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# Irreducible Green function theory for ferromagnets with first- and second-neighbour exchange

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**Abstract.** A conceptually new version of the irreducible Green function (IRG) formalism is applied to study a Heisenberg ferromagnet with first-neighbour exchange ( $J_1$ ) and second-neighbour exchange ( $J_2$ ). The most important quantity which appears in IRG formalism is the commutator average  $\lambda = \langle [I_{kk'}, S_{q'}^-] \rangle$  (where  $k$ ,  $q'$  and  $k'$  refer to the incoming, outgoing and internal momentum lines, respectively), which is found to be not only non-zero but also independent of  $k'$  in a natural way. This replaces the old irreducibility condition  $\lambda = 0$  and enables one to recast the equation of motion into the exact Dyson form. For the estimation of self-energy the reducible operators are mapped onto irreducible observables, which introduces a parameter  $\xi$  into the self-energy operator. The values of  $\xi$  for various ratios  $J_2/J_1$  and for several spins have been found from the results of exact high-temperature series. From the least-squares fit of these values of  $\xi$  against  $1/S$ , we obtain an estimate of  $\xi$  for  $S = \infty$ . This is then used to evaluate the Curie temperature for  $S = \infty$  and a FCC lattice. The result is found to be in good agreement with the series result. The theory is then applied to EuS which corresponds to a  $S = \frac{7}{2}$  FCC lattice. Using the experimental values of  $T_C$  the exchange parameters  $J_1$  and  $J_2$  have been computed. The results agree very well with the series results and with those obtained from spin-wave analysis.

## 1. Introduction

The irreducible Green function (IRG) approach has been adopted in the past by several workers to study some simple and complicated problems of condensed-matter theory (Plakida 1971, 1973, Micnas and Kawalewski 1979, Kuzemsky 1978, 1989, Marvakov *et al* 1985, Chakraborty 1988, 1989). In all these calculations, a mean-field or a generalized mean-field contribution is extracted from the higher-order Green function so that the residual Green function is made irreducible by means of a formal irreducibility condition  $\lambda = \langle [I_{kk'}, S_{q'}^-] \rangle = 0$ , where  $I_k$  is the Fourier-transformed irreducible operator,  $S_{q'}^-$  is a Fourier-transformed spin operator, and  $k$ ,  $q'$  and  $k'$  refer to the incoming, outgoing and internal momentum lines, respectively. The above condition was employed with the aim of recasting the equation of motion in the form of the exact Dyson equation in which the irreducible self-energy appears. However, in the course of carrying out the derivation by IRG formalism for any problem, we observed that there is neither any reason nor any need to put  $\lambda$  equal to zero, and that there exists an exact condition which appears in the analysis in a natural way and which is not based on any assumption. This condition states that  $\lambda$  is independent of  $k'$ . This simple condition enables one to accomplish the task of recasting the equation of motion in the form of the exact Dyson equation. The advantage of the present condition is that one does not need to include unknown parameters and the residual

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Green function is written by extracting the contributions estimated from known decoupling approximations applied to the problem concerned. The exact Dyson equation derived in this way for a Heisenberg ferromagnet with first- and second-nearest-neighbour exchange consists of a self-energy operator  $\Sigma$ , the computation of which seems to be extremely difficult because of the appearance of a Green function such as  $\langle\langle I_k; I_{q'} \rangle\rangle$ , where  $I_k$  and  $I_{q'}$  are the irreducible operators. Some time ago, one of the present authors (Chakraborty 1988, 1989) decoupled such a Green function by the random-phase approximation (RPA), but strictly speaking the estimation of the self-energy in this way is grossly inaccurate. For accurate estimation the reducible operators are mapped onto irreducible observables so that we need to use a parameter  $\xi$  which has been determined by matching with the known values of Curie temperature obtained from the exact high-temperature series expansion. By extrapolation to  $S \rightarrow \infty$  the value of  $\xi$  for a classical Heisenberg ferromagnet has been derived. This value of  $\xi$  provides an accurate estimate of the Curie temperature for  $S = \infty$ . The theory is then applied to estimate the values of the exchange constants for EuS, a member of the europium chalcogenide series. The results agree well with those obtained from other theories.

## 2. The Hamiltonian and the irreducible Green function theory

We consider the Heisenberg model with first- and second-neighbour exchange described by the following Hamiltonian:

$$H = -\mu H \sum_i S_i^z - \sum_{i,j_1} J_{ij_1} S_i \cdot S_{j_1} - \sum_{i_2,j_2} J_{i_2j_2}^{(2)} S_{i_2} \cdot S_{j_2} \quad (1)$$

where  $\mu$  is the magnetic moment per site and  $H$  is the applied magnetic field. The first sum in equation (1) extends to first neighbours and the second sum to second neighbours.  $J_{ij_1}^{(1)}$  and  $J_{i_2j_2}^{(2)}$  represent the nearest- and next-nearest-neighbour exchange integrals, respectively.

We use here a Zubarev Green function  $\langle\langle S_f^+; S_g^- \rangle\rangle$ , where  $f$  and  $g$  are lattice sites. The Fourier-transformed equation of motion in momentum space is

$$\begin{aligned} (\omega - \mu H) \langle\langle S_k^+; S_{q'}^- \rangle\rangle &= \frac{\langle S_{k-q'}^z \rangle}{\pi \sqrt{N}} + \frac{2}{\sqrt{N}} \sum_{k'} J_{k'}^{(1)} \langle\langle S_{k'}^z S_{k-k'}^+ - S_{k-k'}^z S_{k'}^+; S_{q'}^- \rangle\rangle \\ &+ \frac{2}{\sqrt{N}} \sum_{k''} J_{k''}^{(2)} \langle\langle S_{k''}^z S_{k-k''}^+ - S_{k-k''}^z S_{k''}^+; S_{q'}^- \rangle\rangle. \end{aligned} \quad (2)$$

At this point we introduce a residual Green function  $\langle\langle \phi_k; S_{q'}^- \rangle\rangle$  defined by

$$\langle\langle \phi_k; S_{q'}^- \rangle\rangle = \langle\langle (S_{k'}^z S_{k-k'}^+ - S_{k-k'}^z S_{k'}^+) - C_{mf} - C_{emf}; S_{q'}^- \rangle\rangle \quad (3)$$

where  $C_{mf}$  denotes the mean-field contribution and  $C_{emf}$  denotes the extra-mean-field contribution:

$$C_{mf} \equiv \langle S_{k'}^z \rangle S_{k-k'}^+ - \langle S_{k-k'}^z \rangle S_{k'}^+ \quad (4)$$

$$C_{emf} \equiv (A_{k'} - A_{k-k'}) S_k^+. \quad (5)$$

In the old IRG approach the  $A$ -values are determined from the assumed irreducibility condition:  $\lambda = 0$ . In the new approach it does not matter whether we put  $A_{k'} = A_{k-k'} = 0$ .

or  $A_{k'} \neq A_{k-k'} \neq 0$ . In the case when  $A_{k'} = A_{k-k'} = 0$  the zeroth-order Green function contains only the mean-field contribution and the rest is accumulated in the self-energy operator of the Dyson equation. When  $A_{k'} \neq A_{k-k'} \neq 0$ , more contributions are allowed to be included in the zeroth-order Green function. The extent to which these contributions exceed the mean-field contribution depends on the  $A$ -values. We here choose, in accordance with the Callen (1963) decoupling scheme,

$$A_{k'} = \frac{\langle S^z \rangle}{2S^2} \langle S_{k-k'}^- S_{k-k'}^+ \rangle. \quad (6)$$

With this choice we arrive at

$$(\omega - \omega_k) \langle\langle S_k^+; S_{q'}^- \rangle\rangle = \frac{m}{\pi} \delta_{k-q'} + \frac{2}{N^{1/2}} \sum_{k'} (J_{k'}^{(1)} + J_{k'}^{(2)}) \langle\langle \phi_k; S_{q'}^- \rangle\rangle \quad (7)$$

where  $m = \langle S^z \rangle$  and

$$\omega_k = \mu H + 2m(J_0^{(1)} - J_k^{(1)} + J_0^{(2)} - J_k^{(2)}) + \frac{m}{S^2 \sqrt{N}} \sum_{k'} (J_{k'}^{(1)} - J_{k-k'}^{(1)} + J_{k'}^{(2)} - J_{k-k'}^{(2)}) \langle S_k^- S_k^+ \rangle. \quad (8)$$

Equation (7) consists of a Green function  $\langle\langle \phi_k; S_{q'}^- \rangle\rangle$  which can be eliminated by means of differentiation a second time so that the equation of motion reads

$$\omega \langle\langle \phi_f; S_q^- \rangle\rangle = \frac{\langle[\phi_f, S_q^-]\rangle}{2\pi} + \langle\langle \phi_f; [H, S_q^-] \rangle\rangle. \quad (9)$$

Considering  $H$  as given by equation (1) we obtain the Fourier-transformed equation in momentum space:

$$\langle\langle \phi_k; \psi_{q'} \rangle\rangle = \langle\langle \phi_k; (S_{k'}^2 S_{k-k'}^+ - S_{k-k'}^2 S_{k'}^+) - C'_{mf} - C'_{cmf} \rangle\rangle. \quad (10)$$

With  $C'_{mf}$  and  $C'_{cmf}$  as in (4) and (5) we obtain

$$\begin{aligned} (\omega - \mu H) \langle\langle \phi_k; S_{q'}^- \rangle\rangle &= \frac{\lambda}{2\pi} + \frac{2}{\sqrt{N}} \sum_{k'} (J_{k'}^{(1)} + J_{k'}^{(2)}) \langle\langle \phi_k; \psi_{q'} \rangle\rangle \\ &+ 2m[J_0^{(1)} - J_{q'}^{(1)} + J_0^{(2)} - J_{q'}^{(2)}] \langle\langle \phi_k; S_{q'}^- \rangle\rangle \\ &+ \frac{m}{S^2 N^{1/2}} \sum_{k'} (J_{k'}^{(1)} - J_{k-k'}^{(1)} + J_{k'}^{(2)} - J_{k-k'}^{(2)}) \langle S_k^- S_k^+ \rangle \langle\langle \phi_k; S_{q'}^- \rangle\rangle \end{aligned} \quad (11)$$

with

$$\lambda = \langle[\phi_k; S_{q'}^-]\rangle.$$

At this point of the analysis our conceptually different version of IRG formalism emerges. We note that the first term on the right-hand side of equation (11) does not contain the summation over  $k'$ , implying that no internal momentum indices appears in this term and

hence  $\lambda$  must be regarded as independent of internal momentum  $k'$ . Substituting (11) in (7), we obtain

$$\begin{aligned}
 (\omega - \omega_k) \langle\langle S_k^+; S_{q'}^- \rangle\rangle &= \frac{m}{\pi} \delta_{k-q'} + \frac{\lambda(\omega - \omega_{q'})^{-1}}{\pi\sqrt{N}} \sum_{k'} (J_{k'}^{(1)} + J_{k'}^{(2)}) \\
 &+ \frac{4}{N} (\omega - \omega_{q'})^{-1} \sum_{k'k''} (J_{k'}^{(1)} + J_{k'}^{(2)}) (J_{k''}^{(1)} + J_{k''}^{(2)}) \langle\langle \phi_k; \psi_{q'} \rangle\rangle.
 \end{aligned} \tag{12}$$

The second term on the right-hand side vanishes because  $\sum_{k'} (J_{k'}^{(1)} + J_{k'}^{(2)}) = 0$  and hence it is not necessary to put  $\lambda$  equal to zero. Thus we can write equation (12) in the form of a matrix Dyson equation

$$G = G^0 + G^0 P G^0 \tag{13}$$

where  $G^0$  is the zeroth-order Green function:

$$G^0 = \frac{m/\pi}{\omega - \omega_k} \tag{14}$$

and  $P$  is the polarization operator by

$$P = \frac{4\pi^2}{m^2} \frac{1}{N} \sum_{k'k''} (J_{k'}^{(1)} + J_{k'}^{(2)}) (J_{k''}^{(1)} + J_{k''}^{(2)}) \langle\langle \phi_k; \psi_{q'} \rangle\rangle. \tag{15}$$

Defining  $\Sigma = P(1 + P G^0)^{-1}$  as the self-energy we arrive at the exact Dyson equation

$$G = G^0 + G^0 \Sigma G^0. \tag{16}$$

The IRG formalism is now complete and up to this point exact; equation (16) allows one in principle, to compute the thermodynamic quantities exactly.

### 3. Self-energy and the renormalized spectra

Although we have been able to devise an exact IRG formalism, it does not seem possible at this stage to perform the exact computation of self-energy. For its estimation we present the following method.

It is worth noting that a mapping of reducible observables into the irreducible operator  $A_r \rightarrow A_{ir}$  may be defined such that the commutation relations are preserved. That is, if  $[A_r, B_r] = C_r$ , then  $[A_{ir}, B_{ir}] = C_{ir}$  is true. In addition to this, one must require  $\langle A_r \rangle = L \langle A_{ir} \rangle$ ,  $L$  being a scale factor. A well known example of such mapping is the Holstein-Primakoff and Dyson transformations, where the spin operators (reducible) are transformed to boson operators (irreducible). In accordance with such mapping we can write, in general,

$$\langle\langle A_{ir}; B_{ir} \rangle\rangle = \xi^2 \langle\langle A_r; B_r \rangle\rangle \tag{17}$$

$\xi$  being a spin-dependent parameter (Mitra and Chakraborty 1994).

Following (17) the expression for the self-energy can be written, to leading order, in the form

$$\sum_k = 4\pi^2 G_k \xi^2 (J_0^{(1)} - J_k^{(1)} + J_0^{(2)} - J_k^{(2)})^2. \quad (18)$$

Using this, the normalized Green function can be expressed as

$$G_k = \frac{b}{2\pi} \left( \frac{1}{\omega - E_1} + \frac{1}{\omega - E_2} \right) \quad (19)$$

where

$$E_{1,2} = \omega_k \pm 2b\xi J^{(1)} Z_1 R_1 \quad (20)$$

$$R_1 = 1 - \gamma_1(k) + \alpha[1 - \gamma_2(k)] \quad (21)$$

with  $\alpha = J^{(2)} Z_2 / J^{(1)} Z_1$  and

$$\gamma_1(k) = \frac{1}{Z_1} \sum_k \exp(ik \cdot \delta_1) \quad \gamma_2(k) = \frac{1}{Z_2} \sum_k \exp(ik \cdot \delta_2) \quad (22)$$

$\delta_1$  and  $\delta_2$  being the nearest- and next-nearest-neighbour vectors, respectively.

#### 4. Results for the Curie temperature

An expression for the Curie temperature can be derived in the usual manner from the relation

$$\langle S^z \rangle = \frac{S(S+1)}{3\Phi} \quad (23)$$

$$\Phi = \frac{1}{N} \sum_k \frac{1}{\exp(\beta\omega_k) - 1} \quad (23a)$$

in which it is necessary to evaluate the quantity

$$K' = \frac{\langle S^z \rangle}{S^2 \sqrt{N}} \sum_{k'} (J_{k'}^{(1)} + J_{k'}^{(2)} - J_{k-k'}^{(1)} - J_{k-k'}^{(2)}) \langle S_{k'}^- S_{k'}^+ \rangle. \quad (24)$$

$K'$  can be written as

$$K' = \frac{\langle S^z \rangle}{S^2} J_1 Z_1 \{ f_1 [1 - \gamma_1(k)] + \alpha f_2 [1 - \gamma_2(k)] \} \quad (25)$$

where

$$f_1 = \frac{1}{\sqrt{N}} \sum_k \frac{J_{(k)}^{(1)} / J_{(0)}^{(1)}}{\exp(\beta\omega_k) - 1} \quad (26a)$$

$$f_2 = \frac{1}{\sqrt{N}} \sum_k \frac{J_{(k)}^{(2)} / J_{(0)}^{(2)}}{\exp(\beta\omega_k) - 1}. \quad (26b)$$

Putting  $f_1 \simeq f_2$  and taking the limit  $(S^2) \rightarrow 0$ , we arrive at the following expression for the Curie temperature:

$$t_C(\alpha) = \frac{k_B T_C}{Z_1 J_1} = \frac{4S+1}{9F(\alpha)} [f(\xi) + f(-\xi)] \quad (27)$$

with

$$f(\xi) = a(S+1) + 3SF(\alpha)(1+\xi) \quad (27a)$$

$$a = (1+\alpha)F(\alpha) - 1 \quad (27b)$$

$$F(\alpha) = \frac{1}{\sqrt{N}} \sum_k \frac{1}{1 - \gamma_1(k) + \alpha[1 - \gamma_2(k)]} \quad (27c)$$

For  $S = \infty$  we obtain

$$t_C(\infty) = \frac{k_B T_C}{J_1 Z_1 S^2} \Big|_{S \rightarrow \infty} = \frac{4}{9F^2(\alpha)} \left( \frac{1}{a + 3(1+\xi)F(\alpha)} + \frac{1}{a + 3(1-\xi)F(\alpha)} \right). \quad (28)$$

Both equation (27) and equation (28) contain the parameter  $\xi$ . The extended Watson sum  $F(\alpha)$  has been computed in the literature. The values of  $\xi$  for different values of  $\alpha$  and  $S$  are determined by matching the values of  $t_C(s)$  obtained from equation (27) with those obtained from the exact high-temperature series expansion (HTE) carried out by Wood and Dalton (1967) for a Heisenberg ferromagnet with first- and second-neighbour exchange. These values are shown in table 1 where  $\alpha$  has been considered from 0 to 1 and  $S = \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}$  and 3. It is to be noted from table 1 that each row approximately obeys a linearity relation  $\xi = a + b/s$ ,  $a$  and  $b$  being the parameters to be determined by least-squares fitting. The values of  $a$  and  $b$  for various values of  $\alpha$  are shown in table 2. Extrapolating to  $S \rightarrow \infty$ , we have estimated the values of  $\xi$  for various values of  $\alpha$ . We utilize this value of  $\xi$  in equation (28) and the values of  $t_C(\alpha)$  have been calculated. These are shown in table 2 where the exact series results are also quoted for comparison. The agreement between the calculated values and HTE results is indeed satisfactory.

Table 1. The value of  $\xi_s(\alpha)$  obtained by matching the exact series estimates of Curie temperature with the values obtained from the present theory.

$\alpha$	$\xi_s(\alpha)$					
	$S = \frac{1}{2}$	$S = 1$	$S = \frac{3}{2}$	$S = 2$	$S = \frac{5}{2}$	$S = 3$
0	0.661	0.452	0.360	0.302	0.273	0.247
0.1	0.714	0.485	0.405	0.362	0.324	0.305
0.2	0.769	0.546	0.453	0.405	0.376	0.346
0.3	0.827	0.588	0.493	0.444	0.413	0.392
0.4	0.881	0.633	0.537	0.487	0.456	0.435
0.5	0.939	0.677	0.578	0.526	0.494	0.472
0.6	0.979	0.719	0.617	0.564	0.531	0.509
0.7	1.054	0.764	0.656	0.600	0.567	0.544
0.8	1.113	0.805	0.695	0.637	0.614	0.578
0.9	1.170	0.849	0.732	0.672	0.635	0.612
1.0	1.230	0.891	0.769	0.706	0.669	0.644

**Table 2.** The value of  $k_B T_C / Z_1 J_1 S^2$  for  $S = \infty$  calculated from the present theory for the FCC lattice. The results are compared with those obtained from the HTE. The values of  $\xi_\alpha(\infty)$  extrapolated to  $S = \infty$  are also shown.  $a$  and  $b$  are the least-square parameters, the values of which are obtained from table 1 from a fitting with the equation  $\xi = a + b/s$ .

$\alpha$	$a$	$b$	$\xi_\infty(\infty)$	$k_B T_C(S \rightarrow \infty) / Z_1 J_1 S^2$	
				Calculated	Exact
0	0.1819	0.2456	0.1819	0.5229	0.5308
0.1	0.2346	0.2424	0.2346	0.5567	0.5631
0.2	0.2787	0.2495	0.2787	0.5921	0.5995
0.3	0.3140	0.2599	0.3140	0.6244	0.6313
0.4	0.3538	0.2666	0.3538	0.6563	0.6667
0.5	0.3864	0.2791	0.3864	0.6880	0.6944
0.6	0.4178	0.2919	0.4178	0.7196	0.7310
0.7	0.4481	0.3054	0.4481	0.7509	0.7578
0.8	0.4811	0.3175	0.4811	0.7790	0.7937
0.9	0.5051	0.3346	0.5051	0.8123	0.8251
1.0	0.5313	0.3513	0.5313	0.8430	0.8530

## 5. Application to experimental results

We have seen in the previous section that the present IRG theory is able to reproduce, with a good degree of accuracy, the values of Curie temperature for an  $S = \infty$  Heisenberg ferromagnet for several different values of the parameter  $\alpha$  and for all lattice structures, the parameter  $\xi$  being determined by matching with the exact values for several spin values and then extrapolating to  $S \rightarrow \infty$ . For a more crucial experimental test of IRG results, many observed data are available for the europium chalcogenide series in which both first- and second-nearest neighbour exchange interactions are believed to exist to an appreciable extent. For such verification we concentrate only on one member of the europium chalcogenide series, namely EuS, for which  $S = \frac{7}{2}$ ,  $\alpha = -0.4$ ,  $Z_1 = 12$  and  $Z_2 = 6$ .

To carry out the experimental test it is of prime necessity to have an estimate of  $\xi$  for EuS and for such an estimate we need to proceed as in the previous section. The values for  $T_C$  for  $S = \frac{7}{2}$  from the exact series expansion are not available in the literature. Hence we carry out an extrapolation of the HTE results of Wood and Dalton. To begin with we note that in table 1 the rows obey a least-squares fit relation, which is distinctly different from that obeyed by the columns. In the former case,  $\alpha$  remains fixed and in the latter  $S$  is fixed. For the rows we attempt to get a least-squares fit with the following relation:

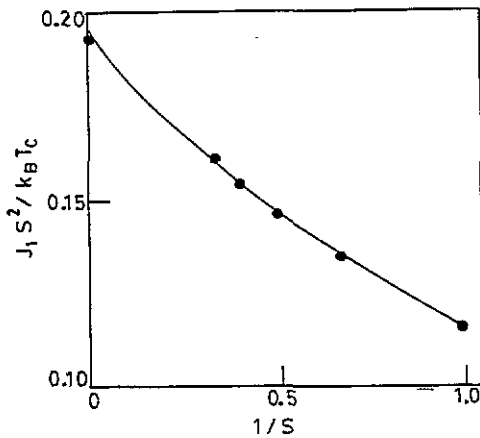
$$\frac{J_1 S^2}{k_B T_C} = A + \frac{B}{S^{3/4}}. \quad (29)$$

Considering any particular row we can determine the least-squares fit parameters  $A$  and  $B$ . Evidently, for different  $\alpha$ , the values of  $A$  and  $B$  are different. We are primarily interested in the value  $\alpha = -0.4$  since it corresponds to EuS. Exact values of  $J_1 S^2 / k_B T_C$  in this case, obtained by Wood and Dalton, are shown in table 3 for  $S = 1, \frac{3}{2}, 2, \frac{5}{2}$  and 3. Using these values the parameters  $A$  and  $B$  have been determined, so that the extrapolated values for  $S = \frac{7}{2}$  can be calculated. The value of  $J_1 S^2 / k_B T_C = 0.196$  for  $S = \infty$  which is close to the exact value, 0.193. Equation (29) has been plotted in figure 1. The extrapolated values are shown by the full curve and the HTE data are shown by full circles. It is interesting to see that the average error is not larger than 1.2%, and equation (29) can be comfortably used to calculate the Curie temperature for  $\frac{S}{2}$ .

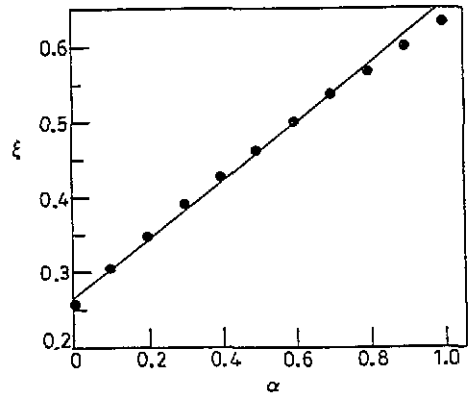


**Table 3.** Extrapolation of the exact high-temperature series expansion (EHTE) for a FCC lattice according to the equation  $J_1 S^2/k_B T_C(\alpha) = A + B/S^{3/4}$ , where  $A$  and  $B$  are least-squares parameters. The result for  $S = \frac{7}{2}$  obtained from table 2 are compared with the EHTE. Here the extrapolation has been performed with five values of spin:  $S = 1, \frac{3}{2}, 2, \frac{5}{2}$  and 3. All results refer to the case  $\alpha = -0.4$ .

$S$	$A$	$B$	$J_1 S^2/k_B T_C(\alpha)$	
			Exact	EHTE
1	0.196	-0.081	0.116	0.115
$\frac{3}{2}$			0.135	0.136
			0.147	0.148
2			0.155	0.155
			0.162	0.160



**Figure 1.** The least-squares fit of  $J_1 S^2/k_B T_C$  against  $1/S$  according to equation (29): —, extrapolated values; ●, HTE data.



**Figure 2.** The least-squares fit with the  $\xi = A' + \alpha B'$  against  $\alpha$ , the calculated values of  $A'$  and  $B'$  are shown in table 4.

The columns of table 1 enable us to estimate  $\xi$  for a particular spin value. The values of  $\xi_s(\alpha)$  for any particular  $S$  for different  $\alpha$  can be obtained from the fitting relation  $\xi = a + b/s$ ,  $a$  and  $b$  being taken from table 2. In this way the values of  $\xi_{7/2}(\alpha)$  have been calculated. These values of  $\xi_{7/2}(\alpha)$  are shown in table 4 for  $\alpha$  from 0 to 1. If one plots these values of  $\xi$  against  $\alpha$ , we note as a whole that the fitting curve should deviate slightly from linearity but, if we look at the first six and the last six values separately, the curve reduces to linear in two separate cases. Since we are chiefly interested in the case  $\alpha = -0.4$  we concentrate on the first six values. As these values fall approximately on a straight line, we attempt to carry out a least-squares fit with the relation  $\xi = A' + \alpha B'$  (figure 2). The calculated values of the parameters  $A'$  and  $B'$  are shown in table 4. These values yield  $\xi_{7/2}(-0.4) = 0.1117$  which may thus be regarded as the value corresponding to EuS.

We can now use the value of  $\xi$  for EuS as measured above in equation (23) to obtain the value of the exchange constants  $J_1/k_B$  and  $J_2/k_B$  if we know the value of  $T_C$  for EuS. Moruzzi and Teaney (1963) reported from specific heat data that  $T_C = 16.3$  K. By comparison of spin-wave theory with low-temperature magnetization and specific heat data, Charp and Boyd (1964) found that  $J_1/k_B = 0.20$  K,  $J_2/k_B = -0.08$  K. Using these values

**Table 4.** Least-squares fit of  $\xi = A' + \alpha B'$  for  $S = \frac{7}{2}$ .

	$\xi_{7/2}(\alpha)$	$A'$	$B'$	$\xi_{7/2}(-0.4)$
0.0	0.2521	0.2581	0.4247	0.1117
0.1	0.3039			
0.2	0.3500			
0.3	0.3883			
0.4	0.4300			
0.5	0.4661			
0.6	0.5012			
0.7	0.5354			
0.8	0.5684			
0.9	0.6007			
1.0	0.6317			

of the exchange constants, Callen and Callen (1964) deduced within the framework of the cluster approximation, that  $T_C = 16.9$  K. Here we shall consider the case the other way round. Using the experimental value of  $T_C$  obtained by Moruzzi and Teaney, the exchange constants  $J_1/k_B$  and  $J_2/k_B$  have been estimated. These values shown in table 5 are in good agreement with those obtained from the EHTE and from spin-wave analysis. It is to be noted that the molecular-field approximation (MFA) yields much lower values. It is necessary to remark that the cluster approximation for the model considered by Callen and Callen (1964) gave  $T_C = 16.9$  K using the values given by Charp and Boyd (1964) for the exchange constants. Finally, we would like to point out that the experimental magnetization curves and the susceptibility data can be satisfactorily reproduced in a straightforward way using the IRG values of the exchange constants given in table 5. We do not, however, present these results here.

**Table 5.** The values of  $J_1/k_B$  and  $J_2/k_B$  for EuS obtained from IRG. For comparison the values obtained from EHTE, MFA and spin-wave analysis are also shown.  $T_C$  has been taken to be 16.3 K.

$J_1/k_B$	$J_2/k_B$	Source
0.24	-0.096	IRG
0.22	-0.088	EHTE
0.20	-0.08	Spin wave
0.16	-0.064	MFA

## 6. Concluding remarks

The IGF theory presented in the preceding sections differs from former approaches in two essential aspects.

(i) The derivation of the exact Dyson equation is carried out without using any *ad-hoc* irreducibility condition  $\lambda = \langle [I_k, S_q^-] \rangle = 0$ . Since  $\lambda$  depends on the incoming and the outgoing momentum lines and since it does not depend on the internal momentum index  $k'$ , the equation of motion reduces, in a natural way, to the exact Dyson equation.

(ii) The self-energy appearing in the Dyson equation contains a Green function of irreducible operators. For decoupling this type of Green function, we perform a mapping

of the reducible operator  $A_r$  onto the irreducible operator  $A_{ir}$  in the form  $A_r = LA_{ir}$ ,  $L$  being a scale factor depending on spin. This type of mapping is analogous to the Holstein-Primakoff transformation of the spin operator (reducible) to the boson (irreducible) operator. However, we have no knowledge at present of the explicit form of the spin-dependent scale factor  $L$  and so we had to introduce parameter  $\xi$  into the estimation of self-energy. Since we have considerable knowledge about the accurate values of the Curie temperature from the exact series expansion analysis we found the values of  $\xi$  in a straightforward way. In future investigations we shall attempt to devise a procedure for determining the values of  $\xi$  in a fundamental way.

Furthermore, we would like to draw attention to the earlier work of Chakraborty (1988, 1989) where in fact the commutator average was assumed to vanish, not to enable calculation of the arbitrary parameters, but rather to enable one to recast the equation of motion in the Dyson form. That assumption has been found here to be unnecessary. Furthermore in those studies the IRG appearing in the self-energy operator were simply decoupled by the RPA, i.e. in the light of the present theory the parameter  $\xi$  had been assumed to be unity. This is quantitatively erroneous. However, since no exact high-temperature expansion for a biquadratic coupling ferromagnet is available, the estimation of  $\xi$  cannot be made as is done in the present paper.

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