Solitons in quasi-one-dimensional magnetic materials and their study by neutron scattering

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A review is made of theoretical concepts from nonlinear dynamics of quasi-one-dimensional magnetic materials and of experimental investigations of solitons by inelastic neutron scattering and of studies of anomalies of thermodynamic quantities such as the specific heat, magnetization, susceptibility, etc. The main investigated substances are the quasi-one-dimensional ferromagnet $CsNiF_3$ and the antiferromagnet tetramethylammonium manganese chloride (TMMC) which share the same crystal structure. They can be regarded as quasi-one-dimensional magnetic materials with easy-plane anisotropy. The spin dynamics of such a system subjected to an external magnetic field applied in the easy plane can be reduced to the sine-Gordon equation. A detailed analysis is given of the recent experiments on $CsNiF_3$ and TMMC carried out using unpolarized and polarized neutrons and demonstrating that in a certain range of temperatures and fields this dynamics includes nonlinear excitations which can be described qualitatively as solitons of the sine-Gordon equation. Another group of quasi-one-dimensional crystals with easy-axis anisotropy is considered: it belongs to Ising-like magnetic materials. In the absence of an external field these materials exhibit soliton-type nonlinear excitations in the form of antiphase domain walls. The available experimental data confirm the concept of a soliton gas of excitations in quasi-one-dimensional magnetic materials.

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INTRODUCTION

Over a decade ago Krumhansl and Schrieffer[1] considered a one-dimensional model of an atomic chain with a two-well potential (ϕ^4 model) and showed that nonlinear localized states (domain walls) predicted by this model can be regarded as elementary excitations of the system present in addition to linear small-amplitude excitations (phonons). Domain walls represent localized entities (solitons) which are in thermodynamic equilibrium with one another and with phonons, so that at sufficiently low temperatures, when the soliton density is low, the system can be described as a gas of solitons and phonons. It was later demonstrated[2] that the concept of a gas of localized and nonlocalized quasiparticles can be applied to various one-dimensional systems which can be described by, for example, the sine-Gordon (SG) or some other nonlinear equation. It has been found that the interaction of solitons with linear excitations reduces simply to a phase shift as a result of scattering of these excitations by a soliton.

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An experimental check of the concept of an ideal gas of solitons in quasi-one-dimensional systems is easiest to carry out using magnetic materials such as quasi-one-dimensional ferromagnets and antiferromagnets, because if a crystal is sufficiently anisotropic, we can readily ensure conditions under which such a magnetic system behaves as if one-dimensional. In 1978 Mikeska[3] showed that the dynamics of a quasi-one-dimensional ferromagnet with easy-plane anisotropy, subjected to an external field in this anisotropy plane, reduces to the SG equation which has a soliton solution describing localized rotation by 2π of the magnetic moments lying in the easy plane as they move along a chain. The dynamic structure of a soliton governing the inelastic neutron scattering cross section was calculated and it was found that the scattering by a soliton gives rise to a central (quasielastic) peak with a Gaussian distribution of the transferred energies. In the same year Kjems and Steiner[4] observed such a peak in a well-known quasi-one-dimensional ferromagnet $CsNiF_3$ and this was regarded as the first experimental observation of a soliton in a quasi-one-dimensional magnetic system. However, soon after Reiter[5] put forward a series of objections against the soliton interpretation of the observed effect, because two-magnon scattering (accompanied by simultaneous emission and absorption of a magnon) should also give rise to a central peak with a similar dependence of its width on the transferred momentum.

These investigations provided the stimulus for intensive experimental[6-15] and theoretical[16-24] studies of solitons in $CsNiF_3$. The use of polarized neutrons made it possible to separate the contributions made to the dynamic structure factor by longitudinal and transverse (relative to the applied magnetic field) components of the spin and thus find the structure of a soliton along two orthogonal directions.

The theoreticians then faced a number of problems, the most important of which were initially the following two: how to allow for interference of solitons and magnons and how valid are the simplifications adopted for $CsNiF_3$, which reduce the spin dynamics of a Heisenberg spin chain to the SG equation. Solution of the first problem[17] was foreshadowed already in the first general treatment,[2] whereas the second problem was found to split into a number of separate difficult problems such as allowance, in the case of a finite anisotropy, for fluctuations which bring spins out of the easy plane,[25] the role of quantum effects for a chain with finite values of the spin,[19,26,27] and the role of the discrete structure.[21,28]

Nevertheless, it has been shown theoretically[29] and experimentally[30] that the soliton contribution to thermo-dynamics results in a characteristic behavior of the temperature and field dependences of the specific heat, so that investigation of anomalies of thermodynamic quantities has become a complementary (to neutron spectroscopy) means for the investigation of solitons in quasi-one-dimensional magnetic materials.

The range of materials being investigated at present has become much wider. Thus, it has been shown theoretically[31] that the dynamics of a quasi-one-dimensional antiferromagnet with easy-plane anisotropy can also be reduced to the SG equation, but only with rotation of the spin by half the total revolution (π soliton), and the anomalies associated with this circumstance have been revealed in neutron scattering experiments[32,33] in the well-known quasi-one-dimensional antiferromagnet TMMC. Various experimental methods have been used to investigate many quasi-one-dimensional magnetic materials and the experimental data obtained in this way have shown that the dynamics of these materials can be explained, in a certain range of temperatures and fields, without invoking the concept of a soliton as a quasiparticle. It should be added that nonlinear excitations have been investigated both theoretically[34] and experimentally[35] also in other types of quasi-one-dimensional systems with easy-axis anisotropy (Ising magnetic materials) in the absence of an applied field.

It should be noted that nonlinear objects in three-dimensional crystals with modulated magnetic structures (soliton gratings) have been investigated by neutron scattering,[36-39] but these are structure elements with macroscopic numbers of spins in each element and they cannot make an intrinsic contribution to the dynamics and to inelastic neutron scattering, respectively. Only in quasi-one-dimensional systems does a soliton behave as a mobile quasiparticle and may manifest itself in inelastic neutron scattering and in thermodynamics of such systems.

The purpose of the present review is to provide a systematic account of the theory and use it to analyze the available numerous experimental data obtained in investigations of nonlinear dynamics of quasi-one-dimensional magnetic materials. The conclusions drawn from these investigations are very illuminating and they largely determine the general behavior of nonlinear excitations in quasi-one-dimensional systems.

1. NONLINEAR DYNAMICS OF A QUASI-ONE-DIMENSIONAL FERROMAGNET WITH EASY-PLANE ANISOTROPY IN A MAGNETIC FIELD

1.1. Reduction of the dynamics to the sine-Gordon equation

We shall consider a one-dimensional chain of atoms along the direction of a unit vector $\mathbf{n} = (0, 0, 1)$ and we shall assume that it is subjected to a magnetic field $\mathbf{H}$. The simplest Hamiltonian which includes the exchange interaction and single-ion anisotropy,

$$\mathcal{H} = -J \sum_l \mathbf{S}_l \mathbf{S}_{l+1} + A \sum_l S_l^{z} - g\mu_0 \mathbf{H} \sum_l \mathbf{S}_l, \qquad (1.1)$$

describes an easy-plane ferromagnet if $J > 0$ and $A > 0$.

In the classical limit ($S \gg 1$) the spin dynamics is described by the general equation

$$\hbar \frac{d\mathbf{S}_l}{dt} = [\mathbf{S}_l \mathbf{H}_{2\mathrm{eff}}], \qquad (1.2)$$

where the effective field

$$\mathbf{H}_{2\mathrm{eff}} = -\frac{\partial \mathcal{H}}{\partial \mathbf{S}_l} = J(\mathbf{S}_{l-1} + \mathbf{S}_{l+1}) - 2AS_l^z \mathbf{n} + g\mu_0 \mathbf{H} \qquad (1.3)$$

itself depends on the vectors $\mathbf{S}_l$, so that the equation of motion for a spin becomes nonlinear. We shall write down this equation in a polar coordinate system with the z axis directed along the chain vector $\mathbf{n}$:

$$\mathbf{S}_l = S(\sin\theta_l \cdot \cos\varphi_l,\ \sin\theta_l \cdot \sin\varphi_l, \cos\theta_l). \qquad (1.4)$$

In the continuum limit (when the lattice parameter $a \to 0$) a system of difference equations reduces to a pair of differential equations for the angles $\theta(z,t)$ and $\varphi(z,t)$. We shall now consider the case when the external field is applied in the anisotropy plane (along the x axis) and the following conditions are satisfeid:

$$g\mu_0 H \ll A \ll J. \tag{1.5}$$

Under these conditions the equations for θ and φ become

$$\hbar \frac{\partial}{\partial t}\cos\theta = -g\mu_0 H \sin\theta\cdot\sin\varphi + Sa^2 J\frac{\partial}{\partial z}\left(\sin^2\theta\frac{\partial\varphi}{\partial z}\right),$$
$$\hbar\frac{\partial\varphi}{\partial t} = 2AS\cos\theta. \tag{1.6}$$

In the case of a strong anisotropy the spins should lie mainly in the anisotropy plane because the angle is $\theta \approx \pi/2$, i.e., $\sin\theta \approx 1$. Combining the two equations of the system (1.6) and replacing $\sin\theta$ with 1, we obtain an approximate equation for the azimuthal angle $\varphi(z,t)$ (Ref. 3):

$$\frac{\partial^2\varphi}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2\varphi}{\partial t^2} = k_0^2 \sin\varphi, \tag{1.7}$$

where we have introduced constants c with the dimensions of velocity and k_0 with the dimensions of reciprocal length:

$$c^2 = \frac{2AJS^2a^2}{\hbar^2}, \quad k_0^2 = \frac{g\mu_0 H}{SJa^2}. \tag{1.8}$$

Therefore, the motion of the magnetic moment (spin) vector in the anisotropy plane is governed by the familiar nonlinear SG equation. Its particular solutions are of the type $\varphi(z,t) = \varphi(\xi)$, where $\xi = z - vt$, and they can be readily obtained by integration of the left- and right-hand sides of Eq. (1.7) with respect to φ. When the boundary conditions are such that

$$\frac{d\varphi}{d\xi} = 0 \quad \text{for} \quad \varphi = 0,\ 2\pi \tag{1.9}$$

these equations become

$$\varphi(z, t) = 4\ \mathrm{acrtg}\exp\left[\pm k_0\gamma(z - vt - z_0)\right], \tag{1.10}$$

where $\gamma = [1 - (v^2/c^2)]^{-1/2}$, and v and z_0 are constants of integration representing the velocity and the initial coordinate, respectively.

Both solutions describe a localized change in the phase of two physically equivalent values of $\varphi = 0$ and $\varphi = 2\pi$ (Fig. 1), which implies rotation of the spin vector S in the plane by an angle 2π in an interval ξ of the order of $1/k_0\gamma$ (Fig. 2). These localized solutions are called a soliton and an antisoliton.

We shall calculate the energy E_{sol} of formation of a spin perturbation in a chain described by a soliton of Eq. (1.10). Writing down the Hamiltonian of Eq. (1.1) in the continuum limit and adopting approximations corresponding to the conditions of Eq. (1.5), we obtain

$$\frac{\mathcal{H}}{S^2Ja} = \int_{-\infty}^{\infty} dz\left\{\frac{1}{2}\left[\left(\frac{\partial\varphi}{\partial z}\right)^2 + \frac{1}{c^2}\left(\frac{\partial\varphi}{\partial t}\right)^2\right] + k_0^2(1-\cos\varphi)\right\}. \tag{1.11}$$

It should be noted that minimization of this energy functional gives the SG equation for the phase and using these we obtain the one-soliton solution

$$\frac{E_{sol}}{S^2Ja} = k_0\gamma\int_{-\infty}^{\infty} d\xi\left(\frac{d\varphi}{d\xi}\right)^2 = 8k_0\gamma. \tag{1.12}$$

The nature of the solution of Eq. (1.10) makes it possible to interpret a soliton as a "relativistic" particle of rest energy $\varepsilon_s = 8k_0S^2Ja$ with a mass $m_s = \varepsilon_s/c^2$ moving at a velocity v and localized at a point z_0. Then, in the nonrelativistic limit ($v \ll c$), we obtain the soliton energy:

$$E_{sol} = \varepsilon_s\gamma = \varepsilon_s + \frac{m_s v^2}{2} + \dots . \tag{1.13}$$

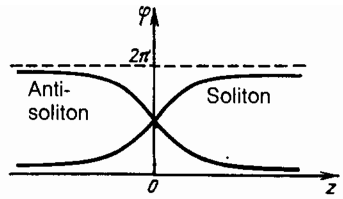

FIG. 1. Soliton and antisoliton deduced from the sine-Gordon (SG) equation.

The limiting velocity c represents the velocity of linear fluctuations of the phase of the magnetic moment (magnons) described by the linearized SG equation:

$$\frac{\partial^2\varphi}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2\varphi}{\partial t^2} = k_0^2\varphi, \tag{1.14}$$

which corresponds to the dispersion law of frequencies

$$\omega_k = c(k_0^2 + k^2)^{1/2}. \tag{1.15}$$

It therefore follows that the dynamics of the magnetic moment of a one-dimensional easy-plane magnetic material in a magnetic field transverse to a chain can be described by linear nonlocalized excitations (spin waves) and nonlinear localized excitations (solitons). Apart from the simplest solution of Eq. (1.10), the SG equation has many other nonlinear solutions. In the class of localized solutions (in the soliton sector) there are two types of solution: n-solitons and breathers.[40] The first of them can be regarded as a set of n separate solitons, each with its own parameters v_j and z_{0j} representing the velocity and coordinate of the center which satisfy the principle of asymptotic superposition. This principle predicts that individual solitons recover their profile after collisions, so that the only result of a collision is a change in the phase. It is this circumstance that allows us to treat the n-soliton solution (with a low density of solitons in the system) as a superposition of independent quasiparticles.[1,2]

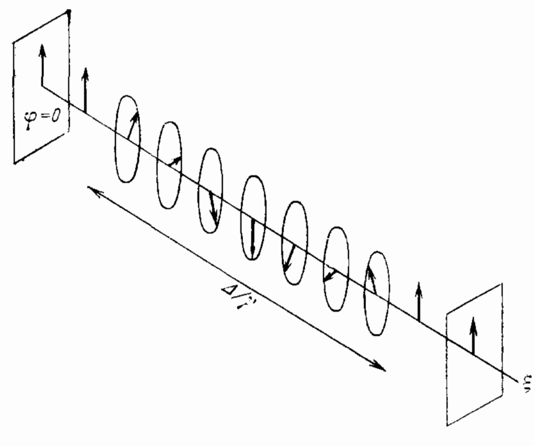

FIG. 2. Soliton in a one-dimensional chain of spins with easy-plane anisotropy.

The second type of solution is represented by breathers which represent localized states with certain internal degrees of freedom and can in a sense be regarded as bound soliton (soliton + antisoliton states).

In contrast to the solitons of Eq. (1.10), breathers depend on two parameters v and ω (Ref. 41):

$$\varphi_B(z,\ t) = 4\,\mathrm{arctg}\frac{[(\omega_0^2/\omega^2)-1]^{1/2}\sin\{\gamma\omega\,[t-(vz/c^2)]\}}{\mathrm{ch}\,\{k_0\gamma\,(z-vt)\,[1-(\omega^2/\omega_0^2)]^{1/2}\}},$$

one of which is the velocity v and the other the precession frequency ω; we know that $v<c$ and $\omega<\omega_0$, where $\omega_0 = \omega_{k=0}$ is the minimal frequency of the spin waves. The breather energy E_B is related to the soliton energy by

$$E_B = 2E_{sol}\left(1-\frac{\omega^2}{\omega_0^2}\right)^{1/2}.$$

The rest energy of a breather varies from $2E_{sol}$ to 0 as ω is varied and its width then changes from $1/k_0$ to ∞. Therefore, these two nonlinear excitations (soliton and breather) have very different properties: a soliton always remains a localized excitation, whereas a breather is gradually converted from a localized to a delocalized state in the limit when $\omega\to\omega_0$.

Linear nonlocalized solutions described by plane waves should change on increase in the excitation amplitude, but in the case of moderately low amplitudes this change can be regarded as a perturbation due to the interaction with solitons. Thus, in general the magnetic state of a ferromagnetic chain of spins should be regarded as a set of spin waves, solitons, and breathers which interact with one another.

We shall study the dynamics of such a system at low temperatures ($kT \ll E_{sol}$), when the number of thermally excited solitons is small and in the zeroth order approximation can be regarded as a gas of particles that do not interact with one another or with spin waves.

1.2. Dynamic structure factors of a soliton

Mikeska[3] was the first to show how nonlinear excitations of a magnetic chain, described as solitons of the SG equation, appear in the inelastic neutron scattering. The inelastic magnetic scattering cross section is governed by a dynamic structure factor $S^{\alpha\beta}(\mathbf{q},\ \omega)$, which represents a Fourier component of spatial-temporal variables of a correlation function of the magnetic (spin) moment

$$G_{ll'}^{\alpha\beta}(t) = \langle S_l^\alpha(t)\, S_{l'}^\beta(0)\rangle; \tag{1.16}$$

here $\langle ...\rangle$ represents statistical averaging of the system using the total Hamiltonian $\mathscr{H}$.

We introduce structure factors $S^{\parallel}(\mathbf{q},\omega)$ and $S^{\perp}(\mathbf{q},\omega)$, corresponding to correlations of longitudinal (relative to the magnetic field) spin components $\langle S_l^x(t)S_{l'}^x(0)\rangle$ and transverse components $\langle S_l^y(t)S_{l'}^y(0)\rangle$. Assuming that the polar angle is $\theta\approx\pi/2$ in Eq. (1.4), we shall consider the quantities

$$S^{\parallel}(\mathbf{q},\ \omega) = S^2\frac{1}{(2\pi)^2}\int dz\,dt\,\exp[i(\mathbf{q}z-\omega t)] \times\langle\cos\varphi(z,\ t)\cos\varphi(0,\ 0)\rangle, \tag{1.17}$$

$$S^{\perp}(\mathbf{q},\ \omega) = S^2\frac{1}{(2\pi)^2}\int dz\,dt\,\exp[i(\mathbf{q}z-\omega t)] \times\langle\sin\varphi(z,\ t)\sin\varphi(0,\ 0)\rangle, \tag{1.18}$$

carrying full information on the scattering by excitations of a chain for which all the spins are retained in the anisotropy plane.

We shall calculate initially these integrals when only one soliton is excited thermally in a chain. It is then easy to go over to a system of a finite low density of solitons in the case when $kT\ll E_{sol}$. When one soliton is present in this system, the average in $\langle ...\rangle_1$ implies integration with respect to z_0 and p (p is the momentum conjugate to the coordinate z_0), i.e., with respect to the phase space of a soliton with a statistical weight representing the Gibbs distribution function, i.e.,

$$\langle \ldots\rangle_1 = \frac{1}{Z_1}\int\int\frac{dp\,dz_0}{B}(\ldots)\,e^{-E_{sol}(v)/kT}, \tag{1.19}$$

$$Z_1 = \int\int\frac{dp\,dz_0}{B}\,e^{-E_{sol}(v)/kT}, \tag{1.20}$$

where B is a certain normalization constant and the index 1 shows that there is one soliton in a chain.

We shall first calculate Z_1. The equation $\dot z_0 = v = dE_{sol}/dp$ and the expression $E_{sol} = \varepsilon_s\gamma$ yield a relationship between p and v: $dp = (1/c^2)\varepsilon_s\gamma^3 dv$. It is convenient to go over from integration with respect to v to integration with respect to a variable x defined by $v/c = \tanh x$. It then follows from Eq. (1.20) that

$$Z_1 = \frac{\varepsilon_s}{Bc}L\int_0^\infty dx\cosh x\, e^{-\varepsilon_s \mathrm{ch}\, x/kT} = \frac{\varepsilon_s L}{Bc}K_1\left(\frac{\varepsilon_s}{kT}\right),$$

where $K_1(z)$ is a modified Hankel function. If we take the asymptote for higher arguments $K_1(z)\to(\pi/2z)^{1/2}e^{-z}$, we obtain the low-temperature limit

$$Z_1 = \frac{L}{Bc}\sqrt{\frac{\pi}{2}}\,\varepsilon_s\left(\frac{kT}{\varepsilon_s}\right)^{1/2}e^{-\varepsilon_s/kT}.$$

We shall now find the relationship between Z_1 and the average number of solitons N. We shall assume that the soliton density is low and that solitons therefore do not interact with one another, so that the following expression can be written down for the partition function of a soliton gas:

$$Z = \sum_{n=0}^{\infty}\frac{1}{n!}Z_1^n e^{\mu n/kT} = \exp(Z_1 e^{\mu/kT}),$$

where μ is the chemical potential of solitons. Applying a familiar thermodynamic identity, we obtain

$$N = -\frac{\partial F}{\partial\mu} = kT\frac{\partial\ln Z}{\partial\mu} = Z_1 e^{\mu/kT}. \tag{1.21}$$

We therefore find that $N\propto Z_1$. The coefficient of proportionality, which is governed by the chemical potential, can be deduced by calculating the total partition function of an SG system. In the transfer matrix method this coefficient can be calculated explicitly and then Eq. (1.21) can be reduced to the following expression for the soliton density[1]:

$$n_s = \frac{N}{L} = 4k_0\left(\frac{\varepsilon_s}{2\pi kT}\right)^{1/2}e^{-\varepsilon_s/kT}. \tag{1.22}$$

Equation (1.22) describes both solitons and antisolitons. Sometimes n_s represents the density of solitons alone and then the corresponding expression is half that given by Eq. (1.22).

The dynamic structure factors can be calculated by substituting the one-soliton solution of Eq. (1.10) into Eqs. (1.17) and (1.18). We thus obtain

$$\cos\varphi = 1 - 2\,\mathrm{sech}^2\,[k_0\gamma\,(z - vt - z_0)]. \qquad (1.23)$$

Substituting this expression in Eq. (1.17), it is convenient first to integrate with respect to t and z, and then with respect to z_0 and p, i.e., it is convenient to average over a statistical ensemble. This gives the following response[3]:

$$S^{\parallel}(q,\omega) = S^2\left(1 - 8\frac{n_s}{k_0}\right)\delta(q)\,\delta(\omega) + \frac{8n_sS^2}{\pi^2k_0^2}\left(\frac{2\pi\varepsilon_s}{c^2q^2kT}\right)^{1/2}\exp\left(-\frac{\varepsilon_s}{2c^2q^2kT}\omega^2\right)\frac{(\pi q/2k_0)^2}{\mathrm{sh}^2\,(\pi q/2k_0)}. \qquad (1.24)$$

We can obtain this expression by multiplying the contribution of one soliton by the total number of solitons in a system and replacing the factor $1/L$ that appears in calculation of Eq. (1.17) with one soliton by a factor $N/L \propto n_s$.

We can similarly calculate the transverse dynamic factor of Eq. (1.18) (Ref. 15):

$$S^{\perp}(q,\omega) = \frac{8n_sS^2}{\pi^2k_0^2}\left(\frac{2\pi\varepsilon_s}{c^2q^2kT}\right)^{1/2}\exp\left(-\frac{\varepsilon_s}{2c^2q^2kT}\omega^2\right)\frac{(\pi q/2k_0)^2}{\cosh^2(\pi q/2k_0)}. \qquad (1.25)$$

It should be noted that Eqs. (1.24) and (1.25) are obtained using the nonrelativistic approximation of Eq. (1.13) for the soliton energy, which gives rise to a Gaussian distribution with respect to the frequency ω. If we retain the complete Lorentz-invariant expression for the soliton energy $E_{\mathrm{sol}} = \varepsilon_s\gamma$, we obtain a more complex frequency distribution. For example, in the case of the function $S^{\perp}(q,\omega)$, we have

$$S^{\perp}(q,\omega) = \frac{16S^2\varepsilon_s}{\pi^2k_0kT}\frac{1}{cq\,[1-(\omega^2/q^2c^2)]^{1/2}} \times \exp\left[-\frac{\varepsilon_s}{kT}\left(1-\frac{\omega^2}{q^2c^2}\right)^{-1/2}\right]\left\{\frac{(\pi q/2k_0)\,[1-(\omega^2c^2q^2)]^{1/2}}{\cosh\{(\pi q/2k_0)\,[1-(\omega^2/c^2)]^{1/2}\}}\right\}^2$$

and similarly for $S^{\parallel}(q,\omega)$ if we replace cosh with sinh in the denominator.[6,42]

We shall now turn to Eqs. (1.24) and (1.25) which determine, at low temperatures, the frequency and angular dependences of the scattering by solitons. We can see that the longitudinal dynamic factor describes an elastic Bragg peak and a quasielastic peak of Gaussian profile and of width

$$\delta\omega = cq\left(\frac{kT}{\varepsilon_s}\right)^{1/2}, \qquad (1.26)$$

which has a characteristic dependence on T and q.

We can similarly calculate the dynamic structure factor $S^{zz}(q,\omega)$, which governs out-of-plane correlations. It follows from the second equation in the system (1.6), which can be rewritten in the form $S^z\,(\hbar/2A)\varphi$, that these correlations are of dynamic nature because the component of the spin S^z appears entirely due to a change in the phase φ with time. Employing the explicit form of the solution of Eq. (1.10), we obtain

$$\dot{\varphi} = \mp\frac{2k_0\gamma v}{\cosh\,[k_0\gamma\,(z-vt-z_0)]},$$

which allows us to calculate the correlation function $S^{zz} \propto \langle\dot{\varphi}\dot{\varphi}\rangle$ and also the correlation functions S^{yz} and S^{xz}.

The complete set of the correlation functions S^{xx}, S^{yy}, S^{zz}, S^{yz}, and S^{zy} calculated in the nonrelativistic approximation can be written in the form

$$S^{\alpha\beta}_{\mathrm{sol}}(q,\omega) = n_s\frac{8S^2}{\pi^2k_0^2}\left(\frac{2\pi\varepsilon_s}{c^2q^2kT}\right)^{1/2} \times \exp\left(-\frac{\varepsilon_s}{2c^2q^2kT}\omega^2\right)f_\alpha(q)\,f^*_\beta(q), \qquad (1.27)$$

where

$$f_x(q) = \frac{\pi q/2k_0}{\sinh(\pi q/2k_0)}, \quad f_y(q) = i\frac{\pi q/2k_0}{\cosh(\pi q/2k_0)},$$

$$f_z(q) = \frac{(\pi k_0/4q)\,\hbar\omega/A}{\cosh(\pi q/2k_0)}$$

are the form factors of a soliton along the various directions. Along the chain the form factor is dynamic and it vanishes for $\omega = 0$. The correlation functions S^{xz} and S^{xy} (and those symmetric to them) vanish because of summation over solitons and antisolitons, which make contributions of opposite signs.

1.3. Interference between solitons and magnons

Equations (1.24) and (1.25) were derived completely ignoring linear magnons. Interference between solitons and magnons gives rise to important corrections that alter considerably the scattering intensity by both localized and nonlocalized quasiparticles. We can allow for these corrections at low temperatures ($kT \ll \varepsilon_s$) using the nature of the nonlocalized solution of the SG equation with a wave vector q and a frequency ω_q in the presence of one soliton moving at a velocity v_j and initially, at the moment $t=0$, present at a point z_{0j}:

$$\psi_q(z,t) = \exp\,[i\,(qz - \omega t)]\,A_{qj}(z,t)\exp(i\Phi_{qj}(z,t)), \quad (1.28)$$

where the amplitude and phase considered in the nonrelativistic limit ($v_j \ll c$) are given by the expressions[17,43]

$$A_{qj}(z,t) = \left\{1 - k_0^2\frac{1-\tanh^2[k_0(z - v_jt - z_0j)]}{[q - (v_j\omega_q/c^2)]^2 + k_0^2}\right\}^{1/2}, \quad (1.29)$$

$$\Phi_{qj}(z,t) = \mathrm{arctg}\,\frac{k_0\,\mathrm{th}\,[k_0\,(z - v_jt - z_{0j})]}{q - (v_j\omega_q/c^2)} + \mathrm{arctg}\,\frac{k_0\tanh(k_0z_{0j})}{q - (v_j\omega_q/c^2)}. \quad (1.30)$$

We can see that perturbation of the magnon solution $\exp[i(qz - \omega t)]$ reduces to the lowering of magnon amplitude near a soliton center and an asymptotic shift of the phase (for a soliton at rest):

$$\Delta\Phi_q = 2\,\mathrm{arctg}\,\frac{k_0}{q}. \qquad (1.31)$$

This shift represents a change in the density of states in a continous spectrum[2]

$$\rho(q) = \frac{L}{2\pi} + \frac{1}{2\pi}\frac{d\Delta\Phi_q}{dq} = \frac{L}{2\pi}\left(1 - \frac{2}{L}\frac{k_0}{q^2+k_0^2}\right). \qquad (1.32)$$

When the soliton density n_s is finite, the quantity $1/L$ should be replaced with n_s and, instead of Eq. (1.32), we now have

$$\rho(q) = \frac{L}{2\pi}\left(1 - 2n_s\frac{k_0}{q^2+k_0^2}\right). \qquad (1.33)$$

At low temperatures, in the first order with respect to n_s, it is sufficient to allow only for those configurations in which the distance between solitons is much greater than the soliton width, so that the one-soliton solution given by Eq. (1.28) can be generalized to the case of N solitons as follows:

$$\psi_q(z,t)=\exp[i(qz-\omega_q t)]\prod_{j=1}^{N}A_{qj}(z,t)\exp(i\Phi_{qj}(z,t)). \tag{1.34}$$

Interference between solitons and magnons can be investigated by representing the field φ as a linear superposition of N one-soliton solutions of the SG equation and delocalized magnon solutions with arbitrary amplitudes:

$$\varphi(z,t)=\sum_{j=1}^{N}\varphi_{\mathrm{sol}}^{j}(z-v_j t-z_{0j})+\mathrm{Re}\sum_q \eta_q\psi_q(z,t). \tag{1.35}$$

We can readily describe the contribution made to the longitudinal correlation function of Eq. (1.17) by a series in powers of η_q. Calculations accurate to η_q^2 allow us to write down $S^{\parallel}(q,\omega)$ in the form of three contributions[17]:

$$S^{\parallel}(q,\omega)=S_{\mathrm{Bragg}}(q,\omega)+S_{\mathrm{sol}}^{\parallel}(q,\omega)+S_{\mathrm{m}}^{\parallel}(q,\omega), \tag{1.36}$$

where

$$S_{\mathrm{Bragg}}(q,\omega)=\left(1-\frac{kT}{2S^2Jak_0}-8\frac{n_s}{k_0}+\frac{13}{3}\frac{n_s}{k_0}\frac{kT}{S^2Jk_0a}\right)\delta(q)\delta(\omega), \tag{1.37}$$

$$S_{\mathrm{sol}}^{\parallel}(q,\omega)=\left[1-\frac{kT}{2S^2Jak_0}\left(1-\frac{k_0^2+q^2}{12k_0^2}\right)+\ldots\right]S_{\mathrm{sol}}^{0\parallel}(q,\omega); \tag{1.38}$$

here, $S_{\mathrm{sol}}^{0\parallel}$ represents the second term in Eq. (1.24).

The magnon contribution $S_m^{\parallel}(q,\omega)$ is a complex expression and we shall give only $S_m^{\parallel}(q)$ representing an integral with respect to the energy ω. In the limit of large wave vectors $\pi q \gg 2k_0$ we find that the expression for $S_m^{\parallel}(q)$, becomes very simple:

$$S_{\mathrm{m}}^{\parallel}(q)=\frac{8}{3}\frac{n_s}{k_0}\frac{q^2}{q^2+k_0^2}S_{\mathrm{m}}^{\perp}(q), \tag{1.39}$$

where $S_m^{\perp}(q)$ is the integral contribution to the magnon part of the transverse correlation function $S^{\perp}(q,\omega)$.

Equations (1.37)–(1.39) were obtained by averaging the magnon amplitudes $\langle|\eta_k|^2\rangle$ using the Gibbs distribution with the energy of the magnon subsystem

$$E_{\mathrm{m}}=\frac{S^2Ja^3}{2}\int \mathrm{d}k\,(k^2+k_0^2)\,|\eta_k|^2, \tag{1.40}$$

which appears as a result of linearization of the functional of Eq. (1.11). Such averaging reduces to a calculation of an elementary Gaussian continuum integral and gives the following answer:

$$\langle|\eta_k|^2\rangle=\frac{kT}{S^2Ja}\frac{1}{k^2+k_0^2}. \tag{1.41}$$

Moreover, in calculation of the sums over the wave vectors of magnons we integrate the continuous spectrum

$$\sum_k \ldots=\int \mathrm{d}k\,\rho(k)\ldots$$

with a density of states of Eq. (1.33) perturbed by solitons.

We shall now consider the results described by Eqs. (1.36)–(1.39). The expressions for the intensities of the Bragg and quasielastic soliton peaks include corrections proportional to kT as a measure of the density of magnons in the classical limit. In the case of a Bragg peak the presence of solitons and magnons reduces its intensity on increase in the density of these quasiparticles, but there is a term $\sim kTn_s$ describing interference of solitons with magnons, which slows down attenuation of the elastic coherent peak.

This magnon scattering results in considerable suppression of the quasielastic peak, so that at a temperature $kT=2JS^2(k_0a)$ it formally vanishes, but at such high temperatures we should include in the series of Eq. (1.38) and also in Eq. (1.37) the higher powers of temperature because of the anharmonic corrections, so that the expressions represented by Eqs. (1.36)–(1.39) should be regarded as the first terms of the series

$$S^{\parallel}(q,\omega)\propto\sum_{n=0}^{\infty}c_nT^ne^{-\varepsilon_s/kT}. \tag{1.42}$$

Another manifestation of the soliton–magnon interference is the appearance of a magnon contribution in the longitudinal correlation function of intensity proportional to the magnon density. We shall not give the spectral dependence of this contribution to $S^{\parallel}(q,\omega)$ but simply note that in addition to the central distribution near $\omega=0$, which is described by the soliton contribution of Eq. (1.38), there are also side distributions around $\omega=\pm\omega_q$, the intensity of which is described by Eq. (1.39).

The transverse correlation function has two contributions:

$$S^{\perp}(q,\omega)=S_{\mathrm{sol}}^{\perp}(q,\omega)+S_{\mathrm{m}}^{\perp}(q,\omega). \tag{1.43}$$

The soliton contribution is renormalized exactly as $S^{\parallel}(q,\omega)$, namely

$$S_{\mathrm{sol}}^{\perp}(q,\omega)=\left[1-\frac{kT}{2S^2Jk_0a}\left(1-\frac{k_0^2+q^2}{12k_0^2}\right)+\ldots\right]S_{\mathrm{sol}}^{0\perp}(q,\omega), \tag{1.44}$$

where $S_{\mathrm{sol}}^{0\perp}$ is the expression used in the zeroth order approximation of Eq. (1.25).

The magnon contribution to the transverse correlation function is the dominant one; in the frequency distribution $S_m^{\perp}(q,\omega)$ there are peaks at $\omega=\pm\omega_q$ and the integral intensity is given by the expression

$$S_{\mathrm{m}}^{\perp}(q)=\left[1-\frac{2n_sk_0}{q^2+k_0^2}\left(1+\frac{4}{3}\frac{q^2}{k_0^2}\right)+\ldots\right]S_{\mathrm{m}}^{0\perp}(q). \tag{1.45}$$

The reduction in the intensity of the magnon contribution to the transverse correlation function is due to the appearance of the magnon contribution in the longitudinal correlation function. A measure of smallness of both effects is $\sim n_s$.

It is shown in Ref. 17 that interference between magnons and solitons broadens the magnon peaks by an amount

$$\Gamma_q=2\frac{n_s}{k_0}\omega_q\left(\frac{k_0c}{\omega_q}\right)^3\left[\frac{1}{2}\left(\frac{kT}{\pi S^2Jk_0a}\right)^{1/2}+\frac{c|q|}{\omega_q}\right]. \tag{1.46}$$

These expressions provide a complete description of the soliton-magnon interference in the lowest order with respect to the soliton density. In the case of the intensities of the various contributions to the correlation function they are described by corrections $\sim n_sT$ or T. The terms $\sim T^2$ can appear only because of the anharmonicity of the magnon system. These effects will be obtained by representing the functional of Eq. (1.11) in the form $\mathscr{H}=\mathscr{H}_0+\mathscr{H}_{\mathrm{anh}}$, where $\mathscr{H}_0$ corresponds to linear magnons and $\mathscr{H}_{\rm anh}$ contains terms $\sim\varphi^4$ because of the expansion of $\cos\varphi$ in Eq. (1.11).

The usual calculations yield[17]

$$S_{2m}^{\parallel}(q,\omega)=\left(\frac{c^2}{2S^2J}\right)^2\frac{1}{2\pi N}\sum_k\frac{n_{k-(q/2)}n_{k+(q/2)}}{\omega_{k-(q/2)}\omega_{k+(q/2)}}$$
$$\times\left[\delta\left(\omega_{k-(q/2)}-\omega_{k+(q/2)}-\omega\right)\right.$$
$$+\frac{1}{2}\delta\left(\omega_{k-(q/2)}+\omega_{k+(q/2)}-\omega\right)$$
$$\left.+\frac{1}{2}\delta\left(\omega_{k-(q/2)}+\omega_{k+(q/2)}+\omega\right)\right],\qquad(1.47)$$

where n_k is the Bose distribution function, which should be taken in the classical approximation $n_k = kT/\hbar\omega_k$. We can see that there are two types of two-magnon processes. One is accompanied by simultaneous emission and absorption of a spin wave and gives rise to a distribution about an energy $\omega = 0$, whereas the other two represent simultaneous creation or annihilation of two spin waves. They begin from threshold energies $\omega = \pm 2\omega_{q/2}$. The integrated intensities of these two contributions can be calculated directly from Eq. (1.47):

$$\int_{-cq}^{cq}d\omega S_{2m}^{\parallel}(q,\omega)=2\int_{2\omega_{q/2}}^{\infty}d\omega S_{2m}^{\parallel}(q,\omega)$$
$$=\frac{1}{32\pi k_0}\left(\frac{kT}{S^2Jak_0}\right)^2\frac{1}{1+(q/2k_0)^2}.\qquad(1.48)$$

The spectral distribution $S_{2m}^{\parallel}(q,\omega)$ is shown in Fig. 3. We can see that the frequency dependence of the central peak is very weak right up to $\omega\approx cq$, where the distribution terminates quite abruptly. The width of this peak depends linearly on the wave vector, but is independent of temperature (in this classical limit). The width of the distribution of the soliton contribution [Eq. (1.25)] also depends linearly on q, but there is a strong temperature dependence. Separation of the soliton and two-magnon contributions to the quasielastic central peak represents clearly an important problem in the interpretation of neutron experiments.

A similar allowance for the anharmonicity in the problem of the transverse correlation function yields the following contribution for the magnon part:

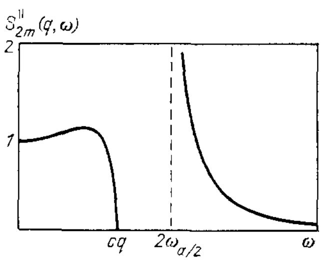

FIG. 3. Two-magnon (2m) contribution to the longitudinal correlation function $S^{\parallel}(q,\omega)$ (Ref. 17). The scale on the ordinate is arbitrary. The assumed parameters are $q=\pi/10a$ and $ak_0=0.185$.

$$S_m^{\perp}(q,\omega)$$
$$=\left\{1-\frac{kT}{2S^2Jk_0a}\left[1-\frac{1}{2}\frac{1}{1+(q^2/k_0^2)}\right]+\ldots\right\}S_m^{0\perp}(q,\omega).\qquad(1.49)$$

We again see that a correction term $\sim T$ appears. The integrated intensity of this contribution at $q = 0$,

$$\int_{-\infty}^{\infty}d\omega S_m^{\perp}(0,\omega)=\frac{kT}{2\pi k_0S^2Jak_0}\left(1-\frac{kT}{4S^2Jak_0}\right)+O(T^3),$$

is in agreement with the sum rule given in Ref. 44.

We can readily derive a quantum analog of Eq. (1.46) (Ref. 5). The quantum expression leads to a temperature dependence of the width of the central peak: this width increases strongly on increase in T and rapidly reaches saturation.

We shall conclude with a discussion of the importance of breathers in this description of the statistical behavior of a system obeying the SG equation. Breathers are localized excitations of width greater than k_0^{-1} and with a rest energy varying from zero to $2\varepsilon_s$. Since their spectrum is distributed continuously and begins from zero, their contribution to thermodynamic quantities should be described by a power law and it should be similar to the magnon contribution (for $kT\gg c\hbar k_0$). At low temperatures ($kT\ll\varepsilon_s$), which will be the only temperatures that we shall consider, the contribution made by solitons is nonanalytic in respect of temperature and is $\sim\exp(-\varepsilon_s/kT)$, whereas in the case of magnons and breathers it should be analytic (described by a power law). This means that it can be deduced from perturbation theory if we include the anharmonic corrections to the energy functional of Eq. (1.11). This is precisely the point demonstrated above where we have obtained corrections of the order of T and T^2. After such calculations however, there is no need for any special search of the contribution of the breathers to thermodynamics: their contribution has been allowed for implicitly already in a power series of the type described by Eq. (1.42).[17]

The dynamic structure factors of breathers and the feasibility of picking out the corresponding contribution to the inelastic neutron scattering is discussed in Refs. 78–80.

This theory will be used in later sections to consider the results of an experimental investigation of solitons by the inelastic neutron scattering method.

2. INVESTIGATION OF SOLITONS IN A QUASI-ONE-DIMENSIONAL FERROMAGNET $CsNiF_3$ BY NEUTRON SCATTERING METHODS

2.1. General expressions for the scattering cross section

The double differential cross section for magnetic scattering accompanied by the transfer of a momentum **Q** and an energy ω is described by the following familiar expression[45]

$$\frac{d^2\sigma}{d\omega d\mathbf{Q}}\propto\sum_{\alpha\beta}\left(\delta_{\alpha\beta}-e_\alpha e_\beta\right)S^{\alpha\beta}(\mathbf{Q},\omega),\qquad(2.1)$$

where $\mathbf{S}^{\alpha\beta}(\mathbf{Q},\omega)$ is the dynamic structure factor representing a Fourier component of the spin correlation function of

Eq. (1.16) and e_α is the projection of the unit scattering vector $\mathbf{e} = \mathbf{Q}/Q$.

The angular factor in Eq. (2.1) is such that the cross section contains only the correlation functions of the spin vector components perpendicular to the scattering vector

$$\mathbf{e}=(1,0,0):\ S^{yy}+S^{zz},\quad \mathbf{e}=(0,1,0):\ S^{xx}+S^{zz},$$

$$\mathbf{e}=(0,0,1):\ S^{xx}+S^{yy}. \tag{2.2}$$

Therefore, in experiments carried out using unpolarized neutrons we can just determine a sum of two structure factors. In order to understand what information on solitons can be deduced from such measurements, we shall write down the main expressions of a theoretical analysis describing the contributions made to the dynamic structure factor by solitons and by two-magnon (2m) processes. It follows from Eqs. (1.24) and (1.25) that the intensity (integrated with respect to the transferred energy) of the scattering by solitons

$$I_{\rm sol}^{\parallel}=\int S_{\rm sol}^{\parallel}(q,\omega)\,d\omega\propto n_s\left[\frac{\pi q/2k_0}{\sinh(\pi q/2k_0)}\right]^2, \tag{2.3}$$

$$I_{\rm sol}^{\perp}=\int S_{\rm sol}^{\perp}(q,\omega)\,d\omega\propto n_s\left[\frac{\pi q/2k_0}{\cosh(\pi q/2k_0)}\right]^2, \tag{2.4}$$

is governed by the square of the structure factor of a soliton in the appropriate direction relative to the magnetic field. The quantity q represents the component of the scattering vector $\mathbf{Q}$ along the direction of a chain. The integrated contribution to $S^{zz}(q,\omega)$ is small compared with $I_{\rm sol}^{\parallel}$ and $I_{\rm sol}^{\perp}$ because $S^{zz}(q,\omega)$ contains an additional small factor proportional to ω^2. The contribution to the scattering by 2m processes is contained only in the longitudinal correlation function and the integrated intensity of these processes deduced from Eq. (1.48) is

$$I_{2m}^{\parallel}\propto\left(\frac{kT}{JS^2ak_0}\right)^2\frac{1}{1+(q/2k_0)^2}. \tag{2.5}$$

It is clear from the above discussion that in order to separate the contribution made by solitons, we have to determine first the $S^{\perp}(q,\omega)$ structure factor, because 2m processes make no contribution to this factor. The quantity $S^{\parallel}(q,\omega)$ contains the contributions of both solitons and 2m processes.

2.2. Experiments with unpolarized neutrons

An ideal object for an experimental investigation based on the nonlinear dynamics described above is $CsNiF_3$. A crystal of this compound consists of chains of Ni ions surrounded by F octahedra which are directed along the hexagonal axis and are separated from one another by the large Cs ions.[46] The distance between the Ni chains is 6.3 Å and that between the Ni atoms along the chain is only 2.6 Å. In view of such a strong anisotropy the difference between the exchange interactions along the chain and between the chains is enormous ($\sim 10^3$). At $T_N = 2.61$ K a crystal becomes antiferromagnetically ordered because of a weak negative interaction between the chains, whereas along the chains the positive exchange interaction imposes a parallel orientation of the spins. At temperatures $T > T_N$ the long-range order between the chains is destroyed and a crystal can be regarded as a set of independent one-dimensional Ni chains with the ferromagnetic interaction.

The Hamiltonian of a single chain is assumed to have the form of Eq. (1.1) with the following parameters:

$$\frac{J}{k}=23\,\text{K},\quad \frac{A}{k}=5\,\text{K},\quad S=1,\quad g=2.4, \tag{2.6}$$

which are deduced from an interpretation of the linear dynamics of magnons on the basis of a classical treatment of the system (although the magnitude of the spin does not satisfy the condition $S \gg 1$).[47] If $T < (AJ/k)^{1/2} \approx 10$ K, the spins are oriented mainly in a plane, so that in the temperature range $3\,\text{K} \lesssim T \lesssim 17$ K a chain can be regarded as an easy-plane quasi-one-dimensional ferromagnet.

The first investigations of $CsNiF_3$ demonstrated the existence of a quasielastic central peak[4] and subsequent studies[6-14] have made it possible to compare the experimental results with the theory and to provide a convincing interpretation in terms of the scattering by solitons. We shall now discuss some of the main results on neutron scattering.[11]

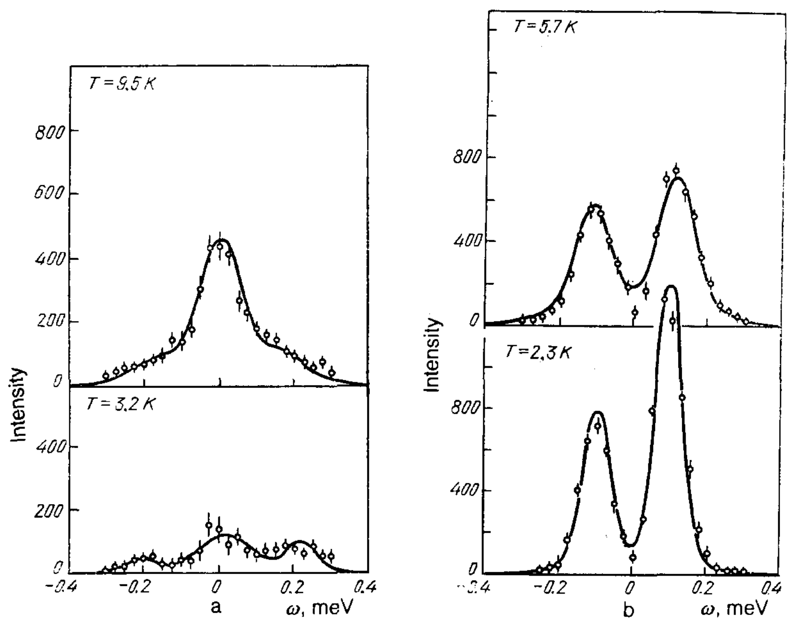

FIG. 4. Neutron spectra of $CsNiF_3$ obtained for different orientations of the scattering vector $\mathbf{Q} = (0.275; 0; 0)$ in a field $H = 3$ kOe: a) $\mathbf{Q} \perp \mathbf{H}$; b) $\mathbf{Q} \parallel \mathbf{H}$ In Fig. 4a the results represent counting for a period of 12 min, whereas in Fig. 4b they represent counting for a period of 11 min (Ref. 11).

Figures 4 and 5 show the results of an inelastic neutron scattering study of $CsNiF_3$ at different temperatures or for different wave vectors. It is clear from Fig. 4a that the quantity $S^{\parallel} + S^{zz}$ has a central peak which increases with temperature. Two side peaks observed at $T = 3.2$ K representing the scattering by spin waves. Figure 4b shows the behavior of $S^{\perp} + S^{zz}$. We can clearly see side peaks but there is no central peak, which is in agreement with Eq. (2.4) according to which we should have $S^{\perp}_{sol} = 0$ at $q = 0$. For finite values of q there should be a central peak in this scattering geometry and the intensity of this peak passes through a maximum, as observed in Fig. 5. The integrated intensity of the central peak is plotted as a function of the wave vector in Fig. 6. The continuous and dashed curves were calculated using Eq. (2.4) and the experimental value of the intensity for $q = 0.045$ and at $T = 12$ K. Therefore, this behavior of the central peak of $S^{\perp}(q,\omega)$ was in good agreement with the theory of solitons based on the SG equation approximation.

Interpretation of the central peak of $S^{\parallel}(q,\omega)$ requires an analysis of the contribution of solitons and 2m processes. A strong temperature dependence of the width of the peak indicates a considerable contribution of solitons, because 2m processes are characterized by a peak with a temperature-independent width. The results of different measurements of the integrated intensities of neutrons scattered by $CsNiF_3$, calibrated always against the intensity of the scattering by spin waves (under the same conditions) are collected in Fig. 7. Using the measured values of $I^{\perp}_{sol}(q)$ the authors of Refs. 9 and 11 found that the contribution to the central peak made by $S^{\parallel}(q,\omega)$ at $q = 0$ and $T = 12$ K is 1/3 and 2/3 for solitons and 2m processes, respectivity. The dotted curve in this figure is theoretical and is calculated from the expressions for $I^{\parallel}_{sol}(q)$ and $I_{2m}(q)$ on the assumption that the intensities at $q = 0$ are in the same ratio of 1/3 to 2/3.

We can thus see that a convincing proof of observation of solitons in $CsNiF_3$ is available.

A detailed investigation of the soliton contribution is reported in Ref. 9. The temperature and q dependences of the width of the central peak $\delta\omega$ show that it should be the result of a superposition of two processes: scattering by solitons and two-magnon (2m) scattering.

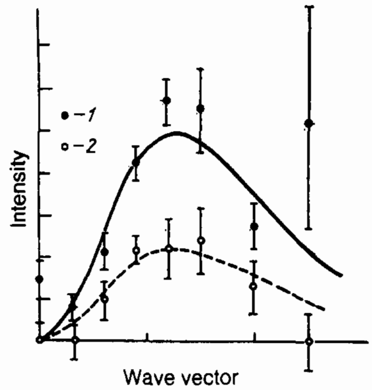

FIG. 6. Intensity of the central component in the case when $\mathbf{Q}_{\parallel}\mathbf{H}$ plotted as a function of q (Ref. 11) for $\mathbf{Q} = (0.6; 0; -q)$ and $H = 10$ kOe. $T = 12$ K (1) and 9 K (2).

2.3. Experiments with polarized neutrons

A theoretical analysis of the scattering by solitons is based entirely on the SG equation approximation which ignores fluctuations of the components of the spins perpendicular to the easy plane. However, a numerical modeling demonstrates the importance of these fluctuations in the case of $CsNiF_3$ (Ref. 48). In an experimental investigation of these fluctuations it is necessary to separate the contribution made to the inelastic scattering process by the correlations $S^{zz}(q,\omega)$. The individual correlations can be found by investigating polarized neutron scattering.

There are various methods for using polarized neutrons and they have the advantage that they make it possible to separate weak magnetic scattering from the nuclear process or to include in the scattering new correlation functions of spins in the same scattering geometry by altering the polarization of the neutron beam.

The cross section for the scattering of a neutron beam, with the polarization $\mathbf{p}_0$ and described by a density matrix $\rho = (1 + \mathbf{p}_0\boldsymbol{\sigma})/2$, is given by[45]:

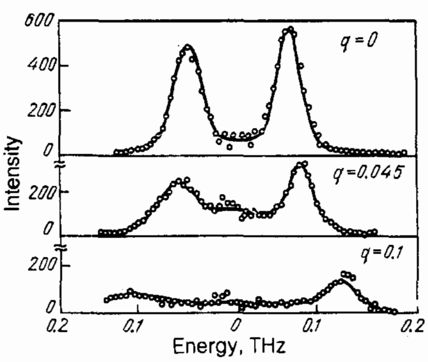

FIG. 5. Neutron spectra of $CsNiF_3$ obtained for different scattering vectors[11] [$\mathbf{Q}_{\parallel}\mathbf{H}$, $\mathbf{Q} = (0.6; 0; -q)$, $H = 10$ kOe, $T = 12$ K]. The results were obtained by counting for 348 s.

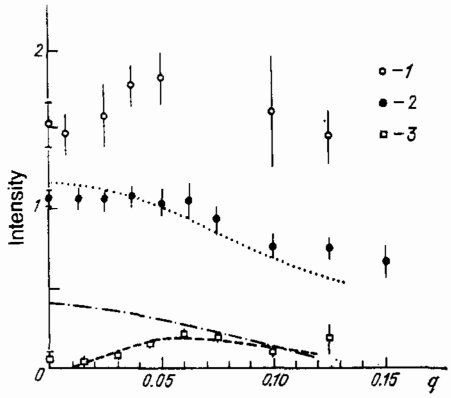

FIG. 7. Dependence of the integrated intensity of the central peak on q plotted for different correlation functions on the basis of the results obtained in $H = 10$ kOe at $T = 12$ K (Ref. 11): 1) $(S^{\parallel} + S^{\perp})$; 2) $(S^{\parallel} + S^{zz})$ 3) $S^{\perp}$ (relative units along the ordinate).

$$\frac{d^2\sigma}{d\omega\, dQ} \propto \sum_{\alpha,\beta}\sum_{\gamma,\gamma'} K^{\gamma\gamma'}(\delta_{\alpha\gamma}-e_\alpha e_\gamma)(\delta_{\beta\gamma'}-e_\beta e_{\gamma'})\, S^{\alpha\beta}(Q,\omega), \tag{2.7}$$

where

$$K^{\gamma\gamma'} = \mathrm{Sp}\,(\sigma^{\gamma'}\rho\sigma^{\gamma}) = \delta_{\gamma\gamma'} + i\varepsilon_{\gamma\gamma'\mu}p_\mu^0, \tag{2.8}$$

$\varepsilon_{\gamma\gamma'\mu}$ is a unit antisymmetric tensor and σ^α are the Pauli matrices. The relationship (2.7) represents the dependence of the scattering cross section on the polarization of the incident beam; for $p_0 = 0$, Eq. (2.7) reduces to Eq. (2.1) for unpolarized neutrons. A change in the orientation of the vector p_0 can alter different combinations of the correlations $S^{\alpha\beta}$.

Another approach involves a polarization analysis of the scattered beam. We can introduce the operator $\hat{K}^{\gamma\gamma'}$ representing a 2×2 matrix in the spin space of the scattered beam:

$$\hat{K}^{\gamma\gamma'} \equiv \sigma^{\gamma'}\rho\sigma^{\gamma} = \frac{1}{2}\,[\delta_{\gamma\gamma'}(1-\mathbf{p}_0\sigma) + p_0^\gamma\sigma^{\gamma'} + p_0^{\gamma'}\sigma^\gamma + i\varepsilon_{\gamma'\gamma\mu}(\sigma^\mu - p_0^\mu)]. \tag{2.9}$$

Then, an expression of the type given by Eq. (2.7) modified by the substitution $K^{\gamma\gamma'} \to \hat{K}^{\gamma\gamma'}$ defines the matrix $d^2\hat{\sigma}/d\omega dQ$ in the same space. We can easily write down its matrix elements labeling them with the indices $+$ and $-$. We shall denote the coordinate axes of the vector by ξ, η, and ζ. We shall select the polarization vector $\mathbf{p}_0 = (0, 0, 1)$ and identify the corresponding projection in the spin space by the symbol $(+)$. It follows from Eq. (2.9) that

$$\frac{d^2\sigma^{++}}{d\omega dQ} \propto \sum_{\alpha\beta}(\delta_{\alpha\zeta}-e_\alpha e_\zeta)(\delta_{\beta\zeta}-e_\beta e_\zeta)\, S^{\alpha\beta}(Q,\omega), \tag{2.10}$$

$$\begin{aligned}\frac{d^2\sigma^{+-}}{d\omega dQ} \propto \sum_{\alpha\beta} [&(\delta_{\alpha\xi}-e_\alpha e_\xi)(\delta_{\beta\xi}-e_\beta e_\xi) \\ &+ (\delta_{\alpha\eta}-e_\alpha e_\eta)(\delta_{\beta\eta}-e_\beta e_\eta) \\ &- i(\delta_{\alpha\xi}-e_\alpha e_\xi)(\delta_{\beta\eta}-e_\beta e_\eta) \\ &+ i(\delta_{\alpha\eta}-e_\alpha e_\eta)(\delta_{\beta\xi}-e_\beta e_\xi)]\, S^{\alpha\beta}(Q,\omega).\end{aligned} \tag{2.11}$$

Selecting now $p_0 = (0, 0, -1)$ and assigning to this polarization the projection $(-)$ in the spin space, we find two other matrix elements:

$$\frac{d^2\sigma^{--}}{d\omega\, dQ} = \frac{d^2\sigma^{++}}{d\omega\, dQ}, \quad \frac{d^2\sigma^{-+}}{d\omega\, dQ} = \frac{d^2\sigma^{+-}}{d\omega\, dQ}\bigg|_{i\to -i}. \tag{2.12}$$

Each of the four expressions in Eqs. (2.10), (2.11), and (2.12) can be determined separately with a spectrometer fitted with additional devices in the form of two flippers which can reverse the direction of the polarization of the incident and scattered beams. The four possible states of the flippers correspond to the quantities σ^{++}, σ^{+-}, σ^{-+} and σ^{--}. We note that the scattering cross section of unpolarized neutrons corresponds to averaging over the initial states and summing over the final states in the spin space:

$$\frac{d^2\sigma}{d\omega\, dQ} = \frac{1}{2}\left(\frac{d^2\sigma^{++}}{d\omega\, dQ} + \frac{d^2\sigma^{--}}{d\omega\, dQ} + \frac{d^2\sigma^{+-}}{d\omega\, dQ} + \frac{d^2\sigma^{-+}}{d\omega\, dQ}\right),$$

which gives Eq. (2.1).

We shall now write down the general relationships (2.10) and (2.11) for the polarization analysis of the scattering by $CsNiF_3$. The direction of the magnetic field (x axis) sets the direction of the polarization vector (ζ axis). We shall identify the coordinate system (ξ, η, ζ) with (y, z, x). In view of the symmetry of the model under the substitution $S_y \to -S_y$, $S_z \to -S_z$ the correlation functions become $S^{xy} = S^{yx} = S^{zx} = S^{xz} = 0$ so that for two specific orientations of the scattering vector Eqs. (2.10) and (2.11) are quite simple[23]:

$$\mathbf{e}\parallel x{:}\quad \frac{d^2\sigma^{++}}{d\omega\, dQ} = 0, \quad \frac{d^2\sigma^{+-}}{d\omega\, dQ} \propto S^{yy} + S^{zz} - i(S^{yz} - S^{zy}), \tag{2.13}$$

$$\mathbf{e}\parallel y{:}\quad \frac{d^2\sigma^{++}}{d\omega\, dQ} \propto S^{xx}, \quad \frac{d^2\sigma^{+-}}{d\omega\, dQ} \propto S^{zz}. \tag{2.14}$$

Therefore in the $\mathbf{Q}\perp\mathbf{H}$ geometry the scattering cross sections σ^{++} and σ^{+-} are governed by the separate correlation functions in contrast to unpolarized neutrons, when the cross section depends on a sum of two correlation functions. The correlation functions occurring in these expressions contain soliton and magnon contributions. The magnon contributions due to out-of-plane fluctuations are contained in S^{yz} and S^{zz}. They were investigated in Refs. 13 and 14 in the $\mathbf{Q}\parallel\mathbf{H}$ geometry. It was found that the experimental data for the cross sections σ^{+-} and σ^{-+} are described well by a planar model which postulates that the spins are confined to the easy plane and their projections perpendicular to this plane are small. In the range of fields $H \leqslant 10$ kOe the compound $CsNiF_3$ does not exhibit any instability of the system which might be induced by such fluctuations.

In addition to the spin-wave peak of σ^{+-}, which was observed only for $\omega > 0$, there is also a contribution from a soliton peak contained in S^{zz} and S^{yz} and the latter is asymmetric with respect to ω [which follows from Eq. (1.27)]. Figure 8 shows the experimental values of $d^2\sigma^{+-}/d\omega dQ$ obtained for $q = 0.06$ together with the continuous curve calculated theoretically on the basis of Eq. (2.13) without recourse to any fitting parameters.[23] The excellent agreement between this curve and the experimental results supports the correctness of the approximations used in the description of the spin dynamics in $CsNiF_3$.

The polarization analysis is carried out in Ref. 15 in the $\mathbf{Q}\perp\mathbf{H}$ geometry. According to the expressions in Eq. (2.14), the cross section σ^{++} contains only the longitudinal correlation function. The experimental points in Fig. 9 represent the observed central peak and the continuous curve is the theoretically calculated contribution of two-magnon scattering. The rest is the contribution made by solitons. The ratio of intensities of the two contributions $I_{sol}/I_{2m} = 1/2$ is in good agreement with the data on unpolarized neutrons, but the absolute contribution of solitons is much smaller (representing approximately one-fifth of the theoretical value obtained in the SG equation approximation).

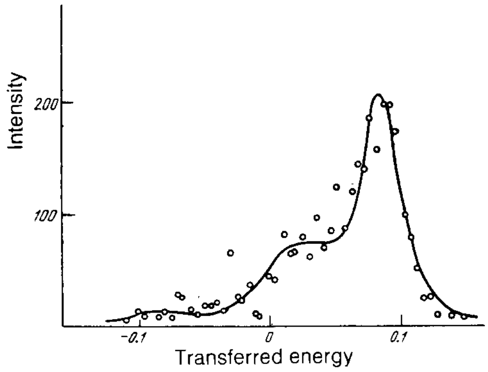

FIG. 8. Experimental and theoretical dependences of the scattering cross section $d^2\sigma^{+} \; /d\omega \cdot d\mathbf{Q}$ in the $\mathbf{Q}\|\mathbf{H}$ geometry ($H = 10$ kOe, $T = 12$ K). The abscissa is in units of terahertz and the ordinate gives the results of counting for 40 min (Ref. 14).

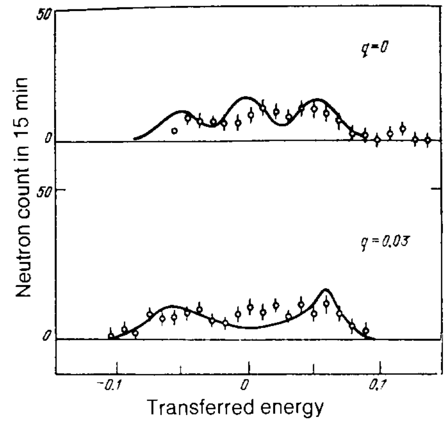

FIG. 10. Scattering cross section $d^2\sigma^{+}/d\omega \cdot d\mathbf{Q}$ obtained inthe $\mathbf{Q}\perp\mathbf{H}$ geometry ($H = 10$ kOe, $T = 12$ K). The abscissa is in units of terahertz and the ordinate gives the results of counting for 15 min (Ref. 15).

The cross section σ^{+-} includes in its pure form a weak magnetic scattering contribution, which is due to out-of-plane fluctuations (Fig. 10). The continuous curves in this figure are the theoretically calculated soliton and magnon contributions to S^{zz}. In particular, the central peak is calculated using Eq. (1.27). Once again the agreement with the experimental results is reasonable.

3. THERMODYNAMICS OF A QUASI-ONE-DIMENSIONAL FERROMAGNET WITH A FINITE ANISOTROPY

3.1. Fluctuations with emergence of spins out of the basal plane

Neutron spectroscopy may be the most direct, but it is not the only method for investigating solitons in quasi-one-dimensional systems. The presence of a gas of new quasi-particles (solitons) in a system makes specific contributions to thermodynamics and gives rise to anomalous temperature and field dependences of the specific heat and other quantities. We shall discuss this in the present section and begin by calculating first the free energy allowing for two types of excited states in a system: magnons and solitons.

We must point out immediately that we have considered so far only the case of extremely high anisotropy so that spins are confined to the easy plane. When the anisotropy parameter A is finite, the spins may project out of this plane so that the motion of the magnetic moment becomes three-dimensional. We shall still be interested in nonlinear objects of the spin system, i.e., in domain walls (solitons), but we shall allow for the possibility of small fluctuations relative to soliton configurations with spins projecting out of the easy plane.[25]

We shall consider excitation of a one-soliton configuration in which spins deviate in the plane by δS and are tilted out of the plane by $\delta S_\perp$. The Hamiltonian of a weakly excited state is described by the quadratic form

$$\mathcal{H} = E_s + \frac{1}{2} \int \frac{dz}{a} (\delta S \cdot M \, \delta S + \delta S_\perp \cdot M_\perp \, \delta S_\perp), \qquad (3.1)$$

where the operators

$$M = JS^2a^2 \left[-\frac{d^2}{dz^2} + k_0^2 \left\{ 1 - \frac{2}{\cosh[k_0(z-z_0)]} \right\} \right], \qquad (3.2)$$

$$M_\perp = JS^2a^2 \left[-\frac{d^2}{dz^2} + 2\alpha a^{-2} + k_0^2 \left\{ 1 - \frac{6}{\cosh[k_0(z-z_0)]} \right\} \right] \qquad (3.3)$$

are the quantum Hamiltonians of a particle which is in a potential well of shape governed by the shape of an SG soliton. [Here, $\alpha = A/J$ and k_0^2 is still given by the previous expression (1.8).]

The eigenvalues and the eigenfunctions of both operators are well known.[49] The operator M has a continuous spectrum and one discrete level:

$$E_k = JS^2a^2 (k^2 + k_0^2), \quad E_0 = 0, \qquad (3.4)$$

whereas the operator $M_\perp$ not only has a continuous spectrum, but also two discrete levels:

$$E_k^\perp = JS^2a^2 (k^2 + k_0^2 + 2\alpha a^{-2}),$$
$$E_0^\perp = JS^2a^2 (2\alpha a^{-2}), \qquad E_1^\perp = JS^2a^2 (2\alpha a^{-2} - 3k_0^2). \qquad (3.5)$$

The continuous spectra E_k and $E_k^\perp$ are identical with the spectra of linear excitations of the zero-soliton configuration, i.e., of a state of all the spins oriented along the magnetic field when E_k describes the spectrum of linear spin waves when all the spins are confined to the anisotropy plane, whereas $E_k^\perp$ corresponds to spin waves with the spins projecting out of the anisotropy plane.

The wave functions of excitations in the zero-soliton configuration are plane waves and for one-soliton configura-

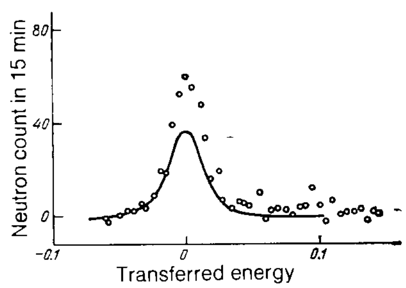

FIG. 9. Scattering cross section $d^2\sigma^{+} \; /d\omega \cdot d\mathbf{Q}$ obtained in the $\mathbf{Q}\|\mathbf{H}$ geometry ($H = 10$ kOe, $T = 12$ K). The abscissa is in units of terahertz and the ordinate gives the results of counting for 15 min (Ref. 15).

tion they are distorted in the region of localization of a soliton. A discrete level E_0 corresponds to a translational mode which restores the translational symmetry disturbed by the dependence of the one-soliton configuration on the coordinate z_0 at the center of the soliton. According to the Goldstone theorem, the energy of such a mode should vanish. The level $E_0^\perp$ belongs to a localized mode describing an oscillation of a one-soliton configuration in which spins project out of the anisotropy plane because of rotation around the field direction (in the absence of the anisotropy, i.e., in the case of an isotropic Heisenberg magnetic material this mode is of the Goldstone type and it rotates relative to the magnetic field). Finally, the level $E_1^\perp$ represents a localized rocking (tilting) mode and the spins again project out of the anisotropy plane.

These results are easily generalized to an n-soliton configuration with a low density of solitons. Obviously, the states in the discrete spectrum are n-fold degenerate. In the continuous spectrum we have to allow for the change in the density of states $\rho(k)$ due to dropping out of n levels E_0 and in $\rho^\perp(k)$ due to dropping out of n levels $E_0^\perp$ and n levels $E_1^\perp$. This change in the continuous spectrum can be expressed in terms of shifts of the phase of the wave function as a result of scattering by a soliton. In the case of the operators M and $M_\perp$ considered here the change in the density of states is given by[25]

$$\rho(k)=\rho_0-n\frac{1}{\pi}\frac{k_0}{k^2+k_0^2},$$
$$\rho_\perp(k)=\rho_0-n\frac{1}{\pi}\frac{k_0}{k^2+k_0^2}-n\frac{1}{\pi}\frac{2k_0}{k^2+4k_0^2},\qquad(3.6)$$

where $\rho_0=L/2\pi$ is the density in the spectrum of excitations of zero-soliton vacuum.

3.2. Manifestation of solitons in thermodynamics of magnetic material

We shall now write down the partition function Z. At low temperatures we have to include all the contributions of n-soliton spin configurations which minimize the Hamiltonian as well as spin fluctuations near local minima representing a specific spin configuration.[2,50,51,75] We shall represent Z as a sum of such configurations in which each term represents a continuum integral with respect to the appropriate fluctuations δS and $\delta S_\perp$ (Ref. 25):

$$Z=\sum_{n=0}^{\infty}e^{-n\varepsilon_s/kT}\frac{1}{n!}\sum_{\varepsilon_1,\ldots,\varepsilon_n}\int\delta S(z)\,\delta S_\perp(z)$$
$$\times\exp\left[-\frac{JS^2a}{2kT}\int dz\,(\delta S\cdot M^{(n)}\delta S+\delta S_\perp\cdot M_\perp^{(n)}\delta S_\perp)\right].\qquad(3.7)$$

The factor $1/n!$ allows for the identity of solitons in an n-soliton configuration; $\Sigma_{\varepsilon_1,\ldots,\varepsilon_n}$ represents summation over solitons of different helicity (topological charge), i.e., over solitons and antisolitons. The operators $M^{(n)}$ and $M_\perp^{(n)}$ represent generalization of the one-soliton expressions (3.2) and (3.3) in which we have to replace z_0 with z_{0i} (representing the coordinate of the center of the ith soliton) and then sum with respect to i between 1 and n.

The eigenfunctions of the operators $M^{(n)}$ and $M_\perp^{(n)}$ are derived in a trivial manner from the eigenfunctions of one-soliton operators. Since they form a complete set of functions, any fluctuation δS or $\delta S_\perp$ can be expanded as a series in eigenfunctions of the operators $M^{(n)}$ and $M_\perp^{(n)}$; then, the integration in Eq. (3.7) is in fact carried out over the coefficients of the expansions and the resultant Gaussian integral yields

$$Z=\sum_{n=0}^{\infty}e^{-n\varepsilon_s/kT}\frac{1}{n!}(8ak_0)^{n/2}N^n2^n\left(\frac{\pi kT}{E_0^\perp}\right)^{n/2}\left(\frac{\pi kT}{E_1^\perp}\right)^{n/2}$$
$$\times\exp\left(\frac{1}{2}\sum_k\ln\frac{2\pi kT}{E_k}+\frac{1}{2}\sum_k\ln\frac{2\pi kT}{E_k^\perp}\right)\equiv Z_{\rm sol}Z_{\rm m}.\qquad(3.8)$$

The factor $(8ak_0)^{n/2}$ appears as a result of integration with respect to the translational mode.[52]

The sum over n represents the contribution of solitons and of associated local modes:

$$Z_{\rm sol}=\exp\left[N\frac{8}{\sqrt{\pi}}\left(\frac{JS^2}{kT}\right)^{1/2}\left(\frac{g\mu_0H}{JS}\right)^{3/4}G\left(\frac{2AS}{g\mu_0H}\right)e^{-\varepsilon_s/kT}\right],\qquad(3.9)$$

where

$$G(\beta)=\frac{[1+(1+\beta)^{1/2}]\,[2+(1+\beta)^{1/2}]}{(\beta-3)^{1/2}\beta^{1/2}}\qquad(3.10)$$

is a function which allows for the anisotropy. In the limit of a strong anisotropy $A\to\infty$ we find that the above function becomes $G(\beta)\to1$ and we obtain the results of the SG equation approximation.

The quantity $Z_{\rm m}$ associated with the continuous spectrum of fluctuations is calculated using the function representing the density of states in a discrete spectrum:

$$Z_{\rm m}=\left(\frac{2e^2kT}{\pi JS^2}\right)^N\exp\left\{-\frac{1}{2}\left[\left(\frac{g\mu_0H}{JS}\right)+\left(\frac{g\mu_0H}{JS}+\frac{2A}{J}\right)^{1/2}\right]\right\}.\qquad(3.11)$$

Since Z has multiplicative properties, the free energy at low temperatures ($kT\ll\varepsilon_s$) consists of the magnon $F_{\rm m}$ and soliton $F_{\rm sol}$ contributions:

$$\frac{F_{\rm m}}{N}=kT\left[-\ln\frac{\pi JS}{2e^2kT}+\frac{1}{2}\left(\frac{g\mu_0H}{JS}\right)^{1/2}+\frac{1}{2}\left(\frac{g\mu_0H}{JS}+\frac{2A}{J}\right)^{1/2}\right],\qquad(3.12)$$

$$\frac{F_{\rm sol}}{N}=-kTn_s,\qquad(3.13)$$

where

$$n_s=\frac{8}{\sqrt{\pi}}\left(\frac{JS^2}{kT}\right)^{1/2}\left(\frac{g\mu_0H}{JS}\right)^{3/4}G\left(\frac{2AS}{g\mu_0H}\right)e^{-\varepsilon_s/kT}\qquad(3.14)$$

is the density of solitons found in the case of a finite anisotropy.

The spin-wave part of F has the temperature dependence $F_{\rm m}\propto NT\ln T$ which is typical of a classical system with a continuous spectrum of modes characterized by two degrees of freedom per spin. The relationships

$$E=F+TS,\quad S=-\frac{dF}{dT}\qquad(3.15)$$

yield the average energy and entropy per spin:

$$\frac{E_m}{N}=kT, \quad \frac{S_m}{N}\sim \ln T.$$

The first relationship agrees with the value of $kT/2$ per degree of freedom in an ideal gas of particles if we bear in mind that there are two types of such particles representing in-plane and out-of-plane spin fluctuations. We can see that the entropy diverges at absolute zero. This violation of the Nernst theorem is due to the classical treatment of the system that completely ignores the quantum corrections.

The soliton part F_{sol} of the free energy allows for the existence of a gas of magnons by a preexponential factor in Eq. (3.14) describing the density of solitons. The mechanism of this influence is discussed in detail in a fundamental paper on the subject[25] and consists, in the present system, of capture by a soliton of three modes from a spin-wave reservoir. These modes becomes localized and are manifested by a translational mode in the anisotropy plane and by two out-of-plane modes representing rotation and rocking (tilting). The translational mode gave rise to a factor $T^{-1/2}$, which is very typical of one-dimensional systems described by solitons,[2,53] but the field dependence $H^{3/4}$ is specific to the model. If we represent the preexponential factor in Eq. (3.13) by some exponential function, we can then interpret the presence of localized modes as renormalization of the soliton energy.

It should be pointed out that when the magnetic field is sufficiently strong to satisfy

$$H>H_c=\frac{2}{3}\frac{AS}{g\mu_0} \tag{3.16}$$

the anisotropic function diverges indicating an instability of a soliton at rest in the case of motion via a localized rocking (tilting) mode.[54]

We can use Eqs. (3.12)–(3.14) to calculate the specific heat using the thermodynamic relationship $C/N = -T\dfrac{d^2F}{dT^2}$. We then obtain the following expression:

$$\frac{C}{N}=k+k\frac{1}{\sqrt{8\pi}}G\left(\frac{2AS}{g\mu_0H}\right)\frac{\varepsilon_s}{JS^2}\left(\frac{\varepsilon_s}{kT}\right)^{5/2}e^{-\varepsilon_s/kT}. \tag{3.17}$$

Hence, we can write down the quantity $\Delta C = C(H) - C(0)$ in the following form:

$$\Delta C=k\left(\frac{\varepsilon_s}{kT}\right)^2 n_s, \tag{3.18}$$

where

$$n_s=\frac{1}{\sqrt{8\pi}}\frac{\varepsilon_s}{JS^2}\left(\frac{\varepsilon_s}{kT}\right)^{1/2}G\left(\frac{2AS}{g\mu_0H}\right)e^{-\varepsilon_s/kT} \tag{3.19}$$

is the expression for the soliton density equivalent to Eq. (3.14).

We can thus see that the temperature dependence of ΔC exhibits a maximum. Recalling that $\varepsilon_s = 8S(SJg\mu_0H)^{1/2}$, we can see that the dependence of ΔC on the magnetic field also has a maximum. This behavior of the specific heat suggests that experimental observations of these maxima can be used as evidence of the existence of thermally excited solitons in one-dimensional easy-plane magnetic materials. Experiments reported in Ref. 30 did indeed reveal a maximum of the field dependence of the specific heat of $CsNiF_3$, but its position differed greatly from that calculated using Eq. (3.18). The amplitudes of the observed maxima (in a certain range of temperatures) is an order of magnitude less than that found by calculation. This discrepancy raises doubts about the approximations used in discussing a spin system described by the Hamiltonian of Eq. (1.1), mainly the transition to the continuum approximation, the concept of an ideal gas of solitons, and the steepest-descent method in the calculation of a partition function. The origin of the discrepancies was studied by calculating the specific heat on the basis of the classical Hamiltonian of Eq. (1.1) using the Monte Carlo method.[29] The results of such calculations are compared with the experimental data in Fig. 11. We can see that there are considerable quantitative differences between all groups of curves. The difference between the two theoretical approaches becomes even greater when we calculate the temperature dependence of ΔC_s (Fig. 12).[55] It should be noted that the maxima of the curves deduced using the continuum theory appear at temperatures where the condition

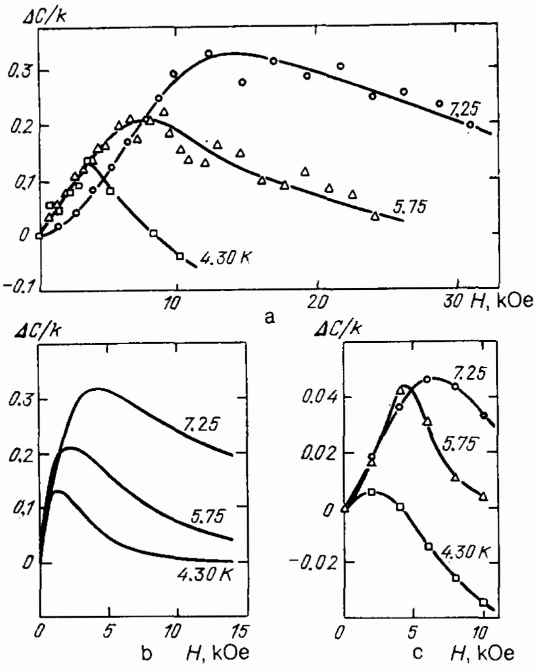

FIG. 11. Field dependences of the specific heat of $CsNiF_3$ at three different temperatures[29]: a) calculations carried out by the Monte Carlo method using a classical discrete Hamiltonian; b) calculations based on Eq. (3.17); c) experimental results.

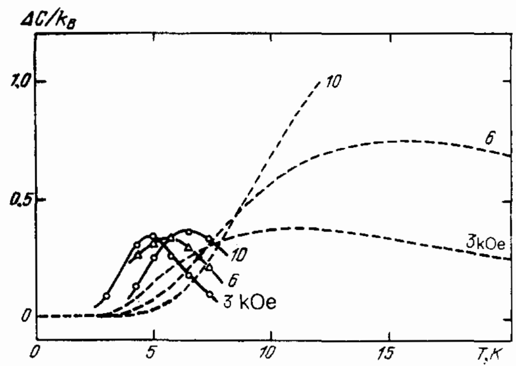

FIG. 12. Temperature dependences of the specific heat of $CsNiF_3$ calculated by the Monte Carlo method (continuous curves) and using the continuum approximation (dashed curves).[55]

$kT \ll \varepsilon_s$ is already disobeyed. There are general doubts whether the peaks of the specific heat predicted by the Monte Carlo calculations or found experimentally are associated with solitons. Moreover, the specific heat peaks are predicted by other models, such as that of an isotropic chain in a field. In this model the low-temperature contribution to thermodynamics is governed primarily by linear spin waves.[56]

In the case of the anomaly predicted by the continuum model for the critical field of Eq. (3.16), it is obviously the result of the adopted approximations. In fact, for the parameters of $CsNiF_3$ the critical field is $H_c \sim 18$ kOe. In the light of the investigations reported in Refs. 20 and 54 it is clear that the anomaly due to the divergence of the anisotropic function $g(\beta)$ at $\beta = 3$ is the result of the static approximation. In the critical field a static soliton is coupled to a moving soliton via a tilting mode and the free energy together with its derivatives with respect to H and T can be represented by smooth functions in the region of the "critical" field H_c. There are no anomalies in the system, as predicted by the classical Monte Carlo calculations.[29]

The discrepancy in the behavior of the specific heat between the numerical results of the classical model (1.1) and the experiments mentioned above is even greater. It therefore follows that the quantum effects should play an important role, at least in the case of $CsNiF_3$. This hypothesis is confirmed by numerical calculations carried out using the quantum model of a one-dimensional magnetic material.[57]

4. ALLOWANCE FOR QUANTUM CORRECTIONS AND DISCRETE NATURE OF A CHAIN

4.1. Quantum corrections in the semiclassical approximation

We calculated earlier the partition function Z of an easy-plane one-dimensional ferromagnet using the classical approximation. At low temperatures ($kT \ll \varepsilon_s$) the main contribution to Z comes from thermally excited static soliton configurations corresponding to local minima of the Hamiltonian $\mathscr{H}$ and from linear static fluctuations of these configurations.

Calculation of Z for a quantum chain of spins in a magnetic field presents serious problems, but it has been suggested that in the limit of high spins $kT \ll \varepsilon_s$ the semiclassical approximation can be used. Assuming the existence of an ideal gas of solitons at temperatures δS^z, we find it possible to consider solitons as classical objects and to quantize only linear excitations of soliton configurations (magnons).[26]

It is convenent to introduce action and angle variables (operators δS^z and $\delta\varphi$) satisfying the commutation relationship[58]

$$[\delta S^z(x),\ \delta\varphi(y)] = -i\delta(x-y); \tag{4.1}$$

where δS^z is the projection of the spin along a chain and $\delta\varphi$ is the azimuthal angle representing out-of-plane and in-plane fluctuations. We can use the general expression (3.11) in these variables to write down the Hamiltonian of a one-soliton configuration in the form

$$\mathscr{H} = E_{\text{sol}} + \frac{1}{2}\int \frac{dx}{a}\,(\delta\varphi\cdot M\,\delta\varphi + \delta S^z\cdot M_\perp\,\delta S^z), \tag{4.2}$$

where the operators M and $M_\perp$ are defined by Eqs. (3.2) and (3.3).

The quadratic form of Eq. (4.2) with the operators δS^z and $\delta\varphi$ can be diagonalized by the familiar unitary approximation, which yields the Hamiltonian of quantum oscillators

$$\mathscr{H} = E_{\text{sol}} + \frac{1}{2}\sum_\nu (p_\nu^2 + \omega_\nu^2 q_\nu^2), \tag{4.3}$$

with the commutation properties $[p_\nu, q_\mu] = -i\hbar\delta_{\nu\mu}$. The frequencies are found from the equation for the eigenvalues

$$M_\perp^{1/2} M M_\perp^{1/2}\psi_\nu = (\hbar\omega_\nu)^2\,\psi_\nu. \tag{4.4}$$

It is found that the spectrum consists of a band of continuous frequencies ω_k and two discrete frequencies ω and 0, which represent linear spin waves, a local mode, and a translational mode, respectively (Fig. 13). The energies are[26]

$$\hbar\omega_k = JSa^2\,[(k^2 + k_0^2 + 2\alpha a^{-2})(k^2 + k_0^2)]^{1/2}, \tag{4.5}$$

$$\hbar\omega = \hbar\Delta\left(1 - \frac{8}{9}\beta^{-2} + \dots\right), \tag{4.6}$$

where $\hbar\Delta = \hbar\omega_{k=0}$ is the magnon gap and the parameter is $\beta = 2AS/q\mu_0 H$. The eigenvalues of the quantum Hamiltonian (4.3) can now be written in the form

$$\mathscr{H} = \varepsilon_s + \frac{p^2}{2m_s} + \hbar\omega(\nu+\gamma) + \int dk\,\rho(k)\,\hbar\omega_k(\nu_k + \gamma_k), \tag{4.7}$$

where $\nu, \nu_k = 0, 1, 2, \dots$, and γ and γ_k are quantum parameters which are indeterminate in the semiclassical quantization; p and m_s are the momentum and mass of a soliton. We shall represent $\rho(k)$ in the form

$$\rho(k) = \frac{N}{2\pi} + \Delta\rho(k),$$

and rewrite Eq. (4.7) in the form of an effective Hamiltonian describing the interaction between a gas of magnons, a localized mode, and a single soliton:

$$\mathscr{H} = E_s + \frac{p^2}{2m_s} + \hbar\omega n + N\int \frac{dk}{\pi}\,\hbar\omega_k\nu_k + \int dk\,\Delta\rho(k)\,\hbar\omega_k\nu_k, \tag{4.8}$$

where

$$E_s = \varepsilon_s + \hbar\omega\gamma + \int dk\,\Delta\rho(k)\,\hbar\omega_k\gamma_k \tag{4.9}$$

is the renormalized energy of a soliton due to zero-point oscillations of local and continuous spin waves.

In the calculation of the partition function we have to integrate with respect to the soliton momenta and the quantum numbers ν and ν_k. This yields the expression

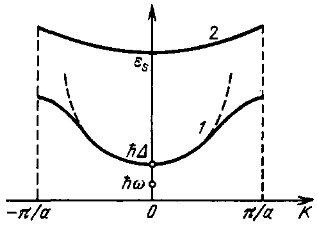

FIG. 13. Continuous spectrum of excited states of a quasi-one-dimensional ferromagnet: 1) magnons; 2) solitons.

$$Z = \exp\left[-N\int \frac{dk}{2\pi}\ln\left(1-e^{-\hbar\omega_k/kT}\right)\right]$$
$$\times\sum_{n=0}^{\infty}\frac{1}{n!}2^nN^n(2\pi kTm_s)^{n/2}\frac{1}{(2\pi\hbar)^n}e^{-nE_s/kT}(1-e^{-\hbar\omega/kT})^{-n}$$
$$\times\exp\left[-n\int dk\,\Delta\rho(k)\ln\left(1-e^{-\hbar\omega_k/kT}\right)\right] \tag{4.10}$$

in full analogy with the classical expression (3.8). The numerical factor 2^n is due to summation over the soliton parity (soliton, antisoliton).

Hence, we can easily show that the specific heat C consists of two additive terms: C_m representing spin waves and C_{sol} representing solitons, where

$$C_m = ka\int\frac{dk}{2\pi}\left[\frac{\hbar\omega_k/2kT}{\sinh(\hbar\omega_k/2kT)}\right]^2, \tag{4.11}$$

$$C_{sol} = k\frac{2a}{2\pi\hbar}(2\pi m_s kT)^{1/2}\left(1-e^{-\hbar\omega/kT}\right)^{-1}\left(\frac{E_s}{kT}\right)^2 e^{-E_s/kT}$$
$$\times\exp\left[-\int dk\,\Delta\rho(k)\ln\left(1-e^{-\hbar\omega_k/kT}\right)\right]. \tag{4.12}$$

The last factor in Eq. (4.12) allows for the interference between spin waves and solitons via the quantity $\Delta\rho$ expressed in terms of the shift of the phase of a spin wave resulting from its scattering by a soliton. As shown in Ref. 2, in the approximation of a low density of a soliton gas, the change in the density of states in the continuous spectrum of linear excitations is the only effective interference with a soliton that contributes to the thermodynamics of such a system at low temperatures.

These expressions together with the formulas for ω_k and ω, and also for $\Delta\rho$ (Ref. 26) are assumed to be valid subject to the conditions

$$S\gg 1,\ kT\ll E_s,\ k_0a\ll 1,\ \beta\gg 1. \tag{4.13}$$

The classical limit of C is obtained for $S\to\infty$ (conserving JS^2, k_0, and a at their fixed values), i.e., when $\omega_k + 0, \omega\to 0$, $E_s\to\varepsilon_s$. In this limit Eqs. (4.11) and (4.12) give

$$C_{sol} = k + k\frac{2a}{2\pi\hbar}(2\pi m_s kT)^{1/2}\frac{kT}{\hbar\omega}\left(\frac{\varepsilon_s}{kT}\right)^{-\varepsilon_s/kT}$$
$$\times\exp\left(-\int dk\,\Delta\rho(k)\ln\frac{\hbar\omega_k}{kT}\right), \tag{4.14}$$

which is in full agreement with Eq. (3.17). In the limit of strong anisotropy $\beta\to\infty$ the spin-wave energy of Eq. (4.5) becomes

$$\hbar\omega_k \to JSa\alpha^{1/2}(k^2+k_0^2)^{1/2}, \tag{4.15}$$

whereas the soliton mass becomes $m_s\to 4\hbar^2\dfrac{k_0}{Aa}$ and we obtain Eq. (3.17) when $g(\beta)\to 1$, i.e., we obtain the result of the SG equation approximation. Retaining in Eq. (4.14) terms of the order of $1/\beta$, we obtain again Eq. (3.17) where the anisotropic function $g(\beta)$ [for a definition see Eq. (3.11)] appears in the leading order with respect to this parameter, i.e., $g(\beta) = 1 + 3\beta^{-1/2}$.

In an explicit calculation of the field or temperature dependence of the soliton contribution to the specific heat on the basis of Eq. (4.12) we have to know the phase shifts $\Delta\rho(k)$ of spin waves. They were calculated in the first Born approximation in Ref. 26 and the results for C_{sol} are plotted in Fig. 14.

We can see a considerable reduction in C_{sol} which is due to inclusion of the quantum effects. Nevertheless, even when we allow for the quantum corrections, a comparison with the experimental data on the field dependence of C_{sol} of $CsNiF_3$ and with the temperature dependence of C_{sol} in various fields shows considerable quantitative discrepancies. The theory overestimates the specific heat. The reason for these discrepancies is clearly the unsatisfactory nature of the semiclassical approximation for this magnetic material characterized by the atomic spin $S=1$. Experiments indicate that the role of the quantum effects is even greater.

We can use the semiclassical approach to calculate readily also the correlation functions. For example, in the case of the longitudinal components of spins the soliton part of the dynamic correlation function has the same frequency dependence as in the case of the classical SG equation approximation [see Eq. (1.24)]:

$$S^{\parallel}_{sol}(q,\omega)\propto n_s e^{-m_s\omega^2/2q^2kT}, \tag{4.16}$$

where n_s is the soliton density. The expression for this density follows directly from Eq. (4.10) describing the partition function:

$$n_s = \frac{2}{2\pi\hbar}(2\pi m_s kT)^{1/2}\frac{1}{1-e^{-\hbar\omega/kT}}e^{E_s/kT}$$
$$\times\exp\left[-\int dk\,\Delta\rho(k)\ln\left(1-e^{-\hbar\omega_k/kT}\right)\right]. \tag{4.17}$$

A comparison of the calculations carried out using the classical and semiclassical approximations demonstrates a reduction in the quantum correlation function by about 50% compared with the classical one (Fig. 15). A similar tendency is exhibited also by other correlation functions. For example, the transverse function $S^{\perp}(q,\omega)$ consists of a central component associated with solitons and two side peaks due to spin waves. The central peak decreases strongly when quantum calculations are made, but the side peaks are not affected.

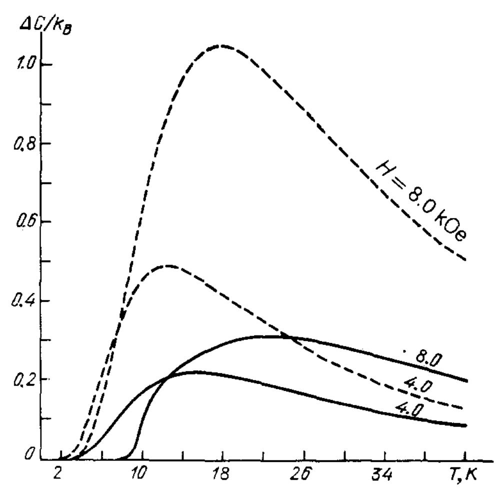

FIG. 14. Temperature dependences of the soliton contribution to the specific heat of $CsNiF_3$ calculated in the semiclassical (continuous curves) and classical (dashed curves) approximations.

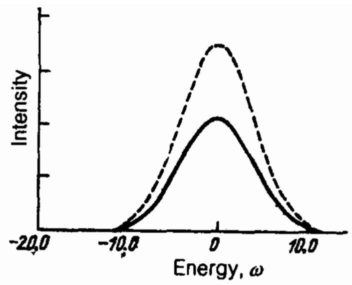

FIG. 15. Longitudinal correlation function calculated for $CsNiF_3$ in the semiclassical (continuous curve) and classical (dashed curve) approximations ($T = 10$ K, $H = 10$ kOe).

4.2. Beyond the semiclassical approximation

An allowance for the quantum corrections beyond the limits of the semiclassical approximation is a difficult task. It is shown in Refs. 19 and 27 that, within the semiclassical approach, a measure of the quantum nature of the system is the parameter $g^2 = \frac{1}{S}\left(\frac{2A}{J}\right)^{1/2}$ or the renormalized parameter $g'^2 = g^2[1 - (g^2/8\pi)]^{-1}$. In the continuum approximation the reduction in the soliton energy due to quantum effects, found in the first order with respect to $1/S$, represents $\sim 10\%$ (Ref. 19), which is approximately half the value reported for $CsNiF_3$ in Ref. 8.

A more rigorous analysis of the role of the quantum corrections can be based on the exact solutions for a quantum spin chain (see, for example, Ref. 59). It is known that in the continuum approximation an anisotropic Heisenberg chain is equivalent to a quantum SG system,[60] the spectrum of which had been thoroughly investigated.[61,62]

Such a system contains not only solitons but also Bose-like particles with a discrete spectrum of masses

$$M_n = M \sin \frac{ng'^2}{16} \; (n = 1, 2, \ldots) < 8\pi g'^{-2}, \qquad (4.18)$$

which can be regarded as bound states of a soliton and an antisoliton. They correspond to quantization of breathers in the classical SG system in which the state of a breather is characterized by a continuous parameter ω (see Sec. 1); in a quantum system such a state corresponds to a discrete index n. The state with $n = 1$ is a renormalized magnon[62] and, therefore, breathers represent all the Bose excitations in a quantum SG system. The Lorentz invariance of the SG equation makes it possible to write down the energy spectrum of particles with a mass described by Eq. (4.18):

$$E_n = (M_n c^4 + c^2 p^2)^{1/2}. \qquad (4.19)$$

These breathers make a thermodynamic contribution which at low temperatures is not of the power-law type, but exponential as in the case of a classical system. However, we must bear in mind that there are certain difficulties in reducing the dynamics of a quantum Heisenberg chain in a transverse magnetic field to the quantum SG equation.[60] Therefore, at present there is no self-consistent quantum theory of a quasi-one-dimensional ferromagnet of the $CsNiF_3$ type.

4.3. Solitons in a discrete ferromagnetic chain

In our theoretical analysis we have used so far the continuum approximation valid when $k_0^{-1} \gg a$ (i.e., when the width of a soliton is much greater than the lattice parameter). If the field is sufficiently high, the dimensionless parameter $k_0 a$ may become of the order of 1 and we have to allow then for the discrete nature of a spin chain. Therefore, this parameter is a measure of the importance of the discrete effects in a system.[21,28]

The most thorough treatment of these effects can be found in a recent paper[21] dealing with a one-dimensional classical ferromagnetic chain exhibiting easy-plane anisotropy and also exchange anisotropy. The equation describing an equilibrium spin configuration with all the spins confined to a plane is

$$\sin(\phi_{l+1} - \phi_l) - \sin(\phi_l - \phi_{l-1}) = (ak_0)^2 \sin \phi_l, \qquad (4.20)$$

where ϕ_l is the azimuthal angle measured from the direction of the field (it is found that such a configuration is always static).

There are two soliton kink-type solutions of this equation differing in respect of the symmetry: one of them (which we shall call S) has a center localized at a lattice site and the other (which we shall call B) has a center half-way between the sites. These solutions are naturally indistinguishable in the continuum limit and we then have a unique one-soliton solution of the SG equation. Numerical solution of Eq. (4.20) demonstrates that a B soliton exists only for values of $(ak_0)^2$ smaller than a certain critical value $(ak_{0c})^2 = 0.2723\ldots$. The difference between the energies of the S and B solitons is described by the expression $\Delta E = E_S(k_0) - E_B(k_0)$ and in a fixed field this difference is very small. For example, if $(ak_0)^2 < 0.2$, then $\Delta E/E_s > 2 \cdot 10^{-5}$ and near k_{0c} it reaches a value of just 10^{-3}. Perturbation theory utilizing the parameter k_0 (Ref. 21) gives an estimate

$$\Delta E \propto JS^2 e^{-\pi^2/k_0 a}. \qquad (4.21)$$

This quantity, which governs the scale of the difference between the energies due to a change in the position of a soliton within one lattice parameter, is known as the soliton pinning energy.[63] The appearance of this quantity is one of the important effects of the discrete nature of a chain.

An analysis shows that an S soliton is unstable in the presence of fluctuations in the easy plane and this is true throughout the range of existence of the above solution. A B-type soliton is stable for all values $k_0 < K_{0c}$. Out-of-plane fluctuations make a lattice soliton unstable at a certain (quite small) value of the anisotropy parameter α.

A moving soliton in a discrete chain was investigated in Ref. 21 by the molecular dynamics method. The critical field, at which a soliton becomes unstable, falls rapidly on increase in the soliton velocity v. An increase in the magnetic field results in narrowing and pinning of a moving soliton until it breaks up.

We shall conclude by noting that the main effects of the discrete nature of a ferromagnetic chain, which are the decay of solitons in strong fields and pinning, appear provided the condition $k_{0a} \sim 1$ is satisfied. This condition is difficult to satisfy in neutron diffraction experiments on $CsNiF_3$, so that an analysis of the current experiments can be made using the continuum approximation.

5. SOLITONS IN A QUASI-ONE-DIMENSIONAL ANTIFERROMAGNET WITH EASY-PLANE ANISOTROPY

5.1. Reduction of the dynamics to the sine-Gordon equation

We shall now consider the case of a quasi-one-dimensional antiferromagnet with the easy-plane anisotropy. The Hamiltonian of such a system is still given by Eq. (1.1), but the exchange integral is now $J<0$. As in the case of a ferromagnet, we shall assume that a magnetic field is applied in the easy plane at right-angles to the chain and we shall seek soliton solutions of dynamic equations along the x axis. It is found that the Landau-Lifshitz equation reduces again to the SG equation when the parameters satisfy the conditions given by Eq. (1.5), but this conclusion is not as trivial as in the ferromagnetic case and the spatial distribution of the magnetic moment in a state with one soliton differs considerably from such a state for a ferromagnet.[31,64,65]

Although there is no long-range magnetic order in a one-dimensional chain if $J<0$, a strong correlation is observed and this correlation creates an antiparallel alignment of the neighboring spins, so that at $T=0$ we can speak of two antiparallel sublattices which are oriented (mainly along the y axis) at right-angles to the applied field with a slight bending along the magnetic field because of the smallness of $g\mu_0 H/JS$.

We shall also assume the existence of such dynamic configurations of the system in which spins may be inclined at any angles relative to the y axis. The vectors representing two neighboring spins in a chain are given by an expression (Fig. 16):

$$S_{2l} = S\{\sin(\theta_{2l}+\vartheta_{2l})\cdot\cos(\Phi_{2l}+\varphi_{2l}),\ \sin(\theta_{2l}+\vartheta_{2l})\cdot\sin(\Phi_{2l}+\varphi_{2l}),\ \cos(\theta_{2l}+\vartheta_{2l})\} \tag{5.1}$$

and an analogous expression for S_{2l+1} where the substitutions $S\to -S$, $\vartheta\to-\vartheta$, and $\varphi\to-\varphi$ are made.

We shall assume that any pair of neighboring spins differs little from the mutual antiparallel orientation because of the smallness of $g\mu_0 H$ and AS compared with $|J|S$, i.e., we shall assume that the angles φ and ϑ are small, whereas the angle θ is close to $\pi/2$. Going over to the continuum limit in Eq. (1.1), we find that in the first nonvanishing order with respect to ϑ, φ, and $\theta_s=(\pi/2)-\theta$, as well as with respect to spatial gradients of ϑ and φ, we obtain the following energy functional:

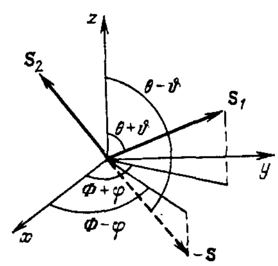

FIG. 16. Definitions of the angles specifying an arbitrary orientation of the neighboring spins in an antiferromagnetic chain.

$$\mathcal{H} = \frac{|J|S^2a}{2}\int dz\left[a^2\left(\frac{d\theta_s}{dz}\right)^2 + 4\vartheta^2 + a^2\left(\frac{d\Phi}{dz}\right)^2 + 4\varphi^2 + 2\alpha(\theta_s^2+\vartheta^2) + 2\varkappa_0 a\varphi\sin\Phi\right], \tag{5.2}$$

where

$$\varkappa_0 = \frac{g\mu_0 H}{|J|Sa}. \tag{5.3}$$

We shall now derive equations of motion of the spin (1.2) for the functional (5.2). We shall write down the Landau-Lifshitz equation (1.2) in terms of the action-angle variables[66]:

$$\hbar\dot{S}_l^z = \frac{\delta\mathcal{H}}{\delta\psi_l},\quad \hbar\dot{\psi}_l = -\frac{\delta\mathcal{H}}{\delta S_l^z}, \tag{5.4}$$

where the spin vector can be expressed in terms of the component S^z and the angle ψ:

$$S_l = \{(S^2-S_l^{z^2})^{1/2}\cos\psi_l,\ (S^2-S_l^{z^2})^{1/2}\sin\psi_l,\ S_l^z\}.$$

The system of equations (5.4) is equivalent to the Hamiltonian equations

$$\hbar\dot{S}_l^z = \{\mathcal{H}, S_l^z\},\quad \hbar\dot{\psi}_l = \{\mathcal{H}, \psi_l\} \tag{5.5}$$

with the Poisson bracket

$$\{S_l^z, \psi_{l'}\} = \delta_{ll'}. \tag{5.6}$$

Using the definition of the angles based on Eq. (5.1) for S_{2l} and the corresponding relationship for S_{2l+1}, we find that Eq. (5.6) yields the following expressions for all the necessary Poisson brackets in the continuum approximation if we allow for the smallness of the angles ϑ, φ, and θ_s:

$$\{\theta_s(z), \varphi(z')\} = \frac{a}{2S}\delta(z-z'),\ \{\Phi(z), \vartheta(z')\} = \frac{a}{2S}\delta(z-z'),$$
$$\{\vartheta(z), \varphi(z')\} = 0,\quad \{\theta_s(z), \Phi(z')\} = 0. \tag{5.7}$$

We shall now use these relationships to write down the equations of motion $\hbar\dot{\theta}_s = \{\mathcal{H}, \theta_s\}$ and $\hbar\dot{\Phi} = \{\mathcal{H}, \Phi\}$, and then find the values of ϑ and φ:

$$\vartheta = -\frac{\hbar}{2|J|S}\frac{1}{1+\alpha/2}\dot{\Phi},$$
$$\varphi = -\frac{\hbar}{2|J|S}\dot{\theta}_s - \frac{1}{2}ak_0\sin\Phi. \tag{5.8}$$

We could compare directly the equations of motion for the other two quantities θ_s and Φ, but it is more convenient to adopt a different procedure which involves substitution of Eq. (5.8) into Eq. (5.2) and derivation of the energy functional for the main variables θ_s and Φ:

$$\mathcal{H} = \frac{|J|S^2a}{2}\int dz\left[\left(\frac{\partial\theta_s}{\partial z}\right)^2 + \frac{1}{c_m^2}\left(\frac{\partial\theta_s}{\partial t}\right)^2 + 2\alpha a^{-2}\theta_s^2 + \left(\frac{\partial\Phi}{\partial z}\right)^2 + \frac{1}{c^2}\left(\frac{\partial\Phi}{\partial t}\right)^2 - \varkappa_0^2\sin^2\Phi\right], \tag{5.9}$$

where there are two parameters with the dimensions of velocity:

$$c_m = \frac{|J|Sa}{\hbar},\quad c = \left(1+\frac{\alpha}{2}\right)^{1/2}\frac{|J|Sa}{\hbar}. \tag{5.10}$$

We can see that the Hamiltonian is separable in terms of the variables θ_s and Φ; the first part describes linear excitations which are spin waves characterized by the dispersion law

$$\omega_k = c_m (k^2 + 2\alpha a^{-2})^{1/2}, \qquad (5.11)$$

whereas the second part in terms of the variable $\psi = 2\Phi - \pi$ assumes the form of the Hamiltonian of an SG system:

$$\mathcal{H}_{SG} = \frac{|J| S^2 a}{4} \int dz \left[\frac{1}{2} \left(\frac{\partial \psi}{\partial z} \right)^2 + \frac{1}{2c^2} \left(\frac{\partial \psi}{\partial t} \right)^2 + \varkappa_0^2 (1 - \cos \psi) \right]. \qquad (5.12)$$

Taking the solution for ψ in the form of Eq. (1.10), we obtain Eq. (1.12) for the soliton energy $E_{sol} (|J| S^2 a/4)^{-1} = 8\varkappa_0 \gamma$ and hence, in the nonrelativistic approximation, we find that

$$E_{sol} = g\mu_0 H S \gamma = \varepsilon_s + \frac{m_s v^2}{2}. \qquad (5.13)$$

Therefore, in an antiferromagnet the energy of an SG soliton is a linear function of H, in contrast to a ferromagnet when we have $E_{sol} \propto H^{1/2}$.

Another important distinction of an antiferromagnet is a different spatial distribution of the x projection of the spin in a soliton given by

$$\cos \Phi = \operatorname{sech} [\varkappa_0 \gamma (z - z_0 - vt)], \qquad (5.14)$$

in contrast to a ferromagnet when the corresponding expression is $\cos \Phi = 1 - 2\operatorname{sech}^2 [k_0 \gamma (z - z_0 - vt)]$. This gives rise to the following form factor:

$$\int dz e^{iqz} \cos \Phi (z) = \frac{\pi}{\varkappa_0} \operatorname{sech} \frac{\pi q}{2\varkappa_0}, \qquad (5.15)$$

in contrast to the form factor given by Eq. (1.24).

5.2. Characteristics of dynamic structure factors

The longitudinal correlation function is of the alternating (variable-sign) type because of the antiferromagnetic ground state

$$\langle S_l^x (t) S_0^x (0) \rangle = S^2 (-1)^l \langle \cos \Phi_l (t) \cos \Phi_0 (0) \rangle,$$

so that a Fourier component contains the wave vector of the antiferromagnetic structure π/a along the direction of a chain

$$S_{=} (q, \omega) = \frac{S^2}{(2\pi)^2} \int dz\, dt \exp \left[i \left(q + \frac{\pi}{a} \right) z + i\omega t \right]$$
$$\times \langle \cos \Phi (z, t) \cos \Phi (0, 0) \rangle.$$

Calculation of this expression is carried out in the usual manner (as in Sec. 1) and it gives

$$S^{\parallel} (q, \omega) = S^2 \frac{\varepsilon_s}{kTq_a c} \frac{1}{\varkappa_0} e^{-\varepsilon_s/kT} e^{-\varepsilon_s \omega^2/kTc^2 q_a^2} \frac{1}{\cosh^2 (\pi q_a/2\varkappa_0)}, \qquad (5.16)$$

where q_a is measured from π/a.

Calculation of the transverse correlation function

$$S^{\perp} (q, \omega) = \frac{S^2}{(2\pi)^2} \int dz\, dt \exp \left[i \left(q + \frac{\pi}{a} \right) z + i\omega t \right]$$
$$\times \langle \sin \Phi (z, t) \sin \Phi (0, 0) \rangle \qquad (5.17)$$

is not so trivial because

$$\sin \Phi (z, t) = \pm \operatorname{th} [\varkappa_0 (z - z_0 - vt)] \qquad (5.18)$$

(the "+" and "−" signs refer to a soliton and an antisoliton, respectively) and in the presence of several solitons the contribution to Eq. (5.17) cannot be represented by a sum of contributions of the individual solitons. However, a soliton of Eq. (5.18) describes a kink (domain wall). In the case of an antiferromagnet this is an antiphase wall of two equivalent states. The correlation function in Eq. (5.17) can be calculated in the limit of a very thin domain wall ($k_0^{-1} \sim a$), when

$$\operatorname{th} [\varkappa_0 (z - z_0 - vt)] \to \operatorname{sign} (z - z_0 - vt), \qquad (5.19)$$

and the presence of a soliton or an antisoliton reduces to a change in the sign of a quantity of the Ising type $\sigma(z, t) = \sin\Phi(z, t) \pm 1$. Similar correlation functions have already been calculated in the one-dimensional Φ^4 model[1] and the method involves calculation of the average value of the quantity $\sigma(z, t)\sigma(0, 0) = (-1)^m$, where m is the number of solitons in the space-time interval between the points (z, t) and $(0, 0)$. Since for a soliton gas the probability $p(m)$ of the appearance of m solitons, when their average value is N, obeys the Poisson distribution $p(m) = (N^m/m!) e^{-N}$, we obtain the following relationship:

$$\langle \sigma (z, t) \sigma (0, 0) \rangle = \langle (-1)^m \rangle = \sum_m p(m) (-1)^m = e^{-2N(z, t)}, \qquad (5.20)$$

which is the correlation function of interest to us in terms of the quantity $N(z, t)$. We find that $N(z, t)$ consists of the average number of solitons which at a time $t = 0$ are within the interval $[0, z]$, apart from those which have crossed the point z in a time t, and also of solitons which at $t = 0$ are outside the interval $[0, z]$ and in a time t travel a distance z. Allowing for the Gibbs probability of the soliton velocity distribution

$$n(v) = \frac{2\varepsilon_s \varkappa_0}{\pi kTc} \exp \left[- \frac{\varepsilon_s + (m_s v^2/2)}{kT} \right], \qquad (5.21)$$

we obtain

$$N (z, t) = \left(\int_{-\infty}^{0} dv \int_0^{z-vt} dz_0 + \int_0^{z/t} dv \int_0^{z-vt} dz_0 + \int_{z/t}^{\infty} dv \int_{z-vt}^{0} dz_0 \right) n(v)$$
$$= \int_{-\infty}^{\infty} dv\, |z - vt|\, n(v) = 2n_s ut f \left(\frac{z}{ut} \right), \qquad (5.22)$$

where $u = c(2kT/\varepsilon_s)^{1/2}$ is a parameter with the dimensions of velocity and

$$f(y) = \frac{1}{\sqrt{\pi}} \left(e^{-y^2} + 2y \int_0^y dz e^{-z^2} \right).$$

Therefore, in the limit of thin domain walls we can calculate the transverse correlation function

$$\langle \sin \Phi (z, t) \sin \Phi (0, 0) \rangle = \exp \left\{ -4n_s ut f \left(\frac{z}{ut} \right) \right\}.$$

If we approximate $f(y)$ by the function $(1/\sqrt{\pi})(1+\sqrt{\pi}y)$,[31] (Ref. 31) we readily obtain the dynamic structure factor

$$S^{\perp}(q,\omega)=\frac{S^2}{\pi^2}\frac{\Gamma_q}{q_a^2+\Gamma_q^2}\frac{\Gamma_\omega}{w^2+\Gamma_\omega^2}, \tag{5.23}$$

where $\Gamma_q = 4n_s$, and $\Gamma_\omega = 4n_s u/\sqrt{\pi}$ are the widths of the distributions of the wave vector and energy. A different approximation of $f(y)$ by $1/\sqrt{\pi}[1+(\sqrt{\pi}y)^2]^{1/2}$ (Ref. 32) gives the expression

$$S^{\perp}(q,\omega)=\frac{S^2}{2\pi}\frac{\Gamma_\omega^2/\Gamma_q}{[\omega^2+(\Gamma_\omega^2/\Gamma_q^2)\,q_a^2+\Gamma_\omega^2]^{3/2}}, \tag{5.24}$$

which also has maxima at $q_a = 0$ and $\omega = 0$, but the width of the peak along the ω scale depends on q_a and vice versa.

Derivation of $S_\perp(q,\omega)$, which yields Eqs. (5.23) and (5.24), is based on the approximation that $\sin\Phi = \pm 1$. Allowance for the finite thickness of a domain wall gives rise to a factor $\langle\sin^2\Phi\rangle$, in these expressions and this factor can be described by the following series[65] if $\frac{\varepsilon_s}{kT}\ll 1$:

$$\langle\sin^2\Phi\rangle = 1-\frac{kT}{\varepsilon_s}-\frac{1}{4}\left(\frac{kT}{\varepsilon_s}\right)^3-\dots.$$

The theoretical results presented above are illustrated in Fig. 17.

We can see from Eqs. (5.23) and (5.24) that the transverse correlation function for an antiferromagnet is of a different nature than for a ferromagnet, because in the latter case it is determined by a structure factor of one soliton at right-angles to the field. In particular, in the case of an antiferromagnet the widths of the distributions along q_a and ω are proportional to the soliton density, indicating that interference effects occur in the scattering process, so that the central peak is not associated with the scattering by a single soliton. A quantity which is a reciprocal of the width of the distributions along q is the correlation length, which characterizes the average size of an antiferromagnetic region between two domain walls. Neutrons are scattered coherently by these regions in a chain.

The different nature of the transverse correlations in ferromagnetic and antiferromagnetic chains is manifested by different temperature dependences of the intensity of the central peak. In the case of an antiferromagnet this dependence shows an increase with T as the soliton density is increased, whereas in the case of an antiferromagnet there is a reduction inversely proportional to Γ_q, i.e., to the soliton density. The longitudinal correlations in an antiferromagnet are entirely due to the structure factor of one soliton and behave similarly to a ferromagnet. Therefore, in the range of the parameters where the intensity of the transverse correlation is high, the corresponding intensity for the longitudinal correlations should be low.

The characteristics of the scattering in an antiferromagnet predicted by this theory have been confirmed by careful neutron investigations of tetramethylammonium manganese chloride (TMMC).[32]

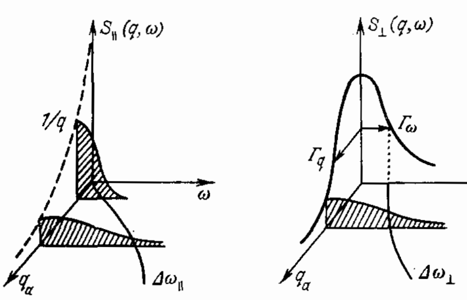

FIG. 17. Longitudinal and transverse dynamic structure factors for a quasi-one-dimensional antiferromagnet.[32] The widths of the distributions along the energy scales are $\Delta\omega_\parallel \propto q$ and $\Delta\omega_\perp \propto [1+(q^2/\Gamma_q^2)]^{1/2}$, based on Eq. (5.24).

5.3. Investigation of spin dynamics in a TMMC crystal by inelastic neutron scattering methods

Tetramethylammonium manganese chloride (TMMC) has the formula $(CH_3)_4NMnCl_3$ and the same hexagonal structure as $CsNiF_3$, if we replace Cs with $(CH_3)_4N$. In a crystal of this compound there are chains formed by Mn atoms and the distances between these atoms are 3.25 Å inside a chain and 9.15 Å between the chains. The antiferromagnetic ordering (Néel) temperature of this crystal is $T_N = 0.85$ K, so that at $T > T_N$ it can be regarded as a quasi-one-dimensional antiferromagnet. Earlier investigations of the linear dynamics of this quasi-one-dimensional antiferromagnet have shown that it is of the easy-plane type with the following parameters of the Hamiltonian of Eq. (1.1):

$$\text{TMMC:}\ \frac{J}{k}=-13\text{ K},$$
$$\frac{A}{k}=0.15\text{ K},\quad S=\frac{5}{2},\quad g=2, \tag{5.25}$$

so that its dynamics can be described by the SG equation at temperatures $T \lesssim 5$ K.

Reported investigations[32] carried out in magnetic fields $H = 0$–50 kOe at temperatures $T = 1.5$–5 K have shown that in the range $H/T \gtrsim 10$ kOe/K the observed effects are in good agreement with the theory. In particular, the values of Γ_q and Γ_ω representing the widths of the central peak along the q and ω scales depend exponentially on the ratio H/T, in full agreement with the expressions for Γ_q and Γ_ω (Fig. 18).

However, the soliton energy does not agree so well with the experimental results. According to the theoretical expression given by Eq. (5.13), in the case of TMMC we should have

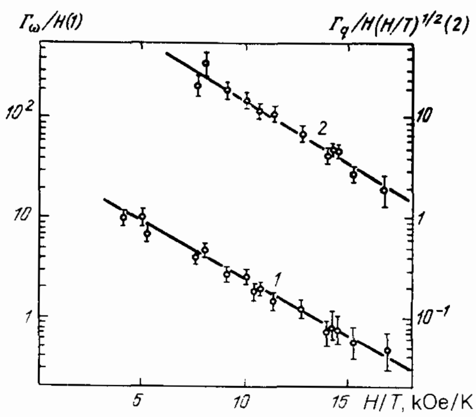

FIG. 18. Dependences of the width of the distributions (along the momentum q and energy ω scales) of the transverse central peak of TMMC on the magnetic field and temperature.[32]

$$\frac{\varepsilon_s}{k}=\frac{g\mu_0 S}{k}H\equiv bH,\quad b=0.336\ \mathrm{K\cdot kOe^{-1}}. \tag{5.26}$$

The considerable difference between the experimental value $b_{ex}=0.26\pm0.02$ k/kOe and the theoretical one given above is clearly due to the fact that certain quantum corrections have been ignored.

The fact that the atomic spin in TMMC is fairly large ($S=5/2$) explains why the classical description of an antiferromagnetic chain agrees with the experimental results. If the spin had been $S=1/2$, we would have been completely unable to describe a quasi-one-dimensional antiferromagnet by the classical approach. The problem of the ground state and classification of the spectrum of excitations of an isotropic Heisenberg antiferromagnetic chain with the spin $S=1/2$ had been solved exactly using the Bethe ansatz.[81] It follows from this solution that the ground state is a singlet and can be represented as a superposition of $N/2$ spin waves on a state with parallel spins. This does not yet describe completely the structure of the ground state, which can be dealt with fully only by a correlation function at $T=0$. Correlation functions for this case are not known, but we can expect sharp maxima in the wave-vector dependence at $q=\pi/a$, i.e., in the middle of the one-dimensional Brillouin zone.

In a three-dimensional system such maxima are manifested in neutron scattering by Bragg peaks and they indicate the existence of a long-range antiferromagnetic order, whereas in a one-dimensional system they are evidence of a short-range order. The observation of such maxima does not imply the existence of magnetic sublattices (or of the Néel classical state), but is a manifestation of antiferromagnetic correlations in the investigated system. The inability to provide a classical description in the case of an antiferromagnet with $S=1/2$ is thus related not to the absence of magnetic sublattices, but to the discrete nature of the spin space of states which is manifested more and more strongly as the atomic spin decreases.

In the next section we shall discuss a different class of antiferromagnets with spin 1/2, but we shall describe them using a quantum and not a classical approach and we shall base this quantum approach on a special variant of perturbation theory.

We have discussed very fully the results of experimental investigations of solitons in the easy-plane ferromagnet $CsNiF_3$ and in the antiferromagnet TMMC. These are not the only representatives of the class of quasi-one-dimensional magnetic materials exhibiting a significant contribution of solitons. The most thoroughly investigated among other magnetic materials of this kind is a quasi-one-dimensional ferromagnet $(C_6H_{11}NH_3)CuBr_3$ (usually abbreviated to CHAB).[71]

Three-dimensional magnetic ordering appears in this compound at $T_N=1.5$ K, and at temperatures right up to 16 K the behavior of CHAB is the same as that of an easy-plane magnetic material with exchange anisotropy and with the following parameters:

$$\frac{J}{k}=110\ \mathrm{K},\quad \frac{J_{zz}-J}{J}=-0.05,\quad S=\frac{1}{2}.$$

At temperatures $1.5\ \mathrm{K}<T<10$ K and in fields $0<H<7$ kOe the temperature and field dependences of the specific heat exhibit maxima similar to those found for $CsNiF_3$. Measurements of the longitudinal spin relaxation time by the NMR method also reveal typical behavior predicted by the soliton theory.[71] The agreement with the classical theory based on the SG approximation is more than qualitative, and this is surprising because CHAB should be a typical quantum magnetic material with spin 1/2.

Similar anomalies of the specific heat are reported for TMMC in Ref. 72 confirming the soliton dynamics of this antiferromagnet deduced from neutron scattering.

6. SOLITONS IN A QUASI-ONE-DIMENSIONAL ANTIFERROMAGNET WITH EASY-AXIS ANISOTROPY

6.1. Nonlinear dynamics of a quasi-one-dimensional ferromagnet of the Ising type

We have considered so far magnetic materials with the anisotropy tending to confine the spins in the basal plane. There is another limiting case when the anisotropy tends to orient spins along a chain. If the anisotropy constant is high, a magnetic material of this kind is Ising-like; if the spin is $S=1/2$, such a material is described by a Hamiltonian of the type

$$\mathscr{H}=-\frac{J}{4}\sum_l\left[\sigma_l^z\sigma_{l+1}^z+\varepsilon\left(\sigma_l^x\sigma_{l+1}^x+\sigma_l^y\sigma_{l+1}^y\right)\right], \tag{6.1}$$

where $|\varepsilon|\ll1$ and σ^α are the Pauli matrices.

If $J<0$, we find that since $|\varepsilon|$ is small, the ground state $|0\rangle$ is nearly of the Néel type in which the directions of spins form an antiferromagnetic sequence

$$|0\rangle=|+-+-+-\ldots\rangle.$$

An elementary excitation is a state with two parallel neighboring spins

$$\left|n+\frac{1}{2}\right\rangle=|\underset{1}{+}\underset{2}{-}\ \ldots\ +-\underset{n}{+}--+\ \ldots\rangle, \tag{6.2}$$

which can be specified conveniently by identifying the point $n+1/2$ separating two domains in a Néel structure. Therefore, $|n+\frac{1}{2}\rangle$ is a state with one antiphase wall.

We can easily describe the matrix element of the Hamiltonian linking the functions (6.2) (when the energy is measured from the energy of a Néel state $\frac{|J|N}{4}$):

$$\left\langle n+\frac{1}{2}\right|\mathscr{H}\left|n'+\frac{1}{2}\right\rangle$$

$$=\frac{|J|}{2}\{\delta_{n,n'}+\varepsilon(\delta_{n',n+2}+\delta_{n',n-2})\}, \tag{6.3}$$

which shows that a linear superposition

$$|k\rangle=\frac{1}{N^{1/2}}\sum_{n=1}^{N}\exp\left[-ik\left(n+\frac{1}{2}\right)a\right]\left|n+\frac{1}{2}\right\rangle \tag{6.4}$$

is an eigenfunction of the Hamiltonian with an eigenvalue

$$\varepsilon_k=\frac{|J|}{2}(1+2\varepsilon\cos2ak). \tag{6.5}$$

The state of Eq. (6.4) describes the motion of a domain wall with an energy that includes the activation energy $|J|/2$ and the dispersion $\sim\varepsilon$.

We shall calculate the correlation function $\langle\sigma_q^z\sigma_{-q}^z(t)\rangle$ using functions with one antiphase boundary. A convenient expression for the matrix element

$$\left\langle l+\frac{1}{2}\right|\sigma_n^z\left|l'+\frac{1}{2}\right\rangle=\delta_{l,l'}(-1)^n\,\mathrm{sign}\left(n-l-\frac{1}{2}\right)$$

together with the equation of motion $\dot{\sigma}_n^z=(i/\hbar)[\mathscr{H},\sigma_n^z]$

for the operator σ_n^z yield

$$\langle\sigma_q^z\sigma_{-q}^z(t)\rangle_1=\frac{1}{ZN}\sum_k\frac{\exp[-(\varepsilon|J|/kT)\cos 2ak]}{\cos^2(qa/2)}$$
$$\times\exp\left\{i\frac{2}{\hbar}\varepsilon|J|t\sin qa\cdot\sin[(2k-q)a]\right\},\qquad(6.6)$$

where

$$Z=\frac{1}{N}\sum_k\exp\left(-\frac{\varepsilon|J|}{kT}\cos 2ak\right).$$

The symbol $\langle...\rangle_1$ denotes averaging over the states with one boundary (we shall assume it is a soliton). The total correlation function for the states with N_s solitons is obtained by multiplying Eq. (6.6) by $N_s=Ln_s$, where n_s is the density of solitons:

$$\langle\sigma_q^z\sigma_{-q}^z(t)\rangle=Ln_s\langle\tau_q^z\sigma_{-q}^z(t)\rangle_1.\qquad(6.7)$$

We can find n_s by comparing this expression at $t=0$ with those which are readily obtained in the $\varepsilon=0$ approximation, when we have

$$\langle\sigma_n^z\sigma_{n+m}^z\rangle=\frac{\mathrm{Tr}\left\{\sigma_n^z\sigma_{n+m}^z\exp\left[(J/4kT)\sum_l\sigma_l^z\sigma_{l+1}^z\right]\right\}}{\mathrm{Sp}\exp\left[(J/4kT)\sum_l\sigma_l^z\sigma_{l+1}^z\right]}$$
$$=\left(\tanh\frac{J}{4kT}\right)^m=(-1)^m e^{-\varkappa m},$$

where $e^{-\varkappa}=\tanh(|J|/4kT)$. Hence, we obtain an expression valid at low values of $\varkappa$ (low T):

$$\langle\sigma_q^z\sigma_{-q}^z\rangle=\frac{1-e^{-2\varkappa}}{(1-e^{-\varkappa})^2+4e^{-\varkappa}\cos^2(qa/2)}\approx\frac{2\varkappa}{\varkappa^2+4\cos^2(qa/2)}.\qquad(6.8)$$

At $t=0$ for $\cos^2(qa/2)\gg\varkappa^2$ we can expect Eq. (6.7), subject to Eq. (6.6), to be identical with Eq. (6.8). Comparing them, we find that $n_s=\varkappa/2a$.

Calculation of the Fourier transform in Eq. (6.6) with respect to time gives the final expression for the longitudinal correlation function[34]:

$$S^{zz}(q,\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dte^{-i\omega t}\langle S_q^zS_{-q}^z(t)\rangle$$
$$=\frac{1}{4\pi Z}\frac{2\varkappa}{\varkappa^2+4\cos^2(qa/2)}\frac{1}{(\Omega_q^2-\omega^2)^{1/2}}e^{\hbar\omega/2kT}$$
$$\times\mathrm{ch}\left[\frac{\hbar(\Omega_q^2-\omega^2)^{1/2}}{2kT}\mathrm{ctg}\,qa\right]\qquad(6.9)$$

for the case when $|\omega|<|\Omega_q|$; when frequencies are in the range $|\omega|>|\Omega_q|$, this correlation function vanishes. We have used above the notation

$$\Omega_q=\frac{2\varepsilon|J|}{\hbar}\sin qa.\qquad(6.10)$$

Moreover, we have introduced $Z=I_0(\varepsilon|J|/kT)$, where $I_0(x)$ is a Bessel function with an imaginary argument and the small quantity is $\varkappa\approx 2e^{-|J|2kT}$.

The transverse correlation function obtained using the same approximations is[67]

$$S^{\perp}(q,\omega)=\frac{\varkappa}{2\pi Z}e^{\hbar\omega/2kT}$$
$$\times\left\{\frac{1}{(\Omega_q^2-\omega^2)^{1/2}}\cosh\left[\frac{\hbar(\Omega_q^2-\omega^2)^{1/2}}{2kT}\mathrm{ctg}\,qa\right]\right.$$
$$\left.-\frac{1}{\Omega_q}\sinh\left[\frac{\hbar(\Omega_q^2-\omega^2)^{1/2}}{2kT}\mathrm{ctg}\,qa\right]\right\}.\qquad(6.11)$$

It follows from Eq. (6.9) that the longitudinal correlation function exists in a frequency interval $-\Omega_q<\omega<\Omega_q$, at the edges of which there is a square-root singularity with a flat minimum in the middle. The corresponding correlations are due to the motion of antiphase domain walls which are assumed to be noninteracting. An allowance for collisions of domain walls broadens the singularities at $\omega=\pm\Omega_q$. The width of the broadening is $\delta\omega\propto 1/\tau$, where τ is the average time between collisions. It can be estimated from $\tau=1/n_s|v_k|$, where $1/n_s$ is the average distance between the walls and

$$v_k=\frac{d\varepsilon_k}{dk}=\frac{2a\varepsilon|J|}{\hbar}\sin(2ka)$$

is the wall velocity. A domain wall of energy $\omega=\pm\Omega_q$ has a momentum $k=q/2\pm\pi/4$, [see Eqs. (6.10) and (6.5)], so that the following estimate can be obtained from the above discussion:

$$\delta\omega=\frac{|\varepsilon J\cos qa|}{\hbar}\varkappa.\qquad(6.12)$$

Equations (6.9) and (6.10) are invalid when $q\approx 0$ or $q\approx\pi/a$. These ranges of q can be investigated using a phenomenological description of thin domain walls moving without collisions, which is used in Sec. 5 in a description of an antiferromagnet. By analogy with Eq. (5.20) we obtain

$$\langle S^z(0,0)S^z(z,t)\rangle=\frac{1}{4}e^{-2N(z,t)},\qquad(6.13)$$

where the factor $N(z,t)$ has the same meaning as in Sec. 5 and is given by an expression of the (5.22) type:

$$N(z,t)=\frac{a}{2\pi}\int_{-\pi/a}^{\pi/a}dk\,|z-v(k)t|\,n(k),\qquad(6.14)$$

where $n(k)$ is the density of solitons with a momentum k given by the Boltzmann factor:

$$n(k)=\frac{1}{a}e^{-\varepsilon_k/kT}.$$

The complex function $N(z,t)$ can be approximated by

$$N(z,t)=\bar{n}_s(z^2+u_0^2t^2)^{1/2},$$

where

$$\bar{n}_s=\frac{1}{a}e^{-|J|/2kT}I_0\left(\frac{\varepsilon|J|}{kT}\right),\quad u_0=\frac{4kTa}{\pi\hbar}\frac{\sinh(|J|\varepsilon/kT)}{I_0(|J|\varepsilon/kT)}$$

are parameters with the dimensions of density and velocity. A calculation of the Fourier transform of Eq. (6.13) gives[68]

$$S^{zz}(q,\omega)=\frac{1}{4}\frac{\Gamma_\omega^2/\Gamma_q}{[\omega^2+(\Gamma_\omega^2/\Gamma_q^2)q_a^2+\Gamma_\omega^2]^{3/2}},\qquad(6.15)$$

where $\Gamma_q=2\bar{n}_s$ and $\Phi_\omega=2\bar{n}_s,u_0$. The quantity $\bar{n}_s$ for $kT\gg\varepsilon|J|$ is identical with n_s representing the density of solitons, so that Eqs. (6.15) and (5.24) are essentially identical.

We thus can see that the dynamic structure factor of an Ising-like antiferromagnet is described by Eq. (6.9). The momenta q are not close to 0 or π/a, whereas in the vicinity of 0 or π/a we can use Eq. (6.15). Both results are valid in the temperature range defined by $\varepsilon|J| \ll kT \ll \varepsilon|J|$. The behavior of $S^{zz}(q, \omega)$ in the (q, ω) plane is demonstrated qualitatively in Fig. 19.

6.2. Investigation of spin dynamics in $CsCoCl_3$ and $CsCoBr_3$ crystals

Both $CsCoCl_3$ and $CsCoBr_3$ have the same crystal structure as $CsNiF_3$. At low temperatures both compounds exhibit a three-dimensional antiferromagnetic ordering with the Néel temperature $T_N = 21$ K ($CsCoCl_3$) or $T_N = 28.3$ K ($CsCoBr_3$). A study of the linear spin dynamics at low temperatures shows that the spin system in these compounds is described by the Hamiltonian (6.1) with the following parameters:

$$CsCoCl_3: \frac{J}{k} = -150\ \mathrm{K}, \quad \varepsilon = 0.12\ (\text{Ref. } 69) \tag{6.16}$$

$$CsCoBr_3: \frac{J}{k} = -155.2\ \mathrm{K}, \quad \varepsilon = 0.137\ (\text{Ref. } 67) \tag{6.17}$$

Thorough neutron scattering studies of the spin dynamics of $CsCoCl_3$ were reported in Refs. 69 and 70 and the corresponding studies of $CsCoBr_3$ are described in Refs. 35 and 67; the experimental results obtained in these studies are in good agreement with the theory given above. For example, Fig. 20 shows the inelastic neutron scattering spectra of $CsCoBr_3$ (Ref. 35). More accurately, it gives the results of measurements of the neutron scattering intensity by the ω = const. method. We can see from a schematic representation in Fig. 19 that at low values of ω there should be a scattering peak at $q = \pi/a$; as ω increases, two symmetrically distributed peaks gradually appear and they represent the scattering by solitons (moving domain walls), whereas the intensity of the central peak decreases in accordance with Eq. (6.15). This is precisely the scattering behavior which is demonstrated in Fig. 20.

Experimental and theoretical integrated intensities of the scattering of neutrons by the longitudinal and transverse spin components, considered as a function of the wave vector, are reported in Ref. 67. There is a strong increase in the scattering by the longitudinal components near $q = \pi/a$, in agreement with the theoretical predictions. The results obtained in the range of the wave vectors near π/a confirm Eq. (6.15) for the frequency and q dependences of $S^{zz}(q, \omega)$ in the form of a Lorentzian with a power exponent $-\frac{3}{2}$ (Ref. 67).

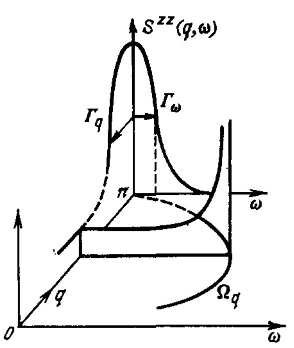

FIG. 19. Dynamic structure factor of longitudinal fluctuations for an Ising-like antiferromagnet.[69]

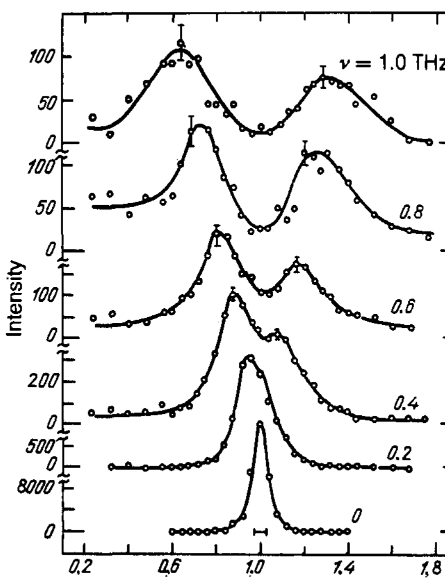

FIG. 20. Intensity of inelastic neutron scattering in $CsCoBr_3$ plotted for different transferred energies ω as a function of the transferred momentum q [$T = 35$ K, $Q = (1.45; 0; q)$].[35]

CONCLUSIONS

We shall now consider the question of quantitative agreement between theory and experiment. The most thoroughly investigated ferromagnet $CsNiF_3$ with $S = 1$ is usually analyzed on the basis of the classical SG theory. We pointed out above that there are considerable quantitative differences between the theory and experiment. One of the most important is the absolute "intensity" of the longitudinal dynamic structure factor, which is several times smaller than predicted by the SG theory. These discrepancies may be due to a number of factors such as the use of the continuum approximation, insufficient allowance for out-of-plane fluctuations, classical approach to a system with a small value of the atomic spin, and finally also an insufficiently well-grounded concept of an ideal soliton gas as a thermodynamic description of a nonlinear system.

Only one of the aspects of the approximations used in the description of the system with the Hamiltonian (1.1) is considered in Ref. 73, namely the treatment of a magnetic material as a classical spin system. The transfer matrix method is used in a numerical calculation of such characteristics as the temperature and field dependences of the magnetization, specific heat, correlation length of spin waves, and susceptibility. In spite of the fact that the continuum approximation and the SG equation are not used in these calculations, it is found that there are still considerable quantitative discrepancies in the case of all these properties of $CsNiF_3$ when calculations are compared with the experimental results. This investigation is a direct proof of the importance of the quantum effects in $CsNiF_3$. The results for $CsNiF_3$ differ greatly from the situation in the case of TMMC (Ref. 74), when the classical model describes better the specific heat[75] and susceptibility[76] data for the simple reason that the atomic spin of TMMC is considerably greater ($S = 5/2$). The difference between the predictions of the SG approximation and the experiments on TMMC is explained in Ref. 76 by the important role of out-of-plane fluctuations, which are allowed for in the quantum approach when calculating the specific heat and the correlation length of spin waves.

It is thus found that the classical SG model used widely in the explanation of the behavior of quasi-one-dimensional magnetic materials can be regarded only as a first approximation which provides a qualitative understanding of the nonlinear dynamics of the spin system. A quantitative theory requires allowance for all the factors discussed above.[82] Since some form of perturbation theory is usually employed, it would be of major interest to investigate various systems by numerical methods of molecular dynamics in order to check the theoretical approximations. Such calculations have already been carried out for classical models[77]; it would be very desirable if such calculations were to be made also for the quantum model. The number of experimental investigations of quasi-one-dimensional magnetic materials for which the nonlinear dynamics of the spin system is important will undoubtedly increase.

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