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SELF-CONSISTENT MANY BODY THEORY FOR THE STANDARD BASIS OPERATOR GREEN'S FUNCTIONS

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ABSTRACT

We propose a self-consistent many body theory for the standard basis operator Green's functions and obtain an exact Dyson type matrix equation for the interacting many level systems. A zeroth order approximation, which neglects all the damping effects, is investigated in detail for the anisotropic Heisenberg model, the isotropic quadropolar system and the Hubbard model. In case of the anisotropic Heisenberg ferromagnet with both exchange and single-ion anisotropy the low-temperature renormalization of the spin-waves for the uniaxial ordering agrees with the Bloch-Dyson theory. For the spin-1 easy plane ferromagnet, the critical parameters for the phase transition at zero temperature are determined and compared with other theories. The elementary excitation spectrum of the spin-1 isotropic quadrupolar system is calculated and compared with the random phase approximation and Callen's like decoupling schemes. Finally, the theory is applied to the study of the single-particle excitation spectrum of the Hubbard model.

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1. INTRODUCTION

In the study of elementary excitations and thermodynamic proporties of the condensed matter systems, it is a commom practice to use the double-time temperature dependent Green's functions [1]. The equation of motion of these Green's functions leads to an infinite set of equations which couple the original Green's functions to the higher-order ones. Approximate solutions are obtained by decoupling of the higher-order Green's functions, at certain stage, to set up a closed system of equations for the original Green's functions The decoupling procedure suffers from the problem that one hardly knows an error involved in this procedure. The quality of such an approximation is often justified on physical intuition, by comparison with the theories wich are certainly valid for limited values of parameters or by comparison with the experiment.

Recently, it has been realized that it is possible to develop a systematic approach called the self-consistent many body theory to the double-time Green's function with an exact Dyson type equation [2,3]. The idea to derive a Dyson equation is a straightforward extension of the Zwanzig-Mori projection operator technique [4,5,6]. As it was previously discussed, this theory ensures the self-consistent results in every order of perturbation, [2,3]. The self-consistent may-body theory (SMT) has already been applied to the study of single-particle and spin-wave excitations in the itinerant electron systems [2,3,7]. An essentially equivalent approach called the irreducible Green's function method has also been independently developed and applied to the localized electron systems [8-10].

In this paper, we apply the SMT to the study of the elementary excitations in the interacting many level systems, using the standard basis operator (SBO) Green's functions, originally introduced by Hubbard [11].

For an ensemble of interacting systems (for example, atoms, ions or moleculs in solids) having a finite and discrete set of energy levels, the Hamiltonian can be written in a very simple form in terms of the SBO's. All the Hamiltonians, containing one or more-than one system operators, have the identical algebraic structure in the SBO's and moreover since the SBO's form a closed algebra under the multiplication rules hence the technique is especially useful in making model independent approximation schemes. Moreover in this method all the terms in the Hamiltonian corresponding to the single system operators are always treated exactly. The Gree'ns functions of the SBO's enable us to determine a large class of elementary excitations in a well defined and consistent manner.

In the previous applications of the double-time Green's functions method, the random phase approximation (RPA) decoupling schemes for the anisotropic Heisenberg ferromagnet with S=1, gave some inconsistencies [12], which were more clearly demonstrated by Halley and Erdös [13] in the language of the SBO's. These inconsistence correspond to the breaking of the multiplication rules for the SBO's, called monotopic restriction or kinematic rules,and lead to nonunique solutions for the order parameters. Furthemore,it appeared that these inconsistencies are quite common in the Green's function method, and that they are specially manifested in the many-level interacting systems, like strongly anisotropic magnets or the systems with higher-order exchange couplings [14-20]. The partial solution of this problem has recently been given by Yang and Wang within the framework of the high-density expansion perturbation technique formulated in the terms of SBO's [21-22]. They demonstrated for the S=1 Heisenberg ferromagnet with uniaxial anisotropy that it is possible to fulfil the kinematic rules for the SBO's in the first order of perturbation with respect to the reciprocal interaction volume. Nevertheless, the problems of kinematic consistency still awaits the positive solution and we hope that the SMT for SBO's Green's functions proposed by us in this paper will be helpful in the solution of this question.

In Section 2, after describing the general properties of SBO's, we give a brief derivation of the SMT for interacting many-level systems. We obtain the Dyson equation for the matrix Green's functions of the SBO's. The zeroth order approximation in our approach corresponds to preserving the first two moments of the spectral density exactly [23-25]. All the damping effects being included in the self-energy operator.

The formalism developed in Section 2 is then applied in Section 3 to the study of spin-waves for the S=1 Heisenberg model with exchange and single-ion anisotropy, in the case of uniaxial ordering. In the zeroth order of approximation in the SMT we show that, the low temperature renormalization of the spin-wave spectrum is in agreement with Bloch-Dyson theory.

Section 4, deals with an easy plane ferromagnet. Here we present the results concerning the critical properties at the ground state as well as for the finite temperature. We also completed the RPA solution and gave the comparison with the SMT results.

In Section 5 we study the elementary excitation spectrum of the isotropic quadrupolar system. We compare our results with those of the RPA and Callen like decoupling schemes. [18, 14-15] .

Finally, in Section 6, we determine the single particle excitations in the Hubbard model and show the equivalence of our zeroth order approximation to that given by Roth [26] .

2. STANDARD BASIS OPERATORS AND THE SELF-CONSISTENT MANY-BODY THEORY

The SBO's and their properties have been described in detail by Hubbard [11] and later on by Halley and Erdös [13]. However, for the sake of completeness, we should mention some of their properties relevant to our purposes.

The SBO's are defined by

$$L^{i}_{\alpha\beta} = | i, \alpha > < i, \beta | \tag{2.1}$$

Where the state vectors $| i, \alpha >$, corresponding to the many-level system i, in the energy state α, form a complete set. They act as raising or lowering operactors when $\alpha > \beta$ or $\alpha < \beta$, respectively, and thus generate interstate transitions. The diagonal operator $L^{i}_{\alpha\beta}$ measures the probability that the state $| i, \alpha >$ is occupied. The multiplications rules for the SBO's are evident

$$L^{i}_{\alpha\beta} \, L^{i}_{\gamma\delta} = \delta_{\beta\gamma} \, L^{i}_{\alpha\delta} \tag{2.2}$$

the commutation rules are the following:

$$[L^i_{\alpha\alpha'}, L^j_{\beta\beta'}]_n = \delta_{ij} (\delta_{\alpha'\beta} L^i_{\alpha\beta'} + n\, \delta_{\beta'\alpha} L^i_{\beta\alpha'}),\ n = \pm , \qquad (2.3)$$

where + sign is used when both operators have fermion character, and the - sign if one or both operators have boson charater. The diagonal SBO's satisfy the normalization condition

$$\sum_{\alpha} L^i_{\alpha\alpha} = 1 \qquad (2.4)$$

Anny operator O_i can be expressed in terms of $L^i_{\alpha\beta}$ according to

$$O_i = \sum_{\alpha\beta} < i\alpha | O_i | \ i\beta > L^i_{\alpha\beta} \qquad (2.5)$$

To study the elemetary excitations and thermodynamics of the interacting many level system having m discrete levels we consider the Green's functions of the off-diagonal SBO's operators defined by [1]

$$G^{\alpha\beta,n}_{ij}(t) = << L^i_{\alpha,\alpha+n} | L^{j(t)}_{\beta+n,\beta} >> =$$

$$= i\Theta(t) < [L^i_{\alpha,\alpha+n}, L^j_{\beta+n,\beta}(t)]_n >;\ n = \pm , \qquad (2.6)$$

where $\Theta(t)$ is the Heaviside step function, and

$$\alpha + n \leq m,\ \beta + n \leq m.$$

The SBO's are the members of the set $\{L^i_{\alpha,\ \alpha+n}\}$, corresponding to a particular type of elementary excitation to be studied. This point will be more clear in the subsequent sections. The operator $L^j_{\beta'\beta}(t)$ is given the Heisenberg representation.

$$L^j_{\beta'\beta}(t) = e^{iHt} L^j_{\beta'\beta} e^{-iHt} , \qquad (2.7)$$

where H is the Hamiltonian of the ensemble of the interacting many level systems;

The SBO's Green's functions will be obtained by SMT, which is described briefly as follows. The equation of motion of the Green's functions (2.6) is given by

$$- i \frac{d}{dt} G_{ij}^{\alpha\beta, n}(t) = < [L^{i}_{\alpha, \alpha+n}, L^{i}_{\alpha+n, \alpha}]_n > \delta_{ij}\, \delta_{\alpha\beta}\, \delta(t)$$

$$+ i\, \Theta(t) < [L^{i}_{\alpha, \alpha+n}, \mathcal{L}\, L^{j}_{\beta+n, \beta}\ (t)]_n > , \tag{2.8}$$

where $\mathcal{L}$ is the Lioville operator defined by

$$\mathcal{L}\, \chi = [H, \chi] \ ; \tag{2.9}$$

for any orbitrary operator χ.

The operator $L^{j}_{\beta+n, \beta}(t)$ is broken into two parts

$$L^{j}_{\beta+n, \beta}\ (t) = P_n\, L^{j}_{\beta+n, \beta}\ (t) + (1 - P_n)\, L^{j}_{\beta+n, \beta}\ (t) \tag{2.10}$$

where the projection operator P_n is chosen as

$$P_n = \sum_{i\alpha} P^{n}_{i\alpha} , \tag{2.11}$$

and

$$P^{n}_{i\alpha}\, \chi = \frac{L^{i}_{\alpha+n, \alpha} < [L^{i}_{\alpha, \alpha+n}, \chi]_n >}{< [L^{i}_{\alpha, \alpha+n}, L^{i}_{\alpha+n, \alpha}]_n >} \tag{2.12}$$

By introducing the Fourier time transform

$$G_{ij}^{\alpha\beta; n}(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{iEt}\, G_{ij}^{\alpha\beta; n}(E)\, dE , \tag{2.13}$$

it can be shown that [2, 3]

$$E\, G_{ij}^{\alpha\beta;n}(E) = < [L^{i}_{\alpha,\alpha+n}, L^{i}_{\alpha+n,\alpha}]_{\eta} > \delta_{ij}\,\delta_{\alpha\beta}$$

$$+ \sum_{\ell\gamma} (\Omega_{i\ell}^{\alpha\gamma;n} + \Gamma_{i\ell}^{\alpha\gamma;n}(E))\; G_{\ell j}^{\gamma\beta;n}(E) \tag{2.14}$$

where

$$\Omega_{i\ell}^{\alpha\gamma;n} = \frac{-<[\mathcal{L}\, L^{i}_{\alpha,\alpha+n}, L^{\ell}_{\gamma+n,\gamma}]_{\eta}>}{<[L^{\ell}_{\gamma,\gamma+n}, L^{\ell}_{\gamma+n,\gamma}]_{\eta}>}\,, \tag{2.15}$$

$$\Gamma_{i\ell}^{\alpha\gamma;n}(E) = \int \Gamma_{i\ell}^{\alpha\gamma;n}(t)\, e^{-iEt}dt\,, \tag{2.16}$$

$$\Gamma_{i\ell}^{\alpha\gamma;n}(t) = \frac{-i\Theta(t) <[\mathcal{L}\, L^{i}_{\alpha,\alpha+n}, e^{it(1-P_n)\mathcal{L}}(1-P_n)\mathcal{L} L^{\ell}_{\gamma+n,\gamma}]_{\eta}>}{<[L^{\ell}_{\gamma,\gamma+n}, L^{\ell}_{\gamma+n,\gamma}]_{\eta}>} \tag{2.17}$$

For translationally invariant systems, we can define the Fourier transforme like

$$f_{ij} = \frac{1}{N} \sum_{\vec{k}} f_{\vec{k}}\, e^{i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)}\,, \tag{2.18}$$

then (2.14) becomes

$$E\, G_{k}^{\alpha\beta;n}(E) = < [L_{\alpha,\alpha+n}, L_{\alpha+n,\alpha}]_{\eta} > \delta_{\alpha\beta}$$

$$+ \sum_{\gamma} (\Omega_{k}^{\alpha\gamma;n} + \Gamma_{k}^{\alpha\gamma;n}(E))\; G_{k}^{\gamma\beta;n}(E)\,. \tag{2.19}$$

In matrix form, it can be rewritten as

$$(\omega\, I - B_k^{n}(E))\, G_k^{n}(E) = A^{n}\,, \tag{2.20}$$

where I is the unit matrix, and the matrix elements of $B_k^n(\omega)$ and A^n are given by :

$$B_k^{\alpha\beta;\,n}(E) = \Omega_k^{\alpha\beta;\,n} + \Gamma_k^{\alpha\beta;\,n}(E) \quad , \tag{2.21}$$

$$A^{\alpha\beta;\,n} = \langle \left[L_{\alpha,\alpha+n},\ L_{\alpha+n,\alpha} \right] \rangle \, \delta_{\alpha\beta} \quad . \tag{2.22}$$

Equation (2.20) can be transformed into a Dyson type equation by defining the zeroth order Green's functions as

$$(\omega I - \Omega_k^n)\, G_k^{o,\,n}(E) = A^n \ . \tag{2.23}$$

Using eq. (2.23) and eqs. (2.20 - 2.21) one gets

$$G_k^n(E) = G_k^{o,\,n}(E) + G_k^{o,\,n}(E) \sum_k^n(E)\, G_k^n(E) \ , \tag{2.24}$$

where

$$\sum_k^n(E) = (A^n)^{-1}\, \Gamma_k^n(E) \tag{2.25}$$

Eqs. (2.23 - 2.25) together with eqs. (2.16 - 2.17) constitute the required Dyson type equation. In the present formulation, all the damping effects are included in the self-energy operator $\sum_k^n(E)$.

3. ANISOTROPIC HEISENBERG FERROMAGNET: UNIAXIAL ORDERING

As a concret application of the results of Section 2, we consider the Heisenberg ferromagnet in the presence of both exchange and single-ion aisotropy. The Hamiltonian of the system is assumed to be ot the form

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

$$- \frac{1}{2} \sum_{ij} K_{ij} S_i^z S_j^z , \qquad (3.1)$$

where h is the external magnetic field, D is the single-ion anisotropy constant and K_{ij} is the anisotropic exchange parameter. In this Section, we consider a case of uniaxial ordering.

The SBO's (2.1) can be defined in terms of the states of the molecular field approximation (MFA) $| i\alpha > = | i, S - m + 1 >$ of the many level systems (ions) corresponding to the Hamiltonian

$$H_i^o = - h S_i^z - D(S_i^z)^2 \quad , \qquad (3.2)$$

and m, takes the values form + S to - S. From eq. (2.5) the spin operators can be expressed by the SBO's, as follows

$$S_i^+ = \sum_\alpha A_\alpha L^i_{\alpha, \alpha+1} \quad , \qquad (3.3)$$

$$S_i^- = \sum_\alpha A_\alpha L^i_{\alpha+1, \alpha} \quad , \qquad (3.4)$$

$$S_i^z = \sum_\alpha B_\alpha L^i_{\alpha\alpha} \quad , \qquad (3.5)$$

where

$$A_\alpha = [\alpha(2S - \alpha + 1)]^{1/2} , \qquad (3.6)$$

$$B_\alpha = S - \alpha + 1 , \qquad (3.7)$$

and $\alpha = 1, 2 \ldots, 2S + 1$.

The Hamiltonian (3.1) expressed in terms of the SBO's takes the following form:

$$H = - \sum_{i\alpha} h_{\alpha\alpha} L^{i}_{\alpha\alpha} - \frac{1}{2} \sum_{ij} \sum_{\substack{\alpha\alpha' \\ \beta\beta'}} M^{ij}_{\alpha\alpha';\,\beta\beta'} L^{i}_{\alpha\alpha'} L^{j}_{\beta\beta'} \quad , \tag{3.8}$$

where

$$h_{\alpha\alpha} = hB_{\alpha} + DB^{2}_{\alpha} \quad , \tag{3.9}$$

$$M^{ij}_{\alpha\alpha',\beta\beta'} = \frac{1}{2} J_{ij} (A_{\alpha} A_{\beta-1}\, \delta_{\alpha,\alpha'-1}\, \delta_{\beta,\beta'+1} + A_{\alpha-1} A_{\beta}\, \delta_{\alpha,\alpha'+1}\, \delta_{\beta,\beta'-1})$$

$$+ K_{ij}\, B_{\alpha}\, B_{\beta}\, \delta_{\alpha\alpha'}\, \delta_{\beta\beta'} \, . \tag{3.10}$$

A Dyson type equation for the off-diagonal Gree's functions is given quite generally by Eqs. (2.23 - 2.24). Here we shall consider only the zeroth order theory which neglects the self-energy operator $\sum^{n}_{k} (E)$. For $\Omega^{\alpha\gamma;\,n}_{k}$ we obtain

$$\Omega^{\alpha\gamma;\,n}_{k} = (h_{\alpha\alpha} - h_{\alpha+n,\,\alpha+n} + n\, K_{0} \sum_{\sigma} B_{\sigma}\, D_{\sigma})\, \delta_{\alpha\gamma}$$

$$- \frac{1}{2}\, J_{k}\, A_{\gamma}\, A_{\alpha}\, (D_{\alpha} - D_{\alpha+1})\, \delta_{n,\,1} + \frac{R^{\alpha,\,\alpha+n;\,\gamma+n,\,\gamma}_{k}}{D_{\gamma} - D_{\gamma+n}} \, , \tag{3.11}$$

where

$$D_{\alpha} = < L_{\alpha\alpha} > \tag{3.12}$$

In derivation of eq. (3.11) we have used the following definitions

$$L^{k}_{\alpha\alpha'} = N^{-1/2} \sum_{j} e^{-i\vec{k}\cdot\vec{R}_j} L^{j}_{\alpha\alpha'} , \tag{3.13}$$

$$J_k = \sum_{j} e^{-i\vec{k}\cdot(\vec{R}_i - \vec{R}_j)} J_{ij} , \tag{3.14}$$

$$K_o = \sum_{i} K_{ij} , \tag{3.15}$$

and the commutation rules for the SBO's in the $\vec{K}$ space, i.e.

$$\left[L^{k_1}_{\alpha\alpha'}, L^{k_2}_{\beta\beta'} \right] = N^{-1/2} \left[L^{k_1+k_2}_{\alpha\beta'} \delta_{\alpha'\beta} - L^{k_1+k_2}_{\beta\alpha'} \delta_{\beta'\alpha} \right]. \tag{3.16}$$

The first and second terms in Eq. (3.11) give the RPA expressions for the collective excitation spectrum, for arbitrary spin value. For $S = 1$, they are in the agreement with those given previously [13]. The last term in eq. (3.11) is expressed in the terms of irreducible correlation functions and goes beyond the RPA. An explicit form of $R_k^{\alpha\alpha;\,\beta\beta'}$ is given in Appendix. The transitions with $n = 1$ are the spin-waves that consist of 2S branches due to the non-equal distance between the molecular field states. The transitions with $n > 1$ correspond to the single-ion-bound states. The quantities $R_k^{\alpha\alpha';\,\beta\beta'}$ describe a scattering of the excitations on longitudinal and transversal fluctions of the angular momenta.

Since the results for arbitrary spin value are rather lengtly, we present here $S = 1$ case, only. $\Omega_k^{\alpha\gamma;\,n}$ are now given by

$$\Omega_k^{11;1} = h+D - J_k D_{12} + K_0 D_{13} + \frac{R_k^{12;21}}{D_{12}} \quad , \qquad (3.17a)$$

$$\Omega_k^{12;1} = - J_k D_{12} + \frac{R_k^{12;32}}{D_{23}} \quad , \qquad (3.17b)$$

$$\Omega_k^{21;1} = - J_k D_{23} + \frac{R_k^{23;21}}{D_{12}} \quad , \qquad (3.17c)$$

$$\Omega_k^{22;1} = h - D - J_k D_{23} + K_0 D_{13} + \frac{R_k^{23;32}}{D_{23}} \quad , \qquad (3.17d)$$

and

$$R_k^{12;21} = \frac{1}{N} \cdot \sum_q J_q \langle L_{23}^{q} \, (L_{21}^{-q} + L_{32}^{-q})\rangle + \frac{2}{N} \sum_q J_q \langle L_{21}^{q}(L_{12}^{-q} + L_{23}^{-q})\rangle$$

$$- \frac{1}{N} \sum_q K_{q-k} \langle L_{12}^{q} \, L_{21}^{-q}\rangle - \frac{1}{N} \sum_q J_{q-k} \langle L_{13}^{q} L_{31}^{-q}\rangle$$

$$+ \frac{1}{N} \sum_q J_{q-k} \langle(\tilde{L}_{22}^{q} - \tilde{L}_{11}^{q}) \, (\tilde{L}_{11}^{-q} - \tilde{L}_{22}^{-q})\rangle$$

$$+ \frac{1}{N} \sum_q K_q \langle(\tilde{L}_{11}^{q} - \tilde{L}_{22}^{q}) \, (\tilde{L}_{11}^{-q} - \tilde{L}_{33}^{-q})\rangle \qquad (3.18a)$$

$$R_k^{12;32} = - \frac{1}{N} \sum_q J_q \langle(L_{12}^{q} + L_{23}^{q}) \, (L_{21}^{-q} + L_{32}^{-q})\rangle$$

$$- \frac{1}{N} \sum_q K_{q-k} \langle L_{23}^{q} \, L_{21}^{-q}\rangle + \frac{1}{N} \sum_q J_{q-k} \langle L_{13} \, L_{31}^{-q}\rangle$$

$$- \frac{1}{N} \sum_q J_{q-k} \langle(\tilde{L}_{22}^{q} - \tilde{L}_{33}^{q}) \, (\tilde{L}_{11}^{-q} - \tilde{L}_{22}^{-q}) \rangle \quad , \qquad (3.18b)$$

$$R_k^{23;21} = R_k^{12;32} \quad , \qquad (3.18c)$$

$$R_k^{23;32} = \frac{1}{N}\sum_q J_q < L_{12}^q \, (\tilde{L}_{21}^{q} + L_{32}^{-q}) \; + \frac{2}{N}\sum_q J_q < L_{32}^q \, (L_{12}^{-q} + L_{23}^{-q}) >$$

$$- \frac{1}{N}\sum_q K_{q-k} < L_{23}^q \, L_{32}^{-q} > - \frac{1}{N}\sum_q J_{q-k} < L_{13}^q L_{31}^{-q} >$$

$$- \frac{1}{N}\sum_q J_{q-k} < (\tilde{L}_{22}^q - \tilde{L}_{33}^q) \, (\tilde{L}_{22}^{-q} - \tilde{L}_{33}^{-q}) >$$

$$+ \frac{1}{N}\sum_q K_q < \tilde{L}_{22}^q - \tilde{L}_{33}^q) \, (\tilde{L}_{11}^{-q} - \tilde{L}_{33}^{-q}) \quad . \tag{3.18d}$$

In Eqs. (3.18a-d) we denote $\tilde{L}_{\alpha\alpha}^k = L_{\alpha\alpha}^k - < L_{\alpha\alpha}^k >$ and we have assumed that $< L_{\alpha\beta}^k > = \delta(k)\, \delta_{\alpha\beta} < L_{\alpha\alpha}^0 >$.

The equation of motion for the Green's functions given by eq. (2.23) takes the following form:

$$\begin{pmatrix} E - \Omega_k^{11;1}, & -\Omega_k^{12;1} \\ -\Omega^{21;1}, & E-\Omega_k^{22;1} \end{pmatrix} \begin{pmatrix} << L_{12}^k | \, L_{21}^{-k} >>_E, & << L_{23}^k \, | \, L_{21}^{-k} >>_E \\ << L_{23}^k | \, L_{21}^{-k} >>_E, & << L_{23}^k \, | \, L_{32}^{-k} >>_E \end{pmatrix}$$

$$= \begin{pmatrix} D_{12} & 0 \\ 0 & D_{23} \end{pmatrix} \tag{3.19}$$

where $D_{\alpha\beta} = D_\alpha - D_\beta$, $<< L_{\alpha,\alpha+n}^k | \, L_{\beta+n,\,\beta}^k >>_E$ is the matrix element of the $G_k^{0,1}(E)$.

The spectrum of spin-waves is then given by

$$E_k^{\pm} = \frac{1}{2}\,(\Omega_k^{11;1} + \Omega_k^{22;1}) \pm \frac{1}{2}\,\Omega_k, \tag{3.20}$$

where

$$\Omega_k = \{(\Omega_k^{11;1} - \Omega_k^{22;1})^2 + 4\,\Omega_k^{12;1}\;\;\Omega_k^{21;1}\,\}^{1/2}. \tag{3.21}$$

Apart from the spin-wave excitations we have the collective excitations with n=2 which are given by the poles of the Green's function

$$\langle\langle L_{13}^{k} \mid L_{31}^{-k} \rangle\rangle_E = \frac{D_{13}}{E - \Omega_k^{11;2}}, \tag{3.22}$$

with

$$\Omega_k^{11;2} = 2h + K_o D_{13} + \frac{R_k^{13;31}}{D_{13}}, \tag{3.23}$$

and

$$\begin{aligned} R_k^{13;31} &= \frac{1}{N} \sum_q J_{q-k} \; \langle (L_{23}^q - L_{12}^q)\,(L_{21}^{-q} - L_{32}^{-q}) \rangle \\ &+ \frac{1}{N} \sum_q J_q \langle (L_{21}^q + L_{32}^q)\,(L_{12}^{-q} + L_{23}^{-q}) \rangle \\ &- \frac{4}{N} \sum_q K_{q-k} \langle L_{13}^q \, L_{31}^{-q} \rangle + \\ &+ \frac{2}{N} \sum_q K_q \langle (\tilde{L}_{11}^q - \tilde{L}_{33}^q)\,(\tilde{L}_{11}^{-q} - \tilde{L}_{33}^{-q}) \rangle . \end{aligned} \tag{3.24}$$

It is worthy to stress that this collective excitation is dispersive, in contrary to the RPA.

The temperature dependence of the spectrum is determined through the correlation function. By making use of eqs. (3.17a - 3.21) and applying the spectral theorem, we get the off-diagonal correlation

.functions from:

$$< L_{21}^{-k} L_{12}^{k} > = \frac{D_{12}}{2} \left[(1 + \psi_k) f (E_k^+) - (1 - \psi_k) f (E_k^-) \right], \qquad (3.25)$$

$$< L_{21}^{-k} L_{23}^{k} > = < L_{32}^{-k} L_{12}^{k} > = \frac{D_{12} \quad \Omega_k^{21;1}}{\Omega_k} \left[f(E_k^+) - f(E_k^-) \right], \qquad (3.26)$$

$$< L_{32}^{-k} L_{23}^{k} > = \frac{D_{23}}{2} \left[(1 - \psi_k) f (E_k^+) + (1 + \psi_k) f (E_k^-) \right], \qquad (3.27)$$

where

$$\psi_k = \frac{\Omega_k^{11;1} - \Omega_k^{22;1}}{\Omega_k}, \qquad (3.28)$$

and $E_k^{\pm}$ and Ω_k are given by eqs. (3.20) and (3.21), respectively.

For $< L_{31}^{-k} L_{13}^{k} >$ one has

$$< L_{31}^{-k} L_{13}^{k} > = D_{13} f(E_k), \qquad (3.29)$$

where $E_k = \Omega_k^{11;2}$ is given by eq. (3.23) and f(x) is the Bose-Einsten distribution function

$$f(x) = (\exp (\beta x) - 1)^{-1}, \ \beta = (k_B \ T)^{-1}. \qquad (3.30)$$

As concerns the irreducible diagonal correlation functions, they creat much more difficult problem and their calculation certainly requires more sophisticated procedure. An eventual line of attack may be chosen by using an approach analogous to that of Liu, in the case of the isotropic Heisenberg mode [27]. In the following we neglect we neglect them. This approximation is reasonable in the low-temperature regime, where they do not play an important role.

It is easy to see from eq. (3.26) that we have nonvanishing values of $<L^{i}_{21}L^{i}_{23}>$ and $<L^{i}_{32}L^{i}_{12}>$, which break the multiplication rules of the SBO's. This problem has already been discussed in the literature [13 - 21] . Although in our approach we found that it is minimal compared to the previous theories, nevertheless this does not resolve the difficulty. We feel that, to answer this question, one should take into account the self-energy operator Σ^{n}_{k} (E) rather than use additional conditions as proposed previously [13-15] .

The low-temperature renormalization of the spin-wave spectrum in our method can be given as follows. Firstly, to obtain the off-diagonal correlation function (3.25-3.27) and (3.29) we approximate them by the corresponding RPA expressions (the first iteration step in the full self-consistent solution)and get

$$<L^{-k}_{32}\ (L^{k}_{12}+L^{k}_{21})>\simeq D_{23}\ \{(A^{-}_{k}-B_{k})\ f(\omega^{+}_{k}) + (A^{+}_{k}+B_{k})\ f(\omega^{-}_{k})\} \quad ,$$

$$<L^{-k}_{21}\ (L^{k}_{12}+L^{k}_{23})>\simeq D_{12}\ \{(A^{-}_{k}+B_{k})\ f(\omega^{+}_{k}) + (A^{+}_{k}-B_{k})\ f(\omega^{-}_{k})\} \quad ,$$

$$<L^{-k}_{21}\ L^{k}_{23}> = <L^{-k}_{32}\ L^{k}_{12}> = -\frac{D_{12}\ D_{23}}{\beta_{k}}\left[f(\omega^{+}_{k}) - f(\omega^{-}_{k})\right] \quad , \qquad (3.31)$$

where

$$A^{\pm}_{k} = \frac{1}{2}(1-D_{13}\ \beta^{-1}_{k}) \quad , \qquad (3.32)$$

$$B_k = \frac{D}{J_k}\,\beta_k^{-1} \tag{3.33}$$

$$\beta_k = \sqrt{D_{13}^2 + \frac{4D}{J_k}\left(\frac{D}{J_k} + 3D_2 - 1\right)} \quad , \tag{3.34}$$

and

$$\omega_k^{\pm} = h + \left(K_o - \frac{1}{2}J_k\right) D_{13} \pm \frac{1}{2} J_k \beta_k \quad , \tag{3.35}$$

$\omega_k^{\pm}$ are the spin-wave energies in the RPA.

Since the third branch of excitations given by eq. (3.23) is independent on the wave-vector in the RPA, then by making use of the fact that $\sum_{\vec{q}} J_{\vec{q}} = 0$, the contribution from $\frac{1}{N}\sum_q J_{q-k} \langle L_{13}^{q} L_{31}^{-q} \rangle$ vanishes.

Secondly, neglecting the upper branch ω_k^{+} and taking the RPA values for D_α in the low temperature regime as given by:

$$D_1 = 1-\Phi \ , \quad D_2 = \Phi \ , \quad D_3 = 0 \ , \tag{3.36}$$

$$\Phi = \frac{1}{N}\sum_k f(\omega_k) \quad , \tag{3.37}$$

$$\omega_k = h+D+K_o-J_k \quad , \tag{3.38}$$

and using eqs. (3.20 - 3.21), we finally arrive at the following expression for the lower branch of excitations, for the small D limit

$$E_k^{-} = \omega_k - \frac{1}{N}\sum_q \left[\, 2D + K_o - J_k + K_{q-k} - J_q \,\right] f(\omega_q) \tag{3.39}$$

If K=J, eq.(3.39) agress with that of Kaschenko et al [28] obtained within the framework of the high-density expansion diagrammatic technique.

Eq. (3.39) reproduces exactly the Bloch-Dyson spin wave theory [29-30]. In particular, for the isotropic Heisenberg model the renomalization of the spin-waves turn out to be $\sim T^{5/2}$ instead of $\sim T^{3/2}$ RPA prediction. The result (3.39) can be generalized for arbitrary spin-value by simple replacement

$$D \rightarrow D(2S - 1). \tag{3.40}$$

4 . EASY PLANE FERROMAGNET

Another interesting application of our formalism concerns the easy planes ferromagnet. Let us consider, for simplicity, the paramagnetic phase and zero external field. If $D>0$, the doublet is a ground state and system orders along z - axis no matter how weak the exchange interaction is. On the other hand if $D<0$, the singlet is a ground state and one needs the critical value of exchange interaction, even at T=0K, to obtain an ordering in the X-Y plane. In the simple non-self-consistent RPA-MFA theory, the phase transition takes place if $|D|/J_0 < 2$ and this is a typical soft-mode phase transition (See, for example, [19] and references therein).

Here we present an improved analysis and we will approach the critical point from the paramagnetic side. The equations of Section 3 still apply to this case provided that $D \rightarrow -|D|$ and $h = 0$.

We begin with our self-consistent RPA expressions. On putting $D_1 = D_3$ in eq. (3.35) we get for the excitation spectrum

$$\omega_k = \sqrt{|D|(|D| + 2qJk} \tag{4.1}$$

where

$$q \doteq \frac{3}{2} < (S^z)^2 > - 1 = D_{12} . \tag{4.2}$$

A gap in the spectrum vanishes for

$$|D| = - 2q J_o . \tag{4.3}$$

To determine the critical value $|D|/J_o$ as well as the critical temperature one needs to solve the self-consistent equation for q which can be obtained from RPA Eqs. (3.31) which, in the present case, take the from:

$$< L^i_{21}(L^i_{12} + L^i_{23}) > = \frac{q}{2} [- 1 - |D| \Phi], \tag{4.4}$$

$$< L^i_{32}(L^i_{12} + L^i_{23}) > = \frac{q}{2} [1 - |D| \Phi], \tag{4.5}$$

$$< L^i_{21} L^i_{23} > = < L^i_{32} L^i_{12} > = \frac{q^2}{2} \frac{1}{N} \sum_k \frac{J_k}{\omega_k} \coth (\frac{\omega_k}{2k_BT}), \tag{4.6}$$

where

$$\Phi = \frac{1}{N} \sum_k \frac{1}{\omega_k} \coth (\frac{\omega_k}{2k_BT}), \tag{4.7}$$

and ω_k is given by (4.1)

With the multiplicatin rules and the normalization condition $2D_1 + D_2 = 1$, we can obtain equation for q. Since such a procedure is not unique, we apply two versions of RPA (for detailed discussion, see [18-19]).

In the first version of RPA (RPA*), we follow a prescription given by Halley and Erdös [13] . In this prescription one uses only eqs. (4.4) and (4.5) and apply the external condition $<L^i_{21}L^i_{23}>$ = $<L^i_{32}L^i_{12}>$ = 0. It yields us

$$q = \frac{2}{1-3\ |D|\Phi} \quad , \tag{4.8}$$

and Φ is given by eq. (4.7). By making use of eq. (4.3) and eq.(4.8), one has the following equation for the critical temperature $T_c = k_B T/J_o$

$$X = \frac{-4}{1-3F} \quad , \tag{4.9}$$

where

$$F = \frac{1}{N} \sum_k \frac{1}{\sqrt{1-\gamma_k}} \coth \frac{x\sqrt{1-\gamma_k}}{2T_c} \quad , \tag{4.10}$$

$$x = \frac{|D|}{J_o} \quad \text{and} \quad \gamma_k = \frac{J_k}{J_o} \quad ,$$

The critical value od x for transition at the ground state is obtained by putting $T_c \to 0$ in (4.10) and is given by

$$X_c = \frac{4}{3G-1} \tag{4.11}$$

where

$$G = \frac{1}{N} \sum_k \frac{1}{\sqrt{1-\gamma_k}} \tag{4.12}$$

The zero point reduction of q amounts $-\frac{1}{2}X_c$.

In the second version of RPA (RPA** or symmetrized RPA), we use all three equations (4.4 - 4.6) to determine q and get:

$$q = \frac{2}{1-3\psi}, \tag{4.13}$$

where

$$\psi = \frac{1}{N}\sum_k \frac{|D| + qJ_k}{\omega_k}\coth\frac{\omega_k}{2k_BT}, \tag{4.14}$$

and ω_k given by (4.1). The critical temperature is given now by eq. (4.9) with

$$F = \frac{1}{2N}\sum_k \frac{2-\gamma_k}{\sqrt{1-\gamma_k}}\coth\frac{x\sqrt{1-\gamma_k}}{2T_c} \tag{4.15}$$

Similarly critical value of x is given by eq. (4.11), with

$$G = \frac{1}{2N}\sum_k \frac{2-\gamma_k}{\sqrt{1-\gamma_k}}. \tag{4.16}$$

The critical values of X for the three cubic lattices haves been calculated numerically, and results are given in Table I. The X_c in RPA are less than the MFA and clearly depend on the topology of lattice. The reduction of q due to the zero point motion at $X = X_c$ is just $-1/2X_c$, and from Table I we conclude that the condition $<(S^z)^2> \geq 0$ is preserved in both versions of RPA. In Fig. 1 we ploted for comparison the phase diagram of the system in RPA and MFA for FCC lattice. Let us emphasize that although the RPA gives better results than those of MFA, the theory is not dependent on the longitudinal coupling, i.e. the phase transition takes place for the same value of X for both the X-Y and the Heinsenberg model. This shortcoming of the RPA theory can be overcome by the SMT as we shall show below.

Since in the paramagnetic phase $D_1=D_3$, the third branch of excitations does not contribute. Retaining only the off-diagonal correlation functions and using eqs. (3.17-3.19), we obtain for $\Omega_k^{\alpha\gamma;1}$:

$$\Omega_k^{11;1} = \alpha_k = -|D| - J_k q + \frac{R_k^{12;21}}{q} \quad , \qquad (4.17.a)$$

$$\Omega_k^{12;1} = \beta_k = - J_k q - \frac{R_k^{12;32}}{q} \quad , \qquad (4.17b)$$

$$\Omega_k^{21;1} = -\beta_k \quad , \qquad (4.18c)$$

$$\Omega_k^{22;1} = -\alpha_k \quad , \qquad (4.17d)$$

where

$$R_k^{12;21} = \frac{1}{N}\sum_p J_p \langle L_{32}^{-p}\,(L_{23}^{p}+L_{12}^{p})\rangle$$

$$+ \frac{2}{N}\sum_p J_p \langle L_{21}^{p}(L_{12}^{-p} + L_{23}^{-p})\rangle - \frac{1}{N}\sum_p K_{p-k} \langle L_{12}^{p}L_{21}^{-p}\rangle \quad , \qquad (4.18a)$$

$$R_k^{12;32} = -\frac{1}{N}\sum J_p < (L_{21}^{p} + L_{23}^{p})\,(L_{21}^{-p} + L_{32}^{-p}) >$$

$$-\frac{1}{N}\sum_p K_{p-k} < L_{23}^{p}\, L_{21}^{-p} > \quad , \tag{4.18b}$$

and the correlation functions are determined self-consistently from

$$< L_{21}^{-k}\, L_{12}^{k} > = -\frac{q}{2} + \frac{q}{2}\,\frac{\alpha_k}{E_k}\,\coth\left(\frac{\beta E_k}{2}\right) \quad , \tag{4.19a}$$

$$< L_{21}^{-k}\, L_{23}^{k} > = < L_{32}^{-k}\, L_{12}^{k} > = \frac{-q}{2}\cdot\frac{\beta_k}{E_k}\,\coth\left(\frac{\beta E_k}{2}\right) \quad , \tag{4.19b}$$

$$< L_{32}^{-k}\;\; L_{23}^{k} > = \frac{q}{2} + \frac{q}{2}\,\frac{\alpha_k}{E_k}\,\coth\left(\frac{\beta E_k}{2}\right) \quad . \tag{4.19c}$$

The spectrum E_k is given by

$$E_k = \sqrt{\alpha_k^2 - \beta_k^2} \tag{4.20}$$

To derive eqs. (4.18-4.19) we used the fact that

$$\sum_q J_q < L_{12}^{q}\, L_{21}^{-q} > = \sum_q J_q < L_{23}^{q}\, L_{32}^{-q} > \tag{4.21}$$

for the considered case.

Introducing the notation

$$f_1 = \frac{1}{qN} \sum_p J_p < L_{12}^p \, L_{21}^{-p} > \qquad , \tag{4.22}$$

$$f_2 = \frac{1}{qN} \sum_p J_p < L_{21}^p \, L_{23}^{-p} > \qquad , \tag{4.23}$$

and using the Callen-Bloch theorem for the cubic lattices with inverse symmetry [29,31]

$$\frac{1}{N} \sum_p J_{k+p} \; f(p) = \gamma_k \frac{1}{N} \sum_p \; J_p \; f(p) \qquad , \tag{4.24}$$

as well as the property $\sum_p J_p = 0$, we get for α_k and β_k

$$\alpha_k = - \mid D \mid - J_k q + 3(f_1 + f_2) - \eta f_1 \gamma_k \qquad , \tag{4.25}$$

$$\beta_k = - J_k q + 2(f_1 + f_2) + \eta f_2 \gamma_k) \qquad , \tag{4.26}$$

and

$$\eta = K/J.$$

A litte inspection of eqs. (4.19) and (4.25-4.26) shows that $\alpha_k - \beta_k$ has a constant sign provided that $\eta<1$. Then the gap vanishes for

$$\alpha_o + \beta_o = 0 \tag{4.27}$$

We can estimate the critical value using the RPA as the first interation step. Taking f_1 and f_2 as given RPA, one has

$$\alpha_k + \beta_k = |D| + 2q\, J_k + \frac{5}{2}\Phi - \eta\left(\frac{1}{2}\Phi + \Phi_1\right)\gamma_k \quad , \tag{4.28}$$

$$\alpha_k - \beta_k = |D| + \frac{1}{2}\Phi\,(1 - \eta\,\gamma_k) \quad , \tag{4.29}$$

where

$$\Phi = \frac{1}{N}\sum_p \frac{|D|J_p}{\omega_p}\coth\left(\frac{\beta\omega_p}{2}\right) \quad , \tag{4.30}$$

$$\Phi_1 = \frac{1}{N}\sum_p q\,\frac{J_p^2}{\omega_p}\coth\left(\frac{\beta\omega_p}{2}\right) \quad , \tag{4.31}$$

and ω_p is given by eq. (4.1). The criterion for softening now reads:

$$|D| + 2qJ_o + \frac{5}{2}\Phi - \frac{1}{2}\eta\Phi - \eta\Phi_1 = 0 \quad . \tag{4.32}$$

Eq. (4.32) supplemented by equation for q in RPA should be solved self-consistently. Here we present the results for only two cases $\eta = 0$ and $\eta = 1$

i) η=0, the X-Y model

For the X-Y model after some algebra, we obtain the following integral equation for the critical value

$$X_c = 2|q| - \frac{5}{2N}\sum_p \frac{x_c\gamma_p}{\sqrt{x_c(x_c - 2|q|\gamma_p)}} \tag{4.33}$$

with q given in RPA, i.e., by eq. (4.8) or (4.13) depending on the versious of RPA we prefer. We have estimated the critical ratio x taking on the RHS of (4.33) X_c as given in RPA i.e., $X_c = 2\,|q|$. This leads to

$$X_c = X_c^{RPA} - \frac{5}{2N} \sum_p \frac{\gamma_p}{\sqrt{1-\gamma_p}} \quad . \tag{4.34}$$

The corresponding value of X_c are given in Table II.

ii) For the isotropic Heisenberg model $\eta = 1$, we obtain the following equation for X_c

$$x_c = 2|q| - \frac{2}{N} \sum_p \frac{x_c \gamma_p}{\sqrt{x_c [x_c - 2|q|\gamma_p]}} - \frac{1}{N} \sum_p \frac{|q|\gamma_p^2}{\sqrt{x_c [x_c - 2|q|\gamma_p]}} \tag{4.35}$$

In the first interation step, one has

$$x_c = x_c^{RPA} - \frac{5}{2N} \sum_p \frac{\gamma_p}{\sqrt{1-\gamma_p}} + \frac{1}{2N} \sum_p \gamma_p \sqrt{1-\gamma_p} \quad . \tag{4.36}$$

Since $\frac{1}{N} \sum_p \gamma_p \sqrt{1-\gamma_p}$ is negative, then the critical value for the Heisenberg model is less then for the X-Y. One should notice this property from the general physical considerations. Table III* contains also comparison with the recent results given by Lines [32] obtained by the correlated effective field theory (CEF). Our values for $\eta = 1$ lie slightly higher than those given by Lines. Eventual improvement can be done by the full solution of above integral equations.

* shows the results for x_c in SMT and

5. S=1 QUADRUPOLAR SYSTEM

In this Section we present application of general formalism developed in Section II to the isotropic S=1 quadrupolar system, characterized by the following Hamiltonian:

$$H = - \sum_{ij} \sum_{m=-2}^{2} J_{ij} \; O_2^m (i) O_2^{-m} (j) \quad , \tag{5.1}$$

where O_2^m are the tensor operators for S=1 and are given by

$$O_2^0 (i) = \sqrt{\frac{3}{2}} \left[(S_i^z)^2 - \frac{2}{3} \right] \quad ,$$

$$O_2^{\pm 1} (i) = \frac{1}{2} \left[S_i^z \, S_i^{\pm} + S_i^{\pm} \, S_i^z \right] \quad ,$$

$$O_2^{\pm 2} (i) = \frac{1}{2} (S_i^{\pm})^2 \; . \tag{5.2}$$

A variety of physical situations can be described in terms of effective quadrupolar coupling, among them the structural phase transitions induced by magnetic ordering in rare-earth compounds and the molecular hydrogen, see e.q. [18] and refs. therein. Although real compounds exhibit anisotropic quadrupolar coupling, for the sake of simplicity we shall consider the idealized system with Hamiltonian (5.1). The MFA gives quadrupolar ordering characterized by on order parameter $q = \sqrt{\frac{3}{2}} < O_2^0 >$, with ground state as a non-magnetic singlet $|0>$ and next level as a doublet $| \pm 1 >$. We shall study the collective excitations (librons) which are the Goldstone modes and correspond to a transition between molecular field states [18]. To describe the dynamics of the system (5.1), several authors have used a new set of pseudo-boson operators introduced by Raich and Etters [33-34], [14-15]. Here we apply the formalism of Section II and derive a Dyson like equation in terms of the SBO's.

The tensor operators can be expressed in terms of the SBO's as follows:

$$O_2^0\ (i) = \sqrt{\frac{3}{2}}\,(L^i_{11} + L^i_{33} - \frac{2}{3}) \quad ,$$

$$O_2^1\ (i) = \frac{1}{\sqrt{2}}\,(L^i_{12} - L^i_{23}) \quad ,$$

$$O_2^{-1}\ (i) = \frac{1}{\sqrt{2}}\,(L^i_{21} - L^i_{32}) \quad ,$$

$$O_2^2\ (i) = L^i_{13}\ ,\ O_2^{-2}(i) = L^i_{31} \quad , \tag{5.3}$$

and after the Fourier transformation the Hamiltonian (5.1) takes the following form

$$H = -\frac{1}{3} N J_o + J_o\sqrt{N}\,(L^0_{11} + L^0_{33}) - \frac{3}{4}\sum_k J_k(L^k_{11} + L^k_{33})\ (L^{-k}_{11} + L^{-k}_{33})$$

$$-\frac{1}{2}\sum_k J_k\ (L^k_{12} - L^k_{23})\ (L^{-k}_{21} - L^{-k}_{32})\ - \sum_k\ J_k L^k_{13} L^{-k}_{31} \quad , \tag{5.4}$$

where $L^k_{\alpha\beta}$ and J_k are defined by (3.13) and eq. (3.14), respectively.

As earlier, the Dyson equation for the Green's functions of the off-diagonal SBO's with $n=1$ is given by eqs.(2.23-2.25). For the zeroth order approximation Green's function, we get

$$\begin{pmatrix} E-\Omega_k^{11;1}, & -\Omega_k^{12;1} \\ -\Omega_k^{21;1} & , E-\Omega_k^{22;1} \end{pmatrix} \begin{pmatrix} \langle\langle L_{12}^k \mid L_{21}^{-k} \rangle\rangle_E , & \langle\langle L_{12}^k \mid L_{32}^{-k} \rangle\rangle_E \\ \langle\langle L_{23}^k \mid L_{21}^{-k} \rangle\rangle_E , & \langle\langle L_{23}^k \mid L_{32}^{-k} \rangle\rangle_E \end{pmatrix}$$

$$= q \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \tag{5.5}$$

where for the considered system $D_1 = D_3$ and $q = D_{12}$.

$\Omega_k^{\alpha\beta;1}$ are given by

$$\Omega_k^{11;1} = \omega_k + \frac{R_k^{12;21}}{q} , \tag{5.6a}$$

$$\Omega_k^{12;1} = -\Omega_k^{21;1} = \bar{\omega}_k - \frac{R_k^{12;32}}{q} , \tag{5.6b}$$

$$\Omega_k^{22;1} = -\omega_k - \frac{R_k^{23;32}}{q} , \tag{5.6c}$$

In eqs. (5.6a - c)

$$\omega_k = J_0 - \frac{1}{2} q\, J_k \tag{5.7a}$$

$$\tilde{\omega}_k = \frac{1}{2} q\, J_k \tag{5.7b}$$

and

$$R_k^{12;21} = -\frac{1}{2N}\sum_q J_p \Big[\langle L^p_{23}(L^{-p}_{21} - L^{-p}_{32})\rangle - 2\langle L^p_{21}(L^{-p}_{12} - L^{-p}_{23})\rangle$$

$$- 2\langle L^{-p}_{13} L^p_{31}\rangle\Big]$$

$$- \frac{3}{2N}\sum_p J_{p-k}\Big[\langle L^p_{12} L^{-p}_{21}\rangle + \frac{1}{3}\langle L^p_{13} L^{-p}_{31}\rangle + \frac{2}{3}\langle L^p_{23} L^{-p}_{32}\rangle\Big]$$

$$+ \frac{3}{2N}\sum_p J_p \langle(\tilde{L}^p_{11} - \tilde{L}^p_{22})(\tilde{L}^{-p}_{11} + \tilde{L}^{-p}_{33})\rangle$$

$$- \frac{1}{2N}\sum_p J_{p-k} \langle(\tilde{L}^{-p}_{11} - \tilde{L}^{-p}_{22})(\tilde{L}^p_{11} - \tilde{L}^p_{22})\rangle \quad , \tag{5.8a}$$

$$R_k^{12;32} = \frac{1}{2N}\sum_p J_p \Big[\langle L^p_{12}(L^{-p}_{21} - L^{-p}_{32})\rangle - \langle(L^{-p}_{12} - L^{-p}_{23}) L^p_{32}\rangle\Big]$$

$$+ \frac{3}{2N}\sum_p J_{p-k}\Big[\langle L^p_{12} L^{-p}_{32}\rangle + \frac{2}{3}\langle L^{-p}_{12} L^p_{32}\rangle - \frac{1}{3}\langle L^p_{13} L^{-p}_{31}\rangle\Big]$$

$$- \frac{1}{2N}\sum_p J_{p-k} \langle(\tilde{L}^{-p}_{22} - \tilde{L}^{-p}_{33})(\tilde{L}^p_{11} - \tilde{L}^p_{22})\rangle \quad , \tag{5.8b}$$

$$R_k^{23;32} = -\frac{1}{2N}\sum_p J_p\left[2<(L_{12}^{-p}-L_{23}^{-p})L_{32}^{p}> - <L_{12}^{p}(L_{21}^{-p}-L_{32}^{-p})>\right.$$

$$\left. - 2<L_{13}^{-p}L_{31}^{p}>\right]$$

$$-\frac{3}{2N}\sum_p J_{p-k}\left[<L_{23}^{p}L_{32}^{-p}> + \frac{1}{3}<L_{13}^{p}L_{31}^{-p}> + \frac{2}{3}<L_{12}^{-p}L_{21}^{p}>\right]$$

$$-\frac{3}{2N}\sum_p J_p <(\tilde{L}_{22}^{p}-\tilde{L}_{33}^{p})(\tilde{L}_{11}^{-p}+\tilde{L}_{33}^{-p})>$$

$$-\frac{1}{2N}\sum_p J_{p-k}<(\tilde{L}_{22}^{-p}-\tilde{L}_{33}^{-p})(\tilde{L}_{22}^{p}-\tilde{L}_{33}^{p})>, \qquad (5.8c)$$

where

$$\tilde{L}_{\alpha\alpha}^{k} = L_{\alpha\alpha}^{k} - <L_{\alpha\alpha}^{k}>$$

For the considered system the correlation function $<L_{13}^{k}L_{31}^{-k}>$ does not contribute, and the following equality holds

$$\sum_p J_p <L_{12}^{p}L_{21}^{-p}> = \sum_p J_p <L_{23}^{p}L_{32}^{-p}> \qquad (5.9)$$

Having this in mind and neglecting the diagonal irreducible correlation functions in (5.8a-c), we obtain for the Green's functions

$$\begin{pmatrix} <<L_{12}^{k}|L_{21}^{-k}>>_E, & <<L_{12}^{k}|L_{32}^{-k}>>_E \\ <<L_{23}^{k}|L_{21}^{-k}>>_E, & <<L_{23}^{k}|L_{32}^{-k}>>_E \end{pmatrix} = \frac{q}{E^2-E_k^2}\begin{pmatrix} E+\Omega_k^{11;1}, & -\Omega_k^{12;1} \\ -\Omega_k^{12;1}, & -E+\Omega_k^{11;1} \end{pmatrix}$$

$$(5.10)$$

where

$$\Omega_k^{11;1} = \dot{\omega}_k + \frac{3}{2} (f_1-f_2) - \frac{5}{2} f_1\gamma_k \quad , \tag{5.11}$$

$$\Omega_k^{12;1} = \hat{\omega}_k - (f_1-f_2) - \frac{5}{2} f_2\gamma_k \quad , \tag{5.12}$$

and

$$f_1 = \frac{1}{qN} \sum_p J_p < L_{21}^{-p} L_{12}^{p} > \quad , \tag{5.13}$$

$$f_2 = \frac{1}{qN} \sum J_p < L_{21}^{-p} L_{23}^{p} > \quad , \tag{5.14}$$

To obtain (5.11-16) we have also used the Callen-Bloch theorem (4.24). The collective excitation spectrum is given by

$$E_k^2 = \left[J_0 q + \frac{5}{2} (f_1 - f_2) \right] \left[J_0 q + \frac{1}{2} (f_1 - f_2) - \right.$$

$$\left. - \frac{5}{2} (f_1 + f_2)\, \gamma_k \right] (1 - \gamma_k), \tag{5.15}$$

which of course is gapless as required by the Goldstone theorem [18]. The correlations functions f_1 and f_2 can be given explicitely by using the spectral theorem and eq. (5.10). The result is given below.

$$\begin{pmatrix} \langle L_{21}^{-k} L_{12}^{k} \rangle , & \langle L_{32}^{-k} L_{12}^{k} \rangle \\ \vdots & \\ \langle L_{21}^{-k} L_{23}^{k} \rangle , & \langle L_{32}^{-k} L_{23}^{k} \rangle \end{pmatrix} =$$

$$\frac{q}{2} \begin{pmatrix} \frac{\Omega_k^{11;1}}{E_k} \coth\left(\frac{\beta E_k}{2}\right) - 1, & -\frac{\Omega_k^{12;1}}{E_k} \coth\left(\frac{\beta E_k}{2}\right) \\ -\frac{\Omega_k^{12;1}}{E_k} \coth\left(\frac{\beta E_k}{2}\right), & \frac{\Omega_k^{11;1}}{E_k} \coth\left(\frac{\beta E_k}{2}\right) - 1 \end{pmatrix} \qquad (5.16)$$

As concerns q, it can be given explicitely by using eq. (5.16). To estimate the zero-temperature corrections to the spectrum we take the-off diagonal correlation functions and q as given in RPA. We will use the RPA** since this version is best suited to the considered system [18]

In RPA** one has [18] $\Omega_k^{11;1} = \omega_k$, $\Omega_k^{12;1} = \tilde{\omega}_k$ and for f_1, f_2 we get

$$f_1 = J_0 \frac{1}{4N} \sum_k \frac{\gamma_k(2-\gamma_k)}{\sqrt{1-\gamma_k}} \coth \frac{\beta J_0 q \sqrt{1-\gamma_k}}{2} , \qquad (5.17)$$

$$f_2 = -J_0 \frac{1}{2N} \sum_k \frac{\gamma_k^2}{\sqrt{1-\gamma_k}} \coth \frac{\beta J_0 q \sqrt{1-\gamma_k}}{2} , \qquad (5.18)$$

and q is given by

$$q = \frac{4}{1+3Q} \quad , \tag{5.19}$$

where

$$Q = \frac{1}{2N} \sum_K \frac{2-\gamma_k}{\sqrt{1-\gamma_k}} \coth \frac{\beta J_0 q \sqrt{1-\gamma_k}}{2} \quad . \tag{5.20}$$

For $T \to 0^0K$ one has for the spectrum:

$$E_k^2 = J_0^2 \, (q + 5F) \, (q + F - 5H\gamma_k) \, (1-\gamma_k) \quad , \tag{5.21}$$

where

$$F = - \frac{1}{4N} \sum_k \frac{\gamma_k}{\sqrt{1-\gamma_k}} \quad , \tag{5.22}$$

$$H = - \frac{1}{4N} \sum_k \gamma_k \cdot \sqrt{1-\gamma_k} \quad , \tag{5.23}$$

and q is given eqs. (5.19-5.20). In Fig. 2 we have plotted the zero-temperature spectrum of a simple-cubic lattice and have compared it with those of RPA-MFA and RPA**. [18]. A difference between the SMT and RPA** is roughly of the same order as between the RPA** and RPA-MFA. In the present method, we determine the two first-moment of the spectral density without any restrictions. In analogous method, based on the Callen-like decoupling scheme of the equation of motion for the Green's functions, Barma [14] as well as Fittipaldi and Tahir-Kheli [15] have introduced external conditions in order to fulfil the kinematic rules. Our results, in the first iteration step, are in fact not distinguishable from those of Barma [14]. Eventual improvement of our zeroth-order results can be done by the full self-consistent calculation of the spectrum and inclusion of the self-energy $\sum_k^1 (E)$ in order to chek the fulfilment of kinematic rules as well as to get a damping of excitations.

6. THE HUBBARD MODEL

After studying the various applications of SMT of SBO's in localized electron systems, we shall, now, apply it to the itinerant electron system deseribed by the Hubbard model [35]. In the past, this model has been extensively studied in connection with the correlation effects in magnetism and metal-non metal transitions in narrow bands [36]. In the language of SBO's, the Hubbard model, described by the Hamiltonian

$$H = \sum_{i\sigma} T_{ij} \; a_{i\sigma}^{+} \; a_{j\sigma} + \frac{I}{2} \sum_{i\sigma} n_{i\sigma} \, n_{i-\sigma} \qquad , \tag{6.1}$$

can be written as

$$H = \sum_{i\alpha} \varepsilon_{i\alpha} \; L_{\alpha\alpha}^{i} + \sum_{\substack{ij \\ \alpha\beta\gamma\delta}} T_{ij}^{\alpha\beta\gamma\delta} \; L_{\alpha\beta}^{i} \; L_{\gamma\delta}^{j} \qquad , \tag{6.2}$$

where $\varepsilon_{i\alpha}$ is the eigenvalue corresponding to the state $|i\alpha>$ of the Hamiltonian

$$H_i = \sum_{\sigma} \left(T_{ii} \, a_{i\sigma}^{+} \, a_{i\sigma} + \frac{I}{2} \; n_{i\sigma} \, n_{i-\sigma} \right) \tag{6.3}$$

and

$$T_{ij}^{\alpha\beta\gamma\delta} = \sum_{\sigma} T_{ij} \langle i\alpha \mid a_{i\sigma}^{+} \mid i\beta\rangle \langle j\gamma \mid a_{j\sigma} \mid j\delta\rangle \qquad (6.4)$$

The Hamiltonian (6.3) has four eigenstates denote as $|i,1\rangle$; $|i,2\rangle$; $|i,3\rangle$; and $|i,4\rangle$ corresponding to $n_+ = n_- = 0$; $n_+ = 1$, $n_- = 0$; $n_+ = 0$, $n_- = 1$; $n_+ = n_- = 1$, respectively. Here n_σ is the eigenvalue of the number operator $n_{i\sigma}$. The eigenvalues $\epsilon_{i\alpha}$ corresponding to the above four states are $\epsilon_{i1} = 0$; $\epsilon_{i2} = \epsilon_{i3} = T_{ii}$ and $\epsilon_{i4} = 2T_{ii} + I$. For convenience, here after we shall denote states $|i2\rangle \equiv |i,1+\rangle$ and $|i,3\rangle \equiv |i,1_-\rangle$. Then from Eq. (2.5) the anihilation and creations operators for the single particle excitations are given as

$$a_{i\sigma} = L^{i}_{1,1\sigma} + \sigma L^{i}_{1-\sigma,4} \qquad (6.5a)$$

and

$$a_{i\sigma}^{+} = L^{i}_{i\sigma,1} + \sigma L^{i}_{4,1-\sigma} \qquad (6.5b)$$

By multiplying (6.5a) and (6.5b), and applying multiplication rules (2.2), SBO's can be written as a product of two fermions operators.

Now we shall use our SMT to obtain the single particle Green's function $\langle\langle a_{i\sigma} | a_{j\sigma}^{+} \rangle\rangle$ from which one obtain the single particle excitations and many thermodynamic quantities [1]. From (6.5a) and 6.5b), the Green's function $\langle\langle a_{i\sigma} | a_{j\sigma}^{+} \rangle\rangle_E$ can be written as a sum of four SBO's Green's functions

$$\begin{aligned} <<a_{i\sigma} \mid a^{+}_{j\sigma}>>_E \; = \; & <<L^{i}_{1,1\sigma} \mid L^{j}_{1\sigma,1}>>_E \\ & + <<L^{i}_{1,1\sigma} \mid L^{j}_{4,1-\sigma}>>_E \\ & + <<L^{i}_{1-\sigma,4} \mid L^{j}_{1\sigma,1}>>_E \\ & + <<L^{i}_{1-\sigma,4} \mid L^{j}_{4,1-\sigma}>>_E \end{aligned} \tag{6.6}$$

The SBO's Green's functions, appearing on the right hand side of Eqs. (6.6), can be obtained from the matrix equations (2.23-2.25) by putting $\alpha,\beta \equiv 1,1\sigma$ and $n = \delta_{\sigma+} + 2\delta_{\sigma-}$. In the zeroth order aproximation, the calculations are straightfowatd. It is found that our results are the same as that of the two pole approximations of Roth [26]. However, when one obtains the correlations functions from the SBO's Green's functions the monotopic restrictions are violated. This fact was not noticed earlier. We realized that if we approximate the self energy $\sum_k^{\alpha\beta;n}(E)$ in such a way that $\sum_k^{\alpha\beta;n}(E) = 0$ for $\alpha = \beta$ and $\sum_k^{\alpha\beta,n}(E) = -\Omega_k^{\alpha\beta,n}$ for $\alpha \neq \beta$ our results reduce to that of Ikeda et al. [37] and satisfy the monotopic restrictions. Recently Ikeda et al. [38] theory has been applied to the doped semiconductors to calculated the specific heat [38] and found to be in good agreement with the experiment.

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APPENDIX

Here we give the explicity form $R_k^{\alpha\alpha';\beta\beta'}$ for arbitrary spin value, which is obtained by calculating of the double commutator in eq. (2.15)

$$R_k^{\alpha\alpha';\beta\beta'} = \frac{1}{2N} \sum_q J_q A_{\alpha-1} [A_\beta \tilde{M}^{k+q}_{\alpha-1,\alpha';\beta+1,\beta'} - A_{\beta'-1} \tilde{M}^{k+q}_{\alpha-1,\alpha';\beta,\beta'-1}]$$

$$+ \frac{1}{2N} \sum_q \sum_\gamma J_q A_{\alpha-1} A_{\gamma-1} [\tilde{M}^q_{\alpha-1,\beta';\gamma,\gamma-1} \delta_{\alpha'\beta} - \tilde{M}^q_{\beta\alpha';\gamma,\gamma-1} \delta_{\beta',\alpha-1}]$$

$$- \frac{1}{2N} \sum_q J_q A_{\alpha'} [A_\beta \tilde{M}^{k+q}_{\alpha,\alpha'+1;\beta+1,\beta'} - A_{\beta'-1} \tilde{M}^{k+q}_{\alpha,\alpha'+1;\beta,\beta'-1}]$$

$$- \frac{1}{2N} \sum_q \sum_\gamma J_q A_{\alpha'} A_{\gamma-1} [\tilde{M}^q_{\alpha,\beta';\gamma,\gamma-1} \delta_{\alpha'+1,\beta} - \tilde{M}^q_{\beta,\alpha'+1;\gamma,\gamma-1} \delta_{\beta'\alpha}]$$

$$+ \frac{1}{2N} \sum_q J_q A_\alpha [A_{\beta-1} \tilde{M}^{k+q}_{\alpha+1,\alpha';\beta-1,\beta'} - A_{\beta'} \tilde{M}^{k+q}_{\alpha+1,\alpha';\beta,\beta'+1}]$$

$$+ \frac{1}{2N} \sum_q \sum_\gamma J_q A_\alpha A_\gamma [\tilde{M}^q_{\alpha+1,\beta';\gamma,\gamma+1} \delta_{\alpha'\beta} - \tilde{M}^q_{\beta\alpha';\gamma,\gamma+1} \delta_{\alpha+1,\beta'}]$$

$$- \frac{1}{2N} \sum_q J_q A_{\alpha'-1} [A_{\beta-1} \tilde{M}^{k+q}_{\alpha,\alpha'-1;\beta-1,\beta'} - A_{\beta'} \tilde{M}^{k+q}_{\alpha,\alpha'-1;\beta,\beta'+1}]$$

$$- \frac{1}{2N} \sum_q \sum_\gamma A_{\alpha'-1} A_\gamma [\tilde{M}^q_{\alpha,\beta';\gamma,\gamma+1} \delta_{\alpha'-1,\beta} - \tilde{M}^q_{\beta,\alpha'-1;\gamma,\gamma+1} \delta_{\beta'\alpha}]$$

$$+ \frac{1}{N} \sum_q K_q \, (B_\alpha - B_{\alpha'}) \, (B_\beta - B_{\beta'}) \, \tilde{M}^{k+q}_{\alpha\alpha';\beta\beta'}$$

$$+ \frac{1}{N} \sum_q \sum_\gamma K_q \, (B_\alpha - B_{\alpha'}) \, B_\gamma \, [\, \tilde{M}^q_{\alpha,\beta';\gamma\gamma} \, \delta_{\alpha'\beta} - \tilde{M}^q_{\beta\alpha';\gamma\gamma} \, \delta_{\beta'\alpha} \,] \, ,$$

where A_α and B_α are given by eqs. (3.6-3.7) respectively, and

$$\tilde{M}^k_{\alpha\alpha',\beta\beta'} = \langle (L^k_{\alpha\alpha'} - \langle L^k_{\alpha\alpha'} \rangle) \, (L^{-k}_{\beta\beta'} - \langle L^{-k}_{\beta\beta'} \rangle) \rangle \, ,$$

and we assume that $\langle L^k_{\alpha\alpha'} \rangle = \sqrt{N} \; D_\alpha \; \delta(k) \, \delta_{\alpha\alpha'}$.

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TABLE I

Critical values of $|D|/J_o$ for the X-Y or Heisenberg model in MFA and RPA

LATTICE	$X_c = \|D\|/J_o$		
	MFA	RPA*	RPA**
S.C	2	1.715	1.878
B.C.C	2	1.777	1.907
F.C.C.	2	1.8075	1.918

TABLE II

Critical values of $|D|/J_o$ for the X-Y model in SMT .

LATTICE	$X_c = \|D\|/J_o$	
	RPA* as a starting point	RPA** as a starting point
S.C	1.375	1.519
B.C.C.	1.538	1.649
F.C.C.	1.595	1.7055

TABLE III

Critical Values of $|D|/J_0$ for the isotropic Heisenberg model in SMT.
The results of CEF are given for comparison [32]

LATTICE	S M T		
	RPA* as a starting point	RPA** as a starting point	CEF
S.C.	1.330	1.474	1.148
B.C.C.	1.504	1.615	1.294
F.C.C.	1.571	1.681	1.359

FIGURE CAPTIONS

Fig. 1 - Curie temperature $k_B T_c/J_o$ as a function of $|D|/J_o$ calculated by the MFA and by the RPA** and RPA*.

Fig. 2 - Zero temperature excitation spectrum for $\vec{k} = (0,0,k)$ plotted for a simple cubic lattice. SMT refers to the lowest iteration step in this method. RPA** and RPA-MFA spectra are given by $E_k/J_o = |q| \sqrt{1-\gamma_k}$ where $|q| = 1$ in MFA whereas in RPA** q is given by eqs. (5.19-20) for T = 0 k.

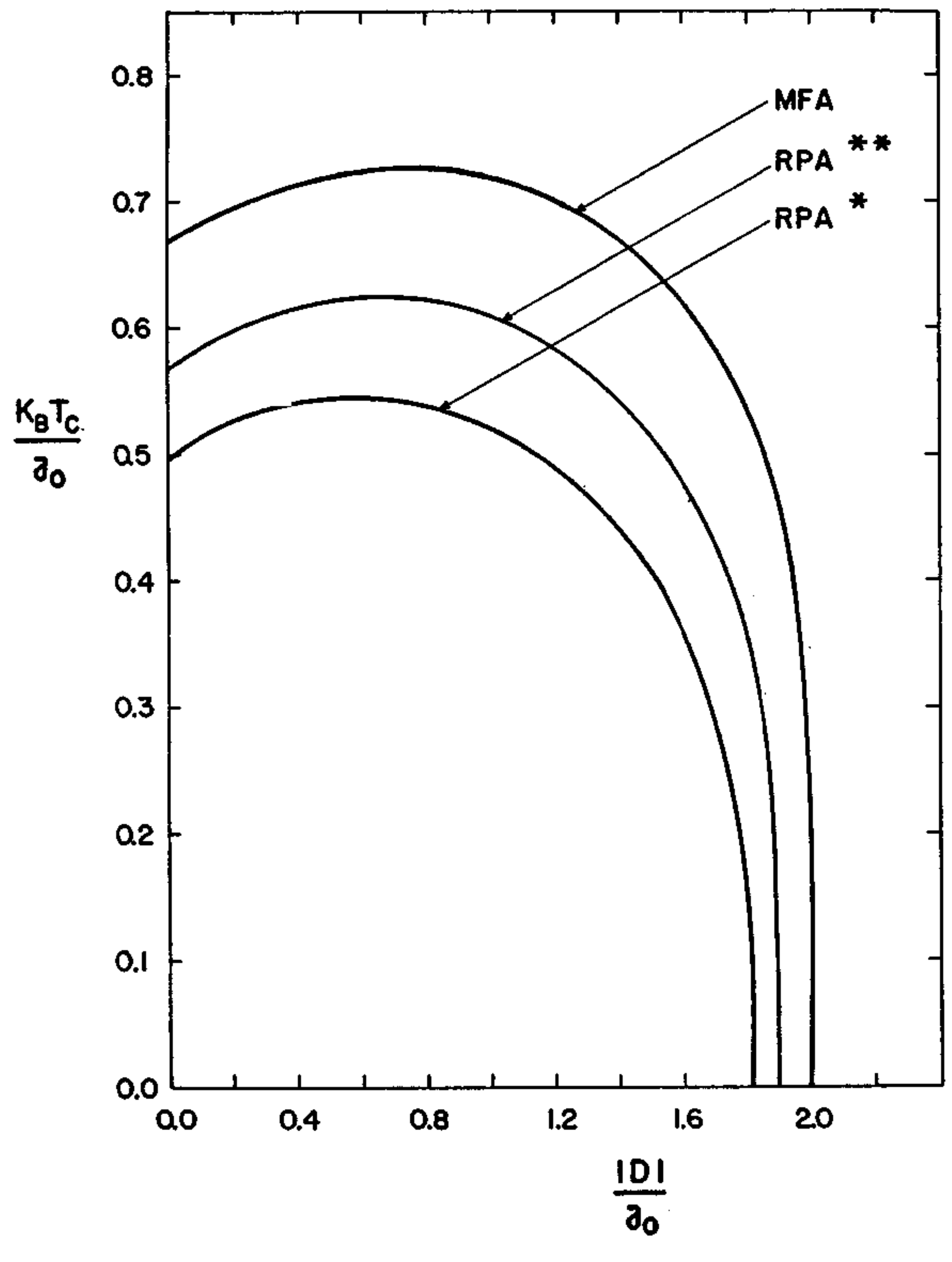

Fig. 1 R. Micnas et al

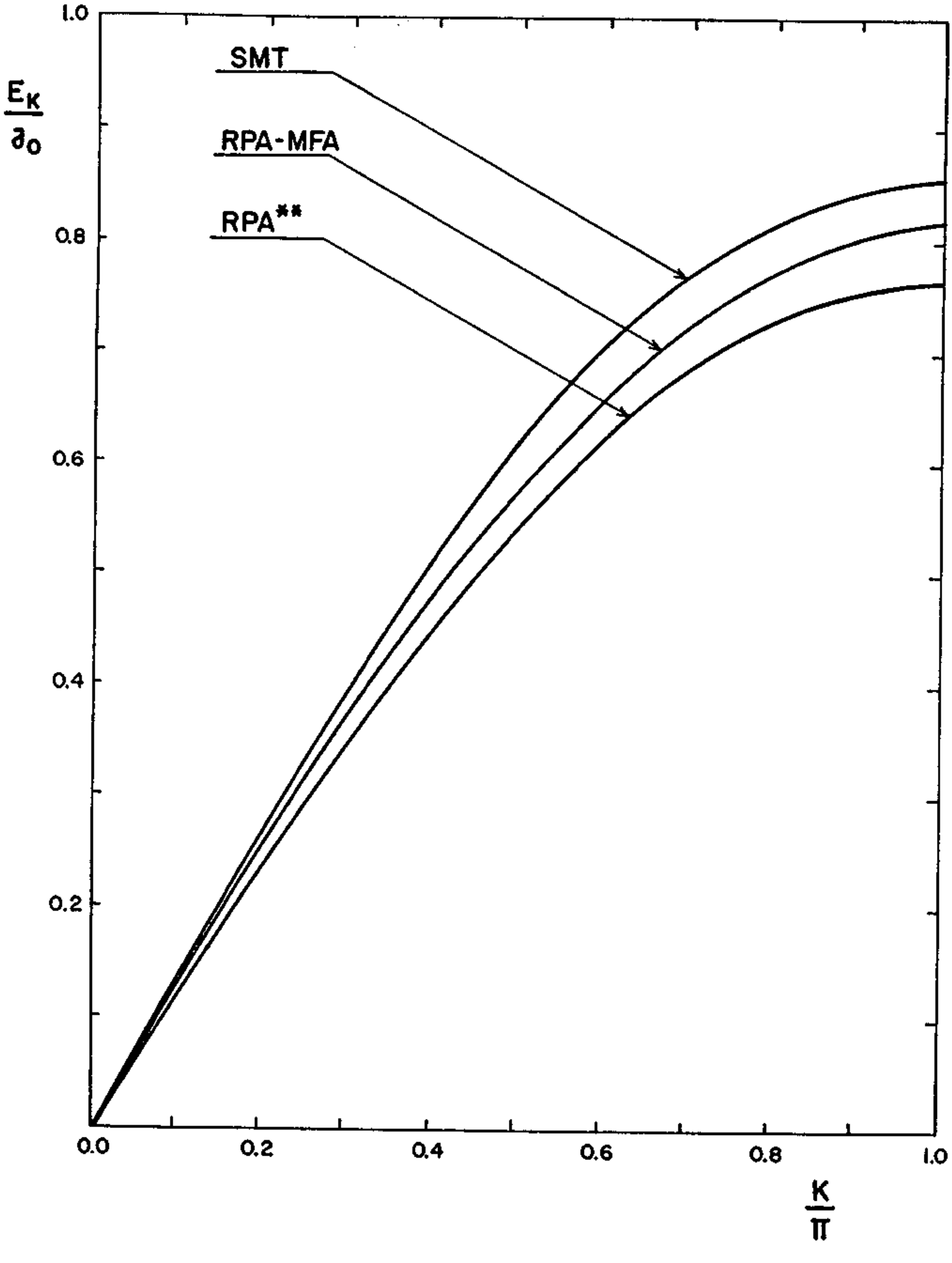

Fig. 2 R. Micnas et al