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1989 J. Phys.: Condens. Matter 1 2691

(http://iopscience.iop.org/0953-8984/1/16/005)

J. Phys.: Condens. Matter 1 (1989) 2691–2701. Printed in the UK

Irreducible Green function theory for a biquadratic coupling system

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Received 23 March 1988, in final form 17 August 1988

Abstract. A Heisenberg ferromagnet with biquadratic exchange and single-ion anisotropy is studied by the irreducible Green function formalism. Equations of motion for different Green functions are solved by means of irreducible operators and the exact matrix Dyson equation is derived. The low-temperature results for spin-wave damping and energy shift are discussed. It is found that the spin-wave modes in the quadrupolar state of the system disappear under certain conditions. The expressions for such modes are also found. The variation of Curie temperature with respect to the strength of the biquadratic exchange and single-ion anisotropy is also studied.

1. Introduction

Theoretical investigations carried out over the past few decades have clearly revealed our inability to perform exact calculations of the statistical mechanical properties of quantum spin models, like Heisenberg models. Even those methods which can provide the best estimates of various thermodynamic properties of some Ising models are not comfortably applicable to the Heisenberg models. If the Heisenberg Hamiltonian contains biquadratic exchange and single-ion anisotropy, the problem becomes much more complicated. To date, no attempts have been made to treat such problems by a high-temperature series expansion technique, a renormalisation group formalism and a Monte Carlo simulation method. It is believed that by these methods it is possible to get the best estimates for statistical quantities of any system. However, it is also possible, in principle, to achieve systematically a reasonably accurate solution of the problem by means of a diagrammatic perturbation formalism. But such calculations for a biquadratic exchange system are extremely complicated and have not been carried out successfully. Some low-temperature results were obtained by Westwansky and Skrobis (1977). The diagram technique they proposed is based on a Wick-like reduction theorem for the standard basis operators. This Wick-like reduction theorem uses the priority principle of Yang and Wang (1975) which leads to ambiguous results in several cases. This difficulty was faced by Chakraborty and Tucker (1987) in evaluating the higher-order semi-invariants while calculating the high-temperature contributions to the self-energy for a Heisenberg model with spin–phonon coupling. Also, it is now generally felt that the use of standard basis operators for developing a diagrammatic theory complicates the problem unnecessarily. Furthermore, Westwansky and Skrobis (1977) did not derive the high-temperature results and so in this sense their work may be regarded as incomplete. The extension of their work to high temperatures is extremely complicated and seems to be intractable. However, a Heisenberg model can be conveniently studied by yet another method, commonly known as the irreducible Green function (IRG) formalism, first introduced by Plakida (1971, 1973) and employed by other authors to study specific problems (Kuzmensky 1978, Marvakov *et al* 1985, Chakraborty 1988). The purpose of the present paper is to employ the IRG formalism to study a Heisenberg ferromagnet with biquadratic exchange and single-ion anisotropy, at all temperatures. We consider a system of spins ($S=1$) arranged over a translationally invariant 3D lattice and governed by the following Hamiltonian

$$H=-\omega_0\sum_i S_i^z - D\sum_i (S_i^z)^2 - \sum_{ij} J_{ij}[(\boldsymbol{S}_i\cdot\boldsymbol{S}_j)+\alpha(\boldsymbol{S}_i\cdot\boldsymbol{S}_j)^2] \tag{1}$$

where $\omega_0=g\mu_B H_a$, g being the Landé splitting factor, μ_B the Bohr magneton, H_a the external magnetic field, D the strength of the single-ion anisotropy, J_{ij} the bilinear exchange integral and α the biquadratic exchange parameter defined by the ratio of the biquadratic exchange to bilinear exchange. A special case of the model ($D=0$) was studied elaborately in the past using the constant-coupling approximation (Brown 1971) and molecular-field approximation (MFA) (Nauciel-Bloch *et al* 1972). The Green function equation-of-motion method with various decoupling procedures was also attempted (Chakraborty 1976, 1977, Munro and Girardeau 1976, Adler *et al* 1976, Adler and Oitmaa 1979, Micnas 1976, Kumar and Sharma 1977, Stewart and Adler 1980, Tiwari and Srivastava 1980). The results obtained from all these calculations differ quantitatively, sometimes qualitatively. In addition to this, the so-called redundancy problem of Murao and Matsubara (1968) prevailing in these calculations render the results doubtful.

2. Equation of motion for the Green functions and irreducible operators

We define the two-time temperature-dependent retarded Green function $\langle\langle A;B\rangle\rangle$ by

$$\langle\langle A;B\rangle\rangle = -\mathrm{i}\theta(t-t')\langle[A(t),B(t')]\rangle \tag{2}$$

where A, B are spin operators, $\theta(x)$ is a step function, t and t' being the time variables. Differentiating with respect to the first time t and taking the time–Fourier transform we can write the equation of motion for the Green function as

$$\omega\langle\langle A;B\rangle\rangle_\omega = (\langle[A,B]\rangle)/(2\pi) + \langle\langle[A,H];B\rangle\rangle \tag{3}$$

where we put $\hbar=1$. Hereafter we omit the suffix ω.

In the present problem we have four independent Green functions, $\langle\langle S_f^+;S_g^-\rangle\rangle$, $\langle\langle \sigma_f^+;S_g^-\rangle\rangle$, $\langle\langle S_f^+;\sigma_g^-\rangle\rangle$, $\langle\langle \sigma_f^+;\sigma_g^-\rangle\rangle$, where f and g are lattice sites and

$$\sigma_f^\pm = S_f^z S_f^\pm + S_f^\pm S_f^z. \tag{4}$$

Using (3) and the Fourier transforms

$$S_i^z = (1/\sqrt{N})\sum_k S_k^z \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}) \tag{5a}$$

$$S_i^\pm = (1/\sqrt{N})\sum_k S_k^\pm \exp(\mp\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}) \tag{5b}$$

$$J_{ij} = (1/N) \sum_k J_k \exp[-\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{R}_i - \boldsymbol{R}_j)] \tag{5c}$$

we arrive at the following equations for the spin-1 case:

$$\begin{aligned}(\omega - \omega_0)\langle\langle S_k^+ ; S_{q'}^- \rangle\rangle = {} & \langle S_{k-q'}^z \rangle/\pi N^{1/2} + D\langle\langle \sigma_k^+ ; S_{q'}^- \rangle\rangle \\ & + (2/N^{1/2})(1 - \tfrac{1}{2}\alpha) \sum_{k'} J_{k'} \langle\langle (S_{k'}^z S_{k-k'}^+ - S_{k-k'}^z S_{k'}^+); S_{q'}^- \rangle\rangle \\ & + (\alpha/N^{1/2}) \sum_{k'} J_{k'} \langle\langle (\lambda_{k'} \sigma_{k-k'}^+ - \sigma_{k'}^+ \lambda_{k-k'}); S_{q'}^- \rangle\rangle \end{aligned} \tag{6a}$$

$$\begin{aligned}(\omega - \omega_0)\langle\langle \sigma_k^+ ; S_{q'}^- \rangle\rangle = {} & \langle \lambda_{k-q'} \rangle/\pi N^{1/2} + (D + \tfrac{8}{3}\alpha J_0)\langle\langle S_k^+ ; S_{q'}^- \rangle\rangle + (2/N^{1/2})(1 - \tfrac{3}{2}\alpha) \\ & \times \sum_{k'} J_{k'} \langle\langle (S_{k'}^z \sigma_{k-k'}^+ - [\tfrac{1}{2}\alpha/(1 - \tfrac{3}{2}\alpha)] S_{k-k'}^z); S_{q'}^- \rangle\rangle - (2/N^{1/2})(1 - \tfrac{1}{2}\alpha) \\ & \times \sum_{k'} J_{k'} \langle\langle (\lambda_{k-k'} S_{k'}^+ - [\tfrac{1}{6}\alpha/(1 - \tfrac{1}{2}\alpha)] \lambda_{k'} S_{k-k'}^+); S_{q'}^- \rangle\rangle \end{aligned} \tag{6b}$$

$$\begin{aligned}(\omega - \omega_0)\langle\langle S_k^+ ; \sigma_{q'}^- \rangle\rangle = {} & \langle \lambda_{k-q'} \rangle/\pi N^{1/2} + D\langle\langle \sigma_k^+ ; \sigma_{q'}^- \rangle\rangle \\ & + (2/N^{1/2})(1 - \tfrac{1}{2}\alpha) \sum_{k'} J_{k'} \langle\langle (S_{k'}^z S_{k-k'}^+ - S_{k-k'}^z S_{k'}^+); \sigma_{q'}^- \rangle\rangle \\ & + (\alpha/N^{1/2}) \sum_{k'} J_{k'} \langle\langle (\lambda_{k'} \sigma_{k-k'}^+ - \lambda_{k-k'} \sigma_{k'}^+); \sigma_{q'}^- \rangle\rangle \end{aligned} \tag{6c}$$

$$\begin{aligned}(\omega - \omega_0)\langle\langle \sigma_k^+ ; \sigma_{q'}^- \rangle\rangle = {} & \langle S_{k-q'}^z \rangle/\pi N^{1/2} + (D + \tfrac{8}{3}\alpha J_0)\langle\langle S_k^+ ; \sigma_{q'}^- \rangle\rangle + (2/N^{1/2})(1 - \tfrac{3}{2}\alpha) \\ & \times \sum_{k'} J_{k'} \langle\langle (S_{k'}^z \sigma_{k-k'}^+ - [\tfrac{1}{2}\alpha/(1 - \tfrac{3}{2}\alpha)] S_{k-k'}^z \sigma_{k'}^+); \sigma_{q'}^- \rangle\rangle - (2/N^{1/2})(1 - \tfrac{1}{2}\alpha) \\ & \times \sum_{k'} J_{k'} \langle\langle (\lambda_{k-k'} S_{k'}^+ - [\tfrac{1}{6}\alpha/(1 - \tfrac{1}{2}\alpha)] \lambda_{k'} S_{k-k'}^+); \sigma_{q'}^- \rangle\rangle. \end{aligned} \tag{6d}$$

Each of the above four equations is a non-linear one containing higher-order Green functions on the right-hand side. These equations are usually linearised by means of decoupling approximations. In the IRG formalism this procedure is avoided. In the present paper the mean-field contributions are extracted out and the rest is kept accumulated in irreducible operators. Here we introduce the following irreducible operators $\varphi_1, \varphi_2, \varphi_3, \varphi_4$ defined by

$$\begin{aligned} \varphi_1 &= (S_{k'}^z S_{k-k'}^+ - S_{k-k'}^z S_{k'}^+)^{\mathrm{ir}} \\ \varphi_2 &= (\lambda_{k'} \sigma_{k-k'}^+ - \lambda_{k-k'} \sigma_{k'}^+)^{\mathrm{ir}} \\ \varphi_3 &= (S_{k'}^z \sigma_{k-k'}^+ - [\tfrac{1}{2}\alpha/(1 - \tfrac{3}{2}\alpha)] S_{k-k'}^z \sigma_{k'}^+)^{\mathrm{ir}} \\ \varphi_4 &= (\lambda_{k-k'} S_{k'}^+ - [\tfrac{1}{6}\alpha/(1 - \tfrac{1}{2}\alpha)] \lambda_{k'} S_{k-k'}^+)^{\mathrm{ir}} \end{aligned} \tag{7}$$

such that

$$(S_{k'}^z)^{\mathrm{ir}} = S_{k'}^z - bN^{1/2}\delta_{k'} \qquad b = \langle S^z \rangle.$$

The above operators satisfy the following conditions:

$$\langle [\varphi_f, S_g^-] \rangle = 0 \qquad \langle [\varphi_f, \sigma_g^-] \rangle = 0. \tag{8}$$

With the use of (7), equations (6) can be simplified. For example, from φ_1 we get using (8)

$$\langle\langle (S^z_{k'}S^+_{k-k'} - S^z_{k-k'}S^+_{k'}); X\rangle\rangle = \langle\langle \varphi_1 + bN^{1/2}(\delta_{k'}S^+_{k-k'} + \delta_{k-k'}S^+_{k'}); X\rangle\rangle. \tag{9}$$

Similarly from φ_2 and φ_3 the higher-order Green functions appearing on the right-hand sides of equations (6) are simplified in the above manner. The new equations of motion now consist of the Green function like $\langle\langle\varphi; x\rangle\rangle$ in addition to other two-spin Green functions representing the mean-field contributions. After simplifications we can express these equations in the following forms:

$$[\omega - \omega_0 - 2b(1-\tfrac{1}{2}\alpha)(J_0 - J_k)]\langle\langle S^+_k; S^-_{q'}\rangle\rangle = (b/\pi)\delta_{k-q'} + D_1\langle\langle\sigma^+_k; S^-_{q'}\rangle\rangle + (2/N^{1/2})\sum_{k'} J_{k'}\langle\langle[(1-\tfrac{1}{2}\alpha)\varphi_1 + \tfrac{1}{2}\alpha\varphi_2]; S^-_{q'}\rangle\rangle \tag{10}$$

$$\{\omega - \omega_0 - 2b[(1-\tfrac{3}{2}\alpha)J_0 - \tfrac{1}{2}\alpha J_k]\}\langle\langle\sigma^+_k; S^-_{q'}\rangle\rangle = (\lambda/\pi)\delta_{k-q'} + D_2\langle\langle S^+_k; S^-_{q'}\rangle\rangle + (2/N^{1/2})\sum_{k'} J_{k'}\langle\langle[(1-\tfrac{3}{2}\alpha)\varphi_3 - (1-\tfrac{1}{2}\alpha)\varphi_4]; S^-_{q'}\rangle\rangle \tag{11}$$

$$[\omega - \omega_0 - 2b(1-\tfrac{1}{2}\alpha)(J_0 - J_k)]\langle\langle S^+_k; \sigma^-_{q'}\rangle\rangle = (\lambda/\pi)\delta_{k-q'} + D_1\langle\langle\sigma^+_k; \sigma^-_{q'}\rangle\rangle + (2/N^{1/2})\sum_{k'} J_{k'}\langle\langle[(1-\tfrac{1}{2}\alpha)\varphi_1 + \tfrac{1}{2}\alpha\varphi_2]; \sigma^-_{q'}\rangle\rangle \tag{12}$$

$$\{\omega - \omega_0 - 2b[(1-\tfrac{3}{2}\alpha)J_0 - \tfrac{1}{2}\alpha J_k]\}\langle\langle\sigma^+_k; \sigma^-_{q'}\rangle\rangle = (b/\pi)\delta_{k-q'} + D_2\langle\langle S^+_k; \sigma^-_{q'}\rangle\rangle + (2/N^{1/2})\sum_{k'} J_{k'}\langle\langle[(1-\tfrac{3}{2}\alpha)\varphi_3 - (1-\tfrac{1}{2}\alpha)\varphi_4]; \sigma^-_{q'}\rangle\rangle \tag{13}$$

with

$$D_1 = D + \alpha\lambda(J_0 - J_k) \qquad D_2 = D + \tfrac{8}{3}\alpha J_0 + 2\lambda[\tfrac{1}{6}\alpha J_0 - (1-\tfrac{1}{2}\alpha)J_k].$$

We now employ the Green function

$$\langle\langle\varphi_f; S^-_g\rangle\rangle = -\mathrm{i}\theta(t-t')\langle[\varphi_f(t), S^-_g(t')]\rangle \tag{14}$$

where φ_f is an irreducible expressed in terms of lattice sites. Differentiating with respect to the second time variable t' we get the equation of motion as

$$\omega\langle\langle\varphi_f; S^-_g\rangle\rangle = \langle\langle\varphi_f; [H, S^-_g]\rangle\rangle. \tag{15}$$

Similarly for $\langle\langle\varphi_f; \sigma^-_g\rangle\rangle$. Calculating the commutator and Fourier transforming to momentum space we arrive at

$$(\omega - \omega_0)\langle\langle\varphi_k; S^-_{q'}\rangle\rangle = D\langle\langle\varphi_k; \sigma^-_{k'}\rangle\rangle + (2/N^{1/2})(1-\tfrac{1}{2}\alpha)\sum_{k'} J_{k'}\langle\langle\varphi_k; (S^z_{k'}S^-_{k'+q'} - S^z_{k'-q'}S^-_{k'})\rangle\rangle + (\alpha/N^{1/2})\sum_{k'} J_{k'}\langle\langle\varphi_k; (\lambda_{k'}\sigma^-_{k'+q'} - \lambda_{k'-q'}\sigma^-_{k'})\rangle\rangle \tag{16}$$

$$(\omega - \omega_0)\langle\langle\varphi_k; \sigma^-_{q'}\rangle\rangle = (D + \tfrac{8}{3}\alpha J_0)\langle\langle\varphi_k; S^-_{q'}\rangle\rangle + (2/N^{1/2})(1-\tfrac{3}{2}\alpha) \times \sum_{k'} J_{k'}\langle\langle\varphi_k; S^z_{k'}\sigma^-_{k'+q'} - [\tfrac{1}{2}\alpha/(1-\tfrac{3}{2}\alpha)]S^z_{k'-q'}\sigma^-_{k'}\rangle\rangle - (2/N^{1/2})(1-\tfrac{1}{2}\alpha) \times \sum_{k'} J_{k'}\langle\langle\varphi_k; \lambda_{k'-q'}S^-_{k'} - [\tfrac{1}{6}\alpha/(1-\tfrac{1}{2}\alpha)]\lambda_{k'}S^-_{k'+q'}\rangle\rangle. \tag{17}$$

We now introduce the following irreducible operators

$$\begin{aligned}\psi_1 &= (S^z_{k''} S^-_{k''+q'} - S^z_{k''-q'} S^-_{k''})^{\mathrm{ir}}\\ \psi_2 &= (\lambda_{k''}\sigma^-_{k''+q'} - \lambda_{k''-q'}\sigma^-_{k''})^{\mathrm{ir}}\\ \psi_3 &= (S^z_{k''}\sigma^-_{k''+q'} - [\tfrac{1}{2}\alpha/(1-\tfrac{3}{2}\alpha)] S^z_{k''-q'}\sigma^-_{k''})^{\mathrm{ir}}\\ \psi_4 &= (\lambda_{k''-q'} S^-_{k''} - [\tfrac{1}{6}\alpha/(1-\tfrac{1}{2}\alpha)]\lambda_{k''} S^-_{k''+q'})^{\mathrm{ir}}.\end{aligned} \tag{18}$$

Using (18) in (16) and (17) we get

$$[\omega - \omega_0 - 2b(1-\tfrac{1}{2}\alpha)(J_0 - J_{q'})]\langle\langle \varphi_k; S^-_{q'}\rangle\rangle$$
$$= D_1\langle\langle \varphi_k; \sigma^-_{q'}\rangle\rangle + (2/N^{1/2})\sum_{k'} J_{k'}\langle\langle \varphi_k; (1-\tfrac{1}{2}\alpha)\psi_1 + \tfrac{1}{2}\alpha\psi_2\rangle\rangle \tag{19}$$

$$\{\omega - \omega_0 - 2b[(1-\tfrac{3}{2}\alpha)J_0 - \tfrac{1}{2}\alpha J_{q'}]\}\langle\langle \varphi_k; \sigma^-_{q'}\rangle\rangle$$
$$= D_2\langle\langle \varphi_k; S^-_{q'}\rangle\rangle + (2/N^{1/2})\sum_{k'} J_{k'}\langle\langle \varphi_k; (1-\tfrac{3}{2}\alpha)\psi_3 - (1-\tfrac{1}{2}\alpha)\psi_4\rangle\rangle. \tag{20}$$

Solving the above two equations we can express the Green functions $\langle\langle \varphi_k; S^-_{q'}\rangle\rangle$ and $\langle\langle \varphi_k; \sigma^-_{q'}\rangle\rangle$ in the following forms:

$$\langle\langle \varphi_k; S^-_{q'}\rangle\rangle = (2/N^{1/2})\sum_{k'} EJ_{k'}\langle\langle \varphi_k; \{\omega - \omega_0 - 2b[(1-\tfrac{3}{2}\alpha)J_0 - \tfrac{1}{2}\alpha J_{q'}]$$
$$\times [(1-\tfrac{1}{2}\alpha)\psi_1 + \tfrac{1}{2}\alpha\psi_2]\} + D_1[(1-\tfrac{3}{2}\alpha)\psi_3 - (1-\tfrac{1}{2}\alpha)\psi_4]\rangle\rangle \tag{21}$$

$$\langle\langle \varphi_k; \sigma^-_{q'}\rangle\rangle = (2/N^{1/2})\sum_{k'} EJ_{k'}\langle\langle \varphi_k; D_2[(1-\tfrac{1}{2}\alpha)\psi_1 + \tfrac{1}{2}\alpha\psi_2]$$
$$+ [\omega - \omega_0 - 2b(1-\tfrac{1}{2}\alpha)(J_0 - J_{q'})][(1-\tfrac{3}{2}\alpha)\psi_3 - (1-\tfrac{1}{2}\alpha)\psi_4]\rangle\rangle \tag{22}$$

where E is given by

$$E = [(\omega - \omega^+_{q'})(\omega - \omega^-_{q'})]^{-1}. \tag{23}$$

Utilising equations (21) and (22) we can express equations (10)–(13), after some rearrangements, in the form of a matrix Dyson equation. This is

$$\mathbf{G} = \mathbf{G}^0 + \mathbf{G}^0\mathbf{P}\mathbf{G}^0 \tag{24}$$

where

$$\begin{aligned}G_1 &= \langle\langle S^+_k; S^-_{q'}\rangle\rangle_\omega\\ G_2 &= \langle\langle \sigma^+_k; S^-_{q'}\rangle\rangle_\omega\\ G_3 &= \langle\langle S^+_k; \sigma^-_{q'}\rangle\rangle_\omega\\ G_4 &= \langle\langle \sigma^+_k; \sigma^-_{q'}\rangle\rangle_\omega.\end{aligned} \tag{25}$$

The G_i^0 may be called the mean-field Green functions given by

$$
\begin{aligned}
G_1^0 &= \frac{b\{\omega - \omega_0 - 2b[(1-\frac{3}{2}\alpha)J_0 - \frac{1}{2}\alpha J_k]\} + \lambda D_1}{\pi(\omega - \omega_k^+)(\omega - \omega_k^-)} \\
G_2^0 &= \frac{\lambda[\omega - \omega_0 - 2b(1-\frac{1}{2}\alpha)(J_0 - J_k)] + bD_2}{\pi(\omega - \omega_k^+)(\omega - \omega_k^-)} \\
G_3^0 &= \frac{\lambda\{\omega - \omega_0 - 2b[(1-\frac{3}{2}\alpha)J_0 - \frac{1}{2}\alpha J_k]\} + bD_1}{\pi(\omega - \omega_k^+)(\omega - \omega_k^-)} \\
G_4^0 &= \frac{b[\omega - \omega_0 - 2b(1-\frac{1}{2}\alpha)(J_0 - J_k)] + \lambda D_2}{\pi(\omega - \omega_k^+)(\omega - \omega_k^-)}.
\end{aligned}
\tag{26}
$$

The P are the polarisation operators given by

$$P_1 = \left(\frac{2\pi\{\omega - \omega_0 - 2b[(1-\frac{3}{2}\alpha)J_0 - \frac{1}{2}\alpha J_k]\}}{b\{\omega - \omega_0 - 2b[(1-\frac{3}{2}\alpha)J_0 - \frac{1}{2}\alpha J_k]\} + \lambda D_1}\right)^2 I_{k'k''} \tag{27}$$

$$P_2 = \frac{4D_2\pi^2\{\omega - \omega_0 - 2b[(1-\frac{3}{2}\alpha)J_0 - \frac{1}{2}\alpha J_k]\}}{\{bD_2 + \lambda[\omega - \omega_0 - 2b(1-\frac{1}{2}\alpha)(J_0 - J_k)]\}^2} I_{k'k''} \tag{28}$$

$$P_3 = \frac{4D_2\pi^2\{\omega - \omega_0 - 2b[(1-\frac{3}{2}\alpha)J_0 - \frac{1}{2}\alpha J_k]\}}{\{bD_1 + \lambda[\omega - \omega_0 - 2b((1-\frac{3}{2}\alpha)J_0 - \frac{1}{2}\alpha J_k)]\}^2} I_{k'k''} \tag{29}$$

$$P_4 = \left(\frac{2\pi D_2}{\lambda D_2 + b[\omega - \omega_0 - 2b(1-\frac{1}{2}\alpha)(J_0 - J_k)]}\right)^2 I_{k'k''} \tag{30}$$

where

$$
\begin{aligned}
I_{k'k''} = (1/N)\sum_{k'k''} J_{k'}J_{k''}\langle\langle &[(1-\tfrac{1}{2}\alpha)\varphi_1 + \tfrac{1}{2}\alpha\varphi_2] + y[(1-\tfrac{3}{2}\alpha)\varphi_3 - (1-\tfrac{1}{2}\alpha)\varphi_4]; \\
&[(1-\tfrac{1}{2}\alpha)\psi_1 + \tfrac{1}{2}\alpha\psi_2] + y[(1-\tfrac{3}{2}\alpha)\psi_3 - (1-\tfrac{1}{2}\alpha)\psi_4]\rangle\rangle
\end{aligned}
\tag{31}
$$

with

$$y = D_1/\{\omega - \omega_0 - 2b[(1-\tfrac{3}{2}\alpha)J_0 - \tfrac{1}{2}\alpha J_k]\}. \tag{32}$$

$\omega_k^\pm$ determine the energy spectra of the system given by

$$\omega_k^\pm = \omega_0 + b[2(1-\alpha)J_0 - J_k] \pm M(k) \tag{33}$$

with

$$M(k) = \{b^2[\alpha J_0 - (1-\alpha)J_k]^2 + D_1D_2\}^{1/2}. \tag{34}$$

In the absence of biquadratic exchange, (33) reduces to the form:

$$\omega_k^\pm = \omega_0 + 2bJ_0 - bJ_k \pm [b^2J_k^2 + D(D - 2\lambda J_k)]^{1/2}. \tag{35}$$

3. Low-temperature properties

Equation (23) can be expressed as the exact Dyson equation

$$\mathbf{G} = \mathbf{G}^0 + \mathbf{G}^0\Sigma\mathbf{G}$$

where Σ is the self-energy operator given by $\Sigma = (P)^c$, c denoting the connected or proper part. Assuming that the approximate poles of G are at $\omega_k^{\mp} + \mathrm{i}\varepsilon$, $\varepsilon \to 0$ we can write

$$G_m(k, \omega) = \frac{A_m^+}{\omega - E_m^+(k)} + \frac{A_m^-}{\omega - E_m^-(k)} \tag{36}$$

where $E_m(k)$ stand for the renormalised energy given by

$$E_m^{\pm}(k) = \omega_k^{\pm} + A_m^{\pm}\Sigma_m(k, \omega_k^{\pm} + \mathrm{i}\varepsilon) \tag{37}$$

with $m = 1, 2, 3, 4$ and

$$A_1^{\mp} = [2\pi M(k)]^{-1}\{b[\omega_k^{\mp} - \omega_0 - 2b((1 - \tfrac{3}{2}\alpha)J_0 - \tfrac{1}{2}\alpha J_k)] + \lambda D_1\} \tag{38a}$$

$$A_2^{\mp} = [2\pi M(k)]^{-1}\{b[\omega_k^{\mp} - \omega_0 - 2b((1 - \tfrac{1}{2}\alpha)(J_0 - J_k))] + \lambda D_2\} \tag{38b}$$

$$A_3^{\mp} = [2\pi M(k)]^{-1}\{bD_2 + \lambda[\omega_k^{\mp} - \omega_0 - 2b(1 - \tfrac{1}{2}\alpha)(J_0 - J_k)]\} \tag{39a}$$

$$A_4^{\mp} = [2\pi M(k)]^{-1}\{bD_1 + \lambda[\omega_k^{\mp} - \omega_0 - 2b((1 - \tfrac{3}{2}\alpha)J_0 - \tfrac{1}{2}\alpha J_k)]\}. \tag{39b}$$

The spin-wave energy shift and spin-wave damping Γ_k are given by

$$\Delta\omega_k^{\mp}(m) - \mathrm{i}\Gamma_k^{\mp}(m) = A_m^{\mp}\Sigma_m(k, \omega_k^{\mp} + \mathrm{i}\varepsilon). \tag{40}$$

Exact calculation of the energy shift, spin-wave damping and other physical properties of the model is extremely difficult, perhaps impossible at this stage. However, the ground-state properties can be estimated exactly and some low-temperature results can be calculated comfortably. We shall confine our attention to finding out the effects of biquadratic exchange on the energy shift and spin-wave damping. First, we discuss some interesting features of the dispersion relation.

At low temperatures, when $\lambda \simeq b$, one can write the dispersion relation

$$\omega_k^{\mp} = \omega_0 + b[2(1 - \alpha)J_0 - J_k] \pm \{D^2 + \tfrac{4}{3}\alpha J_0(2 + b)(D + \alpha b J_0) - 2bJ_k[D + \alpha J_0(1 + b) + \tfrac{1}{3}\alpha^2 J_0(1 - b)] + b^2 J_k^2\}^{1/2}. \tag{41}$$

For $\alpha = 0$, the term within the square root becomes a perfect square and we get

$$\omega_k^{\mp} = \omega_0 + b(2J_0 - J_k) \pm (D - bJ_k). \tag{42}$$

ω_k^- is k-independent and hence we may ignore this excitation. But if $\alpha \neq 0$ the term within the square root does not become a perfect square and both the modes are k-dependent. However, at sufficiently low temperatures such that $\lambda \simeq b \simeq 1$, one will find

$$\omega_k^+ = \omega_0 + 2(J_0 - J_k) + D \tag{43}$$

$$\omega_k^- = \omega_0 + 2J_0(1 - 2\alpha) - D. \tag{44}$$

ω_k^- is again k-independent and ω_k^+ is the same as that in the absence of biquadratic exchange. In such a case

$$G_1^0 = G_2^0 = G_3^0 = G_4^0 = G^0(k) = (1/\pi)/[\omega - \omega_0 + D - 2(J_0 - J_k)] \tag{45}$$

which is α-independent. At $T = 0$, the exact energy spectra are

$$\omega_k^+ = \omega_0 + D \qquad \omega_k^- = \omega_0 - D + 2J_0(1 - 2\alpha). \tag{46}$$

Equation (45) shows that the resonance frequency is independent of biquadratic exchange. The expressions for energy shift and spin-wave damping can easily be found to be

$$\Delta\omega_k^+ = (4\pi/N)\sum_{k'} \frac{(J_{k'} - J_{k+k'})^2}{J_{k-k'} - J_k} \langle S_{k'}^z S_{k'}^z \rangle \tag{47}$$

$$\Gamma_k^+ = (4\pi^2/N)\sum_{k'} (J_{k'} - J_{k+k'})^2 \langle S_k^z S_{k'}^z \rangle \delta(J_{k-k'} - J_k). \tag{48}$$

Γ_0^+, which is related to resonance linewidth, is thus zero.

It was observed by Westwansky and Skrobis (1977) that for a biquadratic coupling system two different low-temperature states should be distinguished: one is the ferromagnetic state ($b = \lambda = 1$) and the other is the quadrupolar state ($b = 0, \lambda = -2$). Consequently, (43) and (44) refer to the spin waves in the ferromagnetic state. For the quadrupolar state we have

$$\omega_k^2/J_0 = [\alpha' - 2\alpha(J_k/J_0)][\alpha' + 2\alpha + 4(1 - \tfrac{1}{2}\alpha)(J_k/J_0)] \tag{49}$$

where the parameter α' stands for D/J_0. In the absence of single-ion anisotropy ($\alpha' = 0$) the spin-wave modes in the quadrupolar state vanish for $k = 0$ and thus the Goldstone theorem is satisfied. Furthermore, it is interesting to note that the spin-wave excitations also disappear even for $k \neq 0$ if the following condition is satisfied:

$$\alpha' = \alpha_c' = 2\alpha[1 - (J_k/J_0)]. \tag{50}$$

This condition is exactly identical with the condition obtained from equation (33) of the paper of Westwansky and Skrobis (1977). Equation (49) also shows that the spin-wave modes in the quadrupolar state are not possible for $\alpha' < \alpha_c'$. Since in all real systems the biquadratic exchange is, in general, believed to be much smaller than the single-ion anisotropy, one may expect that the above kinds of modes may be easily detected.

4. Results for Curie temperature

In this section we shall calculate some approximate results for Curie temperature. The use of the spectral theorem yields the following approximate relations for a weakly interacting system:

$$\tfrac{4}{3} - b - \lambda/3 = 2\pi N^{-1} \sum_k (A_m^+ n_m^+ + A_m^- n_m^-) \tag{51}$$

$$b - \lambda = 2\pi N^{-1} \sum_k (A_r^+ n_r^+ - A_r^- n_r^-) \tag{52}$$

with $m = 1, 4$, $r = 2, 3$ and $n_x^\pm = [\exp(\beta E_x^\pm) - 1]^{-1}$. The above equations contain four equivalent sets of identities. One can calculate the physical properties of the model from just one of these four sets. We choose here the set for $m = 1$, $r = 2$. For this we need to calculate $I_{k'k''}(\omega)$ from

$$I_{k'k''}(\omega) = \frac{1}{N}\sum_{k'k''} J_{k'}J_{k''}\frac{1}{2\pi}\int \frac{\mathrm{d}\omega'}{\omega-\omega'}(\mathrm{e}^{\beta\omega'}-1)\int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega' t} I_{k'k''}(t) \tag{53}$$

with $\beta = (k_B T)^{-1}$, k_B being the Boltzmann constant. Using a decoupling of the form

$$\langle \lambda_{k''-q'} S^-_{\bar{k}''} S^z_{k'}(t) S^+_{k-k'}(t)\rangle \sim \langle \lambda_{k''-q'} S^z_{k}(t)\rangle\langle S^-_{\bar{k}''} S^+_{k-k'}(t)\rangle \tag{54}$$

and approximating the right-hand side as

$$\langle \lambda_{k'} S^z_{k'}\rangle\langle S^-_{\bar{k}+k'} S^+_{k-k'}(t)\rangle \delta_{k'',k'+q'}$$

and replacing G by G^0 we can calculate $I_{k'k''}(\omega)$, which is then used to calculate the self-energy. Finally, taking the limit $b \to 0$, and using $\lambda/b \simeq 0$, we get for $\omega_0 = 0$, the following equations determining the Curie temperature:

$$(4-\lambda)/3 = U_\alpha(\beta_C) + W^\alpha_1(\beta_C) \tag{55}$$

$$1 = U_\alpha(\beta_C) - \lambda V_\alpha(\beta_C) + W^\alpha_2(\beta_C) \tag{56}$$

where

$$U_\alpha(\beta_C) = (1/N)\sum_k [D/M_0(k)]\coth[\tfrac{1}{2}\beta_C M_0(k)] \tag{57}$$

$$V_\alpha(\beta_C) = (1/N)\sum_k \{[J_0/M_0(k)]\coth[\tfrac{1}{2}\beta_C M_0(k)] + aL\} \tag{58}$$

$$W^\alpha_1(\beta_C) = (1/N)\sum_k \{[\alpha\lambda^2(J_0-J_k)/M_0(k)]\coth[\tfrac{1}{2}\beta_C M_0(k)] + \lambda L(D_1 f_1 + D_2 f_2)\} \tag{59}$$

$$W^\alpha_2(\beta_C) = (1/N)\sum_k [\tfrac{2}{3}\alpha J_0(4-\lambda)/M_0(k)]\coth[\tfrac{1}{2}\beta_C M_0(k)] + [LD_2/M^4_0(k)] \times \{2[D-\lambda J_k] + \tfrac{2}{3}\alpha J_0(4-\lambda)(D_1 f_1 + D_2 f_2) - M^2_0(k)(f_1+f_2)\} \tag{60}$$

with

$$a = 4(1-\alpha)J_0 - 2J_k \qquad L = \beta_C E/(E-1)^2 \qquad E = \exp[\beta_C M_0(k)]$$

$$f_1 = \langle (S^z)^2\rangle (1-\tfrac{1}{2}\alpha)^2 (J_0 - J_k)^2 + [\lambda^2 D_1^2/M_0^2(k)][\tfrac{1}{8}\alpha J_0 - (1-\tfrac{1}{2}\alpha)J_k]$$

$$f_2 = \tfrac{1}{4}\alpha^2\lambda^2(J_0-J_k)^2 + \{\langle (S^z)^2\rangle D_1^2[(1-\tfrac{3}{4}\alpha)J_0 - \tfrac{1}{2}\alpha J_k]^2\}/M_0^2(k).$$

We assume that α' is much greater than α. Considering the MFA result as the first step of iteration, we can solve (55) and (56). The result may be written down in the following simplified form:

$$XK_C^2 + YK_C + Z = 0 \tag{61}$$

where

$$K_C = \beta_C J \qquad \beta_C = (k_B T_C)^{-1}$$

$$X = [2P^2 W(1-\alpha)]/(\nu\alpha' Q)$$

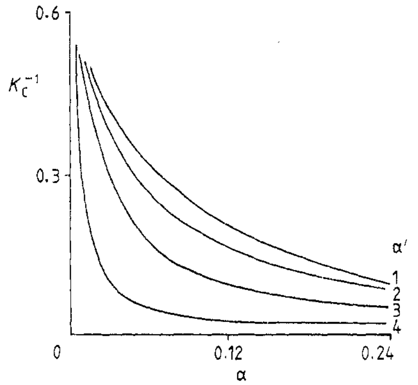

Figure 1. The variation of K_C^{-1} with respect to α for several values of α'.

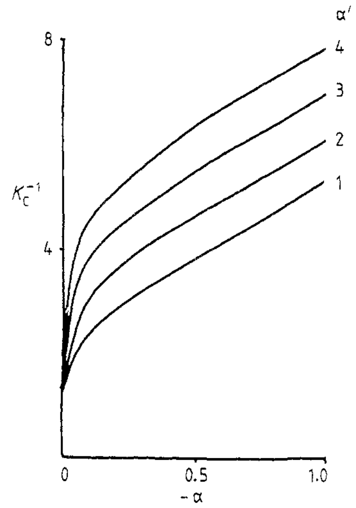

Figure 2. The variation of K_C^{-1} against negative α for several values of α'.

$$Y = 4P\{1 - \alpha + [L(2MW - V)/(8\alpha' Q)]\}$$
$$Z = -\nu FP - (\tfrac{1}{2} + \tfrac{1}{4}Q)[(8\alpha)/(3\alpha')](1 + \nu P)$$

with

$$P = 1 - (2/\nu) \qquad Q = 1 - (3/\nu) \qquad \nu = 2 + \exp(-\beta_C D)$$

and

$$M = 1 + (2Q/\alpha') + (1 + \tfrac{1}{2}Q)[(8\alpha)/(3\alpha')]$$
$$V = 4Q^2(1 - \tfrac{2}{3}\alpha)^2 + \tfrac{2}{3}(1 - Q)(1 - 2\alpha)^2$$
$$W = 4Q^2(1 - \tfrac{2}{3}\alpha)^2 + \tfrac{2}{3}(1 - Q)(1 - 2\alpha)^2 R$$
$$R = 1 + [(8\alpha)/(3\alpha')] + (4Q/\alpha')(1 - \tfrac{2}{3}\alpha).$$

Equation (61) can easily be computed. The variation of Curie temperature T_C against α for several values of α' has been estimated for a simple cubic lattice ($z = 6$) and the results are summarised in figure 1. The results obtained in the present treatment are found to agree, in the first place, with those of the earlier Green function calculations, at least qualitatively. It is seen that the Curie temperature T_C decreases as the biquadratic coupling strength increases. But the results differ very much from a quantitative point of view. It may be noted that in the present calculation the Curie temperature is highly sensitive to very small values of α. As α is increased from zero to a very small value, T_C drops appreciably, but as α increases more, T_C gradually becomes more insensitive. Furthermore, it has also been found that there exists a critical value of α' beyond which the above equation for T_C has no solution. This critical value of α' depends on the strength of the single-ion anisotropy. For $\alpha' > 5$, there is no solution for T_C except at $\alpha = 0$. Since our approximation is based on large positive α' this result may be believed to be true. The solution of T_C is also obtained for negative α as shown in figure 2.

5. Conclusions

Calculations presented here on the basis of the irreducible Green function formalism have been found to yield results which are sometimes drastically different from the earlier conventional Green function theories. Such differences are caused primarily by the arbitrariness in so-called decoupling approximations. However, there are some limitations in carrying out the calculation of physical properties within the framework of irreducible Green function theory. For example, in the present paper it has not been possible to have systematic quantitative estimates for the thermal variation of magnetisation and quadrupolar ordering parameter. Although a rough estimate is possible on the basis of approximations of small b and λ and for large D, no consistent series can be obtained like one available, in principle, from a diagrammatic theory. This would become possible if one could express the self-energy systematically, say, in powers of $1/z$ or in powers of other physically accessible parameters. At present, such method of calculation is not available.

Acknowledgments

The author wishes to thank Dr J W Tucker, Department of Physics, University of Sheffield, for helpful discussions regarding the irreducible Green function formalism, during his stay in Sheffield.

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