Solitons in one-dimensional antiferromagnetic chains

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We study the quantum-statistical mechanics, at low temperatures, of a one-dimensional antiferromagnetic Heisenberg model with two anisotropies. In the weak-coupling limit we determine the temperature dependences of the soliton energy and the soliton density. We have found that the leading correction to the sine-Gordon (SG) expression for the soliton density and the quantum soliton energy comes from the out-of-plane magnon mode, not present in the pure SG model. We also show that when an external magnetic field is applied, the chain supports a new type of kink, where the sublattices rotate in opposite directions.

I. INTRODUCTION

The thermodynamical properties of the one-dimensional classical antiferromagnet described by the Hamiltonian

$$\mathcal{H}=2J\sum_n [\mathbf{S}_n\cdot\mathbf{S}_{n+1}-\delta S_n^z S_{n+1}^z+b(S_n^x)^2]-g\mu_B H\sum_n S_n^x \tag{1.1}$$

have been studied in Ref. 1 using the transfer matrix method. Results have been obtained for the static correlation functions, correlation length, neutron-scattering intensity integrated over energy, etc., and an excellent agreement with experimental data has been found for tetramethyl ammonium manganese trichloride for (TMMC). To interpret physically the experimental results at low temperatures a soliton model has been proposed[2] and this model has been largely studied in the literature.[3–11] Recently Gaulin,[12] using a Monte Carlo calculation, has found evidence for soliton excitations in Hamiltonian (1.1). To accept the soliton model, however, we should be able to show that a phenomenological theory based in this classical model would agree with the transfer matrix result. We should also be able to calculate the quantum corrections to the model.

A phenomeonological treatment for Hamiltonian (1.1) is very difficult, so we will consider the case $H=0$. However, in Sec. II we will present the equations of motion for the full Hamiltonian in order to show the origin of the difficulties involved. We will also discuss a new type of soliton predicted by Gerling *et al.*[13] using a Monte Carlo calculation. In Sec. III we will consider the quantum corrections to the classical model and calculate phenomenologically the soliton density using a quantum approach.

II. EQUATIONS OF MOTION

For a small magnetic field we expect that two neighboring spins are almost antiparallel to each other at low temperature. Making use of the angle variable introduced by Mikeska[5]

$$\mathbf{S}_i=(-1)^i S\{\sin[\theta_i+(-1)^i v_i]\cos[\phi_i+(-1)^i\alpha_i],\sin[\theta_i+(-1)^i v_i]\sin[\phi_i+(-1)^i\alpha_i],\cos[\theta_i+(-1)^i v_i]\}\ , \tag{2.1}$$

where θ and ϕ are the angles giving the sublattice magnetization, and v and α describe the deviations from perfect antialignment and can be assumed to be small at low temperatures. In the continuum limit the equations of motion are[1]

$$\frac{\partial^2\theta}{\partial z^2}+\frac{1}{c^2}\frac{\partial^2\theta}{\partial t^2}=-\frac{h}{2JS}\sin^2\theta\cos\phi\left[\frac{\partial\phi}{\partial t}\right]+\sin\theta\cos\theta\left[\left[\frac{\partial\phi}{\partial z}\right]^2-\frac{1}{c^2}\left[\frac{\partial\phi}{\partial t}\right]^2\right]+\sin\theta\cos\theta[(h^2+2b)\cos^2\phi-2\delta]\ , \tag{2.2}$$

$$\frac{\partial^2\phi}{\partial z^2}-\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2}=-2\cot\theta\left[\frac{\partial\phi}{\partial z}\frac{\partial\theta}{\partial z}-\frac{1}{c^2}\frac{\partial\phi}{\partial t}\frac{\partial\theta}{\partial t}\right]+\frac{h}{2JS}\cos\phi\frac{\partial\theta}{\partial t}-(h^2+2b)\sin\phi\cos\phi\ , \tag{2.3}$$

where $c=4JS$, $h=g\mu_B H/4JS$ and we have chosen the z direction along the chain. The static limit of (2.2) and (2.3) agrees with the corresponding limit for the equations of motion for a ferromagnet with two anisotropies.[6] The dynamics, however, is different for the two models. At low temperatures, however, where only low-velocity solitons are excited we should expect that the thermodynamics of the two models are nearly equivalent. This equivalence has been discussed in details by Gouvea and Pires.[1,14]

Two static solutions to (2.2) and (2.3) can be given immediately:

xy soliton

$$\theta=\pi/2,\quad \sin\phi=\tanh\tilde{h}z\ , \tag{2.4}$$

with energy

$$E^0_{xy}=4JS^2\tilde{h}\ , \tag{2.5}$$

where $\tilde{h}^2=h^2+2b$;

yz soliton

$$\phi=\pi/2,\quad \sin\theta=\tanh\sqrt{2\delta}z\ , \tag{2.6}$$

with energy

$$E^0_{yz}=4JS^2\sqrt{2\delta}\ . \tag{2.7}$$

Dynamic solutions have been studied in details in Refs. 1, 6, 8, and 9. As shown by Wysin *et al.*[9] when $b=0$ the xy solitons are stable above and below the critical field $h_c=\sqrt{2\delta}$. Even for $h>h_c$ they show no tendency to decay to lower-energy yz solitons. At the critical field there is a continuum of xy solitons all with the same energy and velocity. For small velocities $v \ll c$, the sine-Gordon theory adequately describes the yz branch. The static yz solitons are stable only if $h>h_c$, and the dynamic yz solitons require a minimum applied field to be stable, this minimum field decreasing with the increase of velocity. For $h<h_c$ the static yz soliton decays toward a configuration involving a lower energy xy soliton.

For $\tilde{h}<\sqrt{2\delta}$ the xy soliton is the lowest energy soliton and is stable. We will be concerned with this case. The behavior of small oscillations in the presence of a single static soliton $\phi_0(z)$ is determined by solutions to (2.2) and (2.3) of the form

$$\begin{aligned}\theta(z,t)&=\pi/2+\theta_1(u)+\tilde{\theta}(z,t)\ ,\\ \phi(z,t)&=\phi_0(z)+\xi(z,t)\ ,\end{aligned} \tag{2.8}$$

where $\theta_1(u)$ the out-of-plane deviation is given by[6]

$$\theta_1(u)=u\tilde{h}^2(4JS\delta)^{-1}\operatorname{sech}[\tilde{h}(z-ut)]\ , \tag{2.9}$$

and u is the soliton velocity. Substitution of (2.8) in (2.2) and (2.3), linearization in $\tilde{\theta}$ and ξ, and writing $\tilde{\theta}$ and ξ as

$$\tilde{\theta}(z,t)=s(z)e^{i\omega t},\quad \xi(z,t)=r(z)e^{i\omega t} \tag{2.10}$$

leads to the following eigenvalue equations:

$$\frac{d^2r}{dz^2}+\frac{\omega^2}{c^2}r=\tilde{h}^2(1-2\operatorname{sech}^2\tilde{h}z)r+i\frac{2h}{c}\omega s\operatorname{sech}\tilde{h}z\ , \tag{2.11}$$

$$\frac{d^2s}{dz^2}+\frac{\tilde{\omega}^2}{c^2}s=\tilde{h}^2(1-2\operatorname{sech}^2\tilde{h}z)s-i\frac{2h\omega r}{c}\operatorname{sech}\tilde{h}z\ , \tag{2.12}$$

where $\tilde{\omega}^2=\omega^2-(2\delta-\tilde{h}^2)c^2$.

The dispersion relation is determined by the behavior far from the soliton center. We find

$$\omega_1^2(q)=(2\delta+q^2)c^2,\quad \omega_2^2(q)=(\tilde{h}^2+q^2)c^2 \tag{2.13}$$

in agreement with Endoh *et al.*[15] for the frequencies of spin waves excitations in an anisotropic antiferromagnet in an external field (in the limit of small q). Physically, one of the two modes, $\omega_2(q)$, represents the spin fluctuations against the external field (in-plane mode), while the other mode $\omega_1(q)$, is the fluctuation out of the easy plane (out-of-plane mode).

We have been unable to solve Eqs. (2.11) and (2.12) for $h\neq 0$. For this reason we will consider just the case of two anisotropies, i.e., we put $h=0$ in (2.11) and (2.12). Now Eq. (2.11) possesses a bound-state solution with $\omega_2=0$ as in the SG problem.[16] Equation (2.12) has the same form only now $\tilde{\omega}=0$ gives a bound state with frequency

$$\omega_b^2=2(\delta-b)c^2\ . \tag{2.14}$$

As we see ω_b^2 has to be positive for the out-of-plane motion, this means $b<\delta$. Out-of-plane here means fluctuations in the z direction. The bound state becomes soft at the crossover anisotropy $b=\delta$, i.e., the plane becomes unstable. Similarly to the ϕ^4-kink model, the localized mode ω_b should give rise to absorption at $\omega=\omega_b$, the density of states for this magnon mode being proportional to the soliton density. Both (2.11) and (2.12) for $h=0$ have the same phase shift $\Delta(q)$ for the continuum states. We have[16]

$$\Delta(q)=2\tan^{-1}(\sqrt{2b}/q)\ . \tag{2.15}$$

We leave the phenomenological calculation of the soliton density, in the line of Currie *et al.*[16] to Sec. III where we will treat the problem from the quantum mechanical point of view.

Now we will study analytically the existence of a new type of kink which, although its existence was demonstrated by Gerling *et al.*[13] for the classical XY model through a Monte Carlo calculation, was not predicted by early theories.

In the ground state for $h\neq 0$, $b=0$, $h^2<2\delta$, the spins arrange in a spin-flop phase, where all spins from one sublattice align at an angle $+\alpha$ to the x axis and the spins from the other sublattice at an angle $-\alpha$ to the x axis. The angle α is given by[17]

$$\alpha=\cos^{-1}(h/2)\ \text{ if } h\le 2,\quad \alpha=0\ \text{ if } h\ge 2\ . \tag{2.16}$$

At nonzero temperatures the spins fluctuate around this ground state. Obviously the parametrization (2.1) is not suitable when the applied magnetic field is very large, because the spin-flop angle will be large and the antialignment destroyed, thus a two sublattice approach is more indicated. Of course both parametrizations are equivalent to one another. We will then write the Hamiltonian (1.1) as[7]

$$\begin{aligned}\mathcal{H}=\sum_l\{&2J[\mathbf{S}^A(l)\cdot\mathbf{S}^B(l)+\mathbf{S}^A(l)\cdot\mathbf{S}^B(l+1)]\\ &+D[S_z^A(l)^2+S_z^B(l)^2]-g\mu_BH[S_x^A(l)+S_x^B(l)]\}\ ,\end{aligned} \tag{2.17}$$

where the superscripts A and B denote the two sublattices and $D=2J\delta$. If D is large the motion of the spins are largely confined to the xy plane.

After obtaining the equation of motion by using

$$i\dot{\mathbf{S}}=[\mathbf{S},\mathcal{H}]\ , \tag{2.18}$$

we treat the spin components as classical vectors with spherical components

$$\mathbf{S}^A(l)=S(\sin\alpha_l\cos\zeta_l,\sin\alpha_l\sin\zeta_l,\cos\alpha_l) ,$$
$$\mathbf{S}^B(l)=S(\sin\beta_l\cos\Phi_l,\sin\beta_l\sin\Phi_l,\cos\beta_l) . \tag{2.19}$$

Obtaining[7]

$$\dot\alpha_l=2JS[\sin\beta_l\sin(\Phi_l-\zeta_l)+\sin\beta_{l+1}\sin(\Phi_{l+1}-\zeta_l) +2h\sin\zeta_l] , \tag{2.20}$$

$$\dot\zeta_l=-2JS[\cot\alpha_l\sin\beta_l\cos(\zeta_l-\Phi_l) +\cot\alpha_l\sin\beta_{l+1}\cos(\zeta_l-\Phi_{l+1}) -2\delta\cos\alpha_l+2h\cot\alpha_l\sin\zeta_l] , \tag{2.21}$$

with corresponding forms for $\dot\beta_l$ and $\dot\Phi_l$ on the other sublattice.

Since it is very difficult to obtain a time-dependent solution for the above equations, we will consider only the static limit, i.e., $\dot\alpha_l=\dot\zeta_l=0$. We then get

$$\sin(\Phi_{l+1}-\zeta_l)+\sin(\Phi_l-\zeta_l)+2h\sin\zeta_l=0 , \tag{2.22}$$

$$\sin(\Phi_l-\zeta_{l-1})+\sin(\Phi_l-\zeta_l)-2h\sin\Phi_l=0 , \tag{2.23}$$

and $\alpha_l=\beta_l=\pi/2$.

Those equations represent a static kink in the XY plane. If we impose the condition that D is very large we reach the XY limit. In this limit there is no dynamical solution and Eqs. (2.22) and (2.23) represent exact equations for the model.

As pointed out by Gerling *et al.*[13] there are two topologically distinct π solitons in the XY limit. In the first type one sublattice experiences a phase jump of 2α and the other $2\pi-2\alpha$. This type of soliton, for small magnetic field, corresponds to the sine-Gordon solition already studied in details in the literature. For large fields this soliton has a more complicated structure, quite different from the sine-Gordon solution. In the second type the two sublattices interchange direction by rotating through angles $\pm2\alpha$, respectively. We will study this type below. In principle, we can construct yet another "π-like" soliton in which the sublattices rotate through angles $\pm(2\pi-2\alpha)$, but these have such high energy that they have never been observed in the Monte Carlo calculation. Since the spins remain more or less antiparallel in the first type of soliton, we expect that this type should be favored for low magnetic fields in which case the antiferromagnetic spin-spin is dominant. As the field is increased, the second type of soliton should become more common since both spins maintain components in the same direction as the applied field. A 2π soliton where the spins in one sublattice rotate through 2π and the phase of the other sublattice is unchanged is also possible.

Following the work of Gerling *et al.*[13] we look for solutions of the type

$$\Phi_l=\Psi_{2n} ,$$
$$\zeta_l=-\Psi_{2n+1} , \tag{2.24}$$

this is, the spins are in a spin-flop state and the kink is produced by allowing the sublattices to rotate in opposite direction in the xy plane, until the sublattices are interchanged. In this case Eqs. (2.22) and (2.23) reduce to

$$\sin(\Psi_{i+1}+\Psi_i)+\sin(\Psi_i+\Psi_{i-1})-2h\sin\Psi_i=0 . \tag{2.25}$$

Taking the continuum limit we obtain

$$\Psi''\cos2\Psi+2\sin2\Psi-2h\sin\Psi=0 , \tag{2.26}$$

where Ψ is confined to the interval

$$|\Psi|\le\alpha,\quad h<2 ,$$
$$|\Psi|=0,\quad h\ge2 . \tag{2.27}$$

The kink solution to Eq. (2.26) can be written as

$$z=\pm\int_0^{\Psi}\frac{d\Psi_1}{\sqrt{V(\alpha)-V(\Psi_1)}} , \tag{2.28}$$

where

$$V(\Psi_1)=-2\ln\cos2\Psi_1-h\ln\left|\frac{1+\sqrt2\cos\Psi_1}{1-\sqrt2\cos\Psi_1}\right| , \tag{2.29}$$

and the center of the kink was chosen at the origin $z=0$. We have calculated the integral in (2.28) numerically and in Fig. 1 we show $\Psi(z)$ for $\alpha=20°$, 30°, and 40°. We also show, for comparison, the results obtained directly from Eq. (2.25). This figure is similar to Fig. 5A of Ref. 13.

As pointed out by Gerling *et al.*[13] this kink solution is quite different from the sine-Gordon soliton obtained when we allow the sublattices to rotate in the same direction. Of course the continuum approximation (2.26) has limitations. For example, it clearly breaks down for fields

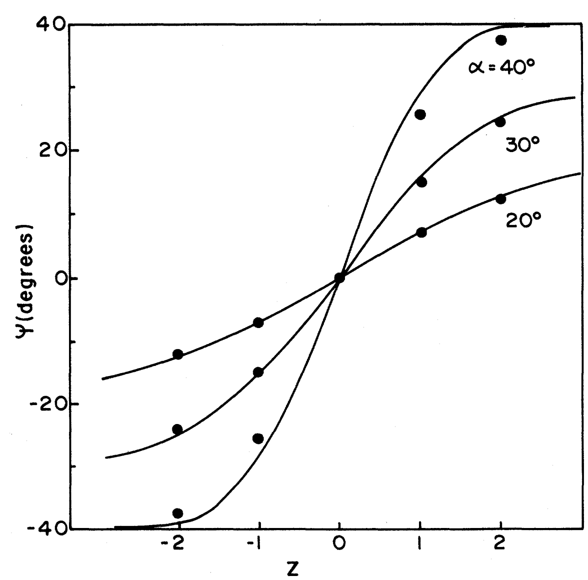

FIG. 1. $\psi(z)$ calculated in the continuum approximation (solid line) and using the discrete model (circles). Here z is measured in units of the lattice parameter.

such that $\alpha > \pi/4$. However, the discrete equation (2.25) always holds.

In Fig. 2 we show the kink energy E_k, calculated numerically, using the discrete Eq. (2.25), as a function of the magnetic field. As we can see the energy decreases as the field increases and is zero for $h \geq 2$.

Now let us discuss the energetics and stability of the model. As we have seen before, for small magnetic fields and any value of the anisotropy the xy soliton has the lowest energy given by $E_{xy}^0 = 4JS^2 h$, and is stable. Now if D/J is small, as it usually is, for $h > \sqrt{2\delta}$ the xy soliton becomes unstable and the yz soliton is the lowest energy soliton and is stable. For small values of h we have $E_{yz}^0 = 4JS^2\sqrt{2\delta}$. If we suppose that only the spin component in the yz plane is effective in the calculation of E_{yz}^0 we can write

$$E_{yz}^0 = 4JS^2\sqrt{2\delta}\sin^2\alpha = 4JS^2\sqrt{2\delta}(1-h^2/4) \; .$$

At least the two limits $h \to 0$ and $h = 2$ are correct since for $h = 2$ we have complete alignment of the spins with the field and $E_{yz}^0 = 0$. Also our estimate for E_{yz}^0 is in agreement with Ref. 9 where this expression for E_{yz}^0 was obtained by using a two-parameter variational ansatz for the YZ soliton. Therefore, for small values of D/J, as is the case for TMMC, the $\pm 2\alpha$ kink has energy larger than the yz soliton and a numerical analysis shows that it is unstable to the yz soliton. We can therefore neglect this type of kink in the calculations done in this paper.

Increasing the value of D/J we will reach a point where E_k will be smaller than E_{yz}^0. This will happen for very large values of δ, ($\delta > 1.12$). Now if we use for the energy of the xy soliton the expression given in Ref. 9, $E_{xy}^0 = 4JS^2 h(1-h^2/6)$ we see, from Fig. 2, that for $h \geq 0.77$ we have $E_k < E_{xy}^0$. For very large values of δ and h a numerical analysis shows that the $\pm 2\alpha$ kink is stable.

We have not discussed the $\pm(2\pi - 2\alpha)$ kink since as pointed out in Ref. 13 these have a higher energy than the $\pm 2\alpha$ soliton. However, when the spins are approximately aligned to the field we should have a 2π soliton similar to the soliton for the ferromagnetic model. In fact, if in Eq. (2.22) we consider the angle between adjacent spins to be small, i.e., $\phi_l \sim \phi_{l+1} \sim \zeta_l = \phi$ we can expand ϕ_l and ϕ_{l+1} in series around ζ_l to obtain in the continuum limit

$$\frac{\partial^2\phi}{\partial z^2} + h\sin\phi = 0 \; , \tag{2.30}$$

the static sine-Gordon equation. For the soliton energy we have

$$E = 4JS^2\sqrt{h} \; . \tag{2.31}$$

However, for TMMC $h = 2$ corresponds to $H \simeq 10^3$ kOe, a value much higher than the fields available in laboratories today.

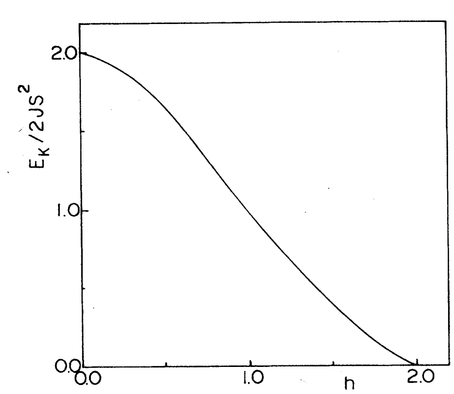

FIG. 2. Soliton energy as a function of the applied magnetic field.

III. QUANTUM CORRECTIONS

The aim of the present section is to present a quantum-statistical mechanics of soliton excitations in the antiferromagnetic linear chain described by Hamiltonian (1.1) when $H = 0$. We will rely on the earlier works of Maki and Takayama[18] where they treated the pure SG model.

Before treating the quantization of the soliton we will briefly discuss the quantization of the magnon modes. In order to do that we shall transform the Hamiltonian into the Villain representation[19]

$$\begin{aligned} S_n^+ &= e^{i\phi_n}[S(S+1) - S_n^z(S_n^z+1)]^{1/2} \; , \\ S_n^- &= [S(S+1) - S_n^z(S_n^z+1)]^{1/2} e^{-i\phi_n} \; , \end{aligned} \tag{3.1}$$

we shall rotate the ϕ_n separately for each sublattice such that the azimuthal angle is measured with respect to the position of the spins in the ground state. Thus we let

$$\phi_n = (-1)^n \pi/2 + \Psi_n \; . \tag{3.2}$$

Following Riseborough and Reiter[17] we take the classical easy plane antiferromagnetic state as the zeroth approximation, and expand in powers of the amplitude of the out-of-plane fluctuations $\langle (S_n^z)^2 \rangle / \tilde{S}^2$ where $\tilde{S}^2 = S(S+1)$, and in-plane fluctuation $\langle (\Psi_n)^2 \rangle$. On expanding in powers of $S_n^z/\tilde{S}$ and Ψ_n we obtain

$$\mathcal{H} = E_0 + \mathcal{H}_0 + \mathcal{H}_1 + \mathcal{H}_2 + \cdots \; , \tag{3.3}$$

where $E_0 = -2JN\tilde{S}^2$ is the energy of the classical ground state and $\mathcal{H}_0$ is the harmonic Hamiltonian. The remaining terms represent interactions between spin waves, and also provides quantum renormalizations of the spin-wave dispersion relations. At very low temperatures, where the number of excited spin waves is extremely small, only the quantum renormalizations are important. Since these are of order $1/\tilde{S}$, they vanish in the classical limit. The harmonic Hamiltonian $\mathcal{H}_0$ can be diagonalized by Fourier transforming and using the canonical transformation

$$\begin{aligned} \Psi_q &= \alpha_q(a_q^\dagger - a_{-q}) \; , \\ S_q^z &= i\beta_q(a_q^\dagger - a_{-q}) \; , \end{aligned} \tag{3.4}$$

where $\alpha_q\beta_q=\frac{1}{2}$. We thus obtain

$$\mathcal{H}_0=\sum_q \frac{\hbar\omega_q}{q}(a_q^\dagger a_q+a_q a_q^\dagger) , \tag{3.5}$$

where

$$\hbar\omega_q=4J\tilde{S}\{[(1+\delta)+\cos q][(1+b)-\cos q]\}^{1/2} , \tag{3.6}$$

and

$$\alpha_q^2=\frac{1}{2\tilde{S}}\left[\frac{1+\delta+\cos q}{1+b-\cos q}\right]^{1/2} ,$$
$$\beta_q^2=\frac{\tilde{S}}{2}\left[\frac{1+b-\cos q}{1+\delta+\cos q}\right]^{1/2} . \tag{3.7}$$

The fluctuations $\langle (S_n^z)^2\rangle$ and $\langle (\Psi_n)^2\rangle$ can be calculated directly from (3.4), we obtain

$$\langle \Psi_n^2\rangle=\frac{1}{N}\sum_q \alpha_q^2(2n_q+1) , \tag{3.8}$$

$$\langle (S_n^z)^2\rangle=\frac{1}{N}\sum_q \beta_q^2(2n_q+1) , \tag{3.9}$$

where

$$n_q=(e^{\omega_q/T}-1)^{-1} . \tag{3.10}$$

The classical limit is obtained by setting $n_q\rightarrow T/\omega_q$, $n_q+\frac{1}{2}\rightarrow T/\omega_q$, (where we have taken $k_B=1$). Equations (3.8) and (3.9) yields the classical result

$$\langle \Psi_n^2\rangle_c=\frac{\tilde{S}^2 T}{4J\sqrt{2b}} , \tag{3.11}$$

$$\langle (S_n^z)^2\rangle_c=\frac{\tilde{S}^2 T}{4J\sqrt{2\delta}} , \tag{3.12}$$

valid to leading order in T. In the classical case $\langle (S_n^z)^2\rangle$ vanishes for $T\rightarrow 0$ and increases linearly with T, whereas in the quantum case at $T=0$ the out-of-plane fluctuations are very large: $\langle (S_n^z)^2\rangle\simeq 0.3$ for TMMC, to be compared with the value 0.5 for the isotropic Heisenberg model. The thermal increment is extremely slow for temperatures up to 10 K. The large discrepancy at $T=0$ occurs due to fact that we have neglected the zero-point energy in Eqs. (3.8) and (3.9) to get the classical limit. In the quantum approach that we will use in this section to treat the soliton sector we will include the zero-point energy of both in-plane and out-of-plane fluctuations. Note that in the pure quantum sine-Gordon model the out-of-plane fluctuations are ignored, thus showing the inadequacy of a mapping of Hamiltonian (1.1) to this model.

Expressed in terms of creation and annihilation operators the interaction terms in the Hamiltonian $\mathcal{H}_1$ in Eq. (3.3) are not normally ordered. On forcing the interactions into a normal ordered form, the commutators produce lower-order interactions and quadratic terms. The application of this procedure, as in the case of the ferromagnet,[20] will generate renormalized values for J, δ, and b (renormalized magnon mass). For instance the δ value calculated for TMMC on the basis of a full Ewald sum for the classical magnetic dipole-dipole coupling alone is $\delta=0.019$. The renormalized value,[21,22] at $q=0$, is $\delta_1=0.0086$ in agreement with experimental data from low-temperature EPR measurement.[23] For b the experimental renormalized value is[24] $b=2.6\times 10^{-4}$ which would correspond to the bare value $b=1.0\times 10^{-3}$.

Now to study the quantum-mechanical corrections to the soliton sector we must be very careful to appropriately count the modes and subtract the vacuum energy for each mode.[25] We compute the difference between the quantum corrections to the ground-state energy of the ordering vacuum and the ground-state energy of the soliton. In the absence of the soliton, the energy of the vacuum comes only from continuum states (magnons modes). When the soliton is introduced, the first two continuum states disappear to become states with $\omega=0$ and $\omega=\omega_b$, as we have seen in Sec. II. This is, the first state ($q=0$) of $\omega_1(q)$ becomes the bound state $\omega=0$ (translation mode) and the first state ($q=0$) of $\omega_2(q)$ becomes the bound state $\omega=\omega_b$. The contribution of these two states to the energy of the soliton will then be

$$E_b=\tfrac{1}{2}(0-m_1c)+\tfrac{1}{2}(\omega_b-m_2c) , \tag{3.13}$$

where

$$m_1^2=2b,\quad m_2^2=2\delta . \tag{3.14}$$

The contribution from the other states, which remain in the continuum in the presence of the kink, will be

$$E_{\text{cont}}=\tfrac{1}{2}\left[\sum_{n=1}[\omega_1(q_n)-\omega_1(k_n)] + \sum_{n=1}[\omega_2(q_n)-\omega_2(k_n)]\right] , \tag{3.15}$$

where q_n is the wave number of the nth mode in the continuum in the presence of the kink, and k_n the wave number in the vacuum. Since we have used a periodix box of length L, q_n and k_n are related by the periodic boundary condition

$$Lq_n+\Delta(q_n)=2n\pi=k_nL , \tag{3.16}$$

where $\Delta(q)$ was given in Eq. (2.15). From Eq. (3.16) we obtain

$$\omega(q)\simeq\omega(k)-\frac{\Delta(k)}{L}\frac{\partial\omega}{\partial k} . \tag{3.17}$$

In the limit $L\rightarrow\infty$ the discrete sum (3.15) becomes an integral

$$E_{\text{cont}}=-\frac{1}{2\pi}\int_0^\Lambda \Delta(k)\frac{\partial\omega_1}{\partial k}dk-\frac{1}{2\pi}\int_0^\Lambda \Delta(k)\frac{\partial\omega_2}{\partial k}dk , \tag{3.18}$$

where Λ is the ultraviolet cutoff, given by the lattice spacing. Integrating (3.18) by parts, adding Eq. (3.13) and doing a few manipulations we find

$$E_b+E_{\rm cont}=-\frac{2\omega_1(0)}{\pi}+\tfrac{1}{2}\omega_b-\frac{m_1c}{\pi}\left[\int_0^\Lambda\frac{dk}{(m_2^2+k^2)^{1/2}}+\int_0^\Lambda\frac{dk}{(m_1^2+k^2)^{1/2}}+\int_0^\Lambda\frac{(m_2^2-m_1^2)dk}{(k^2+m_1^2)(k^2+m_2^2)^{1/2}}\right]. \tag{3.19}$$

Although we have a discrete chain (finite Λ) it is well known that one loop correction to the magnon mass[22] is equivalent to normal ordering of the Hamiltonian. This contributes with terms

$$\int_0^\Lambda dk(m_i^2+k^2)^{1/2},\quad i=1,2\ .$$

So the first two integrals on the right-hand side of Eq. (3.19) are canceled by the ordinary mass renormalization counterterms discussed early. Collecting all the finite terms, we arrive finally to the static soliton energy, at zero temperature,

$$E_s^0=E_{xy}^0-\frac{2}{\pi}m_1c+\tfrac{1}{2}\omega_b-\frac{m_1c}{\pi}\int_0^\Lambda\frac{(m_2^2-m_1^2)dk}{(k^2+m_1^2)(k^2+m_2^2)^{1/2}}\ , \tag{3.20}$$

or

$$E_s^0=E_{xy}^0\left[1+\frac{1}{\pi S}+\frac{1}{2S}\left[\frac{m_2^2}{m_1^2}-1\right]^{1/2}-\frac{(m_2^2-m_1^2)}{\pi S}\int_0^\Lambda\frac{dk}{(k^2+m_1^2)(k^2+m_2^2)^{1/2}}\right]. \tag{3.21}$$

For the SG model the soliton energy is given by[25]

$$E_s^0=E_{xy}^0\left[1-\frac{1}{\pi S}\right]. \tag{3.22}$$

For $\delta=b$, Eq. (3.21) becomes

$$E_s^0=E_{xy}^0\left[1-\frac{2}{\pi S}\right]. \tag{3.23}$$

In this limit the Hamiltonian (1.1) is equivalent to the following Hamiltonian:

$$\mathcal{H}=2J\sum_n[\mathbf{S}_n\cdot\mathbf{S}_{n+1}-\delta(S_n^y)^2]\ , \tag{3.24}$$

which at low temperatures has an Ising-like behavior. The difference from the correction to the SG model comes from the extra degree of freedom represented by the out-of-plane fluctuations. For TMMC we find

$$E_s^0=0.88E_{xy}^0\ . \tag{3.25}$$

Now, to study the quantum corrections to the soliton sector, at finite temperatures, we start from the thermodynamic potential of this sector given by

$$\Omega_s=E_{xy}^0+\beta^{-1}\left[\sum_n\ln\left[2\sinh\frac{\beta}{2}\omega_1(q_n)\right]+\sum_n\ln\left[2\sinh\frac{\beta}{2}\omega_2(q_n)\right]-\sum_n\ln\left[2\sinh\frac{\beta}{2}\omega_1(k_n)\right]-\sum_n\ln\left[2\sinh\frac{\beta}{2}\omega_2(k_n)\right]\right], \tag{3.26}$$

where we have subtracted the thermodynamic potential of the magnon sector and considered a static soliton.

Following steps similar to the ones used before we obtain

$$\Omega_s=E_{xy}^0+\beta^{-1}\left\{\ln\left[2\sinh\frac{\beta}{2}\omega_b\right]-\frac{1}{\pi}\left[2\beta m_1c-\int_0^\Lambda\ln\left[2\sinh\frac{\beta\omega_1}{2}\right]\frac{d\Delta}{dk}dk-\int_0^\Lambda\ln\left[2\sinh\tfrac{1}{2}\beta\omega_2(k)\right]\frac{d\Delta}{dk}dk\right]\right\}. \tag{3.27}$$

From Eq. (2.15) we have

$$\frac{d\Delta}{dk}=-\frac{2m_1c^2}{\omega_1^2(k)}\ . \tag{3.28}$$

Substituting (3.28) into (3.26) we find after a straightforward calculation

$$\Omega_s=E_s^0+T\ln(1-e^{-\beta\omega_b})+2T(F_1+F_2)-\frac{2m_1c^2\omega_b^2T}{\pi}\int_0^\infty\frac{\ln(1-e^{-\beta\omega_2})dk}{\omega_1^2(k)\omega_2^2(k)}\ , \tag{3.29}$$

where

$$F_i=-\frac{m_1c^2}{\pi}\int_0^\infty\omega_i^{-2}(k)\ln(1-e^{-\beta\omega_i(k)})dk\ , \tag{3.30}$$

and E_s^0 is given by Eq. (3.21). At $T=0$, Ω_s is the soliton energy E_s^0. At finite temperatures, we can extract the soliton energy from Ω_s by

$$E_s=\Omega_s-T\left[\frac{d\Omega_s}{dT}\right]. \tag{3.31}$$

If we neglect the temperature dependence of m_i coming from the "normal product" at finite temperatures we have

$$E_s = E_s^0 + \frac{\omega_b}{e^{\beta\omega_b}-1} - 2m_1c^2(F_1^0+F_2^0) - \frac{2m_1c^2\omega_b^2}{\pi}\int_0^\infty \frac{dk}{\omega_1^2(k)\omega_2(k)(e^{\beta\omega_b}-1)} ,$$

where

$$F_i^0 = \frac{1}{\pi}\int_0^\infty \frac{dk}{\omega_i(k)}\frac{1}{(e^{\beta\omega_i(k)}-1)} . \tag{3.32}$$

At the absolute zero of temperature, the energy of the moving solition is readily obtained by the Lorentz transformation

$$E_s^0(v) = E_s^0(1-v^2)^{1/2} = E_s^0(1+v^2/2) . \tag{3.33}$$

However, at finite temperatures, this is not necessarily true, as the thermal magnons establish a preferred frame (i.e., $v=0$). Here we follow Mikeska and Frahm,[26] writing for the thermodynamic potential for a moving soliton with velocity v the following expression:

$$\beta\Omega_s(v) = \beta E_s^0(v) + \Sigma(T) , \tag{3.34}$$

where

$$\Sigma(T) = \ln(1-e^{-\beta\omega_b}) + 2(F_1+F_2) - \frac{2m_1c^2\omega_b^2}{\pi}\int_0^\infty \frac{\ln(1-e^{-\beta\omega_2})dk}{\omega_1^2(k)\omega_2^2(k)} . \tag{3.35}$$

Here we have used the phase-shifts and magnon frequencies at zero soliton velocity, although they could be calculated from Lorentz invariance also for finite velocities. The difference, however, is of higher order in E_s^0/T.

The probability of finding one soliton with velocity v is given by

$$n_s(v) = e^{-\beta\Omega_s(v)} , \tag{3.36}$$

in the dilute-soliton-gas limit. Then the total probability of finding one soliton (i.e., the soliton density) is given by

$$n_s = \frac{1}{2\pi}\int dp\, n_s(v) . \tag{3.37}$$

Substituting Eqs. (3.34) and (3.36) into Eq. (3.37) we obtain

$$n_s = \frac{1}{\pi}\int_0^\infty dp\, \exp\{-\beta E_s^0[1+p^2c^2/(E_s^0)^2]^{1/2} - \Sigma\} , \tag{3.38}$$

which can be written

$$n_s = e^{-\Sigma}\frac{E_s^0}{c}\frac{1}{\pi}\int_0^\infty e^{-\beta E_s^0(1+x^2)^{1/2}}dx . \tag{3.39}$$

The integral can be performed exactly giving

$$n_s = \frac{E_s^0}{\pi c}\{\beta E_s^0[K_0(\beta E_s^0)+K_1(\beta E_s^0)]+K_1(\beta E_s^0)\}e^{-\Sigma} , \tag{3.40}$$

where K_0 and K_1 are modified Bessel functions. In the nonrelativistic limit ($\beta E_s^0 \gg 1$) Eq. (3.40) becomes

$$n_s = \frac{1}{\sqrt{2\pi}}\frac{(E_s^0)^{1/2}}{\pi}\frac{e^{-\beta E_s^0-\Sigma}}{c} . \tag{3.41}$$

At high temperatures, $T \gg m_1c$, (but $T < m_2c$ such that the effect of the xz soliton can be neglected) we can take

$$1-e^{-\beta\omega_i} \simeq \beta\omega_i ,$$

in Eq. (3.35) to obtain

$$\Sigma = -\ln[2\beta m_1(m_2+m_1)c^2\omega_b^{-1}] . \tag{3.42}$$

Inserting Eq. (3.42) into Eq. (3.41) we find

$$n_s = n_{SG}\frac{(1+\sqrt{b/\delta})}{(1-b/\delta)^{1/2}} , \tag{3.43}$$

where n_{SG} is the soliton density for the pure SG model (with the soliton) energy renormalized by quantum effects) given by

$$n_{SG} = \frac{2\sqrt{2b}}{\sqrt{2\pi}}(\beta E_s^0)^{1/2}e^{-\beta E_s^0} . \tag{3.44}$$

Equation (3.43) agrees to order $\sqrt{b/\delta}$ with exact transfer integral result[1] for Hamiltonian (1.1). We see that for small b/δ the leading correction to the SG result comes from fluctuations out of the easy xy plane.

At lower temperature ($T \ll m_1c$), taking $\ln(1-e^{-\beta\omega_i})=0$ such that $\Sigma(T)=0$, Eq. (3.41) reduces to

$$n_s = \left[\frac{E_s^0}{2\pi\beta}\right]^{1/2} e^{-\beta E_s^0} . \tag{3.45}$$

Equation (3.45), with E_s^0 the energy of a sine-Gordon soliton, was first obtained by Trullinger.[27]

The case $b \gg \delta$ is identical to the one studied above by just interchanging b and δ. For $\delta = b$, Eqs. (2.2) and (2.3) present a rotational degeneracy, that is, we have a dynamic SG soliton in any plane passing through the x axis. So solitons with all possible phase value ϕ_0 may be excited. For low temperature most of the solitons are then at rest and effects of the velocity can be neglected to lowest order. Now $\omega_1(q)=\omega_2(q)$ and $\omega_b=0$. For $T \gg m_1c$ we obtain from Eq. (3.39)

$$n = (32JS^2b/T)e^{-\beta E_s^0} , \tag{3.46}$$

where E_s^0 is now given by Eq. (3.23). Taking for E_s^0 the classical value, Eq. (3.46) agrees with exact transfer integral result for Hamiltonian (1.1) in the Ising limit.[1] The difference in the temperature dependence of (3.43) and (3.46) is due to the fact that for $\delta = b$ the system has an "Ising-like" behavior with the phase ϕ_0 delocalized. Decreasing b, the system crosses over to the "planar-like" model where $\theta \simeq \pi/2$.

IV. CONCLUSION

From our results we conclude that quantum corrections for Hamiltonian (1.1) with $H=0$ lead to a reduction of the soliton energy. We have also shown that at temperatures $T<m_1c$, where m_1c is the energy of the lowest energy magnon at $q=0$, the calculated soliton density agrees with the classical statistical-mechanics results, as obtained from the transfer matrix approach, if the soliton energy in the classical theory is replaced by the renormalized one of the present theory.

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