A Wick Theorem for Spin-One Operators*

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A generalization to all spin magnitudes of the drone-fermion representation (previously known for spin $\frac{1}{2}$), is presented, and the resulting eigenstates investigated. Linear combinations of products of fermion operators acting on a vacuum state can always be found which correspond to spin states which are eigenvectors of $\mathbf{S}^2$ and S^z. It is then shown that for the case of spin 1 (units of $\hbar$) it is possible to construct a Wick theorem which is analogous to the usual temperature form for standard fermion creation and destruction operators.

1. INTRODUCTION

SINCE the establishment of the principal perturbation techniques of quantum field theory by Feynman, Dyson, and others, it has been natural to try to extend them to the range of problems in solid-state physics. These have been notably successful everywhere, except in those problems where it is necessary to manipulate spin operators explicitly. The crux of these difficulties is the absence of a simple analog of Wick's theorem.[1] This is the step which reduces multiple products of operators in a thermal average over the free eigenstates of the individual operators to products of pairs of operators (these are normally just creation and destruction field operators).

Several attempts at this problem have been made, especially around 1960. Davis[2] used Schwinger's coupled-boson representation of the spin operators (valid for all S) to derive a useful linked-cluster theorem without the use of diagrams. However, the method must carefully take into account the finite number of spin states, as the bosons, of course, have an infinite number. Indeed, this is the major problem in almost all attempts at a spin Wick theorem.

Mills *et al.*[3] in their treatment of the antiferromagnet, for spin $\frac{1}{2}$, introduced operators which had fermion properties on the same site but boson properties with respect to different sites. This involved the use of diagrams with additional partially overlapping lines, producing rather unconventional structures.[4] In fact, Wang *et al.*[5] have rederived these results in establishing a theorem for spin $\frac{1}{2}$ at zero temperature, leading to retarded spin propagators.

In 1965, Yolin[6] used a spin Wick theorem, again for spin $\frac{1}{2}$, and involving the coupled-fermion spin representation, to investigate spin-phonon interactions in paramagnets. Again the anomalous states were responsible for complications. This time they were in the form of weighting factors which limited its application to retaining the site index; i.e. in general, no Fourier momentum transform was possible. Indeed, this normalization difficulty occurs in the present work for $S=1$ but *not* for $S=\frac{1}{2}$.

Abrikosov[7] generalized the last method to all spin values by introducing the $2S+1$ coupled-fermion representation in an investigation of the Kondo problem of anomalous resistivity behavior in dilute metallic alloys, and he overcame the difficulty of the anomalous states (of which there are now a large but finite number), but there were still normalization difficulties. Doniach[8] also investigated the Kondo problem with the aid of a new Wick theorem for general spin operators at zero temperature. This was a generalization of the usual Wick approach and resulted in special diagrams corresponding to commutators of more than one pair of operators. The central point here is that techniques like the linked-cluster theorems are not readily available. A form of Wick's theorem for spin operators has been introduced in the work of Giovannini *et al.*,[9] which involves "remembering" all the previous commutations which have been carried out. This appears to be a finite-temperature method related to the zero-temperature theory of Doniach. Although a linked-cluster theorem was established, their diagrams lacked the elegance of the Feynman graphical technique.

Very recently Lewis and Stinchcombe[10] generalized the work of Wang *et al.*[5] to finite temperatures for the case of $S=\frac{1}{2}$ and applied their new techniques to the Heisenberg ferromagnet, again resulting in a somewhat unconventional diagrammatic formulation.

The first purpose of the present paper is to generalize

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[1] G. C. Wick, Phys. Rev. **80**, 268 (1950). Recently, T. Arai and B. Goodman [Phys. Rev. **155**, 514 (1967)] have shown that this is a cumulant (semi-invariant) expansion.
[2] H. L. Davis, Phys. Rev. **120**, 789 (1960).
[3] R. L. Mills, R. P. Kenan, and J. Korringa, Physics **26**, S204 (1960).
[4] In fact, R. P. Kenan [J. Appl. Phys. **37**, 1453 (1966)] has also treated the antiferromagnet using the drone-fermion representation with the drones playing the role of the "contracted lines" in Ref. 3, rather than by the general method established in Ref. 12.
[5] Yang-li Wang, S. Shtrikman, and H. Callen, Phys. Rev. **148**, 419 (1966).
[6] E. M. Yolin, Proc. Phys. Soc. (London) **85**, 759 (1965).
[7] A. A. Abrikosov, Physics **2**, 5 (1965).
[8] S. Doniach, Phys. Rev. **144**, 382 (1966).
[9] B. Giovannini, M. Peter, and S. Koide, Phys. Rev. **149**, 251 (1966).
[10] W. W. Lewis and R. B. Stinchcombe, Proc. Phys. Soc. (London) (to be published).

the drone-fermion representation, introduced by Mattis[11] for $S=\frac{1}{2}$, to all spin values. This is done in the next section, and the resulting eigenstates are investigated. The main section will demonstrate that averages over the spin states for $S=1$ are directly proportional to averages over the corresponding C space. This then results in a Wick theorem for spin-one operators.

2. GENERALIZED DRONE REPRESENTATION

In an earlier paper[12] it was shown that a simple Wick theorem for spin-$\frac{1}{2}$ operators resulted from an analysis of the drone-fermion representation for $S=\frac{1}{2}$. In this section this representation is generalized to all spin values S. The result is slightly less elegant than in the previous case, and its principal use is to demonstrate that numerical coefficients in certain expressions take the value S rather than $\frac{1}{2}$, which might result from only using the simplest form.

The drone-fermion representation is generalized by associating with each localized spin operator $\mathbf{S}_i$ (sites labeled i, j, etc.) $2S$ spin-$\frac{1}{2}$ operators $\mathbf{S}_{i\alpha}$ each of which can be represented algebraically by a pair of fermion operators $c_{i\alpha}$ and $d_{i\alpha}$ (and their adjoints).

$$S_{i\alpha}^z = c_{i\alpha}^\dagger c_{i\alpha} - \tfrac{1}{2}; \qquad S_{i\alpha}^+ = c_{i\alpha}^\dagger \phi_{i\alpha};$$
$$\phi_{i\alpha} = d_{i\alpha} + d_{i\alpha}^\dagger. \tag{1}$$

The complete anticommutation rules are

$$[c_{i\alpha}, c_{j\beta}^\dagger]_+ = [d_{i\alpha}, d_{j\beta}^\dagger]_+ = \delta_{ij}\delta_{\alpha\beta}. \tag{2}$$

All other pairs of operators anticommute.
Each site (and representation, α) is associated with a vector space spanned by four basic vectors

$$|0,0\rangle, \qquad |0,1\rangle, \qquad |1,0\rangle, \qquad |1,1\rangle, \tag{3}$$

where the entry on the left in each ket of the C_α space is the c_α occupation number, and that on the right is the d_α occupation number (the site label has been omitted for the present). The joint vacuum state $|0,0\rangle$ is defined by

$$c_\alpha |0,0\rangle = d_\alpha |0,0\rangle = 0. \tag{4}$$

Because of the drones, the $S_\alpha^z = -\frac{1}{2}$ state for each α corresponds to *two* independent "vacuum" states $|0,0\rangle$ or $|0,1\rangle$, while the $S_\alpha^z = +\frac{1}{2}$ state corresponds to the two independent states with one c_α present, i.e., $|1,0\rangle$ and $|1,1\rangle$. For each spin $\mathbf{S}_i$ we now associate the direct-product space (C) for $\alpha = 1, \cdots, 2S$ of the four-dimensional space Eq. (3). Corresponding to the original spin operators are the C-space operators

$$\mathbf{S}_i = \sum_{\alpha=1}^{2S} \mathbf{S}_{i\alpha}. \tag{5}$$

[11] D. C. Mattis, *Theory of Magnetism* (Harper and Row, New York, 1965).
[12] H. J. Spencer (to be published).

The spin computation rules

$$[S_i^+, S_j^-] = 2\delta_{ij} S_i^z; \qquad [S_i^z, S_j^+] = \delta_{ij} S_i^+ \tag{6}$$

are preserved [this may be checked directly using $\phi_{i\alpha}^\dagger = \phi_{i\alpha}$ and $(\phi_{i\alpha})^2 = 1$]; without the ϕ operators these would be anticommutation rules. A basis vector in the larger C space (for each site) can be written in the following manner

$$|c_{2S} d_{2S} \cdots c_2 d_2 c_1 d_1\rangle, \tag{7}$$

where each c_α or d_α is either 0 or 1. This convention for their normal order is necessary to preserve the sign of these vectors as the operators are fermions. Now any one of these states with all $c_\alpha = 0$ is an independent eigenstate $|S, -S\rangle$ of $\mathbf{S}^2$ and S^z, and defines a $2S+1$ multiplet $|S, M\rangle$ by repeatedly using the following equation to generate the complete multiplet.

$$S^+ |S, M\rangle = \{(S-M)(S+M+1)\}^{1/2} |S, M+1\rangle. \tag{8}$$

It should be emphasized that this procedure assigns *all* the states specified by Eq. (7) to the same $|S, M\rangle$ multiplet in the form of 2^{2S} independent spin-equivalent series—unlike the $2S$—fermion representation, which forms all multiplets for $\mathbf{S}^2 = 0$ to $S(S+1)$. The square-root coefficient in Eq. (8), which is a direct consequence of the general spin commucation rules, is also the required normalization of the states in the C space.

3. WICK THEOREM FOR $S=1$

In order to demonstrate the Wick theorem for $S=1$, the complete set of C-space states for $S=1$ are needed. There are now four independent operators, namely, c_1, c_2, d_1, d_2 (again the site label will be dropped for the present). The four independent triplets, which are normalized and satisfy Eq. (8), are listed in Table I. It is at this point that one can see the difficulty of deriving a general Wick theorem for finite-temperature averages, for although they all contribute to the same multiplet, some of these states are only present in linear combinations and so have different normalization factors. This means there cannot be a general correspondence between a trace over spin states and a trace over the states in C space, each of which, by definition, has the same statistical weight. This difficulty can be avoided for the case of $S=1$ by noting that the "underweight" states in each triplet only occur for $M=0$, so the two spaces will only be related by a simple constant Y. The crucial property here is that for all these states $S^z|c\rangle = 0$. Then if $X(S^z)$ is expressible as a power series in S^z,

$$\mathrm{Tr}_s X(S^z) = \tfrac{1}{4}\mathrm{Tr}_c X(S^z) - X(0). \tag{9}$$

The factor 4 arises from overcounting the four independent triplets, and the operators on the right-hand

TABLE I. The four independent sets of C states for one site corresponding to the three spin states $|S, M\rangle$ for $S=1$ and $M=\pm1, 0$. The notation of Eq. (7) of the text is used.

The spin states	The equivalent C-D states 1	2	3	4
$\|1,-1\rangle$	$\|0000\rangle$	$\|0001\rangle$	$\|0001\rangle$	$\|0101\rangle$
$\|1,0\rangle$	$2^{-1/2}(\|0011\rangle+\|1100\rangle)$	$2^{-1/2}(\|0010\rangle+\|1101\rangle)$	$2^{-1/2}(\|1000\rangle+\|0111\rangle)$	$2^{-1/2}(\|1001\rangle+\|0110\rangle)$
$\|1,+1\rangle$	$\|1111\rangle$	$\|1110\rangle$	$\|1011\rangle$	$\|1010\rangle$

side take their C-space form (5). This latter result is also true for exponential functions, in particular, the partition function Z^0, evaluated in the interaction representation of the two spaces. If the Hamiltonian is diagonalized with respect to S^z in the usual form $H_0=\omega_0 S^z$, with ω_0 a nonvanishing constant, then $Z^0=\operatorname{Tr}\exp(-\beta\omega_0 S^z)$, where $\beta^{-1}=kT$. The corresponding equation is then

$$Z_s^0=\tfrac{1}{4}Z_c^0-1 \tag{10}$$

with

$$Z_c^0=4[\exp(\beta\omega_0)+\exp(-\beta\omega_0)+2]$$
$$=4[\exp(\beta\omega_0)+1][\exp(-\beta\omega_0)+1]. \tag{11}$$

This latter factorization is crucial to the whole argument, for it helps to cancel out the Fermi factors

$$f^{\pm}=\{\exp(\mp\beta\omega_0)+1\}^{-1}. \tag{12}$$

Moreover the factor $\frac{1}{2}$ in the C form of S^z is just sufficient to introduce an inverse Bose factor in the $\langle S^z\rangle_0{}^c$-type averages. This eventually will relate the fermion anticommutation rules of the C operators with the bosonlike commutation rules of the actual spin operators. (The term "bosonlike" is used to indicate that the spins obey commutation rules rather than anticommutation rules.) Now, as can be checked by either explicit calculation or cycling one of the C operators around the trace (see later), one has

$$\operatorname{Tr}_c[\exp(-\beta\omega_0 S^z)c_\alpha{}^\dagger c_\alpha]=4[1+\exp(-\beta\omega_0)]. \tag{13}$$

So, upon defining averages with respect to the C space by

$$\langle c_\alpha{}^\dagger c_\alpha\rangle_0{}^c=(Z_c{}^0)^{-1}\operatorname{Tr}_c\{\exp(-\beta\omega_0 S^z)c_\alpha{}^\dagger c_\alpha\}=f^-(\omega_0), \tag{14}$$

using Eqs. (14) and (6) for $S=1$, we get

$$\langle S^z\rangle_0{}^c=2f^-(\omega_0)-1=\mu\left\{\frac{1-\exp(\mu\beta\omega_0)}{1+\exp(\mu\beta\omega_0)}\right\}. \tag{15}$$

In the last form, the notation $\mu=\pm1$ has been introduced for later use. The magnetization in the two spaces can now be related by using Eq. (9):

$$\langle S^z\rangle_0{}^s=(Z_s{}^0)^{-1}\operatorname{Tr}_s\{\exp(-\beta\omega_0 S^z)S^z\}$$
$$=(4Z_s{}^0)^{-1}\operatorname{Tr}_c\{\exp(-\beta\omega_0 S^z)S^z\}. \tag{16}$$

Then, multiplying and dividing by $Z_c{}^0$ and using Eq. (15), one may introduce the normalization factor $Y(\omega_0)$,

$$\langle S^z\rangle_0{}^s=Y(\omega_0)\langle S^z\rangle_0{}^c, \tag{17}$$

where

$$Y(\omega_0)=Z_c{}^0(4Z_s{}^0)^{-1}=\{f^+f^-Z_s{}^0\}^{-1}. \tag{18}$$

Moreover for $S=1$, one can always use the following closure relations for products of S^z, (for any integer n)

$$(S^z)^{2n+1}=S^z \quad\text{or}\quad (S^z)^{2n}=(S^z)^2. \tag{19}$$

So if $X(0)=0$, then

$$\langle X(S^z)\rangle_0{}^s=Y\langle X(S^z)\rangle_0{}^c. \tag{20}$$

This is the equation which restricts the proof to $S=1$ and $S=\frac{1}{2}$. In the latter case $Y=1$.[12]

The next stage of the proof is to generalize this to products of the raising and lowering operators S^μ (remembering $\mu=\pm1$). So, on rewriting Eq. (6) for one site in the useful form,

$$[S^\mu, S^{-\mu}]=2\mu S^z \quad\text{and}\quad [S^z, S^\mu]=\mu S^\mu. \tag{21}$$

Since spin averages are diagonal in S^z, there must be an equal number of S^μ and $S^{-\mu}$ operators. The general proof is inductive, so one starts out with the simplest products $\langle S^+S^-\rangle_0{}^s$ or $\langle S^-S^+\rangle_0{}^s$ and uses the property of cyclically transferring the operators around the trace, then "passing" them through the operator $\exp(-\beta\omega_0 S^z)$ using

$$\exp(\lambda S^z)S^\mu\exp(-\lambda S^z)=e^{\lambda\mu}S^\mu, \tag{22}$$

then finally commuting them back to their usual position in the product. The final result is

$$\langle S^\mu S^{-\mu}\rangle_0{}^s=2\mu\langle S^z\rangle_0{}^s[1-\exp(\mu\beta\omega_0)]^{-1}. \tag{23}$$

This approach can be equally well applied to the spin operators in their C-D form since the trace now covers the complete representation of the C-D states and so maintains the cyclic property; so immediately

$$\langle S^{\mu}S^{-\mu}\rangle_0{}^c = 2\mu\langle S^z\rangle_0{}^c[1-\exp(\mu\beta\omega_0)]^{-1}. \quad (24)$$

Upon multiplying by the factor Y and using Eq. (17),

$$\langle S^{\mu}S^{-\mu}\rangle_0{}^s = Y\langle S^{\mu}S^{-\mu}\rangle_0{}^c. \quad (25)$$

The same argument gives

$$\langle S^{\mu}S^{-\mu}S^z\rangle_0{}^s = 2\mu\langle (S^z)^2\rangle_0{}^s/[1-\exp(\mu\beta\omega_0)] + \langle S^{\mu}S^{-\mu}\rangle_0{}^s/[1-\exp(-\mu\beta\omega_0)], \quad (26)$$

and an identical form for

$$\langle S^{\mu}S^{-\mu}S^z\rangle_0{}^c.$$

Using Eqs. (20) and (25) one gets

$$\langle S^{\mu}S^{-\mu}S^z\rangle_0{}^s = Y\langle S^{\mu}S^{-\mu}S^z\rangle_0{}^c. \quad (27)$$

So it has been shown that a product of n spin operators can be reduced to ones involving $(n-1)$ spin operators. Then the rest of the proof is simply inductive and need not be stated here; this immediately leads to the central result of this paper for a general product of spin operators

$$\langle X(S^{\mu}, S^{-\mu}, S^z)\rangle_0{}^s = Y\langle X(S^{\mu}, S^{-\mu}, S^z)\rangle_0{}^c, \quad (28)$$

where the operators on the right-hand side take their C-D form for $S=1$ (Eq. 5). The corresponding result for a product of spin operators referring to N different sites is to convert Y to Y^N on the right-hand side of Eq. (28).

This equation also holds for P-ordered products of spin operators (no sign change) written in the interaction representation, that is by Eq. (22),

$$S^{\mu}(t) = \exp(iH_0t)S^{\mu}\exp(-iH_0t) = \exp(i\mu\omega_0t)S^{\mu}. \quad (29)$$

Moreover as the fermions in this representation occur in pairs, the P-ordering can be immediately converted to a T-ordered product (minus sign for each permutation) of the individual fermion operators so that

$$\langle PX(S^{\mu}, S^{-\mu}, S^z)\rangle_0{}^s = Y\langle TX(S^{\mu}, S^{-\mu}, S^z)\rangle_0{}^c. \quad (30)$$

After establishing this fundamental correspondence between the two spaces, the usual proof of Wick's theorem can be applied to the C and D operators since they are averaged with respect to a complete set of their states. The easiest method is that of Gaudin,[13] who used the cyclic argument employed above for the individual operators.

4. CONCLUSION

We have established a very simple procedure for handling thermal averages of spin operators for $S=1$, which may be further manipulated through the techniques of quantum field theory.[14] It must be emphasized that, apart from the additional multiplicative factor Y, the present method is a direct extension of such techniques to $S=1$ operators and does not necessitate any specialized manipulation or diagrams in contrast to most other spin-Wick treatments.

The present result is applied, along with the simpler result for $S=\frac{1}{2}$ previously established,[12] to the problem of the Heisenberg model of the ferromagnet in the following paper.

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