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" SELF-CONSISTENT MANY BODY THEORY FOR STANDARD BASIS OPERATOR GREEN'S FUNCTION: AN APPLICATION TO ANISOTROPIC FERROMAGNETS"

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16.Summary/Notes

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ABSTRACT

A self-consistent many body theory developed by Fedro and Wilson and extended by Kishore is used to obtain exact Dyson type equation of the retarded Green's function for the standard basic operators. These Green's functions are used to obtain elementary excitations and thermodynamic properties of the Heisenberg ferromagnet with uniaxial anisotropy.

The equation of motion method using double time temperature dependent Green's functions has received widespread use in various approximations to predict the thermodynamics of condensed-matter systems. Nevertheless this method suffers from the lack of systematic procedure like diagram technique. To resolve this question it is possible to develop a variant of self-consistent many-body theory with exact Dyson type equation for the Green's functions (Fedro and Wilson, 1975; Kishore,R., 1979).

Here we consider the application of the self-consistent many-body theory for interacting many-level systems. The generalization of Fedro and Wilson (1975) projection operator technique can be done after Kishore (Kishore,R., 1979) in the following way. Let us consider a many-body system having m discrete levels. The thermodynamics of the system can be conveniently described by adapting the standard basis operator method (Hubbard, 1965; Haley and Erdös,P.,1972).

We define the Green's function (Hubbard,1965; Halley and Erdös, 1972)

$$G_{ij}^{\alpha\,\beta\,n}(\omega) = \langle\langle L^{i}_{\alpha\;\alpha+n} ; \; L^{j}_{\beta+n,\beta} \rangle\rangle \qquad \eta=-1 \tag{1}$$

where

$$\alpha + n \leqslant m \;, \quad \beta + n \leqslant m \tag{2}$$

$m \equiv$ total number of states in a complete set of states
$\alpha =$ 1, ... m-n
$\beta =$ 1, ... m-n

It should be noted that

$$[\, L^{i}_{\alpha,\alpha+n} \,,\, L^{j}_{\beta+n,\,\beta} \,] = (L^{i}_{\alpha,\alpha} - L^{i}_{\alpha+n,\,\alpha+n})\, \delta_{\alpha\beta}\delta_{ij} \tag{3}$$

By defining a projection operator

$$P_n = \sum_{i\alpha} P^n_{i\alpha} \tag{4}$$

$$P^n_{i\alpha}\,\chi = \frac{L^i_{\alpha+n,\alpha} < [L^i_{\alpha,\alpha+n},\chi] >}{<[L^i_{\alpha,\alpha+n}\;,\;L^i_{\alpha+n,\alpha}]>} \tag{5}$$

the self consistent many-body theory gives (Fedro and Wilson,1975; Kishore 1979)

$$\omega\, G^{\alpha\beta\;n}_{ij}(\omega) \;=\; (<L_{\alpha\alpha}>-<L^i_{\alpha+n,\;\alpha+n}>)\,\delta_{ij}\;\delta_{\alpha\beta} +$$

$$+ \sum_{\ell\gamma}\;(\Omega^{\alpha\gamma,n}_{i\ell} + \gamma^{\alpha\gamma\;n}_{i\ell}(\omega)G^{\gamma\beta\;n}_{\ell j}(\omega) \tag{6}$$

where

$$\Omega^{\alpha\gamma\;n}_{i\ell} = -\,\frac{<[L\;L^i_{\alpha,\alpha+n}\;,\;L^\ell_{\gamma+n,\gamma}]_->}{<[L^\ell_{\gamma,\gamma+n}\;,\;L^\ell_{\gamma+n,\gamma}]_->} \tag{7}$$

$$\gamma^{\alpha\gamma\;n}_{i\ell}\;(\omega) \;=\; \int \gamma^{\alpha\gamma\;n}_{i\ell}(t)\;e^{-i\omega t}\;dt \tag{8}$$

$$\gamma^{\alpha\gamma\;n}_{i\ell}(t) \;=\; \frac{-\Theta(t)<[L\;L^i_{\alpha,\alpha+n},e^{it(1-P_n)L}(1-P_n)L\;L^\ell_{\gamma+n,\gamma}]_->}{<\;[L^\ell_{\gamma,\gamma+n},\,L^\ell_{\gamma+n,\gamma}]_->} \tag{9}$$

$$LX \equiv [\;H,X\;]_- \tag{10}$$

For translationally invariant systems we can define Fourier transform like

$$f_{ij} = \frac{1}{N}\sum_k f_k\;e^{ik.\;(\bar{R}_i\;-\;\bar{R}_j)} \tag{11}$$

then (6) becomes

$$\omega\, G_k^{\alpha\beta\ n}(\omega) = (\langle L_{\alpha\alpha}\rangle - \langle L_{\alpha+n,\ \alpha+n}\rangle)\,\delta_{\alpha\beta} +$$
$$+ \sum_{\gamma} (\Omega_{\bar{k}}^{\alpha\gamma\ n} + \gamma_{\bar{k}}^{\alpha\gamma\ n}(\omega))\, G_k^{\gamma\beta\ n}(\omega) \tag{12}$$

In matrix form it can be rewritten as

$$(\omega\, I - B_k^n(\omega))\, G_k^n(\omega) = A^n \tag{13}$$

Where I is the unit matrix and the matrix element of B_k^n and A^n are

$$B_k^{\alpha\beta\ n}(\omega) = \Omega_{\bar{k}}^{\alpha\beta\ n} + \gamma_{\bar{k}}^{\alpha\beta\ n}(\omega) \tag{14}$$

and

$$A^{\alpha\beta\ n} = (\langle L_{\alpha\alpha}\rangle - \langle L_{\alpha+n,\ \alpha+n}\rangle)\delta_{\alpha\beta} \tag{15}$$

From the theory of linear equation, solution of (13) is

$$G_k^{\alpha\beta\ n}(\omega) = \frac{D_{k\alpha\beta}^n}{D_k^n} \tag{16}$$

Where D_k^n is the determinant

$$D_k^n = |\ \omega\, I - B_k^n(\omega)\ | \tag{17}$$

$$= \begin{vmatrix} \omega - B_k^{11\ n}(\omega) & B_k^{12\ n}(\omega) & \cdots & B_k^{1\ m-n\ n}(\omega) \\ B_k^{21\ n}(\omega) & \omega - B_k^{22\ n}(\omega) & \cdots & B_k^{2\ m-n\ n}(\omega) \\ \vdots & & & \\ B_k^{m-n,1\ n}(\omega) & B^{m-n,2;n}(\omega) & \cdots & \omega - B_k^{m-n,\ m-n;n}(\omega) \end{vmatrix} \tag{18}$$

and $D^n_{k\alpha\beta}$ is the determinant obtained from D^n_k by replacing its 2^{nd} column (containing coefficients)

$$[B_k^{1\alpha,n}(\omega) \quad \omega - B_k^{2\alpha,n}(\omega),\ B_k^{3\alpha,n}(\omega) \ \ldots \ B_k^{m-n\ \alpha\ n}(\omega)]$$

by the column of the members $A^{1\beta\ n}$, $A^{2\beta\ n}$ ... $A^{m-n,\beta;n}$

For example

$$D^n_{k\alpha\beta} = \begin{vmatrix} \omega - B_k^{11\ n}(\omega) & A^{1\beta\ n} & \ldots & B_k^{1\ m-n;n}(\omega) \\ B_k^{21\ n}(\omega) & A^{2\beta\ n} & \ldots & B^{2\ m-n;n}(\omega) \\ B_k^{m-n,1\ n}(\omega) & A^{m-n\beta;n} & \ldots & \omega - B_k^{m-n,\ m-n;\ n}(\omega) \end{vmatrix}$$

As a concrete application of the above general results we consider the Heisenberg ferromagnet in the presence of both exchange and single-ion anisotropy:

$$H = h \sum_i S_i^z - D \sum_i (S_i^z)^2 - \frac{1}{2} \sum_{ij} J_{ij}(S_i^x S_j^x + S_i^y S_i^y) - \frac{1}{2} \sum_{ij} K_{ij} S_i^z S_j^z \tag{19}$$

where h is the external magnetic field, D is the single-ion anisotropy and K_{ij} is the anisotropic exchange. The standard basis is taken as the molecular-field basis and is given by

$$|\alpha> = |S-\alpha+1> \quad \text{where} \quad \alpha = -S, \ldots, S \tag{20}$$

The spin operators are given by

$$S^+ = \sum_\alpha A_\alpha \ L_{\alpha,\alpha+1} \tag{21}$$

$$S^- = \sum_\alpha A_\alpha \ L_{\alpha+1,\alpha} \tag{22}$$

$$S^z = \sum_\alpha B_\alpha L_{\alpha\alpha} \tag{23}$$

Where

$$A_\alpha = | \alpha(2S- +1)|^{1/2} \tag{24}$$

$$B_\alpha = S-\alpha+1 \tag{25}$$

The off-diagonal standard basis operators cause the transitions between the molecular-field states and due to non-equal distance between these states one obtains several branches of the collective excitations. For example, for S=1, one has two magnon branches generated by the operators L^k_{12} and L^k_{23}, and one branch of excitations by L^k_{13}.

The Dyson equation for off-diagonal Green's functions is given quite generally by eq. (6). Since the results for arbitrary spin value are rather lengthy we present here only S=1 case. For $\Omega_k^{\alpha,n}$ we obtain

$$\Omega_k^{11,1} = h - J_k D_{12} + K_0 D_{13} + \frac{R^k_{11}}{D_{12}} + D \tag{26}$$

$$\Omega_k^{12,1} = -J_k D_{12} + \frac{R^k_{12}}{D_{23}} \tag{27}$$

$$\Omega_k^{21,1} = -J_k D_{23} + \frac{R^k_{21}}{D_{12}} \tag{28}$$

$$\Omega_k^{22,1} = h- J_k D_{23} + K_0 D_{13} + \frac{R^k_{22}}{D_{23}} - D \tag{29}$$

Where J_k is the Fourier transform of exchange integral

$$D_{\alpha\beta} = D_\alpha - D_\beta = \langle L_{\alpha\alpha}\rangle - \langle L_{\beta\beta}\rangle \tag{30}$$

and

$$K_0 = \sum_j K_{ij} \tag{31}$$

If we neglect in eqs. (26-29) $R^k_{\alpha\beta}$ contributions our results reduce to those obtained in the Random Phase Approximation (RPA) (Halley and Erdos, 1972). The quanities $R^k_{\alpha\beta}$ are expressed by the irreducible correlation functions of the standard basis operators and represent nontrivial contribution beyond RPA. The general expression for the collective excitations is given by

$$E^{\pm}_k = \frac{1}{2} (\Omega^{11,1}_k + \Omega^{22,1}_k) \pm \frac{1}{2} \Omega_k \tag{32}$$

where

$$\Omega_k = \left\{ (\Omega^{11,1}_k - \Omega^{22,1}_k)^2 + 4\Omega^{12,1}_k \Omega^{21,1}_k \right\}^{1/2} \tag{33}$$

The results obtained are close to those obtained recently by Yang and Wang by usiny the high-density expansion diagramatic technique (Yang and Wang, 1975). The contributions beyond RPA represent the scattering of spin waves on the longitudinal and transversal fluctuations of angular momenta.

In the low temperature limit the results are in agreement with those given by Kaschenko et al (1973). Also the low temperature renormalization of spin waves for the D=0, and K=J is predicted to be $T^{5/2}$ in agreement with Dyson theory (Dyson, 1956; Bloch, 1963).

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