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Semiclassical and variational approximations for spin-1 magnetic chains

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We discuss some refinements of semiclassical calculations for the spin-wave excitation spectrum of easy-plane ferromagnets such as $CsNiF_3$ and examine their validity for low-spin values. We also introduce a new overcomplete set of spin states, which is used to derive integral representations and variational approximations for the partition function of magnetic chains with positive uniaxial anisotropy.

I. INTRODUCTION

One-dimensional magnetic systems have been the subject of intensive experimental and theoretical study in recent years.[1,2] Since exact results are scarce for all but spin-$\frac{1}{2}$ models, theoretical predictions have been based primarily on approximate semiclassical calculations. The validity of semiclassical approximations is often questioned for low-spin magnetic systems. A typical example is the spin-1 magnetic chain observed in $CsNiF_3$, which is described by the effective Hamiltonian

$$\mathscr{H}=-J\sum_n \vec{S}_n\cdot\vec{S}_{n+1}+A\sum_n (S_n^z)^2\,, \tag{1.1}$$

where J and A are positive constants. The purpose of this work is to examine the domain of applicability of semiclassical calculations, and to present a new variational method for the study of easy-plane ferromagnets such as (1.1).

Thus, in Sec. II we discuss various refinements of semiclassical results for the spin-wave excitation spectrum of (1.1). A coherent-state approach is shown to lead directly to a renormalization of the anisotropy constant familiar from the work of Lindgard and Kovalska.[3] We also find that, if a magnetic field parallel to the anisotropy axis is introduced, transition to an ordered state occurs above a critical field value $B_{||}=B_{||}^c$. For $CsNiF_3$, the critical value lies in the experimentally accessible region: $B_{||}^c=56$ kG. We further examine the first quantum correction to the spin-wave dispersion of (1.1) calculated within the conventional $1/s$ expansion. We have found that both the Villain[4] and the Holstein-Primakoff[5] (HP) transformation lead to the same result for the spectrum, despite claims in the literature that the HP theory is inadequate for the description of systems without long-range order. It should be noted, however, that the Villain transformation offers definite calculational advantages for systems with azimuthal symmetry. We finally show that the quantum corrections remain small throughout the spectrum, and that agreement with experiment is obtained using the currently accepted values for $J=23.6k$ and $A=9k$.

In Sec. III we introduce a new overcomplete set of "planar" spin states, which shares some properties with the more familiar overcomplete set of coherent states.[6,7] However, planar states differ from coherent states in an important way: They are not minimum-uncertainty states. Rather, they favor spin configurations lying in a plane, which suggests that planar states may be used to advantage in the study of easy-plane ferromagnets.

It is notable that overcomplete sets containing the coherent states as a special case were introduced within a general framework developed long ago by Klauder.[8] The same author emphasized that judicious choices of overcomplete sets, designed to accommodate special characteristics of a given physical system, may prove profitable in the study of dynamical questions. The example described here may be thought of as a concrete illustration of Klauder's ideas, even though some important differences arise that were not anticipated by the general treatment. For instance, path integrals derived on the basis of planar states lead to singular classical mechanics. Nonetheless, integral representations for the partition function are obtained that can be used to derive variational bounds through the Peierls-Bogoliubov inequality. Hence, the results of Sec. III are used in Sec. IV to derive a variational approximation for the partition

function of (1.1). At zero temperature this procedure leads to a Hartree-Fock approximation for the ground state, whereas the calculation at finite temperature is effected by a transfer matrix technique analogous to that developed previously for classical spin systems.[9,10] The results are compared with semiclassical calculations, and the potential as well as the limitations of the present method are discussed.

Current interest in magnetic chains such as $CsNiF_3$ is centered around possible observation of nonlinear (soliton) modes.[2] This subject is not addressed directly in the present paper, but some of the techniques discussed here might prove useful in the study of difficult questions involved in that issue.

II. SURVEY OF SEMICLASSICAL RESULTS

Path-integral representations have already been used for the derivation of semiclassical approximations for spin systems.[11–13] They are most directly derived on the basis of spin-coherent states. Consider a system described by a Hamiltonian $\mathscr{H}$ that is a function of the spin operators $\vec{S}_n$, $n=1,2,\ldots,N$. We restrict ourselves to equal spin for all sites, namely, $\vec{S}_n^2=s(s+1)$ for all n. A coherent state associated with such a system is then defined as the direct product of coherent states for individual spins:

$$|\Omega\rangle=\bigotimes_{n=1}^{N}|\Omega_n\rangle\ , \qquad (2.1)$$

$$|\Omega\rangle=\left[\cos\frac{\theta_n}{2}\right]^{2s}\exp\left[\left[\tan\frac{\theta_n}{2}\right]e^{i\phi_n}S_n^-\right]|s\rangle_n\ ,$$

$$0\le\theta_n\le\pi\ ,\quad 0\le\phi_n\le 2\pi$$

where S_n^- is the usual lowering operator and $|s\rangle_n$ is the state with maximal weight.

The resolution of unity in terms of the overcomplete set of the (normalized) coherent states (2.1) is given by

$$\int d\Omega\,|\Omega\rangle\langle\Omega|=I\ , \qquad (2.2)$$

$$d\Omega=\prod_n\left[\frac{2s+1}{4\pi}\sin\theta_n d\theta_n d\phi_n\right]\ ,$$

whereas traces of operators may be transformed into integrals over diagonal matrix elements in the basis (2.1). For instance, the trace of the evolution operator may be written as

$$Z(T)=\mathrm{Tr}e^{-i\mathscr{H}T}=\int d\Omega\langle\Omega|e^{-i\mathscr{H}T}|\Omega\rangle\ . \qquad (2.3)$$

The identity

$$e^{-i\mathscr{H}T}=\lim_{\Lambda\to\infty}\left[1-i\frac{T}{\Lambda}\mathscr{H}\right]^{\Lambda}\ , \qquad (2.4)$$

and repeated application of (2.2), may be used to convert (2.3) into the path-integral representation

$$Z(T)=\int\prod_{t\in[0,T]}d\Omega(t)\exp\left[i\int_0^T dt\left[\sum_{n=1}^{N}s\cos\theta_n\dot{\phi}_n-\langle\Omega|\mathscr{H}|\Omega\rangle\right]\right]\ . \qquad (2.5)$$

A careful short-time definition of (2.5) and discussion of related ordering problems, boundary conditions, etc., are not necessary for the Gaussian approximation we consider below. Equation (2.5) may then be interpreted as follows: The system is described by the effective Hamiltonian

$$\mathscr{H}(\Omega)=\langle\Omega|\mathscr{H}|\Omega\rangle=\mathscr{H}(\pi_n,\phi_n)\ , \qquad (2.6)$$

quantized with the commutation relations

$$[\pi_n,\phi_m]=\frac{1}{i}\delta_{nm}\ ,\quad \pi_n=s\cos\theta_n\ . \qquad (2.7)$$

Given an operator Hamiltonian $\mathscr{H}$, such as (1.1), the effective Hamiltonian is obtained by calculating the diagonal matrix elements of $\mathscr{H}$ in the coherent-state basis (2.1). The following table of matrix elements taken from Ref. 11 will be sufficient for our current calculation:

$$\begin{aligned}&\langle S_n^x\rangle=s\sin\theta_n\cos\phi_n\ ,\\ &\langle S_n^y\rangle=s\sin\theta_n\sin\phi_n\ ,\\ &\langle S_n^z\rangle=s\cos\theta_n\ ,\\ &\langle(S_n^z)^2\rangle=s(s-\tfrac{1}{2})\cos^2\theta_n+s/2\ .\end{aligned} \qquad (2.8)$$

Extending (1.1) to incorporate a magnetic field $B_\perp$ in the x direction, we write

$$\mathscr{H}=J\sum_n[-\vec{S}_n\cdot\vec{S}_{n+1}+\alpha(S_n^z)^2-b_\perp S_n^x]\ , \qquad (2.9)$$

$$\alpha=A/J\ ,\quad b_\perp=g\mu_B B_\perp/J\ .$$

The corresponding effective Hamiltonian is calculated with the aid of Eq. (2.8):

$$\mathscr{H}(\Omega)=J\sum_n \{-s^2[\cos\theta_n\cos\theta_{n+1}+\sin\theta_n\sin\theta_{n+1}\cos(\phi_n-\phi_{n+1})] +\alpha[s(s-\tfrac{1}{2})\cos^2\theta_n+s/2]-sb_\perp\sin\theta_n\cos\phi_n\} , \tag{2.10}$$

which should be viewed as a function of the coordinates ϕ_n and the canonical momenta $\pi_n=s\cos\theta_n$.

To derive the Gaussian approximation, we expand (2.10) around its minimum at $\theta_n=\pi/2$ and $\phi_n=0$, or $\pi_n=0$ and $\phi_n=0$, and keep terms that are at most quadratic:

$$\mathscr{H}(\Omega)\simeq J(-s^2+\alpha s/2-sb_\perp)+\mathscr{H}_0 ,$$
$$\mathscr{H}_0=J\sum_n \left[\left[1+\bar{\alpha}+\frac{b_\perp}{2s}\right]\pi_n^2-\pi_n\pi_{n+1} +s^2\left[1+\frac{b_\perp}{2s}\right]\phi_n^2-s^2\phi_n\phi_{n+1}\right] , \tag{2.11}$$
$$\bar{\alpha}=\alpha(1-1/2s) .$$

The c-number term in the above expansion is the leading contribution to the ground-state energy. $\mathscr{H}_0$ may be diagonalized by the standard Bogoliubov transformation to yield the magnon spectrum

$$E_p=2sJ\left[\left[1-\cos p+\frac{b_\perp}{2s}\right]\times\left[1-\cos p+\frac{b_\perp}{2s}+\bar{\alpha}\right]\right]^{1/2} ,$$
$$\bar{\alpha}=\alpha(1-1/2s)=\frac{A}{J}\left[1-\frac{1}{2s}\right] , \tag{2.12}$$
$$b_\perp=g\mu_B B_\perp/J .$$

The magnon dispersion (2.12) differs from Villain's[4] classical dispersion only by a "renormalization" of the anisotropy constant, $\alpha\to\bar{\alpha}=\alpha(1-1/2s)$, which occurs also in the work of Lindgard and Kowalska.[3] The importance of this renormalization in the analysis of experimental data for $CsNiF_3$ is discussed in Ref. 14.

The case of a magnetic field parallel to the anisotropy axis, $\vec{B}=(0,0,B_{||})$, may be treated in a similar manner. The operator Hamiltonian is now given by

$$\mathscr{H}=J\sum_n [-\vec{S}_n\cdot\vec{S}_{n+1}+\alpha(S_n^z)^2-b_{||}S_n^z] ,$$
$$b_{||}=\frac{g\mu_B B_{||}}{J} , \tag{2.13}$$

and the associated effective Hamiltonian is found to be

$$\mathscr{H}(\Omega)=J\sum_n \{-s^2[\cos\theta_n\cos\theta_{n+1} +\sin\theta_n\sin\theta_{n+1}\cos(\phi_n-\phi_{n+1})] +\alpha[s(s-\tfrac{1}{2})\cos^2\theta_n+s/2]-sb_{||}\cos\theta_n\} . \tag{2.14}$$

A translationally invariant minimum of (2.14) is given by $\phi_n=\phi$ (arbitrary constant) and $\theta_n=\theta$, minimizing the function

$$\mathscr{H}(\theta)=NJ\left[-s^2+\frac{\alpha s}{2}+\alpha s(s-\tfrac{1}{2})\cos^2\theta -sb_{||}\cos\theta\right] . \tag{2.15}$$

This leads to the algebraic equation

$$(2s\bar{\alpha}\cos\theta-b_{||})\sin\theta=0 ,$$
$$\bar{\alpha}=\alpha(1-1/2s) , \tag{2.16}$$

which possesses the solution ($s\neq\frac{1}{2}$)

$$\cos\theta=\frac{b_{||}}{2s\bar{\alpha}} , \tag{2.17}$$

a local minimum for magnetic field strengths below a critical value $B_{||}^c$:

$$\frac{b_{||}}{2s\bar{\alpha}}\leq 1 \Rightarrow B_{||}\leq(2s-1)A/g\mu_B\equiv B_{||}^c . \tag{2.18}$$

For $B_{||}\geq B_{||}^c$, the second root of (2.16), $\sin\theta=0$, becomes a local minimum describing an ordered (ferromagnetic) state in the z direction. Notice that the ordered state is an exact eigenstate of (2.13) for all values of the magnetic field $B_{||}$. In general,

however, it is not the ground state. The preceding semiclassical argument indicates that level crossing occurs at $B_{||}=B_{||}^c$, so the ordered state becomes the ground state of the system for $B_{||}\geq B_{||}^c$.

To probe the validity of the above picture we calculate the magnon dispersion in both regions. For $B_{||}\leq B_{||}^c$, the Gaussian approximation is obtained by expanding (2.14) around its minimum, shifting fields according to $\pi_n\rightarrow\pi_n+s\cos\theta$ and $\phi_n\rightarrow\phi_n+\phi$. Dropping inessential constants and higher-order terms, a straightforward calculation yields

$$\mathscr{H}(\Omega)\simeq J\sum_n\left[\frac{(1+\bar{\alpha}\sin^2\theta)\pi_n^2-\pi_n\pi_{n+1}}{\sin^2\theta}+s^2\sin^2\theta(\phi_n^2-\phi_n\phi_{n+1})\right], \tag{2.19}$$

which leads to the magnon dispersion

$$E_p=2sJ[(1-\cos p)(1-\cos p+\bar{\alpha}\sin^2\theta)]^{1/2},$$
$$\bar{\alpha}\sin^2\theta=\frac{2s-1}{2s}\frac{A}{J}\left[1-\left[\frac{B_{||}}{B_{||}^c}\right]^2\right],\quad B_{||}\leq B_{||}^c. \tag{2.20}$$

The critical behavior revealed by the preceding calculation could, in principle, be an artifact of the employed approximations. However, an argument due to Alevizos (private communication) suggests that the critical-field value given by Eq. (2.18) may be exact, even though (2.20) is an approximation to the spectrum. As mentioned earlier the state with all spins aligned in the z direction is an exact eigenstate of the original Hamiltonian. Furthermore, the exact one-magnon excitation around the ordered state may be derived in complete analogy with the case of an ideal ferromagnet:

$$E_p=2sJ(1-\cos p)+[g\mu_B B_{||}-(2s-1)A]. \tag{2.21}$$

The energy gap $E_{p=0}=g\mu_B B_{||}-(2s-1)A$ ceases to be positive below the field value $B_{||}=(2s-1)A/g\mu_B$, which coincides with the critical value found in (2.18). This coincidence suggests that the critical field $B_{||}^c$ may actually be exact. It should be noted, however, that the above argument does not prove that ordering occurs for $B_{||}\geq B_{||}^c$; it merely establishes that the ordered state cannot be the ground state for $B_{||}\leq B_{||}^c$.

The critical field for $CsNiF_3$ is found by using the values[14] $s=1$, $g=2.4$, and $A=9k$ in Eq. (2.18), which yields the relatively low value $B_{||}^c=55.8$ kG. Experimental verification of the above result should thus be possible and might provide further tests of the model. Already at $B_{||}\simeq 40$ kG, the dispersion (2.20) differs appreciably from the free-field result, and from the magnon dispersion for a magnetic field in the easy plane, Eq. (2.12).

The Gaussian approximation discussed so far may be extended to include higher-order corrections obtained by a loop expansion of the path integral (2.6). Such calculations require special care to avoid ordering problems and will not be described here. Instead, quantum corrections will be considered later in this section within more conventional operator techniques. As it stands the path integral (2.6) might, however, prove useful for WKB quantization of space-time–dependent extrema of the associated classical action. These are solutions of the classical equations for an effective anisotropy $\alpha\rightarrow\bar{\alpha}=\alpha(1-1/2s)$ and spin magnitude equal to s. In the continuum limit the relevant classical equations are those studied by Long and Bishop,[15] with minor modifications to incorporate the effective anisotropy $\bar{\alpha}$. Notice that the classical spin magnitude is equal to s rather than $\hat{s}=\sqrt{s(s+1)}$. The latter choice is often considered to be more appropriate in order to account for quantum effects. Our calculations do not support such a choice. Rather, quantum corrections are properly handled as small fluctuations around classical configurations and by the appearance of the renormalized anisotropy $\bar{\alpha}$. Similarly, Lieb's semiclassical bound for the partition function[11]

$$Z_Q=\mathrm{Tr}e^{-\beta\mathscr{H}}=\int d\Omega\langle\Omega|e^{-\beta\mathscr{H}}|\Omega\rangle,$$
$$Z_Q\geq\int d\Omega e^{-\beta\langle\Omega|\mathscr{H}|\Omega\rangle}\equiv Z_C, \tag{2.22}$$

may be calculated by the transfer matrix technique developed for this system in Ref. 16, modulo the reinterpretation of parameters discussed in the preceding paragraph.

We finally turn to a brief description of quantum corrections to the ground-state energy and the magnon dispersion, without giving calculational details. Anharmonic corrections have already been calculated by Mikeska and Patzak.[17] The reason we reconsider such calculations is to provide more detailed expressions than those given in Ref. 17, and to discuss a few theoretical points concerning

the method of calculation. We only consider the case of vanishing magnetic field for which closed-form results may be given. Thus, the $1/s$ expansion of the ground-state energy of (1.1) reads

$$E_{\rm gr}=NJs^2[\epsilon_0+\epsilon_1/s+\epsilon_2/s^2+O(s^{-3})]\ ,$$

$$\epsilon_0=-1\ , \tag{2.23}$$

$$\epsilon_1=\frac{2}{\pi}\left[\left[\frac{\alpha}{2}\right]^{1/2}+\left[1+\frac{\alpha}{2}\right]\arctan\left[\frac{2}{\alpha}\right]^{1/2}\right]-1\ ,$$

$$\epsilon_2=\frac{\alpha}{\pi^2}\left[\frac{\alpha}{2}\right]^{1/2}\arctan\left[\frac{2}{\alpha}\right]^{1/2}-\tfrac{1}{4}\epsilon_1^2\ ,$$

$$\alpha\equiv A/J$$

whereas the magnon dispersion is given by

$$E_p=2sJ[(1-\cos p)(1-\cos p+\alpha)]^{1/2}\times[1+\delta_p/s+O(s^{-2})]\ ,$$

$$\delta_p=-\frac{(1-\cos p)C_1(\alpha)+C_2(\alpha)}{1-\cos p+\alpha}\ , \tag{2.24}$$

$$C_1(\alpha)=\frac{1}{\pi}\left[\left[\frac{\alpha}{2}\right]^{1/2}+\arctan\left[\frac{2}{\alpha}\right]^{1/2}-\frac{\pi}{2}\right]\ ,$$

$$C_2(\alpha)=\frac{\alpha}{2\pi}\left[\left[\frac{\alpha}{2}\right]^{1/2}+\left[3+\frac{\alpha}{2}\right]\times\arctan\left[\frac{2}{\alpha}\right]^{1/2}-\pi\right]\ .$$

Reexpansion of the above expressions in inverse powers of $\hat{s}=\sqrt{s(s+1)}$ is straightforward using

$$s=\hat{s}\left[1-\frac{1}{2\hat{s}}+\frac{1}{8\hat{s}^2}+\cdots\right]\ . \tag{2.25}$$

For instance, the ground-state energy (2.23) may be written in the form

$$E_{\rm gr}=NJ\hat{s}^2\left[\epsilon_0+\frac{\epsilon_1-\epsilon_0}{\hat{s}}+\frac{\epsilon_2+(\epsilon_0-\epsilon_1)/2}{\hat{s}^2}+O(\hat{s}^{-3})\right]\ , \tag{2.26}$$

whereas re-expansion of (2.24) leads to expressions that can be compared with the explicit results of Ref. 17, concerning the region $p\simeq 0$; agreement is thus obtained. However, a closer examination of (2.26) suggests that the $1/\hat{s}$ expansion may not be preferable to the $1/s$ expansion given by Eq. (2.23). Applied for $\alpha=0.38$ the series (2.23) reads

$$E_{\rm gr}=NJs^2\left[-1+\frac{0.15609}{s}+\frac{0.013373}{s^2}+\cdots\right]\ ,$$

which is a smooth series that should give reliable estimates even for $s=1$. In turn, the series (2.26) yields

$$E_{\rm gr}=NJ\hat{s}^2\left[-1+\frac{1.15609}{\hat{s}}-\frac{0.56467}{\hat{s}^2}+\cdots\right]\ ,$$

which is too irregular to provide reliable results for $\hat{s}=\sqrt{1(1+1)}=\sqrt{2}$. From the mathematical point of view the above series are identical in the sense that they should both reach the same limit if a sufficient number of terms are included. In practice, however, only a few terms of the expansion can be calculated, so the choice of the expansion parameter becomes a pragmatic issue. Within the limits of the current calculation the $1/s$ expansion yields faster convergence; it will thus be used for the comparison of (2.24) with experimental data for $CsNiF_3$.[14,18] Table I contains the results for $s=1$, $J=23.6k$, and $\alpha=A/J=0.38$. Notice that the quantum correction δ_p remains small (and negative) throughout the spectrum; its largest values occur in the region $p\simeq 0$ because of the delicate infrared structure of this theory.

We conclude this section with some comments about the method of calculation of (2.23) and (2.24). They were obtained with the standard HP transformation, which was shown to lead to the same $1/s$ expansion for the energy spectrum with the Villain transformation used in Ref. 17. Infrared divergences appear in intermediate stages of the calculation, reflecting the metastability of the classical configuration upon which the derivation of the $1/s$ series is based. Nonetheless, infrared terms cancel each other in a consistent $1/s$ expansion of the energy and the remaining finite contributions are identical to those found by the Villain theory. The latter theory is computationally preferable only because it exploits in a natural manner the azimuthal symmetry of this problem.

III. OVERCOMPLETE SET OF PLANAR STATES

The remainder of this paper is the result of our effort to derive independent approximation methods that could be used to check the consistency of semiclassical calculations. Experimentation with simple variational functions for the ground state of (1.1) suggested to us a new overcomplete

TABLE I. Predictions of (2.24) and comparison with experimental data for $CsNiF_3$.

p/π	0.1	0.25	0.35	0.45	0.55	0.65	0.75
δ_p	−0.141 03	−0.092 768	−0.069 571	−0.054 574	−0.045 071	−0.039 041	−0.035 265
E_p (meV)	0.506	1.638	2.691	3.906	5.177	6.382	7.406
Experimental[a]	0.45	1.7	2.7	3.9	5.15	6.4	7.45

[a]Reference 18.

set of spin states, which appears to be suitable for the description of easy-plane ferromagnets. This section is devoted to the study of some formal properties of such states.

To simplify the notation we first consider the case of one degree of freedom $\vec{S}=(S^x,S^y,S^z)$. Generalization to many degrees of freedom is straightforward and will be worked out in Sec. IV along with some concrete applications. For spin $s=\frac{1}{2}$, a discrete basis is provided by the usual linearly in dependent states $|\pm\frac{1}{2}\rangle$ defined by the relations

$$\begin{aligned}
&\vec{S}^2|\pm\tfrac{1}{2}\rangle=\tfrac{1}{2}(\tfrac{1}{2}+1)|\pm\tfrac{1}{2}\rangle\ ,\\
&S^z|\pm\tfrac{1}{2}\rangle=\pm\tfrac{1}{2}|\pm\tfrac{1}{2}\rangle\ ,\\
&S^+|\tfrac{1}{2}\rangle=0\ ,\quad S^+|-\tfrac{1}{2}\rangle=|\tfrac{1}{2}\rangle\ ,\\
&S^-|\tfrac{1}{2}\rangle=|-\tfrac{1}{2}\rangle\ ,\quad S^-|-\tfrac{1}{2}\rangle=0\ .
\end{aligned}\tag{3.1}$$

We now consider an one-parameter family of normalized states $|\Phi\rangle$, which are linear superpositions of the basic vectors $|\pm\frac{1}{2}\rangle$ with *real* coefficients:

$$\begin{aligned}
&|\Phi\rangle=\cos\left[\frac{\phi}{2}\right]|\tfrac{1}{2}\rangle+\sin\left[\frac{\phi}{2}\right]|-\tfrac{1}{2}\rangle\ ,\\
&\langle\Phi|\Phi\rangle=1\ ,\quad 0\le\phi\le 2\pi\ .
\end{aligned}\tag{3.2}$$

The restriction of the angle $\phi/2$ to the upper semicircle was dictated by the observation that states in the lower semicircle are already contained in (3.2) up to an overall sign.

The family of states (3.2) shows some formal analogies with the coherent states (2.1), which simplify to

$$|\Omega\rangle=\cos\left[\frac{\theta}{2}\right]|\tfrac{1}{2}\rangle+\sin\left[\frac{\theta}{2}\right]e^{i\phi}|-\tfrac{1}{2}\rangle\ ,\qquad 0\le\theta\le\pi\ ,\quad 0\le\phi\le 2\pi \tag{3.3}$$

for spin $s=\frac{1}{2}$. Notice that the above superposition contains complex coefficients in contrast to (3.2). Nevertheless, the family of states (3.2) forms an overcomplete set in analogy with the coherent states. Thus, the resolution of unity reads

$$\int d\Phi\,|\Phi\rangle\langle\Phi|=I\ ,\quad d\Phi=\frac{1}{\pi}d\phi\ ,\qquad 0\le\phi\le 2\pi\ . \tag{3.4}$$

This may be verified by substituting (3.2) in (3.4) and by using the completeness relation $|\frac{1}{2}\rangle\langle\frac{1}{2}|+|-\frac{1}{2}\rangle\langle-\frac{1}{2}|=I$. Putting it differently, a state $|\psi\rangle=\alpha|\frac{1}{2}\rangle+\beta|-\frac{1}{2}\rangle$, where α and β are arbitrary *complex* coefficients, may be represented as

$$|\psi\rangle=\int d\Phi\,|\Phi\rangle\langle\Phi|\psi\rangle\ . \tag{3.5}$$

In order to understand the structure of the states (3.2) in more detail, we calculate simple matrix elements between the states $|\Phi\rangle$ and $|\Phi'\rangle$:

$$\begin{aligned}
&\langle\Phi|\Phi'\rangle=\cos\left[\frac{\phi-\phi'}{2}\right]\ ,\\
&\langle\Phi|S^x|\Phi'\rangle=\tfrac{1}{2}\sin\left[\frac{\phi+\phi'}{2}\right]\ ,\\
&\langle\Phi|S^y|\Phi'\rangle=\frac{i}{2}\sin\left[\frac{\phi-\phi'}{2}\right]\ ,\\
&\langle\Phi|S^z|\Phi'\rangle=\tfrac{1}{2}\cos\left[\frac{\phi+\phi'}{2}\right]\ .
\end{aligned}\tag{3.6}$$

Restriction of the above expressions to diagonal matrix elements leads to the result:

$$\langle\Phi|S^x|\Phi\rangle=\tfrac{1}{2}\sin\phi\ ,\quad \langle\Phi|S^y|\Phi\rangle=0\ ,$$
$$\langle\Phi|S^z|\Phi\rangle=\tfrac{1}{2}\cos\phi\ . \tag{3.7}$$

Therefore, the average spin in the y direction vanishes, which suggests the name "planar" for the family of states (3.2). This terminology should not create the impression that planar states span only a submanifold of spin states; as is shown in Eq. (3.4), (3.2) is an overcomplete set in the sense that it provides an integral representation for the resolution of unity.

Further insight is obtained by examining rotations of the states $|\Phi\rangle$ around the y axis:

$$|\Phi_\omega\rangle=e^{-i\omega S^y}|\Phi\rangle\ ,$$
$$e^{-i\omega S^y}=\cos\left[\frac{\omega}{2}\right]-\sin\left[\frac{\omega}{2}\right](S^+-S^-)\ . \tag{3.8}$$

Explicit calculation using the definition (3.2) in Eq. (3.8) yields the simple result

$$|\Phi_\omega\rangle=\cos\left[\frac{\phi+\omega}{2}\right]|\tfrac{1}{2}\rangle +\sin\left[\frac{\phi+\omega}{2}\right]|-\tfrac{1}{2}\rangle\ , \tag{3.9}$$

whereas rotations around the x and z axis act in a complicated manner. Hence, the kinematical properties of planar states appear to be suitable for the description of systems with azimuthal symmetry.

We next consider generalization to the more complicated spin-1 case. The usual discrete basis is defined by

$$\vec{S}^2|\pm1\rangle=1(1+1)|\pm1\rangle\ ,$$
$$\vec{S}^2|0\rangle=1(1+1)|0\rangle\ ,$$
$$S^z|\pm1\rangle=(\pm1)|\pm1\rangle\ ,$$
$$S^z|0\rangle=0\ , \tag{3.10}$$
$$S^-|1\rangle=\sqrt{2}|0\rangle\ ,\quad S^-|0\rangle=\sqrt{2}|-1\rangle\ ,$$
$$S^-|-1\rangle=0\ ,\quad S^+|1\rangle=0\ ,$$
$$S^+|0\rangle=\sqrt{2}|1\rangle\ ,S^+|-1\rangle=\sqrt{2}|0\rangle\ .$$

A family of normalized planar states is sought in the form

$$|\Phi\rangle=C_1|1\rangle+C_0|0\rangle+C_{-1}|-1\rangle\ ,$$
$$C_1^2+C_0^2+C_{-1}^2=1\ , \tag{3.11}$$

where $C_{\pm1}$ and C_0 are real coefficients.

To find a natural parametrization of (3.11), we examine a general rotation around the y axis,

$$|\Phi_\omega\rangle=e^{-i\omega S^y}|\Phi\rangle\ , \tag{3.12}$$

which can be explicitly calculated using the identity

$$e^{-i\omega S^y}=1-\tfrac{1}{2}\sin\omega(S^+-S^-) +\tfrac{1}{4}(1-\cos\omega)(S^+-S^-)^2\ , \tag{3.13}$$

valid for $s=1$. The result of a direct calculation may be presented in the matrix form

$$\begin{bmatrix}C_1'\\C_0'\\C_{-1}'\end{bmatrix}=\begin{bmatrix}\frac{1+\cos\omega}{2} & -\frac{\sin\omega}{\sqrt{2}} & \frac{1-\cos\omega}{2}\\ \frac{\sin\omega}{\sqrt{2}} & \cos\omega & -\frac{\sin\omega}{\sqrt{2}}\\ \frac{1-\cos\omega}{2} & \frac{\sin\omega}{\sqrt{2}} & \frac{1+\cos\omega}{2}\end{bmatrix}\begin{bmatrix}C_1\\C_0\\C_{-1}\end{bmatrix}\ , \tag{3.14}$$

where the primed coefficients are defined from

$$|\Phi_\omega\rangle=C_1'|1\rangle+C_0'|0\rangle+C_{-1}'|-1\rangle\ . \tag{3.15}$$

Inspection of (3.14) suggests the parametrization

$$C_1=\frac{\cos\theta+\cos\phi\sin\theta}{\sqrt{2}}\ ,\quad 0\le\theta\le\frac{\pi}{2}$$
$$C_0=\sin\phi\sin\theta\ ,\quad 0\le\phi\le2\pi \tag{3.16}$$
$$C_{-1}=\frac{\cos\theta-\cos\phi\sin\theta}{\sqrt{2}}\ ,$$

so that Eq. (3.14) takes the simple form

$$C_1'=\frac{\cos\theta+\cos(\phi+\omega)\sin\theta}{\sqrt{2}}\ ,$$
$$C_0'=\sin(\phi+\omega)\sin\theta\ , \tag{3.17}$$
$$C_{-1}'=\frac{\cos\theta-\cos(\phi+\omega)\sin\theta}{\sqrt{2}}\ .$$

Without loss of generality, the parameters θ and ϕ in Eq. (3.16) have been restricted to the upper

hemisphere.

The family of states defined by Eqs. (3.11) and (3.16) forms an overcomplete set in the sense that the resolution of unity reads

$$\int d\Phi\,|\Phi\rangle\langle\Phi| = I\ ,$$
$$d\Phi = \frac{3}{2\pi}\sin\theta\, d\theta\, d\phi\ , \qquad (3.18)$$
$$0\le\theta\le\frac{\pi}{2}\ ,\quad 0\le\phi\le 2\pi$$

as can be established by a simple calculation, in analogy with the spin-$\frac{1}{2}$ case discussed earlier in this section.

It is now a simple matter to calculate useful matrix elements such as

$$\begin{aligned}
\langle\Phi|\Phi'\rangle &= \cos\theta\cos\theta' \\
&\quad + \sin\theta\sin\theta'\cos(\phi-\phi')\ , \\
\langle\Phi|S^x|\Phi'\rangle &= \sin\phi\sin\theta\cos\theta' \\
&\quad + \sin\phi'\sin\theta'\cos\theta\ , \\
\langle\Phi|S^y|\Phi'\rangle &= i\sin(\phi-\phi')\sin\theta\sin\theta'\ , \\
\langle\Phi|S^z|\Phi'\rangle &= \cos\phi\sin\theta\cos\theta' \\
&\quad + \cos\phi'\sin\theta'\cos\theta\ .
\end{aligned} \qquad (3.19)$$

Restriction to diagonal matrix elements results in

$$\begin{aligned}
&\langle\Phi|S^x|\Phi\rangle = \sin\phi\sin 2\theta\ ,\quad \langle\Phi|S^y|\Phi\rangle = 0\ , \\
&\langle\Phi|S^z|\Phi\rangle = \cos\phi\sin 2\theta\ ,
\end{aligned} \qquad (3.20)$$

where we again note that the average spin in the y direction vanishes. Nevertheless, the variance of S^y does not vanish:

$$\langle\Phi|(S^y)^2|\Phi\rangle = \sin^2\theta\ , \qquad (3.21)$$

a fact that will be important for the dynamical calculations of Sec. IV.

Before considering specific applications of the preceding kinematical results, we briefly indicate a generalization to arbitrary spin. An overcomplete family of planar states may then be defined from

$$|\Phi\rangle = \sum_{\mu=-s}^{s} C_\mu\,|s\mu\rangle\ , \qquad (3.22)$$

where the C_μ's are real coefficients satisfying the normalization constraint

$$\sum_{\mu=-s}^{s} C_\mu^2 = 1\ . \qquad (3.23)$$

A natural parametrization of the $(2s+1)$-dimensional sphere of unit radius defined by (3.23) should again be found by examining a rotation around the y axis. We do not work out the details here but merely indicate that the definition of planar states requires a number of parameters that increases with spin, in contrast to the coherent states (2.1) that are specified by two real parameters for arbitrary spin.

We now assume that a dynamical system is described by the Hamiltonian $\mathscr{H}=\mathscr{H}(S)$. The corresponding partition function may then be expressed as an integral over diagonal matrix elements in the basis of planar states:

$$Z_Q = \mathrm{Tr}\,e^{-\beta\mathscr{H}} = \int d\Phi\langle\Phi|e^{-\beta\mathscr{H}}|\Phi\rangle\ . \qquad (3.24)$$

An immediate application of (3.24) is the derivation of a lower bound for the partition function through the Peierls-Bogoliubov inequality

$$Z_Q \ge \int d\Phi\, e^{-\beta\langle\Phi|\mathscr{H}|\Phi\rangle}\ , \qquad (3.25)$$

which is studied in Sec. IV. The rest of this section concerns possible elaboration of Eq. (3.24) to derive path-integral representations following the general treatment of Klauder,[8] to which the interested reader is referred for a detailed exposition of the procedure.

The interval $[0,\beta]$ is partitioned into Λ equal links of length $\epsilon=\beta/\Lambda$. To each site $i=0,1,2,\ldots$ one associates a variable $\Phi(i)$ that defines a planar state $|\Phi(i)\rangle$. Using an identity analogous to (2.4), and repeated application of the completeness relation (3.4) or (3.18), leads to the multiple-integral representation for the partition function:

$$\begin{aligned}
Z_Q &= \lim_{\substack{\epsilon\to 0\\(\Lambda\to\infty)}} \int \prod_{i=0}^{\Lambda} d\Phi_i\, e^{-I_\Lambda}\ , \\
I_\Lambda &= \sum_{i=0}^{\Lambda}\left[-\ln\langle\Phi(i+1)|\Phi(i)\rangle\right. \\
&\quad \left. + \epsilon\langle\Phi(i+1)|\mathscr{H}|\Phi(i)\rangle\right]\ , \\
&\quad \Phi(\Lambda+1)\equiv\Phi(0)\ .
\end{aligned} \qquad (3.26)$$

By construction, the limit $\epsilon\to 0$ $(\Lambda\to\infty)$ of (3.26) should reach the exact partition function of the system described by the Hamiltonian $\mathscr{H}$. It is thus instructive to examine the formal continuum limit of the effective action I_Λ appearing in Eq. (3.26). This is accomplished by the replacement

$$\epsilon\sum_i \langle\Phi(i+1)|\mathscr{H}|\Phi(i)\rangle \sim \int_0^\beta d\tau\langle\Phi|\mathscr{H}|\Phi\rangle\ ,$$

and by explicit calculation of the continuum limit of the kinematical terms appearing in (3.26). For $s=\frac{1}{2}$, we may use Eq. (3.6) to write

$$-\sum_i \ln\langle\Phi(i+1)\,|\,\Phi(i)\rangle=-\sum_i \ln\cos\left[\frac{\phi_{i+1}-\phi_i}{2}\right]$$
$$\sim\frac{\epsilon}{4}\int_0^\beta d\tau\dot{\phi}^2\,,$$

where the dot denotes differentiation with respect to the continuous Euclidean time τ. Hence, the continuum limit of the effective action (3.26) is presumably

$$I(s=\tfrac{1}{2})=\int_0^\beta d\tau\left[\frac{\epsilon}{4}\dot{\phi}^2+\langle\Phi\,|\,\mathscr{H}\,|\,\Phi\rangle\right]. \tag{3.27}$$

A similar calculation for $s=1$, using Eq. (3.19), yields

$$I(s=1)=\int_0^\beta d\tau\left[\frac{\epsilon}{2}(\dot{\theta}^2+\sin^2\theta\dot{\phi}^2)+\langle\Phi\,|\,\mathscr{H}\,|\,\Phi\rangle\right]. \tag{3.28}$$

Comparison of the explicit formal limits (3.27) and (3.28) with the general results of Ref. 8 reveals a surprise: Terms containing first-order derivatives have dropped out of Eqs. (3.27) and (3.28) while second-order derivatives are weighted with the small parameter ϵ, which will eventually be set equal to zero at the end of the calculation. One may then conclude that the "classical" mechanics associated with the overcomplete set of planar states is singular, or that the c-number configurations relevant for the evaluation of the multidimensional integral (3.26) become singular in the continuum limit. Although several methods have been developed in recent years for handling such singular problems (singular perturbation theory, boundary layers, multiple-scale analysis, etc.), we have not yet been able to directly explore the path-integral representation (3.26). We shall thus restrict ourselves to the study of the variational bound provided by Eq. (3.25).

IV. VARIATIONAL METHOD

The kinematical discussion of the preceding section suggests that planar states may be useful for the study of easy-plane ferromagnets, whose dynamics favors planar spin configurations. More precisely, one should be able to derive approximations that are sensitive to the planar behavior induced by the dynamics.

In order to exploit the properties of planar states the Hamiltonian (1.1) is written in the physically equivalent form

$$\mathscr{H}=J\sum_{n=1}^N[-\vec{S}_n\cdot\vec{S}_{n+1}+\alpha(S_n^y)^2]\,, \tag{4.1}$$

which is taken to describe a system with spin $s=1$. We further generalize the spin-1 planar states defined by Eqs. (3.11) and (3.16) to an arbitrary number of degrees of freedom:

$$|\Phi\rangle=\bigotimes_{n=1}^N|\Phi_n\rangle\,,$$
$$|\Phi_n\rangle=C_{1,n}\,|1\rangle_n+C_{0,n}\,|0\rangle_n+C_{-1,n}\,|-1\rangle_n$$
$$C_{1,n}=\frac{\cos\theta_n+\cos\phi_n\sin\theta_n}{\sqrt{2}}\,, \tag{4.2}$$
$$C_{0,n}=\sin\phi_n\sin\theta_n\,,$$
$$C_{-1,n}=\frac{\cos\theta_n-\cos\phi_n\sin\theta_n}{\sqrt{2}}\,.$$

The resolution of unity reads

$$\int d\Phi\,|\,\Phi\rangle\langle\Phi\,|=I\,,$$
$$d\Phi=\prod_{n=1}^N\left[\frac{3}{2\pi}\sin\theta_n d\theta_n d\phi_n\right], \tag{4.3}$$
$$0\le\theta_n\le\frac{\pi}{2}\,,\quad 0\le\phi_n\le 2\pi\,.$$

The statistical sum for the system (4.1) may then be written in the integral form

$$Z_Q=\mathrm{Tr}e^{-\beta\mathscr{H}}=\int d\Phi\langle\Phi\,|\,e^{-\beta\mathscr{H}}\,|\,\Phi\rangle\,, \tag{4.4}$$

which is an exact representation for the quantum partition function.

A variational approximation is obtained by applying the Peierls-Bogoliubov inequality

$$Z_Q\ge\int d\Phi e^{-\beta\langle\Phi\,|\,\mathscr{H}\,|\,\Phi\rangle}\equiv Z_P\,. \tag{4.5}$$

The free energy defined in terms of Z_P is a rigorous upper bound for the free energy of the quantum system. It will be taken here to define an approximation to the thermodynamics of (4.1).

Therefore, our task will be to evaluate explicitly the multidimensional integral (4.5). The explicit form of the diagonal matrix elements of the Hamiltonian appearing in (4.5) is obtained by a simple generalization of Eqs. (3.20) and (3.21) to many degrees of freedom:

$$\mathscr{H}(\Phi)\equiv\langle\Phi\,|\,\mathscr{H}\,|\,\Phi\rangle=J\sum_{n=1}^{N}[-\sin(2\theta_n)\sin(2\theta_{n+1})\cos(\phi_n-\phi_{n+1})+\alpha\sin^2\theta_n]\ . \tag{4.6}$$

The zero-temperature ($\beta\to\infty$) limit of (4.5) is dominated by stationary points of the effective Hamiltonian $\mathscr{H}(\Phi)$. This is equivalent to a Hartree-Fock approximation for the ground state corresponding to a variational state of the form (4.2). A translationally invariant minimum is found by setting $\theta_n=\theta$ and $\phi_n=\phi$ in Eq. (4.6). The variable ϕ drops out of the energy as a result of the underlying azimuthal symmetry. Thus,

$$\mathscr{H}(\Phi)=NJ[-\sin^2(2\theta)+\alpha\sin^2\theta]=\mathscr{H}(\theta)\ . \tag{4.7}$$

Extrema of the function $\mathscr{H}(\theta)$ are roots of the algebraic equation

$$\left[\cos2\theta-\frac{\alpha}{4}\right]\sin2\theta=0\ ,\quad 0\le\theta\le\frac{\pi}{2}\ . \tag{4.8}$$

Restricting our attention to minima of $\mathscr{H}(\theta)$ we find that

$$\begin{aligned}&\cos2\theta=\frac{\alpha}{4}\quad\text{for }\alpha\le4\ ,\\ &\sin\theta=0\quad\text{for }\alpha\ge4\ .\end{aligned} \tag{4.9}$$

The variational energy is then given by

$$E_{\rm gr}/NJ=\begin{cases}-\left[1-\dfrac{\alpha}{4}\right]^2 & \text{for }\alpha\le4\\ 0\ \text{ for }\alpha\ge4\end{cases} \tag{4.10}$$

and the corresponding variational ground state by

$$|\Phi\rangle=\bigotimes_n|\Phi_n\rangle\ ,$$

$$\begin{aligned}|\Phi_n\rangle=&\tfrac{1}{4}(\sqrt{4+\alpha}+\cos\phi\sqrt{4-\alpha})\,|\,1\rangle_n\\ &+\frac{1}{2\sqrt{2}}\sin\phi\sqrt{4-\alpha}\,|\,0\rangle_n\\ &+\tfrac{1}{4}(\sqrt{4+\alpha}-\cos\phi\sqrt{4-\alpha})\,|\,-1\rangle_n\\ &\qquad\text{for }\alpha\le4\\ |\Phi_n\rangle=&\frac{1}{\sqrt{2}}(|\,1\rangle_n+|\,-1\rangle_n)\quad\text{for }\alpha\ge4\ ,\end{aligned} \tag{4.11}$$

where the symbol $\otimes_n$ again denotes the direct product. The arbitrary parameter ϕ in (4.11) reflects the azimuthal degeneracy of the variational state and may be set equal to zero:

$$\begin{aligned}|\Phi_n\rangle=&\tfrac{1}{4}(\sqrt{4+\alpha}+\sqrt{4-\alpha})\,|\,1\rangle_n\\ &+\tfrac{1}{4}(\sqrt{4+\alpha}-\sqrt{4-\alpha})\,|\,-1\rangle_n\\ &\qquad\text{for }\alpha\le4\ .\\ |\Phi_n\rangle=&\frac{1}{\sqrt{2}}(|\,1\rangle_n+|\,-1\rangle_n)\quad\text{for }\alpha\ge4\ .\end{aligned} \tag{4.12}$$

In Fig. 1 we compare the predictions of the simple variational result (4.10) with Lieb's semiclassical bound for the ground-state energy, which can be extracted from Eqs. (2.11) and (2.22) applied for $s=1$; $E_{\rm gr}/NJ=-1+\alpha/2$, and with the predictions of the $1/s$ expansion summarized in Eq. (2.23). It is notable that all three approximations coincide in the weak-anisotropy region, where $E_{\rm gr}/NJ\simeq-1+\alpha/2$. However, the semiclassical bound deteriorates rapidly for strong anisotropy, while the results of the $1/s$ expansion remain fairly consistent with the present variational bound over a wide range of values for α. Ultimately, the predictions of three terms of the $1/s$ expansion also become inadequate, as is shown in Fig. 1. Notice that our variational result establishes that the ground-state energy cannot be positive for any α.

The simple variational state (4.12) has shown unusual resistance to improvements. We have tried to lower the energy by the moment method, which consists of constructing a new variational state

$$|\psi_\lambda\rangle=|\Phi\rangle+\lambda\mathscr{H}\,|\,\Phi\rangle\ , \tag{4.13}$$

where $|\Phi\rangle$ is the state (4.11) or (4.12), $\mathscr{H}$ is the Hamiltonian operator (4.1), and λ is the new variational parameter. The energy is then obtained as the minimum of

$$E_\lambda=\frac{\langle\psi_\lambda\,|\,\mathscr{H}\,|\,\psi_\lambda\rangle}{\langle\psi_\lambda\,|\,\psi_\lambda\rangle}\ . \tag{4.14}$$

A nontrivial solution ($\lambda\neq0$) is normally guaranteed by the nonvanishing of the variance of the Hamil-

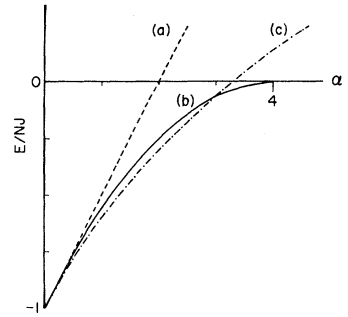

FIG. 1. Ground-state energy for the spin-1 chain: (a) semiclassical bound, (b) variational bound, Eq. (4.10), and (c) predictions of three terms of the $1/s$ expansion applied for $s=1$, Eq. (2.23).

tonian in the approximate ground state $|\Phi\rangle$, namely, by

$$\langle\Phi|\mathscr{H}^2|\Phi\rangle-\langle\Phi|\mathscr{H}|\Phi\rangle^2\neq 0 .$$

However, using the variational state (4.12) as input in Eqs. (4.13) and (4.14) does not lead to improvement of the energy. Technically, this is due to the vanishing of the variance of the Hamiltonian in the state (4.12). A lengthy calculation shows that

$$\lim_{N\to\infty}\frac{1}{N^2}[\langle\Phi|\mathscr{H}^2|\Phi\rangle-\langle\Phi|\mathscr{H}|\Phi\rangle^2]=0 , \tag{4.15}$$

which renders the moment method inapplicable. On the other hand, Eq. (4.15) and application of the Schwarz inequality would seem to imply that the state (4.12) is an exact eigenstate; this can be disproved by a direct calculation. The resolution of the paradox apparently lies in the $N\to\infty$ limit involved in Eq. (4.15). While (4.15) implies that the variance per site vanishes, the variance itself is of order N, $\langle\mathscr{H}^2\rangle-\langle\mathscr{H}\rangle^2=O(N)$.

We now return to the evaluation of the approximate statistical sum for any temperature, accomplished by a transfer matrix method analogous to that developed for the study of a classical version of this theory.[16,19] Using a periodic lattice, the integral (4.5) may be written in the symmetrized form

$$Z_P=\int\prod_{n=1}^{N}d\Phi_n G(\Phi_n,\Phi_{n+1}) , \tag{4.16}$$

$$G(\Phi_n,\Phi_{n+1})=e^{-1/2\alpha\bar{\beta}\sin^2\theta_n}\times e^{\bar{\beta}\sin2\theta_n\sin2\theta_{n+1}\cos(\phi_n-\phi_{n+1})}\times e^{-1/2\alpha\bar{\beta}\sin^2\theta_{n+1}} ,$$

where we have used the notation $\bar{\beta}=\beta J$. The problem then reduces to finding the eigenvalues of the integral equation

$$\int d\Phi' G(\Phi,\Phi')f_n(\Phi')=\lambda_n f_n(\Phi) . \tag{4.17}$$

Thanks to the azimuthal invariance of the kernel, eigenfunctions of (4.17) may be sought in the form

$$f_n(\Phi)=f_n(\theta,\phi)=\begin{bmatrix}\cos m\phi\\ \sin m\phi\end{bmatrix}\psi_{n,m}(\theta) , \quad m=0,1,2,\ldots . \tag{4.18}$$

Inserting (4.16) and (4.18) in (4.17) and performing the azimuthal integrations[10] leads to the eigenvalue problem

$$\int_0^{\pi/2}\sin\theta' d\theta' G_m(\theta,\theta')\psi_{n,m}(\theta')=\tfrac{1}{3}\lambda_{n,m}\psi_{n,m}(\theta) , \tag{4.19}$$

$$G_m(\theta,\theta')=I_m(\bar{\beta}\sin2\theta\sin2\theta')e^{-1/2\alpha\bar{\beta}(\sin^2\theta+\sin^2\theta')} ,$$

where we have used the phase space defined in Eq. (4.3), and $I_m(x)$ is the modified Bessel function of the first kind. Only the largest eigenvalue of (4.19) contributes to the statistical sum, in the limit $N\to\infty$, which corresponds to vanishing azimuthal quantum number ($m=0$):

$$\int_0^{\pi/2}\sin\theta' d\theta' G_0(\theta,\theta')\psi_{n,0}(\theta')=\tfrac{1}{3}\lambda_{n,0}\psi_{n,0}(\theta) . \tag{4.20}$$

In terms of the largest eigenvalue of (4.20), which we denote by $\lambda_{0,0}=\lambda_0$, the variational statistical sum is given by

$$Z_P=\lim_{N\to\infty}(\lambda_0)^N . \tag{4.21}$$

The explicit calculation of $\lambda_0=\lambda_0(\alpha,\bar{\beta})$ is effected by a numerical method that exploits the special structure of the kernel in (4.20). Using the Taylor expansion for the Bessel function

$$I_0(x)=\sum_{k=0}^{\infty}\frac{(x/2)^{2k}}{(k!)^2} , \tag{4.22}$$

which converges for all x, the kernel G_0 may be written in the quasidegenerate form

$$G_0(\theta,\theta')=\sum_{k=0}^{\infty}M_k(\theta)M_k(\theta') , \tag{4.23}$$

$$M_k(\theta)=\frac{1}{k!}\left[\frac{\bar{\beta}}{2}\right]^k(\sin2\theta)^{2k}e^{-1/2\alpha\bar{\beta}\sin^2\theta} .$$

Therefore, an iterative numerical scheme may be derived by truncating the infinite sum in (4.23) according to

$$G_0^{(L)}=\sum_{k=0}^{L-1} M_k(\theta)M_k(\theta') \tag{4.24}$$

and by calculating successive approximations to the eigenvalues through diagonalization of the $L\times L$ matrix ($L=1,2,\ldots$):

$$A_{kl}^{(L)}=\int_0^{\pi/2}\sin\theta\, d\theta\, M_k(\theta)M_l(\theta)$$
$$=\frac{1}{k!l!}\left[\frac{\bar\beta}{2}\right]^{k+l}\int_0^{\pi/2}\sin\theta\, d\theta(\sin2\theta)^{2k+2l}$$
$$\times e^{-\alpha\bar\beta\sin^2\theta}, \tag{4.25}$$

$k,l=0,1,\ldots,L-1$. The integral in (4.25) may be expressed in terms of known special functions:

$$A_{kl}^{(L)}=\frac{2^{k+l-1}}{k!l!}\bar\beta^{k+l}e^{-\alpha\bar\beta}B(k+l+1,k+l+\tfrac{1}{2})$$
$$\times\Phi(k+l+\tfrac{1}{2},2k+2l+\tfrac{3}{2},\alpha\bar\beta), \tag{4.26}$$

where $B(\mu,\nu)$ is the β function and $\Phi(\mu,\nu,z)$ is the degenerate (confluent) hypergeometric function. In practice, the integral in (4.25) was calculated numerically for a variety of values for k, l, α and $\bar\beta$.

To summarize, the maximal eigenvalue of $A_{kl}^{(L)}$ was computed by numerical diagonalization and its convergence for $L=1,2,\ldots$ was examined. The procedure was stopped after the result had stabilized to six figures. Apparently because the modified Bessel function I_0 is an entire function, the algorithm converges very rapidly. A few iterations suffice in the region $\bar\beta\lesssim 1$. An increasing number of iterations is necessary for larger values of $\bar\beta$, but matrices not larger than 25×25 are required in the low-temperature region $\bar\beta\simeq15$. In the extreme low-temperature limit $\bar\beta\to\infty$, λ_0 may be obtained analytically by a steepest descent calculation analogous to that described in Ref. 16:

$$\lambda_0\simeq\frac{\gamma(\alpha)}{\bar\beta}e^{\bar\beta(1-\alpha/4)^2},$$
$$\gamma(\alpha)=\frac{3\sqrt{2}}{4}\{(1+\alpha/4)$$
$$\times[1+\sqrt{1-(\alpha/4)^4}]\}^{-1/2}, \tag{4.27}$$

where we recognize in the exponent the variational ground-state energy obtained in Eq. (4.10).

An independent verification of the results was carried out with the numerical method of Ref. 16, where the integral equation is transformed into a matrix eigenvalue problem using Simpson integration. While the results of the former calculation were confirmed, the latter algorithm was much slower. It should be noted, however, that the current method does not apply to the classical-spin problem because the corresponding kernel cannot be written in a quasidegenerate form.

We shall not tabulate values for λ_0 but calculate the specific heat

$$C/kN=\bar\beta^2\frac{\partial}{\partial\bar\beta^2}\ln\lambda_0 . \tag{4.28}$$

The second derivative was obtained numerically on the basis of results for λ_0 that were eventually accurate within five or six figures. The accuracy demanded for (4.28) was better than 1%, which allowed us to plot the magnetic specific heat versus temperature for $\alpha=0.38$ and $\alpha=2$; see Fig. 2. The general structure of the curves obtained is qualitatively similar to the classical results of Ref. 16, especially because the variational specific heat also reaches the unphysical value $C/kN=1$ (instead of zero) at low temperatures, as could have been anticipated from the asymptotic result (4.27). The detailed predictions of the current calculation are, of course, different from the classical results. Notice that the low-temperature peak of the specific heat is suppressed for large values of the anisotropy constant α.

Analogous computations may be performed for various correlation functions along the lines of the earlier work on the classical model. The validity of such calculations would be difficult to defend on general grounds. Strictly speaking, the only solid result of this calculation is the derivation of a rigorous upper bound for the free energy. The structure of the variational ansatz and the discussion of the ground-state energy earlier in this section suggest that the present bound is superior to the semiclassical bound. We thus hope that, aside from its methodological interest, our calculation will provide a valuable guide for checking the consistency of future approximation schemes. It may also prove useful for the study of models similar to the model discussed in this paper. For example, the spin-1 planar magnetic chain with uniaxial anisotropy described by the Hamiltonian

$$\mathcal{H}=J\sum_n[-(S_n^xS_{n+1}^x+S_n^zS_{n+1}^z)+\alpha(S_n^y)^2] \tag{4.29}$$

is often considered in the literature.[20] The variational bound derived in this section for the Hamiltonian (4.1) applies to (4.29) without modification

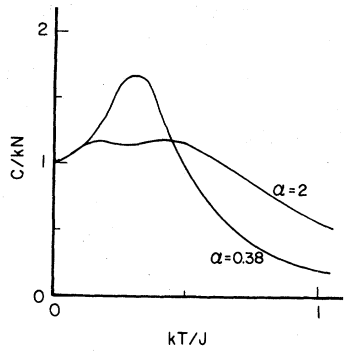

FIG. 2. Variational results for the magnetic specific heat of the spin-1 model.

because diagonal matrix elements of the spin component S_n^y in the basis of planar states vanish [see Eq. (3.20)], so that $\langle\Phi|S_n^yS_{n+1}^y|\Phi\rangle=0$. Within the limits of the variational calculation, the system (4.29) is identical to (4.1). In fact, the planar states discussed in Sec. III appear to be ideally suited for systems such as (4.29).

The difficulties of the classical, as well as the present, model in the low-temperature region may partly be attributed to the suppression of correlations in the ground state; both approximations lead to a variational ground state for the Hartree-Fock type. The construction of a more sophisticated variational ansatz including correlations turns out to be a complicated problem. The following remarks might prove helpful in that direction. One may search for an exactly solvable model that possesses the basic qualitative features of the system described by the Hamiltonian (1.1). This is a nontrivial task for spin $s=1$. However, it should be possible to diagonalize the spin-1 Hamiltonian

$$\mathcal{H}_\gamma=J\sum_n[-(S_n^aS_{n+1}^a+\tfrac{1}{2}T_n^{ab}T_{n+1}^{ab})+\gamma(S_n^z)^2], \tag{4.30}$$

$$T_n^{ab}=S_n^aS_n^b+S_n^bS_n^a,$$

using the Bethe ansatz, as was shown to be the case in the absence of anisotropy ($\gamma=0$) by Sutherland.[21] The applicability of the Bethe ansatz stems from the fact that the operator in the first parenthesis in (4.30) is the exchange operator for $s=1$.[22] It is feasible that Sutherland's solution may be extended to include the single-ion anisotropy term appearing in (4.30). It is further evident that the above system possesses the standard characteristics of an easy-plane ferromagnet (for $J>0$). The exact ground state of (4.30) could then be used as a variational state for (1.1), the variational parameter being γ, in close analogy with the treatment of the polaron problem.[23] This procedure could also provide useful qualitative suggestions concerning the excitation spectrum of (1.1). Thus, the diagonalization of (4.30) for $\gamma=0$ and $J<0$ leads to a twofold spectrum of elementary excitations.[21] While the semiclassical treatment of Sec. II is incapable of detecting a second branch in the spectrum of elementary excitations of $CsNiF_3$, there is no *a priori* theoretical argument that excludes a second branch. It should be kept in mind, of course, that the twofold spectrum may be peculiar to the tensor coupling involved in (4.30). It might also become necessary to reanalyze the whole issue of elementary excitations for spin systems without long-range order in view of the recent observations of Faddeev and Takhtajan.[24]

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[1]M. Steiner, J. Villain, and C. G. Windsor, Adv. Phys. 25, 87 (1976).

[2]See the contributions of M. Steiner and J. Villain, in *Ordering in Strongly Fluctuating Condensed Matter Systems,* NATO Advanced Study Institute Series, edited by T. Riste (Plenum, New York, 1980), pp. 91 and 107.

[3]P. A. Lindgard and A. Kowalska, J. Phys. C 9, 2081 (1976).

[4]J. Villain, J. Phys. (Paris) 35, 27 (1974).

[5]T. Holstein and H. Primakoff, Phys. Rev. 58, 1098 (1940).

[6]F. T. Arecchi, E. Courtens, R. Gilmore, and H. Thomas, Phys. Rev. A 6, 2211 (1972).

[7]A. M. Perelomov, Usp. Fiz. Nauk 123, 23 (1977) [Sov. Phys.—Usp. 20, 703 (1977)].

[8]J. R. Klauder, Ann. Phys. (N.Y.) 11, 123 (1960); and in *Path Integrals,* Proceedings of the NATO Advanced Summer Institute, edited by G. J. Papadopoulos and J. Devreese (Plenum, New York, 1978), p. 5.

[9]M. E. Fisher, Am. J. Phys. 32, 343 (1964).
[10]G. S. Joyce, Phys. Rev. 155, 478 (1967).
[11]E. H. Lieb, Commun. Math. Phys. 31, 327 (1973).
[12]A. Jevicki and N. Papanicolaou, Ann. Phys. (N.Y.) 120, 107 (1979).
[13]J. R. Klauder, Phys. Rev. D 19, 2349 (1979).
[14]M. Steiner and J. Kjems, J. Phys. C 10, 2665 (1977).
[15]K. A. Long and A. R. Bishop, J. Phys. A 12, 1325 (1979).
[16]J. M. Loveluck, S. W. Lovesey, and S. Aubry, J. Phys. C 8, 3841 (1975).
[17]H. J. Mikeska and E. Patzak, Z. Phys. B 26, 253 (1977).
[18]M. Steiner (private communication).
[19]A. R. McGurn and D. J. Scalapino, Phys. Rev. B 11, 2552 (1975).
[20]R. Jullien and P. Pfeuty, J. Phys. A 14, 3111 (1981).
[21]B. Sutherland, Phys. Rev. B 12, 3795 (1975).
[22]E. Schrödinger and J. Hamilton, Proc. Ir. Acad. 47, 39 (1941).
[23]R. P. Feynman, *Statistical Mechanics* (Benjamin, Reading, Mass., 1972).
[24]L. D. Faddeev and L. Takhtajan, Phys. Lett. A 85, 375 (1981).