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Amplitude Mode in Quantum Magnets via Dimensional Crossover

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We investigate the amplitude (Higgs) mode associated with longitudinal fluctuations of the order parameter at the continuous spontaneous symmetry breaking phase transition. In quantum magnets, due to the fast decay of the amplitude mode into low-energy Goldstone excitations, direct observation of this mode represents a challenging task. By focusing on a quasi-one-dimensional geometry, we circumvent the difficulty and investigate the amplitude mode in a system of weakly coupled spin chains with the help of quantum Monte Carlo simulations, stochastic analytic continuation, and a chain-mean field approach combined with a mapping to the field-theoretic sine-Gordon model. The amplitude mode is observed to emerge in the longitudinal spin susceptibility in the presence of a weak symmetry-breaking staggered field. A conventional measure of the amplitude mode in higher dimensions, the singlet bond mode, is found to appear at a lower than the amplitude mode frequency. We identify these two excitations with the second (first) breather of the sine-Gordon theory, correspondingly. In contrast to higher-dimensional systems, the amplitude and bond order fluctuations are found to carry significant spectral weight in the quasi-1D limit.

Introduction— The phenomenon of spontaneous symmetry breaking (SSB) represents one of the key notions in modern physics. For a continuous global symmetry, SSB is expected to generate two types of collective excitations – Goldstone modes, describing transverse or phase fluctuations of the order parameter, and Higgs modes, which describe its longitudinal or amplitude fluctuations. In contrast to the gapless Goldstone excitation, which is commonly observed in a variety of condensed matter systems (e.g. magnons in magnetically ordered materials), the observation of the amplitude (longitudinal) mode is more challenging. It is complicated by its intrinsically finite lifetime – an amplitude-mode excitation is allowed to decay into a pair of Goldstone excitations which leads to a strong damping of this excitation. By now several successful experimental sightings of the amplitude mode have been reported in the dimerized [1] and quasi-one-dimensional (1D) quantum magnets KCuF_3 [2, 3], $\text{BaCu}_2\text{Si}_2\text{O}_7$ [4], Ising-like spin chains $\text{SrCo}_2\text{V}_2\text{O}$ and $\text{Yb}_2\text{Pt}_2\text{Pb}$ [5, 6] as well as in superconducting settings [7, 8].

The amplitude mode is a well-defined excitation when its lifetime is long, which requires suppression of the decays into Goldstone modes, the spin waves. Theoretically, such suppression requires weakening of the long range magnetic order, magnitude of which determines spectral weight of the spin waves. Two ways to achieve this have been proposed, through (a) quantum critical points (QCPs) [9–12] and (b) dimensional crossover towards one dimension (1D) [13–16]. The first strategy was recently verified via quantum Monte Carlo model simulations in dimerized antiferromagnet [17–19] and superconductor-insulator transition [20].

In this letter, we explore the second, quasi-1D approach. It has long been proposed that a stable longitudinal mode shall arise in weakly coupled spin chains [14–16]. It should be noted that this 1D critical point is strongly different from

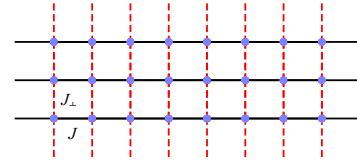


FIG. 1. Coupled antiferromagnetic Heisenberg spin chains with nearest-neighbor spin exchange J (black solid line) and J_\perp (red dashed line).

the $O(3)$ QCP one due to the extreme spatial anisotropy of spin correlations. At the critical point, which corresponds to the limit of decoupled spin chains, excitations propagate only along chains. This feature, combined with unique properties of the spin-1/2 Heisenberg chain, imbues the ordered phase of weakly coupled spin-1/2 chains with the spinon confinement physics which is absent in the spatially isotropic magnetically ordered phase with spontaneously broken $O(3)$ symmetry.

To study the excitation spectrum of the quasi-1D spin system, we utilize quantum Monte Carlo (QMC) simulations and stochastic analytic continuation (SAC) [21–23] to compute the spectral information of weakly-coupled Heisenberg spin-1/2 chains. The predicted amplitude mode is directly observed in numerics as the interchain interaction is reduced towards zero, and the dispersions of all low-energy modes agree nicely with analytic predictions. More importantly, we find that the amplitude mode in quasi-1D systems exhibits two novel features. First, in contrast with higher-dimensional magnets, the amplitude mode in quasi-1D systems is characterized by a spectral weight significantly stronger than the continuum, making it highly visible and easy to detect. Secondly, we find that a quasi-1D spin-1/2 magnet contains *three*, instead of two, low-energy modes. In addition to the phase

and amplitude modes, visible in the dynamic spin correlation functions, an additional scalar mode emerges in the dynamic *bond correlation* function. Similar to the amplitude mode, this scalar mode is singlet-like but exhibits different frequency and momentum dependence.

In higher dimensions, it has been known that the scalar susceptibility serves as a great tool for probing fluctuations in the singlet channel [10] and has been widely used in numerical studies of dimerized antiferromagnets [17–19]. Inside the ordered SSB phase scalar fluctuations overlap with the amplitude ones but with much suppressed damping, and the scalar susceptibility exhibits a sharp peak at the amplitude mode frequency [11]. Quasi-1D limit is different. We show that in contrast to the amplitude mode which corresponds to the “second breather” in the effective sine-Gordon description of the ordered quasi-1D magnet, the scalar mode is represented by the “first breather”, an excitation with smaller frequency which is probed via the dynamic bond-bond correlation function.

The model and the QMC method— The geometry of the problem is shown in Fig. 1. The Hamiltonian reads

$$H = J \sum_{\langle i,j \rangle_x} \mathbf{S}_i \cdot \mathbf{S}_j + J_\perp \sum_{\langle i,j \rangle_y} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i (-1)^i S_i^z, \quad (1)$$

where $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ denotes the spin-1/2 operator on site i and J (J_\perp) is the nearest-neighbor Heisenberg exchange along the x (y) direction. We set $J = 1$ and introduce ratio $g = J_\perp/J$ to control the crossover from decoupled 1D chains, $g = 0$, to the isotropic 2D square lattice, $g = 1$. The last term represents the staggered pinning field h , which explicitly breaks the spin-rotational symmetry.

In our QMC simulations the following three correlation functions are measured: the transverse spin correlation function $G_{S^x}(\mathbf{q}, \tau) = \frac{1}{L^2} \sum_{i,j} e^{-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \langle S_i^x(\tau) S_j^x(0) \rangle$, similarly defined longitudinal S^z correlation function $G_{S^z}(\mathbf{q}, \tau)$, and the bond correlation $G_B(\mathbf{q}, \tau) = \frac{1}{L^2} \sum_{i,j} e^{-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_j)} \langle B_j(\tau) B_i(0) \rangle$. Here $B_i = \mathbf{S}_i \cdot \mathbf{S}_{i+\hat{x}}$ is a spin singlet bond operator (dimerization order parameter) defined on a nearest-neighbor bond of the spin chain, L is the linear system size and $\tau \in [0, \beta]$ is the imaginary time. In the ordered SSB ground state with finite $\langle S^z \rangle \neq 0$ phase fluctuations (spin waves) are probed by G_{S^x} , G_{S^z} measures the amplitude fluctuations, and the scalar correlation function G_B probes correlations between bonds (energy density) [17–19].

It is important to notice that SSB ground state is not possible in the QMC simulation on a finite $L \times L$ system and at finite inverse temperature β . Therefore, in the QMC with $h = 0$, there is no distinction between the phase and amplitude correlation functions, $G_{S^x}(\mathbf{q}, \tau) = G_{S^z}(\mathbf{q}, \tau)$. Finite $h \neq 0$ breaks spin-rotational symmetry and allows one to probe the amplitude mode by measuring G_{S^z} . It also induces the h -dependent gap in the phase mode in G_{S^x} [24–26].

In order to access real-time quantum dynamics and obtain the real-frequency spectral function $A(\mathbf{q}, \omega)$ from the imaginary-time correlation $G(\mathbf{q}, \tau)$, $G(\mathbf{q}, \tau) = \frac{1}{\pi} \int_0^\infty d\omega A(\mathbf{q}, \omega) (e^{-\tau\omega} + e^{-(\beta-\tau)\omega})$, we employ the

stochastic analytic continuation (SAC). This technique, details of which are described in [27–30] and the Supplemental Material (SM) [31], has been successfully applied to a broad range of quantum magnets [32–41].

Analytical Theory— At small $g = J_\perp/J \ll 1$, a variety of exact (Bethe ansatz) and nonperturbative approaches (bosonization and renormalization group) are available. In the $g = 0$ limit elementary excitations of the spin chain are right- and left-moving spinons, neutral spin-1/2 fermions $\psi_{R/L,s}$, which encode an extended $SU(2)_R \times SU(2)_L$ symmetry of chiral rotations at low energies. Staggered part of the lattice spin operator is expressed via spinons as $S_i^a \sim (-1)^i \psi_{R,s}^\dagger \sigma_{ss'}^a \psi_{L,s'} + \text{h.c.}$, where σ^a is the Pauli matrix. The singlet bond operator is staggered as well $B_i \sim (-1)^i \psi_{R,s}^\dagger \psi_{L,s} + \text{h.c.}$. These expressions define physical response functions G_{S^a} and G_B of the chain. When continued to the real frequency, the response is given by the triplet and singlet spinon continua, correspondingly.

Interchain interaction, $g \neq 0$, causes *confinement of spinons*, binding them in triplet and singlet pairs. This is easiest seen with the help of the chain mean-field theory [15, 16, 42, 43] which maps the problem to the 1D sine-Gordon model by approximating J_\perp term in Eq. (1) by the interchain staggered field $2J_\perp m_0 \sum_i (-1)^i S_i^z$ with the self-consistently determined staggered magnetic order $m_0 = (-1)^i \langle S_i^z \rangle$ along the z -axis [31]. This mean-field breaks spin rotational symmetry of the problem (with $h = 0$). The excitation spectrum of the sine-Gordon model consists of solitons and antisolitons of mass Δ_0 , which describe transverse spin excitations, and their bound states, breathers. The amplitude mode, which within the low-energy mapping to the sine-Gordon model is represented by $S^z \sim \cos(\Phi/2)$, is described by the *second* breather, of mass $\sqrt{3}\Delta_0$. The singlet mode, which is represented as $B \sim \sin(\Phi/2)$, is instead described by the *first* breather, of mass Δ_0 , see [31] and [16, 43]. This brief description shows that in the system of weakly coupled spin-1/2 chains the amplitude, S^z , and the scalar, B , modes are distinct and *independent* excitations.

Detailed calculation of spin and bond susceptibilities are presented in SM [31]. The dispersions of the phase (S^x and S^y), amplitude (S^z) and bond (B) modes near $k_x = \pi$ are

$$\omega_{S^x} = \omega_{S^y} = \Delta_0 \sqrt{1 + b_h + \cos k_y + \frac{v^2(k_x - \pi)^2}{\Delta_0^2}} \quad (2)$$

$$\omega_{S^z} = \Delta_0 \sqrt{3(1 + b_h) + \frac{Z_2}{Z_1} \cos k_y + \frac{v^2(k_x - \pi)^2}{\Delta_0^2}} \quad (3)$$

$$\omega_B = \Delta_0 \sqrt{1 + b_h + \frac{v^2(k_x - \pi)^2}{\Delta_0^2}} \quad (4)$$

Here k_x (k_y) is the momentum along the chain (transverse to the chain) and b_h is a dimensionless parameter describing the effect of the external staggered field h , Eq. (S25). At $h = 0$, b_h vanishes and our equations for ω_{S^x} and ω_{S^z} recover the corresponding formulae in Ref. [43]. The velocity v is $\pi J/2$ and the ratio $Z_2/Z_1 \approx 0.491309$.

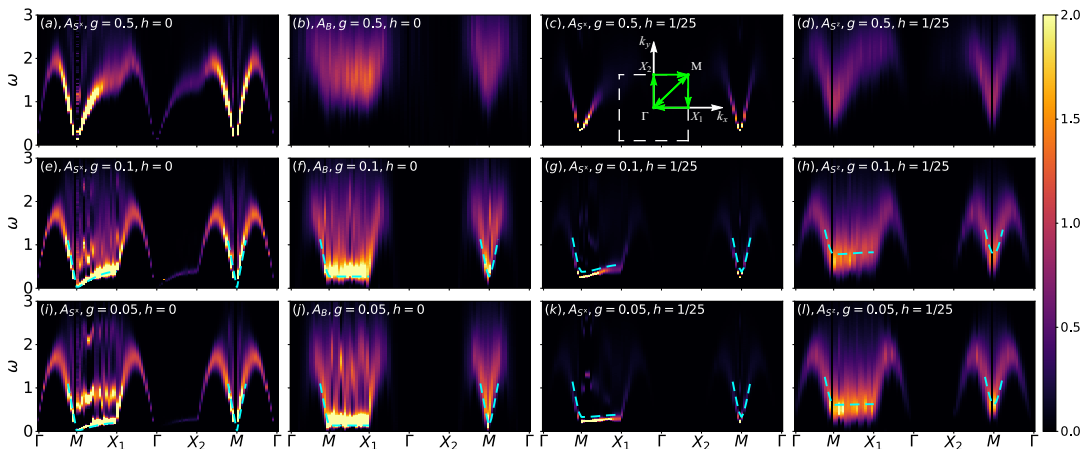


FIG. 2. Spectral functions obtained from QMC-SAC. (a), (e), (i) and (b), (f), (j) show the spectra function of spin and bond operators respectively, $A_{S^x}(\mathbf{q}, \omega)$ and $A_B(\mathbf{q}, \omega)$, without the field, $h = 0$, at different values of $g = J/J_\perp$, with the system size is $L = 36$ and inverse temperature $\beta = 4L$. The dashed cyan curves in (e), (i) and (f), (j) are analytical dispersions in Eqs. (2) and (4) with $b_h = 0$. (c), (g), (k) and (d), (h), (l) show the phase mode spectra $A_{S^x}(\mathbf{q}, \omega)$ and amplitude mode spectra $A_{S^z}(\mathbf{q}, \omega)$ measured in the presence of a weak staggered field $h = 1/25$, with system size $L = 36$ and inverse temperature $\beta = 4L$. The dashed cyan curves in (g), (k) and (h), (l) are analytical dispersions in Eqs. (2) and (3) with finite b_h .

Note that in addition to having a different mass, the dispersion of the bond mode is different from the amplitude one as well. It propagates along the chain with the same velocity v as spin fluctuations but is essentially dispersionless in the transverse k_y direction, see [31].

Numerical Results— In Fig. 2, we present numerical results of spectral functions for spin-spin and bond-bond correlations, with and without the pinning field h and compare them with the dispersions (cyan lines) obtained from analytic theory Eq.(2)-(4). From the top to bottom row, the values of g are 0.5, 0.1 and 0.05, reflecting the dimensional crossover from 2D to quasi-1D. The system has periodic boundary condition $L \times L$ with $L = 36$. The QMC calculations are carried out at inverse temperature $\beta = 4L$. The spectra are plotted along the high-symmetry path indicated in the BZ in panel Fig. 2(c). The first (last) two columns of Fig. 2 are measured in the absence (presence) of the staggered field h .

Key differences between the 2D ($g = 0.5$, Fig. 2 (a-d)) and quasi-1D regimes ($g = 0.1$ for Fig. 2 (e-h) and $g = 0.05$ for Fig. 2 (j-l)) are easily seen. For $g = 0.5$ the phase mode is clearly visible in panels (a) and (c) while the amplitude and scalar fluctuations (d) and (b) exhibit only an over-damped multi-magnon continuum without any sharp modes, as expected [13, 14]. As the system moves towards 1D ($g = 0.1$ and 0.05), the single magnon mode remains sharp and becomes more 1D-like (i.e. less dispersive along the interchain $M - X_1$ direction). At the same time, the spectral weight in the bond (Fig. 2 (f) and (j)) and amplitude (Fig. 2 (h) and (i)) sectors shifts down in energy, resulting in the emergence of the two low energy peaks in corresponding spectral densities.

Let us investigate these differences closer. The first column in Fig. 2 shows A_{S^x} at $h = 0$. Note that simulations in finite size and temperature system are necessarily done in the

symmetric phase with three components of spin susceptibility degenerate $A_{S^x} = A_{S^y} = A_{S^z}$. The minimal spin excitation energy, measured at the M point (π, π) , is small but finite. At $g = 0.05$ it is about 0.004. The dispersion of the lowest energy branch is well described by the pole of the RPA susceptibility Eq. (S35). Notice that in this magnetically disordered phase the gap is $\Delta^2 - 2Z_1 J_\perp > 0$, as discussed above. It vanishes only in the thermodynamic limit $L = \infty$ when the SSB takes place and the spin rotational symmetry gets broken, resulting in different dispersion relations for transverse, Eq. (2), and longitudinal, Eq. (3), modes (with $b_h = 0$).

We also observe noticeable spectral intensity at higher energy, $\omega \approx 0.6 - 0.7$, in Fig. 2 (e) and (i). We assign this to the second breather of the sine-Gordon+RPA theory, Eq. (S36), with the mass $\sqrt{3}\Delta$ [31]. Naturally, this feature is absent in the 2D limit, Fig. 2(a), where our quasi-1D arguments do not apply. This interpretation is further supported by the data for bond spectral function A_B , presented in the 2nd column of Fig. 2. Here, one observes pronounced difference between the 2D, $g = 0.5$, and 1D limits, $g = 0.05$ and 0.1: the broad and over-damped multi-particle continuum evolves into a very structured one with a sharp particle-like peak at the lowest energy for small- g cases, in Fig. 2 (f) and (j). This is the first breather of the sine-Gordon model, describing scalar bond (staggered dimerization) mode, with mass Δ , of weakly coupled spin chains, as described below Eq. (4). As explained in SM [31], its dispersion along k_y is negligible while that along k_x matches Eq. (4) (with $b_h = 0$) very well.

Taken together, our data lend strong support to the description of the spin system in terms of *confined* spinon pairs. The spin susceptibility is described by the triplet of bound spinons and its internal excited state (the second breather) while the scalar susceptibility is represented by bound singlet pairs of

spinons.

To differentiate between the transverse and longitudinal fluctuations we next turn on the staggered field $h \neq 0$ along the z axis. The corresponding QMC data are represented by the last two columns of Fig. 2. Now $A_{S^x} = A_{S^y}$ measures the phase fluctuations of the order parameter (the third column), which are gapped stronger by the finite h , while A_{S^z} gives the amplitude fluctuations (the last column).

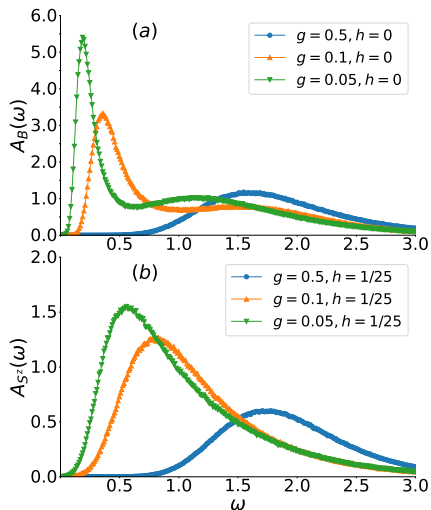


FIG. 3. Frequency dependence of the spectral functions at $\mathbf{k} = (\pi, \pi/2)$ for (a) the bond-bond correlation at $h = 0$ and (b) the amplitude mode at $h = 1/25$.

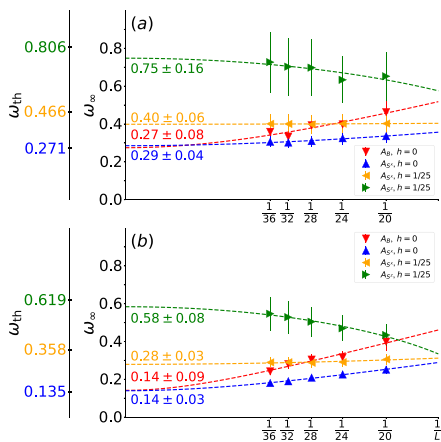


FIG. 4. Finite-size analysis for (a) $g = 0.1$ and (b) $g = 0.05$ at the momentum point $\mathbf{k} = (\pi, \pi/2)$. The vertical ω_∞ -axis shows extrapolation of the numerical data to the $L = \infty$ limit. Values on the left vertical ω_{th} -axis mark analytical predictions for the peak frequencies of different modes. See main text for details.

To illustrate the emergence of the amplitude and scalar modes we plot in Fig. 3 the frequency dependence of these two spectra at different value of g at the wavevector $\mathbf{k} = (\pi, \pi/2)$. In 2D ($g = 0.5$), both spectra exhibit a continuum background from multi-magnon excitations. As g gets smaller, a peak

emerges in the spectral function and becomes sharper as g becomes smaller. It is seen that for the same value of g the peak in A_B is more narrow and occurs at a lower frequency than that in A_{S^z} . The larger linewidth of the amplitude mode is due to the stronger damping it experiences due to decays into the low energy phase fluctuations, in comparison with the bond correlation function [10], while the peak's maxima difference is a unique property of quasi-1D system as equations (3) and (4) show.

In Fig. 4, we present the finite-size analysis and extrapolate the peak frequency of each mode to the thermodynamic limit. Here, we focus on the momentum point $\mathbf{k} = (\pi, \pi/2)$, at which the interchain dispersion vanishes within the RPA approximation, and the frequency of a mode is obtained by fitting the correlation function to an exponential function of the imaginary time $\propto e^{-\omega\tau}$ (several representative cases of such fitting are presented in SM [31]). Given the square-root form of dispersions (2), (3) and (4), we take the following functional form for the extrapolation to infinite size $\omega_L = \sqrt{\omega_\infty^2 + L_0^2/L^2}$, where ω_∞ and L_0 are fitting parameters. The results for so obtained ω_∞ are presented to the right of ω_∞ -axis in Fig. 4. As discussed above, without the staggered field the lowest energy peak in A_{S^x} ($h = 0$) describes coherent 3-fold degenerate mode ω_{S^x} . At finite $h = 1/25$, the degeneracy is removed and ω_{S^x} and ω_{S^z} scale to different limits. Within the sine-Gordon description $\omega_{S^z}/\omega_{S^x} = \sqrt{3}$, see Eqs. (2) and (3). Figure 4 shows that this ratio extrapolates to 1.8 for $g = 0.1$ and to 2.0 for $g = 0.05$ at $L = \infty$. The ω_{th} axis in Fig. 4 shows analytical predictions for $\omega_{S^x}, \omega_{S^z}$, which are calculated as functions of g and h , without any adjustable parameters, in SM [31]. This parameter-free comparison is seen to work reasonably well. In addition, in agreement with analytical predictions, Fig. 4 shows that for $h = 0$, ω_{S^x} and ω_B extrapolate to the same limit, just as equations (2) and (4) with $b_h = 0$ require.

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