(\mathbf{r})$ are plane waves one finds e.g.

$$F_{\gamma}^{p.w}(\mathbf{r}) = \frac{1}{\sqrt{v_0}} \frac{\sin \pi x_1}{\pi x_1} \cdot \frac{\sin \pi x_2}{\pi x_2} \cdot \frac{\sin \pi x_3}{\pi x_3} \text{ with } \mathbf{r} = (x_1 \mathbf{a}_1, x_2 \mathbf{a}_2, x_3 \mathbf{a}_3) \tag{2.11}$$

$F_{\gamma}(\mathbf{r} - \mathbf{R}_l)$ is real because $u_{\mathbf{k}\gamma}^*(\mathbf{r}) = u_{-\mathbf{k}\gamma}(\mathbf{r})$. The hamiltonian now becomes

$$H_0 = \sum_{\sigma\gamma} \sum_{lm} E_{\gamma}(lm) b_{\sigma\gamma}^*(\mathbf{R}_l) b_{\sigma\gamma}(\mathbf{R}_m) \tag{2.12}$$

with

$$E_{\gamma}(lm) = \frac{1}{N} \sum_{\mathbf{k}} E_{\gamma}(\mathbf{k}) e^{i\mathbf{k}\cdot(\mathbf{R}_l - \mathbf{R}_m)}$$

$$H_2 = g\beta_0 \mathcal{H} \sum_{\sigma\gamma l} S_{\sigma}^z b_{\sigma\gamma}^*(\mathbf{R}_l) b_{\sigma\gamma}(\mathbf{R}_l) \tag{2.13}$$

$$H_1 = -\frac{1}{2} \sum W_{\gamma_1\gamma_2}(l_1 l_2 l_3 l_4) b_{\sigma_1\gamma_1}^*(\mathbf{R}_{l_1}) b_{\sigma_2\gamma_2}^*(\mathbf{R}_{l_2}) b_{\sigma_1\gamma_1}(\mathbf{R}_{l_3}) b_{\sigma_2\gamma_2}(\mathbf{R}_{l_4}), \tag{2.14}$$

where the summation now extends over $(\sigma_1\sigma_2\gamma_1\gamma_2 l_1 l_2 l_3 l_4)$ and where

$$W_{\gamma_1\gamma_2}(l_1 l_2 l_3 l_4) = \int_{\Omega} d\mathbf{r}_1 \int_{\Omega} d\mathbf{r}_2 F_{\gamma_1}^*(\mathbf{r}_1 - \mathbf{R}_{l_1}) F_{\gamma_2}^*(\mathbf{r}_2 - \mathbf{R}_{l_2}) V_1(\mathbf{r}_1 - \mathbf{r}_2) F_{\gamma_1}(\mathbf{r}_1 - \mathbf{R}_{l_3}) \cdot F_{\gamma_2}(\mathbf{r}_2 - \mathbf{R}_{l_4}). \tag{2.15}$$

3. *Reduction of the hamiltonian.* From now on we will assume that the *range of the Wannier functions* $F_{\gamma}(\mathbf{r} - \mathbf{R}_l)$ is such that only nearest neighbours are included. Even for a conduction band this is not bad, as is seen from the expression (2.11) of $F_{\gamma}(\mathbf{r})$ for plane waves. A consequence of this

assumption is that $W_{\gamma_1\gamma_2}(l_1l_2l_3l_4)$ is equal to zero, unless one of the following cases holds: the pairs (l_1l_3) and (l_2l_4) are such that for each pair the members of that pair are either

- 1) equal, or are
- 2) nearest neighbours, or
- 3) have a common nearest neighbour.

A second approximation consists of neglecting $W_{\gamma_1\gamma_2}(l_1l_2l_3l_4)$ in case 3). The remaining terms are assembled in three different classes.

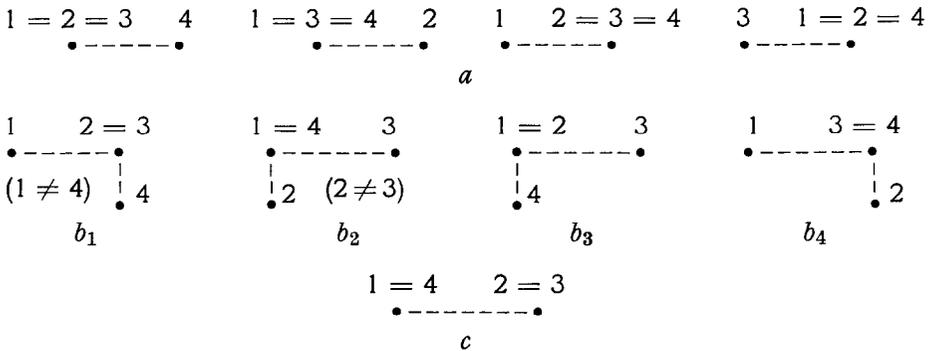
Class I: $l_1 = l_3$ and $l_2 = l_4$. The corresponding part of H_1 is

$$H_1^I = \frac{1}{2} \sum W_{\gamma_1\gamma_2}(l_1l_2l_1l_2) b_{\sigma_1\gamma_1}^*(\mathbf{R}_{l_1}) b_{\sigma_1\gamma_1}(\mathbf{R}_{l_1}) b_{\sigma_2\gamma_2}^*(\mathbf{R}_{l_2}) b_{\sigma_2\gamma_2}(\mathbf{R}_{l_2}). \quad (3.1)$$

The summation is over $(\sigma_1\sigma_2\gamma_1\gamma_2l_1l_2)$ excluding the terms for which simultaneously $\sigma_1 = \sigma_2$, $\gamma_1 = \gamma_2$ and $l_1 = l_2$. The expectationvalue of this H_1^I is the static Coulomb interaction between the electrons. It is infinite, but can be made finite by subtracting its value for a uniform distribution of the electrons over the lattice sites. This in turn is cancelled by the ion-electron interaction.

Class II: Of the remaining terms none of the members of (l_1l_3) is equal to any of the members of (l_2l_4) .

Class III. All other terms. These can be graphically represented as below.



A lattice point is indicated by a dot. Nearest neighbours are connected by a dotted line.

We now make the following *assumption*: the terms of classes I and II are responsible for plasma oscillations and when these are irrelevant, as in the present case, it is allowed to replace all terms of these two classes by those terms of H_1^I (3.1) for which l_1 and l_2 are either equal or nearest neighbours. This assumption amounts to the introduction of a screening of the Coulomb interaction. For a discussion of these effects one should consult the papers of reference 2.

We now discuss the terms of class III, which correspond to the different graphs. In order to obtain simple formulae we *discard* the effects of *band*

exchange, i.e. $W_{\gamma_1\gamma_2} = 0$, unless $\gamma_1 = \gamma_2$. Furthermore we neglect the diagrams b_3 and b_4 , because their effect is either to pile two additional electrons on one atom or to remove two electrons from one atom. After some tedious but straightforward manipulations the contributions of the graphs a , b en c (see page (881) can be written in the following form

$$H^a = -2 \sum_{\gamma l_1 l_2} W_{\gamma\gamma}(l_1 l_1 l_1 l_2) [S_\gamma^z(1) P_\gamma^z(1, 2) - S_\gamma^o(1) P_\gamma^o(1, 2)], \quad (3.2)$$

$$H^b = - \sum_{\gamma l_1 l_2 l_3} W_{\gamma\gamma}(l_1 l_2 l_2 l_3) [S_\gamma(2) \cdot P_\gamma(1, 3) + S_\gamma^o(2) P_\gamma^o(1, 3)], \quad (3.3)$$

$$H^c = - \sum_{\gamma l_1 l_2} W_{\gamma\gamma}(l_1 l_2 l_2 l_1) [S_\gamma(1) \cdot S_\gamma(2) + S_\gamma^o(1) S_\gamma^o(2)]. \quad (3.4)$$

In all summations \mathbf{R}_{l_1} and \mathbf{R}_{l_3} must be nearest neighbours of \mathbf{R}_{l_2} and in H^b one has $\mathbf{R}_{l_1} \neq \mathbf{R}_{l_3}$. We have introduced the followed hermitian operators:

$$\begin{aligned} S_\gamma^x(l) &= \frac{1}{2} \{ b_{+\gamma}^*(\mathbf{R}_l) b_{-\gamma}(\mathbf{R}_l) + b_{-\gamma}^*(\mathbf{R}_l) b_{+\gamma}(\mathbf{R}_l) \}. \\ S_\gamma^y(l) &= \frac{1}{2i} \{ b_{+\gamma}^*(\mathbf{R}_l) b_{-\gamma}(\mathbf{R}_l) - b_{-\gamma}^*(\mathbf{R}_l) b_{+\gamma}(\mathbf{R}_l) \}. \end{aligned} \quad (3.5)$$

$$S_\gamma^z(l) = \frac{1}{2} \{ b_{+\gamma}^*(\mathbf{R}_l) b_{+\gamma}(\mathbf{R}_l) - b_{-\gamma}^*(\mathbf{R}_l) b_{-\gamma}(\mathbf{R}_l) \}.$$

$$S_\gamma^o(l) = \frac{1}{2} \{ b_{+\gamma}^*(\mathbf{R}_l) b_{+\gamma}(\mathbf{R}_l) + b_{-\gamma}^*(\mathbf{R}_l) b_{-\gamma}(\mathbf{R}_l) \}.$$

and

$$\begin{aligned} P_\gamma^x(1, 3) &= \frac{1}{2} \{ b_{+\gamma}^*(\mathbf{R}_{l_1}) b_{-\gamma}(\mathbf{R}_{l_3}) + b_{-\gamma}^*(\mathbf{R}_{l_3}) b_{+\gamma}(\mathbf{R}_{l_1}) + \\ &\quad + b_{-\gamma}^*(\mathbf{R}_{l_1}) b_{+\gamma}(\mathbf{R}_{l_3}) + b_{+\gamma}^*(\mathbf{R}_{l_3}) b_{-\gamma}(\mathbf{R}_{l_1}) \} \\ P_\gamma^y(1, 3) &= \frac{1}{2i} \{ b_{+\gamma}^*(\mathbf{R}_{l_1}) b_{-\gamma}(\mathbf{R}_{l_3}) - b_{-\gamma}^*(\mathbf{R}_{l_3}) b_{+\gamma}(\mathbf{R}_{l_1}) - \\ &\quad - b_{-\gamma}^*(\mathbf{R}_{l_1}) b_{+\gamma}(\mathbf{R}_{l_3}) + b_{+\gamma}^*(\mathbf{R}_{l_3}) b_{-\gamma}(\mathbf{R}_{l_1}) \} \quad (3.6) \\ P_\gamma^z(1, 3) &= \frac{1}{2} \{ b_{+\gamma}^*(\mathbf{R}_{l_1}) b_{+\gamma}(\mathbf{R}_{l_3}) + b_{+\gamma}^*(\mathbf{R}_{l_3}) b_{+\gamma}(\mathbf{R}_{l_1}) - \\ &\quad - b_{-\gamma}^*(\mathbf{R}_{l_1}) b_{-\gamma}(\mathbf{R}_{l_3}) - b_{-\gamma}^*(\mathbf{R}_{l_3}) b_{-\gamma}(\mathbf{R}_{l_1}) \} \\ P_\gamma^o(1, 3) &= \frac{1}{2} \{ b_{+\gamma}^*(\mathbf{R}_{l_1}) b_{+\gamma}(\mathbf{R}_{l_3}) + b_{+\gamma}^*(\mathbf{R}_{l_3}) b_{+\gamma}(\mathbf{R}_{l_1}) + \\ &\quad + b_{-\gamma}^*(\mathbf{R}_{l_1}) b_{-\gamma}(\mathbf{R}_{l_3}) + b_{-\gamma}^*(\mathbf{R}_{l_3}) b_{-\gamma}(\mathbf{R}_{l_1}) \} \end{aligned}$$

The representation (3.5) is analogous to the one with Bose operators³⁾.

In order to study the effects of the interactions H^a , H^b and H^c we consider the operators S and P in some more detail.

If there is no electron or if there are two electrons in the band γ and on the lattice site \mathbf{R}_l the operators $S_\gamma^x(l)$, $S_\gamma^y(l)$ and $S_\gamma^z(l)$ are all zero and $S_\gamma^o(l)$ has the value zero or one respectively. If there is one (up or down) electron in the band γ and on the lattice site \mathbf{R}_l , the operator $S_\gamma^o(l)$ has the value $\frac{1}{2}$, while the others satisfy the commutation relations

$$[S_\gamma^x(l), S_\gamma^y(l')] = i S_\gamma^z(l) \delta_{ll'} \delta_{\gamma\gamma'} \text{ and cyclic}$$

and

$$[S_\gamma^i(l), S_\gamma^o(l')] = 0 \quad (i = x, y, z).$$

$S_\gamma(l)$ is therefore the ordinary spinoperator and, apart from the second term, H_c is therefore the usual exchange interaction. The exchange integral

$$W_{\gamma\gamma}(l_1 l_2 l_2 l_1) = \int_{\Omega} d\mathbf{r}_1 \int_{\Omega} d\mathbf{r}_2 \rho_\gamma^*(\mathbf{r}_1, \mathbf{R}_{l_1}, \mathbf{R}_{l_2}) V_1(\mathbf{r}_1 - \mathbf{r}_2) \rho_\gamma(\mathbf{r}_2, \mathbf{R}_{l_1}, \mathbf{R}_{l_2}),$$

with

$$\rho_\gamma(\mathbf{r}, \mathbf{R}_{l_1}, \mathbf{R}_{l_2}) = F_\gamma^*(\mathbf{r} - \mathbf{R}_{l_2}) F_\gamma(\mathbf{r} - \mathbf{R}_{l_1}),$$

is always positive. So H^c has the tendency to align the spins parallel to each other. The second term in H^c amounts to an attractive Coulomb interaction.

The effect of the P -operators is more complicated and is best discussed by first showing (table I) how they operate on the following complete set of states: (for each of the positions \mathbf{R}_{l_1} (left) and \mathbf{R}_{l_2} (right) it is indicated by an arrow or a dot whether or not the corresponding lattice site is occupied)

$$\begin{aligned} |a\rangle &= \frac{1}{\sqrt{2}} \{ |\uparrow \cdot \rangle + |\cdot \uparrow \rangle \}; & |c\rangle &= \frac{1}{\sqrt{2}} \{ |\uparrow \uparrow \cdot \rangle - |\cdot \uparrow \rangle \}; \\ |b\rangle &= \frac{1}{\sqrt{2}} \{ |\downarrow \cdot \rangle + |\cdot \downarrow \rangle \}; & |d\rangle &= \frac{1}{\sqrt{2}} \{ -|\downarrow \cdot \rangle + |\cdot \downarrow \rangle \}; \\ |e\rangle &= |\uparrow \uparrow \rangle; & |h\rangle &= \frac{1}{\sqrt{2}} \{ |\uparrow \uparrow \cdot \rangle + |\cdot \uparrow \downarrow \rangle \}; \\ |f\rangle &= |\downarrow \downarrow \rangle; & |k\rangle &= \frac{1}{\sqrt{2}} \{ -|\uparrow \downarrow \rangle + |\downarrow \uparrow \rangle \}; \\ |g\rangle &= \frac{1}{\sqrt{2}} \{ |\uparrow \downarrow \rangle + |\downarrow \uparrow \rangle \}; & |l\rangle &= \frac{1}{\sqrt{2}} \{ |\uparrow \downarrow \cdot \rangle - |\cdot \uparrow \downarrow \rangle \}; \\ |m\rangle &= \frac{1}{\sqrt{2}} \{ |\downarrow \downarrow \uparrow \rangle + |\uparrow \downarrow \downarrow \rangle \}; & |r\rangle &= \frac{1}{\sqrt{2}} \{ |\downarrow \downarrow \uparrow \rangle - |\uparrow \downarrow \downarrow \rangle \}; \\ |n\rangle &= \frac{1}{\sqrt{2}} \{ |\uparrow \uparrow \downarrow \rangle + |\uparrow \downarrow \uparrow \rangle \}; & |s\rangle &= \frac{1}{\sqrt{2}} \{ -|\uparrow \uparrow \downarrow \rangle + |\uparrow \downarrow \uparrow \rangle \}. \end{aligned}$$

TABLE I

	a	b	c	d	e	f	g	h	k	l	m	n	r	s
P^+	0	a	0	c	0	$\sqrt{2}h$	0	$\sqrt{2}e$	0	0	n	0	s	0
P^-	b	0	d	0	$\sqrt{2}h$	0	0	$\sqrt{2}f$	0	0	0	m	0	r
P^z	$\frac{1}{2}a$	$-\frac{1}{2}b$	$-\frac{1}{2}c$	$\frac{1}{2}d$	0	0	0	0	l	k	$\frac{1}{2}m$	$-\frac{1}{2}n$	$-\frac{1}{2}r$	$\frac{1}{2}s$
P^0	$\frac{1}{2}a$	$\frac{1}{2}b$	$-\frac{1}{2}c$	$-\frac{1}{2}d$	0	0	h	g	0	0	$\frac{1}{2}m$	$\frac{1}{2}n$	$-\frac{1}{2}r$	$-\frac{1}{2}s$

We have put $P^\pm = P^x \pm P^y$. From table I we immediately read off what the effect of H^b is if an up spin (α) or a down spin (β) in the band γ and on the lattice site \mathbf{R}_{l_2} is combined with any of the states a to s of the neighbouring spins. For the states e, f, g, h, k, l this effect cannot be interpreted as a tendency to spin alignment. For the other states, however, it can. In table II we have listed the eigenvalues of the operator $S^z(2) P^z(1, 3) + S^0(2) P^0(1, 3)$ for all possible combinations, and also whether these combinations

are ferromagnetic or antiferromagnetic. From this table we see that the states of lowest energy are ferromagnetic or antiferromagnetic, irrespective of the sign of the integral $W_{\gamma\gamma}(l_1l_2l_3)$. Further we observe that the states a, b, c, d have less than one electron per lattice site, whereas the states m, n, r, s have more than one. Table II therefore implies that H^b favours a ferromagnetic alignment of neighbouring spins for bands which are less than half filled and an antiferromagnetic alignment for more than half filled bands. We also conclude that, even if this theory is capable of explaining antiferromagnetism at all, the simple antiferromagnetic Heisenberg interaction does not describe it correctly.

TABLE II

αa	$\frac{1}{2}$	f.	αm	$\frac{1}{2}$	a.f.
βa	0	a.f.	βm	0	f.
αb	0	a.f.	αn	0	f.
βb	$\frac{1}{2}$	f.	βn	$\frac{1}{2}$	a.f.
αc	$-\frac{1}{2}$	f.	αr	$-\frac{1}{2}$	a.f.
βc	0	a.f.	βr	0	f.
αd	0	a.f.	αs	0	f.
βd	$-\frac{1}{2}$	f.	βs	$-\frac{1}{2}$	a.f.

H^a has no effect on the magnetic ordering of the spins. The operator $S_\gamma^z(1) P_\gamma^z(1, 2) - S_\gamma^o(1) P_\gamma^o(1, 2)$ has its lowest and highest values for the states m, n, r, s . This shows that because of H^a , and irrespective of the sign of $W_{\gamma\gamma}(l_1l_1l_2)$, the electrons tend to accumulate.

H^a and H^b describe the effects due to polar states.

The terms of class I which we keep after having neglected the plasma oscillations can also be put into a simple form. They can be written as (cf. (3.1))

$$H^I = 2 \sum_{\gamma_1\gamma_2l_1l_2} W_{\gamma_1\gamma_2}(l_1l_2l_1l_2) S_{\gamma_1}^o(l_1) S_{\gamma_2}^o(l_2) \tag{3.7}$$

R_{l_1} and R_{l_2} are equal or nearest neighbours. In H^I the short range effects of the Coulomb interaction are incorporated.

The final form to which the hamiltonian has now been reduced reads

$$H_{\text{red}} = H_0 + H^a + H^b + H^c + H^I + H_2. \tag{3.8}$$

The first five terms on the right hand side are respectively given by (2.12), (3.2), (3.3), (3.4) and (3.7), while H_2 (2.13) can also be written as

$$H_2 = g\beta_0\mathcal{H} \sum_{\gamma l} S_\gamma^z(l)$$

The effect of an external homogeneous electric field E can be taken into account by adding the following term to H_{red} :

$$H_{e1} = \sum_{\sigma\gamma l_1l_2} U_\gamma(l_1l_2) b_{\sigma\gamma}^*(R_{l_1}) b_{\sigma\gamma}(R_{l_2}), \tag{3.9}$$

with

$$U_{\gamma}(l_1l_2) = e(\mathbf{E} \cdot \mathbf{R}_{l_1}) \delta_{l_1l_2} + e \int_{\Omega} d\mathbf{r} (\mathbf{E} \cdot \mathbf{r}) F_{\gamma}^*(\mathbf{r}) F_{\gamma}(\mathbf{r} + \mathbf{R}_{l_1} - \mathbf{R}_{l_2}), \quad (e > 0).$$

Here it is assumed that the ions are not polarized by the external field.

It is felt that in the process of reducing the hamiltonian no major effects are neglected. The present theory should therefore be capable of explaining ferromagnetism. In the following section we will discuss the circumstances under which this is the case.

4. *The molecular field approximation.* Similar to what is done in the Weisz theory of ferromagnetism we truncate the reduced hamiltonian in the following way. All terms in (3.8), which are of fourth order in the creation and absorption operators are reduced to second order terms by replacing a sufficient number of the operators $S_{\gamma}^{\sigma}(l)$ and $\mathbf{S}_{\gamma}(l)$ by their average values as follows

$$S_{\gamma}^{\sigma}(l) \rightarrow \langle S_{\gamma}^{\sigma}(l) \rangle_T = \frac{1}{2}[n_{+}(\gamma) + n_{-}(\gamma)] \tag{4.1}$$

and

$$\mathbf{S}_{\gamma}(l) \rightarrow \langle \mathbf{S}_{\gamma}(l) \rangle_T = \{0, 0, \frac{1}{2}[n_{+}(\gamma) - n_{-}(\gamma)]\}. \tag{4.2}$$

$n_{\sigma}(\gamma)$ is the average number of electrons per atom with spin σ and in the band γ . Because the total number of electrons is NZ we have

$$\sum_{\sigma\gamma} n_{\sigma}(\gamma) = Z. \tag{4.3}$$

In this approximation the reduced hamiltonian becomes

$$\begin{aligned} \tilde{H} = & \sum_{\sigma\gamma} \sum_{lm} E_{\sigma\gamma}(lm) b_{\sigma\gamma}^*(\mathbf{R}_l) b_{\sigma\gamma}(\mathbf{R}_m) + \\ & + \sum_{\gamma l} (A_{\gamma} + B_{\gamma}) b_{+\gamma}^*(\mathbf{R}_l) b_{+\gamma}(\mathbf{R}_l) + \sum_{\gamma l} (A_{\gamma} - B_{\gamma}) b_{-\gamma}^*(\mathbf{R}_l) b_{-\gamma}(\mathbf{R}_l) \end{aligned} \tag{4.4}$$

with the following abbreviations:

$$\begin{aligned} E_{\sigma\gamma}(lm) = & E_{\gamma}(lm) + n_{-\sigma}(\gamma)\{W_{\gamma\gamma}(llm) + W_{\gamma\gamma}(mml)\} - \\ & - \frac{1}{2}n_{\sigma}(\gamma) \sum_j \{W_{\gamma\gamma}(ljjm) + W_{\gamma\gamma}(mjjl)\}; \quad (lj) \text{ and } (mj) \text{ nearest neighbours} \\ A_{\gamma} = & \sum_{\gamma_2 l_2} \lambda_{+}(\gamma_2) W_{\gamma\gamma_2}(ll_2l_2) - \frac{1}{2}\lambda_{+}(\gamma) \sum_{l_2} W_{\gamma\gamma}(ll_2l_2); \end{aligned}$$

In the first term l and l_2 are equal or nearest neighbours. In the second term l and l_2 are nearest neighbours.

$$B_{\gamma} = \frac{1}{2}g\beta_0 \mathcal{H} + \frac{1}{2}\lambda_{-}(\gamma) \sum_{l_2} W_{\gamma\gamma}(ll_2l_2); \quad \lambda_{\pm}(\gamma) = \frac{1}{2}[n_{-}(\gamma) \pm n_{+}(\gamma)].$$

$E_{\sigma\gamma}(lm)$ depends on \mathbf{R}_l and \mathbf{R}_m only through their difference and A_{γ} and B_{γ} are independent of \mathbf{R}_l . This allows us to diagonalize \tilde{H} by again introducing

the Bloch states (2.8). It then takes the form

$$\tilde{H} = \sum_{\sigma\gamma\mathbf{k}} \{E_{\sigma\gamma}(\mathbf{k}) + A_\gamma + \sigma B_\gamma\} b_{\sigma\gamma}^*(\mathbf{k}) b_{\sigma\gamma}(\mathbf{k}), \quad (4.5)$$

with

$$E_{\sigma\gamma}(\mathbf{k}) = \sum_l e^{-i\mathbf{k}\cdot(\mathbf{R}_l - \mathbf{R}_m)} E_{\sigma\gamma}(lm).$$

Since (4.5) is the hamiltonian for a system of free particles it is clear that in the process of deriving it all correlations between the electrons have been neglected. Apart from this defect, however, (4.5) is very useful in that it exhibits very clearly the different effects of the electron-electron interaction. As compared to H_0 (2.5) we see that the band energy has been changed due to H^a and H^b and that this change is proportional to the number of electrons in the band in question. There is also a relative shift A_γ of the bands. This is determined by the short range Coulomb interaction (H^I) and the second term of H^c , which, as remarked before, has the effect of an attractive Coulomb interaction. The main effect (B_γ) is a band shift in different directions for up and for down spins.

The grand partition function of (4.5) can of course be calculated exactly and all thermodynamic quantities can be found in principle. In particular the average values of $S_\gamma^0(l)$ and of $S_\gamma(l)$ can be written down and this leads to implicit equations for $n_+(\gamma)$, $n_-(\gamma)$ and the chemical potential. We will not bother to give all the formulae, but only quote the results, which are the same as those of the collective electron theory of Stoner⁴). It turns out that only those (corrected) bands contribute to the spontaneous magnetization which contain the chemical potential and which are sufficiently narrow. The magnetization at the absolute zero of temperature will in general differ from its saturation value. For very low temperature the magnetization follows a T^2 -law, which is not in accord with the experimentally verified $T^{\frac{1}{2}}$ -law. In order to get the latter behaviour the exchange term in the hamiltonian must be treated in a more exact fashion than is done in the molecular field approximation. For very high temperatures the usual $1/T$ -dependence of the susceptibility is obtained. More accurate results must be found by a machine calculation, but this requires a knowledge of the (original) energy bands.

5. *A new model.* From the foregoing sections we infer that the main features of a ferromagnetic are very likely incorporated in the following hamiltonian

$$H = \sum_{\sigma lm} E(lm) b_\sigma^*(\mathbf{R}_l) b_\sigma(\mathbf{R}_m) - J \sum_{lm} \{\mathbf{S}_l \cdot \mathbf{S}_m + S_l^0 S_m^0\} + g\beta_0 \mathcal{H} \sum_l S_l^z, \quad (5.1)$$

where in the second summation \mathbf{R}_l and \mathbf{R}_m are nearest neighbours. We consider only one band. Apart from two extra terms in the hamiltonian this

model differs also from the usual Heisenberg theory in that we have dropped the condition that there shall be one electron on each lattice site. This is a great advantage because it does away with the difficulty of the intermediate statistics of spin waves in the Heisenberg problem.

In the Bloch wave representation, which is most profitable for the following discussion, our hamiltonian is $H = H_0 + V$, with

$$H_0 = \sum_{\sigma\mathbf{k}} [E(\mathbf{k}) + g\beta_0\mathcal{H}\sigma] b_{\sigma}^*(\mathbf{k}) b_{\sigma}(\mathbf{k}) \tag{5.2}$$

and

$$V = \frac{1}{2N} \sum_{\sigma_1\sigma_2\mathbf{k}_1\dots\mathbf{k}_4} V(\mathbf{k}_1 - \mathbf{k}_2) \Delta(\mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3 - \mathbf{k}_4) b_{\sigma_1}^*(\mathbf{k}_1) b_{\sigma_2}^*(\mathbf{k}_2) b_{\sigma_2}(\mathbf{k}_3) b_{\sigma_1}(\mathbf{k}_4).$$

We have put

$$V(\mathbf{k}_1 - \mathbf{k}_2) = J \sum_{\delta} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \delta},$$

where δ is a vector to a nearest neighbour. The zero point of the energy is fixed by setting $E(\mathcal{U}) = 1/N \sum_{\mathbf{k}} E(\mathbf{k}) = 0$. The completely saturated state

with one down spin on each lattice site is an eigenstate of the hamiltonian (5.1) with energy $E_0 = -\frac{1}{2}NzJ - \frac{1}{2}Ng\beta_0\mathcal{H}$ (z is the number of nearest neighbours). This state, to be denoted by $|\varphi_0\rangle$, is not necessarily the ground-state. For narrow bands, however, $E(\mathbf{k})$ can be considered as a constant (zero) and in this case $|\varphi_0\rangle$ is indeed the state of lowest energy. In the Bloch wave representation $|\varphi_0\rangle$ is the state with all N sites in the first Brillouin zone occupied by down spins.

In the approximation that $E(\mathbf{k}) = 0$ other exact eigenstates are

$$|\mathbf{k}\rangle = \frac{1}{\sqrt{N}} \sum_l e^{i\mathbf{k} \cdot \mathbf{R}_l} S^+(\mathbf{R}_l) |\varphi_0\rangle. \tag{5.3}$$

These states are called spin waves. Their energy is

$$\varepsilon(\mathbf{k}) = E_0 + g\beta_0\mathcal{H} + J[z - \sum_{\delta} \cos(\mathbf{k} \cdot \delta)]. \tag{5.4}$$

Assuming that states of more than one spin wave are to a good approximation still eigenstates of the hamiltonian and that the spin waves satisfy Bose-Einstein statistics one can derive for low temperatures the $T^{\frac{3}{2}}$ -law for the deviation of the magnetization from saturation.

Also in the present case, where $E(\mathbf{k})$ is not a constant, it will be possible to construct exact eigenstates of the hamiltonian. To see this we consider the state

$$|l_1 l_2\rangle = b_+^*(\mathbf{R}_{l_1}) b_-(\mathbf{R}_{l_2}) |\varphi_0\rangle,$$

which has an up spin on site l_1 , no down spin on site l_2 and only down spins

on the remaining sites ($l_1 = l_2$ is not excluded). We now define

$$|\mathbf{k}_1\mathbf{k}_2\rangle = \frac{1}{N} \sum_{l_1 l_2} e^{i(\mathbf{k}_1 \cdot \mathbf{R}_{l_1} + \mathbf{k}_2 \cdot \mathbf{R}_{l_2})} |l_1 l_2\rangle.$$

$|\mathbf{k}_1\mathbf{k}_2\rangle$ represents a state of two quasi particles of two different kinds. The first is a plane wave of up spins, the second is a plane wave of holes in the sea of the down spins. Their interaction is determined by the hamiltonian (5.2) and given by

$$H |\mathbf{k}_1\mathbf{k}_2\rangle = [E(\mathbf{k}_1) - E(\mathbf{k}_2) + E_0 + zJ + g\beta_0\mathcal{H}] |\mathbf{k}_1\mathbf{k}_2\rangle - \frac{J}{N} \sum_{\boldsymbol{\kappa}, \boldsymbol{\delta}} e^{-i(\mathbf{k}_1 + \mathbf{k}_2) \cdot \boldsymbol{\delta}} |\mathbf{k}_1 + \boldsymbol{\kappa}, \mathbf{k}_2 - \boldsymbol{\kappa}\rangle. \quad (5.5)$$

We try to find exact eigenstates of the form

$$|\varphi\rangle = \sum_{\mathbf{k}_1\mathbf{k}_2} \tilde{c}(\mathbf{k}_1, \mathbf{k}_2) |\mathbf{k}_1\mathbf{k}_2\rangle.$$

Introducing the total and the relative (pseudo) momentum $\boldsymbol{\kappa} = \mathbf{k}_1 + \mathbf{k}_2$ and $\mathbf{k} = \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$, the Schrödinger equation $H |\varphi\rangle = W |\varphi\rangle$ leads to the following equation for the coefficients $c(\boldsymbol{\kappa}, \mathbf{k}) = \tilde{c}(\mathbf{k}_1, \mathbf{k}_2)$

$$[E(\boldsymbol{\kappa}, \mathbf{k}) - W] c(\boldsymbol{\kappa}, \mathbf{k}) = \frac{1}{N} f(\boldsymbol{\kappa}) \sum_{\boldsymbol{\kappa}'} c(\boldsymbol{\kappa}, \mathbf{k} - \boldsymbol{\kappa}'), \quad (5.6)$$

where we have put

$$E(\boldsymbol{\kappa}, \mathbf{k}) = E(\mathbf{k}_1) - E(\mathbf{k}_2) + E_0 + zJ + g\beta_0\mathcal{H}$$

and

$$f(\boldsymbol{\kappa}) = J \sum_{\boldsymbol{\delta}} \cos(\boldsymbol{\kappa} \cdot \boldsymbol{\delta}).$$

Equation (5.6) is easily solved. The equation for the energy W becomes

$$\frac{1}{f(\boldsymbol{\kappa})} = \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{E(\boldsymbol{\kappa}, \mathbf{k}) - W} \equiv G_{\boldsymbol{\kappa}}(W). \quad (5.7)$$

The general shape of the function $G_{\boldsymbol{\kappa}}(W)$ is plotted in figure 1. The intersections of the line $f^{-1}(\boldsymbol{\kappa})$ with $G_{\boldsymbol{\kappa}}(W)$ are the roots of equation (5.7). The $N - 1$ roots, which in the limit $N \rightarrow \infty$ form the continuous part of the spectrum, correspond to the scattering states of two quasi particles with a total energy $E(\mathbf{k}_1) - E(\mathbf{k}_2) + zJ + g\beta_0\mathcal{H}$ above the energy of the groundstate. Since the quasi particles always occur in pairs we can assign separate excitation energies

$$\varepsilon_1(\mathbf{k}) = E(\mathbf{k}) + \lambda \quad (5.8)$$

and

$$\varepsilon_2(\mathbf{k}) = -E(\mathbf{k}) + \lambda \quad (2\lambda = zJ + g\beta_0\mathcal{H})$$

to them, as long as they occur in scattering states.

The remaining root $W(\kappa)$ of (5.7) corresponds to a bound state of the two quasi particles. We will call this state a spin wave of momentum κ and denote its excitation energy by

$$\omega(\kappa) \equiv W(\kappa) - E_0. \tag{5.9}$$

We remark that if $f(\kappa)$ is negative the energy of the spin wave lies above the continuous part of the spectrum, so that it may be unstable and decay into two quasi particles if some interaction is taken into account, which has here been neglected.

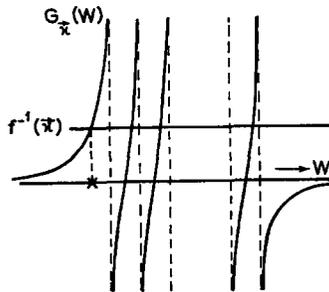


Fig. 1. The roots of equation (5.7).

We will now assume that for low temperatures our ferromagnetic can, to a good approximation, be described in the following way. It is a dilute gas of a variable number of quasi particles – as many of the first as of the second kind. This gas is considered to be an ideal Fermi gas. In addition there is a dilute gas of a variable number of spin waves, to be treated as Bose-Einstein particles, which do not interact, neither among themselves, nor with the quasi particles. The energy E_α of the state α with

$$\begin{aligned} l_k^{(1)} &= 0 \text{ or } 1 \text{ quasi particles of the first kind,} \\ l_k^{(2)} &= 0 \text{ or } 1 \text{ quasi particles of the second kind and} \\ m_k &= 0, 1, 2, \dots \text{ spin waves, for all momenta is} \end{aligned}$$

$$E_\alpha = E_0 + \sum_k \{l_k^{(1)}\epsilon_1(\mathbf{k}) + l_k^{(2)}\epsilon_2(\mathbf{k}) + m_k\omega(\mathbf{k})\}.$$

The grand canonical partition function for this system is

$$Z = \sum_\alpha \exp \beta\mu \sum_k (l_k^{(1)} - l_k^{(2)}) \cdot \exp - \beta(E_\alpha - E_0).$$

This can be evaluated and we find

$$Z = \prod_k [1 - e^{-\beta\omega(\mathbf{k})}]^{-1} [1 + e^{-\beta(E(\mathbf{k})+\lambda-\mu)}] \cdot [1 + e^{\beta(E(\mathbf{k})-\lambda-\mu)}].$$

The condition that on the average there shall be as many quasi particles of the first as of the second kind gives the following equation for the chemical

potential μ

$$\sum_{\mathbf{k}} [1 + e^{\beta(E(\mathbf{k})+\lambda-\mu)}]^{-1} = \sum_{\mathbf{k}} [1 + e^{-\beta(E(\mathbf{k})-\lambda-\mu)}]^{-1}. \tag{5.10}$$

The z -component of the magnetic moment of the state α is

$$M_{\alpha} = \frac{1}{2}Ng\beta_0 - \frac{1}{2}g\beta_0 \sum_{\mathbf{k}} \{l_{\mathbf{k}}^{(1)} + l_{\mathbf{k}}^{(2)} + 2m_{\mathbf{k}}\}.$$

From this we easily find the average magnetization at temperature T to be

$$M(T) = \frac{1}{2}Ng\beta_0 \left[1 - \frac{1}{N} \sum_{\mathbf{k}} \left\{ \frac{1}{1 + \exp \beta(E(\mathbf{k}) + \lambda - \mu)} + \frac{1}{1 + \exp -\beta(E(\mathbf{k}) - \lambda - \mu)} + \frac{2}{\exp \beta\omega(\mathbf{k}) - 1} \right\} \right] \tag{5.11}$$

Let $Nn(E) dE$ be the number of \mathbf{k} -values for which $E < E(\mathbf{k}) < E + dE$ and let $N\rho(\omega) d\omega$ be the number of \mathbf{k} -values for which $\omega < \omega(\mathbf{k}) < \omega + d\omega$. The formula for the magnetization can then be written as

$$M(T) = \frac{1}{2}Ng\beta_0 \left[1 - 2 \int_{-\infty}^{\infty} \frac{n(E) dE}{1 + e^{\beta(E+\lambda-\mu)}} - 2 \int_{-\infty}^{\infty} \frac{\rho(\omega) d\omega}{e^{\beta\omega} - 1} \right], \tag{5.12}$$

while μ must be solved from

$$\int_{-\infty}^{\infty} \frac{n(E) dE}{1 + e^{\beta(E+\lambda-\mu)}} = \int_{-\infty}^{\infty} \frac{n(E) dE}{1 + e^{-\beta(E-\lambda-\mu)}}. \tag{5.13}$$

At absolute zero temperature this equation becomes

$$\int_{-\infty}^{\mu-\lambda} n(E) dE = \int_{\mu+\lambda}^{\infty} n(E) dE,$$

so that μ lies somewhere in the middle of the energy band. If λ is very small compared with the band width the second term in the right hand side of (5.12) is almost equal to one and there is no spontaneous magnetization. In this case, moreover, it is no longer correct to approximate the spin-system by a dilute gas of quasi particles. If the point $\mu - \lambda$ falls outside the energy band (narrow band) the second term in (5.12) will, for low temperatures, depend exponentially on T , so that only the spin wave term affects the magnetization with increasing temperature. If $\mu - \lambda$ falls inside the energy band the second term in (5.12) can, for low temperature, be calculated, using the method of Sommerfeld. We get to lowest order in the temperature

$$\int_{-\infty}^{\mu-\lambda} n(E) dE + \frac{\pi^2}{6} n'(\mu - \lambda)(kT)^2. \tag{5.14}$$

By adjusting the magnetic field it should be possible to let $\mu - \lambda$ fall just inside the energy band, so that the first term in (5.14) becomes small and the quasi particle approximation is applicable. In this case of a nonvanishing magnetic field the spin wave term can be neglected (see below) and the magnetization will depend quadratically on the temperature.

We now discuss the last term in (5.12). From the equation (5.7) one can easily deduce that for small values of the momentum one obtains the conventional form⁵⁾ of the spin wave energy, viz.

$$\omega(\mathbf{k}) = g\beta_0\mathcal{H} + \frac{1}{2}J \sum_{\mathbf{d}} (\mathbf{k} \cdot \mathbf{d})^2.$$

This gives a density of states which, for ω just above $g\beta_0\mathcal{H}$, is of the form

$$\rho(\omega) = a \sqrt{\omega - g\beta_0\mathcal{H}}.$$

If we assume that there are no values of ω less than $g\beta_0\mathcal{H}$, we can evaluate the last integral in (5.12) for low temperatures. If \mathcal{H} is positive ω is also larger than a positive value, so that the integral depends exponentially on T . For $\mathcal{H} = 0$, however, the integral may be approximated by

$$2a \int_0^{\infty} \frac{\sqrt{\omega} d\omega}{e^{\beta\omega} - 1} = 4a(kT)^{\frac{3}{2}} \int_0^{\infty} \frac{x^2 dx}{e^{x^2} - 1}$$

and this is the $T^{\frac{3}{2}}$ -law of Bloch.

Finally we should like to make the following remarks.

Due to the two branches of the spin wave energy, the function $\rho(\omega)$ will in general consist of two bands, separated by an energy gap. This property has not been predicted before and it should be interesting to check experimentally (e.g. by inelastic neutron scattering) what the precise form is of the energy spectrum of spin waves.

Recently⁶⁾ Freeman, Nesbet and Watson suggested that the Heisenberg exchange interaction could not be responsible for the existence of ferromagnetism. It should be worth while to repeat these calculations, but now based on the theory presented in this paper.

We have shown that some terms in the hamiltonian (3.8) correspond to an attractive interaction between the electrons. If large enough, these terms could in principle account for superconductivity without an isotope effect. A similar suggestion was recently made by Falk and Ferrell⁷⁾.

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Note added in proof: Only recently the author's attention was drawn to related work by P. W Anderson, Phys. Rev. **115** (1959) 2.