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# Kinematical Problem in Spin-Wave Theory

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A spin-1/2, nearest neighbor Heisenberg Hamiltonian acting on a periodic, $d$-dimensional lattice is considered. Multi-spin-wave solutions to the Schrödinger equation for a Heisenberg ferromagnet involve an unlimited superposition of spin-reversal operators at sites. This violates the physical restriction that no more than one excitation reside on any one site. This exclusion rule affects spin-wave interaction—the determination of these effects is called the kinematical problem. A general nonperturbative treatment that includes kinematical effects in spin-wave theory is developed along the following lines. Using the property of the Heisenberg Hamiltonian that it does not couple states obeying the single occupation condition at all sites with states that violate the single-occupancy condition at some sites, the unphysical multiply occupied states can be eliminated by a nonunitary transformation of the eigenvalue equation. An overcomplete Hamiltonian matrix is obtained that contains all the physical eigenvalues as a subset of its spectrum. Overcompleteness is shown to be a large part of the kinematical problem and several schemes to handle it are discussed. The remainder of the kinematical problem lies in the nonorthogonality of spin waves. It is shown that a new type of distribution, one that is neither Bose nor Fermi, correctly describes free spin-wave statistics at all temperatures. This formal but nonetheless complete solution to the overcompleteness aspect of the kinematical problem is then carried over, *in toto*, to the boson formulation of the spin Hamiltonian. Application to the calculation of the partition function and to thermal Green's functions is noted.

## 1. INTRODUCTION

The Heisenberg Hamiltonian for a localized fermionic system is the parent of other much-studied spin models (Ising, $X$-$Y$, and spherical models, among others). Accurate analytical calculation of the partition function for the Heisenberg model is limited to the low- and high-temperature regimes by the use of expansions in $T$ and $T^{-1}$. An exact

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quantum mechanical description of dynamics at intermediate temperatures including the critical region would be achieved by solving a spin-wave theory that preserves the original state space of denumerable configurations in which $S^2_{\text{total}}$ is a constant of the motion and $S_z$ is a good quantum number. The two main obstacles to such a solution are the dynamical and kinematical problems. The first is to find a means of solving the Schrödinger equation proceeding without regard to additional physical constraints. Here the spin-wave approach uses plane waves as approximate eigenfunctions about which corrections are computed. The second is to establish a faithful relation between the function space used to solve the equations of motion and the Hilbert space; the problem stems from their different dimensions (see below). The kinematical *problem* arises in spin-wave theory because superpositions of spin-wave creation operators can include components in which spin $S$ wavefunctions are excited more than the maximum $2S$ times. In the case of spin 1/2, such multiple excitations violate the basic restriction of the Heisenberg spin model, in which no more than one electron with either spin up or spin down can occupy a single site. The effect arises because the boson formalism includes states in which there is a superposition of more than $S$ spin excitation operators at a site. The kinematical *interaction*, a term we will reserve for use in the context of the boson formulation, is a complicated coupling interaction that acts in addition to a quartic spin-wave interaction. The kinematical interaction has resisted treatment by perturbative means, that is, the use of expansions in some small parameter.

The kinematical problem is an important factor in any situation where the description of the system includes excited states with occupation numbers that are a substantial fraction of the total system size. In these cases a large number of spin-wave states are affected by the limitation of no more than $S$ spins per site and this restriction cannot be ignored. Such situations are the thermodynamic behavior of Heisenberg spin systems outside the low-temperature regime ($k_B T$ a substantial fraction of $J$), at proportionally lower temperatures for smaller systems (because, in the absence of external fields, the spontaneous magnetization of small systems is metastable with respect to the creation of many zero-wavevector spin waves), and for such phenomena that are described using wave packets that contain a large number of excitations localized in a small region. Despite nearly 30 years and many attempts (Vaks *et al.*, 1968a; Wortis, 1965; Morita and Tanaka, 1965; Marshall and Murray, 1969; Kenan, 1967; Wenzel and Wagner, 1977; Szaniecki, 1965; Parmenter, 1984; Goldhirsch and Yakhot, 1980; Shi-Xun and Rui-Bau, 1980; Silberglitt and Harris, 1968) since Dyson's (1956) original exposition of the kinematical problem, no general solution or even unified picture of kinematical effects has emerged.



This work presents both a complete description and a formal resolution of the kinematical problem in both its spin and Bose Hamiltonian aspects. By distinguishing overcompleteness and nonorthogonality as two independent features, one obtains a deeper understanding of the mathematics of the problem and manner in which it can be solved. However, in this article, the job of developing practical approximation schemes is only begun. An approximation scheme for including the nonorthogonality of spin waves in the perturbative scheme using the boson Hamiltonian and thermal Green's functions will be presented in a separate work.

The following Heisenberg Hamiltonian models the interaction of electrons through an exchange effect proportional to the overlap integral

$$J_{\mathbf{ij}} = \langle \varphi_{a,\mathbf{i}} \langle \varphi_{b,\mathbf{j}} | e^2 / r(\mathbf{i}-\mathbf{j}) | \varphi_{a,\mathbf{j}} \rangle | \varphi_{b,\mathbf{i}} \rangle$$

where $|\varphi_{a,\mathbf{i}}\rangle$ is a one-electron Wannier wave function for electron $a$ centered at site $\mathbf{i}$, $\langle \varphi_{\mathbf{i}} | \varphi_{\mathbf{j}} \rangle = \delta_{a,b}\delta_{\mathbf{ij}}$, and $J_{\mathbf{ij}} = J$ or 0 depending on whether or not $\mathbf{i}$ and $\mathbf{j}$ are nearest neighbors. If $J > 0$ ($<0$), the model is ferromagnetic (antiferromagnetic). we have

$$\hat{H} = -\frac{J}{2} \sum_{\mathbf{j}\boldsymbol{\delta}} \mathbf{S}_{\mathbf{j}} \cdot \mathbf{S}_{\mathbf{j}+\boldsymbol{\delta}} \tag{1}$$

$\sum_{\boldsymbol{\delta}}$ is a sum over nearest neighbor vectors $\boldsymbol{\delta}$. A ground state $|0\rangle$ is chosen with a totally symmetric wave function and a maximum magnetic quantum number $m$; $m = N/2$ for an $N$-electron system ($|0\rangle$ is a lowest energy state for a ferromagnet). In the absence of an external magnetic field this energy is $N$-fold degenerate; in the presence of an external field it is unique. Excited states are labeled with a spin-wave number $n = (N/2 - m)$, $n = N/2$ for states with zero $z$-component magnetization. These states are given by spin creation operators on the ground state,

$$V(n): \quad \left\{ \prod_{\mathbf{k}} (S^+_{\mathbf{k}})^{a_{\mathbf{k}}} |0\rangle : \quad \sum_{\mathbf{k}} a_{\mathbf{k}} = n \right\} \quad \text{unnormalized} \tag{2}$$

with $S^+_{\mathbf{k}}$ given in terms of spin operators according to (5).

The one-spin-wave eigenstates, magnons, are of plane wave form, as was obtained by Bloch (1930). Wortis (1963) obtained the exact two-spin-wave eigenstates by a factoring of the eigenvalue equation into relative and absolute coordinates (separability is a consequence of wavevector conservation). This solution was corrected for the presence of unphysical states by Liu and Chow (1978). Closed-form expressions for the eigenfunctions of a

one-dimensional system have been obtained by Bethe (1931; see also Orbach, 1958) and Gochev (1972).

In the absence of an external **B** field the eigenvalues of (1) may be obtained through spin-algebraic methods (Pauncz, 1979), where the basis is symmetry-adapted to $S_{\text{tot}}^2 = (\sum_i S_i) \cdot (\sum_j S_j)$ with eigenvalues $S(S+1)$, $S = 0, 1, \ldots, N/2$; and $S_{\text{tot}}^z = \sum_j S_j^z$ with eigenvalues $m = +S, \ldots, -S$. The $n$-spin-wave states of equation (2) are constructed as linear combinations of the symmetry-adapted basis vectors with $m = N/2 - n$ and $S = N/2, N/2 - 1, \ldots, N/2 - n$. Only $m$ continues to be a good quantum number. Although this formulation can only be applied in practice to small systems, it shows that the spectrum of $n$-spin-wave excitations contains as a subset all those eigenvalues that occur for $(n' < n)$-spin-wave states. The spectrum at $B = 0$ is highly degenerate; $n$-spin-wave states whose energies are equal to $n'$-spin-wave states, with $n > n'$, can be considered bound states.

Bloch used the one-spin-wave states describing a free-magnon gas to derive the $T^{3/2}$ law for the low-temperature magnetization. Subsequently Dyson (1956), Maleev (1958), and then Wortis (1965) attempted to incorporate the effects of higher spin-wave states on the low-temperature thermodynamics of a ferromagnet, specifically to corrections of the $T^{3/2}$ law. Both authors transform (1) to an effective Hamiltonian $H_B$ written in terms of Bose operators [equation (34)] and employ a Fourier representation that requires an enlargement of the Hilbert space to include states with more than one raising operator at each site, a violation of the exclusion principle. The addition of these improper states adds unphysical eigenvalues that can cause the partition function to diverge (Wortis, 1965). Dyson named the elimination of the effects of these unphysical states the kinematical problem. The object of this paper is to solve the kinematical problem that arises in the boson formulation. The problem is first investigated in the context of spin operators, where techniques are developed that are then applied to the Bose operator formalism.

Essential to the present work is the interdependent role of kinematics and dynamics in the spin problem. It will be seen that the eigenvalues of the system are obtained from a matrix that is itself the product of two component matrices, one containing all the kinematics and another all the dynamics. The strong coupling of spin waves occurs to a large extent because the basis that approximately diagonalizes the dynamical component—the spin-wave basis—fails to approximately diagonalize the kinematic component. The nondiagonality of the kinematic component can be ignored at low temperatures because the thermodynamics is dominated by a subset of states that experience little kinematic interaction. These are highly magnetized states with few quasiparticle excitations. At higher temperatures, where



states with many excitations make a substantial contribution to the thermal behavior, perturbative spin-wave theory generates nonsense. This means that in general we do not have a noninteracting approximation.

My main result is a general spin-wave description of the Heisenberg system, founded on a commutator algebra, that forms an approximately diagonal basis at long wavelengths and at all temperatures. The spin-wave strong coupling problem is not solved completely—strong coupling remains at short wavelengths—but it is pushed back into a more limited domain. We now have a complete and consistent noninteracting approximation based on wavelike excitations for the ferromagnet and related systems. Spin waves can be represented as bosons populating energy levels according to a new, spin distribution function. Interaction among these particles is given by a quartic Hamiltonian (the boson Hamiltonian of Dyson and Maleev) whose coupling is both weak at long wavelengths and generally nonlocal. Standard thermal perturbation theory can be applied in theory—knowing the noninteracting distribution function (the thermal propagator) and having a quartic, Bose interaction Hamiltonian suggest perturbation theory can also be carried out in practice. The quasiparticle approximation I am presenting is to $SU(2)$ systems what noninteracting boson and fermion approximations are to interacting Bose and Fermi systems. Aside from the technical differences, the conceptual and perturbative role that these particles play is the same.

The layout of the paper is as follows. In Section 2 improper states are defined in the spin operator formalism and distinguished from improper states of the boson formulation. Working with finite systems and a matrix representation of the Schrödinger equation, it is shown that the secular equation can be transformed nonunitarily to a simpler expression in which improper states have zero eigenvalues. This is done by rewriting the secular equation, $\text{Det}\{[G]([S] - \lambda)\} = 0$, where $[G]$ is the inner-product matrix and $[S]$ is called the scattering matrix, as $\text{Det}([G][S] - \lambda) = 0$. We are allowed to make this simplification in the case of the Heisenberg Hamiltonian because proper and improper states exhibit a particular lack of coupling. The secular equation for a function $f$ of the Hamiltonian $\hat{H}$ [specifically the function $\exp(-\beta\hat{H})$ as appears in the partition function] is similarly transformed from $\text{Det}([G]\{f([S]) - \lambda\}) = 0$ to $\text{Det}\{[G]f([S]) - \lambda\} = 0$. In this case the improper states again generate zero eigenvalues. It is shown that the secular equation factors into two determinants, one involving only physical (or proper) states and another involving nonphysical (or improper) states. For spin operators, the improper states are shown to represent the extension of the basis to include extra, linearly dependent, degrees of freedom. This represents a reformulation of the kinematical problem from

a case involving unphysical degrees of freedom to one described by an overcomplete state space in which all the independent degrees of freedom are physical.

In Section 3 the effects of overcompleteness (the zero eigenvalues) are removed; this embodies a formal solution to the kinematical problem. This is accomplished through an elimination of dependent degrees of freedom, that is, by a reduction of the state space so as to include only a linearly independent set of states. When the secular equation is written in terms of such a complete set, no extraneous zero eigenvalues appear. We formally obtain a Hamiltonian matrix, in terms of a reduced set of the original spin-wave states, that represents only physical degrees of freedom and generates only physical eigenvalues.

Section 4 considers the problem of realizing the state space reduction crucial to the solution of Section 3. The two approaches to overcompleteness problem considered first are the boson approximation of Bloch and the fermion approximation of Wenzel and Wagner. Because the first effects no state space reduction, while the second effects a reduction but fails to represent the rotational symmetry of the Hamiltonian, a third approach is introduced in Section 5. This final description of the state space embodies the $SU(2)$ structure that is characteristic of quantum spin systems. As a result, we obtain a new distribution function describing spin waves. We conclude that the equilibrium properties of a Heisenberg ferromagnet, at finite temperatures and to lower order, are described by spin-wave excitations that populate the system according to an unusual distribution function that is neither Bose nor Fermi.

Section 6 generalizes these results to the boson Hamiltonian of Dyson and Maleev. It is found that the use of the inner-product matrix as a projection operator factors the problem, as before, into independent physical and nonphysical spaces. The use of the inner-product matrix, described in Sections 2 and 3, and the state space selection of Sections 4 and 5 achieve the elimination of nonphysical dimensions of the boson Hilbert space. With this, we can develop a perturbative formulation of spin-wave theory which includes the correct kinematics.

The bearing these techniques have on the thermal temperature Green's function formalism is noted in Section 6.

## 2. ISOLATION OF IMPROPER STATES

Consider a cubic, periodic lattice of $N^d < \infty$ sites with $d$ any number of dimensions. The discussion is limited to the spin-1/2 case. The Pauli principle is represented by the requirement that no more than one raising operator may be assigned to any site. The Hamiltonian (1) has the wave-



number form

$$k \text{ space} \qquad \hat{H} = -\frac{J}{2}\sum_{\mu=1}^{N} \gamma_\mu \mathbf{S}_\mu \cdot \mathbf{S}_{-\mu} \qquad \gamma_\mu = \sum_{\delta} \exp\left(i\boldsymbol{\delta}\cdot\boldsymbol{\mu}\frac{2\pi}{N}\right) \tag{3}$$

$\delta$ connects nearest neighbor sites. The relevant properties of the spin operators are (with $\hbar = 1$)

$$x \text{ space} \qquad \mathbf{S}_i = \tfrac{1}{2}\boldsymbol{\sigma}_i, \qquad \mathbf{S}_\mathbf{i}^{\pm} = S_\mathbf{i}^x \pm iS_\mathbf{i}^y$$
$$[S_\mathbf{j}^z, S_\mathbf{k}^{\pm}] = \pm\delta_{\mathbf{jk}}S_\mathbf{j}^{\pm}, \qquad [S_\mathbf{i}^+, S_\mathbf{k}^-] = 2\delta_{\mathbf{ik}}S_\mathbf{i}^z \tag{4}$$
$$S_\mathbf{j}^-|0\rangle = 0, \qquad S_\mathbf{j}^z|0\rangle = -\tfrac{1}{2}|0\rangle \qquad \text{for } \mathbf{i}, \mathbf{j}, \mathbf{k} \text{ site labels}$$

with the corresponding $k$-space properties

$$\mathbf{S}_\mu = N^{-d/2}\sum_{\mathbf{j}} \exp\left(i\boldsymbol{\mu}\cdot\mathbf{j}\frac{2\pi}{N}\right)\mathbf{S}_\mathbf{j}$$
$$[S_\mu^z, S_\nu^{\pm}] = \pm N^{-d/2}S_{\mu+\nu}^{\pm}, \qquad [S_\mu^+, S_\nu^-] = 2N^{-d/2}S_{\mu+\nu}^z \tag{5}$$
$$S_\mu^-|0\rangle = 0, \qquad S_\mu^z|0\rangle = -\tfrac{1}{2}N^{d/2}\delta_{\mu,0}|0\rangle$$
$$(S_\mathbf{k}^+)^* = S_{-\mathbf{k}}^-$$

The ground-state energy is $E_0 = -JN^d d/4$, where $d$ is the dimension of the lattice.

The unnormalized basis consists of $n$-spin-wave states, products of raising operators at lattice sites, and is cumulatively assigned a single label $R$,

$$|^n\varphi_{R(\mathbf{i},\mathbf{j},\ldots,\mathbf{k})}\rangle = S_\mathbf{i}^+ S_\mathbf{j}^+ \cdots S_\mathbf{k}^+|0\rangle \tag{6}$$

Capital Latin indices specify a unique nonordered set of site or wavevector subscripts. When all sites in $R$ are different the assignment of spin reversals conforms to the single-occupancy condition. Such $|^n\varphi_R\rangle$ will be called *proper states*. When any two or more of the labels in $R$ are identical, more than one spin-raising operator acts on some site or sites. Let $R(\text{im})$ indicate a labeling of this sort. Because the raising and lowering operators are nilpotent, that is,

$$(S_j^+)^n = (S_j^-)^n = 0 \qquad \text{for any } j \text{ and any integer } n > 1$$

these states $|^n\varphi_{R(\text{im})}\rangle$ vanish. Nevertheless, it will be useful to keep track of where and when such spin arrangements occur. Because the zero state is still a state, we can include a copy of it whenever the assignment of spin operators leads to vanishing states through the nilpotence property. The basis will then include many copies of the zero vector, each assigned a

unique labeling, giving a many-to-one mapping of the space of spin-site assignments onto the space of states. We will refer to these assignments as *improper states* and label them as $|^n\varphi(\text{im})\rangle$. Although all such configurations are represented by the *same* state (i.e., are not linearly independent), it is consistent with standard treatment of overcomplete sets to refer to all the vectors in the set as *different.* This subtlety in nomenclature presents no difficulties as long as the underlying mathematical definition is retained. The essential feature is that the state space now includes and distinguishes two ways of distributing spin reversals among sites.

Proper states in the position space basis, labeled by $R(\text{pr})$ and $R'(\text{pr})$, are orthonormal:

$$\langle^m\varphi_{R(\text{pr})}|^n\varphi_{R'(\text{pr})}\rangle \propto \delta_{m,n}\delta_{R(\text{pr}),R'(\text{pr})}$$

A superposition of $k$-space states can be defined as in equation (2) as the product

$$|^n\varphi_{K(k_1,k_2,\ldots)}\rangle = S^+_{k_1}S^+_{k_2}\cdots S^+_{k_n}|0\rangle \tag{7}$$

As each $S^+_k$ is a sum of operators at sites, according to (5), some of the terms included in this product of sums will contain improper assignments, and hence vanishing components. However, $|^n\varphi_K\rangle$ itself does not vanish. There remains a nonvanishing state $|^n\varphi_K\rangle$ for every distinct $K(k_1, k_2, \ldots, k_n)$. The number of states ${}^nM$ is the number of ways to assign $n$ wavenumber labels where each label takes a value in the first Brillouin zone

$${}^nM = \binom{N^d + n - 1}{n}$$

The number of proper states remains

$${}^nA = \binom{N^d}{n} < {}^nM$$

Thus, there are more approximate eigenvalues to the $k$-space spin-operator problem than proper states of the system despite the vanishing of the improper states.

In addition, $k$-space states are not orthogonal. That is, for $K$ and $K'$ different,

$$\langle^n\varphi_K|^n\varphi_{K'}\rangle = \delta_{K,K'} + \frac{1}{N^d}f(K, K')\delta_{K_{\text{tot}},K'_{\text{tot}}} \tag{8}$$

where $f(K, K')$ is some function of the total $2n$ components described by $K$ and $K'$ and $\delta_{K_{\text{tot}},K'_{\text{tot}}}$ is zero, unless the total wavenumber $K_{\text{tot}} = (k_1 + k_2 + \cdots)_{\text{mod } N}$ is equal for each of the $d$ components of the two states. The vanishing of the improper elements in the Fourier expansion undermines the unitarity of the Fourier transform.



These two effects, overcompleteness and nonorthogonality, which originate in the exclusion principle, constitute the kinematical problem.

In the boson formulation of Dyson and Maleev the spin states (6) and the spin operator Hamiltonian are replaced by boson states and an "equivalent" boson Hamiltonian. The transformation to boson operators is effected by the replacement of $S^+_j$ and $S^-_j$ by boson site creation and annihilation operators $\eta^*_j$ and $\eta_1$, which obey $[\eta^*_j, \eta_1] = \delta_{j,1}$. The ground state $|0\rangle$ is replaced by the state $|0)$, formally defined by the property $\eta_j|0) = 0$. The boson Fock space is spanned by states $|^n\varphi_R)$:

$$|^n\varphi_{R(r_1,\ldots,r_n)}) = \eta^*_{r_1}\cdots\eta^*_{r_n}|0) \tag{9}$$

Unlike the spin operator states, an improper assignment $R(\text{im})$ of boson site-raising operators does not lead to a vanishing state, because the boson operators are not nilpotent. Fourier-transformed states $\alpha^*_\mu$ and $\alpha_\mu$ may be constructed in analogy with the Fourier-transformed spin operators of equation (5). Following (7), we superpose these states to construct a wavenumber basis labeled by $K(\mu_1, \ldots)$. Unlike the spin-operator wavenumber states of equation (8), boson multi-spin-wave states are orthogonal. That is, using

$$\alpha^*_\mu = N^{-d/2}\sum_{\mathbf{j}} \exp\left(i\boldsymbol{\mu}\cdot\mathbf{j}\,\frac{2\pi}{\text{sift}}\mathbf{R}\frac{*}{N}\right)\eta_{\mathbf{j}}$$

where

$$[\alpha^*_\mu, \alpha_\nu] = \delta_{\mu,\nu}, \qquad |^n\varphi_{K(\mu_1,\ldots,\mu_n)}) = \alpha^*_{\mu_1}\cdots\alpha^*_{\mu_n}|0)$$

we have

$$(^n\varphi_K|^m\varphi_{K'}) \propto \delta_{n,m}\delta_{K,K'} \tag{10}$$

If we allow all combinations of boson spin-wave creation operators operating on the state $|0)$ to span the basis, then, in analogy with equation (2), the unnormalized boson spin-wave basis consists of the direct sum of subspaces of $n$ spin waves:

$$B = \sum_{n=0}^{\infty} \oplus B(n) \qquad B(n): \quad \left\{\prod_{\mathbf{k}} (\alpha^*_{\mathbf{k}})^{a_{\mathbf{k}}}|0): \quad \sum_{\mathbf{k}} a_{\mathbf{k}} = n\right\} \tag{11}$$

The boson Hamiltonian is defined by the requirement that when it acts on boson states, it models the scattering of spin operator states generated by the original Heisenberg Hamiltonian. Further discussion of the boson formulation is deferred to Section 4, where ideas developed in this and the following sections are applied in detail. For the moment it will suffice to say that the boson Hamiltonian [which is given by equation (34)] is of quartic form, that the quartic part represents spin-wave interaction, which

is weak at long wavelengths, and that the quadratic part is diagonal in the boson spin-wave basis, with associated free spin-wave eigenvalues.

Before developing features particular to the spin operator space, it is useful to note general features common to both the Bose and spin formalisms. In the spin operator formalism the improperly assigned spin operators act on the vacuum state to give the zero state, while in the boson formalism such an assignment of raising operators doe not give the zero state. While the spin operator formalism is faithful to the exclusion condition, its use in perturbation theory is complicated by spin commutation relations,[2] and by the absence of a natural separation of the Hamiltonian into interacting and noninteracting parts. The boson reformulation was invented as a tool to facilitate the application of perturbation theory. It exactly reproduces the dynamics of the Heisenberg Hamiltonian (in the sense that it reproduces all the same eigenvalues), but inherently violates the exclusion principle. This failure leads to extra eigenvalues and vectors, called unphysical or improper eigenvalues and vectors, which contribute to statistical sums when one computes thermal expectation values. It is remarkable that the inclusion of unphysical states in no way effects the physical eigenvalues or vectors. The explanation for this phenomena will emerge in the course of this analysis. It is just that property of the Heisenberg Hamiltonian that was recognized by Bethe (1931) and resulted in the Bethe ansatz. This ansatz allows closed-form expressions for the eigenfunctions of a linear spin system to be obtained in terms of coupled transcendental equations.

As it has been introduced, kinematics appears distinct from the dynamical aspect of the eigenvalue problem. In addition, it may appear that the kinematical interaction has been defined in such away as to refer only to the boson formulation. Both of these perspectives are incorrect and have led authors to a variety of (often unrecognized) incomplete results (see footnote 2, for example).

The exact solution to the kinematical problem that is developed here shows kinematical effects to exert a complicated influence upon the perturbative solutions of the Schrödinger equation. A key point is that the degree to which the kinematical and dynamical interactions are coupled depends on the approximations used to solve the eigenvalue problem. In an exact solution of the secular equation one can separate dynamical and kinematical effects and solve them independently. However, in a perturbative solution (an expansion in orders of the coupling parameter about free spin-wave states) the two interactions do not separate. Marshall and Murray (1969) have found that only in the low-temperature limit, where $S \to \infty$ and

[2]Two instances of note where a spin operator perturbation theory has been employed are Vaks *et al.* (1968a) and Lewis and Stinchcombe (1967). In neither case has overcompleteness in $k$ space beeen recognized.



operator expansions are truncated at low order, does the kinematical interaction separate from the dynamical interaction and cancel out in the calculation of certain quantities. Wenzel and Wagner (1977) have attempted to incorporate kinematical effects through a reduction of the space of eigenfunctions—eigenfunctions that are obtained as corrections to free spin waves through an expansion in the dynamical interaction alone.

Kinematical effects are not limited to the boson formulation, but also occur in the spin-operator formalism. The kinematical problem consists of two parts: overcompleteness and nonorthogonality. These effects persist for spin waves defined with respect to either Bose or spin operators. The real culprit here is the wavevector description which is at the heart of (the present) perturbation theory—it is in the transformation to the wavevector basis that kinematical restrictions, clear in position space, become truly obscure.

It should be noted that the kinematical effects that give rise to boson improper states and improper eigenvalues are not the same as those that generate the improper states and values that appear in the spin formalism. The boson formalism has nonphysical states that are nonzero and linearly independent; the spin-operator formulation has an overcomplete spin-wave space in which a large number of states are linearly dependent. The context of the discussion will indicate which of these two species of improper phenomena is being addressed.

Turning specifically to the spin operator formalism, recall that the number of spins flipped is a constant of the motion. Since every multi-spin-wave state is some combination of products of spin flips, spin-flip conservation implies that the total number of spin waves is a constant of the motion.

Spaces of different numbers of spin waves are considered independently. The $n$-spin-wave energies are solutions to the Hamiltonian secular equation. The eigenvalue equation $H|^n\varphi_\rho\rangle = \lambda|^n\varphi_\rho\rangle$, written in terms of eigenstates $|^n\varphi_K\rangle = \sum_K Q_{KP}|^n\varphi_K\rangle$, for some unitary transformation $Q_{KP}$, can be written in matrix element form as

$$\sum_{K,K'} \langle {}^n\varphi_K | Q^*_{PK} H Q_{K'P'} | {}^n\varphi_{K'}\rangle = \sum_{K,K'} \langle {}^n\varphi_K | Q^*_{PK} \lambda Q_{K'P'} | {}^n\varphi_{K'}\rangle \tag{12}$$

Using the following expression for the Hamiltonian matrix

$$[H]_{KK'} = \langle {}^n\varphi_K | \sum_{K''} HS_{K''K'} | {}^n\varphi_{K''}\rangle = ([{}^nG][{}^nS])_{KK'} \tag{13}$$

gives the secular equation

$$\mathrm{Det}([Q^+]([{}^nG][{}^nS] - \lambda[{}^nG])[Q]) = 0$$

Hence,

$$\mathrm{Det}([{}^nG]([{}^nS] - \lambda)) = 0 \tag{14}$$

where $[{}^nS]$ is called the scattering matrix and $[{}^nG]$ is the inner-product matrix. $[{}^nG]_{KK'}=\langle {}^n\varphi_K | {}^n\Phi_{K'}\rangle$ (which is not the unit matrix). $[{}^nG][{}^nS]_{KK'}$ is the $K, K'$ component of the product of $[{}^nG]$ and $[{}^nS]$ matrices. Capital letters indicate matrices in the wavevector basis. Transforming to a site representation by inserting inverse Fourier transform matrices $[U]$ and $[U^+]$, where $[U]=[U^+]^{-1}$, and indicating matrices in the site basis by lower case letters, we have

$$\begin{aligned}[{}^nh]_{R,R'} &= ([U]^+[{}^nG][U][U]^+[{}^nS][U])_{R,R'} \\ &= ([{}^ng][{}^ns])_{R,R'} \\ &\to \mathrm{Det}\{[{}^ng]([{}^ns]-\lambda)\}=0 \end{aligned} \tag{15}$$

The dimension of both $[{}^ng]$ and $[{}^nG]$ is ${}^nM$, the number of $n$-spin-wave states. $[{}^ng]$ can be divided into two sectors, an upper left sector of dimension ${}^nA$ that accounts for the inner product of all proper states and a lower right sector containing the inner products of improper states. Since we are in a position space basis,

$$[{}^ng]=\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix} \tag{16}$$

Similarly, $[{}^ns]$ can be broken into four quadrants, which, starting in the upper left and going clockwise, correspond to scattering from proper to proper, proper to improper, improper to improper, and improper to proper states:

$$[{}^ns]=\begin{bmatrix} s^P_{(A)\times(A)} & w^a_{(A)\times(M-A)} \\ w^c_{(M-A)\times(A)} & w^b_{(M-A)\times(M-A)}\end{bmatrix} \tag{17}$$

where the $n$ superscript has been suppressed. These matrix elements are well defined because $H$ acts on a particular assignment of spins to generate "scattering" to other spin assignments, without regard to whether or not the states themselves actually vanish. Distinguishing the $[{}^ns]$ and $[{}^ng]$ factors of the Hamiltonian matrix $[{}^nh]$ effectively separates the properties of the Hamiltonian from the properties of the states. If we use only the properties,

$$S^z_j|0\rangle=-\tfrac{1}{2}|0\rangle \qquad \text{and} \qquad S^-_j|0\rangle=0$$

but not the nilpotence property, then we find

$$\begin{aligned}&\hat{H}\prod_r (S^+_r)^{a_r}|0\rangle \\ &=\sum_{j,\delta}(a_j-\tfrac{1}{2})(a_{j+\delta}-\tfrac{1}{2})\prod_r (S^+_r)^{a_r}|0\rangle \\ &\quad+\sum_{j,\delta}[a_j-\vartheta(a_j-2+\varepsilon)(a_j^2+a_j-4)]\prod_r (S^+_r)^{a_r+\delta_{r,j+\delta}-\delta_{r,j}}|0\rangle \end{aligned} \tag{18}$$



where the $0<\varepsilon<1$, used in conjuction with the theta function, ensures that the $(a_j^2+a_j-4)$ contribution vanishes if $a_j$ is less than two. If the initial state is proper and has single spins raised at some nearest neighbor sites, then the second term above generates an improper state with two creation operators acting on the same site. There is scattering from proper to improper states, but no scattering from improper to proper states. For the latter to occur, all occupation numbers $a_i$ for $i\simeq j$ in the initial state would have to be proper (that is, $\leq 1$), while $a_j=2$ at only one site $j$. Then, as long as at least one of the nearest neighbor sites about site $j$ was unoccupied, the second term of (18) would take a spin from site $j$ and move it to the unoccupied site. However, the coefficient of this second term vanishes whenever $a_j=2$, so this type of scattering has vanishing matrix elements. Thus, the submatrix $w^c_{(M-A)\times(A)}$ in expression (17) vanishes.[3]

Returning to equation (14), notice that since the determinant of a product equals the product of determinants, and since $\mathrm{Det}[{}^ng]=0$, the secular equation reduces to $0=0$. It is the zero norms of the improper states that are responsible. One's first inclination might be to return to a faithful representation of the problem by eliminating all improper degrees of freedom. While this would be a straightforward matter in position space, it remains unclear how this can be effected in $k$ space. Therefore, I propose the following ansatz; replace the secular equation (14) with the following expression;

$$\mathrm{Det}([{}^ng][{}^ns]-\lambda)=0 \tag{19}$$

where $[{}^ng][{}^ns]$ is just the Hamiltonian matrix. Using equation (16), we can write the argument of the determinant as

$$[{}^ng][{}^ns]-\lambda=\begin{bmatrix}([s]-\lambda]_{(A)\times(A)} & [w]_{(A)\times(M-A)} \\ 0 & (-\lambda)_{[M-A)\times(M-A)}\end{bmatrix} \tag{20}$$

so that equation (19) becomes

$$\begin{aligned}&\mathrm{Det}([{}^ns]_{(A)\times(A)}-\lambda)\,\mathrm{Det}(-\lambda)_{(M-A)\times(M-A)} \\ &=(-\lambda)^{M-A}\,\mathrm{Det}([{}^ns]_{(A)\times(A)}-\lambda)=0\end{aligned}$$

The solutions to equation (19) consists of ${}^nA$ proper eigenvalues, identical to those generated from the formulation of the problem that contained no unphysical states, plus ${}^nM-{}^nA$ eigenvalues at zero.

The adoption of equation (19) does not resolve anything in itself, it merely postpones the removal of improper degrees of freedom until after

[3]This was noticed for two-spin-wave interactions by Boyd and Callaway (1965).

the eigenvalue problem has been solved. This is in contrast to the original formulation of equation (12), which requires that improper states be removed before the secular determinant is taken. The advantage of the new formulation is that only one matrix needs to be to diagonalized, the Hamiltonian matrix. It is not necessary to first diagonalize the inner product matrix, remove improper states, and then diagonalize the remaining Hamiltonian matrix. Computations can be carried out using improper states and then their contributions can be removed afterward.

This ansatz can also be applied to the problem of diagonalizing any power series in $\hat{H}$. If the action of $f(\hat{H})$ on $|\varphi\rangle$ is represented by the matrix $[f(\hat{H})]$, then the ansatz tells us to make the following replacement:

$$\mathrm{Det}\{[g](f(\hat{H})]-\lambda)\}=0 \rightarrow \mathrm{Det}\{[g][f(\hat{H})]-\lambda\}=0 \tag{21}$$

Since $f(\hat{H})$ is a power series in $\hat{H}$, the matrix representation for its action on $|\varphi\rangle$ is a power series in $[s]$. If one considers an arbitrary term in this expansion, then

$$\langle\varphi_A|(\hat{H})^m|\varphi_B\rangle=([g][s]^m)_{A,B} \tag{22}$$

Because of the vanishing of matrix elements between improper and proper states,

$$[s]^m=\begin{bmatrix}[s^P]^m_{(A)\times(A)} & [w^a(m)]_{(A)\times(M-A)}\\ 0 & [w^b]^m_{(M-A)\times(M-A)}\end{bmatrix}$$

and

$$\mathrm{Det}\{[g][f(\hat{H})]-1\}=\mathrm{Det}\begin{bmatrix}[f([s^P])]_{(A)\times(A)}-\lambda & 0\\ 0 & (-\lambda)_{(M-A)\times(M-A)}\end{bmatrix} \tag{23}$$

Of the eigenvalues obtained, ${}^nA$ are the same as if the improper states were eliminated initially while the ${}^nM-{}^nA$ unphysical zero eigenvalues remain.

In the present context, $[U]$ is defined as an ${}^nM\times{}^nM$ unitary matrix representing the Fourier transform. The Hamiltonian matrix can be written in a $k$-space basis as

$$\begin{aligned}\langle\varphi_R|[U]\hat{H}[U]^+|\varphi_{R'}\rangle&=\langle\varphi_K|[S]|\varphi_{K'}\rangle\\ &=([G][S])_{K,K'}\\ &=[H]_{K,K'}\end{aligned} \tag{24}$$

where I have used the condensed notation

$$[U]^+|\varphi_{R'}\rangle\equiv\sum_{R'}[U]^+_{R'K}|\varphi_{R'}\rangle=|\varphi_K\rangle$$

The spectrum of $[H]$ consists of ${}^nA$ physical eigenvalues and ${}^nM-{}^nA$ unphysical eigenvalues at zero.



To review, the restructuring of the secular equation given by equation (19) results in a consistent matrix formulation of the Heisenberg Hamiltonian in the spin operator context that includes improper states and generates ${}^nM-{}^nA$ (the dimension of the unphysical sector) improper eigenvalues of value zero.

## 3. OVERCOMPLETENESS AND THE KINEMATICAL PROBLEM

In Section 2, I proposed solving for the eigenvalues of the Hamiltonian matrix of equation (12). It is easy to reobtain the results of Section 2. Notice from equations (16) and (17) that although the order of the matrices $[{}^ng]$ and $[{}^ns]$ is ${}^nM$, the rank of $[{}^ng]$ is only ${}^nA$. The product $[{}^ng][{}^ns]$ must have rank less than or equal to ${}^nA$ because the rank of a product is no larger than the largest rank of its factors.[4] Whenever one diagonalizes a matrix of rank $A$, where $A$ is less than the order of the matrix $M$, one always gets at least $M-A$ zero eigenvalues—this is a consequence of the $M$-dimensional rank-$A$ matrix being overcomplete. While this is evident from equation (20) in the position space basis, it means, on the other hand, that the Hamiltonian matrix in the $k$-space basis is also overcomplete. This means that some of the spin-wave states are linearly independent. A complete basis can be obtained by reducing the dimension of the wavevector basis in such a way that it only includes linearly independent basis vectors. However, this is not as simple as it might seem at first, because properness is not something that is conserved by the Hamiltonian (because $w^a_{(A)\times(M-A)}$ in equation (17) is not zero). Let us consider this in some detail.

Say we find that a particular state $|{}^n\varphi_{K^0}\rangle$ is one of a set of $n$-spin-wave states ${}^nV^e$ that are linearly dependent with respect to a set ${}^nV^s$ of other states in the space. That is to say, all the states in ${}^nV^e$ can be represented in terms of states in ${}^nV^s$. The states $|{}^n\varphi^e\rangle$ and $|{}^n\varphi^s\rangle$ are defined as components of the sets ${}^nV^e$ and ${}^nV^s$. The ${}^nV^e$ corresponds to a set of improper degrees of freedom that can be removed from the initial set of states on which $\hat{H}$ operates. However, the action of $\hat{H}$ on the remaining set ${}^nV^s$ will generate matrix elements from the space of selected states back to the extra set ${}^nV^e$. Consider two-spin-wave states. In this case there are ${}^2M-{}^2A=N^d$ improper degrees of freedom $K^0$ is a two-component array, each component $\mathbf{k}^0_1$ and $\mathbf{k}^0_2$ specifying the wave vectors of the component spin waves,

$$|{}^2\varphi_{K^0}\rangle=S^+_{\mathbf{k}^0_1}S^+_{\mathbf{k}^0_2}|0\rangle$$

The action of $\hat{H}$ on a two-spin-wave state $|{}^2\varphi_K\rangle$ is to scatter it into all channels $|{}^2\varphi_{K'}\rangle$ such that $K'_{\mathrm{tot}}=K_{\mathrm{tot}}$ [i.e., $(\mathbf{k}_1+\mathbf{k}_2)_{\mathrm{mod}\,L}=(\mathbf{k}'_1+\mathbf{k}'_2)_{\mathrm{mod}\,L}$; $\hat{H}$ conserves total wave vector]. Therefore, starting with any state $|{}^2\varphi_K\rangle$ such

[4]Matrix theorems used here can be found in Graham (1979) and Nobel (1969).

that $K_{tot} = K^0_{tot}$, $\hat{H}$ returns a state that is a linear combination of all two-spin-wave states of total wave vector $K_{tot}$, one component of which is $|^2\varphi_{K^0}\rangle$. This contribution cannot be discarded; rather, as it is a linearly dependent state, it must be *projected back* onto the ${}^nV^s$ space.

One can think of $\hat{H}$ as an operator that acts on the vector $|{}^n\varphi^s\rangle$, whose elements $|{}^n\varphi^s_c\rangle$ are states in the set ${}^nV^s$, to change the order, but not the rank, of the set:

$$\hat{H}|{}^n\varphi^s\rangle = [{}^nS^{f,s}]|{}^n\varphi^f\rangle$$

where $|{}^n\varphi^f\rangle$ is a vector with components in the full space ${}^nV^f = {}^nV^s \oplus {}^nV^e$ of dimension ${}^nA$ and order ${}^nM$. Here $[{}^nS^{f,s}]$ is an ${}^nM \times {}^nA$ matrix. The order and rank of a set of states are defined in analogy with order and rank for a matrix as the number of states contained in the set and the number of degrees of fredom represented by states in the set.

The resolution of the overcompleteness problem requires essentially three steps. First, choose a reduced basis of linearly independent states. Second, orthogonalize the reduced basis. And third, act on the states with the Hamiltonian and project the resulting components back on this complete, orthogonalized basis. While various ways of choosing a reduced subspace will be considered in the next section, assume, for the moment, that such a selection has been made: a reduced $n$-spin-wave subspace ${}^nV^s$ has been chosen whose nonorthogonal basis vectors yield the inner-product matrix [cf. equation (8)]

$$[{}^nG^s]_{K,K'} = \langle {}^n\varphi^s_K | {}^n\varphi^s_{K'}\rangle$$

Following Löwdin (1950, 1956), orthogonalize the basis by multiplying the basis vectors, given collectively by $|{}^n\varphi^s\rangle$, by the inverse square root of $[{}^nG^s]$. Writing the transformation for the $b$th component of $|{}^n\varphi^s\rangle$, summing over repeated indices, gives

$$|{}^n\bar{\varphi}^s_b\rangle = [{}^nG^s]^{-1/2}_{cb}|{}^n\varphi^s_c\rangle$$

where

$$\langle {}^n\bar{\varphi}^s_a | {}^n\bar{\varphi}^s_b\rangle = \langle {}^n\varphi^s_a|[{}^nG^s]^{-1}_{cb}|{}^n\varphi^s_c\rangle = \delta_{ab}$$

The orthogonalized reduced basis set provides a projection operator $|{}^n\bar{\varphi}^s\rangle\langle {}^n\bar{\varphi}^s| \equiv \sum_c |{}^n\bar{\varphi}^s_c\rangle\langle {}^n\bar{\varphi}^s_c|$, which reduces the order of an overcomplete matrix. Applying this to the expression for $[{}^nG][{}^nS]$ in equation (14) used in the determination of the eigenvalues [summing over repeated indices, and according to the convention of equation [24]), we obtain

$$\begin{aligned}\langle {}^n\varphi^s_a|\hat{H}|{}^n\varphi^s_b\rangle &= \langle {}^n\varphi^s_a|{}^n\bar{\varphi}^s_c\rangle\langle {}^n\bar{\varphi}^s_c|[{}^nS^{f,s}]|{}^n\varphi^f_b\rangle \\ &= \langle {}^n\varphi^s_a|([{}^nG^s]^{-1/2}|{}^n\varphi^s_c\rangle\langle {}^n\varphi^s_c|[{}^nG^s]^{-1/2})[{}^nS^{f,s}]|{}^n\varphi^f_b\rangle\end{aligned}$$



$$\begin{aligned}&= \langle {}^n\varphi^s_a|{}^n\varphi^f_c\rangle[{}^nS^{f,s}] \\ &= ([{}^nG^{s,f}][{}^nS^{f,s}])_{ab}\end{aligned} \tag{25}$$

The scattering and inner product matrices are ${}^nA$ by ${}^nM$ and ${}^nM$ by ${}^nA$, respectively. There are no improper eigenvalues in the eigenvalue spectrum of this matrix product. Equation (25) embodies a simple and complete solution to the kinematical problem, as will become clear in the next section.

## 4. OVERCOMPLETENESS AND STATE SPACE REDUCTION

In this first treatment of kinematical effects, dynamical interactions are eliminated by replacing the diagonal elements of $[{}^nS^{f,s}]$ with their associated free-spin-wave energies, and by setting off-diagonal elements equal to zero. That is, the magnon approximation will be adopted. Since $[{}^nS^{f,s}]$ is not a square matrix, what I mean by "diagonal matrix elements" are those that appear between states $\langle {}^n\varphi^s_a|$ and $|{}^n\varphi^s_a\rangle$ in the reduced basis. Writing the ${}^nA$-dimensional, square matrix of free-$n$-spin-wave eigenvalues in the reduced basis as $[{}^nD^s]$, we have

$$[{}^nS^{f,s}] = \left[\frac{[{}^nD^s]}{0}\right]$$

Because of the vanishing components in the lower portion of the scattering matrix. in this approximation, the inner-product matrix elements connecting states in ${}^nV^s$ with states in ${}^nV^e$ do not contribute to the product $[G][S]$. Equation (25) reduces to the product of two ${}^nA \times {}^nA$ matrices:

$$[{}^nH^s] = [{}^nG^s][{}^nD^s]$$

In addition, neglect the nonorthogonality effects in $[{}^nG^s]$ by replacing it with the ${}^nA$-dimensional unit matrix. Clearly, the dynamical interaction, nonorthogonality, and overcompleteness are three distinct aspects to the problem of determining the eigenvalues. In this section only overcompleteness is treated. It is worth underscoring the fact that Hamiltonian is *fixed* to be of free-spin-wave form, and this will not be changed by any alterations of the state space. When isolated in this way, the issue of overcompleteness only concerns the choice of sttates that one includes when taking the statistical trace.

Consider the magnon approximation used by Boch to derive the $T^{3/2}$ law for the reduced magnetization at low temperatures (Martin, 1967). There, the population of spin waves at one wavenumber does not depend on the population at another wavenumber. Defining $E(k_0 \notin K')$ as the energy of a set of noninteracting spin waves $K'$, none of which are excited at $k_0$, and $E_{k_0}$ as the energy of a single free spin wave at $k_0$, one can write the

partition function in the Boch approximation as

$$Z=\sum_{K}\exp[-\beta E(K)=\sum_{a_{k_0}}\exp(-\beta a_{k_0}E_{k_0})\sum_{K'}\exp[-\beta E(k_0\notin K')]$$

where $a_{k_0}$ is the number of spin waves excited at $k_0$. The $a_{k_0}$ ranges between 0 and $N$. The thermal expectation value for the number operator at $k_0$ is given in the $N\to\infty$ limit by a boson distribution function.

$$\langle n_{k_0}\rangle_T=\sum_{a_{k_0}}a_{k_0}\exp(-\beta a_{k_0}E_{k_0})\Big/\sum_{a_{k_0}}\exp(-\beta a_{k_0}E_{k_0})=1/[\exp(\beta E_{k_0})-1] \quad (26)$$

This result is a sufficient condition for the derivation of the $T^{3/2}$ law. Bloch's approximation includes contributions from all states in the overcomplete basis; there is no state space reduction. With some hindsight it can now be said that any approach to the kinematical problem that does not perform some state space reduction has, *ab initio*, missed a large part of the physics.

Wenzel and Wagner (1977) were the first to use a reduced spin-wave state space. They were concerned with Raman scattering in an antiferromagnet above the Néel temperature. The drastic change in the temperature dependence of $n_k$ that was brought about by their particular state space reduction brought theoretical predictions into agreement with observed two-magnon Raman spectra for the two-dimensional antiferromagnet $K_2MnF_4$.

I will derive in a simple manner the reduction scheme that they used. Consider the space of excited states, which has been parameterized in Fock space by an array $\boldsymbol{\alpha}$ whose components $\alpha_k$ are the occupation numbers for spin waves at wave vector $k$. A Fock space representation can also be given with respect to a site basis using an array $\mathbf{s}$ whose components $s_j$ label the number of creation operators acting on site $j$ [cf. equations (2) and (11)]. The number of sites in position space is equal to the number of allowable wavenumber values in $k$ space: $N^d$. If a reduced $k$-space basis is constructed by including only states $K=(k_1,k_2,\ldots,k_n)$ where $k_i\neq k_j$ for all $i$ and $j$, which is the same as restricting the components of $\boldsymbol{\alpha}$ to take either the value 0 or 1, the dimension of this reduced space will be ${}^nA$. This follows from the isomorphism of the reduced $k$ space with the site-defined Fock space. In the site-defined Fock space one has $s_j=0$ or 1 and $\sum_j s_j=n$. In this simple scheme the number of wave vector states *eliminated* is exactly equal to the number of linearly *dependent* wave vector states ${}^nM-{}^nA$. Despite its being inexact, as will be shown, this scheme allows for a new closed-form expression for $\langle n_k\rangle_T$. An important ingredient in making this closed form possible is that, as in the unrestricted boson scheme, the number of excitations at wavenumber $k$ is independent of the number of spin waves excited at $k'\neq k$.



If multi-spin-wave states that do not contain excitations at wavenumber $k_0$ are defined as $|\bar{K}\rangle$, then the whole reduced state space is spanned by states that are either of the form $|\bar{K}\rangle$ or $S^+_{k_0}|\bar{K}\rangle$. The partition function for free spin waves is

$$Z=[1+\exp(-\beta E_{k_0})]\sum_{K}\exp[-\beta E(\bar{K})]$$

and the expectation value of the number operator is

$$\langle n_{k_0}\rangle_T=[0\cdot\exp 0+1\cdot\exp(-\beta E_{k_0})]\sum_{\bar{K}}\{\exp[-\beta E(\bar{K})]\}Z^{-1}$$

$$=\frac{1}{\exp(\beta E_{k_0})+1} \quad (27)$$

Considering the nature of the restrictions on the reduced space, equation (27) is the expected result: the Fermi distribution. It is also the result at which Wenzel and Wagner arrived in order to describe the effect of the kinematical interaction, although their derivation followed different lines. At high temperatures the Fermi distribution asymptotically approaches the value 1/2, indicative of a system that cannot support any more excitations at wavenumber $k$. At high $T$ the boson distribution increases without bound. At sufficiently low temperatures, with $k\neq 0$, both distributions are approximately Boltzmannian. This agrees with our expectation that kinematical effects are small at low temperatures.

In order to uncover the error in the fermion scheme, recall that $\hat{H}$ conserves total wavenumber. This allows $[{}^nS]$ to be further broken down into block diagonal form where each block is the scattering submatrix $[{}^{n,p}S]$ for $n$-spin-wave states of total wavenumber $p$ (in a still overcomplete basis). In addition, the inner-product matrix, equation (8), also factors according to subspaces of fixed total wavenumber. The secular equation of equation (19), written in terms of the $k$-space matrices of equation (24), can be written as a product of factors, one factor for each value of the total wavenumber $p$:

$$\mathrm{Det}([{}^nG][{}^nS]-\lambda)=\prod_{p}\mathrm{Det}([{}^{n,p}G][{}^{n,p}S]-\lambda)=0$$

Knowing that the number of states by which the $n$-spin-wave basis is overcomplete is ${}^nM-{}^nA$, one formally defines ${}^nM^p-{}^nA^p$ to be the number of $n$-spin-wave states by which the set consisting of states with all possible wavenumber assignments at total wavenumber $p$ is overcomplete. A closed-form expression for ${}^nM^p-{}^nA^p$ has not been found, but, from looking at small systems (cf. Section 5), it seems to be weakly dependent on $p$, approximately of the form $({}^nM-{}^nA)/N^d$.

The fermion scheme of Wenzel and Wagner is not exact, because it does not remove the correct number of linearly dependent states from the

subspaces of states with fixed excitation number $n$ and total wavenumber $p$. In the fermion scheme, the number of states at fixed $n$ and $p$ does not equal ${}^nM^p - {}^nA^p$. I illustrate this with an example.

Consider a ring of six sites and the set of 2-spin-wave states. There are six subspaces of fixed total wavenumber. The wavenumber assignments of the 2-spin-wave states, divided into $K_{\text{tot}}$ classes, is given as follows:

| $K_{\text{tot}}(\times N/2\pi)$: | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| $(k_1, k_2)$: | (0, 0) | (1, 0) | (1, 1) | (2, 1) | (2, 2) | (3, 2) |
| | (1, 5) | (2, 5) | (2, 0) | (3, 0) | (3, 1) | (4, 1) |
| | (2, 4) | (3, 4) | (3, 5) | (4, 5) | (4, 0) | (5, 0) |
| | (3, 3) | | (4, 4) | | (5, 5) | |

According to the fermion reduction scheme, remove two states from the $K_{\text{tot}} = 0$ subspace, two from the $K_{\text{tot}} = 2$, and two from $K_{\text{tot}} = 4$. No states are removed from subspaces of $K_{\text{tot}} = 1$, 3, or 5. However, if the form of the inner product matrix is worked out,

$$\langle 0|S^-_a S^-_b S^+_c S^+_d|0\rangle = \delta_{a,c}\delta_{b,d} + \delta_{a,d}\delta_{b,c} - \tfrac{1}{3}\delta_{a+b,c+d}$$

one finds that the $3\times 3$ inner product submatrix for the $K_{\text{tot}} = 3$ subspace is overcomplete: it has two eigenvalues at 1 and one at 0, (any zeros in the spectrum of the inner-product matrix indicate overcompleteness). Alternatively, if the states $|2, 1\rangle$, $|3, 0\rangle$, and $|4, 5\rangle$) are expanded in the site basis, one finds $|3, 0\rangle = 2(|1, 2\rangle + |4, 5\rangle)$. The fermion scheme fails to remove linearly dependent states in some cases, while, as it turns out, it eliminates too many states in other cases, (that is, it eliminates linearly *in*dependent states in some cases).

Another argument throws serious doubt on the applicability of the fermion scheme. The fermion scheme discards many exact eigenstates as well as many nearly exact eigenstates in favor of other states which, although linearly independent (modulo the above observations), are poor approximate states. If an exact calculation were done, diagonalizing the Hamiltonian matrix on a computer, this would be unimportant, as any complete basis can be used. However, the kinematical problem never presented any serious difficulty in exact computation, as it is trivially resolved by working in a site representation. In this case, only proper spin-raising assignments are included from the very start. The kinematical problem is serious only in the context of perturbation theory. In such a context it is crucial to work in a basis that nearly diagonalizes the Hamiltonian.

We can go further to put a finger on the physical limitations of the fermion reduction scheme. The fermion scheme eliminates states in which many spin waves are excited at $k = 0$. The $k = 0$ modes are the Goldstone modes that reflect the global rotational symmetry of the problem. By



eliminating these modes, the fermion scheme breaks rotational symmetry. Therefore, it is not clear whether or not, in the fermion scheme, accurate values for high-temperature correlation functions can be obtained, no matter how many terms we include in perturbation theory. It is clear that the fermion scheme cannot be used in the critical region, as there the low-energy rotational modes are important to the restoration of the broken symmetry.

These criticisms aside, judging from the successes of Wenzel and Wagner, it is likely that the fermion model provides an interpolation scheme that is useful for the calculation of certain quantities at temperatures high enough so that rotational degrees of freedom are no longer statistically important. The scale at which this may be the case will have to be determined through reference to experiment.

## 5. CORRECT SPIN-WAVE STATISTICS

I now present a third scheme for reducing the state space, which gives the correct spin-wave statistics at all temperatures. I will refer to this simply as the spin-wave state space and the resulting distribution function as the spin-wave distribution. Although this formulation will not yield immediate, closed-form expressions, it accurately reflects spin-wave properties completely absent from both the Bose and Fermi descriptions.

The spin-wave distribution can be defined by introducing an $n$-dependent upper limit $Q_+(n)$ to the $k$-space sums that appear in the partition function:

$$\left(\sum_{k_1^x=-N/2}^{N/2}\sum_{k_1^y=-N/2}^{N/2}\cdots\right)\cdots\left(\sum_{k_n^x=-N/2}^{N/2}\sum_{k_n^y=-N/2}^{N/2}\cdots\right)$$

$$\to\left(\sum_{k_1^x=-Q(n)/2}^{Q(n)/2}\sum_{k_1^y=-Q(n)/2}^{Q(n)/2}\cdots\right)\cdots\left(\sum_{k_n^x=-Q(n)/2}^{Q(n)/2}\sum_{k_n^y=-Q(n)/2}^{Q(n)/2}\cdots\right)$$

$$\equiv\sum_{{}^nK} \tag{28}$$

where it is required that $k_1^x < k_2^x < \cdots$ for the $x$ as well as for the $y$ and $z$ components. Here ${}^nK$ represents the whole space of these ordered, $n$-spin-wave states.

$Q(n)$ is a short-wavelength cutoff. It most affects states with a large, spin-wave population $n$. Except for the imposition of a $k$-space cutoff, the sums in (28) are boson-like, that is, they allow multiple occupancy. The number of states in an $n$-excitation space, in which the wavevector index runs over $Q(n)$ values and for which multiple occupancy states are allowed, is of the same form as ${}^nM$, except with $N$ replaced by $Q(n)$. The $Q(n)$ is

determined by the condition of equation (29) that the number of district terms in the sum (i.e., terms that differ by more than just a permutation of indices) equal the number of proper states in the $n$-spin-wave subspace,

$$\binom{[Q(n)]^d + n - 1}{n} \equiv \binom{N^d}{n} \tag{29}$$

Thus,

$$Q(n) = (N^d - n + 1)^{1/d} \tag{30}$$

in the continuum limit.

Consider (30) in the two following asymptotic cases. For $n = 1$ there is no state space reduction. This is exact because the set of all possible single-spin-wave states is complete (the single spin waves are eigenstates). At $n = N^d$ the state space reduction eliminates all but the one state at $\alpha_{k=0}(N^d) = 1$. This is correct since at $n = N^d$ (all spins reversed) there is only one possible configuration, and that is the zero-energy state obtained by rotating $|0\rangle$ by 180°.

In addition to equation (30), there is the additional criterion that the summations of equation (28) generate the correct counting for each irreducible subspace of fixed total wave vector. That is, in the spin-wave picture the number of $n$-spin-wave states with $\mathbf{K}_{tot} = (\mathbf{k}_1 + \cdots + \mathbf{k}_n)_{\text{mod } N}$, defined to be $''M(Q(n), \mathbf{k}_{tot})$, must equal the number of linearly independent degrees of freedom in this subspace, $''A(\mathbf{K}_{tot})$.

Unfortunately, no analytic form exists for $''M(Q(n), \mathbf{K}_{tot})$ or $''A(\mathbf{K}_{tot})$. The problem of determining these quantities exactly is related to the problem of finding the number of partitions of an integer $T$ into $n$ additive factors. That is, determining the number of distinguishable sets of integers $t_1$, $t_2, \ldots, t_n$ such that $\sum_{j=1}^{n} t_j = T$. Problems of this kind generally do not admit analytic solutions (Hardn and Wright, 1960).

On the other hand, it can be argued that because there is no quantity to set a scale for an asymmetry in the number of states in different $\mathbf{K}_{tot}$ subspaces, this number must be independent of $\mathbf{K}_{tot}$ in the limit of large systems. Some deviation from exact $\mathbf{K}_{tot}$ indepdence, that is, some breaking of the symmetry, is expected due to the combinatorial requirement that both $''A$ and $''A(\mathbf{K}_{tot})$ be integers.

To support these predictions, the behavior of $''A(\mathbf{K}_{tot})$ was investigated numerically. All values of $K_{tot}$ and $n < N$ with $N = 1$-8 were computed in one dimension. In order to satisfy both the criteria of equation (30) and the requirement that the wavenumber cutoff be integer, it is necessary for the upper and lower cutoff values to differ by one in the cases that $N$ is odd and $n$ is even, or $N$ is even and $n$ is odd. The expectation that $''A(K_{tot})$ differs from $''A/N$ only on a scale of order one [due to the requirement



that all $''A(K_{tot})$ be integers] is borne out in all cases. Table I shows the results for $n = N/2$ or $(N-1)/2$ for $N$ even or odd.

If we accept that $''A(K_{tot})$ approaches $''A/N$ in one dimension in the thermodynamic limit, then this result can be applied to find the limiting form of $''A(K_{tot})$ in any number of dimensions. Since each irreducible subspace is defined by the $d$ components $\mathbf{K}_{tot}$, each component being an independent degree of freedom, the total number of states at fixed $n$ and $N$ must factor:

$$''A(K^1_{tot}, K^2_{tot}, \ldots) = ''A[K^1_{tot}) \cdot ''A(K^2_{tot}) \cdot \cdots \tag{31}$$

From the assumption of the asymptotic form of $''A(K_{tot})$ in one dimension, it follows that in $d$ dimensions, in the thermodynamic limit,

$$''A(K^1_{tot}, K^2_{tot}, \ldots) = ''A/(N)^d \tag{32}$$

It is now necessary to demonstrate that the number of degrees of freedom of the spin-wave space given by equation (32) is equal to the size of this space given by $''M(Q(n), K_{tot})$. The previous argument (that no $K_{tot}$ scale exists that can break the symmetry of $''A(K_{tot})$ in the thermodynamic limit) no longer holds for $''M(Q(n), K_{tot})$ because $Q(n)$ *does* introduce an asymmetry scale. Actual counting of the number of states in the spaces of fixed $K_{tot}$, $n$, and $N$ is easy compared with finding the dimensions of the overcomplete subspaces. Some results are shown in the last column of Table I.

It is found that in one dimension, in every case that $''M(Q(n))$ is evenly divisible by $N$, $''M(Q(n), K_{tot})$ exactly equals $''A/N$. When $''M(Q(n))$ is not evenly divisible by $N$, the values of $''M(Q(n), K_{tot})$ exactly match those of $''A(K_{tot})$ for every value of $n$, $N$, and $K_{tot}$ tested. It is unlikely that this

**Table I.** Exact Number $''A(K)$ of Degrees of Freedom in Spin-Wave Subspaces of Fixed, Total Wavevector $K$ and Excitation Number $n$ for Linear Systems of size $N$, and Number $''M(Q(n), K)$ of Linearly Dependent Spin-Wave States for Fixed $K$, $N$, and $N$ in the Cutoff Space

| $N$ | $n$ | $K$ | $''A(K)$ | $''M(Q(n), K)$ |
|---|---|---|---|---|
| 4 | 2 | 0, 1, 2, 3 | 2, 1, 2, 1 | 2, 1, 2, 1 |
| 5 | 2 | 0, 1, 2, 3, 4 | 2, 2, 2, 2, 2 | 2, 2, 2, 2, 2 |
| 6 | 3 | 0, 1, 2, 3, 4, 5 | 4, 3, 3, 4, 3, 3 | 4, 3, 3, 4, 3, 3 |
| 7 | 3 | 0, 1, 2, 3, 4, 5, 6 | 5, 5, 5, 5, 5, 5, 5 | 5, 5, 5, 5, 5, 5, 5 |
| 8 | 4 | 0, 1, 2, 3, 4, 5, 6, 7 | 10, 8, 9, 8, 10, 8, 9, 8 | 10, 8, 9, 8, 10, 8, 9, 8 |
| 9 | 4 | 0, 1, 2, 3, 4, 5, 6, 7, 8 | 14, 14, 14, 14, 14, 14, 14, 14, 14 | 14, 14, 14, 14, 14, 14, 14, 14, 14 |

behavior is a combinatorial coincidence that holds only at small $N$, because the cutoff model has no scale that distinguishes small- from large-scale combinatorial behavior. In lieu of a rigorous proof, the evidence obtained from small systems can be taken as a strong indication that, at least, ${}^nM(Q(n), K_{tot})$ goes to ${}^nA/N$ in the thermodynamic limit [and is perhaps equal to ${}^nA(K_{tot})$ even for small $N$]. We accept the following likely result for one-dimensional systems:

$$\lim_{\substack{N,n\to\infty \\ (n/N)=\text{const}}} {}^nA(K_{tot}) = \lim_{\substack{N,n\to\infty \\ (n/N)=\text{const}}} {}^nM(Q(n), K_{tot}) \tag{33}$$

In $d$ dimensions the wavevector cutoff can be written as a vector $\mathbf{Q}(n)$, each of its components setting a limit on the corresponding component of the wave vector. The linear independence of the components of $K_{tot}$ then implies that each factor in $\mathbf{Q}(n) = (Q^1(n), Q^2(n), \ldots)$ must be independent. This leads to the analogue of equation (32) for the number of states in the cutoff scheme in $d$ dimensions, namely

$${}^nM(Q(n), \mathbf{K}_{tot}) = {}^nM(Q(n))/N^d$$

which equals ${}^nA/N^d$ in the thermodynamic limit.

Unlike the boson scheme, the spin-wave scheme leads to drastic reductions in the number of states when there is a high occupation number. Unlike the fermion scheme, this scheme retains the full spectrum of $k=0$ excitations in each subspace. By including all the Goldstone modes, the spin-wave space preserves rotational symmetry. This property is crucial in such phenomena as critical behavior, where rotational symmetry exerts a strong effect.

Perhaps most importantly, and also unlike the fermion scheme, this description retains those states of the $n$-spin-wave subspace that are *closest* to being eigenvectors of $H$. This means that the spin-wave space not only resolves the overcompleteness problem, but it also improves the convergence of perturbative expansions in powers of $\hat{H}$ (see below). However, unlike either of the previous schemes, this reduction scheme introduces an $n$ dependence into the number of states that can be created at wavenumber $k$. As a result, the calculation of thermal expectation values, even in the noninteracting, orthogonal spin-wave approximation, is quite difficult.

The three models I have discussed will be summarized using two different pictorial representations. For simplicity, take $d=1$. In a Fock space representation the state of the system is parametrized by wavenumbers $k$ and occupation numbers $\alpha_k$, and $\alpha(k)$ is an integer-valued function of discrete $k$.

The boson state space is defined as the space described by the set of all functions $\alpha(k)$ whose range is bounded by upper and lower limits $N$ and 0, for all values of the argument $k$ that lie in the first Brillouin zone. The total number of excitations $\sum_k \alpha(k)$ is bounded above and below by $N^2$ and 0.



The fermion scheme can be thought of as a "squeezing" of the boson space in a wavenumber-independent manner so as to meet the physical requirement that the total number of excitations not exceed $N$: $\sum_k \alpha_k \le N$. By lowering the maximum number of excitations at any given wavenumber $L_+$, the allowable space of state-defining functions $\alpha(k)$ is restricted to $\alpha_f(k)$. The only $k$-independent value of $L_+$ to meet this criterion is $L_+ = 1$. Any integer-valued function $\alpha_f(k)$ whose range is limited to [0, 1] automatically satisfies $\sum_k \alpha_k \le N$. Thus, the fermion scheme is, in this sense, the simplist state space reduction scheme. The range of $\alpha(k)$ is shown in Figure 1 for both the Bose and Fermi schemes.

The spin-wave scheme for state space reduction goes a step beyond the fermion scheme by introducing an $n$ dependence into the Fock space. While the range of $\alpha_s(k)$ continues to be from 0 to $N^d$, to allow for a realistic low-energy spectrum, its domain is limited to the interval $(-Q_+(n)/2, Q_+(n)/2)$. The state space consists of the direct sum of subspaces of fixed $n$ in which each excitation carries a wavenumber $k_j$ and $j = 1, \ldots, n$. For a one-dimensional system this space is represented using the three axes $n$, $j$, and $k_j$. Each state of the system is represented by a line that runs from $j=1$ to $n$, passing through the points $k_j$, in one of the fixed $n$ planes. The space of states in the Bose and spin-wave schemes is shown in Figure 2.

State space reduction is a large part of the kinematical effect. While nonorthogonality works in conjunction with the dynamical interaction to

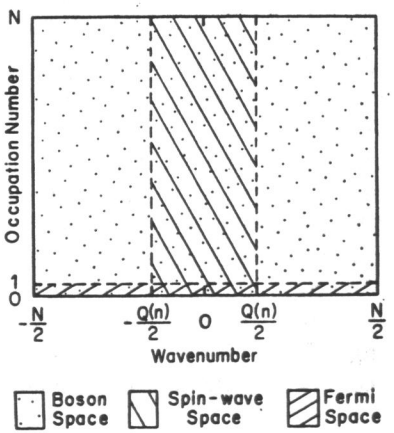


**Fig. 1.** Defining regions of occupation number $\alpha_k$ as a function of wavenumber for Bose, Fermi, and spin-wave state spaces in one dimension. Unlike the Bose and Fermi spaces, it is necessary to include along with this picture of the spin-wave space the additional requirement that $\sum_k \alpha_k \le N$.

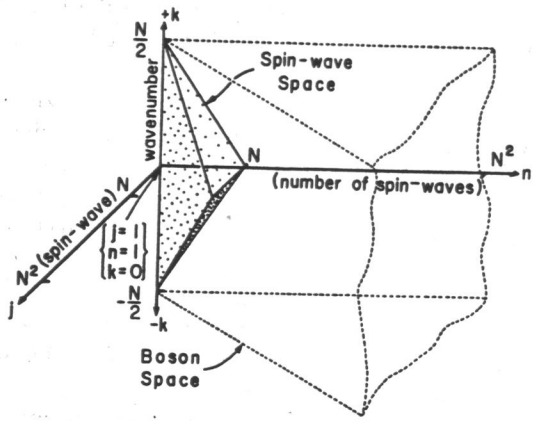


**Fig. 2.** Limits of the Bose and spin-wave state spaces plotted in coordinates where a point $(j, k, n)$ gives the wavenumber $k$ of the $j$th spin wave in an $n$-spine-wave excited state. The $\sum_k \alpha_k \leq N$ requirement in the cutoff scheme is naturally enforced by the geometry of these coordinates.

destabilize noninteracting spin-wave modes, it is likely that below $T_c$ state space reduction has more of an effect on statistics than either the dynamics or nonorthogonality. Vaks *et al.* (1968b) have computed thermal susceptibilities in a non-reduced-state-space scheme, i.e., the boson scheme, and found a weak $K_{\text{tot}}$ dependence for a wide range of $K_{\text{tot}}$ at $T \leq T_c$. They interpret this to mean that spin-wave damping remains small even at $T \simeq T_c$; hence, dynamical and nonorthogonality effects remain small. However, the overcompleteness effects are not small at $T_c$, because $\langle M_z^2 \rangle = 0$ implies the average number of $k \neq 0$ spin waves is at a value of $N/2$ ($k \neq 0$ spin waves must be excited in order to obtain vanishing magnetization squared).

Above $T_c$ the instability of spin waves (Dietrich *et al.*, 1976; Ermolov and Sigov, 1981) is expected to become statistically important. This can also be expressed by saying that soliton modes begin making a significant contribution, in analogy with the role of vortices in the two-dimensional $X$-$Y$ model (Kosterlitz, 1974). The effect of working in the spin-wave state space, rather than the boson space, will remain large, but the combination of dynamical and nonorthogonal effects will become significant as well. The appearance of increasingly numerous and increasingly unstable modes near the edge of the Brillouin zone is usually associated with the breakdown of perturbation theory. However, as the state space reduction removes the least stable of the spin-wave modes (the high-$k$, high-$n$ modes), the destabilizing effects of the nonorthogonal dynamical interactions are somewhat reduced. While nonorthogonal dynamical interactions will need to be included above $T_c$, it is possible that through the elimination of the most



unstable modes perturbative spin-wave theory may still apply to calculations of statistical behavior above $T_c$.

Finally, it should be emphasized that there is no unique state space reduction scheme. *Any* means of removing the linearly dependent states from the basis set will eliminate the unphysical zero eigenvalues. The spin-wave reduction scheme given above can thus be further refined—this will be considered in subsequent papers.

## 6. APPLICATION TO THE BOSON HAMILTONIAN

The boson reformulation of the Heisenberg spin Hamiltonian (to be distinguished from Bloch's boson treatment of the state space) consists in defining a ground state $|0\rangle$ to replace $|0\rangle$ such that $|0)$ is annihilated by boson operators $\alpha_k$. The state space is constructed by replacing spin-raising and -lowering operators with operations $\alpha_k^*$ and $\alpha_k$ that obey boson commutation relations. This second quantized description has been discussed in Section 2, equations (9)–11). The boson operator Hamiltonian $H_B$ is defined so as to reproduce the matrix elements of the scattering matrix of equation (13),

$$\hat{H}_B = E_0 + \frac{J}{2} \sum_{\mathbf{j},\boldsymbol{\delta}} [S|\eta_{\mathbf{j}} - \eta_{\mathbf{j}+\boldsymbol{\delta}}|^2 + \tfrac{1}{2}\eta_{\mathbf{j}}^* \eta_{\mathbf{j}+\boldsymbol{\delta}}^* (\eta_{\mathbf{j}} - \eta_{\mathbf{j}+\boldsymbol{\delta}})^2] \tag{34}$$

Since the boson inner-product matrix $[{}^n g_B]$ is just the unit matrix, the Hamiltonian matrix is given by

$$[{}^n h_B]_{RS} = ({}^n\varphi_R|\hat{H}|{}^n\varphi_S) = [{}^n g_B][{}^n s] = [{}^n s]$$

From the nonhermiticity of $\hat{H}_B$ it follows that $[{}^n h_B]$ is nonunitary and generally has complex eigenvalues. The information contained in the matrix $[{}^n g]$ defined with respect to the spin operators is reintroduced, so that the boson problem becomes identical to the spin-operator problem that has already been solved.

The general spin $S$ formula for the scattering of boson states is

$$\hat{H}_B \prod_{\mathbf{r}} (\eta_{\mathbf{r}}^*)^{a_{\mathbf{r}}}|0) = \left[ E_0 + J \sum_{\mathbf{j},\boldsymbol{\delta}} (S - \tfrac{1}{2} a_{\mathbf{j}+\boldsymbol{\delta}}) a_{\mathbf{j}} \right] \prod_{\mathbf{r}} (\eta_{\mathbf{r}}^{*a_{\mathbf{r}}}|0)$$

$$+ \frac{J}{2} \sum_{\mathbf{j},\boldsymbol{\delta}} [a_{\mathbf{j}} - (2S+1)] a_{\mathbf{j}} \prod_{\mathbf{r}} (\eta_{\mathbf{r}}^{*a_{\mathbf{r}} - \delta_{\mathbf{r},\mathbf{j}} + \delta_{\mathbf{r},\mathbf{j}+\boldsymbol{\delta}}}|0)$$

The second term is nondiagonal in the site basis; it raises or lowers by one the number of creation operators acting on a site. In order to create a proper

state from an improper state in the spin-1/2 case it is necessary, due to the form of this second term, that the initial improper state have no more than one site **b** at which $a_{\mathbf{b}} > 1$. At that site $a_{\mathbf{b}}$ must equal 2 (in order that the state be transformed to one in which $a_{\mathbf{b}} = 1$ by the action of $\hat{H}_B$). But because the off-diagonal contribution vanishes at $a_{\mathbf{b}} = 2$, there is no scattering from improper to proper states.[5] Dividing the state space into proper and improper blocks, we can write

$$[{}^n h] = \begin{bmatrix} [{}^n s^P]_{(A)\times(A)} & [{}^n v^a]_{(A)\times(M-A)} \\ 0 & [{}^n v^b]_{(M-A)\times(M-A)} \end{bmatrix}$$

[cf. equation (20)], and

$$({}^n\varphi^R|(\hat{H}_B)^m|{}^n\varphi^S) = \begin{bmatrix} [{}^n s^P]^m_{(A)\times(A)} & [{}^n v^a(m)]_{(A)\times(M-A)} \\ 0 & [{}^n v^b]^m_{(M-A)\times(M-A)} \end{bmatrix} \equiv [{}^n s_B]^m$$

If $f(\hat{H}_B)$ is a polynomial in $\hat{H}_B$, its eigenvalues are given by [cf. equation (23)]

$$\mathrm{Det}\{f([s_B]) - \lambda\} = \mathrm{Det}\{f([s_B^P]) - \lambda\}\,\mathrm{Det}\{f([v_B^b]) - \lambda\} = 0 \qquad (35)$$

This factoring of the secular equation also hold for general $S$. From equations (23) and (35) one sees that the same proper eigenvalues are generated in the boson scheme as in the spin operator scheme. However, the spin formalism generates $M - A$ zero eigenvalues; the improper eigenvalues of equation (35) are not identically zero. It can also be seen that proper and improper boson states are uncoupled, neither of their eigenvalues are affected by the presence of states in the other subspace, and their eigenvectors will be orthogonal. Therefore, the boson state space can be reduced by eliminating improper components without affecting the proper eigenvalues. This is a different line of reasoning than the one that motivated the removal of spin-wave states in the previous formalism. In contrast with the spin Hamiltonian matrix discussed before, the boson Hamiltonian matrix is not overcomplete. It is not obvious at the start whether or not proper and improper boson states are coupled. It is conceivable, for example, that the boson formalism only reproduced proper eigenvalues through a coupling of proper and improper states.

Rather than removing improper states from the boson state space directly, they can instead be replaced with zero vectors. An overcomplete matrix is obtained whose improper eigenvalues are zero. This is just what $[g]$ does in equation (23). Thus, the solution to the kinematical problem for the boson formulation is exactly the same as in the spin-operator case.

[5] A similar situation was noticed by Wortis with respect to his boson Hamiltonian [Wortis, 1965, Eq. (34)].



The matrix whose eigenvalues we want to compute is

$$[{}^n H_B] = [{}^n G^{s,f}][{}^n S_B^{f,s}] \qquad (36)$$

where, as before, $[{}^n S_B^{f,s}]$ is an ${}^n A \times {}^n M$ matrix with matrix elements between an ${}^n A$-dimensional reduced basis space and the ${}^n M$-dimensional space of all $n$-boson-spin-wave states. Here $[{}^n G^{s,f}]$ is the inner-product matrix defined with respect to the spin-operator basis [cf. equation (8)]. I have taken the circuitous route to this conclusion, rather than just simply stating it to be obvious from equation (19), in order to show what exactly the matrix $[G]$ is doing to the matrix $[S_B]$.

When computing the expectation value of a function of $\hat{H}_B$ one follows equation (21) and computes the eigenvalues of $[g]f([s])$. Note that $[H_B]'$ should not be considered a matrix representation of an effective Hamiltonian; it does not simply replace $[H_B]$; if this were so, then one would diagonalize $f([H_B]')$ instead of $[G]f(H_B])$. The point is that no matter what functional form $H_B$ appears in, the improper eigenvalues are always eliminated by premultiplying the matrix function $f([S_B])$ by $[G]$: $[G]$ is not mixed up in any function dependence, but only plays the role of a projection operator. This is an important fact for arriving at approximations to $[G]$, as it means that the errors inherent in approximating $[G]$ do not become multiplicatively compounded by the appearance of $[G]$ in any power series.

It is possible to approach equation (36) by finding an operator $\hat{G}$ in terms of Bose fields that reproduces $[{}^n G]$. With such an operator $f(\hat{H}_B)$ would be replaced by $\hat{G}f(\hat{H})$. Unfortunately, $\hat{G}$ turns out to be a much more complicated operator than $\hat{H}$. It can be written in terms of $k$-space boson operators $\alpha_k^*$ and $\alpha_k$ as a series in powers of $\alpha_k^*\alpha_k$ up to $(\alpha_k^*\alpha_k)^n$. Its detailed form is sufficiently complicated to warrant individual attention and will appear in a later paper.

The issue of boson state space reduction is exactly the same as is considered in Section 4. There, two schemes to include kinematical effects are described: the fermion state space reduction scheme illustrated in Figure 1 and the spin-wave scheme in Figure 2. The applicability of these schemes does not depend on whether the spaces are spanned by spin or Bose operators. Either can be used in the boson operator formalism, each with its accompanying advantages and disadvantages.

The formal solution to the kinematical problem in the calculation of the partition function in the boson formulation is

$$Z = \underset{\binom{\text{reduced}}{\text{space}}}{\mathrm{Tr}} \langle \hat{G} \exp(-\beta \hat{H}_B) \rangle \qquad (37)$$

This requires a choice of a reduced state space and the inclusion of an

inner-product operator. With the derivation of equation (34) the purpose of the present paper is achieved.

## 7. CONCLUSION

Kinematical effects in the spin operator formalism separate into nonorthogonality effects, embodied in $[G]$, and overcompleteness, as is treated by a state space reduction scheme. Both of these effects are expected to play a major role in intermediate- and high-temperature thermodynamics.

Section 4 presents an analysis of two treatments of the overcomplete state space that have been used to date. The first correct description of the spin-wave state space is described in Section 5. Section 6 turns to the boson model of Dyson and Maleev and shows that the kinematical problem that appears here has the same solution as that derived in the context of spin operators.

The discussion of Section 6 treated the overcompleteness problem independently from the other aspects of the problem. In at least two important instances the statistics of free spin waves appear independently from their dynamics.

The scattering function $S(q, \omega)$ which is the Fourier transform of a spin-pair correlation function, is proportional to the inelastic neutron scattering cross section and is well understood only in the asymptotic regimes of very high and very low temperatures (e.g., Loveluck and Windsor, 1978). One form for $S(q, \omega)$ in the intermediate region is (Cable *et al.*, 1981)

$$S(q,\omega) \propto (1-e^{-\beta E(q)})^{-1}\left(\frac{E(q)\Gamma}{[E(q)-E_0]^2+E(q)^2\Gamma^2}+\frac{E(q)\Gamma}{[E(q)+E_0]^2+E(q)^2\Gamma^2}\right)$$

where $E_0$ and $\Gamma$ are characteristic frequency and damping parameters, respectively. This form of $S(q, \omega)$, used in experimental studies of EuO and Gd,[6] is proportional to the free-particle distribution, in this case the boson distribution, so that alterations in the size of the state space alter this distribution function and affect $S(q, \omega)$ directly.

The effects of state space reduction on $\langle n_k \rangle_T$ in the context of a noninteracting particle approximation is also done with the thermal Green's function formalism in mind (Dietrich *et al.*, 1976; Loveluck and Windsor, 1978). In this approach to thermodynamics the thermal Green's function $G(k, \beta; k', 0)$ plays a central role in terms of which all thermodynamic quantities can be expressed ($\beta - 1/k_B T$). The expansion that is at the heart of thermal Green's function theory is an expansion in powers of an interaction Hamiltonian. $G(k, \beta; k', 0)$ can be written in terms of free-particle

[6]For the study of EuO and EuS see Dietrich *et al.* (1976); for the study of Gd see Loveluck and Windsor (1978).



Green's functions $G^0(k, \beta; k', 0)$ multiplied by powers of the interaction Hamiltonian. If $E_k^0$ is the energy of a single free spin wave of wavenumber $k$, then $G^0(k, \beta; k', 0)$ is written as (see Fetter and Walecka, 1971, p. 233)

$$G^0(k,\beta;k,0) = \frac{\sum_{\text{(reduced space)}} \langle\varphi|\alpha_k^\dagger \alpha_k \exp(-\beta \hat{H}_B^0)|\varphi\rangle}{\sum_{\text{(reduced space)}} \langle\varphi| \exp(-\beta \hat{H}_B^0)|\varphi\rangle}$$

$$= \langle n_k^0 \rangle_T$$

where $\hat{H}_B^0$ is the quadratic (noninteracting) part of $\hat{H}_B$ and the denominator is $Z_0$, the partition function in the noninteracting approximation. The free particle number operator plays a central role, and can be readily incorporated (Wenzel and Wagner, 1977), in the Green's function approach. The inclusion of such kinematical effects on the Green's function formalism is currently being investigated.

The free-spin-wave distribution derives from a zeroth-order approximation to the many-body wave function of the underlying magnetic medium. The multiexcitation free-spin-wave satates are products of individual excitations. The free-spin-wave space consists of all distinct products of spin waves; it does not consist of all possible products: states that have components at wavenumbers too high for the given $n$-particle subspace are excluded. Viewed in terms of spin operators, these excluded states are linearly dependent. This is directly analogous to multi-boson and fermion spaces also composed of all distinct products of independent particle states. The distinctness of a multiparticle state is determined solely by the statistics of the particles or, equivalently, the algebra of the operators that represent them. Thus, the spin space and the distribution function that follows from it are as fundamental to $SU(2)$ algebra systems as are bosons and fermions, and the Bose and Fermi distribution functions, to systems based on commutator and anticommutator algebras. The main result of this work, then, is the identification of what wavevector states are distinct in an $SU(2)$ algebra.

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