Exact boson representation of quantum spin systems and investigation of their critical behavior

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Quantum spin systems are shown to be rigorously equivalent to certain Bose systems. As a result the phase transitions occuring in such systems can be regarded as generalized Bose condensation processes. In those processes it is not the number of bosons that is kept constant but a certain function of it. The problem of degeneracy arising in Bosonizing a spin system is solved in a simple fashion. The low-temperature limit of the Bose systems reproduces the magnon gas with correct interactions. The Bloch sum rule becomes exact at all temperatures, when one replaces the magnon number by the number of bosons. The crossover to classical behavior at criticality is discussed and it is shown that at T_c the quantum S = 1/2 spin systems behave like the corresponding classical $S = \infty$ systems. A classical effective Hamiltonian whose corresponding partition function is equal to the partition function of the quantum spin systems is derived. Finally, possible application to dynamics are briefly discussed.

INTRODUCTION

The powerful tools provided by the renormalization-group approach¹ have been used to investigate the critical behavior of many classical systems. Less attention has been devoted to quantum systems as can be judged from the relatively small number of publications treating the latter.²⁻⁷ Two main reasons seem to be responsible for this state of affairs: the first is a philosophical one and the other is technical in nature. The philosophical reason is that since close to the critical point one can take the Kadanoff-type⁸ blocks to be extremely big, the microscopical quantum nature of the Hamiltonian is lost and one can justify the use of classical Hamiltonians. The technical reason is the additional complication introduced by noncommuting objects.

The philosophy is certainly intuitively appealing yet has never been proven to be true. On the contrary, numerical evidence suggests a different behavior for $S = \frac{1}{2}$ and $S = \infty$ Heisenberg models.⁹ Thus the problem is open and requires investigation. Furthermore, it is a problem of great physical importance since mircroscopical Hamiltonians *are* of quantum nature.

One technical characteristic property of quantum systems whose partition function has been written in path integral form is the fact that the "effective" classical Hamiltonian appearing in the functional integral is a sum of an infinity of terms. This is going to be the case here too and it should be reminiscent of the fact that the (classical) models treated so far are merely a great simplification of physically realistic models. It is not clear a priori whether such Hamiltonians belong to the same universality class as their corresponding classical Hamiltonians. A naive renormalizationgroup (RG) treatment would disregard the higherorder terms $(U_6, U_8, \ldots, \text{ etc.})$ as being irrelevant. This may be particularly useless in case the effective Hamiltonian is written in terms of an order parameter that seems to be of lower dimensionality than it should be (see below). It certainly disregards a possible effect of the higher-order terms. Yet, even in the classical case one assumes a certain form of the effective Hamiltonian in the linear range of the RG, namely, close to T_c , since it is pratically impossible to follow the development of the effective Hamiltonian in the nonlinear range of the RG.

The treatment of quantum spin systems, described in this paper is based upon the author's view that second-order phase transition can be generally described by condensation processes in appropriate Bose systems. Practically speaking, we describe a general method of exact bosonization of spin Hamiltonians that has, in our opinion, many advantages over existing methods.

For example, we need not restrict the Bose operators corresponding to spin operators to act only on a subset of the Bose Hilbert space, hence projection operators are not needed and the way is open to use known techniques for writing the Bose Hamiltonian in path-integral form. In addition the effective Hamiltonian is analytic and can be ex-

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pressed as a converging power series in the order parameters (methods we are aware of contain expansion of logarithms, see, e.g., Ref. 2). As a result one should find this representation useful for numerical methods too.

The main features appearing in the process of writing down the path-integral form of the partition function are (a) the appearance of an additional dimension whose origin is the division of the inverse temperature β into segments (see below); (b) the disappearance of this extra dimension and crossover to the starting dimension when one approaches T_c ; (c) at zero temperature the additional dimension does not disappear; (d) by using the naive renormalization-group approach mentioned above one finds that the quantum Heisenberg Hamiltonian belongs to the universality class of the classical Heisenberg Hamiltonian.

I. BOSONIZATION OF SPIN OPERATORS

In this section we use the results of Agranovich and Toschich¹⁰ to derive a representation of Pauli (spin) operators in terms of bosons. The work has been published in 1968 but to the best of our knowledge it did not attract much attention of people interested in statistical mechanics and quantum theory of magnetism. We believe that the results of Agranovich and Toschich are of great importance and that is why in this section we will follow the main steps which lead to the final formula expressing the spin operators in terms of bosons. In addition we will show a way to simplify this formula by rewriting it in a compact form which is suitable for renormalization-group treatment.

We consider the case $S = \frac{1}{2}$, $S_g = \pm \frac{1}{2}$, and

$$S_i^- S_i^+ + S_i^+ S_i^- = 1, (1.1)$$

where i denotes the lattice sites. Let us introduce (Agranovich-Toschich):

$$S_{i}^{*} = \left(\sum_{\nu=0}^{\infty} a_{\nu} B_{i}^{\dagger \nu} B_{i}^{\nu}\right)^{1/2} B_{i} \text{ and } S_{i}^{*} = B_{i}^{\dagger} \left(\sum_{\nu=0}^{\infty} a_{\nu} B_{i}^{\dagger \nu} B_{i}^{\nu}\right)^{1/2};$$
$$[B_{i}, B_{j}^{\dagger}] = \delta_{ij}, \quad [B_{i}, B_{j}] = [B_{i}^{\dagger} B_{j}^{\dagger}] = 0.$$
(1.2)

This is obviously a generalization of the Holstein-
Primakoff¹¹ transformation. The latter corre-
sponds to
$$a_0 = -a_1 = 1$$
 and $a_\nu = 0$ for $\nu \ge 2$, where a_ν
are real coefficients and B_i^{\dagger} , B_i are the Boson op-
erators. Substituting (1.2) into (1.1) and using
the fact that

$$B_{i}^{\dagger \nu+1} B_{i}^{\nu+1} = (\hat{N}_{i} - \nu) B_{i}^{\dagger \nu} B_{i}^{\nu}, \qquad (1.2')$$

where $\hat{N}_i = B_i^{\dagger}B_i$, and that the term inside the square root sign commutes with \hat{N} , we get

$$S_{i}^{*}S_{i}^{*} + S_{i}^{*}S_{i}^{-} = \sum_{\nu=0}^{\infty} a_{\nu} \left[2B_{i}^{\dagger\nu+1}B_{i}^{\nu+1} + (\nu+1)B_{i}^{\dagger\nu}B_{i}^{\nu} \right] = 1 .$$
(1.3)

Equality (1.3) can be fulfilled if and only if

$$a_{\nu} = -2/(\nu+1)a_{\nu-1}, \quad a_0 = 1$$

or

$$a_{\nu} = (-2)^{\nu} / (1+\nu)!$$

Thus we obtained an Agranovich-Toschich spinboson transformation:

$$S_{i}^{-} = \left(\sum_{\nu=0}^{\infty} \frac{(-2)^{\nu}}{(1+\nu)!} B_{i}^{\dagger\nu} B_{i}^{\nu}\right)^{1/2} B_{i},$$

$$S_{i}^{+} = B_{i}^{\dagger} \left(\sum_{\nu=0}^{\infty} \frac{(-2)^{\nu}}{(1+\nu)!} B_{i}^{\dagger\nu} B_{i}^{\nu}\right)^{1/2}.$$
 (1.4)

The operator for the spin deviation number is just

$$\hat{L}_{i} = S_{i}^{*}S_{i}^{-} = \hat{N}_{i} + \sum_{\nu=1}^{\infty} \frac{(-2)^{\nu}}{(1+\nu)!} \, \hat{N}_{i}(\hat{N}_{i}-1) \cdots (\hat{N}_{1}-\nu).$$
(1.5)

We can see readily that together with (1.1)

 $S_i^{-2} = S_i^{+2} = 0$

holds and thus the transformation (1.4) reproduces all the properties of spin- $\frac{1}{2}$ operators. Equation (1.4) is the result of Agranovich and Toshich.

Now we simplify formula (1.4) and derive the equivalent expression which can be written in a compact form.

It is clear from (1.2') that

$$B_{i}^{\dagger \nu}B_{i}^{\nu} = \hat{N}_{i}(\hat{N}_{i} - 1) \cdots (\hat{N}_{i} - \nu + 1)$$
(1.6')

and thus

$$S_{i}^{*} = B_{i}^{\dagger} \left(\sum_{\nu=0}^{\infty} \frac{(-2)^{\nu}}{(1+\nu)!} \, \hat{N}_{i}(\hat{N}_{i}-1) \cdots \right) \\ \times (\hat{N}_{i}-\nu+1) \right)^{1/2} \equiv B^{\dagger}f(\hat{N}_{i}).$$
(1.6)

Furthermore, a state which is an eigenstate of \hat{N} with eigenvalue N_i is an eigenstate of $f(\hat{N}_i)$ with an eigenvalue $f(N_i)$ given by

$$f^{2}(N_{i}) = \sum_{\nu=0}^{\infty} \frac{(-2)^{\nu}}{(1+\nu)!} N_{i}(N_{i}-1) \cdots (N_{i}-\nu+1). \quad (1.7)$$

(1.7) follows directly from (1.6). We should note that all the terms in the sum (1.7) with $\nu > N_i + 1$ are equal to zero because they contain a zero in the corresponding products. As a result (1.7) can be rewritten

$$f^{2}(N_{i}) = \sum_{\nu=0}^{N_{i}} \frac{(-2)^{\nu}}{(1+\nu)!} \frac{N_{i}!}{(N_{i}-\nu)!} . \qquad (1.7')$$

It is easy to see that (1.7') is equal to

$$f^{2}(N_{i}) = -\frac{1}{2(N_{i}+1)} \sum_{\nu=1}^{N_{i}} (-2)^{\nu+1} {N_{i}+1 \choose \nu+1}$$

and

$$f^{2}(N_{i}) = -\frac{1}{2(N_{i}+1)} \left[\sum_{\nu=0}^{N_{i}+1} (-2)^{\nu} \binom{N_{i}+1}{\nu} - 1 \right]. \quad (1.8)$$

This expression is equal to

$$f^{2}(N_{i}) = -\frac{1}{2(N_{i}+1)} \left[(-1)^{N_{i}+1} - 1 \right] = \frac{1}{N_{i}+1} \frac{(-1)^{N_{i}} + 1}{2}$$
(1.9)

because

$$\sum_{\nu=0}^{N_i+1} (-2)^{\nu} {\binom{N_i+1}{\nu}} = (1-2)^{N_i} = (-1)^{N_i}.$$

We note that

$$\frac{1}{2} \left[1 + (-1)^{N_{i}} \right] = \frac{1}{2} \left[1 + (-1)^{N_{i}} \right]^{1/2}$$

for integer N_i . Thus,

$$f(N_i) = (N_i + 1)^{-1/2} \frac{1}{2} [1 + (-1)^{N_i}].$$
(1.10)

This formula is correct for any integer N_i , i.e., for any possible eigenvalue of \hat{N}_i , hence we can identify $f(\hat{N}_i)$ in (1.6) with

$$(1+\hat{N}_i)^{-1/2} \frac{1}{2} [1+(-1)^{N_i}]$$

As a result we get

$$S_{i}^{*} = B_{i}^{\dagger}(\hat{N}_{i}+1)^{-1/2} \frac{1}{2} [1+(-1)^{N_{i}}],$$

$$S^{-} = (\hat{N}_{i}+1)^{-1/2} \frac{1}{2} [1+(-1)^{\hat{N}_{i}}]B_{i}.$$
(1.11)

To calculate S_i^x we use the fact that for any analytic function h, the following holds:

$$h(\hat{N}_{i})B_{i} = B_{i}h(\hat{N}_{i} - 1).$$
(1.12)

The proof of (1.12) is very simple. We can readily see that

$$\hat{N}_i B_i = B_i (\hat{N}_i - 1),$$

hence for every integer n

$$\hat{N}_i^n B_i = B_i (\hat{N}_i - 1)^n ,$$

which justifies (1.12). We also have

$$h(\hat{N}_{i})B_{i}^{\dagger} = B_{i}^{\dagger}h(\hat{N}_{i}+1).$$
(1.12')

Using (1.12) and (1.12'), we get

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$$N_i!$$
 $S_i^*S_i^* = B_i^*(N_i+1)^{-1/2} \frac{1}{2} [1+(-1)^{\hat{N}_i}] \frac{1}{2} [1+(-1)^{\hat{N}_i}]$

$$\times (\hat{N}_{i} + 1)^{-1/2} B_{i} = \frac{1}{2} [1 + (-1)^{\hat{N}_{i} - 1}]$$
(1.13)

and

$$S_i^* S_i^* = \frac{1}{2} [1 + (-1)^{N_i}].$$
 (1.13')

Hence

$$S_{i}^{z} = \frac{1}{2} [S_{i}^{*}, S_{i}^{*}] = -\frac{1}{2} (-1)^{N_{i}}.$$
(1.14)

The eigenvalues of S_i^z are $\pm \frac{1}{2}$ as expected.

Thus Eqs. (1.11), (1.14), and (1.2) are equivalent representation of spin operators through bosons.

Formulas (1.2) and (1.11) are inconvenient because they represent the Pauli operators in a nonanalytic way. Now we will show that they can be rewritten in an analytic fashion.

To do it we must prove that for any function f(N) there exists an analytic function g(N) which coincides with f(N) for integer values of N. As a result $f(\hat{N})=g(\hat{N})$ as a function of the \hat{N} operator. Define

$$g(N) = \sum_{\nu=0}^{N} b_{\nu} \frac{N!}{(N-\nu)!}$$

= $\sum_{\nu=0}^{\infty} b_{\nu} N_{i} (N_{i} - 1) \cdot \cdot \cdot (N_{i} - \nu + 1).$ (1.15)

The coefficients b_{ν} are determined below. We demand f(N) = g(N) for integer N or

$$f(0) = \frac{0!}{0!} b_0,$$

$$f(1) = \frac{1!}{1!} b_0 + \frac{1!}{0!} b_1,$$

$$f(2) = \frac{2!}{2!} b_0 + \frac{1}{1!} b_1 + \frac{2!}{0!} b_2,$$

$$f(3) = \frac{3!}{3!} b_0 + \frac{3!}{2!} b_1 + \frac{3!}{1!} b_2 + \frac{3!}{0!} b_3,$$

(1.16)

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 successively calculate all the coefficients b_{ν} . Writing

$$g(\hat{N}) = \sum_{\nu=0}^{\infty} b_{\nu} \hat{N}(\hat{N}-1) \cdots (\hat{N}-\nu+1), \qquad (1.17)$$

we have the desired operator $g(\hat{N})$.

We conclude this section by finding a closed formula for b_{ν} . To do so let us define the set of functions $f_N(x)$:

$$f_N(x) = \sum_{\nu=0}^N \frac{N!}{(N-\nu)!} b_{\nu} x^{N-\nu}.$$
 (1.18)

We can see that $f_N(1) = f(N)$ and $f_N(0) = b_N N!$ From (1.18), we have

$$\frac{df_N(x)}{dx} = Nf_{N-1}(x)$$
(1.19)

and

$$\frac{dh_N(x)}{dx} = h_{N-1}(x) , \qquad (1.19')$$

where

$$h_N(x) \equiv f_N(x)/N! \; .$$

The solution of (1.19') is simple:

$$h_N(x) = \int_1^x h_{N-1}(y) \, dy + h_N(1). \tag{1.20}$$

By successive integrations, taking into account that from (1.18) follows that $f_0(y) = f_0(1)$ and hence $h_0(y) = h_0(1)$, we derive

$$h_{1}(x) = (x - 1)h_{0}(1) + h_{1}(1),$$

$$h_{2}(x) = \frac{1}{2}(x - 1)^{2}h_{0}(1) + (x - 1)h_{1}(1) + h_{2}(1),$$

$$h_{3}(x) = (1/3!)(x - 1)^{3}h_{0}(1) + \frac{1}{2}(x - 1)^{2}h_{1}(1)$$

$$+ (x - 1)h_{2}(1) + h_{3}(1).$$
(1.21)

From (1.21) one can see that

$$h_N(x) = \sum_{\mu=0}^N \frac{1}{(N-\mu)!} (x-1)^{N-\mu} h_{\mu}(1). \qquad (1.22)$$

Equation (1.22) can be clearly proven by mathematical induction. Recalling the definition of $h_{x}(x)$, we obtain

$$b_{N} = \frac{1}{N!} \sum_{\mu=0}^{N} {N \choose \mu} (-1)^{N-\mu} f(\mu), \qquad (1.23)$$

since

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

Substituting (1.10) into (1.23) we end up with

$$b_{N} = \frac{1}{N!} \sum_{\mu=0}^{N} {\binom{N}{\mu}} (-1)^{N-\mu} \frac{1+(-1)^{\mu}}{2} \frac{1}{\sqrt{1+\mu}}.$$
 (1.24)

Since only even μ contribute to the sum, we can rewrite (1.24)

$$b_{N} = (-1)^{N} \frac{1}{N!} \sum_{\substack{\mu=0\\ \text{oven}}}^{N} {N \choose \mu} \frac{1}{\sqrt{1+\mu}} . \qquad (1.25)$$

We see that b_N alternates in sign with N. Thus we have the following analytical expression for the spin operators:

$$S_{i}^{*} = B_{i}^{*} \left(\sum_{n=0}^{\infty} b_{n} \hat{N}_{i} (\hat{N}_{i} - 1) \cdots (\hat{N}_{i} - n) \right),$$

$$S_{i}^{-} = \left(\sum_{n=0}^{\infty} b_{n} \hat{N}_{i} (\hat{N}_{i} - 1) \cdots (\hat{N}_{i} - n) \right) B_{i},$$

$$S_{i}^{z} = \sum_{n=0}^{\infty} c_{n} \hat{N}_{i} (\hat{N}_{i} - 1) \cdots (\hat{N}_{i} - n),$$
(1.26)

where c_n is given by substituting $f(\mu) = -\frac{1}{2}(-1)^{\mu}$ [see (1.14)] into (1.23). The result is

$$c_n = 2^{n-1} (-1)^{n+1} / n! . \tag{1.27}$$

Now using (1.6'), we can rewrite (1.26) in normal ordered form:

$$S_{i}^{*} = B_{i}^{\dagger} \left(\sum_{n=0}^{\infty} b_{n} B_{i}^{\dagger n} B_{i}^{n} \right),$$

$$S_{i}^{-} = \left(\sum_{n=0}^{\infty} b_{n} B_{i}^{\dagger n} B_{i}^{n} \right) B_{i},$$

$$S_{i}^{g} = \sum_{n=0}^{\infty} c_{n} B_{i}^{\dagger n} B_{i}^{n},$$
(1.28)

where b_n is given by (1.25) and c_n by (1.27). From the above given derivation it should be clear that expressions (1.28) are built in such a way that their matrix elements between states with welldefined eigenvalues of \hat{N}_i are equal to the corresponding matrix elements of (1.11) and (1.14), respectively, i.e., they coincide on a basis of the Bose-Hilbert space. As a result all their matrix elements coincide, respectively, and we can regard the two Bose representations of the spin operators as equal. Thus we can use each of them according to what we find more convenient.

II. INTUITIVE TREATMENT OF THE QUANTUM HEISENBERG MODELS

The Heisenberg Hamiltonian is

$$\mathcal{H} = \sum_{ij} J_{ij} (\alpha S_i^* S_j^* + S_i^z S_j^z) + h \sum_i S_i^z, \qquad (2.1)$$

where α is a measure of anisotropy ($\alpha = 1$ means isotropic Heisenberg model) and *i*, *j* denote lattice sites.

To treat (1.26) we substitute the representations (1.2) or (1.11) or (1.15) into (1.26) and then we are left with the problem of the interacting Bose gas. This problem was treated by various groups, Pataschinsky and Pokrovsky,¹² for example. We assume that near the critical point only $B_k^*B_k \gg 1$ are of importance, that we can consider the operators as c numbers and that only terms up to the fourth

order must be taken into account. This means that we should plug (1.2) into the Hamiltonian and evaluate the coefficients U_2 and U_4 considering the higher orders as irrelevant. This intuitive scheme will be verified in the next sections while now we shall limit our considerations to this simple procedure.

To illustrate the results we take $J_{ij}=J-$ const. After a simple calculation we get the following:

(a) Isotropic Heisenberg model: $U_2 = U_4$ and

$$\mathfrak{K} = \sum_{k} Jk^{2}a^{2}(|B_{k}^{2}| + |B_{k}^{4}|) \equiv \sum jk^{2}a^{2}(|B_{k}|^{2} + |N_{k}|^{2}).$$

The shape of this Hamiltonian corresponds to three order parameters in the system or in other words to O(3) symmetry. The new U_4 term is assymetric with respect to the order parameters (see Sec. III).

(b) x-y model ($\alpha > 1$):

$$\mathcal{K}=\sum Jk^{2}a^{2}\left|B_{k}^{2}\right|+4J(\alpha-1)\sum \left|B_{k}^{4}\right|$$

and we see that $U_4 > 0$ and the model has two order parameters.

These results, although they are of intuitive quality, show that the quantum and classical Heisenberg models behave in the same way at the critical point because the expressions obtained above repeat the output of the vector-spin-model considerations.

To conclude this section we would like to stress that although our assumption $B \gg 1$ is equivalent to a transition to a classical Bose system the results correspond to the quantum spin system with spin $S = \frac{1}{2}$ in which the straightforward transition to a classical limit is impossible. This can be seen in a simple way: if we neglect the spin commutation relations, going to a "classical limit," it is impossible to derive the spin-Bosons representations derived above and used in the above calculations of U_2 and U_4 coefficients. Thus the classical features of the system near the critical point stems from the fact that near T_c the quantum spin system is equivalent to a classical Bose system which contains the information about the quantum nature of spins (commutation relations, $S = \pm \frac{1}{2}$, etc.).

III. BOSONIZED HEISENBERG MODEL: STATES OVER COUNTING PROBLEM AND ITS SOLUTION

We recall the transformation relating the Boson operators B_i^{\dagger} , B_i to the spin operators:

$$S_{i}^{*} = B_{i}^{*} (1 + N_{i})^{-1/2} \frac{1}{2} [1 + (-1)^{\hat{N}_{i}}],$$

$$S_{i}^{-} = \frac{1}{2} [1 + (-1)^{\hat{N}_{i}}] (1 + \hat{N}_{i})^{-1/2} B_{i},$$
(3.1)

$$S^{z} = -\frac{1}{2}(-1)^{\hat{N}_{i}}.$$
(3.2)

One can easily check that the commutation and anticommutation relations of those operators are in accordance with what is expected of spin $-\frac{1}{2}$ operators. In particular $(S_i^*)^2 = (S_i^-)^2 = 0$. The eigenvalues of S_i^z are $\pm \frac{1}{2}$ as expected.

Now we shall turn to a problem of general nature that appears in every attempt to bosonize any spin model. Any finite lattice having say, N lattice sites, with a $S = \frac{1}{2}$ spin at each site has a finite number of independent states, namely, 2^N , since the state of a spin $\frac{1}{2}$ is always described in terms of two orthogonal states.

In contrast to the spin Hilbert space, a system of bosons always lies in an infinite-dimensional Hilbert space. (For example, $B^{\dagger}|0\rangle$, $(B^{\dagger})^{2}|0\rangle$,... are mutually orthogonal). Thus it is impossible to find a one-to-one correspondence between the basis elements of a spin Hilbert space and any Hilbert space of bosons. However, a multivalued transformation assigning to each basis state in the spin space an infinity of states in the Bose-Hilbert space is possible. To see how this happens let us examine the set of 2^{N} states S defined by

$$S = \{ |m_1, m_2, \dots, m_N \rangle, m_i \in \{n_i, n_i + (-1)^n i \} \},\$$

where n_1, n_2, \ldots, n_N is a given set of integers and m_i denotes the number of bosons associated with lattice site *i*. Now from (3.1) and (3.2) we see that S_i^* changes an even number of bosons to an odd one keeping the norm with the aid of the $(\hat{N}+1)^{-1/2}$ factor] and gives zero for an odd number of bosons. S_i changes an odd m_i into an even m_i but gives zero when acting on an even m_i . S_i^z does not change the boson number at lattice site i. We conclude that the spin operators can connect only states inside the set S but they cannot connect states belonging to different sets S. An even m_i corresponds to $S_i^z = -\frac{1}{2}$ and an odd one to $S_i^z = \frac{1}{2}$. Since the different sets S are mutually exclusive and their union constitutes a basis for the complete Hilbert-Bose space we conclude the following:

(a) In the process of bosonization we have embedded the spin Hilbert space into an infinite-dimensional Bose space.

(b) The infinite-dimensional Bose space is a union of an infinity of mutually orthogonal sub-



FIG. 1. Structure of the bosonized Hamiltonian in the Bose space. Each block is a matrix identical to the Hamiltonian matrix in the spin space.



FIG. 2. Diagonalized form of the bosonized Hamiltonian, in Bose space.

spaces each having the dimension of the original spin space. S gives a possible definition of the basis of such a subspace.

(c) The spin operators are invariant inside every subspace described in (b) and their action there is completely isomorphic to the action of the spin operators in the spin Hilbert space. Inside this subspace the matrices representing the spin-Bose operators are equal to the matrices representing those operators in the spin space, provided the proper correspondence between Bose states and spin states is kept, i.e., even m_i corresponds to $S_i^x = -\frac{1}{2}$ and odd m_i to $S_i^x = \frac{1}{2}$.

(d) It therefore follows that the matrix representing any spin Hamiltonian in the original spin space is equal to the matrix representing it in any of the above defined subspaces.

(e) In conclusion the matrix representing the spin Hamiltonian in the Bose space is of block form, each block matrix being equal to the matrix



FIG. 3. Diagonalized form of the Hamiltonian in Bose space, including the weight function.

representing this Hamiltonian in the original spin space. (See Fig. 1.) Diagonalizing this matrix we get Fig. 2, where E_1, E_2, \ldots, E_{2N} are the eigenvalues of the original spin Hamiltonian. Thus the new partition function is the trace of $e^{-\beta H}$ due to one block, namely, $\sum_{i=1}^{2N} e^{-\beta E_i}$ multiplied by the number of blocks which is infinite. To remedy this point we can assign a different weight to each block such that we get a finite partition function. (This is possible since for a finite lattice the number of blocks is denumerable.) By this we mean calculating $Tre^{-B\mathcal{K}-W}$, where W is chosen so that it commutes with $\mathcal R$ and is constant inside each block. The new "effective" Hamiltonian $\mathcal{K} + (1/\beta)W$ will have the form shown in Fig. 1 when represented in the basis in which 3C is diagonal (see Fig. 3). Denoting by Z_{or} the original Heisenberg partition function we see that the partition function we get for the Bose system with the weight function is

$$e^{-W^{(1)}} \left(\sum_{i=1}^{2^n} e^{-\beta E_i} \right) + e^{-W^{(2)}} \sum_{i=1}^{2^n} e^{-\beta E_i} + \cdots \\ = \sum_{\alpha=0}^{\infty} e^{-W(\alpha)} Z_{\text{or}},$$

where α is an index denoting the number of the block. Now if we choose the W's so that $\sum e^{-W}$ is a finite number M we get that the partition function of the Bose system is MZ_{or} . Thus our Bose system will reproduce the thermodynamical properties of the original spin model. W is not determined uniquely by the requirements mentioned above. We can choose, for example,

$$W = -\mu \sum_{i} [2\hat{N}_{i} + (-1)^{\hat{N}_{i}} + \lambda]^{2},$$

where μ and λ are constants.

Denote the two possible eigenvalues of \hat{N}_i in a certain block by $2n_i$, $2n_i+1$, where n_i is an integer. The $2\hat{N}_i + (-1)^{\hat{N}_i}$ has the same eigenvalue for both of them, i.e., it is actually a constant inside a given block. One can even calculate the constant M (to do so one has to calculate the number of blocks n_W contributing to each eigenvalue of W and then calculate $\sum n_W e^{-W}$). The result is of the order of $N! / \mu N$, where N is the number of lattice sites.

This completes the description of the exact bosonization process we propose for spin systems. Its virtues are its exactness and the fact that one does not need projection operators in order to project a partial Hilbert space out of the whole space, as is done in other bosonization schemes.

Finally we would like to stress the fact that our picture describes the conventional magnon gas in

the low-temperature limit, provided B_k^{\dagger} , B_k are identified as creation and annihilation operators of magnons, respectively. $\sum_i [2\hat{N}_i + (-1)^{\hat{N}_i}]$ is constant in each block and since μ is temperature independent, $\langle \sum_i [2\hat{N}_i + (-1)^{\hat{N}_i}] \rangle = \text{const}$, the latter constant being independent of temperature. Since $S_a^i = -\frac{1}{2}(-1)^{\hat{N}_i}$, we can rewrite this relation as

$$\langle \sum_{k} B_{k}^{\dagger} B_{k} \rangle - M = \text{const},$$
 (3.3)

where $M = \langle \sum_i S_z^i \rangle$ is the total magnetization. Relation (3.3) is the well-known relation of Bloch.¹³ In our picture this relation is exact and true for all temperatures [the sign in (3.3) differs from the one used in Keffer¹³ due to the fact that in our ground state the spins point in the $-\frac{1}{2}$ direction].

IV. PATH-INTEGRAL FORM OF THE QUANTUM-HEISENBERG-MODEL PARTITION FUNCTION

In this section the partition function of the quantum Heisenberg model is rewritten in a path-integral form using Klauder's technique¹⁴ of coherent states. The only difference between what is used here and what Klauder does is the fact that we calculate $\operatorname{Tr} e^{-\beta H}$ for real β whereas Klauder does so for imaginary $\beta(\beta = it)$. Transcribing his *it* into β gives immediately the desired result for the partition function. The reader is reminded that a coherent state is an eigenstate of a Bose operator *B* with given complex eigenvalue λ :

$$B |\lambda\rangle = \lambda |\lambda\rangle, \ \langle \lambda | B^* = \langle \lambda | \lambda^*.$$
(4.1)

Coherent states for different complex λ are not orthogonal but satisfy

$$\langle \mu | \lambda \rangle = e^{-|\mu|^2/2 - |\lambda|^2/2 + \mu^* \lambda}.$$

As a particular case $\langle \lambda | \lambda \rangle = 1$.

The most important property of coherent states is their completeness:

$$\int |\lambda\rangle \frac{d\lambda \, d\lambda^*}{\pi} \, \langle \lambda | = 1,$$

where $d\lambda d\lambda^*$ means now and henceforth $d(\text{Re}\lambda)$ $d(\text{Im}\lambda)$. The extension to many bosons is straightforward. We define

 $|\lambda_1, \lambda_2, \ldots, \lambda_N\rangle = |\lambda_1\rangle |\lambda_2\rangle, \ldots, |\lambda_N\rangle$

and all previously proper described properties of coherent states still hold. In particular,

$$\int \frac{d\lambda_1 d\lambda_1^*}{\pi} \frac{d\lambda_2 d\lambda_2^*}{\pi} \cdots$$

$$\times \frac{d\lambda_N d\lambda_N^*}{\pi} |\lambda_1, \dots, \lambda_N \rangle \langle \lambda_1, \dots, \lambda_N | = 1. \quad (4.3)$$

Now, we wish to calculate $Z = \operatorname{Tr} e^{-\beta H - W}$. Using Trotters formula,¹⁵ we can write

$$Z \cong Z^{(M)} = \operatorname{Tr}\left(1 - \frac{\beta}{M} H - \frac{W}{M}\right)^{M} \equiv \operatorname{Tr}Q^{M}, \qquad (4.4)$$

where

$$Q \equiv 1 - \frac{\beta}{M} H - \frac{1}{M} W.$$

The limit $M \rightarrow \infty$ gives the exact Z. We shall take a finite but very big M to make $Z^{(M)}$ close enough to Z. Let us insert complete sets of coherent states among the members of this product:

$$Z^{(M)} = \langle \lambda^0 | Q | \lambda^1 \rangle \langle \lambda^1 | Q | \lambda^2 \rangle \cdots \langle \lambda^{M-1} | Q | \lambda^0 \rangle.$$
 (4.5)

Summation (integration) over equal indices is understood, $|\lambda^r\rangle$ is defined as a coherent state of N bosons:

$$|\lambda^{\mathbf{r}}\rangle = |\lambda_1^{\mathbf{r}}, \lambda_2^{\mathbf{r}}, \dots, \lambda_N^{\mathbf{r}}\rangle, \quad 0 \leq \mathbf{r} \leq M - 1.$$
(4.6)

Now

(4.2)

$$\begin{split} \left\langle \lambda^{r} \left| Q \right| \lambda^{r+1} \right\rangle &= \left\langle \lambda^{r} \left| 1 - \frac{\beta}{M} \left(H + \frac{W}{\beta} \right) \right| \lambda^{r+1} \right\rangle \\ &= \left\langle \lambda^{r} \left| \lambda^{r+1} \right\rangle \left(1 - \frac{\beta}{M} \frac{\left\langle \lambda^{r} \right|^{H+W/\beta} \left| \lambda^{r+1} \right\rangle}{\left\langle \lambda^{r} \right| \lambda^{r-1} \right\rangle} \right). \end{split}$$

When using coherent states it is convenient to have the Bose operators in normal ordered form since then the B^{\dagger} 's operate on the left and yield complex numbers and the B's operate on the right:

$$\langle \lambda^{r} | B_{i}^{\dagger} B_{j}^{\dagger} \cdots B_{k}^{\dagger} B_{e} B_{m} \cdots B_{n} | \lambda^{r+1} \rangle$$

$$= \langle \lambda^{r} | \lambda^{r+1} \rangle \lambda_{i}^{r+1} \lambda_{j}^{r+1} \cdots \lambda_{k}^{r+1} \lambda_{e}^{\tau} \lambda_{m}^{\tau} \cdots \lambda_{n}^{r}.$$

$$(4.7)$$

Using (1.28) we already have H in normal ordered form and W can be easily rewritten in this form. The conclusion is that in the normal ordered form of $H + W/\beta$, we have

$$\frac{\langle \lambda^{r} | ^{H+W/\beta} | \lambda^{r+1} \rangle}{\langle \lambda^{r} | \lambda^{r+1} \rangle} = H(\lambda^{r+1*}, \lambda^{r}) + \frac{W}{\beta} (\lambda^{r+1*}, \lambda^{r})$$
$$\equiv \tilde{H}(\lambda^{r+1*}, \lambda^{r}).$$
(4.8)

The right-hand part means substitution of λ_i^{r+1*} for B_i^{t} and λ_i^{r} for B_i in both W and H. The definition of \tilde{H} is clear from (4.8). Hence

$$\langle \lambda^{r} | Q | \lambda^{r+1} \rangle = \langle \lambda^{r} | \lambda^{r+1} \rangle \left(1 - \frac{\beta}{M} \tilde{H}(\lambda^{r+1} * \lambda^{r}) \right)$$

$$\sim \langle \lambda^{r} | \lambda^{r+1} \rangle \exp \left(-\frac{\beta}{M} \tilde{H}(\lambda^{r+1} *, \lambda^{r}) \right)$$

$$= \exp[-\frac{1}{2} | \lambda^{r}_{i} |^{2} - \frac{1}{2} | \lambda^{r+1}_{i} |^{2} + \lambda^{r}_{i} * \lambda^{r+1}_{i}$$

$$- (\beta/M) \tilde{H}(\lambda^{r+1} *, \lambda^{r})]$$

$$(4.9)$$

A summation over *i* is understood in (4.9). We have used the smallness of β/M and (4.2).

Now we can write (4.5) as

$$Z^{(M)} = \int \prod_{r=0}^{M-1} \frac{d\lambda^r d\lambda^{r*}}{\pi} \langle \lambda^r | Q | \lambda^{r+1} \rangle$$

with $|\lambda^M\rangle = |\lambda^0\rangle$. Or,
$$Z^{(M)} = \int \exp\left(\sum_{r,i} \left(-\frac{1}{2} |\lambda_i^r|^2 - \frac{1}{2} |\lambda_i^{r+1}|^2 + \lambda_i^{r*} \lambda_i^{r+1}\right) - \frac{\beta}{M} \sum_r \tilde{\mathcal{G}}(\lambda^{r*}, \lambda^{r+1})\right) \prod_{r,i} \frac{d\lambda_i^r d\lambda_i^{r*}}{\pi}$$

(4.10)

The limit $M \rightarrow \infty$ gives a proper path integral (see Klauder⁴).

$$Z = \int \mathfrak{D}\lambda_{i} \exp \left[- \left[\int_{0}^{\theta} \left(\frac{\sum_{i} \lambda_{i}^{r*} (\partial/\partial r) \lambda_{i}^{r}}{2} + \tilde{\mathscr{K}} (\lambda^{r*}, \lambda^{r}) \right) dr \right], \qquad (4.11)$$

where r is a continuous variable $0 < r < \beta$. It should be mentioned that (4.11) is not enough to define the path integral in general and (4.10) should be taken as its proper definition.¹⁴

We would like to illustrate this procedure on a system of free bosons, where we also drop the index i. The partition function is

$$Z^{(M)} = \int \prod_{r} \frac{d\lambda^{r} d\lambda^{r*}}{\pi} \times \exp\left[+ \sum_{r=0}^{M-1} \left(-\frac{\left|\lambda^{r}\right|^{2}}{2} - \frac{\left|\lambda^{r+1}\right|^{2}}{2} + \lambda^{r*} \lambda^{r+1} - \frac{\left(\beta\right)}{M} E \lambda^{r*} \lambda^{r+1} \right) \right],$$

where E is $h\omega$.

Fourier transforming with respect to γ (remember $\lambda^{M} = \lambda^{0}$):

$$\lambda^{r} = \frac{1}{\sqrt{M}} \sum_{n=0}^{M} \exp\left(-i\frac{2\pi}{M} rn\right) \lambda^{\omega_{n}}$$

where λ^{ω_n} is defined as the Fourier transform of λ^r , we get

$$Z^{(M)} = \int \prod_{n=0}^{M-1} \frac{d\lambda^{\omega_n} d\lambda^{\omega_n *}}{\pi} \exp\left[-\sum_n \left|\lambda^{\omega_n}\right|^2 + \sum_n \left(1 - \frac{\beta E}{M}\right) e^{-i(2\pi/M)n} \left|\lambda^{\omega_n}\right|^2\right].$$

Since

$$d\lambda^{\omega n} d\lambda^{\omega n*} = \frac{1}{2} d \left| \lambda^{\omega n} \right| d\phi^n$$

where ϕ^n is the phase of λ^{ω_n} , we get

$$Z^{(M)} = \prod_{n=0}^{M-1} \frac{1}{1 - (1 - \beta E/M)e^{-1(2\pi/M)n}}$$
$$= \frac{1}{(1 - \beta E/M)^{M}} \prod_{n=0}^{M-1} \frac{1}{1/(1 - \beta E/M) - e^{-24\pi n/M}}.$$

Every polynomial P(Z) is proportional to $\Pi_i(Z - Z_i)$ where Z_i are its roots. $e^{2i\pi n/M}$ are the roots of unity, hence

$$Z^{M}-1=\prod_{n=0}^{M-1}(Z-e^{2i\pi n/M}).$$

Hence

$$Z^{(M)} = \frac{1}{(1 - \beta E/M)^{M}} \frac{1}{1/(1 - \beta E/M)^{M^{-1}}}$$
$$= \frac{1}{1 - (1 - \beta E/M)^{M}} \cdot$$

Hence

$$Z = \lim_{M \to \infty} Z^{(M)} = 1/(1 - e^{-\beta E})$$

as it is expected.

V. CLASSICAL EFFECTIVE HAMILTONIAN FOR THE ISOTROPIC HEISENBERG MODEL

The path integral as it stands is very complicated and even the original O(3) symmetry is not obvious in it. In this paragraph we shall show that only a few properties of this representation are really needed to write down a simple O(3) symmetric equivalent classical Hamiltonian for the Heisenberg model.

As we have shown, we can write S_{i}^{*} , S_{i}^{*} , S_{i}^{*} in terms of the Bose operators B_{i}^{\dagger} , B_{i} . Equivalently we can use S_{i}^{*} , S_{j}^{*} , S_{i}^{*} . When those operators are put between the coherent states, we get

$$\langle \lambda^{r+1} \left| S_i^{\alpha} \right| \lambda^r \rangle = \langle \lambda^{r+1} \rangle \langle \lambda^r \left| \lambda^{r+1} \right\rangle S_i^{r,\alpha} (\lambda_i^{r+1*} \lambda_i^r)$$
 (5.1)

where $\alpha = 1, 2, 3$ represents x, y, or z, respectively, and $S_i^{r,\alpha}$ is a function of λ_i^{r+1*} , λ_i^r . The explicit dependence is given in the Appendix. Thus the effective classical Hamiltonian in the former paragraph is

$$\begin{split} \tilde{H}^{\text{eff}} &= \left(-\sum_{\substack{i,j\\\alpha=1,2,3}} J_{ij} S_{i}^{\alpha,r} S_{j}^{\alpha,i} + \sum_{i} T_{i}^{r} (\lambda_{i}^{r*}, \lambda_{i}^{r}, \lambda_{i}^{r+1*}, \lambda_{i}^{r+1}) - \sum_{\substack{i,r\\\alpha=1,2,3}} h_{i}^{\alpha} S_{i}^{r,\alpha}\right) \frac{\beta}{M}, \end{split}$$
(5.2)

where T_i contains both the weight function W_i and the part coming from the norm of the coherent states. The variables appearing in the effective classical Hamiltonian $-\lambda_i^{r,\alpha}$, $\lambda_i^{r,\alpha*}$ carry an additional label with respect to the original variables, i.e., the label r. The latter label stems from the division of the inverse temperature β into segments. Thus we have added, in effect, a new dimension to the system. If the original quantum system was a d-dimensional system, the classical effective Hamiltonian describes a (d+1)-dimensional system, which is finite in the (d+1)th dimension. As we approach criticality we expect a crossover from (d+1)-dimensional behavior to d-dimensional behavior. It is important to note that the last two terms in \mathfrak{R}_{eff} are sums of singleion terms, i.e., they do not couple different spin sites. T_i may however, depend on the r's through $\lambda^{r+1*}\lambda_i$ or $\lambda_i^{r*}\lambda_i$.

We have also added a magnetic field h_i , the purpose of which is to keep track of symmetry. By this we mean that if we have $\bar{\mathbf{h}}_j = \delta_{ij} \bar{\mathbf{h}}$ then the partition function

$$Z = \operatorname{Tr} e^{-(3c_{+}\vec{\mathbf{h}}\cdot\vec{\mathbf{S}}_{i}) - W}$$
(5.3)

should be independent of the direction of h. This results merely from the O(3) symmetry of \mathcal{K} . The same is true for $Z^{(M)}$ as well, because O(3) is not broken in its definition.

Let us write the partition function

$$Z^{(M)} = \int \prod_{i,r} \frac{d\lambda_i^{r*} d\lambda_i^r}{\pi} \exp\left[\frac{\beta}{M} \left(\sum_{i,r,i} J_{ij} \vec{S}_i^r \cdot \vec{S}_j^r + \sum_{i,n} h_i S_i^r + R_i^r\right)\right]. \quad (5.4)$$

Now let us denote by (\bar{X}) the column matrix whose components are the real numbers X_i (1 < i < n) and by (X) the corresponding row matrix. Let A be an $n \times n$ symmetric matrix. Then the following holds:

$$\int \prod_{i} dx_{i} e^{-(X)A(\bar{X})/2 + b\bar{X}} = \left(\frac{(2\pi)^{n}}{\det A}\right)^{1/2} e^{(b)A^{-1}(\bar{b})/2},$$
(5.5)

where b is another n-component vector. Now take

$$A_{ij}^{-1} = J_{ij}$$
 or $A^{-1} = J$,

where J is the (symmetric) matrix whose elements are J_{ij} . J should be invertible (det $J \neq 0$) in order for formula (5.5) to apply. The condition for J to be invertible can be best seen in its Fouriertransformed representation. We can write

$$e^{(b)J(\bar{b})/2} = \exp\left(\frac{1}{2}\sum_{i,j}J_{ij}b_ib_j\right)$$
$$= \exp\left(\frac{1}{2}\sum_{\bar{k}}J(k)b_kb_k\right).$$

Thus we can deduce that the condition det $J \neq 0$ is equivalent to demanding $J(\vec{k}) \neq 0$ for all \vec{k} . If $J(\vec{k})$ does not fulfil this requirement we can add a constant c to it so that the requirement is fulfilled.¹⁶ Since $J(\vec{k})$ is bounded in all cases of interest such a c may be taken as max |J(k)| + 1. Adding this constant to $J(\vec{k})$ amounts to changing J_{ij} to $J_{ij} + c$. Doing so in our original Heisenberg Hamiltonian will have the effect of adding to it a constant term $c\sum_i \vec{S}_i \cdot \vec{S}_j = \frac{3}{4}cN$ only (a different constant is added in the anisotropic case). Henceforth we shall take $J_{ij} + c$ as our new J_{ij} .

Now, define

$$b_i^{r,\alpha} = (2\beta/M)^{1/2} \cdot S_i^{r,\alpha}$$

and $(b^{r,\alpha})$ as the matrix whose components are $b_i^{r,\alpha}$. From Eq. (5.5) it follows that

$$\left(\frac{(2\pi)^{N}}{\det(J^{-1})}\right)^{1/2} \exp\left(\sum_{i,j}\frac{\beta}{M}J_{ij}S_{i}^{r,\alpha}S_{j}^{r,\alpha}\right) = \int \prod_{i} dx_{i}^{r,\alpha} \exp\left(-\frac{1}{2}\sum_{i,j}X_{i}^{r,\alpha}J_{ij}^{-1}X_{j}^{r,\alpha} + \sum_{i}X_{i}^{r,\alpha}\left(\frac{2\beta}{M}\right)^{1/2}S_{i}^{r,\alpha}\right)$$
$$= \left[\left(\frac{2\beta}{M}\right)^{1/2}\right]^{N} \int \prod_{i} dy_{i}^{r,\alpha} \exp\left[\frac{\beta}{M}\left(-\sum_{i,j}J_{ij}^{-1}Y_{i}^{r,\alpha}Y_{j}^{r,\alpha} + 2\sum_{\alpha,i,r}Y_{i}^{r,\alpha}S_{i}^{r,\alpha}\right)\right]$$
(5.6)

where

$$Y_i^{r,\alpha}(2\beta/M)^{1/2} = X_i^{r,\alpha}$$

or

$$\exp\left(\sum_{i,j,r,\alpha}\frac{\beta}{M}J_{ij}S_{i}^{r,\alpha}S_{j}^{r,\alpha}\right) = \left[\frac{1}{\det J} \left(\frac{\beta}{M\pi}\right)^{N}\right]^{3M/2} \int \prod_{i} dy_{i}^{r,\alpha} \exp\left[\frac{\beta}{M} \left(-\sum_{\substack{i,j\\r,\alpha}}J_{ij}^{-1}Y_{i}^{r,\alpha}Y_{j}^{r,\alpha}+2\sum_{i,r,\alpha}Y_{i}^{r,\alpha}S_{i}^{r,\alpha}\right)\right]$$
(5.7)

Now $Z^{(M)}$ can be rewritten

$$Z^{(M)} = G \int \prod_{i,r,\alpha} dy_i^{r,\alpha} \frac{d\lambda_i^{r,\alpha} d\lambda_i^{r,\alpha} *}{\pi} \exp\left[\frac{\beta}{M} \left(-\sum_{\substack{i,j\\r,\alpha}} J_{ij}^{-1} Y_i^{r,\alpha} Y_j^{r,\alpha} + 2\sum_{i,r,\alpha} Y_i^{r,\alpha} S_i^{r,\alpha} + \sum_{i,r,\alpha} h_i^{\alpha} S_i^{r,\alpha} + \sum_{i,r} T_i^{r}\right)\right]$$
(5.8)

with

$$G = \left[\frac{1}{\det J} \left(\frac{\beta}{M\pi} \right)^N \right]^{3M/2}.$$

Thus we have the $S_i^{r,\alpha}$ in the "classical effective Hamiltonian" only in a linear form. The procedure we used is very close to the Hubbard-Stratonovich^{17,18} transformation. For a short-range interaction J_{ij} , the small-k behavior of its Fourier transform J(k) is proportional to $k^2 + r$, where r is a constant so that the asymptotic behavior of J_{ij}^{-1} is given by

$$J_{ij}^{-1} \sim \int \frac{e^{i\vec{\mathbf{k}}(\vec{\mathbf{i}}-\vec{\mathbf{j}})}}{k^2 + \gamma} d^d k \propto e^{-\left|\vec{\mathbf{i}}-\vec{\mathbf{j}}\right| \sqrt{\tau}}; \quad \left|\vec{\mathbf{i}}-\vec{\mathbf{j}}\right| \to \infty$$
(5.9)

i, j denote the lattice vectors corresponding to lat-

tice sites i, j, respectively, and translational invariance is assumed. As a consequence J_{ij}^{-1} is a short-range interaction too. Since the new coupling is $(-J_{ij}^{-1})$ the coefficient of k^2 in the U_2 term is kept positive and we stay in a ferromagnetic problem.

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The term in the effective classical Hamiltonian, containing $S_i^{r_i \, \alpha}$ is

$$\frac{\beta}{M} \sum_{i,r,\alpha} (2Y_i^{r,\alpha} + h_i^{\alpha}) S_i^{r,\alpha}.$$
(5.10)

It is convenient to perform a shift $Y_i^{r,\alpha} - Y_i^{r,\alpha} - \frac{1}{2}h_i$. We shall also denote $\hat{J}_{ij} = -J_{ij}^{-1}$. By a proper choice of the constant C, \hat{J}_{ij} can be made positive. Now, $Z^{(M)}$ can be rewritten

$$Z^{(M)} = G \int \prod_{i, r, \alpha} dy_{i}^{r, \alpha} \frac{d\lambda_{i}^{r, \alpha} d\lambda_{i}^{r, \alpha}}{\pi} \exp\left[\frac{\beta}{M} \left(\sum_{\substack{i, j \\ r, \alpha}} \hat{J}_{ij} Y_{i}^{r, \alpha} Y_{j}^{r, \alpha} + \sum_{\substack{i, j \\ r, \alpha}} \hat{J}_{ij} Y_{i}^{r, \alpha} h_{j}^{\alpha} + \frac{1}{4} \sum_{\substack{r, \alpha \\ i, j}} \hat{J}_{ij} h_{i}^{\alpha} h_{j}^{\alpha} + 2 \sum_{i, r, \alpha} Y_{i}^{r, \alpha} S_{i}^{r, \alpha} + \sum_{i, r} T_{i}^{r}\right)\right].$$

$$(5.11)$$

The term

$$\sum_{\substack{i, \ j \\ r, \alpha}} \hat{J}_{ij} h_i^{\alpha} h_j^{\alpha}$$

is independent of the integration variables and multiplies $Z^{(M)}$ by a constant

$$\exp\left(\beta\sum_{i,j}\hat{J}_{ij}\vec{h}_i\cdot\vec{h}_j\right).$$

The term it adds to the free energy is

$$^{\beta}\sum_{i,j}\hat{J}_{ij}\vec{\mathbf{h}}_{i}\cdot\vec{\mathbf{h}}_{j}.$$

This term does not contribute to the magnetization or susceptibility at zero field and we can therefore either disregard it or absorb it in G.

The only term in the classical effective Hamiltonian that couples different lattice sites (after we omitted the $\vec{h}_i \cdot \vec{h}_i$ terms) is the

$$\frac{\beta}{M}\sum \hat{J}_{ij}Y_i^{r,\,\alpha}Y_j^{r,\,\alpha}$$

terms. The rest are "single-ion" terms. Equation (5.11) can be rewritten in the form

$$Z^{(M)} = G \int \prod_{i} dy_{i}^{r,\alpha} \exp\left[\frac{\beta}{M} \left(\sum_{i,j} \hat{J}_{ij} Y_{i}^{r,\alpha} Y_{j}^{r,\alpha} + \sum_{j,i,r,\alpha} \hat{J}_{ij} Y_{i}^{r,\alpha} h_{j}\right)\right] \times \prod_{i} \left\{ \int \prod_{r,\alpha} \frac{d\lambda_{i}^{r} d\lambda_{i}^{r*}}{\pi} \exp\left[\frac{\beta}{M} \left(\sum_{r,\alpha} S_{i}^{r,\alpha} Y_{i}^{r,\alpha} + \sum_{r} T_{i}^{r}\right)\right]\right\}.$$
(5.12)

The expression in the curly brackets depends only on the index *i* (or lattice point *i*) and since the functional dependence of $S_i^{r,\alpha}$ and T_i^r on the λ 's is independent of *i* (see the Appendix for the explicit dependence of $S_i^{r,\alpha}$), the result of the integration can be written as $\exp[(\beta/M)f(Y_i)]$, meaning that *f* is a function of $Y_i^{r,\alpha}$, $Y_i^{r,\alpha*}$, $(r=0,1,\ldots,M-1;\alpha=1,2,3)$. The form of $Z^{(M)}$ is therefore

$$Z^{(M)} = G \int \prod_{i} dy_{i}^{r, \alpha} \exp\left[\frac{\beta}{M} \left(\sum_{\substack{i, j \\ r, \alpha}} \hat{J}_{ij} Y_{i}^{r, \alpha} Y_{j}^{r, \alpha} + \sum_{\substack{i, j \\ r, \alpha}} \hat{J}_{ij} Y_{j}^{r, \alpha} h_{i}^{\alpha} + \sum_{i} f(Y_{i})\right)\right]$$
(5.13)

The effective classical Hamiltonian here is built as the usually investigated classical spin models are, i.e., it has a quadratic spin-spin coupling term and a sum of single-ion terms.¹⁹ This result follows essentially from the fact that during the process of bosonization and the rewriting of the partition function in terms of the coherent states, the $\vec{S}_i \cdot \vec{S}_j$ part coming from the original Hamiltonian is kept "form invariant." The next step is to Fourier transform the $Y_i^{r, \alpha}$ with respect to r:

$$Y_{i}^{r,\alpha} = \sum_{\omega} e^{i\omega t_{r}} Y_{i}^{\omega,\alpha},$$

$$\omega = (2\pi/\beta)n, \quad n = 0, 1, \dots, M-1$$

$$t_{r} = \beta r/M, \quad r = 0, 1, \dots, M-1.$$
(5.14)

 ω are the Matsubara frequencies.⁸ They correspond to the boundary condition $Y_i^{M_i \alpha} = Y_i^{0_i \alpha}$, which, here, follows from $\lambda_i^{M_i \alpha} = \lambda_i^{0_i \alpha}$. Expressing $Z^{(M)}$ in terms of $Y_i^{\omega, \alpha}$ we get

$$Z^{(M)} = GM^{3MN/2} \int \prod_{i} dy_{i}^{\omega, \alpha} \exp\left[\beta \left(\sum_{\substack{i, j \\ \omega, \alpha}} \hat{J}_{ij} Y_{i}^{\omega, \alpha} Y_{j}^{-\omega, \alpha} + \sum_{\substack{i, j \\ \omega, j}} J_{ij} Y_{j}^{\omega=0, \alpha} h_{i}^{\alpha} + f(Y_{i})\right)\right].$$
(5.15)

The additional term $M^{3MN/2}$ stems from the Jacobian of the transformation $\{Y_i^{\alpha}, \alpha\} \rightarrow \{Y_i^{\alpha}, \alpha\}$. It cancels a

similar term inside G [see Eq. (5.8) thus making it M independent]. We define $G = GM^{3MN/2}$. We observe that the upper cutoff on ω is the only reminiscent of the fact that we divided β into M segments. In the limit $M \rightarrow \infty$, ω will have the values $(2\pi/\beta)n$, where n is any integer from zero to infinity. Thus the limit $M \rightarrow \infty$ of $Z^{(M)}$ in Eq. (5.15) is achieved by letting ω be unbounded as we have explained:

$$Z = \tilde{G} \int_{\substack{i, \ \omega \\ \alpha}} dy_i^{\omega, \alpha} \exp\left[\beta \left(\sum_{\substack{i, \ j \\ \omega, \ \alpha}} \hat{J}_{ij} Y_i^{\omega, \alpha} Y_j^{-\omega, \alpha} + \sum_{i \ j} \hat{J}_{ij} Y_j^{\omega, \alpha} h_i^{\alpha} + f(Y_i)\right)\right], \quad w = \frac{2\pi}{\beta}n, \quad n = 0, 1, 2, \dots$$
(5.16)

Alternatively we could develop a field-theoretical approach and show that the critical behavior of the system described by the above given Hamiltonian is independent of the cutoff on ω , hence one need not take the limit $M \rightarrow \infty$ in order to find this behavior. In the renormalization-group approach it is convenient to have such a cutoff, since then we can regard the system as the 3M-component anisotropic vector model that crosses over to three-component isotropic vector model in the process of renormalization. For details of this approach we refer the reader to Young.²⁰

Another approach within the finite cutoff theory would be (as has already been mentioned in Ref. 2) to regard the r's as an additional dimension in whose direction the system is finite in extent (of size β). Such a system will crossover to the original dimension as has already been explained.²

The common feature of all approaches mentioned so far is the fact that only the $\omega = 0$ component survives renormalization. In Eq. (5.16) we see that the external magnetic field \overline{h} couples only to $Y_i^{\omega=0,\alpha}$. We conclude that the $Y_i^{\omega=0,\alpha}$ component represents the physical spin. At criticality we can replace $\sum_j \hat{J}_{ij} Y_j^{\omega=0,\alpha}$ by a constant c times $Y_i^{\omega=0,\alpha}$, since \hat{J}_{ij} is short ranged. The constant c can be absorbed into the magnetic field h. The interaction with the magnetic field is now $\sum_i Y_i^{\omega=0,\alpha} h_i^{\alpha}$.

It is easy to show that partition function of the isotropic quantum Heisenberg model is a scalar in the \vec{h}_i 's for all temperatures. Thus

$$\frac{\partial^2 Z}{\partial h_i^{\alpha} \partial h_i^{\beta}} \bigg|_{\text{all } h_i=0}$$

is zero for $\alpha \neq \beta$ and does not depend on α for $\alpha = \beta$. As a result the renormalized propagator for the $\omega = 0$ component in our equivalent classical model is proportional to the symmetric tensor $\delta_{\alpha\beta}$. On the basis of those considerations we expect the general form of the renormalized inverse propagator close to T_c to be

$$\left[\delta_{\alpha\beta}k^{2-n}A(\vec{k}^2) + r\delta_{\alpha\beta} + C_{\omega,k}^{\alpha,\beta}\right], \qquad (5.17)$$

where \vec{k} are the vectors in the reciprocal lattice, η is the well-known exponent. A represents corrections to leading scaling behavior, and $C_{\omega,k}$ represent the behavior of $\omega \neq 0$ components. The form is correct in the limit of small k. $C_{\omega,k}$ can be written as

$$C_{\omega k}^{\alpha,\beta} \simeq + \omega Q_k^{\alpha,\beta} + \mathcal{O}(\omega^2) .$$
(5.18)

(The other term of the inverse propagator are regarded as "zeroth order" in ω .) Hence for small ω , k and neglecting corrections to scaling and the k dependence of Q, we have the inverse propagator

$$\delta_{\alpha,\beta} k^{2-\eta} + r \delta_{\alpha,\beta} + \omega Q_{\alpha,\beta} . \tag{5.19}$$

As is shown in various references^{2-5, 7, 20-22} the discrete values of ω lead to disappearance of all but the ω =0 term in a renormalization group procedure. Thus we get an isotropic fixed point in ddimensions. When the temperature goes to zero the values of the ω 's become continuous and then we have exactly a (d + 1)-dimensional system. The crossover from d + 1 to d dimensions is explained in several references^(2-7, 20-22) and we shall not reproduce it here.

We can summarize this chapter as follows:

(a) The classical effective Hamiltonian that reproduces the partition function of the quantum Heisenberg model has been written in the general form of the classical Hamiltonians that we have investigated using RG (see Aharony¹⁹).

(b) Using the O(3) symmetry of the problem it became clear that only an isotropic fixed point with a n = 3 order parameter can exist at a finite temperature.

(c) As T approaches zero we cannot get rid of the ω dependence and the problem becomes essentially a (d+1)-dimensional problem, that is isotropic in the first d dimensions and anisotropic in the (d+1)th dimension.

(d) The derivation of the classical effective Hamiltonian is exact and the only inexact arguments are the RG considerations. But the latter considerations are inexact in any calculation in the sense that one can do calculations only in the linear range of RG and has to assume the form of the effective Hamiltonian in this range. This is usually done assuming universality.

(e) Our "classical limit" has nothing to do with block constructions in the manner of Kadanoff. On the contrary, it is correct at all temperatures and therefore presents a proof that classical Hamiltonians can represent the thermodynamics of small-spin systems, which is a nontrivial result.

VI. ANISOTROPIC HEISENBERG MODEL

Formula (5.6) remains basically correct if J_{ij} depends on α too. One can have $J_{ij}^{\alpha} = \theta^{\alpha} J_{ij}$ with $\theta^{\alpha} = 1$ for $\alpha = 3$ and $\theta^{\alpha} = \theta$ for $\alpha = 1, 2$. As a result we shall have $J_{ij}^{-1}/\theta^{\alpha}$ instead of J_{ij}^{-1} in (5.6) and (5.7). Since the coupling in (5.6) and (5.7) is $-J_{ij}^{-1}$, the corresponding anisotropic coupling is $-J_{ij}^{-1}/\theta^{\alpha}$. If $\theta^{\alpha} > 0(X-Y \text{ anisotropy}) - J_{ij}^{-1}/\theta^{\alpha}$ is bigger in 1, 2 directions than in the third and we still have an X-Y anisotropy. A similar conclusion holds for $\theta^{\alpha} < 1$. Now using the usual RG arguments we arrive at the conclusion that for $\theta^{\alpha} > 1$ we have a X-Y-type critical behavior whereas for $\theta^{\alpha} < 1$ we have an Ising-type critical behavior.

VII. BOSE EFFECTIVE CLASSICAL HAMILTONIAN: HEURISTIC ANALYSIS

It is instructive to examine the Bose effective classical Hamiltonian, i.e., the Hamiltonian expressed in terms of the λ 's. Since we know by now that only the $\omega = 0$ terms are important close to T_c , we shall restrict ourselves to the analysis of those alone. In addition we shall mainly focus our attention on the quadratic and quartic couplings of the Hamiltonian, regarding the higher-order couplings as "irrelevant" (in $4 - \epsilon$ dimensions). We assume therefore that close to T_c one can write

$$Z \propto \int \prod_{i} d\lambda_{i} d\lambda^{*}_{i} \exp\left(-\beta \sum_{i} \Im(\lambda_{i}^{*}, \lambda_{i}) + \sum_{i} W(\lambda_{i}^{*}, \lambda_{i})\right) . \quad (7.1)$$

The label $\omega = 0$ has been omitted in (7.1) and the $\omega = 0$ component coming from the norm of the coherent states is zero. *W* is the weight function (see Sec. III) and it is defined here as

$$\hat{W(N_i)} = -\mu \sum_i \left[\hat{2N_i} + (-1)^{\hat{N_i}} \right]^2.$$
 (7.2)

 $W(\lambda_i^*, \lambda_i)$ denotes $\langle \lambda_i | W | \lambda_i \rangle$ as before,

$$W(\lambda_i^*,\lambda_i) = -\mu \sum_i \left(4 \left|\lambda_i\right|^4 + 4 \left|\lambda_i\right|^2 - 2 \left|\lambda_i\right|^2 e^{-2|\lambda_i|^2}\right).$$

In our crude approach we shall take $W = 4 \mu \Sigma_i (|\lambda_i|^2)$

+ $|\lambda_i|^4$) only since this is the part that is responsible for the convergence of the path integral. *H* is not assumed to be O(3) symmetric:

$$H = -\alpha \sum J_{ij} S_i^* S_j^- - \sum J_{ij} S_i^z S_j^z.$$

Going to momentum space and denoting by U_2 the coefficient of $\lambda_k^* \lambda_{\vec{k}}$ and by U_4 the coefficient of terms of the type $\lambda_{\vec{k}_1}^* \lambda_{\vec{k}_2}^* \lambda_{\vec{k}_3} \lambda_{\vec{k}_4}^*$, we get (in the smallk limit):

$$U_{2} = 4 \mu + 2d\beta J(1 - \alpha) + \beta \alpha J k^{2} a^{2} + O(k^{4}) .$$

$$U_{4} = 4 \mu / N + \beta (4dJ/N)(\alpha - 1) + O(k^{2}) .$$
(7.3)

a is the lattice constant and *N* the number of lattice sites. When $\alpha > 1$, $U_4 > 0$ and we have a *X*-*Y*-type model. The order parameters are λ and λ^* or Re λ and Im λ . When $\alpha = 1$, i.e., in the isotropic case we have $U_4 \rightarrow 4\mu$ when $k \rightarrow 0$. Actually both U_2 and U_4 are $4\mu + O(k^2)$. As we shall see this situation reflects the fact that in this case we have three order parameters. One can see this formally by defining a variable $n_i \equiv |\lambda_i|^2$ and integrating over it with an appropriate σ function expressing this equality.²⁷ In the momentum space we can use

$$\sigma\left((n_{k})^{2}-\left(\sum_{\vec{q}}\lambda_{\vec{k}}^{*}+\vec{a}_{q}\right)^{2}\right), \qquad (7.4)$$

which can be put into the exponent as

$$\exp\left[-b\left|(n_k)^2-\left(\sum_{\vec{q}}\lambda_{\vec{k}_1}^*,\vec{q}\lambda_{\vec{q}}\right)^2\right|^2\right].$$

Rigorously speaking one should use the $b \rightarrow \infty$ limit, but assuming universality we can keep a finite b.¹ We take n_i as the third-order parameter. The quartic part of the Hamiltonian can be expressed as $4\mu + \beta J k^2$ term in the exponent will affect only the U_4 part. The U_2 part is now

$$\left[4\mu+2d\beta J(1-\alpha)+\alpha\beta JK^{2}a^{2}\right]\lambda_{k}^{*}\lambda_{k}^{-}+\left(4\mu+\beta Jk^{2}a^{2}\right)\left|n_{k}\right|^{2}$$

when
$$\alpha = 1$$
 we have just

$$(4\mu + \beta J k^2 a^2)(\lambda_k^* \lambda_{\vec{k}} + |n_{\vec{k}}|^2)$$

corresponding to the usual O(3) symmetry of the Heisenberg Hamiltonian.

When $\alpha < 1$ then the constant (k independent part) corresponding to $|n_k|^2$ in (6.5) is smaller than the constant corresponding to the $\lambda_k^* \lambda_k$ part, which indicates a crossover to Ising-type behavior.

Thus we see that an analysis of the U_2 , U_4 parts alone (dropping higher-order terms as affecting only higher-order corrections in ϵ) already gives the results we got in the last paragraph.

Several remarks about the analysis carried out

above are in order:

(a) The U_4 part is not O(3) symmetric. Yet it is believed from works using the ϵ expansion that the isotropic fixed point is stable. In this case there is no doubt that the exact fixed point is isotropic (see Sec. V).

(b) This remark is concerned with the additional variable $n_i = |\lambda_i|^2$ that we use as the third-order parameter. One should note that the reason one could bosonize the spin operators is the fact that only two of them are independent, say S^* and S^- . S^z is given by $\frac{1}{2} [S^*, S^-]$. Otherwise the two independent operators B^{\dagger} , B would not suffice. The $S_i^z S_j^z$ part of the Heisenberg Hamiltonian can be rewritten in terms of the independent S_i^{\pm} operators as

$$\frac{1}{4} \sum J_{ij} [S_i^+, S_j^-] [S_j^+, S_j^-],$$

showing that the term corresponding to the "thirdorder parameter" is a magnon-magnon interaction term. This explains the identification of n_i as the third-order parameter, and simultaneously shows why the O(3) symmetry of the original Hamiltonian is not obvious in this representation.

(c) In spite of (a), one can make the effective Hamiltonian O(3) symmetric up to any U_{2n} . This is possible since one can trade a $|\lambda_i|^4$ term for a $|n_i|^2$ term and thus transfer terms between U_{2n} and U_{2n+2} . Thus any anisotropy can be pushed into as high U_{2n} as one wishes.

(d) One may note that when $\alpha = 1$ the only k-independent term in (6.5) is μ , i.e., a temperatureindependent constant. However, after the first RG iteration one gets corrections to μ that come from U_4 and higher-order couplings, all of which are proportional to β . Therefore the U_2 term will be of the form $4\mu - c\beta$ and we shall have a term of type $\beta - \beta_c$ as in usual Landau-Ginsburg models.

CONCLUDING REMARKS

The work presented here may be of use in understanding dynamical critical phenomena too. Most of the work done so far in this field²³ is based upon phenomenological Hamiltonians and the use of linear response theory for deriving equations of motion.

Some works (e.g., Ref. 24) have tried to find a microscopic justification of the above mentioned phenomenology, but they were restricted to Boson systems since only there the convenient existence of coherent states and other methods made this task manageable. Similar methods for spin systems lead to extremely complicated²⁵ and non-intuitive expressions. Furthermore if one is not interested only in the linear relaxation process

but in cooling a system below the critical point,²⁶ the situation gets much more complicated. Though it may be true that the phenomenological equations of motion lead to a physically correct description of the systems described by them (even in the nonlinear domain) it is of great importance to justify them from a microscopical point of view.

This paper is not concerned with dynamical problems but since it presents a unified picture of second-order phase transitions as generalized Bose condensation process it may lead to a unified picture of dynamics-as soon as the Bose condensation problem is satisfactorily solved. An important feature of the bosonized systems is the fact that certain quantities are conserved. In the *real* boson system we have a boson-number conservation whereas in the systems corresponding to spin system, some functions of the number of bosons are conserved, as we have seen. Since it is clear that without the existence of conserved quantities one cannot have a condensation process, our method leads to an understanding of the phase transitions in spin systems from a very general point of view.

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APPENDIX: CLOSED FORMULA FOR THE CLASSICAL EFFECTIVE HAMILTONIAN

In this Appendix we calculate the part of the effective classical Hamiltonian (ECH) that comes directly from the original Hamiltonian, i.e., we do not include the norm of the coherent states or the part coming from the weight function. This remaining part is called henceforth the ECH. The formula we derive here should be useful for further analytical and numerical investigation.

First we note that the ECH corresponding to the Heisenberg Hamiltonian can be written as

$$\begin{aligned} \Im \mathcal{C}^{\text{eff}} &= -\sum_{r, i, j} J_{ij} \Big[S_i^+ (\lambda_i^{r+1} *, \lambda_i^r) S_j^- (\lambda_j^{r+1} *, \lambda_j^r) \\ &+ S_i^z \left(\lambda_i^{r+1} *, \lambda_i^r) S_j^z (\lambda_j^{r+1} *, \lambda_j^r) \right]. \end{aligned} \tag{A1}$$

Since always $i \neq j$ in the Hamiltonian S_i^*, S_j^- commute in the original Hamiltonian and thus one can calculate separately the results for S_i^*, S_j^- , and S_i^{ε} .

A. Calculation of S_i^z

From (1.27) and (1.28), we have

$$S_i^z = -\frac{1}{2} \sum_{\nu=0}^{\infty} \frac{(-2)^{\nu}}{\nu!} B_i^{\dagger \nu} B_i^{\nu}.$$
 (A2)

Hence

$$\frac{\langle \lambda^{r+1} | S_i^x | \lambda^r \rangle}{\langle \lambda^{r+1} | \lambda^r \rangle} = -\frac{1}{2} \sum_{\nu=0}^{\infty} \frac{(-2)^{\nu}}{\nu !} (\lambda_i^{r+1*})^{\nu} (\lambda_i^r)^{\nu}$$
$$= -\frac{1}{2} e^{-2\lambda_i^{r+1*} \lambda_i^r}.$$
(A3)

B. Calculation of $S_i^+(\lambda_i^{r+1*},\lambda^r)$

From (1.25) and (1.28) we have:

$$S_i^{\dagger} = B_i^{\dagger} \sum_{n=0}^{\infty} b_n B_i^{\dagger n} B_i^n$$
(A4)

where:

$$b_n = (-1)^n \frac{1}{n!} \sum_{\substack{\mu \text{ even} \\ \mu \text{ even}}}^n \binom{n}{\mu} \frac{1}{\sqrt{1+\mu}} .$$
 (A5)

From (A4) we get in a similar way to (A3)

$$S_i^*(\lambda_i^{r+1*}, \lambda_i^r) = \lambda^{r+1*} \sum_{n=0}^{\infty} b_n (\lambda_i^{r+1*} \lambda_i^r)^n .$$
 (A6)

(A6) can be considered a closed formula for S_i^* .

In what follows we rewrite (A6) in another form, that explicitly shows the convergence of (A6). From (A5) we have

$$b_{n} = (-1)^{n} \frac{1}{n!} \sum_{\substack{\mu = 0 \\ \mu \text{ even}}}^{n} \binom{n}{\mu} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dZ \, e^{-z^{2}(1+\mu)}$$

$$= \frac{(-1)^{n}}{\sqrt{\pi}n!} \int_{-\infty}^{\infty} dZ \left[e^{-z^{2}} \sum_{\substack{\mu = 0 \\ \mu \text{ even}}}^{n} \binom{n}{\mu} e^{-z^{2}\mu} \right]$$

$$= \frac{(-1)^{n}}{\sqrt{\pi}n!} \int_{-\infty}^{\infty} dZ e^{-z^{2}} \left[\sum_{\substack{\mu = 0 \\ \mu = 0}}^{n} \binom{n}{\mu} (e^{-z^{2})^{\mu}} + \sum_{\substack{\mu = 0 \\ \mu = 0}}^{n} \binom{n}{\mu} (-e^{-z})^{\mu} \right] \times \frac{1}{2}$$

$$= \frac{(-1)^n}{2\sqrt{\pi}n!} \int_{-\infty}^{\infty} dZ \, e^{-z^2} [(1+e^{-z^2})^n + (1-e^{-z^2})^n] \,. \, (A7)$$

Substituting (A7) into (A6), we get

$$S_{i}^{*}(\lambda_{i}^{r+1}*,\lambda_{i}^{r}) = \lambda_{i}^{r+1}*\frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} dZ \ e^{-z^{2}} \sum_{n=0}^{\infty} \frac{1}{n!} \{ [-(1+e^{-z^{2}})\lambda_{i}^{r+1}*\lambda_{i}^{r}]^{n} + [-(1-e^{-z^{2}})\lambda_{i}^{r+1}*\lambda_{i}^{r}]^{n} \}$$
$$= \lambda_{i}^{r+1}*\frac{1}{2\sqrt{\pi}} \int_{-\infty}^{\infty} dZ \ e^{-z^{2}} (e^{-(1+e^{-z^{2}})\lambda_{i}^{r+1}*\lambda_{i}^{r}} + e^{-(1-e^{-z^{2}})\lambda_{i}^{r+1}*\lambda_{i})}) .$$
(A8)

So we have

$$S_{i}^{*}(\lambda_{i}^{r+1}*,\lambda_{i}^{r}) = \frac{\lambda_{i}^{r+1}*}{2\sqrt{\pi}} \int_{-\infty}^{\infty} dZ \ e^{-z^{2}}(e^{-e^{-z^{2}}(\lambda_{i}^{r+1}*\lambda_{i}^{r})} (A9)) \times e^{+e^{-z^{2}}(\lambda_{i}^{r+1}*\lambda_{i}^{r})} e^{-\lambda_{i}^{r+1}*\lambda_{i}^{r}}.$$

The last integral can be evaluated by expanding $e^{\pm e^{-z^2}\lambda_i^{r+1*}\lambda_i^r}$

in a power series in e^{-z^2} . The result is

$$S_i^*(\lambda_i^{r+1} * \lambda_i^r) = \lambda_i^{r+1} * \sum_{\substack{m=0\\m \text{ even}}} \frac{(-\lambda_i^{r+1} * \lambda_i^r)^m}{m!\sqrt{1} + m} e^{-\lambda_i^r + 1 * \lambda_i^r}.$$
(A10)

In any case we write

 $S_i^+(\lambda_i^{r+1*},\lambda_i^r) = \lambda_i^{r+1*}f(\lambda_i^{r+1*}\lambda_i^r),$

where f is defined through (A10). f is clearly well defined for every value of $(\lambda_i^{r+1} * \lambda_i^r)$.

(c) $S_i^{-}(\lambda_i^{r+1*}, \lambda_i^r)$ is calculated like S_i^{+} . The result is

$$S_i^{-}(\lambda_i^{r+1*},\lambda_i^r) = f(\lambda_i^{r+1*}\lambda_i^r)\lambda_i^r,$$

where f is the same as in (b).

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