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High density corrections for a Heisenberg antiferromagnet

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Abstract. The high density expansions derived in the two preceding papers for the thermodynamic quantities and correlation functions of the spin half Heisenberg antiferromagnet are here extended to higher order, for the low temperature case. The $(1/z)^2$ terms in the sublattice magnetization, free energy and internal energy are evaluated and contact made with the interacting spin wave theory of Oguchi. The selfconsistency of the method in this order is demonstrated, and the criteria for the validity of the results determined. The spin wave damping in order $(1/z)^2$ is also investigated. This includes spin wave scattering contributions and gives the dominant contribution at low temperatures.

1. Introduction

This paper presents extensions of the work of the preceding two papers (Cottam and Stinchcombe 1970a, b, to be referred to as I and II) to higher order in the high density expansion, for low temperatures.

In section 2 the order $(1/z)^2$ terms in the expansions of the magnetization and free energy of the Heisenberg antiferromagnet are calculated and connection is made with the work of Oguchi (1960). These terms represent small corrections to the leading order results, evaluated in I, if the criteria for the validity of the high density expansion are satisfied. The terms are however of qualitative interest, since they include the first effects of spin wave interactions just as the order $1/z$ terms introduced the leading effect of fluctuations, absent altogether from the molecular field terms.

These are cases where the first one or two terms in the high density expansion give no contribution to a particular quantity and the leading contributions come from terms of quite high order. Other examples where the low order terms in the high density expansion have vanishing coefficients are the expansions of the higher virial coefficients and, as was noted in II, of the low temperature spin wave damping $\Gamma_{\mathbf{k}}$. The leading nonvanishing contributions to $\Gamma_{\mathbf{k}}$ at low temperatures are evaluated in section 3.

2. The magnetization and free energy in order $(1/z)^2$

In this section the magnetization and free energy are evaluated in order $(1/z)^2$ for the low temperature case only, where the results are expected to lead to a description of spin wave interactions. A connection will be made with the work of Oguchi (1960).

The magnetization is here determined by calculating the one particle Green function $C_1(\mathbf{k}, \alpha)$ as in I. It will be shown in subsection 2.1 that the contributions to the magnetization can be obtained as the field derivatives of a set of terms which also occur in the calculation of the corresponding free energy in subsection 2.2. Subsections 2.1 and 2.2 each conclude with an analysis of the results and a direct check of their order in the high density expansion.

2.1. $(1/z)^2$ calculation of $C_1(\mathbf{k}, \tau)$

The renormalization scheme for $C_1(\mathbf{k}, \alpha)$ in order $(1/z)^2$ is illustrated in figure 1. All

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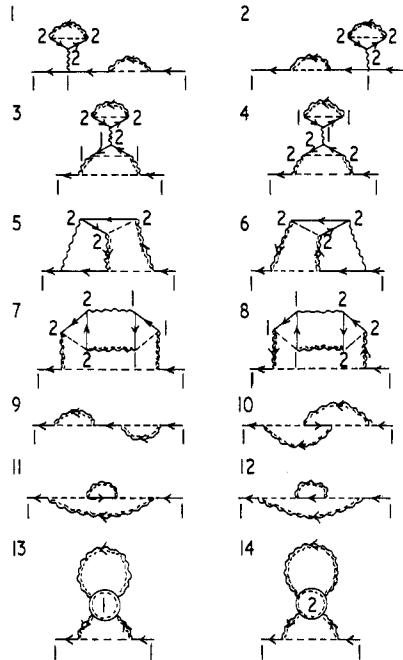


Figure 1. Diagrams contributing to $C_1(\mathbf{k}, \alpha)$ in order $(1/z)^2$ at low temperatures.

constituent lines are renormalized to order $(1/z)^0$, and in diagrams 13 and 14 the vertex part with sublattice label l denotes the semi-invariant ${}^lM_4^{+-}$ of I, appendix B. The calculation is greatly simplified by suitably grouping these diagrams, and expressing the results in terms of a field derivative.

Consider diagrams 1-4. Diagrams 1 and 2 are equal by symmetry, and at low temperatures the total α -dependent part of their contribution gives upon summation

$$\frac{2}{\beta} \sum_{\alpha} \{C_1(\alpha)\}^3 D_1^0(\alpha - \eta) = -\frac{1}{\beta} \frac{\partial}{\partial h_1} \sum_{\alpha} \{C_1(\alpha)\}^2 D_1^0(\alpha - \eta) = \frac{\partial}{\partial h_1} {}^1M_3^{+-}(\eta, \eta, 0) \quad (2.1)$$

where ${}^1M_3^{+-}$ is a semi-invariant defined in appendix B. Hence from equation (2.1) the contribution to $C_1(\mathbf{k}, \tau = 0)$ from 1 and 2 may be written as

$$\frac{(1 + \sigma)}{\beta^2 N^2} \sum_{\substack{\eta \eta' \\ \mathbf{q} \mathbf{q}'}} J(0) J_{11}^T(\mathbf{q}, \eta) J_{22}^T(\mathbf{q}', \eta')^2 M_3^{+-}(\eta', \eta', 0) \frac{\partial}{\partial h_1} {}^1M_3^{+-}(\eta, \eta, 0). \quad (2.2)$$

For diagram 3 the summation over the external frequency α gives a factor

$$\frac{1}{\beta} \sum_{\alpha} \{C_1(\alpha)\}^2 D_1^0(\alpha - \eta) = -\frac{1}{\beta} \frac{\partial}{\partial h_1} \sum_{\alpha} C_1(\alpha) D_1^0(\alpha - \eta) = \frac{\partial}{\partial h_1} {}^1M_2^{+-}(\eta, \eta).$$

By using this result and expressing $J_{11}^T(\mathbf{q}, \eta)$ as

$$\{J_{11}^T(\mathbf{q}, \eta)\}^{-1} = \frac{1}{\frac{1}{4}J^2(\mathbf{q})^2 M_2^{+-}} \{1 - \frac{1}{4}J^2(\mathbf{q})^2 M_2^{+-} M_2^{+-}\}$$

it may be shown that

$$\frac{1}{\beta} \sum_{\alpha} \{J_{11}^T(\mathbf{q}, \eta)\}^2 \{C_1(\alpha)\}^2 D_1^0(\alpha - \eta) = \frac{\partial}{\partial h_1} J_{11}^T(\mathbf{q}, \eta). \quad (2.3)$$

Equation (2.3) enables the contribution to $C_1(\mathbf{k}, \tau = 0)$ from diagram 3 to be expressed as

$$\frac{(1 + \sigma)}{\beta^2 N^2} \sum_{\substack{\eta\eta' \\ \mathbf{q}\mathbf{q}'}} J(0)^1 M_3^{+-z}(\eta, \eta, 0)^2 M_3^{+-z}(\eta', \eta', 0) J_{22}^T(\mathbf{q}'\eta') \frac{\partial}{\partial h_1} J_{11}^T(\mathbf{q}, \eta). \quad (2.4)$$

Equation (2.3) may be generalized to

$$\frac{1}{\beta} \sum_{\alpha} \{C_1(\alpha)\}^2 D_1^0(\alpha - \eta) J_{11}^T(\mathbf{q}, \eta) J_{1\nu}^T(\mathbf{q}, \eta) = \frac{\partial}{\partial h_1} J_{1\nu}^T(\mathbf{q}, \eta) \quad (2.5)$$

which is a constituent in diagrams 3, 4, 7, 8, 13, 14. Using this result the contribution from diagram 4 is

$$\frac{(1 + \sigma)}{\beta^2 N^2} \sum_{\substack{\eta\eta' \\ \mathbf{q}\mathbf{q}'}} J(0)^1 M_3^{+-z}(\eta, \eta, 0)^2 M_3^{+-z}(\eta', \eta', 0) J_{11}^T(\mathbf{q}, \eta) \frac{\partial}{\partial h_1} J_{22}^T(\mathbf{q}', \eta'). \quad (2.6)$$

Equations (2.2), (2.4) and (2.6) may be combined and written in terms of an overall derivative, whence the contribution to the magnetization from diagrams 1–4 is

$$\Delta R = \frac{\partial}{\partial h_1} \left\{ \frac{(1 + \sigma)}{\beta^2 N^2} \sum_{\substack{\eta\eta' \\ \mathbf{q}\mathbf{q}'}} J(0) J_{11}^T(\mathbf{q}, \eta) J_{22}^T(\mathbf{q}', \eta')^1 M_3^{+-z}(\eta, \eta, 0)^2 M_3^{+-z}(\eta', \eta', 0) \right\}. \quad (2.7)$$

In a similar fashion by making use of equations (2.5) and (2.1) (or the analogous equation for $\partial/\partial h_1 M_4^{+--+}$) the remaining diagrams of figure 1 may be grouped and expressed in terms of a derivative with respect to h_1 . The results for diagrams 5–8 are

$$\Delta R = \frac{\partial}{\partial h_1} \left\{ \frac{1 + \sigma}{\beta^2 N^2} \sum_{\substack{\eta\eta' \\ \mathbf{q}\mathbf{q}'}} J(\mathbf{q} - \mathbf{q}')^1 M_3^{+-z}(\eta, \eta', \eta' - \eta)^2 M_3^{+-z}(\eta', \eta, \eta - \eta') J_{12}^T(\mathbf{q}, \eta) J_{12}^T(\mathbf{q}', \eta') \right\} \quad (2.8)$$

For diagrams 9–13,

$$\Delta R = \frac{1}{2} \frac{\partial}{\partial h_1} \left\{ \frac{1}{\beta^2 N^2} \sum_{\substack{\eta\eta' \\ \mathbf{q}\mathbf{q}'}} J_{11}^T(\mathbf{q}, \eta) J_{11}^T(\mathbf{q}', \eta')^1 M_4^{+--+}(\eta, \eta, \eta', \eta') \right\}. \quad (2.9)$$

For diagram 14,

$$\Delta R = \frac{1}{2} \frac{\partial}{\partial h_1} \left\{ \frac{1}{\beta^2 N^2} \sum_{\substack{\eta\eta' \\ \mathbf{q}\mathbf{q}'}} J_{22}^T(\mathbf{q}, \eta) J_{22}^T(\mathbf{q}', \eta') M_4^{+--+}(\eta, \eta, \eta', \eta') \right\}. \quad (2.10)$$

The conclusions of equations (2.7) to (2.10) may be summarized as follows. The low temperature $(1/z)^2$ contribution to the sublattice magnetization may be calculated from

$$\Delta R = \frac{\partial Y}{\partial h_1} \quad (2.11)$$

where Y is equivalent to the sum of the closed diagrams of figure 2. This procedure will now be carried out.

In this calculation it is important to retain all sublattice labels until after the differentiation with respect to h_1 . By applying the usual rules, diagrams 1–4 of figure 2 give contributions

$$Y_1 = - \frac{1}{16N^2} \sum_{\mathbf{q}\mathbf{q}'} (1 + \sigma) J(0) J^2(\mathbf{q}) J^2(\mathbf{q}') \Gamma_1(\mathbf{q}) \Gamma_3(\mathbf{q}')$$

$$Y_2 = \frac{1}{4N^2} \sum_{\mathbf{q}\mathbf{q}'} (1 + \sigma) J(\mathbf{q} - \mathbf{q}') J(\mathbf{q}) J(\mathbf{q}') \Gamma_1(\mathbf{q}) \Gamma_1(\mathbf{q}')$$

$$\begin{aligned}
 Y_3 &= -\frac{1}{8N^2} \sum_{\mathbf{q}\mathbf{q}'} J^2(\mathbf{q}) J^2(\mathbf{q}') \Gamma_2(\mathbf{q}) \Gamma_1(\mathbf{q}') \\
 Y_4 &= \frac{1}{8N^2} \sum_{\mathbf{q}\mathbf{q}'} J^2(\mathbf{q}) J^2(\mathbf{q}') \Gamma_3(\mathbf{q}) \Gamma_1(\mathbf{q}').
 \end{aligned}
 \tag{2.12}$$

In these equations the quantities $\Gamma_i(\mathbf{q})$ are

$$\begin{aligned}
 \Gamma_1(\mathbf{q}) &= \frac{1}{\beta} \sum_{\eta} \frac{1}{(\epsilon_{\mathbf{q}}^+ - i\eta)(\epsilon_{\mathbf{q}}^- - i\eta)} & \Gamma_2(\mathbf{q}) &= \frac{1}{\beta} \sum_{\eta} \frac{1}{(\epsilon_{\mathbf{q}}^+ - i\eta)(\epsilon_{\mathbf{q}}^- - i\eta)(\gamma_1 - i\eta)} \\
 \Gamma_3(\mathbf{q}) &= \frac{1}{\beta} \sum_{\eta} \frac{1}{(\epsilon_{\mathbf{q}}^+ - i\eta)(\epsilon_{\mathbf{q}}^- - i\eta)(\gamma_2 - i\eta)}.
 \end{aligned}
 \tag{2.13}$$

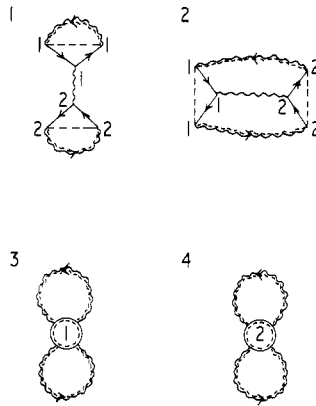


Figure 2. Diagrams contributing to Y .

The result of performing the frequency summations is

$$\begin{aligned}
 \Gamma_1(\mathbf{q}) &= \frac{n(\epsilon_{\mathbf{q}}^+) - n(\epsilon_{\mathbf{q}}^-)}{(\epsilon_{\mathbf{q}}^+ - \epsilon_{\mathbf{q}}^-)} \\
 \Gamma_2(\mathbf{q}) &= \frac{4 \{(\gamma_1 - \epsilon_{\mathbf{q}}^-) n(\epsilon_{\mathbf{q}}^+) - (\gamma_1 - \epsilon_{\mathbf{q}}^+) n(\epsilon_{\mathbf{q}}^-)\}}{J^2(\mathbf{q})(\epsilon_{\mathbf{q}}^+ - \epsilon_{\mathbf{q}}^-)} \\
 \Gamma_3(\mathbf{q}) &= \frac{-4 \{(\gamma_2 - \epsilon_{\mathbf{q}}^-) n(-\epsilon_{\mathbf{q}}^+) - (\gamma_2 - \epsilon_{\mathbf{q}}^+) n(-\epsilon_{\mathbf{q}}^-)\}}{J^2(\mathbf{q})(\epsilon_{\mathbf{q}}^+ - \epsilon_{\mathbf{q}}^-)}.
 \end{aligned}
 \tag{2.14}$$

The derivatives of equation (2.11) with respect to h_1 will involve derivatives of $\Gamma_i(\mathbf{q})$. From equation (2.14) these are

$$\begin{aligned}
 \frac{\partial \Gamma_1}{\partial h_1} &= -\gamma \frac{\partial \Gamma_3}{\partial h_1} = \frac{\gamma n'(\epsilon_{\mathbf{q}})}{2\epsilon_{\mathbf{q}}^2} - \frac{\gamma n(\epsilon_{\mathbf{q}})}{2\epsilon_{\mathbf{q}}^3} + \frac{\gamma}{4\epsilon_{\mathbf{q}}^3} \\
 \frac{\partial \Gamma_2}{\partial h_1} &= \frac{2(\gamma^2 + \epsilon_{\mathbf{q}}^2) n'(\epsilon_{\mathbf{q}})}{J^2(\mathbf{q}) \epsilon_{\mathbf{q}}^2} - \frac{n(\epsilon_{\mathbf{q}})}{2\epsilon_{\mathbf{q}}^3} + \frac{1}{4\epsilon_{\mathbf{q}}^3}
 \end{aligned}$$

where $n'(x)$ denotes the derivative of $n(x)$ with respect to x . Using these results it follows from equation (2.11) that the sublattice magnetization is after much simplification

$$\Delta R = \frac{1}{8N^2} \sum_{\mathbf{q}\mathbf{q}'} \frac{1}{\epsilon_{\mathbf{q}}^3 \epsilon_{\mathbf{q}'}} \{ K_1 n(\epsilon_{\mathbf{q}}) n(\epsilon_{\mathbf{q}'}) + K_2 \epsilon_{\mathbf{q}} n'(\epsilon_{\mathbf{q}}) n(\epsilon_{\mathbf{q}'}) \\ + K_3 n(\epsilon_{\mathbf{q}}) - \frac{1}{2} K_1 n(\epsilon_{\mathbf{q}'}) + K_4 \epsilon_{\mathbf{q}} n'(\epsilon_{\mathbf{q}}) - \frac{1}{2} K_3 \} \quad (2.15)$$

where

$$K_1 = J(\mathbf{q}) J(\mathbf{q}') \{ J(\mathbf{q}) J(\mathbf{q}') - 2(1 + \sigma) \gamma J(\mathbf{q} - \mathbf{q}') \} + 2\gamma J^2(\mathbf{q}) \{ 2\gamma - (1 + \sigma) J(0) \} \\ K_2 = 4\gamma^2 \{ 2(1 + \sigma) \gamma J(0) - J^2(\mathbf{q}) - J^2(\mathbf{q}') \} + 2(1 + \sigma) \gamma J(\mathbf{q}) J(\mathbf{q}') J(\mathbf{q} - \mathbf{q}') \\ K_3 = -\frac{1}{2} J(\mathbf{q}) J(\mathbf{q}') \{ J(\mathbf{q}) J(\mathbf{q}') - 2(1 + \sigma) \gamma J(\mathbf{q} - \mathbf{q}') \} - \frac{1}{2} J^2(\mathbf{q}) \{ 2\gamma - (1 + \sigma) J(0) \} (\gamma - \epsilon_{\mathbf{q}'}) \\ K_4 = \gamma J(\mathbf{q}') \{ 2\gamma J(\mathbf{q}') - (1 + \sigma) J(\mathbf{q}') J(\mathbf{q} - \mathbf{q}') \} + 2\gamma \{ J^2(\mathbf{q}) - 2(1 + \sigma) \gamma J(0) \} (\gamma - \epsilon_{\mathbf{q}'}). \quad (2.16)$$

The terms proportional to $n(\epsilon_{\mathbf{q}}) n(\epsilon_{\mathbf{q}'})$ and $n'(\epsilon_{\mathbf{q}}) n(\epsilon_{\mathbf{q}'})$ describe interactions between two spin waves, and there is a zero point magnetization given by $-(1/16N^2) \sum_{\mathbf{q}, \mathbf{q}'} K_3 / \epsilon_{\mathbf{q}}^3 \epsilon_{\mathbf{q}'}$. The remaining terms give temperature dependent contributions corresponding to single spin wave processes. The general result of equation (2.15) is now considered in several special cases.

If the coupling is only between nearest neighbour sites and the lattice has a centre of symmetry, the results may be simplified by the use of equation (3.15) of II. Applying this to the isotropic case ($\sigma = h = 0$), equation (2.15) becomes

$$\Delta R = \frac{2}{N^2} \sum_{\mathbf{q}\mathbf{q}'} \epsilon_{\mathbf{q}} n(\epsilon_{\mathbf{q}}) n'(\epsilon_{\mathbf{q}}) + \frac{1}{N^2} \sum_{\mathbf{q}\mathbf{q}'} \frac{\{ \frac{1}{2} J(0) - \epsilon_{\mathbf{q}'} \}}{\epsilon_{\mathbf{q}'}} n'(\epsilon_{\mathbf{q}}). \quad (2.17)$$

Using momentum summations evaluated in I, equations (C.4) and (C.5), this result becomes

$$\Delta R = \frac{-192 \rho^2 \zeta(2) \zeta(4)}{\mu^3 J^6(0)} T^6 + \frac{4(\sqrt{2}) \rho \zeta(2)}{\mu^{3/2} J^2(0)} \left\{ \frac{1}{N} \sum_{\mathbf{q}} \frac{\{ \frac{1}{2} J(0) - \epsilon_{\mathbf{q}} \}}{\epsilon_{\mathbf{q}}} \right\} T^2. \quad (2.18)$$

The contribution to the zero point magnetization in this approximation is zero, and the linear spin wave term of order $(1/z)^2$ is proportional to T^2 . The term proportional to T^6 is the spin wave interaction term, first treated by Oguchi (1960), which corresponds to Dyson's leading Born approximation (1956) for the spin wave interaction effects for the Heisenberg ferromagnet.

If the nearest neighbour assumption is not made, the spin wave interaction terms still give a term in ΔR proportional to T^6 . This follows from equation (2.15), using the methods of I, Appendix C, since the momentum summations are dominated by small \mathbf{q} and \mathbf{q}' in the isotropic case, for which K_1 and K_2 are both of order $(qq')^2$. There will also be higher order terms proportional to T^8 . The zero point term is now no longer vanishing but it is expected to be small. The single spin wave terms give contributions proportional to T^2 or T^4 in leading order.

The anisotropic cases are included in the general result of equation (2.15). For equal and opposite anisotropy fields h it is again possible to perform the momentum summations to obtain an expansion for small h provided $h \ll J(0)$ and $hJ(0) \ll T^2$, as was carried out for the order $(1/z)^1$ terms in I, subsection (3.2). The divergence in $(\partial/\partial h)\Delta R$ as $h \rightarrow 0$ still occurs in this order. Anisotropy in the exchange is no longer equivalent to an additional field $h' = \frac{1}{2}\sigma J(0)$ as it was in order $(1/z)^1$.

It is possible to include exchange coupling between sites on the same sublattice as described in I, subsection (3.2). Also the generalization of the $(1/z)^2$ results to higher temperatures is a relatively simple matter in principle, but the calculations are rather lengthy.

The method of I, appendix A, allows a direct check to be made of the order in the $(1/z)$ expansion and the absolute size of the low temperature magnetization result (2.15). In this

equation each momentum summation has a range of order q_0 or less so that the contribution to ΔR is indeed proportional to $(1/z)^2$. Its ratio to the leading order result R_0 is $(1/z)^2$ apart from a constant of order unity, and the result from (2.15) is therefore much smaller than the previous terms in the high density expansion for the magnetization provided the low temperature validity criterion $1/z \ll 1$ of I, subsection (3.4), is satisfied.

2.2. The free energy in order $(1/z)^2$

In this subsection the $(1/z)^2$ terms in the low temperature free energy are determined. It is first shown that these terms in the free energy correspond to the diagrams of figure 2 for Y so that equation (2.11) is equivalent to the usual relation between magnetization and free energy, and the determination in the previous subsection of Y amounts to a determination of the free energy terms within the same approximations.

The calculation of the free energy uses the generalization given in I, appendix D, of the selfconsistent formalism developed by Luttinger and Ward (1960). The method of separating the $(1/z)^2$ terms is analogous to that of I, subsection (4.2) for order $(1/z)^1$. Terms up to and including $(1/z)^2$ will be selfconsistently included, and all higher order terms will be neglected. The self-energy parts are expanded as in I, equation (4.5), and hence neglecting terms of order $(1/z)^3$ the expansions of the Green functions become

$$C_i(\mathbf{k}, \alpha) = C'_i(\mathbf{k}, \alpha) + C'_i(\mathbf{k}, \alpha) \{ \Sigma_i^{(1)}(\mathbf{k}, \alpha) + \Sigma_i^{(2)}(\mathbf{k}, \alpha) \} C'_i(\mathbf{k}, \alpha) + C'_i(\mathbf{k}, \alpha) \Sigma_i^{(1)}(\mathbf{k}, \alpha) C'_i(\mathbf{k}, \alpha) \Sigma_i^{(1)}(\mathbf{k}, \alpha) C'_i(\mathbf{k}, \alpha) \tag{2.19}$$

with an analogous result for $D_i(\mathbf{k}, \alpha)$. The $(1/z)^2$ contribution to the free energy is obtained by submitting these expansions of the self energies and Green functions into I, (4.1) and selecting the $(1/z)^2$ terms

$$\mathcal{F}^{(2)} = Y^{(2)} - \frac{1}{\beta N} \sum_{\mathbf{k}, \alpha, l} e^{i\alpha 0^+} \{ \frac{1}{2} (\Sigma_l^{(1)})^2 C_l^2 + \frac{1}{2} (\Lambda_l^{(1)}) D_l^0 \}^2 + \Sigma_l^{(0)} (\Sigma_l^{(1)})^2 (C_l^2)^3 + \Sigma_l^{(0)} \Sigma_l^{(2)} (C_l^2)^2 \} \tag{2.20}$$

This will be evaluated only in the low temperature approximation where $e^{-1/T}$ factors are neglected, and thus all terms in equation (2.20) involving a $\Sigma_l^{(0)}(\mathbf{k}, \alpha)$ factor may be omitted. The corresponding skeleton self energy parts and contributions to Y are illustrated in figure 3, where all internal lines are selfconsistently renormalized. From these diagrams the quantities $\Sigma_l^{(1)}(\mathbf{k}, \alpha)$, $\Lambda_l^{(1)}(\mathbf{k}, \alpha)$ and $Y^{(2)}$ may readily be derived and substituted into equation (2.20). After much simplification the result is that $\mathcal{F}^{(2)}$ is given by the sum of the four diagrams of figure 2, with the appropriate symmetry numbers. These contributions have already been calculated and are expressed in equations (2.12) and (2.14). Thus in the symmetrical case the result for $\mathcal{F}^{(2)}$ may be written as

$$\mathcal{F}^{(2)} = - \frac{1}{4N^2} \sum_{\mathbf{q}\mathbf{q}'} \frac{1}{\epsilon_{\mathbf{q}}\epsilon_{\mathbf{q}'}} \{ K_5 n(\epsilon_{\mathbf{q}}) n(\epsilon_{\mathbf{q}'}) + K_6 n(\epsilon_{\mathbf{q}'}) + K_7 \} \tag{2.21}$$

where

$$K_5 = 4(1 + \sigma) \gamma^2 J(0) + (1 + \sigma) J(\mathbf{q}) J(\mathbf{q}') J(\mathbf{q} - \mathbf{q}') - 2\gamma J^2(\mathbf{q}) - 2\gamma J^2(\mathbf{q}')$$

$$K_6 = 2\gamma J^2(\mathbf{q}) - (1 + \sigma) J(\mathbf{q}) J(\mathbf{q}') J(\mathbf{q} - \mathbf{q}') - 2 \{ 2(1 + \sigma) \gamma J(0) - J^2(\mathbf{q}') \} (\gamma - \epsilon_{\mathbf{q}})$$

$$K_7 = \frac{1}{4}(1 + \sigma) J(\mathbf{q} - \mathbf{q}') J(\mathbf{q}) J(\mathbf{q}') - J^2(\mathbf{q}') (\gamma - \epsilon_{\mathbf{q}'}) + (1 + \sigma) J(0) (\gamma - \epsilon_{\mathbf{q}}) (\gamma - \epsilon_{\mathbf{q}'})$$

The terms proportional to $n(\epsilon_{\mathbf{q}}) n(\epsilon_{\mathbf{q}'})$ and $n(\epsilon_{\mathbf{q}'})$ describe the two spin wave processes and single spin wave processes respectively, and there is a zero point energy given by $-(1/4N^2) \sum_{\mathbf{q}, \mathbf{q}'} (K_7/\epsilon_{\mathbf{q}}\epsilon_{\mathbf{q}'})$. The general result of equation (2.21) is now considered in several special cases.

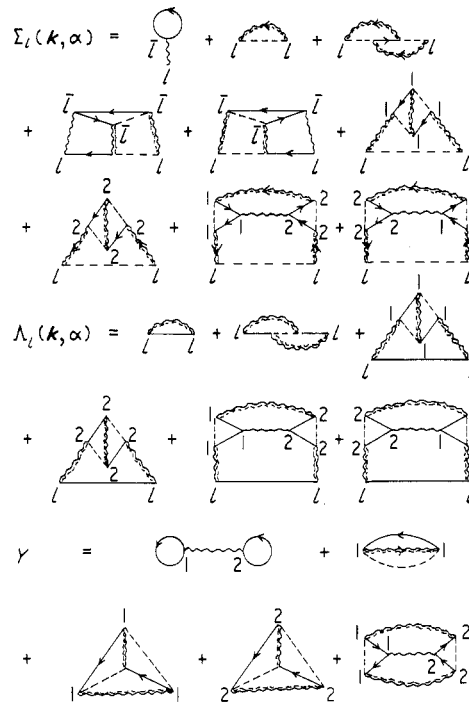


Figure 3. $(1/z)^2$ calculation of \mathcal{F} at low temperatures

In the approximation of nearest neighbour coupling only, II, equation (3.15) may be used and for the isotropic case the result simplifies to

$$\mathcal{F}^{(2)} = -\frac{4}{J(0)} \left\{ \frac{1}{N} \sum_{\mathbf{q}} \epsilon_{\mathbf{q}} n(\epsilon_{\mathbf{q}}) \right\}^2 - \frac{4}{J(0)} \left\{ \frac{1}{N} \sum_{\mathbf{q}} (\frac{1}{2}J(0) - \epsilon_{\mathbf{q}}) \right\} \left\{ \frac{1}{N} \sum_{\mathbf{q}'} \epsilon_{\mathbf{q}'} n(\epsilon_{\mathbf{q}'}) \right\} - \frac{1}{J(0)} \left\{ \frac{1}{N} \sum_{\mathbf{q}} (\frac{1}{2}J(0) - \epsilon_{\mathbf{q}}) \right\}^2. \tag{2.22}$$

This is equivalent to the expression obtained by Oguchi (1960) from spin wave theory. Using I, (C.5) for the momentum summations, the temperature dependent part of (2.22) becomes

$$\mathcal{F}^{(2)} = \frac{-1152 \rho^2 \zeta^2(4)}{\mu^3 J^7(0)} T^8 + \frac{48(\sqrt{2}) \rho \zeta(4)}{\mu^{3/2} J^4(0)} \left\{ \frac{1}{N} \sum_{\mathbf{q}} (\frac{1}{2}J(0) - \epsilon_{\mathbf{q}}) \right\} T^4. \tag{2.23}$$

Hence the interaction term is proportional to T^8 , while the single spin wave term has a T^4 dependence. If the assumption of nearest neighbour coupling is not made the spin wave interaction term in the isotropic case is, from (2.21)

$$-\frac{1}{4N^2} \sum_{\mathbf{q}\mathbf{q}'} \{ J^3(0) + J(\mathbf{q}) J(\mathbf{q}') J(\mathbf{q} - \mathbf{q}') - J(0) J^2(\mathbf{q}) - J(0) J^2(\mathbf{q}') \} \frac{n(\epsilon_{\mathbf{q}}) n(\epsilon_{\mathbf{q}'})}{\epsilon_{\mathbf{q}} \epsilon_{\mathbf{q}'}}. \tag{2.24}$$

The momentum summations are dominated by the behaviour at small \mathbf{q} and \mathbf{q}' for which the factor

$$J^3(0) + J(\mathbf{q}) J(\mathbf{q}') J(\mathbf{q} - \mathbf{q}') - J(0) J^2(\mathbf{q}) - J(0) J^2(\mathbf{q}')$$

is of order $(qq')^2$. This results in a leading temperature dependence again proportional to T^8 . It may also be shown that the term proportional to $n(\epsilon_q)$ in (2.21) still has a leading temperature dependence proportional to T^4 in the isotropic case. The zero point energy has an additional term

$$-\frac{1}{16N^2} \sum_{\mathbf{q}\mathbf{q}'} \frac{J(\mathbf{q})J(\mathbf{q}')}{J(0)} \{J(\mathbf{q}-\mathbf{q}')J(0) - J(\mathbf{q})J(\mathbf{q}')\}. \tag{2.25}$$

The anisotropic cases are included in the general result of equation (2.21)

The $(1/z)^2$ term in the internal energy at low temperatures is obtained by substituting equation (2.21) into the Gibbs-Helmholtz relation. For example in the isotropic case with nearest neighbour coupling only, this becomes

$$U^{(2)} = -\frac{1}{J(0)} \left\{ \frac{1}{N} \sum_{\mathbf{q}} \left(\frac{1}{2}J(0) - \epsilon_{\mathbf{q}} \right) \right\}^2 - \frac{144(\sqrt{2})\rho\zeta(4)}{\mu^{3/2}J^4(0)} \left\{ \frac{1}{N} \sum_{\mathbf{q}} \left(\frac{1}{2}J(0) - \epsilon_{\mathbf{q}} \right) \right\} T^4 + \frac{8064\rho^2\zeta^2(4)}{\mu^3J^7(0)} T^8. \tag{2.26}$$

Equation (2.26) is equivalent to the spin wave result of Oguchi (1960).

In analyzing the free energy result (2.21) the same cases have been considered as for the $(1/z)^2$ magnetization (2.15). The same methods as were used in the discussion of the magnetization have been applicable, essentially because of the relation (2.11). We may likewise confirm, by the use of the momentum summation method of I, appendix A, that the contribution (2.21) to the free energy is of order $(1/z)^2$ times the leading contribution to the low temperature free energy, that given by the molecular field approximation of I, subsection (4.1).

3. The damping $\Gamma_{\mathbf{k}}$ at low temperatures

In the leading order in the high density expansion, given by II (2.17) the transverse Green function has real poles at all temperatures, therefore no damping. In the next order, there is damping, given by II (3.25) but this vanishes at low temperatures where terms of order $e^{-1/T}$ are neglected. The leading terms for the low temperature damping $\Gamma_{\mathbf{k}}$ come from the next higher order and will now be calculated.

The self energy diagrams for calculating $\Gamma_{\mathbf{k}}$ from equation II (3.10) are shown in figure 4,

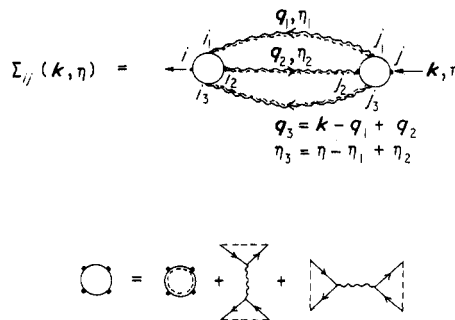


Figure 4. Self energy diagrams for calculating $\Gamma_{\mathbf{k}}$ at low temperatures.

in terms of effective spin wave vertices. They represent spin wave scattering effects analogous to those included in the derivation of the low temperature spin wave damping for the ferromagnet by Tahir-Kheli and ter Haar (1962), and Lewis and Stinchcombe (1967). Each diagram contains two independent momentum labels which are eventually summed

over. The result for $\Sigma_{ij}(\mathbf{k}, \eta)$ which links sublattices i and j may be written as

$$\Sigma_{ij}(p) = \frac{1}{(\gamma_i - i\eta)(\gamma_j - i\eta)} \cdot \frac{1}{\beta^5 N^2} \sum_{\substack{p_1 p_2 p_3 \\ i_1 i_2 i_3 \\ j_1 j_2 j_3}} \left\{ V_{ii_1 i_2 i_3}(p, p_1, p_2, p_3) V_{jj_1 j_2 j_3}(p, p_1, p_2, p_3) \right. \\ \left. J'_{i_1 j_1}(p_1) J'_{i_2 j_2}(p_2) J'_{i_3 j_3}(p_3) \delta(p - p_1 + p_2 - p_3) \right\} \quad (3.1)$$

where p_i denotes the momentum 4-vector $(\mathbf{q}_r, i\eta_r)$ and $p = (\mathbf{k}, i\eta)$. In equation (3.1), V denotes a modified vertex part resulting from absorbing the energy denominators $(\gamma \pm i\eta)$ of the vertex function defined in figure 4 into the spin wave chains to give a modified transverse interaction J'_{im} . These quantities may be expressed as

$$V_{ii_1 i_2 i_3}(p, p_1, p_2, p_3) = 2(-1)^i (2\gamma_i - i\eta - i\eta_2) \delta_{ii_1 i_2 i_3} \\ + J(\mathbf{k} - \mathbf{q}_1) \delta_{ii_1 i_2 i_3} + J(\mathbf{k} - \mathbf{q}_3) \delta_{ii_1 i_2 i_3} \quad (3.2)$$

$$J'_{ij}(p) = T_{ij}(p) - \delta_{ij} M_2^{+-}(p) = \sum_l (Q^{-1})_{il} T_{il}^*(Q^{-1})_{lj} - \frac{\delta_{ij}}{\gamma_i + (-1)^i i\eta} \quad (3.3)$$

In equation (3.2) the notation $\delta_{ii_1 i_2 i_3} = \delta_{ii_1} \delta_{ii_2} \delta_{ii_3}$, etc., has been used. If equation (3.3) is substituted into equation (3.1) there will be several different types of terms resulting from the product of the $J'_{ij}(p)$. For example, the term proportional to $T_{i_1 i_1}^* T_{i_2 i_2}^* T_{i_3 i_3}^*$ may be simplified to

$$\frac{1}{(\gamma_i - i\eta)(\gamma_j - i\eta) \beta^5 N^2} \sum_{\substack{p_1 p_2 p_3 \\ i_1 i_2 i_3}} \left\{ V_{i_1 i_1 i_2 i_3}^{(1)}(p, p_1, p_2, p_3) V_{j_1 j_1 i_2 i_3}^{(1)}(p, p_1, p_2, p_3) \right. \\ \left. T_{i_1 i_1}^*(p_1) T_{i_2 i_2}^*(p_2) T_{i_3 i_3}^*(p_3) \delta(p - p_1 + p_2 - p_3) \right\} \quad (3.4)$$

where

$$V_{i_1 i_1 i_2 i_3}^{(1)}(p, p_1, p_2, p_3) = 2(-1)^i (2\gamma_i - i\eta - i\eta_2) (Q_{\mathbf{q}_1}^{-1})_{i_1 i_1} (Q_{\mathbf{q}_2}^{-1})_{i_2 i_2} (Q_{\mathbf{q}_3}^{-1})_{i_3 i_3} \\ + J(\mathbf{k} - \mathbf{q}_1) (Q_{\mathbf{q}_1}^{-1})_{i_1 i_1} (Q_{\mathbf{q}_2}^{-1})_{i_2 i_2} (Q_{\mathbf{q}_3}^{-1})_{i_3 i_3} \\ + J(\mathbf{k} - \mathbf{q}_3) (Q_{\mathbf{q}_1}^{-1})_{i_1 i_1} (Q_{\mathbf{q}_2}^{-1})_{i_2 i_2} (Q_{\mathbf{q}_3}^{-1})_{i_3 i_3}$$

Advantage has been taken of the diagonal nature of the matrix T^* to reduce the number of summation variables in equation (3.4) to six. Equation (3.4) may be evaluated by replacing the delta function on frequencies by an integral representation

$$\delta_{\eta - \eta_1 + \eta_2 - \eta_3, 0} = \frac{1}{\beta} \int_0^\beta \exp \{i\alpha(\eta - \eta_1 + \eta_2 - \eta_3)\} d\alpha \quad (3.5)$$

This enables the frequency summations of equation (3.4) to be freely carried out. After making the analytic continuation $i\eta \rightarrow \epsilon_{\mathbf{k}} + i\delta$, the imaginary part of equation (3.4) is

$$\frac{\pi(2\delta_{ij} - 1)}{(\gamma_i - \epsilon_{\mathbf{k}})(\gamma_j - \epsilon_{\mathbf{k}}) \beta^2 N^2} \sum_{\substack{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3 \\ i_1 i_2 i_3}} \left\{ V_{i_1 i_1 i_2 i_3}^{(1)}(\mathbf{k}, \mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) V_{j_1 j_1 i_2 i_3}^{(1)}(\mathbf{k}, \mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) \right. \\ \left. X \left((-1)^{i_1} \epsilon_{\mathbf{q}_1}, (-1)^{i_2} \epsilon_{\mathbf{q}_2}, (-1)^{i_3} \epsilon_{\mathbf{q}_3} \right) \delta(\mathbf{k} - \mathbf{q}_1 + \mathbf{q}_2 - \mathbf{q}_3) \right. \\ \left. \delta(\epsilon_{\mathbf{k}} - (-1)^{i_1} \epsilon_{\mathbf{q}_1} + (-1)^{i_2} \epsilon_{\mathbf{q}_2} - (-1)^{i_3} \epsilon_{\mathbf{q}_3}) \right\} \quad (3.6)$$

where the function X is defined by

$$X(x_1, x_2, x_3) = n(x_1) \{n(x_3) - n(x_2)\} + n(x_2) n(-x_3)$$

and $V^{(1)}$ is now a function of the momenta only given by

$$\begin{aligned}
 V_{i_1 i_2 i_3}^{(1)}(\mathbf{k}, \mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) = & 2(\epsilon_{\mathbf{k}} + (-1)^l \epsilon_{\mathbf{q}_2} - 2\gamma) (Q_{\mathbf{q}_1}^{-1})_{i_1} (Q_{\mathbf{q}_2}^{-1})_{i_2} (Q_{\mathbf{q}_3}^{-1})_{i_3} \\
 & + J(\mathbf{k} - \mathbf{q}_1) (Q_{\mathbf{q}_1}^{-1})_{i_1} (Q_{\mathbf{q}_2}^{-1})_{i_2} (Q_{\mathbf{q}_3}^{-1})_{i_3} \\
 & + J(\mathbf{k} - \mathbf{q}_3) (Q_{\mathbf{q}_1}^{-1})_{i_1} (Q_{\mathbf{q}_2}^{-1})_{i_2} (Q_{\mathbf{q}_3}^{-1})_{i_3}.
 \end{aligned}
 \tag{3.7}$$

The result of equation (3.6) may be substituted into II, equation (3.10) to give a contribution to $\Gamma_{\mathbf{k}}$. The contributions from the other terms in $\Sigma_i(p)$ obtained by substituting equation (3.3) into (3.1) may be evaluated by an analogous procedure. The results are similar to equation (3.6) but with one or more of the $\epsilon_{\mathbf{q}}$ replaced by γ .

The temperature dependence of the result for $\Gamma_{\mathbf{k}}$ arising from (3.6) and similar equations comes from the $n(\epsilon_{\mathbf{q}})$ factors. When a summation over \mathbf{q} is carried out, this gives rise to a temperature dependence proportional to a power of T in the isotropic case (as in I, appendix C). This will replace the exponential $e^{-1/T}$ type of behaviour obtained in II, subsection (3.3) from the lowest order calculation. There will also be terms in the self-energy which have no $n(\epsilon_{\mathbf{q}})$ factors, and so there is a possibility of obtaining a zero point contribution to $\Gamma_{\mathbf{k}}$. It may be shown that the only zero point contribution to the imaginary part of the analytically contained self energy is

$$\frac{\pi(2\delta_{ij} - 1)}{(\gamma_i - \epsilon_{\mathbf{k}})(\gamma_j - \epsilon_{\mathbf{k}}) \beta^2 N^2} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3} V_{i_1 i_2 i_3}^{(1)} V_{j_1 j_2 j_3}^{(1)} \delta(\mathbf{k} - \mathbf{q}_1 + \mathbf{q}_2 - \mathbf{q}_3) \delta(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}_1} - \epsilon_{\mathbf{q}_2} - \epsilon_{\mathbf{q}_3}).
 \tag{3.8}$$

All other terms are such that the delta functions cannot be satisfied. The delta functions in equation (3.8) impose a heavy restriction on the functional form of $\epsilon_{\mathbf{q}}$ for there to be a non-zero result. If $\epsilon_{\mathbf{q}}$ is assumed to be a monotone increasing function of q , it may be proved that a necessary condition for a nonzero contribution is that $\epsilon_{\mathbf{q}}$ is a concave function of q

$$\epsilon_{q_1} + \epsilon_{q_2} \leq \epsilon_{q_1 + q_2}
 \tag{3.9}$$

for any \mathbf{q}_1 and \mathbf{q}_2 . This condition is not normally satisfied if there is any anisotropy, or even in the isotropic case for general \mathbf{q} . It may, however, be satisfied in the isotropic case for very small \mathbf{q} where $\epsilon_{\mathbf{q}}$ becomes proportional to q . For a strictly linear spectrum the zero point damping from equation (3.8) is

$$\Gamma_{\mathbf{k}} = \frac{\pi \rho^3 J(0)}{240(\sqrt{2}) \mu^{5/2}} k^4.
 \tag{3.10}$$

The requirements for this result are not likely to be satisfied for most physical cases. The leading temperature-dependent terms are of the form

$$\frac{1}{N^2} \sum_{\mathbf{q}_1 \mathbf{q}_2 \mathbf{q}_3} \frac{n(\epsilon_{\mathbf{q}_1}) f(\mathbf{q}_2 \mathbf{q}_3)}{\epsilon_{\mathbf{q}_1}} \delta(\mathbf{k} - \mathbf{q}_1 + \mathbf{q}_2 - \mathbf{q}_3) \delta(\epsilon_{\mathbf{k}} \pm \epsilon_{\mathbf{q}_1} \pm \epsilon_{\mathbf{q}_2} \pm \epsilon_{\mathbf{q}_3}).$$

They contain only one $n(\epsilon_{\mathbf{q}})$ type of factor. The \mathbf{q}_1 summation will be dominated by the behaviour at small \mathbf{q}_1 , and so each term of this type will be proportional to T^2 in the isotropic case.

4. Conclusions

Calculations have been presented for the sublattice magnetization and free energy in order $(1/z)^2$ and the spin wave damping at low temperatures where terms proportional to $e^{-1/T}$ are neglected. Within this approximation the lowest order nonvanishing contribution to the damping is obtained. At higher temperatures an approximate description of the damping is obtained from lower order terms in the $(1/z)$ expansion as described in paper II. The calculations for the thermodynamic quantities represent an extension of the results in paper I and are equivalent to including the effects of spin wave interactions. The generalization of the results to higher temperatures may be carried out by a similar procedure.

Note added in proof. Following Harris *et al.* (1970) we have shown (Cottam and Stinchcombe 1970c) that the symmetry of the various T^2 terms is such that they mutually cancel for small k , leaving a leading contribution to the low temperature damping proportional to $\epsilon_k T^4$ for $(T/T_N) \ll (\epsilon_k/J(0)) \ll 1$.

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