Dynamical properties of a gas of solitons in one-dimensional quantum antiferromagnets

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The influence of the soliton-magnon coupling on the dynamical properties of quantum antiferromagnets is studied as a function of the external magnetic field and the temperature. The specific case of tetramethyl ammonium manganese chloride is analyzed above and below the transition temperature. The existence of a dissipative regime for the soliton motion is conjectured and its influence on the dynamical structure factor—which might be experimentally detected—is reported.

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I. INTRODUCTION

In the past few decades it has become well established that the physical properties of some magnetic materials, TMMC (tetramethyl ammonium manganese chloride), CsNiF₃ (caesium nickel fluoride), and CuCl₂ 2NC₅H₅ (dichloro-bis-piridine copper II), for instance, have essentially one-dimensional character above their transition temperature. In those kind of materials the distance between magnetic ions along a given direction (magnetic chain direction) is shorter than in the other directions. In such an arrangement the intrachain coupling constant is typically more than two orders of magnitude stronger than the interchain coupling constant. Therefore, the system can be considered as a set of weakly interacting magnetic chains. Due to the relative simplicity of obtaining solitonic or solitary-wave solutions in one-dimensional (1D) systems, these quasi-one-dimensional magnets turn out to be the paradigm for the study of the influence of the nonlinear modes (solitons) on the dynamical properties of such systems at finite temperatures. Although all real magnetic materials investigated are not perfectly one dimensional, the assumption of the 1D behavior is shown to be in good agreement with the experimental results (see Ref. 1 and the references therein).

In magnetic materials solitons or solitary-waves can be regarded as “kinks” or “twists” in the spin space moving with constant speed and carrying a constant topological charge defined by the values of the spin variables at infinity. For low-enough temperatures, when the linear modes (spin-waves) are not excited, the magnetic system can be represented in first approximation by a gas of noninteracting solitons. Using this idea, Mikeska calculated the soliton contribution to the dynamical structure factor of the classical one-dimensional magnets. From both works we learn that the assumption of ballistic motion for solitons is the origin of the “central peak” behavior observed in neutron scattering experiments. A different situation could be found from the quantum field theory point of view when the temperature is raised. In this case the spin-wave (SW) modes are excited, therefore not all of the degrees of freedom of the system contribute to the soliton formation and a residual interaction (which couples the center of mass of the soliton to the spin-wave modes) shows up leading to a stochastic motion for the soliton.

Several theoretical works have been devoted to studying the soliton stochastic motion and its influence on the properties of the systems in different nonlinear theories. For instance, based on the fact that an incoming phonon (the linear modes of the theory) produces only a shift in the soliton position without changing its momentum, Wada and Schriefter estimated the diffusion constant of an isolated domain wall interacting with a phonon thermal bath. In the same spirit, Theodorakopoulos studied the kink-phonon interaction within the framework of perturbation theory and described the dynamics of a noninteracting kink gas as it would be seen in a light-scattering experiment; on the other hand, a stochastic equation of motion for the sine-Gordon soliton in a gas of magnons and the effects of the solitonic sector on the spin correlation function were presented by Fesser. In the above-mentioned works, the motion of the soliton is assumed to be purely diffusive, which is in contradiction with the experimental results reported in Ref. 7 in which the damping process also plays an important role.

The damping of the magnetization carried by a soliton was studied by Sassaki and Maki for antiferromagnets. In this case, the soliton-soliton collisions are responsible for the appearance of the damping. However, in this scenario, the effects of soliton-magnon collisions give no contribution to the damping mechanism. Therefore, it would be important to investigate the contribution of the soliton-“phonon” collisions in the damping process in a more general context and, derive a Langevin equation of motion in the strict sense. In order to do that, the soliton center of mass must be treated as a true dynamical variable. This would give us information about the random force acting on the soliton and could be used to derive the fluctuation-dissipation theorem.

In studying the dissipative stochastic motion of a soliton due to its collisions with the linear modes (LM) of the theory, we have found a mechanism in which the soliton and the LM momenta are coupled. Therefore, our first goal will be the derivation of a soliton-LM interacting Hamiltonian. In practice, the specific form of this interaction can be obtained via the collective coordinate method when the classical Hamiltonian is quantized. From the interacting Hamiltonian we can compute the reduced density operator for the soliton center of mass from which an equation of motion naturally arises. As it will be seen, the soliton-LM coupling results in a dis-
the dissipative regime described by a Langevin equation of motion for the soliton.

The formulation presented here is general enough to be used in any nonlinear theory with solitonic solution, and therefore, can be applied to studying the specific case of the TMMC antiferromagnet. In this material the spin dynamics is described by two different equations depending on the temperature. For temperatures below \(T_N\), the spin dynamics is governed by a double sine-Gordon (2sG) equation and, for \(T > T_N\), the spins evolve in time following a sine-Gordon (sG) equation. Due to collisions with the LM of the theory the solitonic solutions of those equations have different motional regimes, turning the TMMC into a suitable probe for the investigation of the soliton dynamics.

To begin with, in Sec. II we review the models currently applied to the spin dynamics of the TMMC compound, above and below its transition temperature, and also the corresponding classical field theories. Sections III and IV are devoted to the derivation of the soliton-magnon interacting Hamiltonian and to obtaining of the soliton reduced density operator. In Sec. V the calculation of the damping and diffusion constants for the TMMC is presented. Finally, Sec. VI is devoted to the study of the influence of the soliton damped motion on the dynamical structure factor and, our conclusions are presented in Sec. VII.

II. THE MODEL FOR TMMC

The antiferromagnet TMMC has extensively been studied from the theoretical and experimental points of view. The Hamiltonian describing the interacting 3D array of classical spins in this material can be written as

\[
\mathcal{H} = \sum_j H_j - \frac{1}{2} \sum_{i \neq i'} \sum_j S_{i,j} S_{i',j},
\]

where

\[
H_j = \sum_k \left\{ J_{i,j} S_{i,k} S_{j,k+1} + A(S_{i,j}^z)^2 - g \mu_B B S_{i,j}^y \right\}.
\]

The Hamiltonian \(H_j\) describes the nearest-neighbor intrachain interaction between spins with an easy plane anisotropy \((A > 0)\) placed in an external magnetic field \((B)\) in the \(x\) direction. The spins will be treated as classical vectors of length \(S\) and the constants \(J_{||}\) and \(J_{\perp}\), both positive, correspond to the antiferromagnetic and ferromagnetic exchange coupling constants, respectively. The second term on the right-hand side (rhs) of Eq. (1) represents an intrachain interaction between the spins, completing the description of the 3D spin arrangement. Finally, the following values of material parameters will be used: \(J_{||} = 13.4\ \text{K},\ \ S = 5/2,\ \ A/J_{||} = 0.01 - 0.02,\ \ J_{\perp}/J_{||} = 1.5 \times 10^{-5}\), and \(g = 2.01\).

In order to start the classical description of the spin dynamics it is convenient to look at two main different situations; namely, temperatures below and above the transition temperature. For temperatures below \(T_N\) the system described by Eq. (1) displays long-range magnetic order. Therefore the staggered magnetization is not zero and the system can be described in the mean field approximation as a set of noninteracting antiferromagnetic chains with an additional spontaneous magnetization in the \(y\) direction. Explicitly,

\[
H = \sum_i \left\{ J_{||} S_i S_{i+1} + A(S_i^z)^2 - g \mu_B B S_i^y - g \mu_B B_{MF} (-1)^i S_i^y \right\},
\]

where

\[
B_{MF} = \eta J_{\perp} ((-1)^i S_i^y)/g \mu_B,
\]

and \(\eta\) accounts for the presence of neighboring chains in the model. In the specific case of TMMC, \(\eta = 6\). The intrachain mean field \(B_{MF}\) is usually replaced by its saturation value \(B_s = 22.3\ \text{Oe}\) that results from the substitution of \(S_i^y\) in Eq. (4) by its maximum value.

At this point, we can carry on with the classical description of the spin dynamics. In order to do that it is convenient to change the spin variables to the following form

\[
S_{e,o} = \pm S [\sin(\Theta \pm \theta) \cos(\Phi \pm \varphi), \ \sin(\Theta \pm \theta) \sin(\Phi \pm \varphi), \ \cos(\Theta \pm \theta)],
\]

where \(e\) and \(o\) stands for even and odd sites along a chain.

Using the representation (5) a \(\Phi\)-dependent part of the Hamiltonian (3) can be obtained (see Ref. 11 for details). Explicitly,

\[
H^B = \frac{1}{2} J_{||} S^2 \int dz \left[ \frac{1}{c^2} (\partial_t \Phi)^2 + (\partial_x \Phi)^2 \right. \left. + \frac{1}{4} b^2 \sin^2 \Phi - 2 b_\perp \sin \Phi \right],
\]

where

\[
c^2 = 4 + \frac{2A}{J_{||}}, \quad b = \frac{g \mu_B B}{J_{||} S}, \quad b_\perp = \frac{g \mu_B B_{MF}}{J_{||} S},
\]

and the time and length scales are \((J_{||} S)^{-1}\) and the lattice constant, respectively.

It should be stressed that the Hamiltonian (6) is an approximated description of the real TMMC system. To reproduce the experimental results, magnon mass and solitonic energy, for instance, quantum effects and the out-of-plane component of the magnetization must be taken into account. To go on with the classical description of the \(\Phi\)-dependent part of the original Hamiltonian (1) the equation of motion associated to Eq. (6),

\[
\frac{1}{c^2} \partial_{tt} \Phi = \partial_x \Phi + \frac{b^2}{8} \sin 2 \Phi + b_\perp \cos \Phi
\]

has to be solved. Although equation (8) is not completely integrable it has solitonic solutions in the form of \(2\pi\) kinks(antikinks), specifically...
\[ \cos \Phi = \pm 2 \frac{\sqrt{\alpha}}{1 + \alpha \sinh^2 y}, \quad (9) \]

\[ \sin \Phi = 1 - \frac{2}{1 + \alpha \sinh^2 y}, \quad (10) \]

where

\[ \Phi = \begin{cases} 
2 \tan^{-1} \exp[\pm (z-z_0)b/2], \\
2 \tan^{-1} \exp[\pm (z-z_0)b/2] + \pi,
\end{cases} \]

for spin rotations from 0 to \( \pi \)

\[ U(\Phi) = \frac{b^2}{8} \sin 2\Phi + b_\perp \sin \Phi. \quad (14) \]

To quantize the system described by Eq. (13) we need to evaluate

\[ G(t) = \text{tr} \int D\Phi \exp \frac{i}{\hbar} S[\Phi]. \quad (15) \]

where the functional integral has the same initial and final configurations and \( \text{tr} \) means to integrate it over all such configurations. As the functional integral in Eq. (15) is impossible to be evaluated for a potential energy density as in Eq. (14) we must choose an approximation to do it. Since the magnetic moments on the manganese sites in the TMMC are large (5/2), the semiclassical limit will be chosen as the appropriate one in our case. Within the functional integral formalism of quantum mechanics, the semiclassical limit is simply the stationary-phase method applied to Eq. (15) around the solitonic solutions (9), (10) or (12) in which we are interested. When this is done we are left with an eigenvalue problem that reads

\[ \left\{ -\frac{d^2}{dz^2} + U''(\Phi_s) \right\} \psi_s(z-z_0) = k_s^2 \psi_s(z-z_0), \quad (16) \]

where \( \Phi_s \) is denoting the solitonlike solution around which we are expanding \( \Phi(z,t) \) and \( \psi_s(z-z_0) \) are the spin-wave modes in the presence of the soliton.

Now one can easily show that \( d\Phi_s/dz \) is a solution of Eq. (16) with \( k_s=0 \). The existence of this mode is related to the translation invariance of the system and causes a divergence of the functional integral in Eq. (15) in the semiclassical limit (Gaussian approximation). The way out of this problem is the so-called collective coordinate method. This method consists basically in expanding the field configurations about \( \Phi_s(z) \) as

\[ \Phi(z,t) = \Phi_s(z-z_0(t)) + \sum_{n=1}^{\infty} c_n \psi_n(z-z_0(t)). \quad (17) \]
but promoting the $c$-number $z_0$ to a position operator. Using expansion (17), the second quantized version of Eq. (6) can be written as

$$\hat{H} = \frac{1}{2M_s} \left( \hat{P} - \sum_{mn} \hbar g_{mn} b_n^+ b_m \right)^2 + \sum h\Omega_n b_n^+ b_n,$$

(18)

where $\Omega_n = c k_n$.

In the Hamiltonian (18), $\hat{P}$ stands for the momentum canonically conjugated to $\hat{z}_0$.

$$M_s = \frac{2\hbar S^2 a}{c^2} \int_{-\infty}^{+\infty} dz U(\Phi_s(z))$$

(19)

is the soliton mass and the coupling constant $g_{mn}$ is given by

$$g_{mn} = \frac{1}{2i} \left[ \frac{\Omega_m}{\Omega_n} + \sqrt{\frac{\Omega_n}{\Omega_m}} \right] \int dz \psi_m(z) \frac{d\psi_n(z)}{dz}.$$  

(20)

The operators $b^+$ and $b$ are respectively the creation and annihilation operators of the linear excitations of the magnetic system (magnons) in the presence of the soliton. The second term in Eq. (18) is the energy of the noninteracting linear-modes of the theory. On the other hand, the first term can be interpreted as the kinetic energy of the soliton. Notice that

$$\dot{z}_0 = \frac{1}{i\hbar} [\hat{z}_0, \hat{H}] = \frac{1}{M_s} \left( \hat{P} - \sum_{mn} \hbar g_{mn} b_n^+ b_m \right),$$

(21)

and so $\hat{P}$ cannot be the soliton momentum because, since

$$\dot{\hat{P}} = \frac{1}{i\hbar} [\hat{P}, \hat{H}] = 0$$

(22)

it is a constant of motion. From Eq. (21), $M_s \dot{z}_0$ can be interpreted as the soliton momentum, and therefore, $\sum_{mn} \hbar g_{mn} b_n^+ b_m$ is nothing but the momentum of the linear-modes field.

At this point we have reformulated the problem of solitons and LM in the system in such a way that, the momentum associated with the soliton is now coupled to the linear-modes momenta. This interaction suggests that the soliton will behave as a Brownian particle due to its collisions with the linear-modes. It is important to notice that in this formulation both the stochastic and damped motions of the solitons have the same origin as it should be expected due to the fluctuation-dissipation theorem. On the other hand, as the population of magnons is a temperature-dependent quantity, the soliton mobility will be strongly related to the temperature of the system and, its dynamics [determined by Eq. (18)] will be nontrivial.

**IV. EFFECTIVE SOLITON DYNAMICS**

As we are interested in the average values of observables just for the soliton we need to compute its reduced density operator. This can be done by tracing the magnon coordinates out in the density operator for the whole system (soliton plus magnons). Following closely Ref. 13 the soliton density operator can be expressed as

$$\hat{\rho}(x,y,t) = \int dx' dy' J(x,y,t;x',y',0) \hat{\rho}_s(x',y',0),$$

(23)

where $J$ is the Feynman-Vernon superpropagator. Explicitly

$$J = \int_0^T d\tau_1 \int_x^y d\tau_2 \exp \left[ \frac{i}{\hbar} S[x,y] + \frac{1}{\hbar} \Phi^R[x,y] \right],$$

(24)

where

$$S[x,y] = S_0[x] - S_0[y] + \Phi^I[x,y],$$

(25)

and the action associated with the free soliton motion is

$$S_0[x] = \int_0^T \frac{(\dot{x})^2}{2} dt,$$

(26)

with $M_s$ given by Eq. (19). It is convenient to notice that the action $S[x,y]$ for the soliton dynamics does not describe a free particle, and the whole information regarding the soliton-magnon interaction is contained in the functionals $\Phi^I$ and $\Phi^R$.

$$\Phi^I = \int_0^T dt \int_0^t \left\{ (\dot{x}(t') + \dot{y}(t')) \times \Gamma^I(t' - t'') (\dot{x}(t'') - \dot{y}(t'')) \right\} dt'',$$

(27)

and

$$\Phi^R = \int_0^T dt \int_0^t \left\{ (\dot{x}(t') - \dot{y}(t')) \times \Gamma^R(t' - t'') (\dot{x}(t'') - \dot{y}(t'')) \right\} dt''.$$

(28)

Here

$$\Gamma^I(t) = \hbar \Theta(t) \sum_{mn} g_{mn}^2 (\tilde{N}_m - \tilde{N}_n) \sin(\omega_n - \omega_m) t,$$

(29)

$$\Gamma^R(t) = \frac{1}{2} \hbar \Theta(t) \sum_{mn} g_{mn}^2 (\tilde{N}_m + \tilde{N}_n + 2 \tilde{N}_m \tilde{N}_n) \times \cos(\omega_n - \omega_m) t,$$

(30)

with

$$\tilde{N}_m = \frac{1}{\exp(\beta \hbar \omega_m) - 1},$$

(31)

$\Theta(t) = 1(0)$ if $t > 0 (< 0)$ and the form of $g_{mn}$ given by Eq. (20).

In order to understand the meaning of the reduced action for the soliton (25), it is convenient to define the new variables $R = (x + y)/2$ and $r = (x - y)$. In terms of these variables the equations of motion generated from the variation of Eq. (25) can be written as
\[ \dot{R}(t) + \int_0^t \gamma(t-t') \dot{R}(t') dt' = 0, \quad (32) \]

\[ \dot{r}(t) - \int_0^t \gamma(t-t') \dot{r}(t') dt' = 0. \quad (33) \]

As it can be seen, Eqs. (32) and (33) are nothing but the equations for the mean value of the center of the wave packet \( \langle R \rangle \) associated with the soliton and for the spreading of its width \( \langle r \rangle \). In Eq. (32) it is explicit that the mean value of the fluctuating force acting on the soliton is zero. At the same time, equations (32) and (33) tell us that the linear modes act on the soliton not simply as a random force but also as a viscous medium, implying that the soliton motion is not purely diffusive.

The damping function \( \gamma(t-t') \) in Eqs. (32) and (33) is given by

\[ \gamma(t) = \frac{\hbar \Theta(t)}{M_s} \sum_{mn} |g_{mn}|^2 (\overline{\mathcal{N}}_m - \overline{\mathcal{N}}_n) (\omega_n - \omega_m) \times \cos(\omega_n - \omega_m)t. \quad (34) \]

Generally, in the analysis of a stochastic motion one is interested in time scales much longer than \( (\omega_n - \omega_m)^{-1} \). In this case, the damping function can be shown to reduce to the form \(^{34}\)

\[ \gamma(t) = \gamma(t) \delta(t), \quad (35) \]

where we denote by \( \gamma \) the temperature-dependent quantity given by

\[ \gamma = \frac{M_{mg}}{2 \pi \hbar} \int_0^\infty dE \mathcal{R}(E) \frac{\beta E e^\beta E}{(e^{\beta E} - 1)^2}. \quad (36) \]

In Eq. (36) \( \mathcal{R}(E) \) is the reflection coefficient of the “potential” \( U'(\Phi_i) \) of the Schrödinger-like equation (16) and \( M_{mg} \) is the magnon mass. Therefore, within the collective coordinate approach, the soliton dynamics is governed by the way in which the linear modes are scattered by the soliton potential.

To complete the description of the soliton motion we proceed to analyze the real part of the exponent (24). In order to do that, we will assume the long-time approximation when Eqs. (25)–(30) are substituted in Eq. (24). After some manipulations the superpropagator for the soliton can be written as

\[ \mathcal{J} = \int \int dx \int dy \exp \left[ \frac{i}{\hbar} \int_0^t \left( \frac{1}{2M_s} (\dot{x}^2 + \dot{y}^2) - 2M_s \gamma(x\dot{x} - y\dot{y} + x\dot{y} - y\dot{x}) \right) dt' \right. \]

\[ \times \exp \left. \left[ - \frac{1}{\hbar} \int_0^t \int_0^t [x(t') - y(t')] dt' \right] \right] \]

\[ \times \alpha_R(t''-t') [x(t'') - y(t'')] dt' dt''. \quad (37) \]

with

\[ \alpha_R(t''-t') = \frac{2M_s \gamma}{\pi} \int_0^\infty \frac{1}{\coth \frac{\hbar \omega}{2kT} \cos \omega(t''-t')} d\omega. \quad (38) \]

The superpropagator (37) has exactly the same form as that obtained by Caldeira and Leggett in the study of the quantum Brownian motion. \(^{12}\) Therefore, as they demonstrated, \( \alpha_R(t''-t') \) is nothing but the correlation of forces acting on the soliton or

\[ \langle F(t')F(t'') \rangle = \frac{2M_s \gamma}{\pi} \int_0^\infty \frac{1}{\coth \frac{\hbar \omega}{2kT} \cos \omega(t''-t')} d\omega, \quad (39) \]

and it is directly related to the diffusive motion of the soliton, as will be demonstrated later.

On the other hand, is not hard to verify that Eq. (39) reproduce the usual correlation of forces for the Brownian motion in the high-temperature limit (classical regime). In fact, when \( kT \gg \hbar \omega \),

\[ \langle F(t')F(t'') \rangle = 4M_s \gamma kT \lim_{\omega \to \infty} \frac{\sin \omega(t''-t')}{\pi(t''-t')} = 4M_s \gamma kT \delta(t''-t'). \quad (40) \]

Unless we know the main features of the soliton motion we need to proceed further and perform the functional integrations in Eq. (24). Following closely Ref. 15 we get a closed expression for the time evolution of the soliton density operator, namely,

\[ \mathcal{J} = \left( \frac{N(t)}{\pi \hbar} \right)^2 \exp \left[ \frac{i}{\hbar} \left( \frac{K(t) - M_s \gamma}{2} \right) Rr \right. \]

\[ + \left. \left( K(t) + \frac{M_s \gamma}{2} \right) R_i r_i - L(t) R r - N(t) R r_i \right] \]

\[ \times \exp \left. \left[ - \frac{1}{\hbar} \left( A(t)^2 + B(t)^2 R_i r_i + C(t)^2 \right) \right] \right), \quad (41) \]

where the time-dependent functions are given explicitly in Appendix A.

Now we have the tool we need to calculate the time development of the reduced-density operator for the soliton. We can assume, for instance, that initially the soliton center is at the origin and in a pure state described by an initial momentum \( p \) and a width \( \sigma \). The reduced-density operator in this situation is

\[ \tilde{\rho}(R, r, 0) = \frac{1}{\sqrt{2\pi \sigma^2}} \exp \frac{i \eta r_i}{\hbar} \exp \frac{R_i^2 + r_i^2}{2 \sigma^2}, \quad (42) \]

which evolves in time as

\[ \tilde{\rho}(R, r, t) = \int \int dR' dR_i \mathcal{J}(R, r; R', r_i) \tilde{\rho}(R', r_i, 0). \quad (43) \]
Substituting Eqs. (41) and (42) in Eq. (43) and making \( r = x - y = 0 \) we get the time development of the diagonal elements of the reduced-density operator as

\[
\tilde{\rho}(R, t) = \frac{N(t)}{\sqrt{\pi(2\sigma^2 K_1^2(t) + h C_1(t))}} \exp \left[ - \frac{N^2(t)}{2\sigma^2 K_1^2(t) + h C_1(t)} \left( R - \frac{P}{2N(t)} \right)^2 \right].
\]

This expression shows that the soliton center evolves following the path

\[
R(t) = \frac{P}{2M_0^* \gamma}(1 - e^{-2\gamma t}),
\]

which is nothing but the one of a classical damped particle. On the other hand, expression (44) gives us the width of the wave packet at any time as

\[
\sigma^2(t) = \left[ \left( R - R(t) \right) \right]^2 = \frac{2\sigma^2 K_1^2 + h C_1}{2N^2(t)}.
\]

As shown in Ref. 15, this expression automatically obeys the fluctuation-dissipation theorem and allows us to calculate the diffusion constant for this Brownian particle, in the classical limit

\[
D = 2M_0^* \gamma kT.
\]

Now, once we know the solitonic solutions at rest and the reduced-density operator for the soliton center of mass, the time-dependent soliton configurations can be obtained straightforwardly as

\[
S^{(x)}(z(t) - z_0) = \int_{-\infty}^{+\infty} S^{(x)}(z - z_0 - R(t)) \tilde{\rho}(R, t) dR,
\]

where \( z_0 \) denotes the initial position of the soliton center of mass and \( S^{(x)} \) are the components of the spin configurations at rest, given by

\[
S^x = \pm \frac{1}{\cosh(z - z_0)} b/2, \quad S^y = \pm \tanh(z - z_0) b/2
\]

for \( T > T_N \), and

\[
S^z = \mp \frac{\sqrt{\alpha \sinh(z - z_0)}}{1 + \alpha \sinh^2(z - z_0)} \frac{b_+}{\alpha},
\]

\[
S^y = \pm \frac{2}{1 + \alpha \sinh^2(z - z_0)} b_+ / \alpha
\]

for \( T < T_N \) with \( \alpha = b_+ / (b_+ + b_0^2/4) \).

Up to this point we have demonstrated that the superpropagator (24) describes the motion of a Brownian particle in the strict sense. Then, to study the influence of this kind of dynamics on the properties of the system, we can use the time-dependent soliton configurations mentioned above to compute the dynamical structure factor of a set of randomly distributed solitons. In order to do that we will calculate the explicit values of the damping constant (basically the inverse of the mobility) and the spreading of the width for temperatures above and below \( T_N \).

V. SOLITON MOBILITY

In order to compute the soliton mobility we need the explicit form of the potential \( U''(\Phi) \) involved in Eq. (16) to evaluate the reflection coefficient that enters Eq. (36). Let us begin with the simpler case, namely, the situation in which the temperature is above the transition temperature.

A. Soliton mobility for \( T > T_N \)

Performing the calculation of the \( \pi \)-soliton mobility for \( T > T_N \) we simply set \( b_+ \) in the Hamiltonian (6) to zero the and therefore, the equation of motion for the \( \Phi \)-dependent part of the spin degree of freedom (8) becomes a \( s_N \) equation with solitonic solution (12). In this case the potential involved in the Schrödinger-like equation (16) that determines the fluctuations around the soliton solution have the form

\[
U''(z) = \xi^2 (1 - 2 \text{sech}^2 \xi z),
\]

where \( \xi = b/2 \). The spectrum of Eq. (51) contains a bound state with zero energy\(^\dagger\)

\[
\psi_0 = \sqrt{\frac{\eta}{2}} \text{sech}(\xi z), \quad k_0 = 0,
\]

which constitutes the translation mode of the soliton (Goldstone mode), and a continuum of quasiparticles modes (magnons) given by

\[
\psi_n(x) = \frac{1}{\sqrt{L}} \left[ \frac{k_n + i \xi \tanh(\xi z)}{k_n + i \xi} \right] e^{i k_n z},
\]

where

\[
k_n = \frac{2n \pi}{L} - \delta(k_n), \quad \delta(k) = \arctan \left[ \frac{2 \xi k}{k^2 - \xi^2} \right].
\]

On the other hand, the reflection coefficient \( \mathcal{R} \) for a general symmetric potential can be expressed in terms of the corresponding even- and odd-phase shifts\(^\dagger\)

\[
\mathcal{R}(E) = \sin^2\left[ \delta_0(E) - \delta_0(E) \right].
\]

Now, re-expressing Eq. (53) in terms of parity eigenstates it is easy to prove that the potential (51) belongs to the class of reflectionless potentials because its phase shifts are given by

\[
\delta^{\pi}(k) = \arctan(\xi k),
\]

that do not distinguish between odd and even parities. Therefore no matter how high the temperature rises above \( T_N \) the damping coefficient is always zero and as a direct consequence the interaction between soliton and magnons do not modify its motional regime. From this result we can conclude that the damped motion observed above the transition...
temperature in Ref. 7 is due to some other mechanism; that could be the one proposed by Sasaki and Maki in Ref. 8.

**B. Soliton mobility for \( T < T_N \)**

When the temperature drops below \( T_N \), the potential generated by the 2sG soliton that enters the Schrödinger-like equation (16) has the form

\[
U''(\Phi^2_{sG}) = \frac{1}{\lambda^2} \left[ 1 - 2 \tanh^2 \left( \frac{z}{\lambda} + \rho \right) - 2 \tanh^2 \left( \frac{z}{\lambda} - \rho \right) + 2 \tanh \left( \frac{z}{\lambda} + \rho \right) \tanh \left( \frac{z}{\lambda} - \rho \right) \right],
\]

(57)

where

\[
\lambda = \frac{1}{b_\perp + b^2/4}, \quad \cosh \rho = \frac{1}{\sqrt{\alpha}}, \quad \alpha = \frac{b_\perp}{b_\perp + b^2/4}.
\]

As it can be seen, the second and third terms on the rhs of Eq. (57) are the potentials of the noninteracting \( \pi \) solitons located at \( z/\lambda = \pm \rho \) whereas the last term describes the interaction of the two \( \pi \) solitons at \( z/\lambda = \pm \rho \), respectively. When \( b \gg b_\perp \) the third term in Eq. (57) is negligible and as a result we are left with a pair of \( \pi \) solitons that move without dissipation as for \( T > T_N \). As the strength of the external field decreases the \( \pi \) solitons get closer and cannot be treated independently anymore. In that situation of moderate fields the relative motion of these solutions must be taken into account. Now, in the limit of weak external field both \( \pi \) solitons overlap and, as its relative motion can be neglected. In this limit, the potential (57) can be handled in a perturbative fashion as shown below. Another important point about Eq. (57) is that for all finite values of \( \lambda \) and \( \rho \), the system is translationally invariant and, consequently, has a zero-energy state

\[
\psi_0 \propto \tanh \left( \frac{z}{\lambda} + \rho \right) + \tanh \left( \frac{z}{\lambda} - \rho \right),
\]

(59)

which is nothing but the Goldstone mode of the 2\( \pi \) soliton for finite transverse magnetization and finite external field.

In the limit of weak external fields (\( b_\perp \gg b^2/2 \)), when \( \rho \ll 1 \), the Schrödinger-like equation (16) can be written as

\[
-\frac{d^2}{dz^2} + V(z) \psi_n(z) = \kappa_n^2 \psi_n(z), \quad \kappa_n^2 = k_n^2 - \frac{1}{\lambda^2} - \frac{\rho^2}{\lambda^2},
\]

(60)

where

\[
V(z) = V_0(z) + \left( \frac{b_\perp}{\lambda} \right)^2 V_1(z),
\]

(61)

with

\[
V_0(z) = -2 \tanh^2 \left( \frac{z}{\lambda} \right)
\]

(62)

and

\[
V_1(z) = -8 \tanh^2 \left( \frac{z}{\lambda} \right) \tanh^2 \left( \frac{z}{\lambda} \right).
\]

(63)

The potential (57) is now reduced to the sum of two contributions; one coming from the spontaneous staggered magnetization and, the other, from the presence of the weak external field. The calculation of the even and odd phase shifts is reported in Ref. 18 and here we will only show the main results of the numerical solution of the Schrödinger-like equation (60). Figures 1 and 2 show the even- and odd-parity phase shifts for different values of the external field.

The values of \( \delta_e \) and \( \delta_o \) for \( k = 0 \) are in agreement with the 1D version of Levinson’s theorem\(^{19} \) which establishes that

\[
\delta'(k=0) = \pi n^e - \frac{1}{2}, \quad \delta'(k=0) = \pi n^o,
\]

(64)

where \( n^e \) and \( n^o \) are the number of even- and odd-parity bound states.

As it can be seen in Fig. 1 the even-phase shift is \( \pi/2 \) at the origin. This behavior is in complete agreement with the existence of an even bound state corresponding to the Goldstone mode. On the other hand, the odd-phase shift \( \delta_o(0) = \pi \), indicates the presence of an odd bound state. This result was previously obtained by Kivshar et al.\(^{20} \) in the study of the small-amplitude modes around the localized solution of the 2sG equation and shows that there is always an odd bound state in this kind of system. Therefore, the spectrum of...
is composed by: (i) the \( \psi_0 \) solution \((59)\) corresponding to the translation mode of the soliton (Goldstone mode) (ii) an internal mode that appears when the system is perturbed by the external magnetic field and (iii) the \( \psi_k \) solutions that constitute a continuum of modes and correspond to magnons.

In order to find the damping coefficient we must compute the reflection coefficient \( R(k) \). This can be done by inserting the numerical results of the even- and odd-phase shifts into the general expression \((55)\). In Fig. 3, we have plotted \( R \) for different values of the perturbation parameter \( \rho \) for the whole range of \( k \). Having done that, one can immediately integrate the function \( R \) in expression \((36)\) that finally allows us to describe the damping coefficient as a function of the temperature (see Fig. 4). As it can be seen, the damping coefficient is linear for high temperatures. This result can be obtained directly from Eq. \((36)\). In fact, for \( T \) high enough the damping constant can be approximated by

\[
\gamma \approx \frac{M_{ms}}{2\pi M_s} \int_0^\infty dE \frac{R(E)}{E} \propto T, \tag{65}
\]

which is linear in \( T \), independently of the explicit form of \( R(E) \). In the low-temperature regime we can write

\[
\gamma \approx \frac{M_{ms}}{2\pi M_s} \int_0^\infty dE R(E) \beta E e^{-\beta E}, \tag{66}
\]

where \( E \) always presents a gap determined by the presence of the magnetic field and/or the spontaneous staggered magnetization. Here we shall not attempt to write an approximate expression for Eq. \((66)\) because the correct behavior of the reflection coefficient was only numerically determined. As it is shown in Fig. 4, for low-enough temperatures, the damping coefficient drops exponentially to zero due to the existence of the gap. As the temperature increases the damping coefficient rises following a power-law behavior until it becomes linear for high-enough temperatures. This strong temperature dependence of the damping parameter, for \( T \) below the transition temperature, will influence directly the correlation function between the magnetic solitons.

As we have seen, the interaction with magnons leads to the different soliton motional regimes depending on how they are scattered by the solitonic potential. For \( T \) above \( T_N \) the \( \pi \) solitons have infinite mobility so, the magnons do not contribute to the damping process and below the transition temperature the \( 2\pi \) solitons behave like Brownian particles with a finite damping parameter. In the next section we will investigate the influence of the soliton dissipative motion on the dynamical structure factor.

**VI. DYNAMICAL STRUCTURE FACTOR**

The problem of the soliton contribution to the dynamical structure factor (DSF) above and below the transition temperature in the TMMC was studied by Holyst\(^{11}\) within the ideal gas approximation, and therefore no diffusive or damped processes were considered. The diffusive effects and the damping of the magnetization carried by a soliton in this problem for \( T \) above \( T_N \) was reported in Ref. 8. As it was mentioned before, the mechanism responsible for the damping in this case can be attributed to the soliton-soliton colli-
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\[
S^{\|}(q, \omega) = \delta(q) \delta(\omega)S^2[1 - n_sF^\|_0]^2 + \frac{1}{2\pi} n_sS^2|F^\|_0|^2G(q, \omega),
\]

where \(n_s\) is the soliton density and

\[
G(q, \omega) = \sqrt{\frac{2\pi B_E}{q^2\sigma^2}} \exp\left(\frac{\beta E\omega^2}{2c^2q^2}\right),
\]

\[
F^\|_0 = \frac{\pi d}{2} \sinh(qd\sqrt{1 - \alpha/8}),
\]

\[
F^\perp_0 = \frac{\pi d}{2} \sin(qd\sqrt{1 - \alpha/8}),
\]

with

\[
E_s = 2Bg\mu_B\delta[S\sqrt{1 + 4b/\sigma^2 + 4b - 2\sinh^{-1}(bb^{1/2})}],
\]

\[
\sigma = \frac{\sqrt{1 - \alpha}}{8}\ln\left(\frac{2}{\alpha - 1 + \sqrt{1 - \alpha}}\right), \quad d = \frac{8}{b}.
\]

The correlations described by Eq. (69) are induced by single kinks moving from the origin to the position \(z\) in a time interval from 0 to \(t\). As expected, the Maxwellian velocity distribution used to describe the 2\(\pi\)-kink gas is directly reflected in the Gaussian dependence of the longitudinal structure factor with the frequency.

With the previous results in mind we can go further on and study the influence of the dissipative regime in the dynamical properties of the 2\(\pi\)-kink gas. As it was shown before, below the transition temperature the 2\(\pi\) solitons move in a dissipative regime according to

\[
S^{\|}(z(t) - z_0) = \frac{1}{\sqrt{4\pi D|t|}} \int_{-\infty}^{+\infty} S^{\|}(z - z_0 - R) \times \exp\left(-\frac{(R - p |t|/M_s)^2}{2D|t|}\right) dR,
\]

where

\[
f(t) = \frac{1}{2\gamma}(1 - e^{-2\gamma}).
\]

Now, substituting Eqs. (75) and (76) in the general expression (67) and taking the mean value we get

\[
S^\|_0 = \frac{n_sS^2}{2\pi} |F^\perp_0|^2G(q, \omega),
\]

\[
S^\|_0 = \delta(q) \delta(\omega)S^2[1 - n_sF^\|_0]^2 + n_sS^2|F^\|_0|^2G(q, \omega),
\]

where the function \(G(q, \omega)\) is now given by

\[
G(q, \omega) = \sqrt{\frac{2\pi B_E}{q^2\sigma^2}} \exp\left(\frac{\beta E\omega^2}{2c^2q^2}\right),
\]

\[
F^\|_0 = \frac{\pi d}{2} \sinh(qd\sqrt{1 - \alpha/8}),
\]

\[
F^\perp_0 = \frac{\pi d}{2} \sin(qd\sqrt{1 - \alpha/8}),
\]

with

\[
E_s = 2Bg\mu_B\delta[S\sqrt{1 + 4b/\sigma^2 + 4b - 2\sinh^{-1}(bb^{1/2})}],
\]

\[
\sigma = \frac{\sqrt{1 - \alpha}}{8}\ln\left(\frac{2}{\alpha - 1 + \sqrt{1 - \alpha}}\right), \quad d = \frac{8}{b}.
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\]

where

\[
f(t) = \frac{1}{2\gamma}(1 - e^{-2\gamma}).
\]

Now, substituting Eqs. (75) and (76) in the general expression (67) and taking the mean value we get

\[
S^\|_0 = \frac{n_sS^2}{2\pi} |F^\perp_0|^2G(q, \omega),
\]

\[
S^\|_0 = \delta(q) \delta(\omega)S^2[1 - n_sF^\|_0]^2 + n_sS^2|F^\|_0|^2G(q, \omega),
\]

where the function \(G(q, \omega)\) is now given by


\[ G(q, \omega) = \int_{-\infty}^{\infty} \exp \left[ -\frac{q^2c^2}{2E_s \beta} f^2(t) - q^2 D |t| - i \omega t \right] dt. \]

(79)

It is important to notice that when the diffusion and damping constants tend to zero in Eq. (79), we can write

\[ G(q, \omega) = \int_{-\infty}^{\infty} \exp \left[ -\frac{q^2c^2}{2E_s \beta} f^2(t) - i \omega t \right] dt \]

\[ = \sqrt{\frac{2\pi \beta E_s}{q^2c^2}} \exp \left[ -\frac{\beta E_s \omega^2}{2c^2q^2} \right], \]

(80)

which is precisely the result of Eq. (70). On the other hand, to perform the time integration it is convenient to use the expansion

\[ \exp \left[ -\frac{q^2c^2}{2E_s \beta} f^2(t) \right] = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left( \frac{q^2c^2}{2E_s \beta \gamma} \right)^n \]

\[ \times \sum_{m=0}^{2n} (-1)^m C_m^2 e^{-2m \gamma |t|}, \]

(81)

where

\[ C_m^2 = \frac{(2n)!}{m! (2n-m)!}. \]

(82)

Now, substituting Eqs. (81) and (82) in Eq. (79) we get

\[ G(q, \omega) = \sum_{n=0}^{\infty} \sum_{m=0}^{2n} C_m^2 \left( \frac{q^2c^2}{2E_s \beta \gamma} \right)^n \]

\[ \times \frac{4m \gamma + 2q^2 D}{(2m \gamma + q^2 D)^2 + \omega^2}. \]

(83)

which together with Eqs. (77) and (78) define the dynamical structure factor in both directions, namely, parallel and perpendicular to the external magnetic field. In order to get a better idea of the changes introduced by the soliton diffusive and damped motion in the DSF, we show in Fig. 5 a numerical evaluation of Eq. (83) and the corresponding ballistic behavior (69). As it can be seen, the damped/diffusive motion of the solitons (due to interaction with magnons) for temperatures below \( T_N \), changes the behavior of the dynamical structure factor reducing and flattening the central peak in any direction. On the other hand, as the external field becomes weaker (small \( \rho \) values) \( G(q, \omega) \) tends to the ballistic behavior as expected from the results of the \( \pi \)-soliton dynamics.

Although the expression (83) is valid for all finite values of \( q \), it is helpful to study the behavior of Eq. (79) for small momentum and get a simpler expression that can be easily compared to the experiments. Assuming that

\[ q \ll \frac{\gamma}{c} \sqrt{2 \beta E_s}, \]

(84)

the integral in Eq. (79) becomes

\[ G(q, \omega) \approx \frac{2q^2 D}{q^2 D^2 + \omega^2} - \frac{q^2}{2 \pi \beta \gamma^2} \left( \frac{2q^2 D}{q^2 D + \omega^2} \right)^2 \]

\[ + \frac{2q^2 D + 4 \gamma}{(q^2 D + 2 \gamma)^2 + \omega^2} - \frac{2(q^2 D + 2 \gamma)}{(q^2 D + \gamma)^2 + \omega^2}. \]

(86)

Within the approximation of small momentum, the behavior of \( S^{(\perp)}(q, \omega) \) with frequency, changes from the “Gaussian” central peak to a “Lorentzian” dependence. Therefore, as the temperature is lowered below \( T_N \), the central-peak behavior is replaced by a flatter one in the frequency domain. This result is a direct consequence of the dissipative regime of the \( 2\pi \) soliton and, as the damping constant \( \gamma \) can be controlled by changing the temperature and/or the magnetic field, a possible indication of a nonballistic regime has been found.

FIG. 5. The \( G(q, \omega) \) function for \( q=1 \) at \( T=0.5 \) K. The continuous line correspond to the ballistic case while the squares, triangles, and dots correspond to \( \rho=0.14, \rho=0.31 \), and \( \rho=0.50 \) cases, respectively.

\[ G(q, \omega) = \int_{-\infty}^{\infty} \left[ 1 - \frac{q^2}{2E_s \beta \gamma^2} \right] \exp(-q^2 D |t| - i \omega t) dt, \]

(85)
VII. CONCLUSIONS

In this paper we have analyzed the magnetic soliton dynamics from the quantum field theory point of view. We have shown that within this framework, the soliton momentum is coupled to the momentum of the linear excitations of the system (magnons) giving a separate contribution from the soliton-magnon collisions to the damping process. Our results show that the magnetic solitons in the TMMC move as a Brownian particle depending on the system temperature. Two different situations were analyzed separately; the first, above the transition temperature $T_N$ where the $\pi$ soliton moves without dissipation. From this fact we can conclude that the soliton-magnon coupling does not affect the soliton dynamics above $T_N$ and therefore do not contribute to the mechanism proposed by Sassaki and Maki$^8$ to explain the origin of the damped motion in such a situation. On the other hand, when the temperature is below $T_N$ any damping effect should be related to the momentum-momentum coupling between the soliton and the magnons thermal bath since the mechanism proposed in Ref. 8 is no longer valid.

The calculation of the transport properties of the $2\pi$ soliton was performed from the microscopic basis and no phenomenological assumptions were made. The damping and diffusion constants used to describe the soliton dynamics obey the fluctuation-dissipation theorem and are temperature-dependent quantities, since the magnons must be thermally activated in order to scatter the soliton. Although the formulation used to compute the damping parameter is valid for all values of the external magnetic field, we have restricted ourselves to the study of weak fields in order to avoid a more cumbersome treatment. Therefore, some more care is required in the case of moderate fields if one wants to employ more realistic values for the damping and diffusion constants when comparing our results to the experimental data. Nevertheless, the results presented in this work are a clear evidence that the dissipation and/or diffusive effects, coming from the soliton-magnon coupling, tend to flatten off the central peak typical of the ballistic soliton motion.

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APPENDIX CONSTANTS

$$A(t) = \frac{M_s}{\pi} \gamma \int_0^\Omega \nu \coth \frac{\hbar \nu}{2KT} A_s(t) d\nu$$

(A1)

$$A_s(t) = \frac{e^{-2\gamma t}}{\sin^2 \omega t} \int_0^\tau \int_0^\nu \sin \omega \tau \cos \nu(\tau - s) e^{\gamma(\tau + s)} \sin \omega s d\tau ds$$

(A2)

$$B(t) = \frac{M_s}{\pi} \gamma \int_0^\Omega \nu \coth \frac{\hbar \nu}{2KT} B_s(t) d\nu$$

(A3)

$$B_s(t) = \frac{2e^{-\gamma t}}{\sin^2 \omega t} \int_0^\tau \int_0^\nu \sin \omega \tau \cos \nu(\tau - s) e^{\gamma(\tau + s)} \times \sin \omega (t-s) d\tau ds$$

(A4)

$$C(t) = \frac{M_s}{\pi} \gamma \int_0^\Omega \nu \coth \frac{\hbar \nu}{2KT} C_s(t) d\nu$$

(A5)

$$C_s(t) = \frac{1}{\sin^2 \omega t} \int_0^\tau \int_0^\nu \sin \omega (t-\tau) \cos \nu(\tau - s) e^{\gamma(\tau + s)} \times \sin \omega (t-s) d\tau ds$$

(A6)

$$K(t) = \frac{M_s \omega}{2 \cot \omega} \quad L(t) = \frac{M_s \omega e^{-\gamma t}}{2 \sin \omega} \quad N(t) = \frac{M_s \omega e^{\gamma t}}{2 \sin \omega}$$

(A7)