

Anomalous thermal broadening in the Shastry-Sutherland model and $\text{SrCu}_2(\text{BO}_3)_2$ Zhenjiu Wang^{1,2,3,*}, Paul McClarty^{3,4,*}, Dobromila Dankova³, Andreas Honecker⁵, and Alexander Wietek^{3,‡}¹Lanzhou Center for Theoretical Physics, Key Laboratory of Quantum Theory and Applications of MoE, Key Laboratory of Theoretical Physics of Gansu Province, and School of Physical Science and Technology, [Lanzhou University](#), Lanzhou, Gansu 730000, China²Arnold Sommerfeld Center for Theoretical Physics, [University of Munich](#), Theresienstr. 37, 80333 Munich, Germany³Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, Dresden 01187, Germany⁴Laboratoire Léon Brillouin, CEA, CNRS, [Université Paris-Saclay](#), CEA Saclay, 91191 Gif-sur-Yvette, France⁵Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, [CY Cergy Paris Université](#), 95302 Cergy-Pontoise, France

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In the quantum magnet $\text{SrCu}_2(\text{BO}_3)_2$, an anomalous thermal broadening of the triplon modes has been measured at relatively low temperatures compared to the triplon gap Δ using both inelastic neutron scattering and Raman spectroscopy. Given how accurately a broad variety of physical phenomena in $\text{SrCu}_2(\text{BO}_3)_2$ are captured by the spin $S = 1/2$ Shastry-Sutherland model, it remains an open question whether the anomalous thermal broadening is also an intrinsic feature of this minimal model. However, few techniques are available for computing the finite-temperature dynamics of strongly interacting many-body systems. To address this problem, we have developed a broadly applicable numerical simulation method based on matrix-product states to simulate dynamical spectral functions at nonzero temperatures accurately, detailed in a companion paper [[Phys. Rev. B **113**, 024406 \(2026\)](#)]. Using this technique, we demonstrate that the experimentally observed broadening is captured by the Shastry-Sutherland model. Perturbative calculations identify the origin of this phenomenon as singlet bound two-triplon states being thermally excited at an energy scale small compared to the gap Δ to the single triplon excitations at the experimentally relevant model parameters.

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Introduction. All spectroscopic experiments are carried out at finite temperature. Yet, it is very challenging to devise accurate theoretical methods that capture dynamical phenomena in this regime. In particular, there are questions where thermal fluctuations are central.

Here, we address such questions in a case whose history goes back to a two-dimensional quantum spin model that supports an exact dimer ground state over a significant range of exchange couplings [1]. Although the ground state in this $S = 1/2$ “Shastry-Sutherland model” is of simple nature within this regime, it nicely exemplifies the effect of destructive interference on triangular units that is the heart of geometrical frustration, the exploration of which has formed the entire field of frustrated magnetism. Today, studies of highly frustrated magnets range over rich and complex physics on kagome, pyrochlore, and other lattices [2]. There are, however, further pillars to the fame of the Shastry-Sutherland model. One is the discovery, many years after the original theory paper, of a material $\text{SrCu}_2(\text{BO}_3)_2$, that almost perfectly

realizes the dimer phase of the model [3,4]. This material has consistently stood out for the surprises and puzzles that it has generated, and continues to produce over twenty years after the first experiments [3–43]. These include the famous series of magnetization plateaus reaching up to around 100 T [3,5–16], observations of nearly flat triplon excitations about the dimer phase [19,21], infrared, Raman, and neutron studies exploring the triplons and the tower of bound-state excitations [17–23,44,45], topological triplons coming from small exchange anisotropies [22,27–29], experiments observing a plaquette phase in the material at high pressures and investigations of the nature of the phase transition to this phase [32,34–40], including the tantalizing possibility of realizing deconfined criticality on the boundary between Néel order and the plaquette phase [41,42]. The Shastry-Sutherland model has served as suitable framework for understanding these experimental discoveries and both model and material have provided an important proving ground for new numerical and analytical tools. In fact, studies of $\text{SrCu}_2(\text{BO}_3)_2$ have turned out to be almost a microcosm for the development of quantum magnetism as a whole. The low-entanglement dimer phase was an attractive target for tensor network methods, which now have captured much of the complexity of the magnetic field-induced phase diagram as crystals of condensed bound states [33]. Related techniques have also captured the thermodynamics [43] and ground-state spectral functions [46].

In this paper, we consider a further curiosity of $\text{SrCu}_2(\text{BO}_3)_2$ —a dramatic broadening of the triplon modes with increasing temperature uncovered by inelastic neutron scattering [19,21,47] and corroborated by Raman scattering

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[18,23]. Thermal broadening of excitations is entirely to be expected in any correlated magnetic system. The peculiarity of $\text{SrCu}_2(\text{BO}_3)_2$ is its sensitivity to thermal excitations as well as the extent of the effect in the crossover to the paramagnetic state. The triplon excitations are gapped at about 3 meV or about 35 K, and significant broadening is observed by around 5 K, while the Bose factor at this temperature is about 10^{-3} so the triplons are undoubtedly very dilute. By 15 K, the neutron intensity is broadened into a nearly featureless continuum.

In the following, we show how to capture this effect quantitatively and provide insight into the microscopic mechanism that underlies it. Previous work using finite-temperature Lanczos on small cluster sizes up to $N = 20$ sites [48] reported anomalous thermal broadening but such methods are very limited in system size (here $N = 20$) thus providing little momentum space resolution and, relatedly, little room for capturing correlations and especially extended objects such as bound states.

Matrix-product and tensor-network techniques have become increasingly important to quantum many-body physics. By now, they are the technique of choice for studying the ground states of a wide range of interacting systems in one and even two dimensions [16,33,40,49,50]. Recently, developments have shown that such techniques can be adapted to compute dynamical correlators and thermodynamics [43,51–54] with considerable success in capturing experimental results. One important frontier in matrix-product state methods is to extend the methods to computations of dynamics at finite temperature. The basis of this work is our development of just such a method that we expect to be broadly applicable to dynamical correlators at finite temperature. We showcase the method on the problem of thermal broadening of triplons in the Shastry-Sutherland model, showing that the model captures the experimentally observed anomalous broadening semi-quantitatively. We further carry out perturbative calculations of the broadening that provide insight into the microscopic mechanism underlying the phenomenon, albeit without the quantitative success of the matrix-product method.

The Shastry-Sutherland model and its experimental realization. The Shastry-Sutherland model is a localized spin-1/2 model formulated on the lattice illustrated in Fig. 1(a) [1]. The Hamiltonian is given by

$$H = J_D \sum_{\langle i,j \rangle_D} \mathbf{S}_i \cdot \mathbf{S}_j + J \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

where J_D denote the intradimer couplings and J the interdimer couplings. When $J = 0$, the ground state has isolated singlets living on the J_D bonds and canonical excitations are spin $S = 1$ triplets in the local dimers. When J is switched on, each singlet couples via its two component spins to a single site on neighboring singlets. This geometrical frustration endows the singlets with stability such that the dimer covering survives as an exact eigenstate for all couplings and remains the ground state up to $J/J_D \approx 0.67$ as determined numerically [7,49,56,57].

The lowest-lying excited states, for small J/J_D , are coupled triplet excitations called *triplons*. As the model and ground state are spin-rotationally symmetric, the triplons are threefold degenerate. One might expect the coupled triplets to acquire

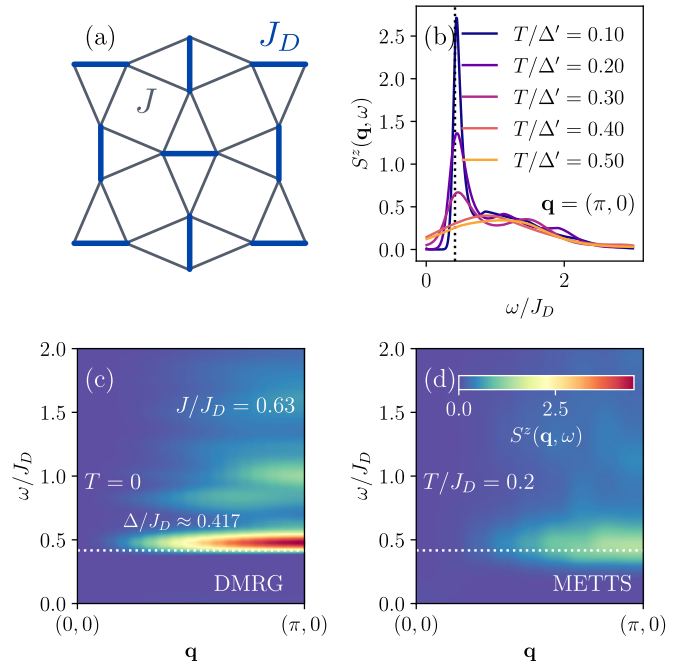


FIG. 1. (a) Geometry of the Shastry-Sutherland lattice. The intradimer couplings J_D are shown in blue and the interdimer couplings J in gray. (b) $S^z(\mathbf{q}, \omega)$ for $\mathbf{q} = (\pi, 0)$ at various temperatures in units of the perturbative triplon gap Δ' from dynamical METTS simulations on a 16×6 cylinder, employing the analytical complex time algorithm at complex angle $\theta = \pi/4$ as proposed in the companion paper [55]. The triplon peak at Δ melts into a broad continuum at temperatures that are a fraction of the triplon gap $\Delta \approx 0.417J_D$. (c), (d) Dynamical spin structure factor $S^z(\mathbf{q}, \omega)$ at $T = 0$ (c) and $T/J_D = 0.2$ (d) from dynamical density matrix renormalization group (DMRG) simulations on a 16×6 cylinder for a cut through the Brillouin zone from $(0, 0)$ to $(\pi, 0)$ exhibiting a flat triplon band at energies around the triplet gap Δ .

some dispersion on the scale of J . However, it turns out that triplon hopping is suppressed by the magnetic frustration with the leading order contribution appearing to $O((J/J_D)^6)$ [7,24,26,58,59], so the triplons are very nearly localized even close to the phase boundary out of the dimer phase, resulting in a flat band of triplon excitations, cf. Fig. 1(c). For the material $\text{SrCu}_2(\text{BO}_3)_2$ at ambient pressure, J/J_D has been experimentally estimated to be 0.63 [7,25,43], so it lies at the edge of the dimer phase. The triplon gap is estimated to be $\Delta \approx 0.417J_D$ from DMRG on the 16×6 cylinder. Given the experimentally measured triplon gap $\Delta = 35$ K, this results in a dimer interaction of $J_D = 7.23$ meV. Observations of the triplons reveal the bandwidth to be about one-tenth of the gap and therefore significantly larger than in the pure Shastry-Sutherland model. This indicates the presence of small anisotropies that are known to be predominantly Dzyaloshinskii-Moriya or antisymmetric exchange that we neglect here. Our results imply that these small corrections to the pristine Shastry-Sutherland model play a negligible role in the thermal broadening to which we now turn.

The sensitivity of the quantum states of $\text{SrCu}_2(\text{BO}_3)_2$ to finite temperatures was first observed from the washing out of magnetization plateaux at around 1 K [3]. Later, the neutron

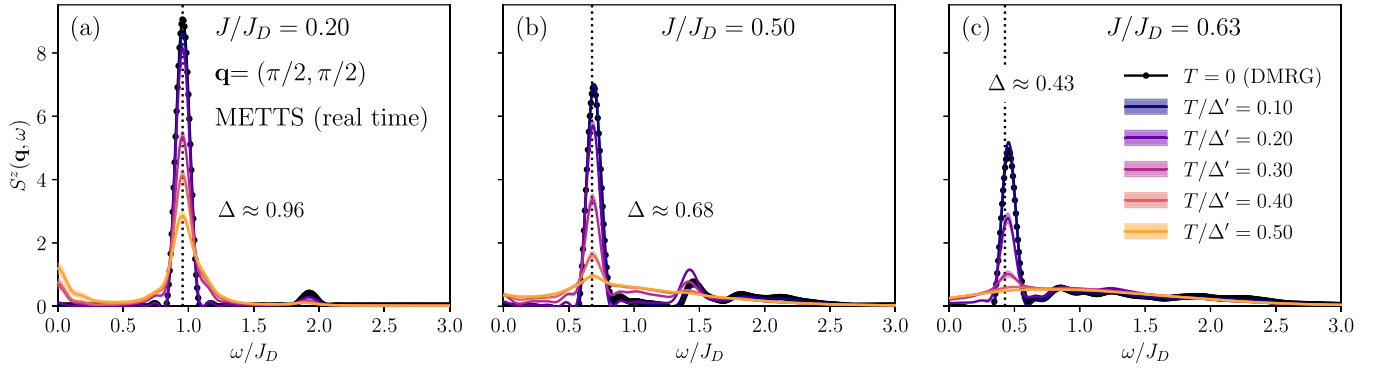


FIG. 2. Dynamical spin-spectral functions evaluated at momentum $\mathbf{q} = (\pi/2, \pi/2)$ from dynamical METTS simulations on the 16×4 cylinder. Results at temperatures that are a fixed ratio of the triplet gap Δ are shown. The triplet gap Δ is shown as the dashed line. (a) $J/J_D = 0.2$, (b) $J/J_D = 0.5$, and (c) $J/J_D = 0.63$. Whereas the dominant peak close to the triplet gap is only weakly broadened for $J/J_D = 0.2$, it completely disappears at temperatures which are small fractions of the triplet gap for $J/J_D = 0.63$ (c).

scattering intensity of the single triplon modes was seen to fall off faster with increasing temperature than would be expected on the basis of the 35 K gap [19,21,47]. Indeed, the triplons are almost completely washed out by about 10 K, leaving a broad continuum of intensity. This behavior is consistent with Raman measurements that are more sensitive to singlet intensity [18,23]. It has been suspected for a long time that the unusual temperature dependence originates from the delicate nature of the frustration-induced dimer formation and, in particular, that only a very dilute concentration of thermal triplet states is sufficient to delocalize the dimers.

Thermal broadening from dynamical METTS. We now demonstrate the dynamics of the pure Shastry-Sutherland model accurately capture the effect of the triplon thermal broadening in $\text{SrCu}_2(\text{BO}_3)_2$ in close agreement with experimental measurements. Our simulation is based on a numerical technique for evaluating dynamical spectral functions at nonzero temperature, based on the idea of minimally entangled typical thermal states [51,52,60,61]. In the companion paper [55], we introduce this technique in detail and benchmark it against more traditional techniques. The principal advantage of dynamical METTS is that it allows one to address significantly larger system sizes than previously possible. The method is performed in two distinct modes. With the real-time evolution algorithm, we directly simulate the dynamical correlation function,

$$C_{AB}(t) = \langle A(t)B \rangle_\beta = \langle e^{iHt} A e^{-iHt} B \rangle_\beta, \quad (2)$$

at nonzero temperature ($T = 1/\beta$) up to a final time Ω , after which a Fourier transform yields the desired spectral function. The dynamical correlation functions can be fully converged on $W = 4$ cylinders at all investigated temperatures for the Shastry-Sutherland model. We also refer to Ref. [55] for the exact definition of lattice constants. Here, we choose a simulation time horizon of $\Omega/J_D = 50$. We use $R = 100$ METTS samples to compute statistical averages and verify convergence in bond dimension up to $\chi = 1000$.

This method yields highly accurate results for smaller cylinders, where even the temperature dependence of secondary and tertiary peaks can be resolved. However, since there are limitations in system size owing to the exponential scaling in cylinder width, we introduce a complex-time

evolution algorithm, where the dynamical correlation function is simulated on a contour in complex time and the spectral function is obtained via stochastic analytic continuation [62–65]. A real-time component mitigates the ill-posedness of the analytical continuation.

Figure 2 shows the dynamical structure factor $S(\mathbf{q}, \omega)$, calculated for fixed $\mathbf{q} = (\pi/2, \pi/2)$ and for different temperatures and various J/J_D . The choice of $\mathbf{q} = (\pi/2, \pi/2)$ is slightly arbitrary as we are probing an approximately flat band and observe similar broadening features at different momenta. For $J/J_D = 0.2$, the principal peak at $\omega/J_D = 0.96$ corresponds to the ground state to single-triplon transition and there is a secondary peak at twice this energy coming mainly from the free two-triplon states. As the temperature increases, the amplitude of both peaks decreases and both broaden and, at the same time, intensity around $\omega \approx 0$ at low-frequencies appears, commonly referred to as quasi-elastic intensity. For larger values of J/J_D , the single-triplon peak comes down in energy and for a fixed temperature it is broader for larger values of J/J_D . Meanwhile, the two-triplon sector broadens into a continuum extending to both higher and lower energies. For $J/J_D = 0.63$ corresponding to the material, the dynamical structure factor is a featureless continuum above around $T/\Delta = 0.4$ corresponding to about 14 K. On the 16×6 cylinder, we analogously observe the melting of the main triplon peak at temperatures $T/\Delta \approx 0.4$ in Figs. 1(b) and 1(d). There, results have been obtained using the complex-time evolution algorithm explained in the companion paper [55].

We now make a more direct comparison of the numerical results and the experiment. Figure 3 shows the cumulative spectral weight up to energy ω for different temperatures. The top panel are the numerical data at fixed momentum and the lower panel are the experimental data taken from Ref. [47]. The lower-temperature data show the single-triplon peak as a rapid upturn in both numerics and experiment. At temperatures of about 40 percent of the triplon gap, the cumulative spectral weight increases almost linearly corresponding to an almost featureless continuum. This plot demonstrates that the numerical technique captures the thermal broadening in the material. In particular, the degree of broadening at a given temperature scale coincides between the simulation and the experiment. Reference [47] points out that

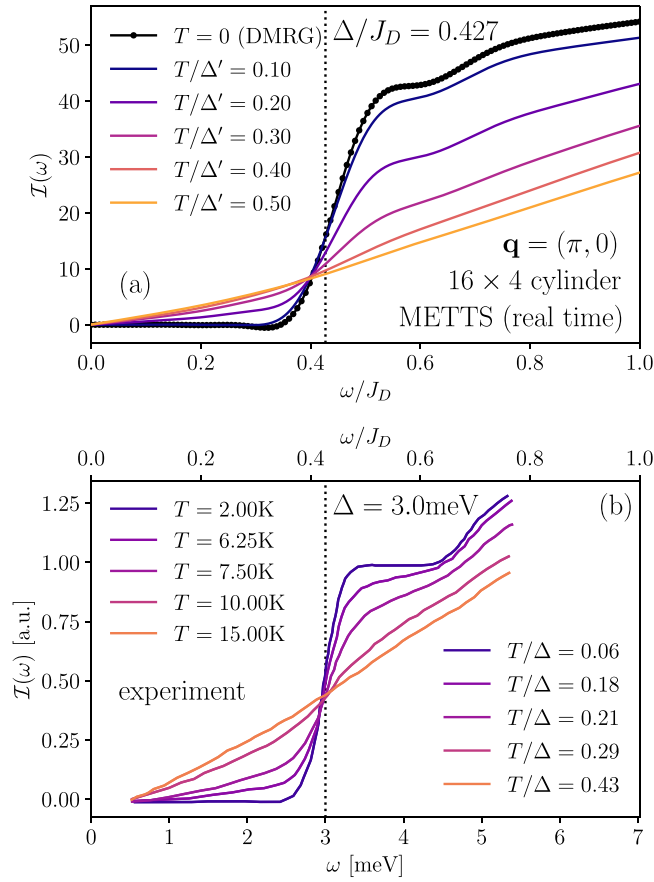


FIG. 3. Temperature dependence of the cumulative spectral weight as a function of energy. The lower panel shows inelastic neutron scattering data (taken from Ref. [47] in arbitrary units) on a powder sample. The data are momentum integrated and resolved in energy. The data at five different temperatures reveal the progressive broadening of the central peak. The top panel shows our numerical result for the cumulative spectral weight at momentum $\mathbf{q} = (\pi, 0)$.

the single triplon peak appears to have one sharp component, whose amplitude decreases with temperature and a broad temperature-dependent component, which is consistent with our numerics. One perceptible discrepancy between the calculation and experiment is the larger relative drop in the integrated spectral weight up to $\omega/\Delta = 5/3$ in the former. On this point, we note that the experimental data are momentum-integrated and that the single-triplon intensity is momentum-dependent and large at $\mathbf{q} = (\pi, 0)$ where the calculation has been performed.

A few comments and caveats are necessary at this point. One is that the zero-temperature peak is a delta function in principle. This is not realized in the numerics because of the inevitable finite-time cutoff in the dynamics. The experimental single-triplon peak also has a width at very low temperatures owing to instrumental resolution. Secondly, one plausible lesson to be drawn from the excellent agreement between theory and experiment is that the relevant physics is rather local. As we shall argue this originates from the almost perfect localization of the single-triplon modes combined with the fact that small system sizes already capture the

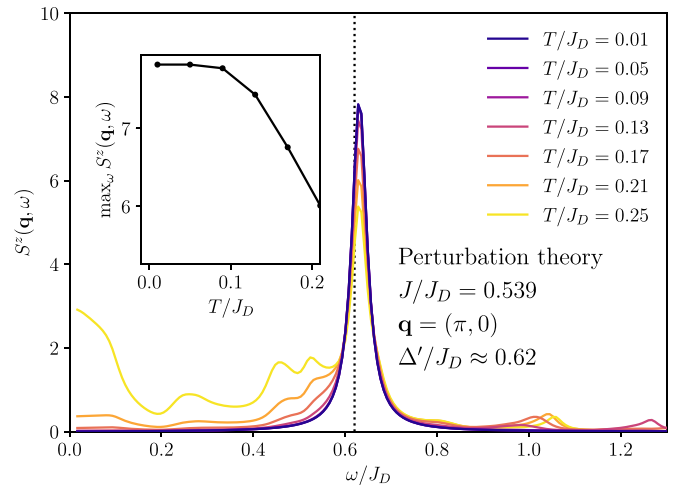


FIG. 4. Dynamical structure factor at $J/J_D = 0.539$ and $\mathbf{q} = (\pi, 0)$ computed from the low-temperature expansion. The inset shows the evolution of the peak height with increasing temperature.

broad spectrum of bound-state modes as the relevant states have a short length scale. Finally, one might be concerned that the material has couplings beyond the Heisenberg model and that these may contribute to the thermal broadening. The good agreement between the numerical results and experiment is, nevertheless, suggestive that the pure Shastry-Sutherland model is largely responsible for the physics. We argue below that indeed the relevant scales are those coming from the Heisenberg model.

Physics of thermal broadening. Having seen that the Shastry-Sutherland model in a nonperturbative analysis leads to thermal broadening similar to that seen in $\text{SrCu}_2(\text{BO}_3)_2$, we now discuss the microscopic origin of this phenomenon. To do so, we discuss the analytical perturbation theory around the non-interacting dimer case. The effects and roles of (multi)triplon states in perturbation theory are detailed in the Supplemental Material [66], where a direct comparison to energetics from ED can be found.

Figure 4 shows the resulting dynamical structure factor from perturbation theory for $J/J_D = 0.539$, where the perturbative singlet-triplon and lowest-lying two-triplon bound-state energies coincide, and for $\mathbf{q} = (\pi, 0)$ where the single-triplon intensity is maximal. This particular value of J/J_D has been chosen, since also for $\text{SrCu}_2(\text{BO}_3)_2$ the triplon and two-triplon bound states are expected to occur at the same energy [22]. Several temperatures are plotted between $T/J_D = 0.01$ up to 0.2 ($T/\Delta' \approx 0.3$), where Δ' refers to the fourth-order perturbative triplon gap (see the Supplemental Material [66]). Notably, the delta peak corresponding to the single-triplon mode remains but its amplitude decreases with increasing temperature as shown in the inset. In addition to the single-triplon peak, there is a broad response originating from the bound states that, as we have mentioned, have a bandwidth of the order of J . This broad component to the dynamical structure factor is bounded, for $J/J_D = 0.539$, by the gap between the triplon mode and the lowermost and uppermost bound-state modes—namely, $\Delta'/J_D = 0.12$ and about 1.5 , respectively.

Thus, the perturbation theory gives an account of the broad inelastic response appearing at energies much smaller than the single triplon gap in the limit $\omega \ll \Delta$. Central to this is the “fine-tuning” in $\text{SrCu}_2(\text{BO}_3)_2$, such that it lies close to a phase boundary and the bound states have anomalously low energy. In “typical” gapped quantum magnets, two-particle states would arise at around 2Δ resulting in an inelastic response from energy Δ . In contrast, in “typical” gapless quantum magnets, a continuum of states and broadening are both to be expected at *zero* temperature so that effects of finite temperature will tend to be quantitative, not qualitative. In this way, we can understand why thermal broadening $\text{SrCu}_2(\text{BO}_3)_2$ stands out among quantum magnets.

Conclusions. We investigated the origin of the anomalous thermal broadening observed in neutron scattering experiments of $\text{SrCu}_2(\text{BO}_3)_2$. By introducing a matrix-product state based technique based on minimally entangled typical thermal states, we demonstrated that this effect is accurately captured by the Shastry-Sutherland model on cylinders

up to width $W = 6$. Moreover, we provide an intuitive explanation where bound states of two triplons proliferate below the single-triplon gap at the experimentally relevant model parameters $J/J_D = 0.63$. By demonstrating the feasibility of studying finite-temperature dynamics using tensor network methods, this work paves the way for future investigations of the dynamics of frustrated quantum magnets at nonzero temperatures.

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