

Paramagnetic half-moon-shaped diffuse scattering arising from three-dimensional magnetic frustration

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We use spin dynamics simulations to determine the origin of the unusual correlated diffuse scattering, characterized by half-moon shapes bridging the magnetic Bragg peaks, observed in the polarized elastic neutron scattering from manganese tungstate, MnWO_4 . We first fit a Heisenberg Hamiltonian with 12 nearest-neighbor exchange interactions and single-ion anisotropy to the experimental ground-state magnon dispersion. We then show via spin dynamics simulations that our model Hamiltonian both reproduces the experimentally observed half-moon features and captures their persistence into the paramagnetic regime. Moreover, we identify the three-dimensional, competing antiferromagnetic interactions driving this behavior. Our work complements earlier studies of half-moon-shaped signatures in pyrochlore and triangular structures, by providing insight into their origin and showing that the half moons in MnWO_4 result from three-dimensional competing exchange interactions, in the absence of the spin-liquid behavior with which they are usually associated.

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I. INTRODUCTION

Neutron scattering measurements on a wide range of geometrically frustrated materials show curved, diffuse signals in reciprocal $\vec{q}$ space. One prevalent signature is “split rings of scattering” [1], also referred to as half moons, found in the metallic spin ice $\text{Pr}_2\text{Ir}_2\text{O}_7$ [2] as well as in kagome classical spin liquids [3]. These dispersive signatures have been variously ascribed to weakly interacting spin loops [2,3], locally ordered domains [4], magnons propagating in a cooperative paramagnetic state [5] or a superposition of zero-energy modes [6]. Such ringlike features in the diffuse signal can be captured by frustrated nearest-neighbor antiferromagnetic (AFM) Heisenberg models, revealing that half moons in spin liquids and ices can be understood as high-temperature dynamical fingerprints of pinch-point correlations [7].

In contrast to these well-studied spin liquids and geometrically frustrated spin ice systems, multiferroic MnWO_4 , which exhibits similar half-moon-shaped signatures in reciprocal space [8], has commensurate magnetic order. Hence, the half moons in MnWO_4 must have a different microscopic origin, which we aim to shed light on in this work. Indeed, while half moons in the scattering from systems with pyrochlore and

triangular lattices have been relatively well studied [1–3,7,9], the similar signals in MnWO_4 are less well understood.

In MnWO_4 , the magnetic Mn^{2+} ions ($S = 5/2$) form zigzag chains along the c axis [8,10] and frustration arises from competing long-range exchange interactions [11]. The half-moon-shaped correlated diffuse scattering is located symmetrically mirrored around $\vec{k}_{ic}^{(ac)} = [-0.21, 0, 0.45]$ and $3 \times \vec{k}_{ic}^{(ac)} = [-0.63, 0, 1.35]$ (fractional coordinates), bridging the magnetic Bragg peaks [8] (Fig. 1), and persisting in the paramagnetic regime to up to 3 times the Néel temperature, T_N [8]. Here, we determine which magnetic interactions in MnWO_4 are responsible for the appearance of this directional diffuse scattering in the paramagnetic regime.

MnWO_4 is paramagnetic at room temperature and undergoes three magnetic phase transitions on cooling in zero magnetic field. The first transition occurs at $T_N = 13.5$ K into the AF3 phase [14], a collinear, antiferromagnetic alignment of moments along the easy axis $\hat{e}_{ac}$, which lies in the ac plane and forms a 37° angle with the a axis [8]. The order is a sinusoidal modulation with an incommensurate propagation vector $\vec{k}_{ic} = [-0.214, 0.5, 0.457]$ [14]. Below 12.3 K, in the AF2 phase, an additional magnetic order develops along the b direction, giving rise to an elliptical spin spiral with the same propagation vector $\vec{k}_{ic}$ as in the AF3 phase. The third phase transition occurs at 8.0 K, below which the system orders in the AF1 ground state, in which the moments are again aligned along $\hat{e}_{ac}$, with a commensurate $\vec{k}_c = [-0.25, 0.5, 0.5]$ magnetic propagation vector [14].

The magnetic dynamics of the AF1 phase have been well characterized. We plot the measured inelastic neutron scattering (INS) spectrum of the AF1 phase from Ref. [11] in the

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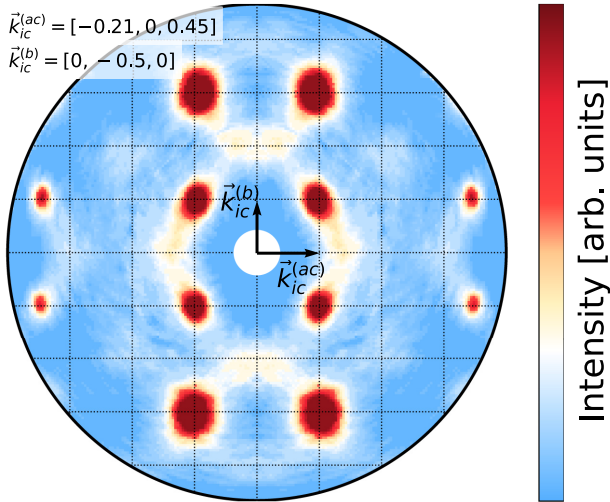


FIG. 1. The elastic scattering map at 14 K in the plane spanned by $\vec{k}_{ic}^{(b)} = [0, -0.5, 0]$ and $\vec{k}_{ic}^{(ac)} = [-0.21, 0, 0.45]$ (fractional coordinates), from Fig. 5.13 in Ref. [8] (reproduced with permission). The signal is purely magnetic, obtained from polarization analysis averaging spin-flip (SF) and non-spin-flip (NSF) channels [8].

left panels of Figs. 2(a) and 2(b), showing the four magnon branches, as well as localized, low-energy signals around $\vec{k}_c$ arising from electromagnons. The measured AF1 magnon dispersions from several experimental studies have been described by an extension of the Heisenberg Hamiltonian with a uniaxial anisotropy term [11–13]:

$$H = - \sum_{i \neq j} J_{ij} \hat{e}_i \cdot \hat{e}_j + D \sum_i (\hat{e}_i \cdot \hat{e}_{ac})^2. \quad (1)$$

Here, J_{ij} are the exchange couplings, as defined in Fig. 3(a), D is the uniaxial single-ion anisotropy, $\hat{e}_{i,j}$ are the normalized magnetic moments, and $\hat{e}_{ac}$ is the direction of the easy axis.

We plot the fitted Hamiltonian parameters from Refs. [11–13] in Fig. 3(b). The initial study in Ref. [13] includes 11 exchange interactions, which we label J_1 – J_{11} , dropping ij for conciseness. Subsequent studies [11,12] find that the quality of the fit improves upon adding a 12th

interaction, J_{12} , with similar values obtained in Refs. [11,12]. Figure 3(b) shows that several long-range interactions are comparable in strength to the AFM nearest-neighbor interaction J_1 , suggesting a considerable degree of magnetic frustration [11]. Indeed, this is corroborated by the frustration index $f = \frac{|\theta_{CW}|}{T_N} \approx 5$, where θ_{CW} is the Curie-Weiss temperature [8,15]. The origin of the frustration lies in the distorted $[\text{MnO}_6]$ octahedra, which have 95° Mn–O–Mn bond angles [8,10,16].

While the magnitude and signs of the exchange interactions are well established, the origin of the half moons in MnWO_4 is not clear. In this work, we aim to capture the short-range correlations giving rise to the half-moon-shaped correlated diffuse scattering by simulating the elastic neutron scattering measured in Ref. [8]. Since previous reports indicate that the half moons in MnWO_4 are not captured by a mean-field model [8], we employ spin dynamics simulations, which successfully have been shown to capture the magnetic domain-wall structures in the AF2 phase of Co-doped MnWO_4 [17].

Our paper is structured as follows. First, we set up an atomistic spin dynamics model with a Heisenberg Hamiltonian that we fit to the experimental AF1 magnon dispersions of MnWO_4 . Next, we calculate structure factors, aiming to reproduce the paramagnetic scattering maps measured in Ref. [8]. Finally, following a similar approach to Ref. [18], we recalculate the structure factor using simplified Hamiltonians, switching off certain exchange interactions. In this way, we can pinpoint the specific exchange interactions that are responsible for the half moons, and provide insight into the interplay between magnetic frustration and correlated diffuse scattering in MnWO_4 .

II. METHODS

We run atomistic spin dynamics simulations as implemented in the UppASD code (version 6.0.1) [19], with a damping coefficient of $\alpha = 0.05$ and 1 fs time steps. The lattice vectors are set to (expressed in Cartesian coordinates and units of Å) $\vec{a} = [4.824, 0, 0]$, $\vec{b} = [0, 5.755, 0]$, and $\vec{c} = [-0.095, 0, 5.001]$ [20,21]. The two symmetry-related manganese atoms occupy the $2f$ Wyckoff positions, which

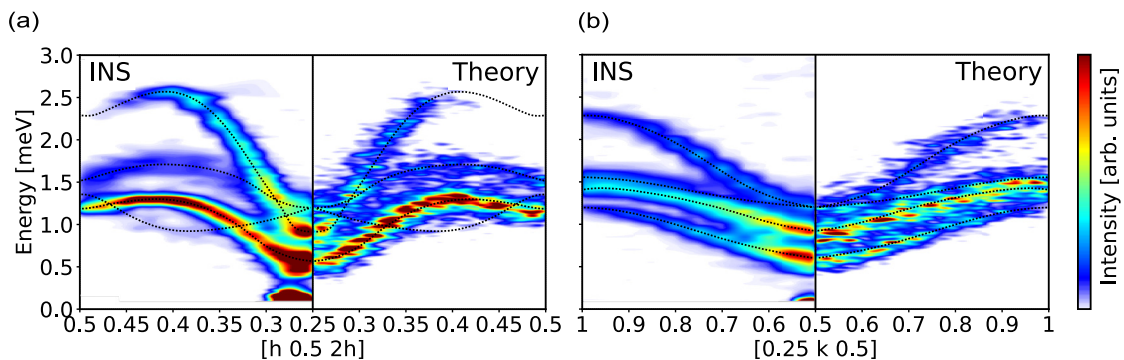


FIG. 2. AF1 magnon dispersions at 1.5 K spanning (a) the $[1\ 0\ 2]$ and (b) $[0\ 1\ 0]$ directions. The left panels in each plot are INS measurements from Ref. [11]. The right panels in each plot show our computed dynamical structure factors $S(\vec{q}, \omega)$. Black dotted lines denote the INS measured branches and are included in the theoretical panels as a guide to the eye.

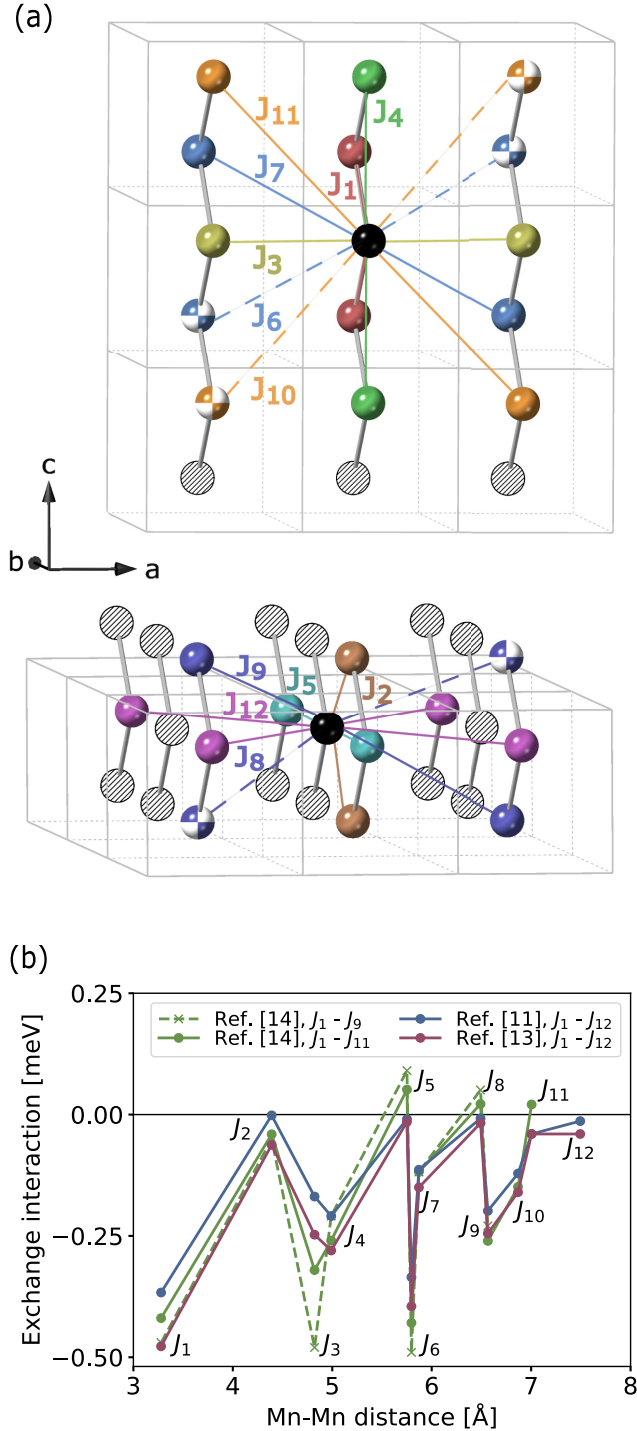


FIG. 3. (a) The 12 nearest exchange interactions between the Mn ions. Top panel: Couplings within one ac layer of zigzag chains. Bottom panel: Couplings across different ac layers of zigzag chains. We show the interactions of a representative black atom, coloring the neighboring atoms according to the respective exchange interaction. Half-colored atoms indicate that they have a Mn-Mn distance very similar to the respective fully colored atom. The exchange interactions are labeled numerically by order of increasing Mn-Mn distance, following Ref. [11]. The gray boxes indicate the structural unit cell. (b) Exchange interactions obtained from Refs. [11–13] from fitting to INS results.

correspond to $[0.5, 0.685, 0.25]$ and $[0.5, 0.315, 0.75]$ in fractional coordinates [20,21]. We set the magnitude of the magnetic moment to $5 \mu_B$, since the electrons of the manganese ions are in the high-spin d^5 configuration [11].

For the ground-state magnon dispersions, we calculate the dynamical structure factor $S(\vec{q}, \omega)$ with an energy resolution of $\Delta E = 0.01$ meV, computing the correlation function every 83 time steps, over a total of 415 000 time steps resulting in 5000 samplings. A $48 \times 48 \times 48$ supercell is initialized in the AF1 configuration at 1.5 K. We linearly interpolate and use a Gaussian smoothing with a standard deviation of 3.

In order to explore the phase transitions, we start from a randomly initialized system and perform Monte Carlo steps from 75 to 18 K, with 20 000 steps performed at 15 log-spaced temperatures. Spin dynamics calculations, with 30 000 initialization steps and 85 000 measurement steps, are run at 1 K intervals between 18 and 11 K, and subsequently at 0.25 K intervals down to 1 K.

To model the correlated diffuse scattering in the paramagnetic phase, we cool the system with spin dynamics steps from 60 K in 2 K steps down to 40 K, followed by 1 K steps down to 14 K. At each temperature, we perform 30 000 initialization steps and 40 000 measurement steps. Since Ref. [8] measures the magnetic elastic scattering, we compute the static structure factor $S(\vec{q})$, with 40 000 initialization and measurement steps each. Since our aim is to capture the signatures of frustration in the presence of thermal fluctuations within the paramagnetic regime, we compare the experimental and our calculated results at the same absolute temperatures, instead of relative to their respective T_N 's. We fit the intensity of the Bragg peaks in our model to the experiment by tuning the postprocessing parameters, using a common setting across temperatures. In this way, we set the Gaussian filter to the standard deviation of 4.

III. MODEL DEVELOPMENT AND VALIDATION

We set up our Hamiltonian adopting the relative magnitudes of the exchange interactions and the single-ion anisotropy given in Ref. [11], but finding that we have to scale the parameters by a factor (Table I) to reproduce the ground-state magnon dispersions. Without rescaling, we do not reproduce the experimental ground state or Néel temperature in our calculations. We suspect that the scaling factor may originate from differences in Hamiltonian conventions or prefactors between the present work and Ref. [11], implying that the same physical system is being simulated. However, the information available in the literature is insufficient to verify this possibility conclusively. We point out that, given that we rescale all the parameters proportionally, we do not change the degree of frustration between the different AFM interactions.

We compare our calculated magnon dispersions, obtained by computing the dynamical structure factor $S(\vec{q}, \omega)$, to the INS-measured magnon dispersions in Figs. 2(b) and 2(c), which show reasonable agreement, confirming the validity of our Hamiltonian. Note that the localized signals at around $[0.25, 0.5, 0.5]$ in the INS-measured spectra arise from electromagnons, which are not captured with Heisenberg

TABLE I. The Hamiltonian parameters used in our spin dynamics model, defined by the Hamiltonian of Eq. (1) and in units of meV. The values are from Ref. [11], but multiplied by 1.6 and -3.2 for J 's and D , respectively.

J_1	J_2	J_3	J_4	J_5	J_6	J_7	J_8	J_9	J_{10}	J_{11}	J_{12}	D
-0.592	-0.0032	-0.272	-0.336	-0.0176	-0.544	-0.176	-0.016	-0.32	-0.192	-0.0672	-0.0256	-0.192

Hamiltonians [11]. The noise in the theoretical calculations, which is spread out in k space, may be reduced by choosing a larger supercell. However, Hamiltonian validation primarily requires a clear picture of the overall shape of the magnon branches, a purpose for which the data quality of Fig. 2 is sufficient—see the overlay with the experimental branches.

As extracted from the temperature dependence of the heat capacity (see Fig. 8 in the Appendix), we locate a phase transition below 11 K, which is reasonably close to the experimental 13.5 K—paramagnetic to AF3—and 12.3 K—AF3 to AF2—transition temperatures [14]. By varying the supercell size and the cooldown speed, our simulation converges to different low-temperature configurations, such as the AF1 phase, the AF2 phase, and various AF1+ spiral phase coexistences (Fig. 9 in the Appendix). Nevertheless, the AF1 state has the lowest energy, indicating that our model correctly identifies the AF1 phase as the ground state.

We point out that, for the purpose of this work, we are not interested in capturing the sequence of the magnetically ordered states. In this context, we note that our model does not reproduce the modulated spin density wave in the AF3 phase, since it does not allow for variations in the magnitude of the magnetic moments.

To further validate our model, we test whether our model at 11 K is consistent with the experimental propagation vector $\vec{k}_{ic}$. Signals at $\vec{k}_{ic}$ are likely to persist in the paramagnetic regime and its associated correlated diffuse scattering. We compute $S(\vec{q})$ across the entire Brillouin zone, and determine the propagation vector from the $\vec{q}$ point with maximum intensity (Fig. 10 in the Appendix). We find for the $36 \times 24 \times 36$ and $48 \times 24 \times 24$ supercells, $\vec{k}_{\text{calc}} = [-0.222, 0.5, 0.444]$ and $\vec{k}_{\text{calc}} = [-0.229, 0.5, 0.458]$, respectively, which are both in reasonable agreement with the experimental $\vec{k}_{ic} = [-0.214, 0.5, 0.457]$.

IV. CORRELATED DIFFUSE SCATTERING AT $T > T_N$

In the following, we show that our spin dynamics model qualitatively reproduces the paramagnetic correlated diffuse scattering measured in Ref. [8]. Figures 4(a)–4(d) compare the computed and experimental scattering maps, showing that the half moons are captured by our model. Furthermore, the computed half moons persist up until 30 K, whereas only background scattering remains at 60 K, consistent with the experiment of Ref. [8].

In this context, we note that, in contrast to the simulated $S(\vec{q})$, the measurements have a significantly higher intensity along the half moon located at $\vec{k}_{ic}^{(ac)}$ than along that at $3 \times \vec{k}_{ic}^{(ac)}$. This is likely due to the anisotropic background caused by the platelike sample holder [8]. There are a number of other possible experimental sources of the quantitative differences between experiment and theory. First, the sample used for the measurements in Ref. [8] contained a small contribution from misaligned crystallites, which can broaden and redistribute diffuse intensity. Second, the finite flipping ratio could introduce channel mixing between NSF and SF channels. Additional discrepancies may arise from finite instrumental resolution and domain averaging. On the theory side, we note that we do not include the magnetic form factor, since our goal is to capture the collective spin-spin excitations that are reflected in the structure factor [22,23], and that interaction terms beyond the model considered here could play a role. We also note that the absolute values of the simulated intensities vary with the number of steps, but the half moons are present regardless of the number of steps (see Fig. 11 in the Appendix), supporting our conclusion that our simulation captures the half moons qualitatively. We point out that we obtain qualitative agreement on including only the competing exchange interactions, concluding that the frustration is a crucial factor in the appearance of the half moons.

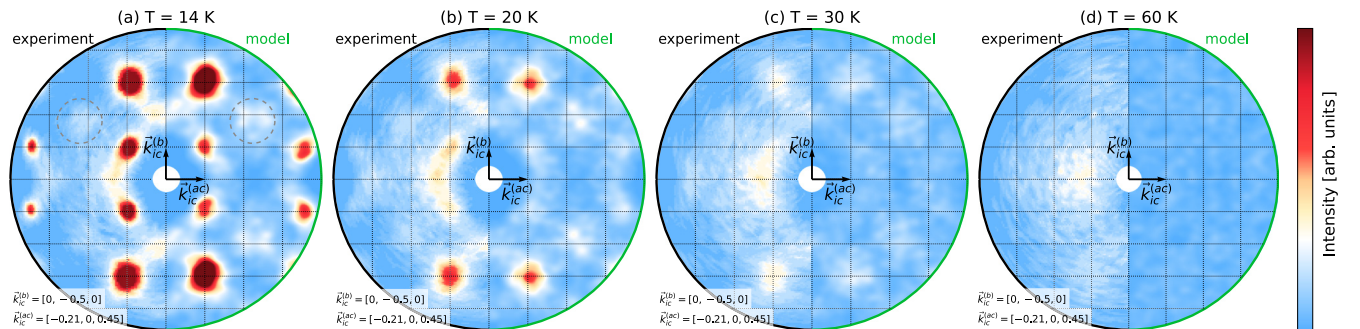


FIG. 4. Comparison between the experimental scattering maps from Fig. 5.13 in Ref. [8] (reproduced with permission) and our calculated $S(\vec{q})$, using the Hamiltonian of Eq. (1) and the parameters from Table I for the $36 \times 24 \times 36$ supercell (see Secs. II and III for details). The reciprocal plane is defined by $\vec{k}_{ic}^{(b)} = [0, -0.5, 0]$ and $\vec{k}_{ic}^{(ac)} = [-0.21, 0, 0.45]$ (or $\vec{k}_{ic}^{(ac)} = [-0.22, 0, 0.44]$ for our model).

A set of weak signals [circled in dashed gray in Fig. 4(a)] is present in both our simulation and the experiment of Ref. [8]. Reference [8] assigns these signals to $2 \times \vec{k}_{ic}$ and attributes them to exchange striction, with the magnetic modulation inducing a lattice modulation of twice the magnetic propagation vector [24]. In fact, the AF2 phase has a $2 \times \vec{k}_{ic}$ lattice modulation and an accompanying $2 \times \vec{k}_{ic}$ magnetic modulation [25–27], remnants of which might persist into the paramagnetic regime [8]. However, we point out that if the signal were at $2 \times \vec{k}_{ic}$, then it should be centered at the grid line intersection in Fig. 4(a). We propose that the signal, found in both our simulation and the measurement of Ref. [8], is more likely to sit at the commensurate $2 \times \vec{k}_c$. Because of this, and the fact that our model does not include exchange striction, we raise the question of the origin of the weak signal at $2 \times \vec{k}_c$ again, and suggest that it could arise from a competing or coexisting order.

We point out that our model captures the characteristic paramagnetic scattering features, including the half moons, regardless of the supercell size and the simulated low-temperature state obtained upon cooling from the paramagnetic state (Fig. 9 in the Appendix). Therefore, we suggest that the short-range correlated features in the paramagnetic regime are not a consequence of the particular pattern of the long-range magnetic order.

We comment that, since $S(\vec{q} = 0) = 0$ in the paramagnetic phase (see Fig. 5), the correlated clusters have no associated magnetic moment. This suggests that the correlated diffuse scattering results from short-range ordered clusters of spins that have zero magnetic moment. Further insight would be gained by studying the response of the diffuse scattering to an external magnetic field, which would couple to a net magnetic moment.

V. SIMPLER HAMILTONIAN MODELS

Next, we identify which interactions give rise to particular scattering signatures, by switching off individual terms in the Hamiltonian in turn and recalculating $S(\vec{q})$ at 20 K, similar to Ref. [18]. Our workflow is presented in Fig. 6.

We start with the full Hamiltonian and remove the single-ion anisotropy (step 0 in Fig. 6). The scattering maps with the anisotropy term [Fig. 7(a)] and without it [Fig. 7(b)] show the same features, indicating that the anisotropy is not responsible for the short-range correlations in the paramagnetic regime, which instead must be caused by the exchange interactions. This finding is consistent with the conclusions of Ref. [14] that exchange interactions dominate at higher temperatures and give rise to the incommensurate AF2 and AF3 spiral orders, whereas the anisotropy prevails at low temperatures and gives rise to the collinear AF1 phase.

Next, we remove the four weakest exchange couplings, J_2 , J_5 , J_8 , and J_{12} , which all couple across different ac layers of Mn zigzag chains (step 1 in Fig. 6). Figure 7(c) shows that the Bragg peaks and the half moons persist with this simpler Hamiltonian, whereas the $2 \times \vec{k}_c$ signals disappear from our calculated structure factor, indicating that the $2 \times \vec{k}_c$ signals are a result of the delicate balance between all 12 exchange interactions.

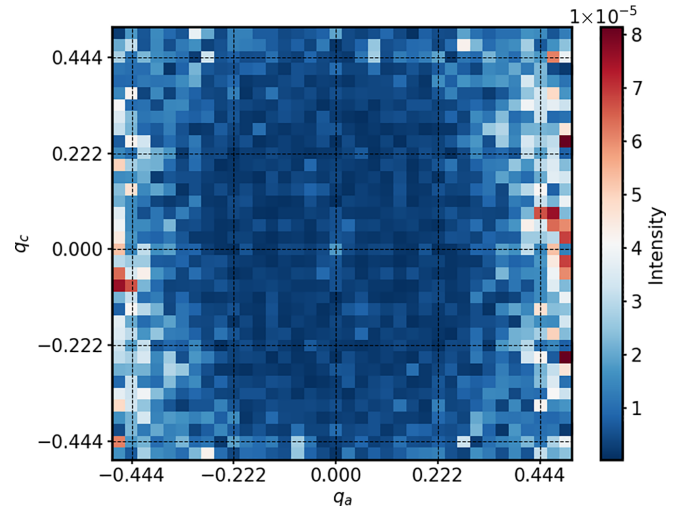


FIG. 5. Computed $S(\vec{q})$ at 11 K and $\vec{k} = [q_a, 0, q_c]$ for the $36 \times 24 \times 36$ supercell.

We can further simplify the Hamiltonian in two distinct ways: either removing the last remaining coupling across different ac layers— J_9 (step 2.a in Fig. 6)—or reducing the frustration within the ac plane by switching off J_3 , J_{10} , J_7 , and J_{11} (step 2.b in Fig. 6). We find that the computed $S(\vec{q})$ for both approaches now lack the dispersive half moons [Figs. 7(d) and 7(e)]. Our calculations show that by removing the frustrating interactions across different ac layers (step 2.a) or by suppressing the interaction within a given ac layer (step 2.b), the half moons disappear. Therefore, we conclude that the half-moon-shaped correlated diffuse scattering is a result of frustration both within and across ac planes.

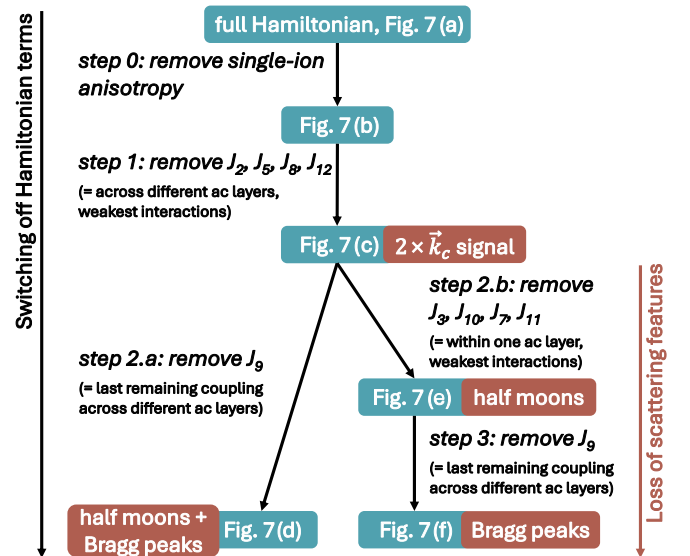


FIG. 6. Our procedure for determining the relevant terms in the Hamiltonian. We start with the full Hamiltonian (top), and then remove terms in a sequence of steps. The blue boxes provide the reference to the corresponding scattering map in Fig. 7. The brown boxes indicate which scattering features disappear.

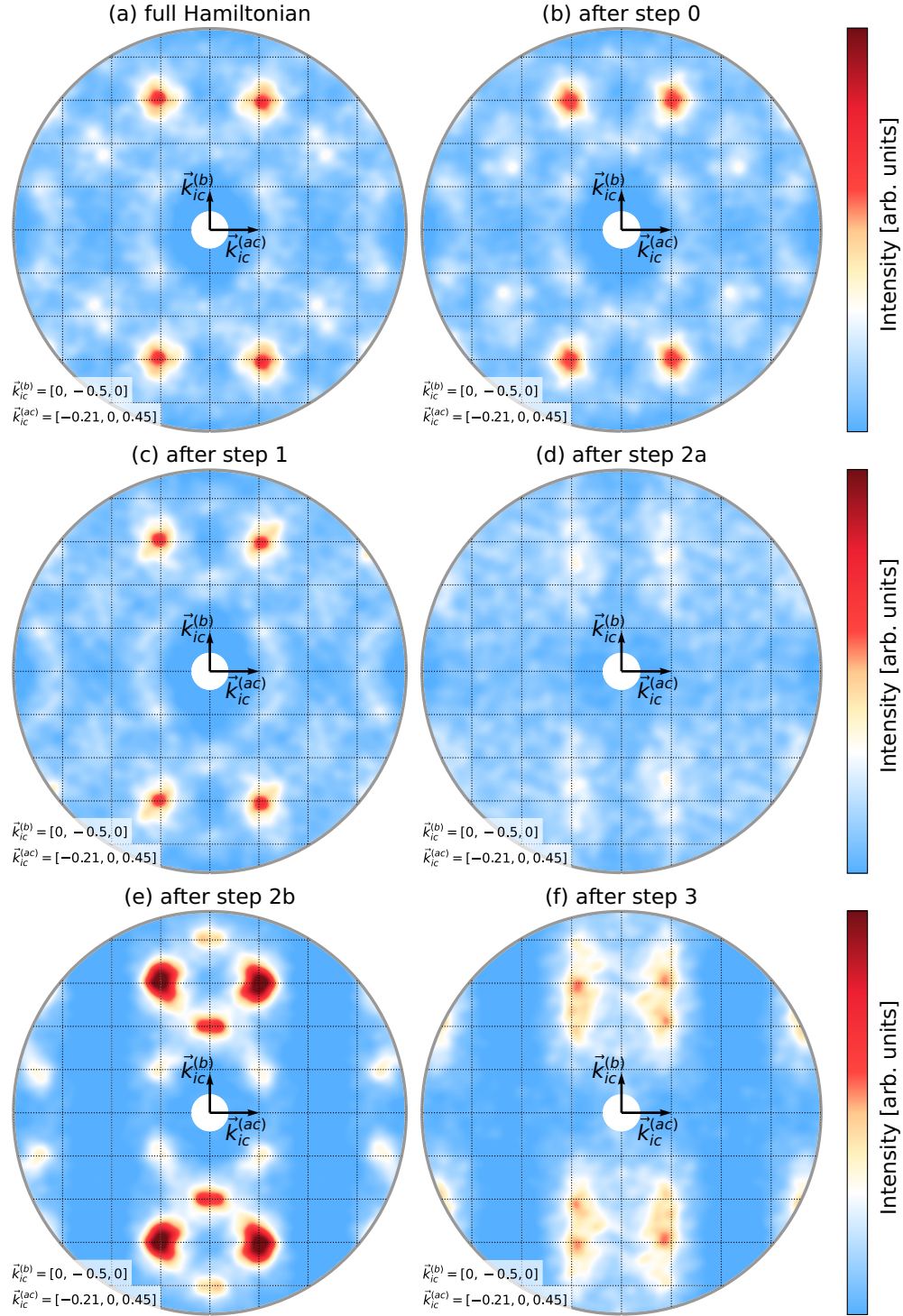


FIG. 7. Simulated $S(\vec{Q})$, computed with a $36 \times 24 \times 36$ supercell at 20 K, for different Hamiltonian models as defined in Fig. 6.

Interestingly, these two approaches do not influence the Bragg peak signal in the same way. A Hamiltonian without J_3 , J_{10} , J_7 , and J_{11} continues to reproduce the magnetic Bragg peak signals [Fig. 7(e)], and only results in their suppression if J_9 is subsequently additionally switched off (step 3 in Fig. 6) [see Fig. 7(f)]. This is not the case when only switching off J_9 (step 2.a), which completely suppresses the magnetic Bragg peaks. We conclude that J_9 , being the dominant coupling

across different ac layers, is vital to the onset of long-range magnetic order.

VI. DISCUSSION AND OUTLOOK

In summary, we find that a Heisenberg model with competing exchange interactions up to the 12th nearest neighbor

captures the paramagnetic half-moon-shaped correlated diffuse scattering in MnWO_4 , including its persistence into the paramagnetic regime, as measured in Ref. [8].

We stress that we achieve agreement with experiment by including only competing symmetric Heisenberg interactions in our Hamiltonian; the Dzyaloshinskii-Moriya interaction [11], single-ion anisotropy [14] and magnetoelastic couplings [27] are not needed to model the half-moon signatures, despite giving rise to INS signatures caused by electromagnons [11] and contributing to the formation of the collinear ground state [14,27]. Furthermore, we note that our model is purely classical, showing that our correlated diffuse scattering arises from classical spin-spin correlations. Interestingly, this type of scattering can also arise from quantum fluctuations, for example, in the spin-1/2 triangular-lattice Heisenberg antiferromagnets, where it has been attributed to intermediate quasiparticle ordering states [28].

We find that the half moons vanish upon removing all frustrating interactions across different *ac* layers of Mn zigzag chains, as well as upon reducing the frustration within one *ac* layer. Thus, our results indicate that frustration is a key player behind the appearance of the half moons, despite the absence of the usual geometric frustration found in pyrochlore and triangular systems.

Moreover, we conclude that the half moons in MnWO_4 are caused by couplings in all three dimensions. Curved correlated diffuse scattering is also measured in MnO and spinel compounds such as ZnCr_2O_4 and MgCr_2O_4 , which are well described by models that include couplings between spins or weakly interacting clusters of spins across all three lattice dimensions [4–6,29,30]. In contrast, the rodlike diffuse scattering in h-YMnO_3 and $\text{NaFe(WO}_4)_2$ is due to correlations in two-dimensional planes [8,22]. Therefore, we suggest that the directionality of the competing exchange interactions in two or three lattice dimensions determines whether the correlated diffuse scattering has a rodlike or half-moon shape, respectively.

Our findings are consistent with previous studies on other frustrated, classical spin systems, such as pyrochlores [2,3,30,31] and MnO [4], which show paramagnetic correlated diffuse scattering associated with cluster formation. Future studies, such as reverse Monte Carlo calculations [4] and energy-resolved $S(\vec{q}, w)$ measurements, could unveil

more details on the microscopic arrangement of spins associated with the correlated diffuse signatures in MnWO_4 since signals from clusters of spins are frequency independent, whereas spin waves appear at well-defined frequencies [22]. We also suggest studying the effect of an applied magnetic field on the correlated diffuse scattering, which would provide insight into any net magnetic moment associated with the correlated regions.

While our study suggests that three-dimensional, magnetically frustrated AFM interactions are at the origin of the half moons in MnWO_4 , several open questions remain. Do the half moons persist below T_N , and what is their energy dependence? Are the short-range correlations associated with the correlated diffuse scattering a prelude to the onset of long-range order, or are these two phenomena independent, as suggested for h-YMnO_3 [22,32]? Since quantum systems can show the same type of scattering features as MnWO_4 , how can one differentiate between classical and quantum signatures in diffuse scattering? We hope that our work inspires future theoretical and experimental investigations on the interplay between correlated diffuse scattering and magnetic phase transitions, in both classical and quantum systems.

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DATA AVAILABILITY

All relevant data for this manuscript are available on the Materials Cloud Archive [33].

APPENDIX

In this appendix, we include additional figures that support the conclusions of the main text (Figs. 8–11).

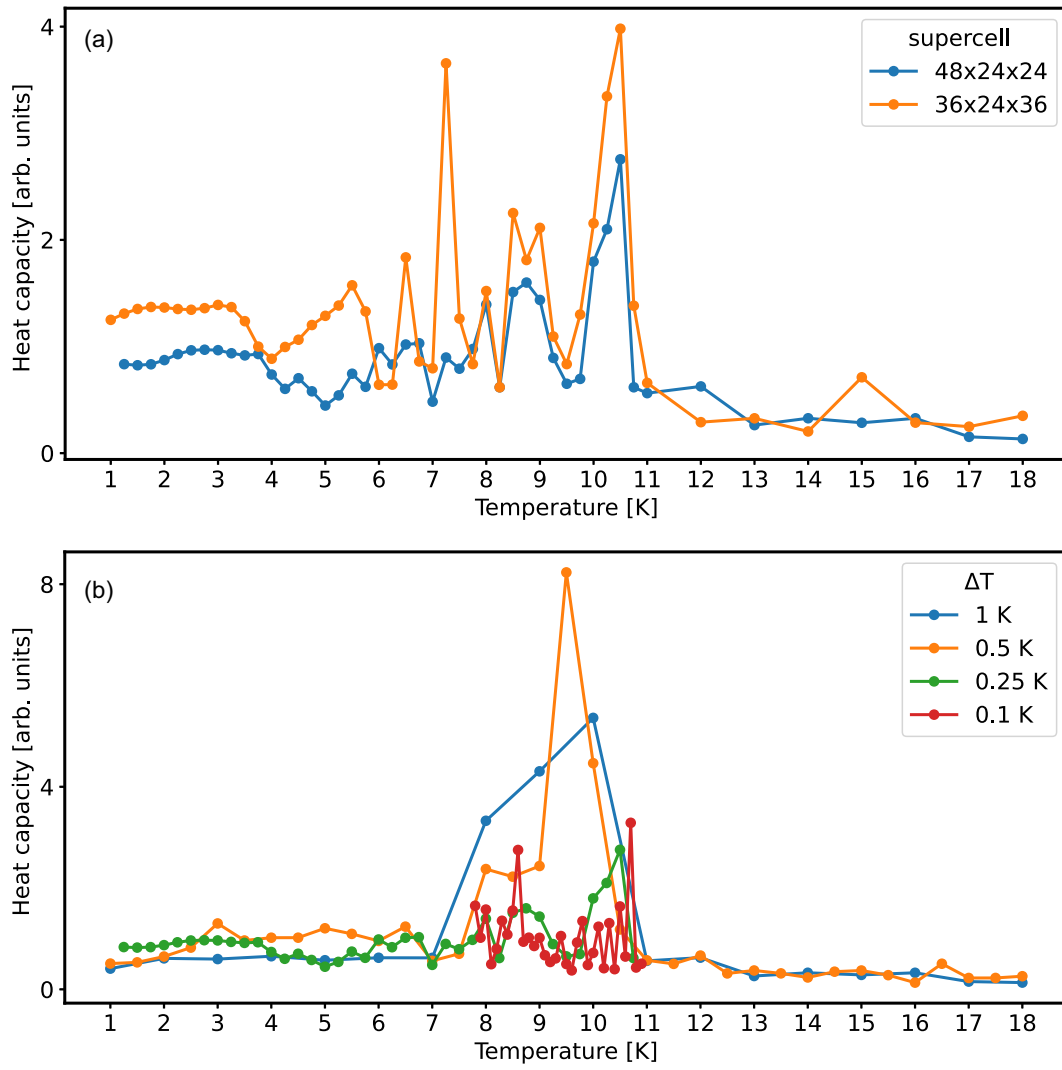


FIG. 8. Calculated heat capacity, at the end of the measurement phase, for different values of the cool down speed and supercell size. (a) The $36 \times 24 \times 36$ and $48 \times 24 \times 24$ supercells at 0.25 K temperature steps, and (b) the $36 \times 24 \times 36$ supercell at 1, 0.5, 0.25, and 0.1 K temperature steps.

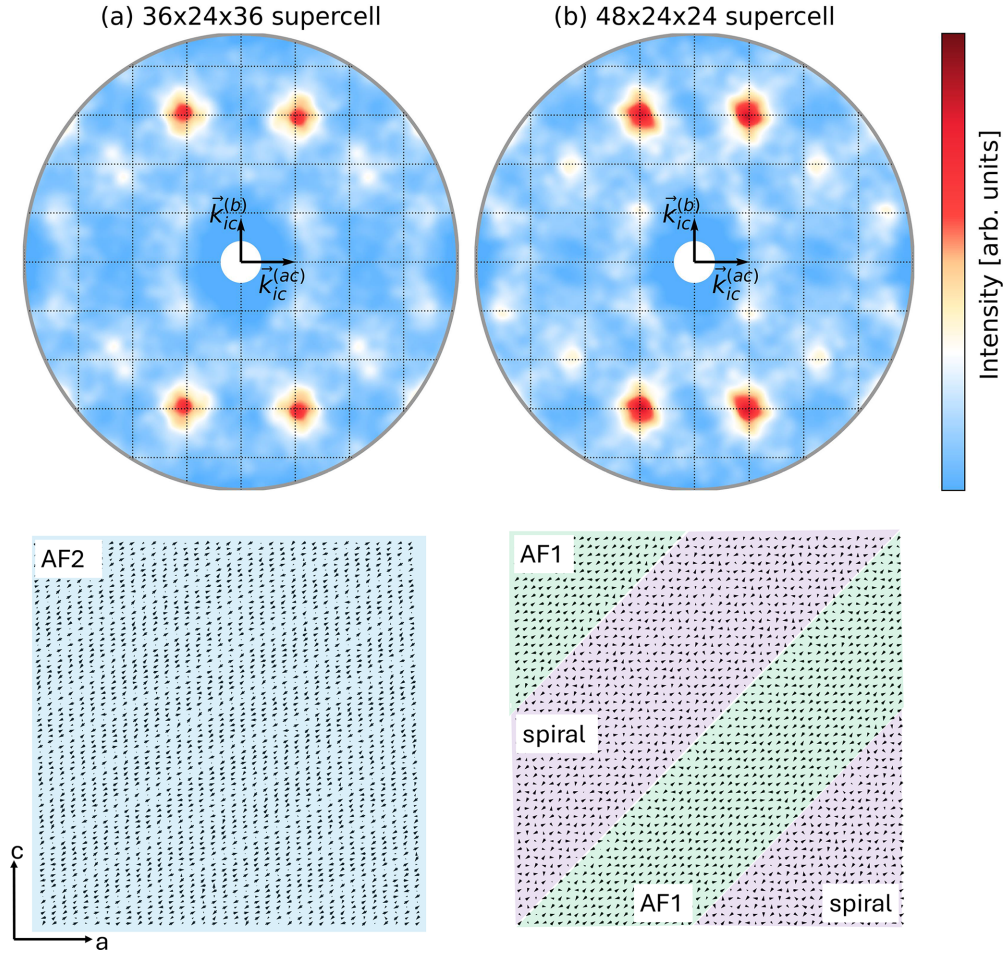


FIG. 9. Comparison of (a) the $36 \times 24 \times 36$ and (b) $48 \times 24 \times 24$ supercells. Top panel: $S(\vec{q})$ at 20 K, with (a) $\vec{k}_{ic}^{(ac)} = [-0.222, 0, 0.444]$ and (b) $\vec{k}_{ic}^{(ac)} = [-0.229, 0, 0.458]$. Bottom panel: Simulated magnetic configurations at 1 K, plotted in the ac plane projection. The orientations of the magnetic moments alternate for subsequent unit cells in the b direction, consistent with $\vec{k}_c$ and $\vec{k}_{ic}$ in the experiment. The configurations are obtained upon cooling from the paramagnetic regime, as described in Sec. II.

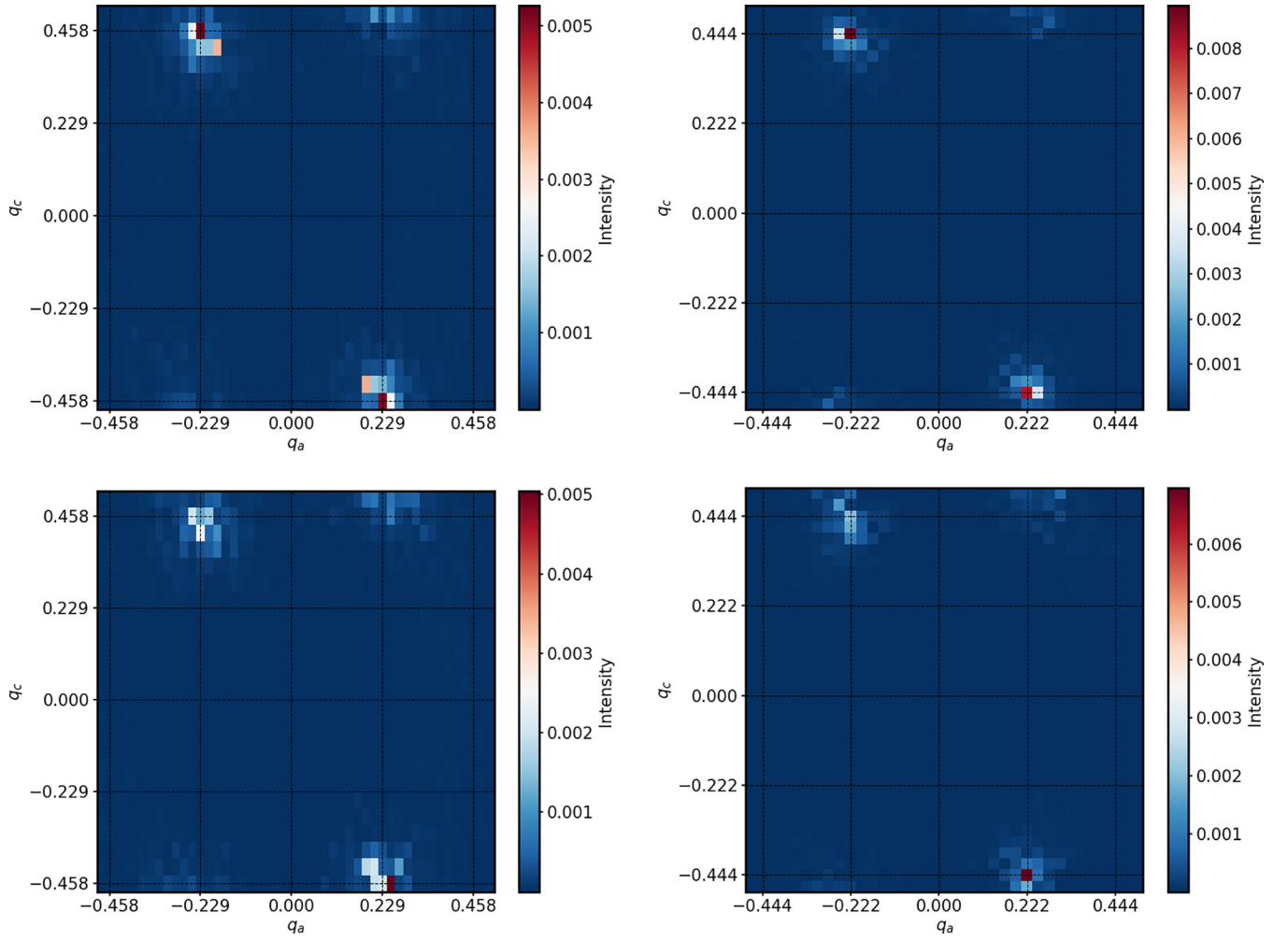


FIG. 10. Computed $S(\vec{q})$ at 11 K in the full Brillouin zone, with the q values given in fractional coordinates. Left: $48 \times 24 \times 24$ supercell; right: $36 \times 24 \times 36$ supercell, at $q_b = 0.5$ (top) and $q_b = 0.458$ (bottom). All other slices with $q_b < 0.5$ and $q_b > 0.5$ have lower intensities.

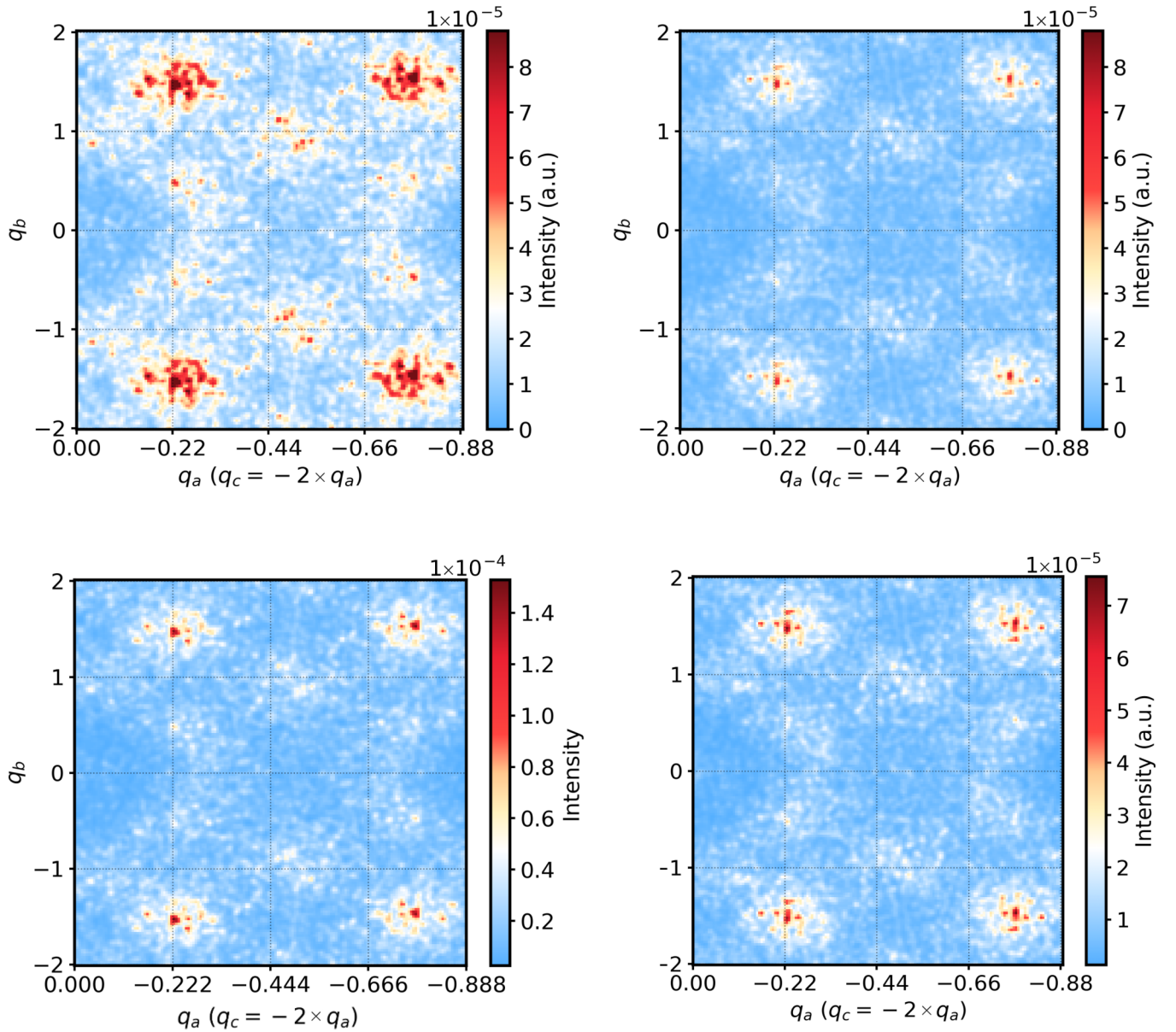


FIG. 11. The scattering maps at 20 K with 40 000 measurement steps (left) and 80 000 measurement steps (right) during the static structure factor calculation. The two plots in the top panel use the same color bars. The two plots in the bottom panel use color bars set by the minimum and maximum values of the respective calculation.

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