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Exact Bose expansion for general spin

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Abstract. An exact Bose expansion for general spin S is presented. It is a generalisation of a previously derived expansion for $S=\frac{1}{2}$. The analysis of the resulting Bose–Hilbert space yields a new understanding of existing Bose expansions and of the meaning of the spin-boson transformations in general. The Bloch sum rule for spin systems is proven rigorously for any value of S and every temperature. It is argued that phase transitions in quantum spin systems can be regarded as generalised Bose condensation processes. Possible applications to quantum spin systems are mentioned.

1. Introduction

In a previous work (Goldhirsch *et al* 1979) it was shown how one can represent quantum spin operators in terms of Bose operators for the case $S=\frac{1}{2}$. It was also shown how the problem of unphysical states appearing in other bosonisation schemes could be avoided, and some properties of quantum spin systems were analysed using the formalism developed. In this work it is shown how these results can be generalised to any spin S, thus yielding a unified picture of the process of Bose expansion of spin operators and its meaning.

The Bloch sum rule is shown to follow trivially from the structure of the Bose–Hilbert space. The formalism is demonstrated for the $S=1$ case. The high-S limit is considered and a way to make a $1/S$ expansion is shown. The Bose expansion can be used in order to write down the partition function of any quantum spin system in terms of a path integral. The path integrals corresponding to quantum spin models are discussed briefly from the point of view of the renormalisation group. The role played by an invariant of the theory, which is a function of the number operator, is shown to be similar to the role of the total particle number in a usual Bose system, when the phase transition is considered. As a result one can argue that phase transitions in quantum spin systems can be described as generalised Bose condensation processes.

2. The spin-boson transformation

In this section the bosonisation of spin operators is defined. First a few definitions are necessary.

Let S^+, S^-, S^z be the usual spin angular momentum operators, satisfying the spin commutation relations

$$[S^+, S^-]=2S^z \qquad [S^z, S^+]=S^+ \qquad [S^z, S^-]=-S^- \tag{1}$$

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and the relation

$$S^+ = (S^-)^\dagger \tag{2}$$

(a dagger means Hermitian conjugate).

In addition, we assume that we are dealing with spin S (or, more rigorously, with a representation corresponding to spin S) so that

$$\tfrac{1}{2}(S^+S^- + S^-S^+) + (S^z)^2 = S(S+1). \tag{3}$$

The operators S^+, S^-, S^z are considered as $(2S+1)\times(2S+1)$ matrices which act on a $(2S+1)$-dimensional linear space, henceforth called the spin space.

We would like to find a set of three operators $\tilde{S}^+, \tilde{S}^-, \tilde{S}^z$ defined in a Bose–Hilbert space, which have the properties (1), (2), (3). These operators will be called the bosonised spin operators. Let the boson operators be denoted by $B, B^\dagger$. Their commutation relations are $[B, B^\dagger] = 1$. The number operator is $\hat{N} \equiv B^\dagger B$. We choose as a basis for the Hilbert space of the bosons the set of normalised eigenstates of $\hat{N}$. An eigenstate of $\hat{N}$ with eigenvalue n will be denoted by the ket $|n\rangle$. Let $F(x)$ be any function defined at least on the set of non-negative integers. Then one defines a function of the operator $\hat{N}$, $F(\hat{N})$, through its matrix elements:

$$\langle n|F(\hat{N})|n'\rangle = \delta_{nn'}F(n). \tag{4}$$

In particular, we shall define

$$f(x) = (2S+1)\left\{\frac{x}{2S+1}\right\} - S \tag{5}$$

where $\{y\}$ means 'the fractional part of y', e.g. $\{1{\cdot}2\} = 0{\cdot}2, \{-0{\cdot}2\} = 0{\cdot}8$.

Now we are in a position to define $\tilde{S}^+, \tilde{S}^-, \tilde{S}^z$:

$$\tilde{S}^+ = B^\dagger\left(\frac{S(S+1) - f(\hat{N})(f(\hat{N})+1)}{\hat{N}+1}\right)^{1/2} \tag{6}$$

$$\tilde{S}^- = \left(\frac{S(S+1) - f(\hat{N})(f(\hat{N})+1)}{\hat{N}+1}\right)^{1/2} B \tag{7}$$

$$\tilde{S}^z = f(\hat{N}). \tag{8}$$

The matrix elements of $\tilde{S}^+, \tilde{S}^-, \tilde{S}^z$ in the Bose space are easily found:

$$\langle n'|\tilde{S}^+|n\rangle = \delta_{n',n+1}[S(S+1) - f(n)(f(n)+1)]^{1/2} \tag{9}$$

$$\langle n'|\tilde{S}^-|n\rangle = \delta_{1+n',n}[S(S+1) - f(n')(f(n')+1)]^{1/2} \tag{10}$$

$$\langle n'|\tilde{S}^z|n\rangle = \delta_{n,n'}f(n).. \tag{11}$$

It should be noted that the square root is always a real number since $S(S+1) - f(n)(f(n)+1) \geqslant 0$ for any integer n, as can be seen from (5).

It is easy to check directly that demands (1), (2) and (3) are satisfied by definitions (6), (7) and (8), using the matrix elements (9), (10) and (11). The same result also follows from the analysis in the following section.

3. The structure of the bosonised spin operators

We shall divide the basis set of the Bose–Hilbert space $|0\rangle, |1\rangle, |2\rangle, \ldots$ into subsets defined as

$$U_m = \{|n\rangle; (2S+1)m \leq n < (2S+1)(m+1)\} \tag{12}$$

where the m's are non-negative integers.

The subsets are mutually exclusive and their union is a complete basis for the Bose–Hilbert space. Each of the subsets spans a $(2S+1)$-dimensional subspace of the Bose–Hilbert space—H_m. We claim that each H_m is closed under the action of $\tilde{S}^+, \tilde{S}^-, \tilde{S}^z$. Moreover, the action of $\tilde{S}^+, \tilde{S}^-, \tilde{S}^z$ inside H_m is isomorphic to the action of S^+, S^-, S^z in the spin space.

Let $|-S\rangle_s|-S+1\rangle_s \ldots |S\rangle_s$ be a basis for the $(2S+1)$-dimensional spin space where the number inside the ket is taken as an eigenvalue of S^z. We define a one-to-one correspondence between H_m and the spin space; to every element $|-S+r\rangle_s$ $(0 \leq r \leq 2S)$ of the spin space we assign a corresponding element in the H_m space, $|(2S+1)m+r\rangle$. In order to prove the isomorphism we have to check the equality of corresponding matrix elements.

From equations (5) and (8) it follows that

$$f(\hat{N})|(2S+1)m+r)\rangle = (r-S)|(2S+1)m+r\rangle \tag{13}$$

or

$$\tilde{S}^z|(2S+1)m+r\rangle = (r-S)|(2S+1)m+r\rangle. \tag{14}$$

Similarly,

$$S^z|-S+r\rangle_s = (-S+r)|-S+r\rangle_s \tag{15}$$

by its definition. Thus

$${}_s\langle -S+r|S^z|-S+r\rangle_s = \langle (2S+1)m+r|\tilde{S}_z|(2S+1)m+r\rangle, \tag{16}$$

which proves the desired equality of matrix elements for S^z and $\tilde{S}^z$. Now we turn to S^+ and $\tilde{S}^+$.

From (5) and (6) it follows that

$$\tilde{S}^+|(2S+1)m+r\rangle = [S(S+1)-(r-S)(r-S+1)]^{1/2}|(2S+1)m+r+1\rangle \tag{17}$$

where we use

$$B^\dagger \frac{1}{(1+\hat{N})^{1/2}}|n\rangle = |n+1\rangle.$$

In the spin space it is well known that

$$S^+|-S+r\rangle_s = [S(S+1)-(-S+r)(-S+r+1)]^{1/2}|-S+r+1\rangle_s. \tag{18}$$

The desired equality of matrix elements follows trivially from (18) and (17). The proof for $\tilde{S}^-$ and S^- is similar to that for $\tilde{S}^+$ and S^+.

In conclusion, the matrices representing S^+, S^-, S^z in the spin space are equal to the matrices representing $\tilde{S}^+, \tilde{S}^-, \tilde{S}^z$ in each of the H_m spaces, provided an appropriate correspondence is chosen between the bases. Thus the matrices representing $\tilde{S}^+, \tilde{S}^-, \tilde{S}^z$ in the Bose space can be written, as shown in figure 1, as block matrices. Each block is a $(2S+1)\times(2S+1)$ dimensional matrix in spin space by repeating it infinitely many times.

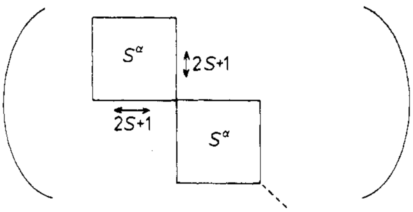

Figure 1. Structure of the bosonised spin operators. Each block is equal to the original matrix in spin space. α denotes either $\pm$ or z.

Several conclusions can be drawn from this analysis.

(*a*) The requirements (1), (2) and (3) are satisfied because of the isomorphism.

(*b*) There is no problem of unphysical states. In usual Bose expansions (Holstein and Primakoff 1940, Dyson 1956) of spin operators such a problem must appear since the Bose space is infinite dimensional, whereas the spin space is $(2S+1)$-dimensional. Thus a one-to-one correspondence between the two is impossible. The usual solution is to define a transformation between the spin space and a subspace of the Bose space, which is always the subspace defined here as H_0 (or $m=0$). All other states, namely $\{|n\rangle; n \geqslant 2S+1\}$ are considered unphysical and are projected out. Here we see that Holstein and Primakoff (1940) worked just in the first block. Our solution is a multivalued transformation between the spin space and the Bose space, which assigns to each state in the spin space an infinity of states in the Bose space. No unphysical states appear in this approach.

(*c*) A new symmetry has emerged in the process of bosonisation, namely the symmetry among the blocks. This symmetry will be shown to be connected to an invariant of the theory.

4. A theorem on functions of the number operator $\hat{N}$

In this section we prove an expansion theorem for functions of the number operator $\hat{N}$ in a Bose space. A similar proof is given in § 1 of Goldhirsch *et al* (1979), and is repeated here for sake of completeness.

According to definition (4), every function $f(x)$, even if it is defined only on the set of non-negative integers, has a corresponding operator $f(\hat{N})$ defined through its matrix elements. In this section we prove that every function $f(\hat{N})$ of the number operator $\hat{N}$ can be expanded as

$$f(\hat{N}) = \sum_{n=0}^{\infty} b_n B^{\dagger n} B^n \tag{19}$$

where the b_n's are a set of numbers which depend on the values $f(n)$ for n as non-negative integers. The expansion (19) is not a Taylor-like expansion of $f(\hat{N})$ (which can be even non-analytic). It just means that the matrix elements of both sides of the equality (19) are equal. In other words,

$$f(m) = \sum_{n=0}^{\infty} b_n \langle m|B^{\dagger n} B^n|m\rangle \tag{20}$$

for every non-negative integer m.

Since $B^n|m\rangle = 0$ for $n > m$ it follows that (20) is equivalent to

$$f(m) = \sum_{n=0}^{m} b_n \langle m|B^{\dagger n}B^n|m\rangle. \tag{21}$$

Using the relation $[B, B^\dagger] = 1$ one can prove by induction in n that

$$B^{\dagger n}B^n = \hat{N}(\hat{N}-1)\ldots(\hat{N}-n+1). \tag{22}$$

Inserting (22) into (21) one gets

$$f(m) = \sum_{n=0}^{m} b_n m(m-1)\ldots(m-n+1)$$

or

$$f(m) = \sum_{n=0}^{m} b_n \frac{m!}{(m-n)!} \tag{23}$$

Equation (23) is therefore equivalent to equation (19). The b_n's should satisfy (23) for every non-negative integer m:

$$\begin{aligned} f(0) &= \frac{0!}{0!} b_o \\ f(1) &= \frac{1!}{1!} b_0 + \frac{1!}{0!} b_1 \\ f(2) &= \frac{2!}{2!} b_0 + \frac{2!}{1!} b_1 + \frac{2!}{0!} b_2 \\ f(3) &= \frac{3!}{3!} b_0 + \frac{3!}{2!} b_1 + \frac{3!}{1!} b_2 + \frac{3!}{0!} b_3, \end{aligned} \tag{24}$$

etc. We see that b_1 is expressed through b_0, b_2 through b_0 and b_1, and so on. Thus we can calculate successively all the coefficients b_n. Moreover, a closed expression for the b_n's can be found. To do this we define a set of functions $f_N(x)$, where N are non-negative integers:

$$f_N(x) = \sum_{\nu=0}^{N} \frac{N!}{(N-\nu)!} b_\nu x^{N-\nu}. \tag{25}$$

One can see that $f_N(1) = f(N)$ and $f_N(0) = b_N N!$ From (25) we have

$$\frac{\mathrm{d} f_N(x)}{\mathrm{d}x} = N f_{N-1}(x) \tag{26}$$

and

$$\frac{\mathrm{d} h_N(x)}{\mathrm{d}x} = h_{N-1}(x) \tag{27}$$

where

$$h_N(x) \equiv f_N(x)/N!. \tag{28}$$

The solution of (27) is simple:

$$h_N(x) = \int_1^x h_{N-1}(y)\,\mathrm{d}y + h_N(1). \tag{29}$$

By successive integrations, taking into account that from (25) it follows that $f_0(y)=f_0(1)$ and hence $h_0(y)=h_0(1)$, we derive

$$\begin{aligned} h_1(x) &= (x-1)h_0(1)+h_1(1) \\ h_2(x) &= \tfrac{1}{2}(x-1)^2h_0(1)+(x-1)h_1(1)+h_2(1) \\ h_3(x) &= \frac{1}{3!}(x-1)^3h_0(1)+\frac{1}{2!}(x-1)^2h_1(1)+(x-1)h_2(1)+h_3(1). \end{aligned} \tag{30}$$

From (30) one can see that

$$h_N(x)=\sum_{\mu=0}^{N}\frac{1}{(N-\mu)!}(x-1)^{N-\mu}h_\mu(1). \tag{31}$$

Equation (31) is simply proven by mathematical induction. Recalling the definition of $h_N(x)$, we obtain

$$b_N=\frac{1}{N!}\sum_{\mu=0}^{N}\binom{N}{\mu}(-1)^{N-\mu}f(\mu) \tag{32}$$

since

$$f(\mu)=f_\mu(1).$$

Formula (32) is the solution of the set of equations (23) or (24).

5. Normal ordered expressions for $\tilde{S}^+, \tilde{S}^-, \tilde{S}^z$

From (6), (7) and (8) it follows that one can write

$$\tilde{S}^+=B^\dagger F(\hat{N}) \tag{33}$$

$$\tilde{S}^-=F(\hat{N})B \tag{34}$$

$$\tilde{S}^z=f(\hat{N}) \tag{35}$$

where $f(x)$ is defined in (5) and

$$F(x)=[S(S+1)-f(x)(f(x)+1)]^{1/2}(1+x)^{-1/2}. \tag{36}$$

According to the previous section, one can write

$$\tilde{S}^+=B^\dagger\left(\sum_{n=0}^{\infty}b_nB^{\dagger n}B^n\right) \tag{37}$$

$$\tilde{S}^-=\left(\sum_{n=0}^{\infty}b_nB^{\dagger n}B^n\right)B \tag{38}$$

$$\tilde{S}^z=\sum_{n=0}^{\infty}C_nB^{\dagger n}B^n \tag{39}$$

where C_n are the coefficients for the function $f(x)$ and b_n those for the function $F(x)$.

In this section we will examine the expansions for $S=\frac{1}{2}$ and $S=1$. In each case we will call the appropriate coefficients b_n, C_n (to avoid additional indexing).

5.1. The case $S=\frac{1}{2}$

In this case

$$\tilde{S}^z = 2\{\tfrac{1}{2}\hat{N}\} - \tfrac{1}{2} \tag{40}$$

or

$$f(n) = \begin{cases} -\frac{1}{2} & n \text{ even} \\ +\frac{1}{2} & n \text{ odd.} \end{cases}$$

Thus, for integer n one can use

$$f(n) = -\tfrac{1}{2}(-1)^n,$$

which shows that we could use the expression

$$\tilde{S}^z = -\tfrac{1}{2}(-1)^{\hat{N}} \tag{41}$$

since both (40) and (41) have the same matrix elements. Using (32) now yields

$$C_n = \frac{1}{N!}\sum_{\mu=0}^{n}\binom{n}{\mu}(-1)^{n-\mu}(-\tfrac{1}{2})(-1)^{\mu}. \tag{42}$$

Equation (42) is a binomial expansion. Hence

$$C_n = (-2)^{n-1}/n!. \tag{43}$$

The function $F(n)$ for this case is (see (36))

$$F(n) = \left(\frac{\frac{1}{2}(\frac{1}{2}+1) - [-\frac{1}{2}(-1)^n][-\frac{1}{2}(-1)^n + 1]}{1+n}\right)^{1/2}. \tag{44}$$

Using $(-1)^{2n} = 1$ for integer n one gets

$$F(n) = \left(\frac{1+(-1)^n}{2}\right)^{1/2}\frac{1}{(1+n)^{1/2}}. \tag{45}$$

For every integer n,

$$\left(\frac{1+(-1)^n}{2}\right)^{1/2} = \frac{1+(-1)^n}{2},$$

hence

$$F(n) = \frac{1}{(1+n)^{1/2}}\,\frac{1+(-1)^n}{2}. \tag{46}$$

This means we could use

$$\tilde{S}^+ = B^\dagger\frac{1}{(1+\hat{N})^{1/2}}\,\frac{1+(-1)^{\hat{N}}}{2} \tag{47}$$

and

$$\tilde{S}^- = \frac{1}{(1+\hat{N})^{1/2}}\,\frac{1+(-1)^{\hat{N}}}{2}B. \tag{48}$$

The b_n's are, according to (32),

$$b_n = \frac{(-1)^n}{n!}\sum_{\substack{\mu=0\\ \mu\ \text{even}}}^{n}\binom{n}{\mu}\frac{1}{(1+\mu)^{1/2}}. \tag{49}$$

Expressions (41), (47) and (48) are the bosonisation transformations derived by Goldhirsch *et al* (1979). The general bosonisation scheme is therefore shown to reduce to the previously derived scheme for $S=\frac{1}{2}$.

5.2. The case $S=1$

In this case

$$\tilde{S}^z = 3\{\tfrac{1}{3}N\}-1 \tag{50}$$

so that

$$f(n)=3\{\tfrac{1}{3}n\}-1. \tag{51}$$

A function equal to $f(n)$ for integer n is

$$\tilde{f}(n)=\frac{\exp(\mathrm{i}\frac{4}{3}\pi n)-\exp[\mathrm{i}\frac{2}{3}\pi(n+1)]}{\exp(\mathrm{i}\frac{2}{3}\pi)-1}. \tag{52}$$

The reader should note that $f(n)$ is periodic with a period of 3, so (52) is merely its representation in terms of Fourier components. In the case of general S one has a period of $2S+1$.

Substitution of (52) in (32) yields

$$C_n=\frac{1}{n!(\exp(\mathrm{i}\frac{2}{3}\pi)-1)}[(\exp(\mathrm{i}\tfrac{4}{3}\pi)-1)^n-\exp(\mathrm{i}\tfrac{2}{3}\pi)(\exp(\mathrm{i}\tfrac{2}{3}\pi)-1)^n],$$

which can be further simplified:

$$C_n=-\frac{1}{n!}\times 2\times 3^{n-1}\sin(\tfrac{5}{6}\pi n+\tfrac{1}{3}\pi). \tag{53}$$

Thus

$$\tilde{S}^z=\sum_{n=0}^{\infty} C_n B^{\dagger n}B^n. \tag{54}$$

The F function, in the case $S=1$, is

$$F(n)=\left(\frac{2-f(n)(f(n)+1)}{1+n}\right)^{1/2} \tag{55}$$

where $f(n)$ is given by (51) or (52). It is easy to check that this function is equal to another function $\tilde{F}(n)$ on the set of non-negative integers:

$$\tilde{F}(n)=\frac{\exp[\mathrm{i}\frac{4}{3}\pi(1+n)]+\exp[\mathrm{i}\frac{2}{3}\pi(1+n)]-2}{(1+n)^{1/2}}\left(-\frac{\sqrt{2}}{3}\right). \tag{56}$$

Hence

$$b_n=-\frac{\sqrt{2}}{3}\frac{1}{n!}\sum_{\mu=0}^{n}\binom{n}{\mu}(-1)^{n-\mu}\frac{\exp[\mathrm{i}\frac{4}{3}\pi(\mu+1)]+\exp[\mathrm{i}\frac{2}{3}\pi(\mu+1)]-2}{(1+\mu)^{1/2}}. \tag{57}$$

The value of C_2 is zero, as can be seen from (53). This is shown in the next section to be part of a general property of our bosonisation, and its meaning is further discussed in § 9.

The sum $\Sigma_{n=0}^{\infty} b_n Z^n$ can be shown to converge for any complex Z. The way to show it is given by Goldhirsch *et al* (1979) for $S=\frac{1}{2}$. Using equation (55) it is a trivial matter to prove the same for $S=1$. Since such an expression appears in the coherent state representation (Klauder 1960) of the Bose operators, it is important to realise that our Bose expansion is convergent with infinite radius of convergence and it is not an expression of the square root appearing in (6) or (7), or the Holstein–Primakoff (1940) transformation.

In conclusion we shall exhibit the first few terms of our expansion for $S=1$,

$$\begin{aligned}\tilde{S}^+ &= \sqrt{2}B^\dagger + (1-\sqrt{2})B^\dagger B^\dagger B + \tfrac{1}{2}(\sqrt{2}-2)B^\dagger B^\dagger B^\dagger BB + \dots \\ \tilde{S}^z &= -1 + B^\dagger B - \tfrac{1}{2}B^\dagger B^\dagger B^\dagger BBB + \dots\end{aligned} \tag{58}$$

compared with the Holstein–Primakoff expansion

$$\begin{aligned}\tilde{S}^+ &= \sqrt{2}B^\dagger - \tfrac{1}{4}\sqrt{2}B^\dagger B^\dagger B - \tfrac{1}{32}\sqrt{2}B^\dagger(B^\dagger B)(B^\dagger B) - \tfrac{1}{128}\sqrt{2}B^\dagger(B^\dagger B)^3) + \dots \\ S^z &= -1 + B^\dagger B.\end{aligned} \tag{59}$$

The agreement is only in the first term for $\tilde{S}^+$ and the first two terms of $\tilde{S}^z$. The normal ordering (59) yields a 5% agreement on the second coefficient of $\tilde{S}^+$.

As we show in the next section, the agreement with Holstein and Primakoff becomes better at higher S, as it should.

6. The case of general S and $1/S$ expansion

Equation (32) shows that if one wishes to know the b_n's up to a certain n, it suffices to know $f(\mu)$ for $\mu \leq n$. Hence if one wishes to know the expansion coefficients up to b_{2S} and C_{2S} one can use functions $\tilde{F}$ and $\tilde{f}$ that coincide with F and f for the integers $0 \leq \mu \leq 2S$ (see § 5 for this notation). In this range of values of μ one can use (see (5))

$$f(\mu) = \mu - S \tag{60}$$

since $\{\mu/(2S+1)\} = \mu/(2S+1)$ in this range. $F(\mu)$ can be calculated using (60) and (36):

$$F(\mu) = \left(\frac{S(S+1) - (\mu - S)(\mu - S + 1)}{\mu + 1}\right)^{1/2}$$

which is equal to

$$F(\mu) = (2S - \mu)^{1/2}. \tag{61}$$

From (60) and (61) we learn that as far as the first $(2S+1)$ coefficients of the expansion are concerned, one could have written

$$\begin{aligned}\tilde{S}^+ &= B^\dagger(2S - \hat{N})^{1/2} \\ \tilde{S}^- &= (2S - \hat{N})^{1/2}B \\ \tilde{S}^z &= \hat{N} - S.\end{aligned} \tag{62}$$

This is exactly the Holstein–Primakoff transformation to which our expansion reduces when only the first $(2S+1)$ coefficients are considered.

Actually, had we used only the first block or the $H_{m=0}$ subspace (see § 2), all matrix elements of the type $B^{\dagger p}B^p$ with $p > 2S+1$ would be zero, since the states in the first block $|n\rangle$ are restricted to $0 \leqslant n \leqslant 2S$. Hence the Holstein–Primakoff transformation is equal to our own when only the first block is concerned. In order to stay in the first block one needs a projection operator in actual calculations. This projection is connected with what is known in the literature (Dyson 1956) as the kinematic interaction.

Using (32) again for the case of general S one gets

$$C_n = -S\delta_{n,0} + \delta_{n,1} \qquad \text{for } 0 < n < 2S$$

or

$$\tilde{S}^z = -S + B^\dagger B + \mathrm{O}(B^{\dagger 2S+1} B^{2S+1}), \tag{63}$$

a special case of which is exhibited in § 5, namely $S = 1$. When $S = \frac{1}{2}$ one has $2S + 1 = 2$ so no coefficient C_n is zero. It is impossible to write down a general expression like (63) for the $\tilde{S}^+$ operator. However, we shall exhibit the first few b_n, calculated using (32) and (61):

$$\begin{aligned} b_0 &= (2S)^{1/2} \\ b_1 &= (2S-1)^{1/2} - (2S)^{1/2} \\ b_2 &= \tfrac{1}{2}[(2S)^{1/2} - 2(2S-1)^{1/2} + (2S-2)^{1/2}] \\ b_3 &= \tfrac{1}{6}[-(2S)^{1/2} + 3(2S-1)^{1/2} - 3(2S-2)^{1/2} + (2S-3)^{1/2}], \end{aligned} \tag{64}$$

etc. Expanding the b_n's in powers of $1/S$ one obtains

$$\begin{aligned} b_0 &= 2S \\ b_1 &= 2S\left(-\frac{1}{4S} - \frac{1}{32S^2} - \frac{1}{128S^3} + \ldots\right) \\ b_2 &= 2S\left(-\frac{1}{32S^2} - \frac{3}{128S^3} + \ldots\right) \\ b_3 &= 2S\left(-\frac{1}{128S^3} + \ldots\right). \end{aligned} \tag{65}$$

The b_n's are therefore of order $1/S^n$. This property can be proved in general as follows. For $\mu < 2S$,

$$\left(1 - \frac{\mu}{2S}\right)^{1/2} = \sum_{m=0}^{\infty} \alpha_m \left(\frac{\mu}{2S}\right)^m \tag{66}$$

where the α_m are the appropriate expansion coefficients. Hence using (32), (62) and (66)

$$b_n = \frac{\sqrt{2S}}{n!} \sum_m \alpha_m \frac{1}{(2S)^m} \left(\sum_{\mu=0}^{n} \binom{n}{\mu} (-1)^{n-\mu} \mu^m \right).$$

The sum in parentheses is equal to

$$\frac{\partial^m}{\partial x^m} \sum_{\mu=0}^{n} \binom{n}{\mu} (-1)^{n-\mu} \, \mathrm{e}^{x\mu} \big|_{x=0}.$$

Hence:

$$\sum_{\mu=0}^{n} \binom{n}{\mu} (-1)^{n-\mu} \mu^m = \frac{\partial^m}{\partial x^m} (\mathrm{e}^x - 1)^n \big|_{x=0}. \tag{67}$$

For $m < n$ the derivative on the right-hand side of (67) is proportional to $e^x - 1$, which goes to zero when $x \to 0$. When $n = m$ one can show from (67) that

$$\sum_{\mu=0}^{n} \binom{n}{\mu} (-1)^{n-\mu} \mu^n = n!;$$

consequently

$$b_n = \sqrt{2S}\alpha_n \frac{1}{(2S)^n} + \text{higher orders in } 1/S \tag{68}$$

for $n \leq 2S$.

To conclude this section we present a closed formula for the coefficients C_n in the expansion of S^z.

From (5) it follows that

$$f(q) = -\sum_{m=1}^{2S} \frac{1}{1-\exp[-i2\pi m/(2S+1)]} \exp[i2\pi mq/(2S+1)]. \tag{69}$$

This formula is just the Fourier representation of $f(x)$. Substituting it into (32) yields

$$C_n = -\frac{1}{n!} \sum_{m=1}^{2S} \frac{1}{1-\exp[-i2\pi m/(2S+1)]} \sum_{\mu=0}^{n} \binom{n}{\mu} (-1)^{n-\mu} \exp[i2\pi m\mu/(2S+1)] \tag{70}$$

from which it follows that

$$C_n = -\frac{1}{n!} \sum_{m=1}^{2S} \exp[i2\pi m/(2S+1)](\exp[i2\pi m/(2S+1)]-1)^{n-1}. \tag{71}$$

Since C_n is real, by its definition, we take the real part of (71) and arrive at

$$C_n = -\frac{2^{n-1}}{n!} \sum_{m=1}^{2S} \cos\left(\frac{2\pi}{2S+1} m(n+1) + \tfrac{1}{2}\pi(n-1)\right)\left(\sin\frac{\pi m}{2S+1}\right)^{n-1}. \tag{72}$$

One can easily check that (72) contains $S = \frac{1}{2}$, $S = 1$ as special cases.

7. Quantum spin models: the Hilbert space

In this section the structure of the Hilbert space for quantum spin models is analysed.

Assume that we have a d-dimensional lattice with three spin operators S_i^+, S_i^-, S_i^z attached to each lattice point i. We define a Hamiltonian as a functional $H[\{S_i^+, S_i^-, S_i^z\}]$ of the spin operators. Aassuming the lattice has $\mathcal{N}$ sites the relevant Hilbert space is $(2S+1)^{\mathcal{N}}$ dimensional, i.e. a direct product of $\mathcal{N}$, $(2S+1)$-dimensional spaces.

Let us analyse the bosonised Hamiltonian, in our notation $H[\{\tilde{S}_i^+, \tilde{S}_i^- \tilde{S}_i^z\}]$. We choose a non-negative integer m_i for each lattice site i. The space spanned by the product $U^{\{m_i\}} = \bigotimes_i U_{m_i}$ (see (12)) is $(2S+1)^{\mathcal{N}}$ dimensional, and since we have proven that the Hilbert spaces spanned by each U_{m_i}, namely H_{m_i}, are invariant under the action of the spin operators $\tilde{S}_i^{\pm}$, $\tilde{S}_i^z$, it follows that the space spanned by $U^{\{m_i\}}$ is closed under the operation of all spin operators on the lattice.

Thus the infinite matrix representing the Hamiltonian in the Bose space can be shown to be made of blocks of size $(2S+1)^{\mathcal{N}} \times (2S+1)^{\mathcal{N}}$. Since as shown in § 2, the action of the bosonised spin operators in each block is isomorphic to the action of the usual spin operators in spin space, it follows that the structure of the bosonised Hamiltonian is one of repeating blocks, each block being equal to the matrix representation of the spin Hamiltonian in the spin space provided one uses the correspondence of basis states mentioned in § 2. Each choice of $\{m_i\}$ fixes a block and thus $\{m_i\}$ can be taken as the index of the block. The union of all $U^{\{m_i\}}$ clearly spans the whole Bose space.

This structure is exhibited in figure (2). It is the same structure as was found for the case $S=\frac{1}{2}$ (see Goldhirsch *et al* (1979) § III).

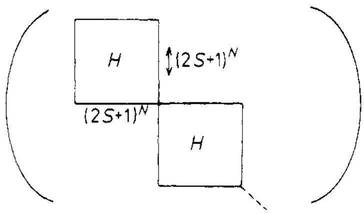

Figure 2. Structure of the bosonised spin Hamiltonian. Each block is equal to the original Hamiltonian matrix in spin space.

This structure of the bosonised spin Hamiltonian contains a new invariant, which we shall call the block invariant. To see it, examine the state $|n_i\rangle$. n_i can always be written as

$$n_i=(2S+1)m_i+r_i \qquad 0\leqslant r_i<2S+1. \tag{73}$$

According to (5) and (8), $|n_i\rangle$ is an eigenstate of $\tilde{S}_i^z$ with eigenvalues r_i-S. Thus $|n_i\rangle$ is an eigenstate of $\hat{N}_i-\tilde{S}_i^z$ with eigenvalue $(2S+1)m_i+S$. The number m_i is typical of a certain block and does not change in it, from state to state.

It follows that $\hat{N}_i-\tilde{S}_i^z$ is an invariant inside each block and as a result it commutes with H. Clearly $\Sigma_i(\hat{N}_i-\tilde{S}_i^z)$ is an invariant in each block also. This invariant is connected with the Bloch sum rule; this is proved in the next paragraph.

8. Quantum spin systems at finite temperature and the Bloch sum rule

Because of the structure of H in the Bose space (see figure 2) the partition function corresponding to H at inverse temperature β can be written as

$$\operatorname{Tr} e^{-\beta H}=\sum_{\text{blocks}} \operatorname{Tr} e^{-\beta H}. \tag{74}$$

This is easily seen in the diagonal representation of H (see figures 3 and 4). Let $\hat{H}$ be the $(2S+1)^{\mathcal{N}}\times(2S+1)^{\mathcal{N}}$ matrix representing the Hamiltonian in spin space. $\operatorname{Tr} e^{-\beta\hat{H}}$ is the partition function of the spin system and will be denoted as Z_{true}. The sum in (74) is thus an infinite sum over the same object, Z_{true}, and hence it is infinite. To remedy this point, one can use the fact that there is a block-invariant $W\equiv\Sigma_i(\hat{N}_i-\tilde{S}_i^z)$ which commutes with the Hamiltonian. We now calculate $\operatorname{Tr} e^{-\beta H-\mu W}$. From $[H, W]=0$ it follows that

$$\operatorname{Tr} e^{-\beta H-\mu W}=\operatorname{Tr} e^{-\beta H} e^{-\mu W}. \tag{75}$$

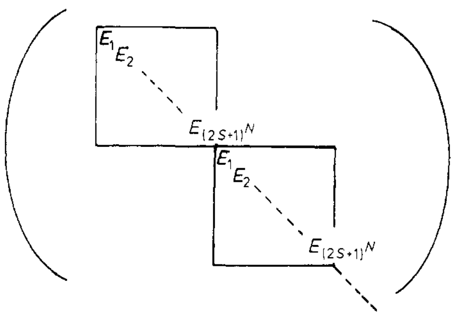

Figure 3. Diagonal representation of H in the Bose space.

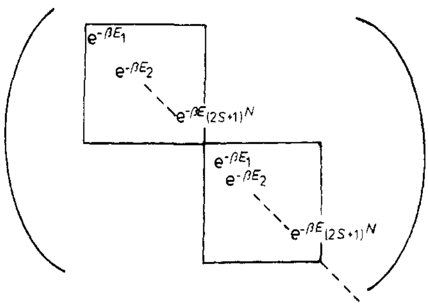

Figure 4. Diagonal representation of $e^{-\beta H}$ in the Bose space.

Equation (75) can be rewritten as

$$\mathrm{Tr}\, e^{\beta H-\mu W} = \sum_{\text{blocks}} \mathrm{Tr}(e^{-\beta H}\, e^{-\mu W}). \tag{76}$$

In each block W is a c number whose value is $\Sigma_i[(2S+1)m_i+S]$, where the set $\{m_i\}$ defines the block (see (73) and § 7). In a given block one can write, instead of W,

$$(2S+1)\sum_i m_i + S\mathcal{N}. \tag{77}$$

Hence

$$\mathrm{Tr}\, e^{-\beta H-\mu W} = Z_{\text{true}} \sum_{\substack{\text{all values}\\ \text{of } m_i}} \exp\Big[-\mu\Big((2S+1)\sum_i m_i + \mathcal{N}S\Big)\Big]. \tag{78}$$

Since the m_i's range over all integers from zero to infinity, one gets

$$Z = Z_{\text{true}}\left(\frac{e^{-\mu S}}{1-e^{-\mu(2S+1)}}\right)^{\mathcal{N}} \tag{79}$$

where Z denotes the left-hand side of (78). As a result, the true partition function of the spin system is proportional to the partition function of the effective Hamiltonians $\bar{H}$ defines as

$$\bar{H} = H + (\mu/\beta)W \tag{80}$$

and the proportionality constant is independent of temperature. Thus $\bar{H}$ and H describe the same physics.

The limit $\mu \to \infty$ projects out the first block (all $m_i = 0$) only, and there one can work with any of the known representations which are valid in this limit. The average $\langle W \rangle$ is given by

$$\langle W \rangle = \frac{\mathrm{Tr}(W\, \mathrm{e}^{-\beta H - \mu W})}{\mathrm{Tr}\, \mathrm{e}^{-\beta H - \mu W}} \tag{81}$$

from which one can easily show that

$$\langle W \rangle = \frac{\mathrm{Tr}\ W\, \mathrm{e}^{-\mu W}}{\mathrm{Tr}\, \mathrm{e}^{-\mu W}}. \tag{82}$$

Hence

$$\langle W \rangle = \mathcal{N} \frac{\Sigma_{m=0}^{\infty} [(2S+1)m + S] \exp\{-\mu[(2S+1)m + S]\}}{\Sigma_{m=0}^{\infty} \exp\{-\mu[(2S+1)m + S]\}}, \tag{83}$$

which leads to

$$\frac{1}{\mathcal{N}} \langle W \rangle = S + \frac{(2S+1)}{\mathrm{e}^{\mu(2S+1)} - 1} \tag{84}$$

or

$$\langle \hat{N}_i - \tilde{S}_i^z \rangle = S + \frac{2S+1}{\mathrm{e}^{\mu(2S+1)} - 1}. \tag{85}$$

The left–hand side of equation (85) is the average number of bosons (or magnons if the two are identified) minus the magnetisation. This quantity is shown in (85) to be a constant independent of temperature. If $\mu \to \infty$, so that one stays in the first block alone, one gets

$$\langle \hat{N}_i - \tilde{S}_i^z \rangle = S \tag{86}$$

which is the usual formulation of Bloch's sum rule (Keffer 1966). (In this reference the average is of $\langle \hat{N}_i + \tilde{S}_i^z \rangle$ since they choose $S^z = S$ as the zero boson states. By making the transformation $\tilde{S}^+ \to \tilde{S}^-$, $\tilde{S}^- \to {}^-\tilde{S}^+$, $\tilde{S}^z \to -\tilde{S}^z$, we can transform to this choice.) Equation (85) is thus a rigorous proof and a generalisation of Bloch's sum rule.

9. Remarks on path integral representation and the critical behaviour of quantum spin systems

Goldhirsch *et al* (1979) showed how the boson representation can be used to write the partition function of a quantum spin system in terms of coherent states. The same can be done here. To get the effective classical Hamiltonian one has just to write H in a normal ordered form, substitute λ_i^{*r} for $B_i^\dagger$ and λ_i^r for B_i (r is the index denoting the 'additional dimension'; see Goldhirsch *et al* (1979)) and add to this the part coming from the norm of the coherent states. Then, using the analysis of Goldhirsch *et al* (1979), one can show that at zero temperature the quantum spin system in d dimensions behaves like an equivalent classical system in $(d+1)$ dimensions, but at finite temperatures a cross-over back to the original dimension must occur. However, there is an important difference between the case $S = \frac{1}{2}$ and any other S. As noted in § 6, the first $(2S+1)$ terms of the Bose expansion are identical to the Holstein–Primakoff expression, thus leading to a magnon-magnon interaction term $U_4 B_{k_1}^\dagger B_{k_2}^\dagger B_{k_3} B_{k_4}$ which does not vanish in the limit of zero momenta. This problem can be solved by going to a non-Hermitian Hamiltonian (Dyson 1956, Maleev 1958). It is interesting to note the role of the term containing μ in this context. From (63) it follows that

$$\tilde{S}^z = -S + B^\dagger B + C_{2S+1} B^{\dagger 2S+1} B^{2S+1} + \text{higher-order terms.} \tag{87}$$

Hence:

$$\hat{N} - \tilde{S}^z = S - C_{2S+1} B^{\dagger 2S+1} B^{2S+1} + \text{higher-order terms.} \tag{88}$$

Thus the lowest-order term in the Bose expansion of the weight function W is of order $B^{\dagger 2S+1} B^{2S+1}$. μ does not appear in any lower term. But, as shown by Goldhirsch *et al* (1979), it is μ that enables one to have a term of the type $T - T_c$, since all other terms are proportional to $\beta(=1/T)$. Thus the 'usual' Landau–Ginzburg free energy can be obtained in the sense of renormalisation group recursion relations only after $(2S+1)$ iterations. In other words, the strength of the Holstein–Primakoff interaction is such that one needs to go to the $(2S+1)$th order in perturbation theory at least in order to obtain a (presumably) small magnon–magnon interaction. The non-unitary transformation of Maleev (1958) which leads to the Dyson–Maleev-type Hamiltonian is probably equivalent to a strong renormalisation of the magnons. Consequently the intuitive approach of § VIII in Goldhirsch *et al* (1979) does not apply to general spin, yet the formal approach of section V of the same reference can be used easily in the general case also, yielding the same results. Consequently, the phase transition in a quantum spin system can be regarded as a generalised Bose condensation in which $W = \Sigma_i (\hat{N}_i - \tilde{S}_i^z)$ is the conserved quantity rather than the total number of particles $\Sigma_i \hat{N}_i$ (Goldhirsch and Yakhot 1979).

The formalism developed above can be applied in a multitude of cases where the fourth- and higher-order interactions of magnons are necessary, e.g. ferromagnetic relaxation theory, renormalisation of magnons, etc.

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