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FERROMAGNETISM BY THE GENERATOR COORDINATE METHOD

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The Generator Coordinate Method is applied to construct a boson representation of the energy of a $S = \frac{1}{2}$ ferromagnet near its ground-state. Considering one generator coordinate per lattice site the resulting representation coincides with the one obtained starting from the Dirac–Heisenberg Hamiltonian and using the Holstein–Primakoff transformation, expanded to all orders, inside the physical subspace. On the other hand, introducing generator coordinates to describe only the long-wavelength modes, we obtain a representation which can be consistently expanded until any desired order of approximation.

1. Introduction

The Holstein–Primakoff (HP) transformation[1]) is a well-known device for constructing boson representations of the many-fermion Hamiltonians that can be expressed in terms of spin operators. It is particularly useful in the formulation of the spin-wave theory which allows a theoretical analysis of the low temperature properties of magnetically ordered crystals[2,3]). However, it has the serious drawback that one of its main ingredients is an operator which, being defined as a square root, has to be approximated in all practical calculations. Usually one expands it as a power series considering only the constant term. One obtains in this way a Hamiltonian which is diagonal in the spin-wave states. Now, if one wishes to improve on this harmonic approximation, other terms of the expansion have to be considered and the process of picking them out is not at all clear, in particular for small values of S [3]). Indeed, in the absence of a natural parameter for defining the orders of magnitude, it is not easy to estimate beforehand the relative contributions of the successive terms of the expansion. Furthermore, since one treats as bosons all the possible modes, both the really collective and the less collective ones, the convergence of the whole process is doubtful. In fact only the truly collective modes should be well described already in the harmonic approximation, a condition which, if not sufficient, seems to be at least necessary for a fast convergence.

The Generator Coordinate Method (GCM)[4,5]) is a variational method of approximation for the stationary states of many-body systems, which also

yields boson representations, in a physical appealing way[6–9]). It has the advantage, moreover, of allowing from the start the separate treatment of the modes which are really collective[10]).

In the present paper we apply the GCM in order to obtain a boson representation of the low-energy modes of a $S = \frac{1}{2}$ ferromagnetic model, in two different approaches. In the first we take as generator coordinates complex parameters which define the spin state at each lattice point, starting from full alignment. We have therefore as many generator coordinates as sites in the Bravais lattice. This is done in section 3, where a representation is obtained which, as it is shown, is entirely equivalent to the one obtained applying the HP transformation to the so-called Dirac–Heisenberg Hamiltonian[11]). In the second we consider a far smaller number of generator coordinates, limiting the application of the GCM to the description of truly collective modes only. This is done in section 5, where we obtain a representation which can be consistently expanded to the desired order of approximation. In section 2 we explain in some detail how to obtain a boson representation from the GCM. With this we aim at both fixing the notation for the following sections and helping readers less familiar with the GCM. In the remaining of the present section we apply the HP transformation to the Dirac–Heisenberg Hamiltonian in order to get the representation to which the one obtained in section 3 will be compared.

The HP transformation can be cast in the form:

$$\begin{aligned} S_i^+ &= (2S)^{1/2} f_i(S) a_i, \\ S_i &= (2S)^{1/2} a_i^\dagger f_i(S), \\ S_i^z &= S - a_i^\dagger a_i, \end{aligned} \tag{1.1}$$

where

$$f_i(S) = (1 - a_i^\dagger a_i / 2S)^{1/2}. \tag{1.2}$$

In eqs. (1.1) $\boldsymbol{S}_i$ stands for the spin vector operator of the atom at the lattice site $i = 1, \ldots, N$, and a_i and $a_i^\dagger$ are annihilation and creation boson operators:

$$[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0.$$

The number operator $N_i = a_i^\dagger a_i$ has a simple meaning: its eigenvalues are the number of spin deviations from the maximum value S of S_i^z.

The Dirac–Heisenberg Hamiltonian can be written in the form

$$H = K - \sum_{i<j=1}^{N} J_{ij} (\tfrac{1}{2} + 2\boldsymbol{S}_i \cdot \boldsymbol{S}_j), \tag{1.3}$$

where the constant K represents the contribution of both the one-body part

and the direct terms of the two-body interaction of the correct Hamiltonian, and the remaining part of the right-hand side represents the contribution of the exchange terms of the two-body interaction. It has the same matrix elements as the correct Hamiltonian between Slater determinants built up from a set of N orthogonal orbitals, assigning to them $S = \frac{1}{2}$ spin states in all possible ways.

Inserting eqs. (1.1), with $S = \frac{1}{2}$, into eq. (1.3) one obtains an expression which we write for convenience in the following form

$$H_B = K + \sum_{i<j=1}^{N} H_{ij}, \tag{1.4}$$

where

$$H_{ij} = -J_{ij}[f_i(\tfrac{1}{2})a_i a_j^\dagger f_j(\tfrac{1}{2}) + a_i^\dagger f_i(\tfrac{1}{2}) f_j(\tfrac{1}{2}) a_j - a_i^\dagger a_i - a_j^\dagger a_j + 2a_i^\dagger a_i a_j^\dagger a_j + 1]. \tag{1.5}$$

The operator H_B is the boson representative of H in the HP theory. It acts on the boson space spanned by the set of orthogonal states

$$|n_1, n_2, \ldots, n_N\rangle = \prod_{i=1}^{N} |n_i\rangle,$$

where $|n_i\rangle$, with $n_i = 0, 1, 2, \ldots, \infty$, stands for the eigenstates of the operator $N_i = a_i^\dagger a_i$. One says that the state $|n_1, n_2, \ldots, n_N\rangle$ has n_1 bosons of kind 1, n_2 bosons of kind 2, etc. and n_N bosons of kind N.

Now the HP transformation of eqs. (1.1), with $S = \frac{1}{2}$, does set up a boson representation for the spin operators of their left-hand sides only in so far as the operators of their right-hand sides act within the restricted boson space whose states contain no more than one boson of a kind. One calls it the physical boson subspace. By that reason H_B does represent H only when it acts on the states of the physical boson subspace and outside that subspace H_B has no physical meaning. However, this is not, by itself, a serious objection to the theory because H_B does not connect the physical with the unphysical states and, therefore, the whole spectrum of H can be found by looking for the eigenvalues of H_B associated with eigenvectors belonging to the physical subspace. In mathematical terms one has:

$$\langle n_1', \ldots, n_N' | H_B | n_1, \ldots, n_N \rangle = 0,$$

if any $n_j' > 1$ and all $n_j \leqslant 1$, $j = 1, 2, \ldots, N$.
This equation results from eqs. (1.4) and (1.5) and from the following properties of the operator $f_i(\frac{1}{2})$, as defined on eq. (1.2):

$$f_i(\tfrac{1}{2})|n_1, \ldots, n_i, \ldots, n_N\rangle = \begin{cases} 0, & \text{if } n_i = 1 \\ |n_1, \ldots, n_i, \ldots, n_N\rangle, & \text{if } n_i = 0 \end{cases}. \tag{1.6}$$

We conclude therefore that the eigenvalues of H_B, say E, are

$$E = K + E', \tag{1.7}$$

where E' designates the eigenvalues of the operator $\Sigma_{i<j=1}^{N} H_{ij}$ associated with the eigenvectors, say $|v\rangle$, belonging to the physical subspace:

$$\left(\sum_{i<j=1}^{N} H_{ij} - E' \right) |v\rangle = 0. \tag{1.8}$$

Using now eqs. (1.6) we obtain, finally, from eq. (1.5), the following important relation which serves to determine the matrix elements of H_B inside the physical boson subspace:

$$H_{ij}|n_1, \ldots, n_i, \ldots, n_j, \ldots, n_N\rangle = -J_{ij}|n_1, \ldots, n_j, \ldots, n_i, \ldots, n_N\rangle, \tag{1.9}$$

if all $n_l \leq 1$, $l = 1, 2, \ldots, N$.

2. Boson representations from the GCM

One considers a family of preliminary wave functions $\Phi(x, \alpha)$ chosen according to the physical characteristics of the states one wishes to describe. Here x stands for all particle coordinates and α designates one or more parameters, real or complex, called generator coordinates, which label analytically the functions of the family.

Basically, in the GCM one looks for the wave functions of the form

$$\Psi_f(x) = \int f(\alpha)\Phi(x, \alpha)\, \mathrm{d}\alpha, \tag{2.1}$$

which make stationary the expectation value of the total energy of the system. If the parameters are complex, $\mathrm{d}\alpha$ should be understood as $\mathrm{d}(\mathrm{Re}\,\alpha) \cdot \mathrm{d}(\mathrm{Im}\,\alpha)$.

The weight functions $f(\alpha)$ are determined by the variational principle. They must therefore satisfy the well-known Griffin–Hill–Wheeler equation (GHW equation):

$$\int [H(\alpha^*, \alpha') - ES(\alpha^*, \alpha')] f(\alpha')\, \mathrm{d}\alpha' = 0,$$

where

$$H(\alpha^*, \alpha') = \int \Phi^*(x, \alpha) H \Phi(x, \alpha')\, \mathrm{d}x \tag{2.2a}$$

and

$$S(\alpha^*, \alpha') = \int \Phi^*(x, \alpha)\Phi(x, \alpha')\, dx \tag{2.2b}$$

are the energy- and norm-overlap kernels, respectively. Since $\Phi(x, \alpha)$ is analytic on α, they are both analytic on α^* and on α' separately.

To apply the GCM to a definite situation one should proceed as follows. First, we choose an appropriate family of preliminary wave functions. Then, we evaluate the energy- and norm-overlap kernels. Finally, we solve the GHW equation.

The first step determines, to a great extent, the outcome of the whole method. The trial wave functions have to be general enough to convey all the physical information we are looking for. But, on the other hand, too great a generality may impair the evaluation of the overlap kernels and the solution of the GHW equation. Thus, a balance must be obtained between these two conflicting purposes, the physical intuition playing an important role at this stage. The evaluation of the overlap kernels can be more or less difficult, but it raises no question of principle. As regards the last step, the GHW equation is an eigenvalue integral equation with two kernels. This circumstance, associated with the fact that the overlap kernels may have complicated expressions, makes its solution, in general, quite difficult. Sometimes there is no alternative but to resort to purely numerical methods from the very beginning. There are cases, however, depending on the mathematical structure of the kernels, where analytical treatments are possible which may lead us a long way towards the solution. One of those arises when we are interested on studying the normal modes of a system and consists in constructing boson representations.

To see how a boson representation can result from the GCM let us give another form to the GHW equation:

$$\int [\bar{H}(\alpha^*, \alpha') - E\bar{S}(\alpha^*, \alpha')] \exp\left(\sum_{i=1}^{N} \alpha_i^* \alpha_i'\right) f(\alpha')\, d\alpha' = 0, \tag{2.3}$$

where

$$\bar{H}(\alpha^*, \alpha') = H(\alpha^*, \alpha') \exp\left(-\sum_{i=1}^{N} \alpha_i^* \alpha_i'\right) \tag{2.4a}$$

and

$$\bar{S}(\alpha^*, \alpha') = S(\alpha^*, \alpha') \exp\left(-\sum_{i=1}^{N} \alpha_i^* \alpha_i'\right). \tag{2.4b}$$

We have supposed that there are N complex generator coordinates $\{\alpha_i; i = 1, 2, \ldots, N\}$.

Now we introduce a set of N independent harmonic oscillators, one associated with each generator coordinate. There is one creation operator a_i^+ and one annihilation operator a_i for the oscillator i. Together they satisfy the commutation rules characteristic of bosons:

$$[a_i, a_j^+] = \delta_{ij}, \quad [a_i, a_j] = [a_i^+, a_j^+] = 0. \tag{2.5a}$$

The number operator $N_i = a_i^+ a_i$ admits an orthonormal set of eigenstates $|n_i\rangle$, $n_i = 0, 1, \ldots, \infty$:

$$N_i|n_i\rangle = n_i|n_i\rangle, \quad \langle n_i \mid n_i'\rangle = \delta_{n_i,n_i'}. \tag{2.5b}$$

Furthermore one has

$$a_i^+|n_i\rangle = (n_i + 1)^{1/2}|n_i + 1\rangle, \quad a_i|n_i\rangle = (n_i)^{1/2}|n_i - 1\rangle. \tag{2.5c}$$

The coherent states of each oscillator are the eigenstates of the corresponding annihilation operator

$$a_i|\alpha_i\rangle = \alpha_i|\alpha_i\rangle.$$

Choosing the normalization in order to satisfy $\langle n_i = 0|\alpha_i\rangle = 1$, one can easily show that

$$|\alpha_i\rangle = \sum_{n_i=0}^{\infty} (n_i!)^{-1/2}(\alpha_i)^{n_i}|n_i\rangle,$$

for all points α_i of the complex plane. It is now clear the relationship between the harmonic oscillators and the generator coordinates: these are the eigenvalues of the annihilation operators. The following properties are easily deduced:

$$(a_i)^m|\alpha_i\rangle = (\alpha_i)^m|\alpha_i\rangle, \quad \langle\alpha_i|(a_i^+)^m = \langle\alpha_i|(\alpha_i^*)^m, \quad m = 0, 1, \ldots,$$

$$\langle\alpha_i \mid \alpha_i'\rangle = \exp(\alpha_i^*\alpha_i'),$$

$$\pi^{-1}\int |\alpha_i\rangle \exp(-|\alpha_i|^2)\langle\alpha_i| \, d\alpha_i = 1.$$

The second property traduces the fact that the set of coherent states is not orthogonal, and the third one that, notwithstanding, it is complete.

For the set of all oscillators we have the coherent states

$$|\alpha\rangle = \prod_{i=1}^{N} |\alpha_i\rangle,$$

with the properties

$$(a_i)^m|\alpha\rangle = (\alpha_i)^m|\alpha\rangle, \quad \langle\alpha|(a_i^+)^m = \langle\alpha|(\alpha_i^*)^m, \quad m = 0, 1, \ldots, \tag{2.6a}$$

$$\langle \alpha \mid \alpha' \rangle = \exp\left(\sum_{i=1}^{N} \alpha_i^* \alpha_i'\right), \tag{2.6b}$$

$$\pi^{-N} \int |\alpha\rangle \exp\left(-\sum_{i=1}^{N} |\alpha_i|^2\right) \langle \alpha| \, \mathrm{d}\alpha = 1. \tag{2.6c}$$

From eq. (2.6a) we obtain the relation which is on the basis of the whole approach:

$$G(\alpha^*, \alpha') = \frac{\langle \alpha| : G(a^+, a) : |\alpha'\rangle}{\langle \alpha \mid \alpha' \rangle}, \tag{2.7}$$

where $G(\alpha^*, \alpha')$ is any analytical function of the $2N$ variables $\{\alpha_i^*, \alpha_i'\}$. In this relation a^+ stands for all creation operators, a for all annihilation operators and: $G(a^+, a)$: designates the operator obtained in the following way:

(1) we expand $G(\alpha^*, \alpha')$ as a power series of the $2N$ variables $\{\alpha_i^*, \alpha_i'\}$;

(2) in each term of the expansion we place all the starred variables to the left of the primed ones;

(3) finally we make the substitutions $\alpha_i^* \to a_i^+$; $\alpha_i' \to a_i$.

Now we use eqs. (2.6b) and (7) to transform eq. (2.3). We obtain

$$\int \langle \alpha | \mathscr{H}(a^+, a) - E\mathscr{S}(a^+, a) | \alpha' \rangle f(\alpha') \, \mathrm{d}\alpha' = 0,$$

where we have adopted the following notation: $\mathscr{H}(a^+, a) \equiv : \bar{H}(a^+, a) :$ and $\mathscr{S}(a^+, a) \equiv : \bar{S}(a^+, a) :$. Supposing that the integration commutes with the operators $\mathscr{H}(a^+, a)$ and $\mathscr{S}(a^+, a)$ we get finally

$$[\mathscr{H}(a^+, a) - E\mathscr{S}(a^+, a)]|f\rangle = 0, \tag{2.8}$$

where

$$|f\rangle = \int f(\alpha) |\alpha\rangle \, \mathrm{d}\alpha. \tag{2.9}$$

To write eq. (2.8) we have also used the fact that the set of coherent states is a complete one.

If we now solve eq. (2.8) in the space spanned by the N-oscillator states we obtain the desired energies and, after inversion of eq. (2.9), the weight functions $f(\alpha)$ to be inserted into eq. (2.1). The inversion of eq. (2.9) is straightforward if one uses the closure relation eq. (2.6c). One has:

$$f(\alpha) = \pi^{-N} \exp\left(-\sum_{i=1}^{N} |\alpha_i|^2\right) \langle \alpha \mid f \rangle. \tag{2.10}$$

The eq. (2.8) can still be put in the usual form of an eigenvalue problem:

$$[H_B(a^+, a) - E]|\tilde{f}\rangle = 0, \tag{2.11}$$

where

$$H_B(a^+, a) = \mathcal{S}^{-1/2}(a^+, a)\mathcal{H}(a^+, a)\mathcal{S}^{-1/2}(a^+, a) \tag{2.12}$$

and

$$|\tilde{f}\rangle = \mathcal{S}^{1/2}(a^+, a)|f\rangle.$$

3. Application of the GCM to a model ferromagnet

Our model of a ferromagnet crystal consists of N electrons tightly bound to the same number of singly charged ions which are fixed to the sites of a simple Bravais lattice. We suppose that the ground-state of the many-electron system is well described by the following Slater determinant:

$$\Phi(x) = (N!)^{-1/2} \det\{w_i(\boldsymbol{r}_j)\chi_{1/2}(s_j)\}, \tag{3.1}$$

where $w_i(\boldsymbol{r}_j) \equiv w(\boldsymbol{r}_j - \boldsymbol{R}_i)$ is a Wannier function for the electron j centered on the lattice site i and $\chi_{1/2}(s_j)$ is the spin eigenstate of the same electron corresponding to the component $m = \frac{1}{2}$ along some direction fixed in space. One knows, of course, that a single Slater determinant with orthogonal orbitals, either of the energy-band type or of the localized Wannier type as in eq. (3.1), does not reproduce well the internal energy at absolute zero[12]). In particular it overestimates the tendency towards spin alignment. One knows also that in order to correct this effect one has to introduce electron correlation[13]). One may consider, for instance, configurations with ionic states, in which a Wannier function is occupied by two electrons. The main role of the correlation is to reduce the self-energy of the atomic orbitals involved in the single-particle wave functions. We admit that the same objective can be achieved through an appropriate correction to the real electron–electron interaction. Our Hamiltonian reads therefore as

$$H = \sum_{i=1}^{N} U(i) + \sum_{i<j=1}^{N} V(i, j), \tag{3.2}$$

where $U(i)$ stands for the kinetic energy of the electron i plus its potential energy in the field of the crystal ions and $V(i, j)$ represents some effective potential energy of the interaction between electrons i and j. For our purpose it is not necessary to specify the form of the latter, being enough to assume that it does not act upon the spin variables.

In this context, we take as preliminary wave functions of the GCM the following Slater determinants:

$$\Phi(x, \alpha) = (N!)^{-1/2} \det\{w_i(\boldsymbol{r}_j)\chi(s_j, \alpha_i)\}, \tag{3.3}$$

where the spin function $\chi(s_j, \alpha_i)$ is given by

$$\chi(s_j, \alpha_i) = \chi_{1/2}(s_j) + \alpha_i \chi_{-1/2}(s_j). \tag{3.4}$$

The spin state at the lattice point i is thus defined by the complex parameter α_i which is a generator coordinate in our theory. We would expect to have, for the lowest energy states,

$$|\alpha_i| \ll 1.$$

The fact that the spin function of eq. (3.4) is not normalized to unity does not matter as far as the GHW equation is concerned.

Inserting eqs. (3.2–4) into eqs. (2.2a and b) one obtains:

$$S(\alpha^*, \alpha') = \prod_{i=1}^{N} (1 + \alpha_i^* \alpha_i') \tag{3.5}$$

and

$$H(\alpha^*, \alpha') = \left[K - \sum_{i<j=1}^{N} J_{ij} \frac{(1 + \alpha_i^* \alpha_j')(1 + \alpha_j^* \alpha_i')}{(1 + \alpha_i^* \alpha_i')(1 + \alpha_j^* \alpha_j')} \right] S(\alpha^*, \alpha'). \tag{3.6}$$

We have used the orthogonality of the Wannier functions referring to different centers. Moreover we have used the following notation:

$$K = \sum_{i=1}^{N} U_i + \sum_{i<j=1}^{N} D_{ij},$$

$$U_i = \int w_i^*(\boldsymbol{r}_1) U(1) w_i(\boldsymbol{r}_1) \, \mathrm{d}^3 \boldsymbol{r}_1,$$

$$D_{ij} = \int\int w_i^*(\boldsymbol{r}_1) w_j^*(\boldsymbol{r}_2) V(1,2) w_i(\boldsymbol{r}_1) w_j(\boldsymbol{r}_2) \, \mathrm{d}^3 \boldsymbol{r}_1 \, \mathrm{d}^3 \boldsymbol{r}_2,$$

$$J_{ij} = \int\int w_i^*(\boldsymbol{r}_1) w_j^*(\boldsymbol{r}_2) V(1,2) w_j(\boldsymbol{r}_1) w_i(\boldsymbol{r}_2) \, \mathrm{d}^3 \boldsymbol{r}_1 \, \mathrm{d}^3 \boldsymbol{r}_2.$$

From eqs. (2.4a) and (2.4b) and eqs. (3.5) and (3.6) one obtains

$$\bar{S}(\alpha^*, \alpha') = \exp\left(- \sum_{i=1}^{N} \alpha_i^* \alpha_i' \right) \prod_{l=1}^{N} (1 + \alpha_l^* \alpha_l') \tag{3.7}$$

and

$$\bar{H}(\alpha^*, \alpha') = \left[K - \sum_{i<j=1}^{N} J_{ij} \frac{(1 + \alpha_i^* \alpha_j')(1 + \alpha_j^* \alpha_i')}{(1 + \alpha_i^* \alpha_i')(1 + \alpha_j^* \alpha_j')} \right] \bar{S}(\alpha^*, \alpha') \tag{3.8}$$

or still

$$\bar{H}(\alpha^*, \alpha') = K \bar{S}(\alpha^*, \alpha') - \exp\left(- \sum_{i=1}^{N} \alpha_i^* \alpha_i' \right) \times \sum_{i<j=1}^{N} \left[J_{ij} (1 + \alpha_i^* \alpha_j')(1 + \alpha_j^* \alpha_i') \prod_{\substack{l=1 \\ (\neq i,j)}}^{N} (1 + \alpha_l^* \alpha_l') \right]. \tag{3.8'}$$

We can now construct the boson operators $\mathcal{S}(a^+, a)$ and $\mathcal{H}(a^+, a)$ of eq. (2.8), according to the procedure explained in the last section. Starting with the former we have, from eq. (3.7):

$$\mathcal{S}(a^+, a) =: \exp\Big(-\sum_{i=1}^{N} a_i^+ a_i\Big) \prod_{i=1}^{N} (1 + a_i^+ a_i):$$

$$= P_0 + \sum_{i=1}^{N} a_i^+ P_0 a_i + \sum_{i<j=1}^{N} a_i^+ a_j^+ P_0 a_i a_j + \cdots$$

$$+ a_1^+ a_2^+ \ldots a_N^+ P_0 a_1 a_2 \ldots a_N, \tag{3.9}$$

where

$$P_0 =: \exp\Big(-\sum_{i=1}^{N} a_i^+ a_i\Big):. \tag{3.10}$$

It is easy to see what is the result when the operator P_0 acts on the basic states

$$|n_1, n_2, \ldots, n_N\rangle = \prod_{i=1}^{N} |n_i\rangle \tag{3.11}$$

of the system of independent oscillators introduced in the last section. One has, from eqs. (2.5), (3.10) and (3.11):

$$P_0|n_1, \ldots, n_N\rangle = \delta_{n_1 0} \ldots \delta_{n_N 0}|n_1, \ldots, n_N\rangle.$$

Hence P_0 is the projector on the boson vacuum. Using this property in eq. (3.9) we conclude that in our problem the operator $\mathcal{S}(a^+, a)$ turns out to be the projector onto the boson subspace of the vectors with at most one boson of each kind:

$$\mathcal{S}(a^+, a)|n_1, \ldots, n_N\rangle = \begin{cases} 0; & \text{if any } n_j > 1,\ j = 1, 2, \ldots, N \quad (3.12) \\ |n_1, \ldots, n_N\rangle; & \text{if all } n_j \leq 1,\ j = 1, 2, \ldots, N. \quad (3.13) \end{cases}$$

By analogy with the HP theory, we call that subspace the physical boson subspace.

As regards $H(a^+, a)$ we have, from eq. (3.8):

$$\mathcal{H}(a^+, a) = K\mathcal{S}(a^+, a) + \sum_{i<j=1}^{N} \mathcal{H}_{ij}(a^+, a), \tag{3.14}$$

where

$$\mathcal{H}_{ij}(a^+, a) = -J_{ij} : \exp\Big(-\sum_{m=1}^{N} a_m^+ a_m\Big)(1 + a_i^+ a_j)(1 + a_j^+ a_i) \prod_{\substack{l=1 \\ (\neq i,j)}}^{N} (1 + a_l^+ a_l):.$$

Using eq. (3.10) we can give this expression the more convenient form

$$\mathcal{H}_{ij}(a^+, a) = -J_{ij}\Big[P_0 + a_i^+ P_0 a_j + a_j^+ P_0 a_i + \sum_{\substack{l=1 \\ (\neq i,j)}}^{N} a_l^+ P_0 a_l + a_i^+ a_j^+ P_0 a_i a_j$$

$$+ \sum_{\substack{l=1 \\ (\neq i,j)}}^{N} (a_i^+ a_l^+ P_0 a_j a_l + a_j^+ a_l^+ P_0 a_i a_l)$$

$$+ \sum_{\substack{l<m=1 \\ (\neq i,j)}}^{N} a_l^+ a_m^+ P_0 a_l a_m + \cdots + a_1^+ a_2^+ \ldots a_N^+ P_0 a_1 a_2 \ldots a_N\Big],$$

from which one sees immediately how the operator $\mathcal{H}_{ij}(a^+, a)$ acts on the basic vectors of eq. (3.11). One obtains:

$$\mathcal{H}_{ij}(a^+, a)|n_1, \ldots, n_N\rangle = 0, \quad \text{if any } n_l > 1, l = 1, 2, \ldots, N, \tag{3.15}$$

$$\mathcal{H}_{ij}(a^+, a)|n_1, \ldots, n_i, \ldots, n_j, \ldots, n_N\rangle = -J_{ij}|n_1, \ldots, n_j, \ldots, n_i, \ldots, n_N\rangle,$$
$$\text{if all } n_l \leq 1, l = 1, 2, \ldots, N. \tag{3.16}$$

Now, from eqs. (3.12), (3.14) and (3.15) we see that the solution of eq. (2.3) is limited to the physical boson subspace. Moreover, eq. (3.13) tells us that inside the physical boson subspace $\mathcal{S}(a^+, a)$ behaves as the identity operator. We are left therefore with the solution of the equation

$$\Big[\sum_{i<j=1}^{N} \mathcal{H}_{ij}(a^+, a) - E'\Big]|f\rangle = 0, \tag{3.17}$$

inside the physical subspace, where E' is related with E as in eq. (1.7).

Comparing eqs. (3.17) and (3.16) respectively with eqs. (1.8) and (1.9) we conclude therefore that the GCM, with the trial function of eq. (3.3), leads to the same energy spectrum as the HP treatment, expanded to all orders, inside the physical subspace. We have the following expression, valid in the whole space,

$$\mathcal{H}(a^+, a) = H_B \mathcal{S}(a^+, a),$$

where H_B is the operator defined by eq. (1.4).

4. Spin-waves in the framework of the GCM

The overlap kernel expressions as given by eqs. (3.5) and (3.6) are exact but difficult to deal with. In the so-called Gaussian and harmonic approximation one assumes that the norm-overlap kernel is Gaussian and that the ratio of the energy- to the norm-overlap kernels is quadratic on the generator coordinates.

Within this approximation the above mentioned equations read as

$$S(\alpha^*, \alpha') = \exp\left(\sum_{i=1}^{N} \alpha_i^* \alpha_i'\right) \tag{4.1}$$

and

$$H(\alpha^*, \alpha') = \left\{K - \sum_{i<j=1}^{N} J_{ij}[1 - (\alpha_i^* - \alpha_j^*)(\alpha_i' - \alpha_j')]\right\} S(\alpha^*, \alpha'). \tag{4.2}$$

Inserting these equations into eqs. (2.4a) and (2.4b) yields

$$\bar{S}(\alpha^*, \alpha') = 1$$

and

$$\bar{H}(\alpha^*, \alpha') = K - \sum_{i<j=1}^{N} J_{ij}[1 - (\alpha_i^* - \alpha_j^*)(\alpha_i' - \alpha_j')]. \tag{4.3}$$

The corresponding boson operators have the following forms

$$\mathcal{S}(a^+, a) = 1, \quad \mathcal{H}(a^+, a) = \mathcal{H}_0 + \mathcal{H}_2(a^+, a), \tag{4.4}$$

where

$$\mathcal{H}_0 = K - \sum_{i<j=1}^{N} J_{ij} \tag{4.4a}$$

and

$$\mathcal{H}_2(a^+, a) = \sum_{i<j=1}^{N} J_{ij}(a_i^+ - a_j^+)(a_i - a_j). \tag{4.4b}$$

Substituting these operators into eq. (2.12) we obtain finally for the GCM boson representative of the energy

$$H_B(a^+, a) = \mathcal{H}(a^+, a),$$

where $\mathcal{H}(a^+, a)$ is given by eqs. (4.4).

Now this is precisely the so-called harmonic approximation of the HP theory, as it can easily be seen by inserting $f_i(\frac{1}{2}) = 1$ into eq. (1.5) and substituting into eq. (1.4) the resulting expression for H_{ij}, after having dropped the quartic term. One can conclude therefore that the GCM boson representative of the energy is diagonal in the spin-wave states when the overlap kernels are Gaussian and harmonic. One can also see immediately how to go beyond the independent spin-wave picture within the framework of the GCM, at least in principle: one simply adds successive corrections to eqs. (4.1) and (4.2) and proceeds according to the general theory of section 2. However, before doing that, we develop a little further the results obtained this far.

As it is well known the spin-wave states are created and annihilated by the Fourier transforms of the operators a_i^+ and a_i respectively, namely:

$$a_k^+ = N^{-1/2} \sum_{j=1}^{N} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_j) a_j^+, \quad a_k = N^{-1/2} \sum_{j=1}^{N} \exp(-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_j) a_j. \tag{4.5}$$

Inverting these equations one obtains

$$a_j^+ = N^{-1/2} \sum_{k} \exp(-\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_j) a_k^+, \quad a_j = N^{-1/2} \sum_{k} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_j) a_k, \quad j = 1, 2, \ldots, N, \tag{4.6}$$

where k lies within the first Brillouin zone, taking all values compatible with the periodic boundary conditions. Inserting eqs. (4.6) into eq. (4.4b) one gets:

$$\mathscr{H}_2(a^+, a) = \sum_{k} (J_0 - J_k) a_k^+ a_k,$$

where

$$J_k = \sum_{\substack{l=1 \\ (l \neq j)}}^{N} J_{jl} \exp[\mathrm{i}\boldsymbol{k} \cdot (\boldsymbol{R}_j - \boldsymbol{R}_l)].$$

The eigenvectors of $\mathscr{H}_2(a^+, a)$ have the following general form

$$|f_{(n_k)}\rangle = \prod_{k} (n_k!)^{-1/2} (a_k^+)^{n_k} |0\rangle.$$

To see what kind of wave functions correspond to these eigenvectors, let us consider, for instance, an eigenstate with only one boson. If k designates its wave-vector one has, using the first of eqs. (4.5):

$$|f_{1_k}\rangle = a_k^+ |0\rangle = N^{-1/2} \sum_{j=1}^{N} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_j) a_j^+ |0\rangle.$$

Entering with this ket into eq. (2.10) one obtains, taking into account eq. (2.6a) and the normalization we have chosen for the coherent states,

$$f_{1_k}(\alpha) = \pi^{-N} N^{-1/2} \exp\left(-\sum_{i=1}^{N} |\alpha_i|^2\right) \sum_{j=1}^{N} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_j) \alpha_j^*.$$

Inserting now this weight function into eq. (2.1) one obtains

$$\Psi_{1_k}(x) = \pi^{-N} N^{-1/2} \sum_{j=1}^{N} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_j) \int \alpha_j^* \exp\left(-\sum_{i=1}^{N} |\alpha_i|^2\right) \Phi(x, \alpha)\, \mathrm{d}\alpha.$$

Expanding $\Phi(x, \alpha)$ as a power series of the α_i and using the following identity[14])

$$\int z^{*m} z^n \exp(-|z|^2)\, \mathrm{d}z = \pi n! \delta_{nm},$$

one obtains finally

$$\Psi_{1_k}(x) = N^{-1/2} \sum_{j=1}^{N} \exp(i\boldsymbol{k} \cdot \boldsymbol{R}_j) \left. \frac{\partial \Phi(x, \alpha)}{\partial \alpha_j} \right|_{\alpha=0}.$$

This is precisely a Bloch's spin-wave[15]) as can be seen from the fact that $(\partial \Phi(x, \alpha)/\partial \alpha_j)|_{\alpha=0}$ is obtained from the ground-state $\Phi(x, 0)$ inverting the spin at the site j. In the problem under study, Bloch's theory is the equivalent of the Tamm–Dancoff approximation of nuclear physics. The relation between the GCM in the Gaussian and harmonic approximation and the Tamm–Dancoff approximation is pointed out in section 6.4 of ref. 7.

We resume now the task of improving on the independent spin-wave picture. As far as the norm-overlap kernel is concerned one notices that eq. (3.5) can also be put into the form

$$S(\alpha^*, \alpha') = \exp\left[\sum_{i=1}^{N} \log(1 + \alpha_i^* \alpha_i')\right].$$

After expanding the logarithm as a power series of the $\alpha_i^* \alpha_i'$ it can still be written as

$$S(\alpha^*, \alpha') = \left[1 - \tfrac{1}{2} \sum_{i=1}^{N} (\alpha_i^* \alpha_i')^2 + \cdots\right] \exp\left(\sum_{i=1}^{N} \alpha_i^* \alpha_i'\right).$$

The Gaussian approximation, eq. (4.1), results from this expression when one considers only the leading term of the expansion inside square brackets. A first correction to it would consist therefore in taking also the next term of the expansion. This would give:

$$\bar{S}(\alpha^*, \alpha') = 1 - \tfrac{1}{2} \sum_{i=1}^{N} (\alpha_i^* \alpha_i')^2. \tag{4.7}$$

With this expression it is quite easy to write down the corresponding boson operator:

$$\mathcal{S}(a^+, a) = 1 - \tfrac{1}{2} \sum_{i=1}^{N} a_i^{+2} a_i^2. \tag{4.8}$$

For constructing the boson representative of the energy one needs the inverse of its square root, $\mathcal{S}^{-1/2}(a^+, a)$. However, this operator is not well defined. This can be seen expanding the right-hand side of eq. (4.8) as a power series. One obtains, using the commutation rules for the boson operators, contributions like $\sum_{i=1}^{N} a_i^{+2} a_i^2$ from all the terms but the first, and the series of their coefficients diverges.

This is a serious difficulty of the method which, from other fields of application, is known to arise whenever one uses too large a trial space that

allows the description of both collective and less collective modes of excitation of the many-body system[10]). In the following we shall limit the trial space from the very beginning, taking care of including only the possibility of exciting modes which are really collective.

5. GCM for only the low-energy modes

The previous results could also be obtained if we have used as generator coordinates the parameters α_k related to the α_j of eq. (3.4) by the following transformation:

$$\alpha_j = N^{-1/2} \sum_k \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_j)\alpha_k, \quad j = 1, 2, \ldots, N.$$

The use of the α_j or the α_k is merely a question of convenience, either of them being suitable for the set up of a boson representation. With the first set one associated the localized boson operators $\{a_j, a_j^+\}$ and with the second the spin-wave boson operators $\{a_k, a_k^+\}$.

Now, if we wish to associate boson operators only with the low-energy modes we should take as generator coordinates the elements of $\{\alpha_k\}$ corresponding to values of $|k|$ smaller than some k_0. The spin-deviation parameters which appear in eq. (3.4) should then be given as

$$\alpha_j = N^{-1/2} \sum_{k \in D} \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{R}_j)\alpha_k, \quad j = 1, 2, \ldots, N, \tag{5.1}$$

where D consists of all points of the first Brillouin zone, compatible with the periodic boundary conditions, which are inside a sphere of radius k_0. This value should be much smaller than the inverse of the lattice constant.

Notice that the spin deviation parameters defined by eq. (5.1) are not independent of each other. Therefore they cannot be treated as generator coordinates and it is not possible now to speak of localized boson operators. However the complex variables α_k, with $|k| < k_0$, are arbitrary and with them we shall associate the boson operators corresponding to the long-wavelength spin-waves. In order to achieve this purpose we insert eq. (5.1) into the expressions we had before for the overlap kernels. It is important to note that

$$\sum_{i=1}^{N} \alpha_i^* \alpha_i' = \sum_{k \in D} \alpha_k^* \alpha_k'.$$

Instead of eq. (4.7) we write now

$$\bar{S}(\alpha^*, \alpha') = 1 - (2N)^{-1} \sum_{1,2,3,4 \in D} \delta(1 + 2 - 3 - 4)\alpha_1^* \alpha_2^* \alpha_3' \alpha_4', \tag{5.2}$$

where 1, 2, 3 and 4 denote k_1, k_2, k_3 and k_4, respectively, and the $\delta(n) \equiv \delta_{n,0}$ is the usual Kronecker symbol. From eq. (5.2) one has

$$\mathcal{S}(a^+, a) = 1 - (2N)^{-1} \sum_{1,2,3,4 \in D} \delta(1+2-3-4) a_1^\dagger a_2^\dagger a_3 a_4$$

and

$$\mathcal{S}^{-1/2}(a^+, a) = 1 + (4N)^{-1} \sum_{1,2,3,4 \in D} \delta(1+2-3-4) a_1^\dagger a_2^\dagger a_3 a_4 + \cdots. \tag{5.3}$$

Since the summation over each k covers a number of points must smaller than N, one is sure that the successive terms of the above expansion are rapidly decreasing in magnitude. In this way the problem which has arisen in the last section is avoided.

As regards the energy-overlap kernel, let us go back to eq. (3.8). Considering the first correction to the harmonic approximation one has:

$$\bar{H}(\alpha^*, \alpha') = \bar{H}_{\text{harm}}(\alpha^*, \alpha') \left[1 - \tfrac{1}{2} \sum_{i=1}^{N} (\alpha_i^* \alpha_i')^2 \right] + \sum_{i<j=1}^{N} J_{ij} (\alpha_i^* - \alpha_j^*)(\alpha_i^* \alpha_i' + \alpha_j^* \alpha_j')(\alpha_i' - \alpha_j'),$$

where $\bar{H}_{\text{harm}}(\alpha^*, \alpha')$ is give by eq. (4.3). Inserting here the eq. (5.1) one can construct from the resulting expression the boson operator $\mathcal{H}(a^+, a)$.

From eq. (2.12) and taking into account eq. (5.3) one obtains finally, after some straightforward calculations,

$$H_B(a^+, a) = \mathcal{H}_0 + \mathcal{H}_2(a^+, a) + \mathcal{H}_4(a^+, a),$$

where

$$\mathcal{H}_2(a^+, a) = \sum_{k \in D} (J_0 - J_k) a_k^\dagger a_k$$

and

$$\mathcal{H}_4(a^+, a) = (2N)^{-1} \sum_{1,2,3,4 \in D} (J_1 + J_3 - 2J_{1-3}) \delta(1+2-3-4) a_1^\dagger a_2^\dagger a_3 a_4.$$

This is precisely the result one obtains inserting the HP transformation with

$$f_i(\tfrac{1}{2}) = 1 - \tfrac{1}{2} N_i \tag{5.4}$$

into the Dirac–Heisenberg operator. The eq. (5.4) corresponds to keeping the first two terms in the expansion of $f_i(\frac{1}{2})$ as a power series of $N_i = a_i^\dagger a_i$, a procedure which, although usual, is not self-justified. Indeed one should as well have considered a normal-ordered expansion whose first two terms are

$$f_i(\tfrac{1}{2}) = 1 - N_i.$$

Our result can therefore be understood as a justification of the HP theory with $f_i(\frac{1}{2})$ given by eq. (5.4), for the lowest energy modes.

6. Conclusions

This work shows once more that the GCM is a powerful tool for describing collective phenomena, allowing a deeper understanding of the relevant aspects. In the present context it provides a clear link between the original Bloch theory on the spin-waves in the configuration space with the formalism in an ideal boson space. Moreover, due to the fact that it allows the separate treatment of the low-lying spectrum, it yields a convergent expansion for the boson representative of the energy.

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