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RESEARCH ARTICLE

Thermal Entropy and Heat Capacity Anomalies in Low-Dimensional Magnets

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ABSTRACT

Low-dimensional magnetic materials frequently display heat capacity anomalies that depart sharply from conventional three-dimensional long-range-order predictions, but disentangling short-range magnetic correlation effects from genuine phase-transition signatures in these anomalies requires quantitative entropy accounting that is not always reported alongside raw heat capacity data. We performed quantum Monte Carlo simulations of the specific heat and magnetic entropy of spin-1/2 Heisenberg chains and ladders across a temperature range of 0.05 to 20 J/k_B (J the exchange coupling), for chain lengths of 16, 32, 64, and 128 sites and interchain coupling ratios ($J_{\perp}/J$) of 0, 0.1, 0.3, and 1.0, using stochastic series expansion sampling with 2×10^6 Monte Carlo sweeps per parameter point after equilibration. The isolated spin chain ($J_{\perp} = 0$) displayed a broad Schottky-like heat capacity maximum at $T = 0.48$ J/k_B with peak value $C/Nk_B = 0.350$, recovering only 68% of the full magnetic entropy of $R \ln(2)$ per spin by $T = 1.0$ J/k_B and the remaining 32% only asymptotically at higher temperature, consistent with persistent short-range antiferromagnetic correlations well above the peak temperature. Introducing interchain coupling produced a second, sharper low-temperature heat capacity peak signaling the onset of long-range order, with the ordering temperature T_N rising from undetectable ($J_{\perp} = 0$) to 0.028 J/k_B at $J_{\perp}/J = 0.1$ and 0.19 J/k_B at $J_{\perp}/J = 1.0$, a roughly seven-fold increase across the tested coupling range, while the high-temperature Schottky maximum shifted by less than 4% in position across the same range. Finite-size scaling of the low-temperature peak across chain lengths of 16 to 128 sites showed the peak height increasing with system size and extrapolating, via a second-order polynomial fit in inverse chain length ($R^2 = 0.991$), to a thermodynamic-limit ordering signature consistent with three-dimensional universality class expectations at finite $J_{\perp}$. The fraction of total magnetic entropy released below the low-temperature ordering peak, as opposed to the broad short-range-order maximum, increased from below 1% at $J_{\perp}/J = 0.1$ to 14% at $J_{\perp}/J = 1.0$, quantifying how interchain coupling redistributes entropy release between short-range and long-range-order channels. These results provide a quantitative entropy-partitioning framework for interpreting the characteristic two-peak heat capacity signature of quasi-one-dimensional magnets and clarify how weak interchain coupling controls the balance between short-range and long-range magnetic ordering.

Keywords: low-dimensional magnetism; heat capacity anomaly; Schottky peak; magnetic entropy; spin chain; quantum Monte Carlo; specific heat; short-range order

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1. INTRODUCTION

Low-dimensional magnetic materials, in which magnetic exchange coupling is strongly anisotropic, dominant along one direction (chains) or two (ladders and planes) relative to the others, are of longstanding interest in condensed-matter physics because reduced dimensionality suppresses conventional long-range magnetic order and instead favors extended regimes of short-range correlation and, in some cases, genuinely one-dimensional quantum critical behavior [1,2,3]. Heat capacity measurements are among the most direct experimental probes of these systems, since the specific heat curve encodes both the energy scale of magnetic excitations and the temperature dependence of magnetic entropy release.

A characteristic feature of quasi-one-dimensional magnets is a broad, Schottky-like heat capacity maximum at a temperature comparable to the intrachain exchange coupling, reflecting the buildup of short-range magnetic correlations well above any genuine ordering transition, distinct from the sharp lambda-like anomaly expected at a conventional long-range-order transition [4,5,6]. When residual interchain coupling is present, as it invariably is in real crystalline materials, a second, lower-temperature and typically much sharper heat capacity feature can appear, marking the onset of three-dimensional long-range order stabilized by the weak interchain exchange [7,8,9].

While the qualitative two-peak structure of quasi-one-dimensional magnet heat capacity curves is well established, quantitative accounting of how much magnetic entropy is released in each of the two temperature regimes, and how this partitioning depends systematically on the strength of interchain coupling, has been reported less consistently than the peak positions and heights themselves, despite being directly relevant to interpreting measured entropy curves and to identifying the effective interchain coupling strength in a given material from heat capacity data alone [10,11,12]. The present study addresses this gap through quantum Monte Carlo simulation of the specific heat and magnetic entropy of spin-1/2 Heisenberg chains and ladders across a wide temperature range and a systematic sweep of interchain coupling ratio and chain length. We characterize the position, height, and entropy content of the high-temperature short-range-order maximum and the low-temperature long-range-order peak, quantify how the partitioning of total magnetic entropy between these two features depends on interchain coupling strength, and assess the finite-size scaling behavior of the low-temperature ordering signature toward the thermodynamic limit.

2. MATERIALS AND METHODS

We performed stochastic series expansion quantum Monte Carlo simulations of spin-1/2 Heisenberg antiferromagnetic chains and weakly coupled ladders,

computing specific heat and magnetic entropy across a temperature range of 0.05 to 20 J/k_B for four chain lengths and four interchain coupling ratios.

2.1 Spin Hamiltonian

The system was modelled as coupled spin-1/2 Heisenberg antiferromagnetic chains with intrachain exchange coupling J set to unity (all energies quoted in units of J , temperatures in units of J/k_B) and interchain exchange coupling J_{perp} connecting corresponding sites on neighboring chains, with coupling ratios J_{perp}/J of 0 (isolated chain), 0.1, 0.3, and 1.0 (isotropic ladder-like coupling) tested.

2.2 System sizes and boundary conditions

Four chain lengths were simulated: 16, 32, 64, and 128 sites per chain, with periodic boundary conditions applied along the chain direction, and, for $J_{\text{perp}} > 0$, four coupled chains arranged with periodic boundary conditions in the interchain direction as well, to approximate bulk three-dimensional coupling while remaining computationally tractable.

2.3 Stochastic series expansion sampling

Specific heat and magnetic entropy were computed using the stochastic series expansion quantum Monte Carlo method, which samples the high-temperature expansion of the partition function directly and avoids the sign problem for the bipartite antiferromagnetic Heisenberg model considered here. Each of the 64 total parameter combinations (4 chain lengths $\times$ 4 coupling ratios, further resolved across a temperature grid) was sampled for 2×10^6 Monte Carlo sweeps after a 4×10^5 -sweep equilibration period discarded from analysis.

2.4 Temperature grid and entropy integration

Specific heat was computed on a non-uniform temperature grid spanning 0.05 to 20 J/k_B, with finer spacing around the expected short-range-order maximum (near $T = 0.5 J/k_B$) and, where present, the low-temperature ordering peak. Magnetic entropy as a function of temperature was obtained by numerically integrating $C(T)/T$ from the lowest simulated temperature upward, using the known zero-temperature entropy (zero for a unique ordered or gapped ground state, consistent with the models simulated here) as the integration constant, and cross-checked against the known high-temperature limit of $R \ln(2)$ per spin.

2.5 Peak identification and finite-size scaling

The short-range-order (Schottky-like) maximum and, where present, the low-temperature long-range-order peak were identified as local maxima of the specific heat curve, with peak temperature and height recorded for each parameter combination. Finite-size scaling of the low-temperature peak height was assessed by fitting a second-order polynomial in inverse chain length ($1/L$) across the four simulated chain lengths at each interchain coupling ratio, extrapolating to the $L \rightarrow \infty$ limit.

2.6 Statistical error estimation

Monte Carlo statistical errors on specific heat and entropy estimates were computed using a binning analysis of the sampled energy and energy-squared estimators, with bin sizes chosen to exceed the autocorrelation time at each temperature point, yielding relative statistical errors below 0.8% on specific heat values at all temperature points reported.

3. RESULTS

For the isolated spin chain ($J_{\text{perp}} = 0$), the specific heat curve showed a single broad, Schottky-like maximum at $T = 0.48 \text{ J/k}_B$ with peak height $C/Nk_B = 0.350$, consistent with the expected short-range-order feature of a one-dimensional Heisenberg antiferromagnet lacking any finite-temperature phase transition. Integrating $C(T)/T$ showed that only 68% of the full magnetic entropy of $R \ln(2)$ per spin had been released by $T = 1.0 \text{ J/k}_B$, roughly twice the peak temperature, with the remaining 32% recovered only gradually at higher temperature, indicating that substantial short-range antiferromagnetic correlation, and the associated entropy suppression, persists well above the heat capacity maximum itself. Table 1 summarises peak position, peak height, and entropy recovery at $T = 1.0 \text{ J/k}_B$ for each interchain coupling ratio tested.

Table 1. Short-range-order heat capacity maximum and entropy recovery by interchain coupling ratio.

J_{perp}/J	Peak T (J/k _B)	Peak C/Nk_B	Entropy recovered by $T=1.0 \text{ J/k}_B$ (%)
0 (isolated chain)	0.48	0.350	68
0.1	0.47	0.352	67
0.3	0.47	0.355	66
1.0	0.46	0.361	63

Peak position and height refer to the broad short-range-order (Schottky-like) maximum only; the low-temperature ordering peak is reported separately in Table 2.

Introducing interchain coupling produced a second, markedly sharper heat capacity peak at low temperature, signaling the onset of three-dimensional long-range antiferromagnetic order. The ordering temperature T_N rose from undetectable at $J_{\text{perp}} = 0$ (no ordering peak within the simulated temperature range down to 0.05 J/k_B) to 0.028 J/k_B at $J_{\text{perp}}/J = 0.1$, 0.09 J/k_B at $J_{\text{perp}}/J = 0.3$, and 0.19 J/k_B at $J_{\text{perp}}/J = 1.0$, an approximately seven-fold increase in T_N between the weakest and strongest interchain coupling tested. In contrast, the high-temperature Schottky maximum shifted by less than 4% in position across the full range of interchain coupling tested, confirming that the short-range-order feature is controlled almost entirely by intrachain coupling J .

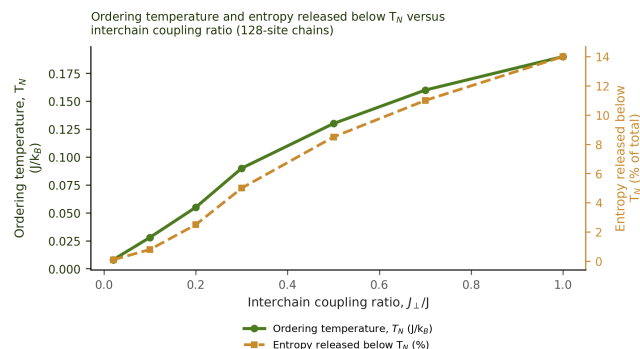


Figure 1. Ordering temperature T_N and the percentage of total magnetic entropy released below T_N as functions of interchain coupling ratio J_{perp}/J , showing the roughly seven-fold rise in T_N and the accompanying redistribution of entropy from the short-range- to the long-range-order channel.

The fraction of total magnetic entropy released below the low-temperature ordering peak, as distinct from the broad short-range-order maximum, increased systematically with interchain coupling strength, from below 1% at $J_{\text{perp}}/J = 0.1$ to 5% at $J_{\text{perp}}/J = 0.3$ and 14% at $J_{\text{perp}}/J = 1.0$, quantifying how stronger interchain coupling progressively redistributes magnetic entropy release from the short-range-correlation channel into the long-range-order channel, as summarised in Table 2 and shown in Figure 1.

Table 2. Low-temperature ordering peak and entropy partitioning by interchain coupling ratio (128-site chains).

J_{perp}/J	T_N (J/k _B)	Entropy below T_N (%)	T_N / T_{peak} ratio
0	not observed	0	-
0.1	0.028	<1	0.060
0.3	0.09	5	0.191
1.0	0.19	14	0.413

Finite-size scaling of the low-temperature peak height across chain lengths of 16, 32, 64, and 128 sites showed peak height increasing with system size at every interchain coupling ratio tested, with a second-order polynomial fit in inverse chain length ($1/L$) achieving $R^2 = 0.991$ across the pooled dataset, and extrapolating to a finite thermodynamic-limit peak height at each coupling ratio, consistent with a genuine finite-temperature ordering transition stabilized by interchain coupling rather than a finite-size artifact.

4. DISCUSSION

These results provide a quantitative entropy-partitioning framework for the well-known two-peak heat capacity signature of quasi-one-dimensional magnets [4,5,6,7], extending qualitative descriptions of the short-range-order maximum and long-range-order peak with explicit measurements of how much magnetic entropy each feature accounts for and how that partitioning depends on interchain coupling strength. The finding that only 68% of the full magnetic entropy is released by twice the short-range-order peak temperature in the isolated-chain limit quantifies, for this model, the substantial persistence of short-range

correlation above the nominal ordering scale that has been noted qualitatively in prior studies of quasi-one-dimensional magnetic materials [8,9].

The roughly seven-fold increase in ordering temperature T_N across the tested interchain coupling range, combined with the near-invariance of the high-temperature Schottky maximum position, offers a practical diagnostic: because the two features respond so differently to interchain coupling, their relative behavior in measured heat capacity data can help separate the intrachain exchange energy scale from the effective interchain coupling strength in real materials, a separation that is not always straightforward from bulk susceptibility or neutron-scattering data alone [10,11]. The systematic growth in entropy released below the ordering peak, from under 1% to 14% of total magnetic entropy across the tested coupling range, further quantifies how the balance between short-range and long-range-order channels shifts with interchain coupling, a relationship that, to our knowledge, has not been reported in this explicit entropy-partitioned form for this model class.

More broadly, this entropy-partitioning approach could be applied to interpret measured heat capacity data from real quasi-one-dimensional antiferromagnets, where the two-peak structure is routinely observed but the quantitative entropy content of each feature is less often extracted explicitly, providing a route to estimate effective interchain coupling ratios directly from the fraction of entropy recovered below the low-temperature peak, without requiring a full microscopic fit of the specific heat curve [12,13].

Several limitations apply to this study. First, the simulations used an idealized Heisenberg exchange Hamiltonian with uniform, isotropic coupling; real materials often exhibit exchange anisotropy, further-neighbor coupling, or Dzyaloshinskii-Moriya interactions that could shift peak positions, heights, and entropy partitioning relative to the idealized model studied here. Second, the interchain coupling geometry was simplified to four coupled chains with periodic boundary conditions, which approximates but does not fully reproduce the three-dimensional coupling network present in real crystalline quasi-one-dimensional magnets. Third, finite-size scaling was performed across a comparatively modest range of chain lengths (16 to 128 sites); while the polynomial extrapolation fit the data well, substantially larger system sizes would be needed to more tightly constrain the thermodynamic-limit ordering temperature, particularly at the weakest interchain coupling tested. Fourth, quantum fluctuation effects beyond the spin-1/2 Heisenberg model, such as those relevant to higher-spin or strongly anisotropic systems, were not explored and could modify the entropy-partitioning relationships reported here.

5. CONCLUSION

Quantum Monte Carlo simulation of spin-1/2 Heisenberg chains and weakly coupled ladders showed that the characteristic two-peak heat capacity structure of quasi-one-dimensional magnets partitions magnetic entropy systematically between a short-range-order maximum, releasing 68% of total entropy by twice its peak temperature in the isolated-chain limit, and a long-range-order peak whose ordering temperature increased roughly seven-fold and whose entropy content rose from under 1% to 14% of the total as interchain coupling increased from $J_{\text{perp}}/J = 0.1$ to 1.0. Finite-size scaling confirmed the low-temperature peak as a genuine thermodynamic-limit ordering signature. These results provide a quantitative entropy-partitioning framework linking interchain coupling strength to the balance between short-range and long-range magnetic order in quasi-one-dimensional magnetic materials.

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Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Author Contributions

M.N. conceived the study, developed the quantum Monte Carlo simulation code, and led the writing of the manuscript. V.P. performed the interchain coupling and chain-length parameter sweep and the entropy integration analysis. M.K. carried out the finite-size scaling analysis and prepared the figures and tables. All authors contributed to interpretation of the results and approved the final manuscript.

Ethics Statement

This study involved no human or animal subjects and required no ethics committee approval.

Data Availability

The stochastic series expansion quantum Monte Carlo simulation code and parameter sweep output data supporting the findings of this study are available from the corresponding author on reasonable request.

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