Soliton energy in an easy-plane quantum spin chain

H. J. Mikeska
Department of Applied Physics, Stanford University, Stanford, California 94305
and Institut für Theoretische Physik, Universität Hannover, West Germany*
(Received 24 February 1982)

We investigate the quantum corrections to the energy of the static soliton in the XY-like ferromagnetic spin chain in a symmetry-breaking external field. We apply a semiclassical continuum approximation which allows us to treat the leading-order deviations from idealized planar behavior. The equivalent quantum-field theory, an extension of the quantum sine-Gordon theory, is renormalized and its soliton energy is shown to depend strongly on this deviation. The quantum-field-theoretical renormalization, however, does not affect the energy of the magnetic soliton, which is calculated to leading order in $1/S$, where S is the spin length. The sine-Gordon limit is found applicable only for very large anisotropies; for realistic anisotropies, the reduction of the soliton energy owing to quantum effects is enhanced and depends only on S. A quantitative calculation for the $S=1$ system $CsNiF_3$ is likely to require higher-order terms in $1/S$.

I. INTRODUCTION

Recently much interest has been devoted to the nonlinear soliton mode of the one-dimensional magnetic system given by the Hamiltonian

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

characterized by an exchange energy $J>0$, a single-ion anisotropy $A>0$, and a magnetic moment $\mu=\mu_B g$. Nonlinear modes of the Hamiltonian (1.1) were originally investigated by applying the classical continuum approximation and assuming very strong xy anisotropy. Under these assumptions the system described by Eq. (1.1) can be mapped[1] to the classical sine-Gordon (SG) chain (a mapping which becomes exact for $A\rightarrow\infty$). The Hamiltonian (1.1) therefore exhibits the well-known nonlinear soliton modes of the SG theory.[2] The implications of this observation have been tested in several investigations, both experimental[3] and by computer simulations.[4,5] From these investigations increasing, although not completely undisputed, evidence has emerged for the importance of the soliton mode in the dynamics of $CsNiF_3$, an $S=1$ magnetic chain compound, which is widely believed to be described by the above Hamiltonian.

In the present paper we will study the quantum aspects of the excitation energy of the soliton mode. The validity of the classical approximation to the Hamiltonian (1.1) has previously been studied qualitatively[6,7] with the result that it requires

$$\frac{1}{2\pi S}\left[\frac{2A}{J}\right]^{1/2}\ll 1\;, \tag{1.2}$$

a condition which is quite well satisfied in $CsNiF_3$. A more quantitative investigation of quantum effects was performed by Maki,[8] using a mapping of the Hamiltonian (1.1) to the quantum SG chain. This field-theory model was then treated in the semiclassical approach of Dashen, Hasslacher, and Neveu[9] (referred to as DHN in the following). The resulting renormalization of the soliton energy of about 20% appeared to be in agreement with experimental findings.

In the following we will investigate quantum effects in the semiclassical approximation including, in addition to the SG approximation, effects from the out-of-plane degree of freedom S^z to lowest order in J/A. At first sight, this seems to be a small correction to the SG approximation; however, there exists a qualitative difference to the SG approach: The quantum correction to the soliton energy as given by DHN for the SG theory[3] is the result of two contributions—the change in the energy of zero-point vibrations between the ground state and the one-soliton state, and the contribution from normal ordering (which is necessary to render the field theory finite). Both contributions are ultraviolet divergent, but the divergences cancel, leaving a finite quantum correction. The ultraviolet behavior, however, is very different for the magnetic chain system and its SG analog: In the continuum limit the frequencies of small vibrations

$\omega(q)$ for large wave vectors q are the following[1]:

$$\omega(q) \sim q \; , \qquad \omega(q) \sim q^2 \; , \tag{1.3}$$

for the SG chain and the planar magnetic chain, respectively. It is the purpose of the present paper to investigate the consequences of this difference for the soliton energy in the realistic magnetic chain with $S=1$; in the course of this work we must also discuss the relevance of the mapping to a continuous field theory for the nonlinear excitations of the Hamiltonian (1.1). In Sec. II, we will apply a semiclassical continuum approximation to Eq. (1.1), which allows us to include the derivations from the idealized planar behavior to leading order in J/A. The resulting Hamiltonian density suggests the structure of an equivalent quantum field theory, which will be studied in Sec. III. We will show that the quantum corrections to the static soliton energy depend strongly on the parameter measuring the strength of the out-of-plane fluctuations in the magnetic analog. In Sec. IV we will make the connection between the magnetic and the field-theory problems. We find that the process of renormalization, which is essential for the continuous field theory, is not relevant for the treatment of the magnetic Hamiltonian (1.1). We will calculate the quantum corrections to the magnetic soliton energy and discuss the application of our results to $CsNiF_3$. A short summary will be given in Sec. V.

II. THE MAGNETIC-CHAIN HAMILTONIAN IN SEMICLASSICAL FORMULATION

In this section we will derive the semiclassical continuum representation of the Hamiltonian (1.1) for large values of the anisotropy energy A. Owing to the easy plane symmetry induced by $A>0$ it is natural to make use of the planar representation of spin operators as introduced by Villain[10]:

$$s_n^+ = e^{i\varphi_n}[1-(s_n^z)^2 - s_n^z/\hat{S}]^{1/2} \; , \tag{2.1}$$

with

$$s_n^\alpha = S_n^\alpha / \hbar \hat{S} \; , \qquad \hat{S}^2 = S(S+1) \; , \qquad [\varphi_m, s_n^z] = \frac{i}{\hat{S}} \delta_{nm} \; . \tag{2.2}$$

We have introduced the operators φ and s^z since in the classical limit they become the quantities φ and $\cos\theta$, which are generally used in a polar-coordinate representation of the classical spin vector. In a formulation starting with Eqs. (2.1) and (2.2), quantum-mechanical corrections arise naturally as an expansion in $1/\hat{S}$. We will now make use of the following approximations to simplify the Hamiltonian (1.1):

(i) the continuum approximation, i.e., expanding in the lattice constant a and keeping only terms which survive the limit $a \to 0$,

(ii) the xy approximation, i.e., expanding in s_n^z and keeping only terms up to second order,

(iii) the semiclassical approximation, i.e., expanding in $\hat{S}^{-1}$ and keeping terms up to second order.

These approximations transform Eqs. (1.1) and (2.2) into ($\hbar$ and a will be set equal to 1 in the following)

$$H = \text{const} + J\hat{S}^2 \int dx \left[\frac{1}{2} \left(\frac{\partial \varphi}{\partial x} \right)^2 + \frac{A}{J}(s^z)^2 - \frac{\mu B}{J\hat{S}} \cos\varphi + \frac{1}{2} \left(\frac{\partial s^z}{\partial x} \right)^2 - \tfrac{1}{2} s^z \left(\frac{\partial \varphi}{\partial x} \right)^2 s^z + \frac{1}{2} \frac{\mu B}{J\hat{S}} s^z \cos\varphi s^z \right] \; , \tag{2.3}$$

$$[\varphi(x), s^z(x')] = \frac{i}{\hat{S}} \delta(x-x') \; . \tag{2.4}$$

In carrying through the semiclassical approximation, all terms in Eq. (2.3) appear multiplied by expressions of the type $1+O(\hat{S}^{-2})$; these corrections, however, must be neglected since they depend on the order of operators in neglected higher-order terms. On the other hand, the occurrence of $\hat{S}$ instead of S in Eqs. (2.3) and (2.4) is significant to the order considered.

It is instructive to illustrate the occurrence of $\hat{S}$ by the following simple example: Consider only the single-particle Zeeman term in Eq. (1.1), $-\mu BS^x$, which evidently has the value in the ground state of $-\mu BS$. However, if we treat this term using Eqs. (2.1) and (2.2) we obtain

$$-\mu B\hat{S}(\cos\varphi-\tfrac{1}{2}s^z\cos\varphi s^z+\cdots),$$

which, to second order in Φ and s^z, is easily diagonalized to give the ground-state energy $-\mu B\hat{S}[1-1/(2\hat{S})+\cdots]$. This agrees with the exact result to $O(S^{-2})$, and higher-order terms will be needed to recover the exact result. This example demonstrates that the occurrence of $\hat{S}$ in Eq. (2.3) is directly connected to the quantum corrections which appear as an expansion in $1/\hat{S}$.

If we consider the limit $A\rightarrow\infty$ in Eq. (2.3) and rescale s^z by $\pi A/J$, we notice that the last three terms in this equation become of order J/A. Thus these terms describe the deviation from ideal planar behavior. In previous treatments[8] along these lines these terms have been neglected. Then the Hamiltonian (2.3) can be transformed to the SG representation,

$$H=\text{const}+J\hat{S}^2g^2\int dx\left[\frac{1}{2}\left[\frac{\partial\Phi}{\partial x}\right]^2+\frac{1}{2}\pi^2-\frac{\mu B}{J\hat{S}}\frac{1}{g^2}\cos g\Phi\right], \quad (2.5)$$

$$[\Phi(x),\pi(x')]=i\delta(x-x'), \quad (2.6)$$

by the transformation

$$\varphi=g\Phi,\;\; s^z=g\left[\frac{J}{2A}\right]^{1/2}\pi, \quad (2.7)$$

$$g^2=\left[\frac{2A}{J\hat{S}^2}\right]^{1/2}. \quad (2.8)$$

Our aim is to perform and to discuss the analogous transformation for the full Hamiltonian (2.3). Before approaching this transformation in Sec. IV, we want to investigate in the next section the field-theory analog of Eq. (2.3) without referring to the magnetic chain.

III. A SINE-GORDON–LIKE FIELD THEORY

The results of the preceding section suggest that the quantum magnetic chain is related to the following field theory:

$$H=E_0g^2\int dx\left\{\frac{1}{2}\left[\frac{\partial\Phi}{\partial x}\right]^2+\frac{1}{2}\pi^2-\frac{m^2}{g^2}\cos g\Phi+\gamma\left[\frac{1}{2}\left[\frac{\partial\pi}{\partial x}\right]^2-\frac{1}{2}g^2\pi\left[\frac{\partial\Phi}{\partial x}\right]^2\pi+\frac{1}{2}m^2\pi(\cos g\Phi)\pi\right]\right\}, \quad (3.1)$$

$$[\Phi(x),\pi(x')]=i\delta(x-x'). \quad (3.2)$$

For the moment we consider E_0, m^2, γ, and g^2 as parameters of the field theory; their relation to the parameters of the quantum magnetic chain will be discussed later. We will investigate the energy of the static soliton solution to Eq. (3.1) for small values of γ, i.e., for small deviations from the SG theory, which is exact for $\gamma=0$. We will do so following the Wentzel-Kramers-Brillouin (WKB) treatment of DHN (Ref. 9) for the SG system, thus restricting the calculation to the weak-coupling limit $g^2\ll 1$. This WKB theory of DHN is based on the use of exactly known classical solutions for the nonlinear excitations of interest. Fortunately, the static classical SG soliton continues to be an exact solution to the classical equations of motion which follow from Eqs. (3.1) and (3.2) for arbitrary values of γ:

$$\frac{\partial\Phi}{\partial t}=\pi-\gamma\left[\frac{\partial^2\pi}{\partial x^2}+g^2\left[\frac{\partial\Phi}{\partial x}\right]^2\pi-m^2(\cos g\Phi)\pi\right], \quad (3.3)$$

$$\frac{\partial\pi}{\partial t}=\frac{\partial^2\Phi}{\partial x^2}-\frac{m^2}{g}\sin g\Phi-\gamma\left[g^2\pi^2\frac{\partial^2\Phi}{\partial x^2}+2g^2\pi\frac{\partial\pi}{\partial x}\frac{\partial\Phi}{\partial x}-\frac{1}{2}m^2\pi^2g\sin g\Phi\right]. \quad (3.4)$$

Here inverse time is measured in units of E_0g^2. An exact static solution of the soliton type to these equations is

$$\Phi_S=\frac{4}{g}\arctan e^{mx}, \quad (3.5)$$

$$\pi_S=0, \quad (3.6)$$

$$E_S^{\text{cl}}=8mE_0. \quad (3.7)$$

In the following we will restrict ourselves to considering the static soliton. Additional approximations would be required to treat a moving soliton, but no drastic changes are expected for a slowly moving soliton.

Following DHN the soliton energy in the semiclassical approximation can be written in the following way:

$$E_S = E_S^{\rm cl} + \delta E_{\rm zp} + \delta E_{\rm no} \; . \tag{3.8}$$

Here,

$$\delta E_{\rm zp} = \tfrac{1}{2} \sum_q (\omega_q - \omega_q^{(0)}) \tag{3.9}$$

is the difference in zero-point (zp) fluctuations in the one-soliton state (frequencies ω_q of small vibrations) and in the ground state (frequencies $\omega_q^{(0)}$). $\delta E_{\rm no}$ is the energy difference owing to normal ordering (no) of the Hamiltonian (3.1), which is necessary to avoid ultraviolet divergences from closed-loop (cl) integrations. In the SG theory, both $\delta E_{\rm zp}$ and $\delta E_{\rm no}$ diverge logarithmically with an ultraviolet cutoff Λ, but these divergences cancel leaving the finite result,

$$E_S = E_S^{\rm cl} \left[1 - \frac{g^2}{8\pi} \right] . \tag{3.10}$$

To carry through this program for the field theory (3.1), we renormalize H by normal ordering which to lowest order in g^2 leads to

$$\begin{aligned} N(H) = E_0 g^2 \int dx \Bigg\{ & \frac{1}{2}(1+\gamma g^2\langle \pi^2\rangle) \left[\frac{\partial\Phi}{\partial x}\right]^2 + \frac{1}{2}\left[1+\gamma g^2 \left\langle \left[\frac{\partial\Phi}{\partial x}\right]^2 \right\rangle \pi^2 \right] \\ & - \frac{m^2}{g^2}(1+\tfrac{1}{2}g^2\langle\Phi^2\rangle + \tfrac{1}{2}g^2\gamma\langle\pi^2\rangle)\cos g\Phi \\ & + \gamma \left[\frac{1}{2}\left[\frac{\partial\pi}{\partial x}\right]^2 - \frac{1}{2}g^2\pi \left[\frac{\partial\Phi}{\partial x}\right]^2 \pi + \frac{1}{2}m^2(1+\tfrac{1}{2}g^2\langle\Phi^2\rangle)\pi\cos g\Phi\pi \right] \Bigg\} . \end{aligned} \tag{3.11}$$

One readily convinces oneself that with these choices of renormalizing factors all one-loop divergences cancel. The additional soliton energy owing to normal ordering is obtained by inserting the classical solution (3.5) and (3.6) into $N(H)-H$, subtracting the ground-state contribution and integrating over all space:

$$\begin{aligned} \delta E_{\rm no} &= E_0 g^2 \left[m^2(\tfrac{1}{2}\langle\Phi^2\rangle + \tfrac{1}{2}\gamma\langle\pi^2\rangle) \int dx (1-\cos g\Phi_S) + \tfrac{1}{2}\gamma\langle\pi^2\rangle \int dx \left[\frac{\partial g\Phi_S}{\partial x}\right]^2 \right] \\ &= 8mE_0 g^2(\tfrac{1}{4}\langle\Phi^2\rangle + \tfrac{3}{4}\gamma\langle\pi^2\rangle) \; . \end{aligned} \tag{3.12}$$

The ground-state expectation values in (3.11) and (3.12) are calculated from the noninteracting part of H as (L is the length of the system)

$$\langle\Phi^2\rangle = \frac{1}{2L}\sum_q 1/\alpha_q \; , \tag{3.13}$$

$$\langle\pi^2\rangle = \frac{1}{2L}\sum_q \alpha_q \; , \tag{3.14}$$

where

$$\alpha_q = \left[\frac{q^2+m^2}{\gamma(q^2+m^2)+1} \right]^{1/2} . \tag{3.15}$$

Thus both $\langle\Phi^2\rangle$ and $\langle\pi^2\rangle$ diverge linearly with the ultraviolet cut-off momentum Λ, and the divergence of $\delta E_{\rm no}$ with Λ is seen to be

$$\delta E_{\rm no} \sim \frac{4m}{\pi} E_0 g^2 \sqrt{\gamma}\Lambda \; . \tag{3.16}$$

In the SG theory, on the other hand, one had to deal only with $\langle\Phi^2\rangle$, which in that case diverges proportional to $\ln\Lambda$.

In order to calculate the contribution $\delta E_{\rm zp}$ to the soliton energy (3.8), we have to find the frequencies of small oscillations $\omega_q^{(0)}$ and ω_q as well as the discrete values of q to be used in the summation in Eq. (3.9). The latter are determined by the asymptotic phase shifts of these phononlike modes. Linearizing Eqs. (3.3) and (3.4) in Φ and π (corresponding to considering small vibrations based on the ground-state configuration) leads to the well-known spin-wave spectrum,

$$\omega_q^{(0)} = E_0 g^2 \sqrt{\gamma} \, [(q^2+m^2)(q^2+m^2+\gamma^{-1})]^{1/2} \; . \tag{3.17}$$

In order to discuss small vibrations based on the one-soliton configuration we linearize Eqs. (3.3) and (3.4) in $\Phi-\Phi_s=\phi$ and π to obtain

$$\frac{\partial\varphi}{\partial t}=\pi-\gamma\left[\frac{\partial^2\pi}{\partial x^2}-m^2(1-6\,\mathrm{sech}^2 mx)\pi\right], \tag{3.18}$$

$$\frac{\partial\pi}{\partial t}=\frac{\partial^2\varphi}{\partial x^2}-m^2(1-2\,\mathrm{sech}^2 mx)\varphi . \tag{3.19}$$

For $\gamma=0$ these equations simplify to the equations of motion for small vibrations in the presence of a SG soliton, which have been solved by Rubinstein[11] with the following results: There exists a bound state with zero frequency, related to translational invariance in the usual way; the remaining states are continuum states with frequencies $\omega_q=\omega_q^{(0)}$ and an asymptotic phase shift

$$\varphi_{\mathrm{SG}}(q)=2\arctan m/q . \tag{3.20}$$

The problem of solving Eqs. (3.18) and (3.19) for finite but small values of γ is treated in the Appendix. The following results are obtained: In addition to the zero-frequency bound state there exists a bound state with frequency

$$\omega_b=\omega_{q=0}^{(0)}(1-\tfrac{8}{9}m^4\gamma^2+\cdots), \tag{3.21}$$

for any $\gamma>0$. The remaining states are continuum states with frequencies $\omega_q^{(0)}$ and an asymptotic phase shift

$$\varphi(Q)=2\arctan 1/Q+\arctan(\alpha-\beta)+\arctan(\alpha+\beta),$$

$$\alpha(Q)=\frac{Q^2+1}{2(Q^2+1)+b^{-1}}\frac{2}{3Q}\left[1+\frac{2Q^2}{1+Q^2}\right], \tag{3.22}$$

$$\beta(Q)=\frac{Q^2+1}{2(Q^2+1)+b^{-1}}\frac{2}{3Q}\frac{\pi Q}{\sinh\pi Q},$$

with

$$Q=q/m,$$

$$b=m^2\gamma .$$

From the knowledge of the phase shifts the contribution of zero-point fluctuations to the soliton energy (3.8) is calculated to be

$$\delta E_{\mathrm{zp}}=-\tfrac{1}{2}\omega_{q=0}^{(0)}+\tfrac{1}{2}(\omega_b-\omega_{q=0}^{(0)})-\frac{1}{2\pi}\int_0^\Lambda dq\,\varphi(q)\frac{d\omega_q^{(0)}}{dq} . \tag{3.23}$$

The divergence with Λ is determined by the behavior for large q of $\varphi(q)\approx 4m/q$ and $d\omega_q^{(0)}/dq\approx E_0g^2\sqrt{\gamma}2q$ and the resulting divergent contribution to δE_{zp} is seen to cancel exactly the divergent term (3.16) in δE_{no}. The remaining corrections are finite and after some rearrangement one obtains

$$\begin{aligned}\delta E_{\mathrm{zp}}+\delta E_{\mathrm{no}}&=\tfrac{1}{2}\omega_b+E_0g^2m\sqrt{b}\\&\quad\times\left\{-\tfrac{1}{4}(1+b^{-1})^{1/2}+\frac{2}{\pi}\int_0^\infty dx\left[\left(\frac{(x^2+1)}{(x^2+1+b^{-1})}\right)^{1/2}-1\right]\right.\\&\quad\left.+\frac{1}{2\pi}\int_0^\infty dx[(1+x^2)(1+x^2+b^{-1})]^{1/2}\left[\frac{d\varphi}{dx}+\frac{2}{x^2+1}+\frac{2}{x^2+1+b^{-1}}\right]\right\}\\&=-8mE_0\frac{g^2}{8\pi}F(b) .\end{aligned} \tag{3.24}$$

Thus the weak-coupling result for the soliton energy is

$$E_S=E_S^{\mathrm{cl}}\left[1-\frac{g^2}{8\pi}F(b)\right]. \tag{3.25}$$

In the limit $b\sim\gamma\to 0$ one can show $F(b)\to 1$. This means that the SG limit is correctly included in the above calculation. For finite b, $F(b)$ has been evaluated numerically and the result is given in Fig. 1. It is obvious that the magnitude of the quantum corrections depends strongly on the value of b. Even for rather small values of this parameter the quantum corrections are considerably suppressed and the soliton energy approaches the classical limit. Since we have obtained our results by expanding in γ we can trust them only for small values of this parameter. The negative values of $F(b)$ in Fig. 1 are probably due to this approximation.

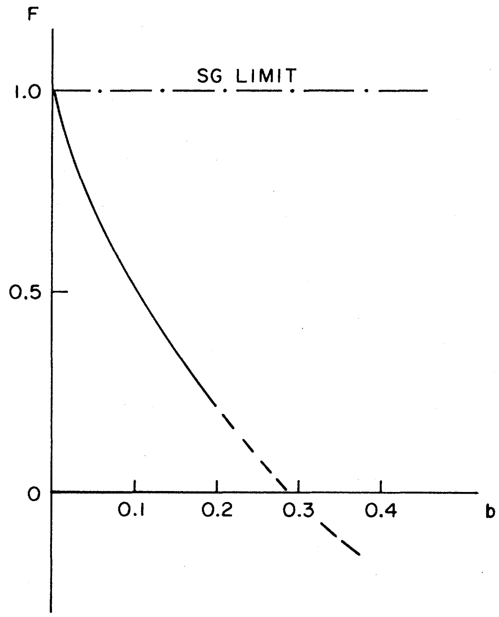

FIG. 1. Relative magnitude of the quantum correction to the soliton energy for the field theory (3.1) for $b=\gamma m^2 \ll 1$.

IV. SOLITON ENERGY IN THE MAGNETIC QUANTUM SYSTEM

We will now make use of the results obtained in the preceding two sections to investigate quantum corrections to the soliton energy for the magnetic quantum chain (1.1). For this purpose we have to establish the relation between the magnetic chain parameters J, A, B, and S and the parameters of the field theory E_0, γ, m^2, and g^2. It is important to note that the magnetic Hamiltonian (1.1) is defined on a discrete lattice. Its continuum version (2.3) therefore has a natural momentum cutoff $\Lambda=\pi/a$. Thus the magnetic Hamiltonian should be mapped to a field theory with a cutoff π/a imposed and both the original form (3.1) and the renormalized form (3.11) can be used, giving identical results for the soliton energy. We prefer to discuss the mapping to the renormalized field theory since it parallels previous treatments.[8]

Mapping Eqs. (2.3) to (3.11) and requiring the commutator (3.2) to be fulfilled by the ansatz

$$\varphi=g\Phi , \tag{4.1}$$

$$s^z=\frac{1}{g\hat{S}}\pi , \tag{4.2}$$

we obtain to leading order

$$E_0=J\hat{S}^2(1-\gamma g^2\langle\pi^2\rangle) , \tag{4.3}$$

$$m^2=\frac{\mu B}{J\hat{S}}(1+\tfrac{1}{2}\gamma g^2\langle\pi^2\rangle-\tfrac{1}{2}g^2\langle\Phi^2\rangle) , \tag{4.4}$$

$$\gamma=\frac{J}{2A} , \tag{4.5}$$

$$g^2=\frac{1}{\hat{S}}\left[\frac{2A}{J}\right]^{1/2} . \tag{4.6}$$

Let us first make use of these results to discuss the limits of validity of our approximations. Actually one discovers a dilemma when one combines the condition for the semiclassical approximation $g^2 \ll 1$ with the condition for planar behavior $\gamma \ll 1$ to obtain

$$\frac{1}{\hat{S}^2} \ll \frac{J}{2A} \ll 1 . \tag{4.7}$$

This means that one would have to resort to the use of unphysically large values of A/J and S to justify the approximations used. The real situation, however, may be more favorable, since previous work[6,7] has suggested that $g^2/2\pi \ll 1$ is a more quantitative condition for semiclassical behavior; likewise, the success of the XY approximation for $CsNiF_3$, where $J/2A \approx 2$, suggests that the condition $\gamma \ll 1$ is too stringent.

Using the above results in Eq. (3.8) we obtain

$$E_S=E_S^{(0)}(1-\tfrac{1}{4}g^2\langle\Phi^2\rangle-\tfrac{3}{4}\gamma g^2\langle\pi^2\rangle) + \delta E_{\text{zp}}+\delta E_{\text{no}} , \tag{4.8}$$

$$E_S^{(0)}=8(\mu B\hat{S}J\hat{S}^2)^{1/2} . \tag{4.9}$$

In the SG limit $\gamma=0$ Eq. (4.8) can be written in the following form [with the use of Eq. (3.24)]:

$$E_S=E_S^{(0)}(1-\tfrac{1}{4}g^2\langle\Phi^2\rangle)\left[1-\frac{g^2}{8\pi}\right] . \tag{4.10}$$

This is equivalent to the statement[8] that the renormalized mass[12]

$$m=m_0\exp(-\tfrac{1}{4}g^2\langle\Phi^2\rangle) , \quad m_0=(\mu B/J\hat{S})^{1/2} , \tag{4.11}$$

must be used (to order g^2) in the calculation of the magnetic soliton energy. The determination of m, of course, requires making use of the discrete lattice cutoff.

However, with the use of Eq. (3.12) in (4.8) it becomes obvious that δE_{no} and the corrections to

$E_S^{(0)}$ cancel exactly, leaving δE_{zp} as the only contribution. The same result would have been obtained simply by mapping Eq. (2.3) directly to the field theory (3.1): The correction terms to $E_S^{(0)}$ and from normal ordering then would not occur, leaving again δE_{zp} as the only quantum correction. The discrete lattice cutoff is again required for the determination of δE_{zp}.

Using the results given in the preceding section, we obtain

$$E_S = E_S^{(0)} + \delta E_{\text{zp}}$$
$$= E_S^{(0)} \left[1 - \frac{g^2}{16\pi}\sqrt{b} \int_0^{\pi/m} dx\, \varphi(x) \frac{d}{dx}[(x^2+1)(x^2+1+b^{-1})]^{1/2} - \frac{g^2}{16}(1+b)^{1/2} \left[1 + \frac{8}{9}b^2 \right] \right] . \quad (4.12)$$

We discuss this expression for large values of the cutoff $\Lambda_0 = \pi/m$ and note that E_S depends strongly on the quantity $b\Lambda_0^2 = \pi^2\gamma$. In the two limiting cases we obtain ($\pi^2\gamma \ll 1$ being the SG limit)

$$E_S = E_S^{(0)} \left[1 - \frac{g^2}{8\pi} \left[\frac{\pi}{2} + \ln\frac{2\pi}{m} \right] \right], \quad \pi^2\gamma \ll 1 \quad (4.13)$$

$$E_S = E_S^{(0)} \left[1 - \frac{g^2}{8\pi} \left[\frac{\pi}{2} + 4\pi\sqrt{\gamma} \right] \right], \quad \pi^2\gamma \gg 1 . \quad (4.14)$$

In this limit the quantum correction to the soliton energy no longer depends on the magnetic field as it does strongly in the SG limit.

A numerical evaluation of Eq. (4.12) for $m = 0.185$ shows that the approximation given in Eq. (4.14) is accurate within a few percent down to $\gamma\pi^2 \approx 1$. For smaller values of $\gamma\pi^2$ the factor of $g^2/8\pi$ gradually settles down to the limiting value given in Eq. (4.13). Numerical evaluation also confirms the statement that for $\gamma\pi^2 \gg 1$ the factor multiplying g^2 in Eq. (4.12) is practically independent of m. Since the value of $\gamma\pi^2$ of acutal interest for a material as $CsNiF_3$ is of the order of 20, Eq. (4.14) is sufficient for all practical purposes, whereas the SG limit (4.13) is of no quantitative value.

For large values of $\gamma\pi^2$ we may actually neglect $\pi/2$ as compared to $4\pi\sqrt{\gamma}$ in Eq. (4.14); with the use of Eqs. (4.5) and (4.6) we thus obtain

$$E_S = E_S^{(0)} \left[1 - \frac{1}{2\hat{S}} + O(\hat{S}^{-2}) \right] . \quad (4.15)$$

In order to identify the quantum correction completely we note that the "classical" soliton energy used in previous approaches[1] is $8(JS^2\mu BS)^{1/2}$. Since, however, in the classical approach the value of the product JS is found from the magnon spectrum, which, according to Eq. (3.17), determines the value of $J\hat{S}$, we have to identify

$$8S(J\hat{S}\mu B)^{1/2} = E_{S,\text{cl}}^{(0)} \quad (4.16)$$

with the soliton energy used in classical theories. Thus we obtain the final result

$$E_S = E_{S,\text{cl}}^{(0)} \frac{1}{S} [\hat{S} - \tfrac{1}{2} + O(1/\hat{S})] . \quad (4.17)$$

Thus, for $S=1$, the soliton energy is about 10% smaller than $E_{S,\text{cl}}^{(0)}$ owing to quantum effects. This, however, cannot be considered a quantitative result for the quantum soliton energy for the following reasons:

(i) The calculation of vibration frequencies and phase shifts has been done in the continuum approximation. Taking into account the discrete lattice will lower the frequencies and probably the quantum correction to the energy as well.

(ii) To the order in the expansion in $1/\hat{S}$ considered here, we find rather substantial corrections. This leads one to guess that higher orders will probably contribute significantly as well.

In spite of these deficiencies we want to emphasize that Eq. (4.17) is the beginning of a consistent expansion. Our approach is actually rather similar to the approximate calculation of the ground-state energy of the linear Heisenberg antiferromagnet with arbitrary spin S.[13] Considering the remarkable success of the expansion in $1/\hat{S}$ in this example and in other previous applications,[6,10] the theory presented here should at least be taken as a qualitatively meaningful first approach to the quantum aspects of the magnetic soliton energy.

V. SUMMARY

We have shown that the quantum correction to the energy of the nonlinear soliton mode for the magnetic chain Hamiltonian (1.1) is given (apart from having to use $[S(S+1)]^{1/2}$ instead of S) to order $1/S$ by the finite sum of differences in zero-point vibration energies. We have verified that the renormalization of the equivalent continuous SG chain (or of a more complicated field theory which takes the out-of-plane degrees of the magnet into account) has no relevance for the magnetic system. This could, of course, have been realized from the outset, since the Hamiltonian (1.1) is well defined owing to the discrete lattice. Nevertheless, we find the method which uses the field-theory approach, given in Sec. III, useful in describing the relation of the magnetic chain Hamiltonian to field-theory models and in clarifying the relation to previous approaches.

Our final result, Eq. (4.17), gives a soliton energy, which for the $S=1$ magnetic chain system $CsNiF_3$ is about 10% below the classical value. Although this is not too far from the experimentally observed[3] difference of about 20% it should not be taken too seriously. Both the use of a continuum model to calculate the vibration frequencies as well as the restriction to the first term of the semiclassical approximation will very probably be sources of errors of the same order of magnitude as the correction obtained here. Thus a quantitative calculation of the energy of the quantum soliton in the $S=1$ magnetic chain considered in this paper remains a challenge for future work.

ACKNOWLEDGMENTS

I wish to thank Dr. K. Maki for a useful discussion and Dr. D. Browne for a critical reading of the manuscript. The hospitality of Dr. S. Doniach and the Department of Applied Physics at Stanford University and financial support from the Bundesministerium für Forschung und Technologie and from the Fulbright Commission is gratefully acknowledged.

APPENDIX

Here we shall discuss the coupled linear eigenvalue problem defined by Eqs. (3.18) and (3.19). We start by rewriting these equations by replacing π with the angular variable (the "out-of-plane" angle) $\theta=\sqrt{\gamma}\pi$ and by introducing the dimensionless space variable $z=mx$ as well as a harmonic time dependence with frequency Ω:

$$-i\Omega\vartheta=\varphi''-(1-2\,\mathrm{sech}^2 z)\varphi\ , \tag{A1}$$

$$i\Omega\varphi=-b^{-1}\vartheta+\vartheta''-(1-6\,\mathrm{sech}^2 z)\vartheta\ . \tag{A2}$$

Ω is the frequency in units of $E_0 g^2\sqrt{\gamma}m^2$ and b has been defined in Eq. (3.22). Equations (A1) and (A2) have the form of coupled Schrödinger equations with $1-2\,\mathrm{sech}^2 z$ and $1-6\,\mathrm{sech}^2 z$ playing the role of an attractive potential. We want to find the eigenfrequencies both in the continuum and of possible bound state and the phase shifts of the continuum states.

In order to calculate the phase shift we have to consider the behavior of the solutions of Eqs. (A1) and (A2) at $z\to\pm\infty$. In these limits we have plane waves, $\phi\sim\theta\sim e^{iQz}$, with frequencies

$$\Omega(Q)=[(1+Q^2)(1+Q^2+b^{-1})]^{1/2}\ , \tag{A3}$$

as already given in Eq. (3.17). We define transition coefficients according to

$$\begin{aligned} &z\to+\infty,\quad \varphi\sim\vartheta\sim e^{iQz}\ ,\\ &z\to-\infty,\quad \varphi\sim\vartheta\sim ce^{iQz}+de^{-iQz}\ . \end{aligned} \tag{A4}$$

From c and d we find the phase shifts χ_+ (χ_-) for solutions which are even (odd) under space reflection,

$$e^{2i\chi_\pm(Q)}=\frac{1\mp d^*(Q)}{c(Q)}\ . \tag{A5}$$

The separation into even and odd solutions restricts the wave vector to values $Q\geq 0$; both even and odd solutions contribute equally to the sum (3.9), which is transformed in the usual way[9] to give the integral in Eq. (3.23) with the phase shift

$$\varphi(Q)=\chi_+(Q)+\chi_-(Q)\ . \tag{A6}$$

For $b\to 0$ (the SG limit) the only term to be considered on the right-hand side of Eq. (A2) is $b^{-1}\theta$. The coupled system of equations then reduces to

$$b\Omega^2\varphi=-\varphi''+(1-v\,\mathrm{sech}^2 z)\varphi\ , \tag{A7}$$

with $v=2$. This eigenvalue problem can be solved exactly[11,14]; the resulting phase shift is

$$\varphi(Q)=2\arctan\frac{1}{Q}\ . \tag{A8}$$

In addition to the continuum there exists a bound state with zero frequency and wave function $\varphi\sim d\Phi_S/dx\sim\mathrm{sech} z$, which is related to translational invariance.[9] This zero-frequency state actually is an eigenstate of the complete system (A1) and (A2), which is solved by $\varphi\sim\mathrm{sech} z$, $\theta=0$. This fact is, of course, related to the observation in Sec. III that the SG soliton continues to be a solution of the equations of motion for $b>0$.

In order to generally investigate Eqs. (A1) and (A2) for $b>0$, we first apply straightforward perturbation theory in b, considering the terms $\theta''-(1-6\,\mathrm{sech}^2 z)\theta$ as perturbation. To lowest order in b, this again leads to an eigenvalue problem of the form (A7) with, however,

$$v=2(1+2\Omega^2 b^2)\ ,$$

and with $b\Omega^2$ on the left-hand side of Eq. (A7) replaced by $b\Omega^2(1-\Omega^2 b^2)$. From the exact treatment of this problem[14] we note that, in addition to the zero-frequency solution discussed before, there now exists a second bound state. It emerges from the continuum threshold $\Omega=\Omega_0$, $\Omega_0^2 b\approx 1$ as soon as $v>2$. The frequency of this state is found to lowest order in b as

$$\Omega=\Omega_0(1-\tfrac{8}{9}b^2\cdots)\ . \tag{A9}$$

One might think that, going beyond perturbation theory, the frequency of this mode will go down to zero at $b=\frac{1}{3}$ to become the dynamical source of the recently discovered[15] instability of the soliton mode [(3.5) and (3.6)] against out-of-plane fluctuations. This is, however, not the case, and an understanding of this stability in terms of the dynamics of the system is actually more subtle and will be published separately.

Use of the above approach to calculate scattering properties is unfortunately restricted to small wave vectors, since θ'' in Eq. (A2) is a small perturbation only for $Q^2 \ll b^{-1}$. Since we need to consider arbitrarily large wave vectors, we now apply a slightly more sophisticated perturbation theory, treating $+4\,\mathrm{sech}^2 z\theta$ in Eq. (A2) as a perturbation. The resulting zero-order equations are the following:

$$-i\Omega\vartheta_0=\varphi_0''-(1-2\,\mathrm{sech}^2 z)\varphi_0\ , \tag{A10}$$

$$i\Omega\varphi_0=-b^{-1}\vartheta_0+\vartheta_0''-(1-2\,\mathrm{sech}^2 z)\vartheta_0\ , \tag{A11}$$

and can be solved to give the continuum states

$$\varphi_0=e^{iQz}(-iQ+\tanh z)\ , \tag{A12}$$

$$\vartheta_0=-i\alpha_Q\varphi_0\ , \tag{A13}$$

$$\alpha_Q=[(Q^2+1)/(Q^2+1+b^{-1})]^{1/2}\ . \tag{A14}$$

In order to treat the perturbation we introduce the integral equation representation equivalent to the system of equations (A1) and (A2):

$$\varphi(z)=\varphi_0(z)+\int dz' G_1(z,z')\mathrm{sech}^2 z'\vartheta(z')\ , \tag{A15}$$

$$\vartheta(z)=\vartheta_0(z)+\int dz' G_2(z,z')\mathrm{sech}^2 z'\vartheta(z')\ . \tag{A16}$$

Here the Green's functions G_i are to be determined from

$$-i\Omega G_2-G_1''+(1-2\,\mathrm{sech}^2 z)G_1=0\ , \tag{A17}$$

$$i\Omega G_1-G_2''+(b^{-1}+1-2\,\mathrm{sech}^2 z)G_2=4\delta(z-z'), \tag{A18}$$

where primes denote derivatives with respect to z. To calculate the Green's functions, we use the ansatz

$$G_i\sim e^{ikz}g_i(\tanh z)\ , \tag{A19}$$

with k to be determined from

$$(k^2+1)(k^2+1+b^{-1})=(Q^2+1)(Q^2+1+b^{-1})\ .$$

Note that this equation has not only real solutions $k_{1,2}=\pm Q$, but also imaginary solutions,

$$k_{3,4}=\pm i(Q^2+2+b^{-1})^{1/2}=\pm i\kappa\ .$$

Thus the Green's functions are linear combinations of four terms of the structure of (A19) with coefficients depending on z'. We finally obtain for $z>z'$,

$$G_i(z,z')=\frac{2\alpha_Q}{1+\alpha_Q^2}\left[\frac{A_i}{Q(1+Q^2)}e^{iQ(z-z')}(iQ+\tanh z')(-iQ+\tanh z)+\frac{B_i}{\kappa(1-\kappa^2)}e^{-\kappa(z-z')}(-\kappa+\tanh z')(\kappa+\tanh z)\right]\ , \tag{A20}$$

with

$$A_1=-1\ ,\ A_2=i\alpha_Q\ ,$$
$$B_1=-i\ ,\ B_2=1/\alpha_Q\ ,$$

whereas for $z<z'$ we have to transform $Q\to -Q$, $\kappa\to -\kappa$ in Eq. (A20) to obtain $-G_i(z,z')$.

We now calculate the phase shifts solving Eqs. (A15) and (A16) in first-order Born approximation, i.e., using θ_0 instead of θ in the integrals. Keeping consistently terms to lowest orders in b, we obtain

$$\chi_{\pm}(Q)=\arctan 1/Q+\arctan[\alpha(Q)\mp\beta(Q)] \quad \text{(A21)}$$

with $\alpha(Q)$ and $\beta(Q)$ given in the main text. It can easily be checked that this result implies that two states are missing in the continuum, and they appear as the two bound states discussed before. We have also checked that the result (A21) for the phase shifts agrees with that from the simple perturbational approach for the small values of Q.

---

*Present address.

[1]H. J. Mikeska, J. Phys. C 11, L29 (1978); for a recent review see H. J. Mikeska, J. Appl. Phys. 52, 1950 (1981).

[2]A. R. Bishop, J. A. Krumhansl, and S. E. Trullinger, Physica D 1, 1 (1980).

[3]J. K. Kjems and M. Steiner, Phys. Rev. Lett. 41, 1137 (1978); M. Steiner, K. Kakurai, W. Knop, R. Pynn, and J. K. Kjems, Solid State Commun. 41, 329 (1982).

[4]W. C. Kerr, D. Baeriswyl, and A. R. Bishop, Phys. Rev. B 24, 6566 (1981); G. Wysin, A. R. Bishop, and P. Kumar J. Phys. C 15, L337 (1982).

[5]T. Schneider and E. Stoll, Phys. Rev. B 23, 4631 (1981); J. M. Loveluck, T. Schneider, E. Stoll, and H. R. Jauslin, Phys. Rev. Lett. 45, 1505 (1980).

[6]H. J. Mikeska and E. Patzak, Z. Phys. B 26, 253 (1977).

[7]A. R. Bishop, J. Phys. C 13, L67 (1980).

[8]K. Maki, Phys. Rev. B 24, 3991 (1981).

[9]R. F. Dashen, B. Hasslacher, and A. Neveu, Phys. Rev. D 10, 4114 (1974); 11, 3424 (1975); R. Rajaraman, Phys. Rep. 21, 229 (1975).

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

[11]J. Rubinstein, J. Math. Phys. 11, 258 (1970).

[12]S. Coleman, Phys. Rev. D 11, 2088 (1975).

[13]P. W. Anderson, Phys. Rev. 86, 694 (1952); H. J. Mikeska, Phys. Rev. B 12, 2794 (1975).

[14]P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), Chap. 12.3.

[15]P. Kumar, Phys. Rev. B 25, 483 (1982); E. Magyari and H. Thomas, *ibid.* 25, 531 (1982).