Recent experiments of the quasi-one-dimensional spin-1/2 antiferromagnet Copper Benzoate established the existence of a magnetic field induced gap. The observed neutron scattering intensity exhibits resolution limited peaks at both the antiferromagnetic wave number and at incommensurate wave numbers related to the applied magnetic field. We determine the ratio of spectral weights of these peaks within the framework of a low-energy effective field theory description of the problem.

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I. INTRODUCTION

Recent experiments\cite{1,2} have investigated the behaviour of the quasi-one-dimensional spin-1/2 antiferromagnet Copper Benzoate in a magnetic field. Neutron scattering experiments\cite{3} established the existence of field-dependent incommensurate low-energy modes in addition to low-energy modes at the antiferromagnetic wave number. The incommensurability was found to be consistent with the one predicted by the exact solution of the Heisenberg model\cite{4} in terms of a massive, relativistic quantum field theory. In a magnetic field the exchange constant is \( \gamma \). The constant \( \gamma \) to describe the low-energy degrees of freedom of the Hamiltonian density

\[
\mathcal{H} = \sum_i J S_i \cdot S_{i+1} - H S_i^z + h(-1)^i S_i^x ,
\]

where

\( h = \gamma H \). (2)

The constant \( \gamma \) is given in terms of the staggered \( g \)-tensor\cite{5} and the DM interaction. For Copper Benzoate the exchange constant is \( J \approx 1.57 \) meV and the induced staggered field is much smaller than the applied uniform field, \( h \ll H \).

As long as \( h \ll J \), or equivalently as long as the field induced gap \( \Delta \) is much smaller than \( J \), it is possible to describe the low-energy degrees of freedom of hamilton in terms of a massive, relativistic quantum field theory. This low-energy effective theory is obtained by abelian bosonization and is given by a Sine-Gordon model with Hamiltonian density

\[
\mathcal{H} = \frac{v}{2} (|\partial_x \Phi|^2 + (\partial_y \Theta)^2) - \mu(h) \cos(\beta \Theta) .
\]

Here \( \Phi \) is a canonical Bose field, \( \Theta \) is the dual field and the coupling \( \beta \) depends on the value of the applied uniform field and has been calculated in Refs.\cite{6,7} by using the results of Ref.\cite{8}. The spin velocity \( v \) also depends on \( H \) and is shown in Fig. 9 of Ref.\cite{9}. It is useful to define

\[
\xi = \frac{\beta^2}{8 \pi - \beta^2} .
\]

The spectrum of the Sine-Gordon model \( \text{SGM} \) in the relevant range of \( \beta \) consists of a soliton-antisoliton doublet and several soliton-antisoliton bound states called “breathers.”\cite{10} The soliton gap as a function of \( H \) and \( h \) was determined in Ref.\cite{11} in the regime \( \Delta \ll H \), where

\[
\frac{\Delta}{J} \approx \left( \frac{h}{J} \right)^{(1+\xi)/2} \times \left[ B \left( \frac{J}{\tilde{H}} \right)^{(2\pi - \beta^2)/4\pi} \left( 2 - \frac{\beta^2}{\pi} \right)^{1/4} \right]^{-\frac{1+\xi}{2}}
\]

with \( B = 0.422169 \). Equation \( \Delta_{\text{deltaRG}} \) is applicable as long as \( H \) is sufficiently smaller than \( J \) or to be more precise as long as the magnetization is small. For magnetic fields comparable to \( J \) it is better to use the following expression\cite{12}

\[
\frac{\Delta}{J} \approx \frac{2\tilde{v}(H) \pi}{\sqrt{\pi}} \Gamma\left( \frac{1}{1+\xi} \right) \left( \frac{c(H) \pi}{\Gamma\left( \frac{1}{1+\xi} \right)} \frac{\tilde{H}}{J} \right)^{(1+\xi)/2}.
\]

Here \( \tilde{v} = v/(Ja_0) \) is the “dimensionless spin velocity”, \( a_0 \) is the lattice constant and \( c(H) \) is given below. The breather gaps are given by

\[
\Delta_n = 2\Delta \sin \left( \frac{\pi \xi n}{2} \right) , \quad n = 1, \ldots, \left[ \frac{1}{\xi} \right] .
\]

II. DYNAMICAL STRUCTURE FACTOR

The staggered/oscillating components of the spin operators are expressed in terms of the continuum fields \( \Phi \)
and $\Theta$ as

$$
S_x^n \sim (-1)^n a(H) \sin \left( \frac{2\pi}{\beta} \Phi - \frac{2\delta}{a_0} x \right),
$$

$$
S_y^n \sim (-1)^n c(H) \cos(\beta \Theta),
$$

$$
S_z^n \sim (-1)^n c(H) \sin(\beta \Theta). \tag{8}
$$

Here $x = n a_0$ and the incommensuration $\delta$ is determined from the exact solution of the Heisenberg model in a uniform magnetic field that is the Hamiltonian hamil for $h = 0$. The amplitudes $a(H)$ and $c(H)$ are at present not known analytically, but can be determined numerically with high accuracy. We note that these amplitudes are also calculated in the absence of a staggered field, the expectation being that the changes due to a small $h \ll H$ will be negligible. The data used in this work are obtained in the scheme of Refs. [1][12]. We calculate the spin polarization $\langle S_x^z \rangle$ and the two-spin correlation function $\langle S_x^n S_y^n \rangle$ in the Heisenberg chain of 200 spins using the density-matrix renormalization group method, and then, fit them to analytic formulas obtained from the abelian bosonization taking $a(H)$ and $c(H)$ as fitting parameters. The results as well as other parameters, which are determined exactly, are listed in Table I for several typical values of the magnetization $m$.

The inelastic neutron scattering intensity is proportional to

$$
I(\omega, k) \propto \sum_{\alpha, \beta} \left( 1 - \frac{k_\alpha k_\beta}{k^2} \right) S^{\alpha \beta}(\omega, k), \tag{9}
$$

where $\alpha, \beta = x, y, z$ and the dynamical structure factor $S^{\alpha \beta}$ is defined by

$$
S^{\alpha \beta}(\omega, k) = \sum_{l=1}^{N} \int_{-\infty}^{\infty} \frac{dt}{2\pi} e^{-ik_\alpha a_0 + i\omega t} \langle S_{l+1}^\alpha(t) S_1^\beta(0) \rangle. \tag{10}
$$

Here $k$ denotes the component of $k$ along the chain direction. A schematic representation of which excited states will contribute to the various components of the dynamical structure factor at $k = \pi/a_0$ and $k = (\pi \pm 2\delta)/a_0$ is shown in Fig. I. At the antiferromagnetic wave number there are several breather excitations and at higher energies multiparticle continua. These contribute to the $xx$ and $yy$ components of the dynamical structure factor, which have been determined in detail in Ref. [7]. At the incommensurate wave numbers $k = (\pi \pm 2\delta)/a_0$ there are soliton and antisoliton states and at higher energies multiparticle scattering continua. In this paper we calculate the single particle soliton/antisoliton contributions to $S^{zz}$ and compare them to the dominant feature in the dynamical structure factor, the contribution of the

| $m$ | $a$ | $c$ | $v$ | $\beta$ | $H$ |
|-----|-----|-----|-----|-------|-----|
| 0.20 | 0.591(3) | 0.4937(3) | 1.54271 | 2.35016 | 0.17599 |
| 0.22 | 0.3813(6) | 0.4764(2) | 1.02184 | 2.06107 | 1.46380 |
| 0.26 | 0.3947(6) | 0.4731(2) | 0.94844 | 2.03735 | 1.54656 |
| 0.28 | 0.3899(6) | 0.4639(2) | 0.79741 | 1.99418 | 1.62134 |
| 0.30 | 0.3864(6) | 0.4578(2) | 0.72074 | 1.99153 | 1.74794 |
| 0.32 | 0.3830(6) | 0.4504(2) | 0.64387 | 1.94775 | 1.80300 |
| 0.34 | 0.3826(6) | 0.4416(2) | 0.56722 | 1.92658 | 1.84575 |
| 0.36 | 0.3820(6) | 0.4310(2) | 0.49116 | 1.90586 | 1.88462 |
| 0.38 | 0.3814(6) | 0.4183(2) | 0.41602 | 1.88559 | 1.91723 |
| 0.40 | 0.3809(6) | 0.4029(2) | 0.34212 | 1.86574 | 1.94930 |
| 0.42 | 0.3807(6) | 0.3841(2) | 0.26973 | 1.84631 | 1.96497 |
| 0.44 | 0.3805(6) | 0.3601(2) | 0.19912 | 1.82727 | 1.98079 |
| 0.46 | 0.3802(6) | 0.3284(2) | 0.13049 | 1.80863 | 1.99168 |
| 0.48 | 0.3801(6) | 0.2802(2) | 0.06407 | 1.79036 | 1.99797 |
| 0.50 | 0.3813(6) | 0.0 | 0 | 1.77245 | 2 |
lightest breather bound state $B_1$ to $S^{yy}$. The lightest breather $B_1$ has a gap $\Delta_1$ and contributes to $S^{yy}$ as

$$S^{yy} \left( \omega, \frac{\pi}{a_0} + q \right) \bigg|_{B_1} = C_y(H) \, \delta \left( \omega^2 - (v q)^2 - \Delta_1^2 \right), \quad (11)$$

where

$$C_y(H) = 2 \tilde{\nu} J \, e^2(H) \left[ 2 \cos(\pi \xi / 2) \sqrt{2 \sinh(\pi \xi / 2)} \exp \left( - \int_0^{\pi \xi} \frac{dt}{2 \sinh t} \right) \right]^2 \left( \frac{\Delta \sqrt{2} \Gamma((1 + \xi)/2)}{\Gamma((\xi)/2)} \right)^{\beta^2 / 2\pi} \times \exp \left[ 2 \int_0^{\infty} \frac{dt}{t} \left( \frac{\sinh^2(2\beta t)}{2 \sinh(\beta^2 t)} \right) \right].$$

(12)

Here we have used the normalizations of Ref. [13]. The leading contributions to the longitudinal structure factor at the incommensurate wave numbers $k = (\pi \pm 2\delta)/a_0$ are due to soliton and antisoliton. Using the results of Ref. [17] we obtain

$$S^{zz} \left( \omega, \frac{\pi \pm 2\delta}{a_0} + q \right) \bigg|_{s, \bar{s}} = C_z(H) \, \delta \left( \omega^2 - (v q)^2 - \Delta^2 \right),$$

(13)

where

$$C_z(H) = \frac{\tilde{\nu} J}{2} \, e^2(H) \left( \frac{C_{15}}{4C_2} \right)^{1/4} \left( \frac{\sqrt{2} \Delta \Gamma \left( \frac{3}{2} + \frac{\xi}{2} \right)}{J^{\beta} \Gamma(\frac{\xi}{2})} \right)^{2\pi / \beta^2} \times \exp \left[ \int_0^{\infty} \frac{dt}{t} \left( \frac{\exp[-(1 + \xi)t] - 1}{2 \sinh(\xi t) \sinh([1 + \xi] t) \cosh(t)} + \frac{1}{2 \sinh(\xi t)} - \frac{2 \pi e^{-2t}}{\beta^2} \right) \right].$$

(14)

Here the constants $C_{1,2}$ are given by

$$C_1 = \exp \left( - \int_0^{\infty} \frac{dt}{t} \frac{\sinh^2(t/2)}{\sinh(t) \sinh([1 + \xi] t) \cosh(t)} \right),$$

$$C_2 = \exp \left( 4 \int_0^{\infty} \frac{dt}{t} \frac{\sinh^2(t/2)}{\sinh(2t) \sinh(t)} \right).$$

(15)

As was pointed out in Ref. [17], at $H = 0$ the low-energy effective theory of the Hamil is SU(2) symmetric. In our notations this implies that

$$\lim_{H \to 0} \frac{C_y}{e^2(H)} = \lim_{H \to 0} \frac{C_z}{e^2(H)}. \quad (16)$$

Equation 2 is easily verified numerically. In order to evaluate $C_{y,z}$ we need to know the constant of proportionality $\gamma$ that relates the induced staggered field $h$ with the applied uniform field $H$. This constant differs from compound to compound. On the other hand, $\gamma$ enters the expressions for $C_{y,z}$ only via the soliton gap $\Delta$. Hence it is useful to isolate the $\gamma$ dependence and consider the quantities

$$C_y'(H) = C_y(H) \left( \frac{\Delta}{J} \right)^{\frac{\Delta^2}{2\pi}} J^{-1},$$

$$C_z'(H) = C_z(H) \left( \frac{\Delta}{J} \right)^{\frac{\Delta^2}{2\pi}} J^{-1}.$$  

(17)

The amplitudes $C_{y,z}'(H)$ are shown as functions of the magnetization in Fig. 2.

### III. COPPER BENZOATE

We are now in a position to determine the ratio between the spectral weights of the first breather (seen in the transverse structure factor $S^{yy}$) and the soliton (seen in the longitudinal structure factor $S^{zz}$). In an ideal situation one would carry out measurements with momentum transfers only along the $y$ and $z$ directions respectively. In practice, the experiments on Copper Benzoate were carried out with momentum transfers $k_{1,2}$ respectively, where

$$k_1 \cdot a, \, k_1 \cdot b, \, k_1 \cdot c = 2\pi (-0.3, 0, 1),$$

$$k_2 \cdot a, \, k_2 \cdot b, \, k_2 \cdot c = 2\pi (-0.3, 0, 1.12).$$

(18)

Here $c$ points along the chain direction and the antiferromagnetic wave number corresponds to $2\pi/c (c = 6.30 A)$.
as there are two copper atoms per unit cell along the $c$-axis. To make contact with our previous notations we need to set $a_0 = c/2$. The measurements with momentum transfers $\mathbf{k}_1$ and $\mathbf{k}_2$ probe the dynamical structure factor around $\pi/a_0$ and the incommensurate wave number $(\pi + 2\delta)/a_0$ respectively. In order to make direct comparisons with the experiments we need to relate the $(a, b, c)$ coordinate system describing the crystal axes to the $(x, y, z)$ spin coordinates. By definition $z$ and $x$ are the directions of the uniform and staggered fields respectively. In the experiments of Ref. [2] the uniform field was applied along the $b$-direction. Based on a polarization analysis it was suggested in Ref. [6] that the staggered field lies in the $ac$ plane and encloses an angle of $\alpha = -72^\circ$ with the $a$-axis. In the vicinity of $\pi/a_0$ the dominant contribution to the structure factor comes from the transverse correlators. This implies that

$$I(\omega, \mathbf{k}_1) \propto (0.083 \cos^2 \alpha + 0.917 \sin^2 \alpha) S^{yy} \left(\omega, \frac{\pi}{a_0}\right) + (0.083 \sin^2 \alpha + 0.917 \cos^2 \alpha) S^{xx} \left(\omega, \frac{\pi}{a_0}\right) \approx 0.84 S^{yy} \left(\omega, \frac{\pi}{a_0}\right) + 0.16 S^{xx} \left(\omega, \frac{\pi}{a_0}\right).$$

(19)

On the other hand at momentum transfer $\mathbf{k}_2$ the dominant contribution to the structure factor is due to the longitudinal component

$$I(\omega, \mathbf{k}_2) \propto S^{zz} \left(\omega, \frac{\pi + 2\delta}{a_0}\right).$$

(20)

As was pointed out in Ref. [6] there are unresolved issues concerning the polarization analysis and the estimate of the angle $\alpha$ should be regarded with some caution. It is possible to infer $\alpha$ by analyzing other experiments such as specific heat and ESR measurements. The analysis of the specific heat data suggests that $\alpha \approx -82^\circ$ which leads to a contribution of about 90% of $S^{yy}$ in $I$.

The neutron scattering experiments of Ref. [2] were performed in a uniform magnetic field of 7 T, which corresponds to a magnetization per site of $m \approx 0.06$. The breather and soliton gaps were observed at

$$\Delta \approx 0.22 \text{ meV}, \quad \Delta_1 \approx 0.17 \text{ meV}.$$  

(21)

Using the expression $\delta \text{RG}$ for the soliton gap we can infer the coefficient of proportionality between the uniform field $H$ and the staggered field $h$ as $\gamma \approx 0.06$. Taking $\gamma = 0.06$ and $m = 0.06$, Eq. $\delta \text{RG}$ gives $\Delta = 0.215 \text{ meV}, \Delta_1 = 0.171 \text{ meV}$ and we will use this set of parameters for our further analysis.

Under the above assumptions we may now determine the spectral weights of the coherent soliton and breather peaks in the dynamical structure factor. The results are shown in Fig. 3.

At a magnetization of $m = 0.06$ we have

$$\frac{C_y(H)}{C_z(H)} \approx 2.88.$$  

(22)

The spectral weights are obtained by integrating the respective structure factors over frequency at fixed momentum, i.e.,

$$I_{B_1} = \int d\omega \, S^{yy} \left(\omega, \frac{\pi}{a_0}\right) \bigg|_{B_1},$$

$$I_s = \int d\omega \, S^{zz} \left(\omega, \frac{\pi + 2\delta}{a_0}\right) \bigg|_s.$$  

(23)

The ratio of spectral weights between the first breather $I_{B_1}$ and the soliton $I_s$ is approximately

$$\frac{I_{B_1}}{I_s} \approx \frac{C_y(H)}{C_z(H)} \Delta_1 \approx 3.64.$$  

(24)
In order to compare to experiment, we need to take into account the different momentum transfers in the measurements of $S^{yy}$ and $S^{zz}$ respectively. From $I_1$ and $I_2$ we arrive at the following theoretical prediction for the ratio of intensities

$$R = 0.84 \frac{I_{B_1}}{I_2} \approx 3.06.$$

(25)

The experimentally observed ratio of peak heights between the breather and soliton peaks is approximately 2.8. This is in reasonable agreement with our result. For a better comparison one should take into account the resolution function of the instrument in both momentum and energy, but this goes beyond the scope of our present analysis.

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