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Solitons in the linear-chain antiferromagnet

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We show that in quasi-one-dimensional antiferromagnets, sine-Gordon solitons should be present as thermal excitations under a range of conditions outlined here. For a class of model spin Hamiltonians which include the influence of a transverse Zeeman field and easy-plane anisotropy, we provide explanations for the soliton rest energy, and its limiting velocity. Also, we examine the statistical mechanics of these systems with emphasis on the form of the soliton contribution to the free energy.

I. INTRODUCTION

It is well known that in condensed-matter physics, many properties of materials are explained simply by the notion that small-amplitude waves (phonons, spin waves, . . .) are the fundamental entities that enter the description of their thermodynamics, and of experiments that probe their dynamical response. Recently, Krumhansl and Schrieffer[1] have suggested that in quasi-one-dimensional materials, solitons may be present as thermal excitations, in addition to the spatially extended, wavelike modes. This question is explored in a number of subsequent theoretical papers.[2]

The nonlinear field theories that enter the description of quasi-one-dimensional solids may be applied also to more nearly isotropic materials. The solitons or solitary waves of interest in one-dimensional physics become domain walls in three dimensions. Since the latter have macroscopically large area, they fail to contribute to the partition function in the thermodynamic limit. Thus, in the absence of spatially localized solutions to the nonlinear field equations in spaces of dimension higher than one, solitons occur as thermal excitations only in the quasi-one-dimensional solid.

Mikeska[3] has pointed out that in one-dimensional systems of spins with ferromagnetic exchange coupling between neighbors, solitons of sine-Gordon form should be present in the appropriate range of temperature and magnetic field. Mikeska supposes a Zeeman field H_0 is applied perpendicular to the axis $\hat{x}$ of the line of spins, and in the analysis strong anisotropy, with $\hat{x}$ a hard axis, keeps the spins nearly confined to the yz plane. Mikeska suggests that $CsNiF_3$ should be a material where these entities can be observed by thermal neutron scattering, and subsequent experimental work by Kjems and Steiner[4] provides direct evidence for their existence, with excitation energy in accord with that predicted from the known parameters in the spin Hamiltonian of $CsNiF_3$. As far as we know, this is the only published report of direct observation of solitons present as thermal excitations in a quasi-one-dimensional solid.

The purpose of this paper is to discuss the existence and properties of sine-Gordon solitons in one-dimensional spin systems with antiferromagnetic coupling rather than ferromagnetic coupling between the spins. Earlier discussions of the surface spin-flop transition[5] and of domain walls[6] in three-dimensional antiferromagnets suggest strongly that solitons should be present in one-dimensional antiferromagnetically coupled spin arrays, though none of these earlier discussions address the case of easy-plane anisotropy encountered predominantly in the one-dimensional materials. Here we examine the linear antiferromagnet to find sine-Gordon solitons under a variety of conditions, including the easy-plane case. We note that Mikeska[7] has discussed some properties of solitons in antiferromagnetically coupled lines of spins, though his attention is directed to the easy-axis case. In the easy-plane case we are able systematically to categorize dynamical quantities by order of magnitude of smallness in a natural parameter of the theory and to establish the existence of stable sine-Gordon solitons under appropriate conditions.

Solitons in quasi-one-dimensional antiferromagnets are of interest for several reasons. First of all, in most one-dimensional magnetic salts, the exchange coupling is antiferromagnetic; $CsNiF_3$ is an exceptional case. Thus, through study of solitons in antiferromagnets, one has the possibility of exploring their properties in a number of materials with a wide range of physical parameters. We shall also see that the solitons in ferromagnetically coupled spin systems and antiferromagnetic ones have very different properties, so different experimental methods may possibly be used to explore them in the two cases.

These differences may be appreciated by a simple physical argument which we give here. A soliton at rest in an easy-plane ferromagnet in a transverse Zeeman field H_0 consists of a 2π rotation of the spins, with the motion of spins largely in the plane perpendicular to the hard axis. If there are N spins in the soliton, its formation has a cost in Zeeman energy of roughly $\mu H_0 NS$, while the cost in exchange energy is $JS^2N(\Delta\theta)^2$, with $\Delta\theta$ the angle between adjacent spins and J the ferromagnetic exchange interaction between nearest neighbors. With $\Delta\theta \simeq 2\pi/N$, the energy of the soliton is minimized when $N=2\pi(JS/\mu H_0)^{1/2}$. This simple argument, familiar from the theory of domain walls in ferromagnets,[8] provides a measure of the size and rest energy of the soliton identical to Mikeska's result, save for numerical prefactors. In $CsNiF_3$ with $H_0=5$ kG, the soliton extends over about five lattice constants, and its rest energy is approximately 30 K.

In the antiferromagnet, with $JS >> \mu H_0$, pairs of adjacent spins are nearly antiparallel. The cost in Zeeman energy per pair of spins is now on the average approximately $\mu H_0 S(\mu H_0/2JS)$, very much smaller than μH_0 because of the near cancellation of the contribution of the two almost antiparallel spins. A spin on a given sublattice rotates through an angle π rather than 2π as one passes through the soliton (see Fig. 1), so the exchange energy per pair is $JS^2(\pi/N)^2$ (we take J to be a positive number). The number of pairs of spins in the wall is now of order $JS/\mu H_0$; the wall is thus very much thicker than in the ferromagnet. The energy of formation of the antiferromagnetic soliton is then of order $\mu H_0 S$, a value much smaller than in the ferromagnetic case in the limit $\mu H_0 << JS$ often encountered in experiments. When the antiferromagnet and the ferromagnet are compared, much larger magnetic fields are required to drive the antiferromagnet into the regime where the soliton rest energy is large compared to $k_B T$ and the solitons form a dilute gas of noninteracting elementary excitations. At lower fields, one may be able to study solitons in antiferromagnets under conditions where soliton-soliton interactions play an important role.

By far the simplest example of a one-dimensional SG (sine-Gordon) system is that of a chain of coupled torsional pendula in a weak gravitational field. In this case the motions are totally restricted to lie in a plane by assumption, and the gravitational field acts as a weak barrier to hinder larger scale rotations of the pendula. From this simple example, one expects that in order for a spin system to satisfy SG dynamics two general criteria must be met—namely, the presence of some kind of plane to which spin motions are largely confined, and the existence of a weak force which slightly hinders rotations in that plane. For the antiferromagnet the hard axis can be established either by single-ion anisotropy, of crystal-field origin, or by exchange. The second criterion can be met with an external magnetic field, single-ion easy axis anisotropies, or exchange anisotropies in the plane of spin rotations.

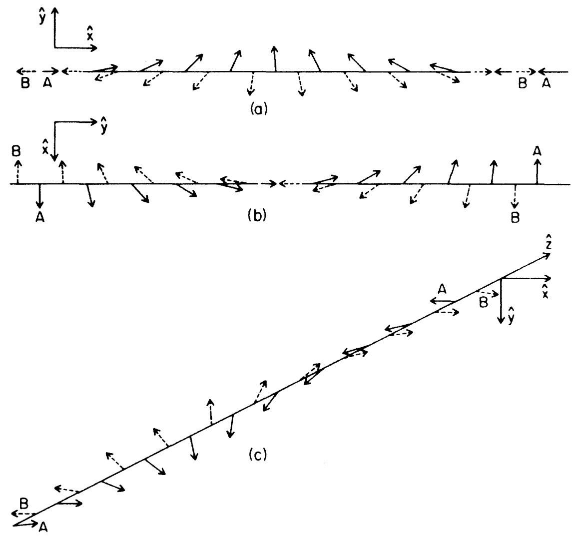

FIG. 1. Position of the spins associated with a single soliton excitation in the linear antiferromagnet. The easy plane is xy, with $\hat{x}$ the easiest direction in that plane, the two sublattices (alternating sites) are labeled A and B, and we have illustrated the situation for the chain direction along each of the coordinate axes. In each case the spins on a given sublattice rotate through an angle π, interchanging the roles of the sublattices at the opposite ends of the soliton. In drawing the figure we have neglected any canting, and Δ in Eq. (2.15) has been taken to be zero.

As will be shown later, the SG soliton here corresponds to spin rotation of π and so interchanges the two sublattices of the antiferromagnet. There is an analogy between this spin structure, shown in Fig. 1, and the sequence of alternating single and double bonds between carbon atoms in polyacetelyne, near the soliton structures described recently by Su, Schrieffer, and Heeger.[9] In our example, in the limits described below, we have solitons described by the sine-Gordon equation, while it is not clear if such a simple mathematical description can be applied to the solitons in polyacetelyne.

In Sec. II, we write down the classical equations of motion for a line of spins with antiferromagnetic coupling in a transverse magnetic field, with easy-plane anisotropy. The model is rather general, including exchange as well as single-ion anisotropy, within the easy plane as well as normal to it. This is of interest, e.g., if the anisotropy is of dipolar origin, and the plane within which the spins rotate contains the axis along which the spins are arranged. Section III is devoted to the statistical mechanics of the system, including the identification of soliton contributions to the free energy, as determined by transfer operator techniques. Section IV summarizes our principal conclusions, and discusses their implications.

II. EQUATIONS OF MOTION

We introduce superscripts A and B to denote the two sublattices of the antiferromagnet and assume in general a model Hamiltonian of the form

$$\mathcal{H} = \sum \mathcal{H}_l \ , \tag{2.1}$$

$$\mathcal{H}_l = \sum_i J_i[S_i^A(l)S_i^B(l) + S_i^A(l)S_i^B(l+1)] + D_z[S_z^A(l)^2 + S_z^B(l)^2] - D_x[S_x^A(l)^2 + S_x^B(l)^2] - g\mu_B H_x[S_x^A(l) + S_x^B(l)] - g\mu_B H_y[S_y^A(l) + S_y^B(l)] \tag{2.2}$$

with i summed over x, y, and z. All coupling parameters here are assumed non-negative, and J_z is no larger than J_x or J_y. Thus, z is a hard axis and the magnetic fields and/or D_x introduce anisotropy into the easy xy plane. This is the standard configuration for which one might anticipate solitons governed by a sine-Gordon or similar equation—namely, motion largely confined to a plane, within which there is a preferred direction and, therefore, an energy barrier to be climbed. We point out that the hard axis may result from either exchange or single-ion anisotropy. It cannot, of course, be established by an external field. On the other hand, the anisotropy within the plane can arise from any one (or a combination) of these three sources. We note, however, that the magnetic field source has the characteristic difference of distinguishing between the two senses of the special axis within the easy plane, which ultimately affects the nature of the nonlinear excitations. We will discuss various cases of interest below.

After finding the equations of motion for the spins, $i\dot{S} = [S,\mathcal{H}]$, we treat the spins as classical vectors, with spherical components

$$\vec{S}^A(l) = S(\sin\alpha_l\cos\zeta_l, \sin\alpha_l\sin\zeta_l, \cos\alpha_l) \ , \tag{2.3a}$$

$$\vec{S}^B(l) = S(\sin\beta_l\cos\phi_l, \sin\beta_l\sin\phi_l, \cos\beta_l) \tag{2.3b}$$

and substitute to obtain four equations of motion at each unit cell l for the angles α, β, ζ, and ϕ. It is convenient further to introduce linear combinations of these angles which will be of more immediate physical relevance in discussing the excitations:

$$\psi_l = \tfrac{1}{2}(\zeta_l + \phi_l), \quad \epsilon_l = \zeta_l - \phi_l - \pi \ , \\ 2\delta_l = \alpha_l + \beta_l - \pi, \quad \gamma_l = \alpha_l - \tfrac{1}{2}\pi \ . \tag{2.4}$$

Thus ψ_l represents the average azimuthal angle of two adjacent spins, whose rotation along the chain through an angle of π (effectively interchanging the roles of the two sublattices) corresponds to an elementary soliton, or "domain wall" or "kink." The other three angles are expected to be small for system parameters in the range which will be of interest to us here, with γ_l indicating motion out of the xy plane and ϵ_l and δ_l deviations from antiparallelism of adjacent spins. At sufficiently low temperatures ($kT \ll JS^2$) the spins will align in a "flopped" configuration—i.e., with nearest neighbors nearly antiparallel and (if there is an external field H_0) a small net moment along H_0 (we assume $g\mu_B H_0 \ll JS$). Then we can expect ϵ_l and δ_l, which represent deviations from perfect antiferromagnetic alignment, to be small. Moreover, the directions of the spins on a given sublattice should vary substantially only over distances large compared to a lattice constant, as long as kT is small compared to exchange energies. This justifies the use of a continuum approximation, where we can replace ψ_{l+1}, e.g., by the first few terms of its Taylor-series expansion about ψ_l. We will assume, and later verify, that ϵ_l, δ_l, and ψ_l' are all of the same order in a suitably defined small parameter r, basically a measure of the ratio of the in-plane anisotropy to exchange energies. Then $\epsilon_l' \sim \delta_l' \sim r^2$, where the prime denotes spatial differentiation with respect to l, now taken to be a continuous variable. Similarly, time derivatives of these quantities will be one order of r smaller than the quantities themselves, since the characteristic velocity divided by the lattice constant is of the order of an exchange frequency. The equations of motion in terms of the angles become

$$\dot{\alpha}_l = \cos(2\delta_l - \gamma_l)(j_+\sin\epsilon_l - j_-\sin2\psi_l) + \cos(2\delta_{l+1} - \gamma_{l+1})\{j_+\sin[\psi_l - \psi_{l+1} + \tfrac{1}{2}(\epsilon_l + \epsilon_{l+1})] - j_-\sin[\psi_l + \psi_{l+1} + \tfrac{1}{2}(\epsilon_l - \epsilon_{l+1})]\} - d_x\cos\gamma_l\sin(2\psi_l + \epsilon_l) - h_x\cos(\psi_l + \tfrac{1}{2}\epsilon_l) - h_y\sin(\psi_l + \tfrac{1}{2}\epsilon_l) \ , \tag{2.5a}$$

$$\dot{\zeta}_l = -\tan\gamma_l \cos(2\delta_l - \gamma_l)(j_+ \cos\epsilon_l - j_- \cos 2\psi_l)$$
$$- \tan\gamma_l \cos(2\delta_{l+1} - \gamma_{l+1})\{j_+ \cos[\psi_l - \psi_{l+1} + \tfrac{1}{2}(\epsilon_l + \epsilon_{l+1})] - j_- \cos[\psi_l + \psi_{l+1} + \tfrac{1}{2}(\epsilon_l - \epsilon_{l+1})]\}$$
$$- j_z[\sin(2\delta_l - \gamma_l) + \sin(2\delta_{l+1} - \gamma_{l+1})] - 2d_x \sin\gamma_l \sin^2(\psi_l + \tfrac{1}{2}\epsilon_l)$$
$$- 2d_z \sin\gamma_l + h_y \tan\gamma_l \cos(\psi_l + \tfrac{1}{2}\epsilon_l) - h_x \tan\gamma_l \sin(\psi_l + \tfrac{1}{2}\epsilon_l) \quad , \tag{2.5b}$$

with corresponding forms for $\dot{\beta}_l$ and $\dot{\phi}_l$ on the other sublattice. The energies introduced here are defined as

$$j_i \equiv J_i S, \quad j_\pm \equiv \tfrac{1}{2}(j_x \pm j_y), \quad d_i \equiv D_i S, \quad h_i \equiv g\mu_B H_i \quad . \tag{2.6}$$

We can immediately obtain the equation for $\dot{\epsilon}_l = \dot{\zeta}_l - \dot{\phi}_l$. The Eqs. (2.5) are exact, but we now make use of the smallness of h_i/j, ϵ_l, δ_l, and γ_l to obtain a more tractable form valid to order r^2

$$\dot{\epsilon}_l \simeq 4[(j_+ - j_z) - j_- \cos 2\psi_l + d_x \sin^2\psi_l + d_z](\delta_l \cos\gamma_l - \sin\gamma_l) \quad . \tag{2.7}$$

As we have already stated, the left-hand side is to be shown below to be self-consistently of order r^2, where δ_l, γ_l, and ϵ_l are of order r, a small parameter of the theory. The factor within square brackets is a sum of terms, each of which describes anisotropy, either between the hard axis and easy plane or within the easy plane. If this factor is of order r^0, as we would expect in general for $(\tilde{j}_z - \tilde{j}_+) + \tilde{d}_z$ (the tilde will henceforth be used to denote energies in units of the largest of the j_i) then $(\delta_l \cos\gamma_l - \sin\gamma_l) \sim O(r^2)$. If, on the other hand, the relative hard-axis anisotropy is only of order r, then the remaining factor, $(\delta_l \cos\gamma_l - \sin\gamma_l)$, must also be of order r, like its separate terms. Under either of these conditions we must have $\gamma_l \sim O(r)$, and to terms of order r we have

$$\dot{\psi}_l \simeq -2\delta_l(j_+ - j_- \cos 2\psi_l + j_z + d_x \sin^2\psi_l + d_z) \tag{2.8}$$

or

$$\dot{\psi}_l \simeq -2\delta_l(j_+ + j_z + d_z), \quad \tilde{j}_-, \tilde{d}_x \leq O(r) \quad . \tag{2.9}$$

This last condition refers to the size of the in-plane anisotropy. In fact we use this condition to *define* r

$$r^2 = \max(\tilde{j}_-, \tilde{d}_x, \tilde{h}_i^2) \tag{2.10}$$

and the reduction of the theory to a sine-Gordon equation (for ψ) will depend on r being small—i.e., on the largest in-plane anisotropy energy being small compared to the largest of the exchange energies j_i. This is certainly a reasonable physical requirement if the motion is going to be confined largely to the neighborhood of the easy plane. The magnetic field, although it also gives anisotropy in the plane, has a weaker influence than the exchange or single-ion anisotropies, j_- and d_x. As pointed out in the introduction, there is substantial cancellation of its effects between the two sublattices; the Zeeman energy of truly antiparallel spins is independent of the alignment of their common axis with the magnetic field. The actual canting angle δ_l of the spins in the plane response to the field is of order (h/J), a familiar result from the standard analysis of spin flop; δ_l is in general of order r. Thus $\dot{\delta}_l$ should be of order r^2; explicit calculation from the above equations of motion gives to this order

$$2\dot{\delta}_l \simeq j_+(\epsilon_l' - \psi_l'') - 2(2j_- + d_x)\sin 2\psi_l + \epsilon_l(h_x \sin\psi_l - h_y \cos\psi_l) \quad . \tag{2.11}$$

The corresponding equation for γ_l is

$$\dot{\gamma}_l = \dot{\alpha}_l \simeq j_+(2\epsilon_l - \psi_l') - (2j_- + d_x)\sin 2\psi_l - h_x \cos\psi_l - h_y \sin\psi_l \quad . \tag{2.12}$$

But this must be of order r^2, which gives immediately

$$\epsilon_l \simeq \tfrac{1}{2}\psi_l' + (h_x \cos\psi_l + h_y \sin\psi_l)/2j_+ \quad . \tag{2.13}$$

If we use these results in the time derivative of Eq. (2.9) for $\dot{\psi}_l$, we obtain finally the dynamical equation for ψ_l

$$\tfrac{1}{2}j_+\psi_l'' - \ddot{\psi}_l/(j_+ + j_z + d_z) = -2(2j_- + d_x)\sin 2\psi_l + \frac{(h_x \cos\psi_l + h_y \sin\psi_l)(h_x \sin\psi_l - h_y \cos\psi_l)}{2j_+} \quad . \tag{2.14}$$

This is a sine-Gordon equation for the quantity $2\psi_l + \Delta$:

$$\psi_l'' - \ddot{\psi}_l/c^2 = \tfrac{1}{2}m^2 \sin(2\psi_l + \Delta) \quad , \tag{2.15}$$

where

$$\Delta = \tan^{-1}\left(\frac{2h_x h_y}{8j_+(2j_- + d_x) + h_y^2 - h_x^2}\right) \quad (2.16)$$

and the velocity c and mass m are given by

$$c^2 = \tfrac{1}{2}a^2 j_+(j_+ + j_z + d_z) \ , \quad (2.17)$$

$$m^2 = \{[8j_+(2j_- + d_x) + h_y^2 - h_x^2]^2 + (2h_x h_y)^2\}^{1/2}/(a^2 j_+^2) \ . \quad (2.18)$$

It will be useful in the following section, in deriving the statistical mechanics, to take advantage of an alternate approach to this result. We can write the Hamiltonian to order r^2 as

$$\frac{\mathcal{H}_l}{S} \simeq \frac{\dot{\psi}_l^2}{2(j_+ + j_z + d_z)} + \frac{j_+(\psi_l')^2}{4} + (2j_- + d_x)\cos 2\psi_l - \frac{(h_x\cos\psi_l + h_y\sin\psi_l)^2}{4j_+} - \tfrac{1}{2}\psi_l'(h_x\cos\psi_l + h_y\sin\psi_l) \quad (2.19)$$

which yields Eq. (2.15) as the field equation for ψ_l.

Let us consider the special case of isotropic exchange ($j_i = j$) and $h_y = 0$, so that anisotropy in the plane is associated with the unique x axis (but is in general due both to the external field h_x and to the single-ion anisotropy d_x). Then the equation of motion (2.15) for ψ_l becomes

$$\psi_l'' - \ddot{\psi}_l/c^2 = \tfrac{1}{2}(aj)^{-2}(8jd_x - h_x^2)\sin(2\psi_l) \ . \quad (2.20)$$

If $h_x^2 < 8jd_x$ then we can write

$$\Phi_l'' - \ddot{\Phi}_l/c^2 = m^2 \sin\Phi_l \ , \quad (2.21)$$

$$m^2 = (8jd_x - h_x^2)/(aj)^2, \quad \Phi_l \equiv 2\psi_l \ . \quad (2.22)$$

The boundary condition for these weak magnetic fields is $\sin\Phi_l = 0$ as $|l| \rightarrow \infty$, or $\zeta_l = 0$, π and $\phi_l = \pi$, 0, so that the spins lie along the $\pm x$ axis far from the kink. On the other hand, if $h_x^2 > 8jd_x$ the equation takes the same form, but

$$m^2 = (h_x^2 - 8jd_x)/(aj)^2, \quad \Phi_l \equiv 2\psi_l - \pi \quad (2.23)$$

and the boundary condition $\sin\Phi_l = 0$ as $|l| \rightarrow \infty$ now corresponds to $\zeta_l = \pm\tfrac{1}{2}\pi$ and $\phi_l = \mp\tfrac{1}{2}\pi$ so that the spins lie along the $\pm y$ axis. The passage, with $m^2 \rightarrow 0$, from one regime to the other is just the phenomenon of spin flop, at the usual critical field value of $h_c^2 = 8jd_x$. Of course, our derivation throughout has assumed $h_x << j$, so the result [Eq. (2.23)] is confined to the region not too far above spin flop, where neighboring spins are still very nearly antiparallel.

The soliton solutions to the sine-Gordon equation (2.15) are by now well known. We restate them here for use later in the paper

$$\psi_l^{(1)} + \tfrac{1}{2}\Delta = 2\tan^{-1} e^{\pm m\gamma(l - ut)} \ , \quad (2.24a)$$

$$\psi_l^{(2)} + \tfrac{1}{2}\Delta = 2\tan^{-1} e^{\pm m\gamma(l - ut)} + \pi \ . \quad (2.24b)$$

Here the velocity u is the soliton velocity $-c \leq u \leq c$ and γ is the Lorentz factor $\gamma = (1 - u^2/c^2)^{-1/2}$.

There are two types of soliton because of the two sublattices in the antiferromagnet; the difference between $\psi_l^{(1)}$ and $\psi_l^{(2)}$ lies only in the boundary conditions imposed (spins on the sublattice labeled A "up" or "down" as $l \rightarrow -\infty$). We point out that ψ_l has been defined so that its meaningful range extends from 0 to 2π. Because of the factor of 2 in front of ψ_l in the argument of the sine potential in Eq. (2.15), the soliton corresponds to a rotation of π for the spins of either sublattice; the roles of the sublattices are interchanged as we pass through the soliton. The soliton energy is given by

$$E_{\text{sol}} = Sj_+ ma \ , \quad (2.25)$$

where ma is given by Eq. (2.18).

III. STATISTICAL MECHANICS

In this section we briefly discuss the classical statistical mechanics of the planar antiferromagnetic chain, with the objective of identifying soliton contributions to the thermodynamic functions such as the free energy. Two different approaches are considered which lead to essentially the same results in appropriate limits. In the first approach, we do not make any *a priori* decomposition of the spin chain into two sublattices. As a result the degeneracy of the ground state (interchange of sublattices) is automatically taken into account in integrating over *all* the spin degrees of freedom. In the second approach we start directly with the approximate Hamiltonian (2.19) and show that it can be mapped onto the canonical sine-Gordon problem considered previously by Currie *et al.*[2] Although this second approach has the disadvantage of requiring a reinstatement of the degrees of freedom suppressed in obtaining Eq. (2.19), it has the advantage of applicability to the general case described in Sec. II, whereas the first approach can only be applied (simply) to the special case of isotropic exchange. These points are discussed further at the end of this section.

In the first approach, we employ a method similar to that of Riseborough and Trullinger,[10] which was developed for the case of a planar *ferromagnetic* chain in an external transverse magnetic field, to consider the special case of isotropic exchange ($J_x = J_y = J_z$) and $D_y = 0$, with the Zeeman field oriented along $\hat{x}$. Using spherical coordinates

$$[\vec{S}_i = S(\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i)] \ ,$$

we may write the Hamiltonian in this case as

$$\mathcal{H} = JS^2 \sum_i [\sin\theta_i \sin\theta_{i+1} \cos(\phi_{i+1} - \phi_i) + \cos\theta_i \cos\theta_{i+1}] - hS \sum_i \sin\theta_i \cos\phi_i + DS^2 \sum_i \cos^2\theta_i \ , \tag{3.1}$$

where $h = g\mu_B H_x$ and $D = D_z$. The partition function is given by

$$Z = \left[\prod_{i=1}^{N} \int_0^{\pi} d\theta_i \sin\theta_i \int_0^{2\pi} d\phi_i \right] \exp[-\beta H(\{\theta_i\}, \{\phi_i\})] \ . \tag{3.2}$$

In the nearly planar limit where $\beta DS^2 >> 1$, the integrations over $\{\theta_i\}$ are dominated by values close to $\frac{1}{2}\pi$, so that the contribution from $DS^2 \cos\theta_i$ can be integrated separately and θ_i set equal to $\frac{1}{2}\pi$ in the exchange and Zeeman terms. Thus,

$$Z \cong [(\pi/\beta DS^2)^{1/2} \operatorname{erf}(\beta DS^2)^{1/2}]^N \left[\prod_{j=1}^{N} \int_0^{2\pi} d\phi_j \right] \exp\left[-\beta JS^2 \sum_{i=1}^{N} \cos(\phi_{i+1} - \phi_i) + \beta hS \sum_{i=1}^{N} \cos\phi_i \right] \ , \tag{3.3}$$

where erf (x) is the error function.[11]

The remaining integrations over the $\{\phi_i\}$ may be carried out using the transfer-integral technique[10,12,13] yielding

$$Z \cong [(\pi/\beta DS^2)^{1/2} \operatorname{erf}(\beta DS^2)^{1/2}]^N \sum_n e^{-N\beta\epsilon_n} \ , \tag{3.4}$$

where ϵ_n are the eigenvalues of the transfer-integral operator:

$$\int_{-\pi}^{\pi} d\phi_i \exp[-\beta JS^2 \cos(\phi_{i+1} - \phi_i) + \beta hS \cos\phi_{i+1}] \Psi_n(\phi_i) = e^{-\beta\epsilon_n} \Psi_n(\phi_{i+1}) \ . \tag{3.5}$$

In this expression Ψ_n is the eigenfunction associated with the eigenvalue ϵ_n. We note that in the thermodynamic limit ($N \to \infty$) only the lowest eigenvalue ϵ_0 is important in the free energy per spin

$$f = -\frac{k_B T}{N} \ln Z$$
$$= -k_B T \ln[(\pi/\beta DS^2)^{1/2} \operatorname{erf}(\beta DS^2)^{1/2}] + \epsilon_0 \ . \tag{3.6}$$

As we shall see, ϵ_0 contains a portion which can be attributed to the solitons discussed in Sec. II.

Although Eq. (3.5) can be converted[10,13] to a matrix eigenvalue problem by Fourier transformation, this approach is not particularly useful for obtaining an analytic approximation to ϵ_0. Instead we proceed in a more direct fashion by converting Eq. (3.5) into a differential equation for $\Psi_n(\phi)$. We first note that *all* solutions Ψ_n of Eq. (3.5) are periodic with period 2π. This property of the solutions will be used repeatedly. We can put Eq. (3.5) in a more convenient form by first shifting ϕ_{i+1} by π

$$\exp(-\beta hS \cos\phi_{i+1}) \int_{-\pi}^{\pi} d\phi_i \exp[\beta JS^2 \cos(\phi_{i+1} - \phi_i)] \Psi_n(\phi_i) = e^{-\beta\epsilon_n} \Psi_n(\phi_{i+1} + \pi) \ . \tag{3.7}$$

Next, we make use of the fact that the integration on ϕ_i covers a full period of the integrand. Thus, we may shift the limits

$$\exp(-\beta hS \cos\phi_{i+1}) \int_{-\pi+\phi_{i+1}}^{\pi+\phi_{i+1}} d\phi_i \exp[\beta JS^2 \cos(\phi_{i+1} - \phi_i)] \Psi_n(\phi_i) = e^{-\beta\epsilon_n} \Psi_n(\phi_{i+1} + \pi) \ . \tag{3.8}$$

The exponential in the integrand is sharply peaked about ϕ_{i+1} when βJS^2 is large. We are thus motivated to Taylor expand $\Psi_n(\phi_i)$ about $\phi_i = \phi_{i+1}$:

$$\Psi_n(\phi_i) = \sum_{l=0}^{\infty} \frac{(\phi_i - \phi_{i+1})^l}{l!} \frac{d^l}{d\phi_{i+1}^l} \Psi_n(\phi_{i+1}) \ . \tag{3.9}$$

Substitution of Eq. (3.9) into Eq. (3.8), approximation of $\cos(\phi_{i+1} - \phi_i)$ by $1 - \frac{1}{2}(\phi_{i+1} - \phi_i)^2$, and extension of the limits to infinity yields simple Gaussian moment integrals with the result

$$\left[\frac{2}{\beta JS^2} \right]^{1/2} \exp(\beta JS^2) \exp(-\beta hS \cos\phi_{i+1}) \left[\sum_{l=0}^{\infty} \frac{1}{l!(2\beta JS^2)^l} \left[\frac{d^2}{d\phi_{i+1}^2} \right]^l \right] \Psi_n(\phi_{i+1}) = e^{-\beta\epsilon_n} \Psi_n(\phi_{i+1} + \pi) \ . \tag{3.10}$$

The quantity in square brackets is just the Taylor representation of the operator $\exp[(1/2\beta JS^2)(d^2/d\phi_{i+1}^2)]$. Thus, dropping the subscript $i+1$, we have

$$\exp(-\beta hS\cos\phi)\exp\left[\frac{1}{2\beta JS^2}\frac{d^2}{d\phi^2}\right]\Psi_n(\phi)=e^{-\beta\tilde{\epsilon}_n}\Psi_n(\phi+\pi) \quad , \tag{3.11}$$

where

$$\tilde{\epsilon}_n \equiv \epsilon_n + JS^2 + \beta^{-1}\ln(2\pi/\beta JS^2)^{1/2} \quad . \tag{3.12}$$

Equation (3.11) does not yet have the form of a differential equation for $\Psi_n(\phi)$ since $\Psi_n(\phi+\pi)$ appears on the right-hand side. This can be remedied by iterating the operator once and using the periodicity of $\Psi_n(\phi)$:

$$e^{\beta hS\cos\phi}\exp\left[\frac{1}{2\beta JS^2}\frac{d^2}{d\phi^2}\right]e^{-\beta hS\cos\phi}\exp\left[\frac{1}{2\beta JS^2}\frac{d^2}{d\phi^2}\right]\Psi_n(\phi)=e^{-2\beta\tilde{\epsilon}_n}\Psi_n(\phi) \quad . \tag{3.13}$$

We can symmetrize the operator on the left-hand side by rewriting Eq. (3.13) as an eigenvalue equation for

$$\Phi_n(\phi)\equiv\exp(-\tfrac{1}{2}\beta hS\cos\phi)\Psi_n(\phi) \quad ,$$

$$e^{A(h)}e^{A(-h)}\Phi_n(\phi)=e^{-2\beta\tilde{\epsilon}_n}\Phi_n(\phi) \quad , \tag{3.14a}$$

where

$$e^{A(h)}\equiv\exp(\tfrac{1}{2}\beta hS\cos\phi)\exp\left[\frac{1}{2\beta JS^2}\frac{d^2}{d\phi^2}\right]\exp(-\tfrac{1}{2}\beta hS\cos\phi) \tag{3.14b}$$

$$\Rightarrow 2\beta JS^2A(h)=\frac{d^2}{d\phi^2}+(\tfrac{1}{2}\beta hS)^2\sin^2\phi+\beta hS\left[\tfrac{1}{2}\cos\phi+\sin\phi\frac{d}{d\phi}\right] \quad . \tag{3.14c}$$

The last term in $A(h)$, odd in h, is of order $(h/JS) \ll 1$. It is a measure of the canting of the spins along the field direction in the ground state, and it can be treated perturbatively. The resultant power series in (h/JS) for the eigenvalue will contain only even powers, since the eigenvalue must be independent of the sign of the field. In particular, the linear terms from the expansion of $A(h)$ and $A(-h)$ are readily seen to cancel, and

$$\epsilon_n(h)=\epsilon_{n0}(|h|)+(h/JS)^2\epsilon_{n1}(|h|)+\cdots \quad .$$

Here we will keep only the leading term; then $A(h)\simeq A(-h)$ and the exponents in Eq. (3.14a) can be added, giving the approximate eigenvalue equation

$$\left[\frac{1}{\beta JS^2}\frac{d^2}{d\phi^2}+\frac{\beta h^2}{8J}(1-\cos 2\phi)\right]\Phi_n(\phi)\simeq-2\beta\tilde{\epsilon}_n\Phi_n(\phi) \quad , \tag{3.15}$$

which is the Mathieu equation,[11] given in standard form as

$$[d^2/d\phi^2+(a-2q\cos 2\phi)]\Phi_n(\phi)=0 \quad , \tag{3.16a}$$

$$a\equiv 2\beta^2JS^2(\tilde{\epsilon}_n+h^2/16J),\quad q\equiv(\beta hS/4)^2 \quad . \tag{3.16b}$$

From the asymptotic formulas[11] for the lowest characteristic Mathieu value (eigenvalue) $a=a_0$, we have for large q

$$\epsilon_0=-JS^2-\beta^{-1}\ln(2\pi/\beta JS^2)^{1/2}-\frac{h^2}{8J}+\frac{h}{4\beta JS}-\left[\frac{2}{\pi}\right]^{1/2}\frac{(hS)^{3/2}}{\beta^{1/2}JS^2}e^{-\beta hS}\quad(\beta hS\gg 1) \quad . \tag{3.17}$$

Here and below the symbol h is intrinsically ≥ 0: $h\equiv|h|$. We note that $-JS^2-h^2/8J\equiv E_0$ is just the ground-state energy per spin, and that $hS\equiv E_{\rm sol}$ is the creation energy of the soliton excitation (Sec. II). Using Eq. (3.6) and the asymptotic form[11] of erf (x) for large x, we finally obtain the low-temperature free energy per spin

$$f-E_0\cong k_BT\left[\frac{h}{4JS}+\ln\frac{(\frac{1}{2}JDS^4)^{1/2}}{\pi k_BT}-\left[\frac{2}{\pi}\right]^{1/2}\frac{h}{JS}\left[\frac{E_{\rm sol}}{k_BT}\right]^{1/2}e^{-E_{\rm sol}/k_BT}\right] \quad . \tag{3.18}$$

The first two terms give precisely the contribution expected[10] from classical spin waves in the absence of solitons, while the last term is interpreted[2] as the soliton contribution

$$f - E_0 \cong f_{\text{spin wave}} - k_B T n_{\text{sol}}^{\text{tot}} \quad . \tag{3.19}$$

Here $n_{\text{sol}}^{\text{tot}}$ is the density of solitons plus antisolitons

$$n_{\text{sol}}^{\text{tot}} = \frac{2}{d_{\text{sol}}} \left[\frac{2}{\pi}\right]^{1/2} \left[\frac{E_{\text{sol}}}{k_B T}\right]^{1/2} e^{-E_{\text{sol}}/k_B T} \tag{3.20}$$

$$(k_B T << E_{\text{sol}}) \quad ,$$

where $d_{\text{sol}} \equiv 2JS/h$ is the characteristic soliton width (in units of the lattice constant, $\frac{1}{2}a$).

We now turn to the second approach to calculating thermodynamic quantities. In this method we start directly from the approximate Hamiltonian (2.19) in discrete form

$$\mathcal{H} = S \sum_{l=1}^{N/2} [\tfrac{1}{4} j_+ (\psi_{l+1} - \psi_l)^2 + \tfrac{1}{2}(j_+ + j_z + d_z)^{-1} \dot{\psi}_l^2 + (2j_- + d_x)\cos 2\psi_l - (1/4 j_+)(h_x \cos\psi_l + h_y \sin\psi_l)^2] \quad . \tag{3.21}$$

We have omitted the last term in the Hamiltonian density (2.19), because it is a perfect derivative with respect to x of a function of ψ, and it therefore vanishes identically upon integration of $\mathcal{H}$ over x when periodic boundary conditions $[\psi(\infty) = \psi(-\infty)]$ are imposed. In the discrete lattice form (if the continuous limit is not taken), it contributes only to higher order in h/J and can still be neglected. Equation (3.21) can be put in the form considered by Currie *et al.*[2]

$$\mathcal{H} = \sum_{l=1}^{N/2} aA [\tfrac{1}{2}\dot{\chi}_l^2 + \tfrac{1}{2}(c^2/a^2)(\chi_{l+1} - \chi_l)^2 + \omega^2(1 - \cos\chi_l)] \quad , \tag{3.22}$$

where

$$\chi_l \equiv 2\psi_l + \Delta \tag{3.23}$$

and

$$A \equiv \frac{S}{4a}(j_+ + j_z + d_z)^{-1}, \quad \omega = mc \quad . \tag{3.24}$$

The constants Δ, c, and m are given by Eqs. (2.16), (2.17), and (2.18), respectively. The constant A sets the energy scale, c is the limiting velocity of the soliton, and ω is a characteristic oscillation frequency ($k = 0$ spin-wave frequency). The "width" of the soliton is $d_{\text{sol}} = c/\omega = m^{-1}$. We have added a constant to $\mathcal{H}$ so that the ground-state configuration ($\chi_l = 0$) has zero energy.

For a linear chain governed by the above Hamiltonian, Currie *et al.*[2] have used the transfer operator technique to obtain the following free energy (per spin *pair*):

$$\tilde{f} = \tfrac{1}{2} k_B T m a + k_B T \ln \left[\frac{\hbar\omega}{k_B T m a}\right] - k_B T 2ma \left[\frac{2}{\pi}\right]^{1/2} \left[\frac{E_{\text{sol}}}{k_B T}\right]^{1/2} e^{-E_{\text{sol}}/k_B T} \quad . \tag{3.25}$$

In this expression E_{sol} is the soliton rest energy given by Eq. (2.25).

In the special case of isotropic exchange and $d_x = 0$, $h_y = 0$, Eq. (3.25) reduces to

$$\tilde{f} = k_B T \left[\frac{h}{2JS} + \ln\left[\frac{JS^2}{k_B T}\right] - 2\left[\frac{2}{\pi}\right]^{1/2} \frac{h}{JS} \left[\frac{E_{\text{sol}}}{k_B T}\right]^{1/2} e^{-E_{\text{sol}}/k_B T}\right] . \tag{3.26}$$

If we compare Eq. (3.26) with Eq. (3.18) (setting $E_0 = 0$), we note two differences. A trivial discrepancy exists between the arguments of the logarithms. This is due to the different phase space normalization employed in Ref. 2. A more subtle difference becomes evident when we recall that $\tilde{f}$ is the free-energy *per spin pair*, whereas f is the free-energy *per spin*. If $\tilde{f}$ is divided by two to give the free-energy per spin, we see that it is, apart from the logarithmic term, the result obtained via the first approach [Eq. (3.18)]. We should make one more logarithmic modification. In the second approach we singled out *one* of the two possible equilibrium configurations and considered excitations with respect to that configuration alone. The partition function should be doubled, and a term $-kT\ln 2$ added to the free energy.

We thus arrive at a result for the free-energy *per spin* in the *general case* at low temperatures

$$f = \tfrac{1}{4} k_B T m a + \tfrac{1}{4} k_B T \ln\left[\frac{j_+(j_+ + j_z + d_z)}{2(k_B T)^2}\right] - k_B T n_{\text{sol}}^{\text{tot}} \quad , \tag{3.27}$$

where the density of solitons plus antisolitons (per spin) is given by

$$n_{\text{sol}}^{\text{tot}} = ma \left[\frac{2}{\pi}\right]^{1/2} \left[\frac{E_{\text{sol}}}{k_B T}\right]^{1/2} e^{-E_{\text{sol}}/k_B T} \tag{3.28}$$

$$(k_B T << E_{\text{sol}}) \quad .$$

It should be noted that Eq. (3.27) for the free-energy density is valid only at temperatures low compared to the soliton activation energy, E_{sol}, (and high compared to the $k = 0$ spin-wave energy in order for quantum corrections[14,15] to be small) so that the soliton density is low. Indeed, Currie *et al.*[2] were able to show that in a phenomenology which regards the solitons as an "ideal gas," the precise form of the free energy could be reproduced, but only in the asymptotic low-temperature limit ($\hbar\omega << k_B T << E_{sol}$). Although the exact classical free energy is in principle obtainable at all temperatures via the transfer operator technique, there is as yet no comparison phenomenology for higher temperatures where, for example, "virial corrections" to the ideal-gas picture are expected to become important.

If one wishes to interpret experimental results, therefore, in terms of a soliton *ideal* gas, one must be sure that $k_B T$ is small compared to E_{sol}. This is particularly important for those planar antiferromagnets where the anisotropy in the easy plane is due solely to the applied magnetic field H (i.e., $J_x = J_y = J_z$, $D_y = 0$). Recall that in this case the antiferromagnetic (AF) soliton energy is $E_{sol}^{AF} = g\mu_B HS$, whereas the analogous soliton energy in planar *ferromagnets*[3,4,10] is $E_{sol}^{F} = 8\ (g\mu_B HJS^3)^{1/2}$. For a 5-kG field applied to the ferromagnet $CsNiF_3$ the soliton energy is[4] $E_{sol}^{F} \cong 34$ K, whereas a 5-kG field applied to the antiferromagnet TMMC[16] [$(CD_3)_4NMnCl_3$] yields a soliton energy of only $E_{sol}^{AF} \cong 1.7$ K. Thus, to be in a dilute gas situation in TMMC, one should use either higher fields or lower temperatures than for $CsNiF_3$.

We emphasize, however, that the low activation energy of the antiferromagnetic soliton, and particularly its linear (instead of square root) dependence on the applied field, can be regarded as an attractive feature in the sense that the antiferromagnetic chain systems could provide an ideal testing ground for future developments in the statistical mechanics of *non*ideal soliton gases, since the soliton density could be varied over a wide range using applied fields which are easily produced in the laboratory.

IV. DISCUSSION AND CONCLUSIONS

We have shown in Sec. II that under appropriate circumstances, the rather general Hamiltonian (2.1) and (2.2) of an antiferromagnetic linear chain, bilinear in the spin operators, can be reduced approximately to a simple sine-Gordon form [Eq. (2.15)]. We collect and reiterate here the conditions necessary for this to be a valid approximation and explore the utility of our approach to the particular quasi-one-dimensional antiferromagnet $(CD_3)_4NMnCl_3$, usually referred to as TMMC.

For the sine-Gordon equation both the spin-wave solutions of the linearized equation and the soliton solutions of the full nonlinear equation are well known. The soliton solutions, given in Eq. (2.24), have spatial logarithmic derivatives of order $m\gamma$. In order for the continuum approximation used in the derivation of the sine-Gordon equation to be valid, these logarithmic derivatives must be small compared to the inverse lattice constant: $am\gamma << 1$. But for the soliton velocity u sufficiently close to the characteristic velocity c [Eq. (2.17)] the factor γ becomes arbitrarily large, and the condition is violated as the soliton length Lorentz contracts to a size of the order of a single lattice spacing. In practice, at sufficiently low temperatures, there are statistically few solitons with $u \simeq c$, since their energies are proportional to $m\gamma$. Moreover, these solitons are expected to slow down as they interact with the discrete lattice and lose energy by radiation of spin waves. (However, their existence can have a significant effect, e.g., on the line shapes of neutron inelastic scattering experiments.[17])

Then the demand of gradual spatial variations on the scale of a few lattice constants requires that ma [or r; compare Eqs. (2.10) and (2.18)] must be small; this is, in fact, the single small parameter of the sine-Gordon theory, as discussed in detail in Sec. II. The need for a sufficiently easy plane further requires that $\tilde{j}_y - \tilde{j}_z$ and/or $\tilde{d}_z$ must not be smaller than order ma. In examining the applicability of the theory to a given material, we must be somewhat more careful, taking account of numerical factors in the equations, some as large as 8.

We turn next then, to an explicit discussion of the antiferromagnet TMMC, the most nearly magnetically one-dimensional of the multitude of magnetic linear-chain compounds known.[18] Furthermore, the large spin ($\frac{5}{2}$) of the magnetic ions, Mn^{++}, can be treated classically to a very good approximation. The effective magnetic interaction between these orbital S-state ions is well described by isotropic Heisenberg exchange; anisotropy is provided almost entirely by the magnetic dipole-dipole interactions. If the latter are truncated beyond the dominant nearest-neighbor interactions, then TMMC can be described by the Hamiltonian in Eqs. (2.1) and (2.2) with $J_x = J_y > J_z$ and $D_x = D_z = 0$. Such a model has proved highly successful in describing both static and dynamic properties[16] of TMMC. Although the anisotropy is small, $(J_y - J_z)/J_y \simeq 0.016$, the development of substantial short-range order with decreasing temperature amplifies its effectiveness, so that the behavior of TMMC turns from isotropic to planar (XY) in character.[16,19] Is it enough to lead to well-defined sine-Gordon solitons? Without loss of generality we can take the external field to be in the y direction. Then Eq. (2.28) gives $ma = g\mu_B H/JS$; for TMMC with $\mathcal{H} = 15$ kOe this gives $ma \simeq 0.1$. Equations (2.11) and (2.13) imply that δ_l and ϵ_l are of order ma, and from Eq. (2.7) we have

$$(\delta_l - \gamma_l) \simeq (ma)^2/4(j - j_z) \simeq 0.16 \ ,$$

so γ_l is also of order ma. For ϵ_l and δ_l, which by definition describe deviations from antiparallelism of adjacent spins, this result is hardly surprising (the canting is expected to be of order $g\mu_B H/JS = ma$). But γ_l describes motion out of the easy plane; it is small not because of the small anisotropy energy of a single spin, but because one must simultaneously tip out of the plane about the number of spins needed to form a soliton—which is of length $\sim m^{-1}$, so the number of spins is of order $(ma)^{-1}$. Then, since ma is linear in the field, at low temperature (well developed short-range order) we expect our theory to be applicable to TMMC for external fields less than a few tens of kilo-oersteds.

There remains the question of the existence of a suitable range of temperature—on the one hand above the three-dimensional antiferromagnetic ordering temperature[20] of about 1 K, where the starting linear-chain Hamiltonian ceases to be applicable, and on the other hand low enough so that the soliton density is sufficiently low to form an approximately ideal gas. The latter demand requires $T << g\mu_B HS/k_B$; for TMMC the right-hand side is approximately 10 K for $H = 25$ kOe. Thus there is a limited accessible range of temperature and magnetic field (approximately 1 K < T < 4 K for $H \sim 20$ kOe) where we would expect to find simple independent soliton behavior at TMMC. At lower fields we would expect to be able to study the effects of soliton interactions as their density increases (while the temperature is still low enough—below 10 K—for the planar anisotropy to be well developed).

Perhaps the most obvious place to look for experimental evidence of solitons in linear-chain antiferromagnets is in the neutron scattering cross section. This was where the corresponding ferromagnetic phenomenon was first experimentally observed,[4] and we have recently become aware of some as yet unpublished results[21] of Boucher *et al.* in TMMC. The model developed here can readily be used to calculate dynamical correlation functions (as Mikeska has done[3] for the ferromagnet) appropriate to the neutron scattering cross sections, at least in the ideal-soliton-gas limit. We also intend to examine the light scattering by spin fluctuations associated with these solitons, an approach which appears promising in the ferromagnetic case,[22] and the solitons may manifest themselves in magnetic resonance phenomena. Finally, we mention our interest in extending these results from the classical spin to the quantum mechanical regime, which is presumably essential in describing spin-$\frac{1}{2}$ linear-chain magnets.

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[1]J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B 11, 3535 (1975).

[2]An extensive discussion of these theories has been presented by J. F. Currie, J. A. Krumhansl, A. R. Bishop, and S. E. Trullinger (unpublished).

[3]H. J. Mikeska, J. Phys. C 11, L29 (1978).

[4]J. K. Kjems and M. Steiner, Phys. Rev. Lett. 41, 1137 (1978).

[5]D. L. Mills, Phys. Rev. Lett. 20, 18 (1968); F. Keffer and H. Chow, Phys. Rev. Lett. 31, 1061 (1973), S. P. Vernon, R. W. Sanders, and A. R. King, Phys. Rev. B 17, 1460 (1978).

[6]A. R. King and D. Paquette, Phys. Rev. Lett. 30, 662 (1973).

[7]H. J. Mikeska (unpublished).

[8]C. Kittel, *Introduction to Solid State Physics*, 5th ed. (Wiley, New York, 1976), p. 488.

[9]W. P. Su, J. R. Schrieffer, and A.J. Heeger, Phys. Rev. Lett. 42, 1698 (1979).

[10]P. S. Riseborough and S. E. Trullinger (unpublished).

[11]M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (U.S. Department of Commerce, Washington, D.C., 1970).

[12]D. J. Scalapino, M. Sears, and R. A. Ferrell, Phys. Rev. B 6, 3409 (1972).

[13]A. Patkos and P. Rujan, Z. Phys. B 33, 163 (1979).

[14]S. E. Trullinger, Solid State Commun. 29, 27 (1979).

[15]K. Maki and H. Takayama, Phys. Rev. B (in press).

[16]L. R. Walker, R. E. Dietz, K. Andres, and S. Darack, Solid State Commun. 11, 593 (1972); D. Hone and A. Pires, Phys. Rev. B 15, 323 (1977).

[17]K. M. Leung and D. L. Huber, Solid State Commun. 32, 127 (1979).

[18]L. J. de Jongh and A. R. Miedema, Adv. Phys. 23, 1 (1974); D. Hone and P. M. Richards, Ann. Rev. Mater. Sci. 4, 337 (1974); M. Steiner, J. Villain, and C. G. Windsor, Adv. Phys. 25, 87 (1976).

[19]J. P., Boucher, L. P. Regnault, J. Rossat-Mignod, J. Villain, and J. P. Renard, Solid State Commun. 31, 311 (1979).

[20]The Néel temperature is remarkably dependent on applied magnetic field in the easy plane: $T_N = 0.85$ K at $H = 0$ and $T_N \simeq 2$ K at $H = 40$ kOe. See F. Borsa, J. P. Boucher, and J. Villain, J. Appl. Phys. 49, 1326 (1978).

[21]J. P. Boucher *et al.*, Solid State Commun. (to be published).

[22]D. L. Mills, P. S. Riseborough, and S. E. Trullinger (unpublished).