Singular ferromagnetic susceptibility of the transverse-field Ising antiferromagnet on the triangular lattice

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A transverse magnetic field $\Gamma$ is known to induce antiferromagnetic three-sublattice order of the Ising spins $\sigma^z$ in the triangular lattice Ising antiferromagnet at low enough temperature. This low-temperature order is known to melt on heating in a two-step manner, with a power-law ordered intermediate temperature phase characterized by power-law correlations at the three-sublattice wavevector $\mathbf{Q}$: $\langle \sigma^z(\mathbf{R})\sigma^z(0) \rangle \sim \cos(\mathbf{Q} \cdot \mathbf{R})/|\mathbf{R}|^{\eta(T)}$ with the temperature-dependent power-law exponent $\eta(T) \in (1/9,1/4)$. Here, we use a newly developed quantum cluster algorithm to study the ferromagnetic easy-axis susceptibility $\chi_u(L)$ of an $L \times L$ sample in this power-law ordered phase. Our numerical results are consistent with a recent prediction of a singular $L$ dependence $\chi_u(L) \sim L^{2-9\eta}$ when $\eta(T)$ is in the range $(1/9,2/9)$. This finite-size result implies, via standard scaling arguments, that the ferromagnetic susceptibility $\chi_u(B)$ to a uniform field $B$ along the easy axis is singular at intermediate temperatures in the small $B$ limit, $\chi_u(B) \sim |B|^{-\frac{4-18\eta}{1-9\eta}}$ for $\eta(T) \in (1/9,2/9)$, although there is no ferromagnetic long-range order in the low temperature state.

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I. INTRODUCTION

The transverse field Ising antiferromagnet on the triangular lattice, with Hamiltonian,

$$H_{\text{Ising}} = J_1 \sum_{\langle \mathbf{R},\mathbf{R'} \rangle} \sigma^z_{\mathbf{R}} \sigma^z_{\mathbf{R'}} - \Gamma \sum_{\mathbf{R}} \sigma^x_{\mathbf{R}} - B \sum_{\mathbf{R}} \sigma^z_{\mathbf{R}}, \quad (1)$$

where $\sigma^z_{\mathbf{R}}$ are Pauli matrices representing $S = 1/2$ moments on sites $\mathbf{R}$ of the triangular lattice, $\langle \mathbf{R},\mathbf{R'} \rangle$ denote the nearest neighbour links of the triangular lattice, $J_1 > 0$ is the antiferromagnetic exchange among easy-axis components of the $S = 1/2$ moments (a factor of $\frac{1}{4}$, appropriate for $S = 1/2$ moments, has been absorbed in the definition of $J_1$), and $B$ and $\Gamma$ are components of the external magnetic field along the easy axis $z$ and transverse direction $\hat{x}$ respectively (a factor of $\frac{2\mu_B}{T}$, appropriate for $S = 1/2$ moments, has been absorbed in the definition of these field components), provides perhaps the simplest example of a quantum “order-by-disorder”\textsuperscript{13} effect, whereby a classical spin liquid develops long-range magnetic order upon the introduction of terms in the Hamiltonian that induce quantum fluctuations.

When $\Gamma = 0$, the zero temperature classical Ising antiferromagnet at $B = 0$ has a macroscopic degeneracy of minimum exchange-energy configurations on the triangular lattice. These are in correspondence with all dimer covers of the dual honeycomb lattice, implying that the entropy-density remains nonzero in this classical zero temperature limit\textsuperscript{13}. At non-zero temperature, thermal fluctuations of $\sigma^z$ allow for defects that take the system out of the minimum exchange-energy dimer subspace. The Ising spins remain in a paramagnetic state all the way down to $T = 0\textsuperscript{10}$ albeit with a diverging correlation length\textsuperscript{11} at the three-sublattice wavevector $\mathbf{Q}$. This provides a simple example of classical spin liquid behaviour, with the $T = 0$ limit characterized by power-law spin correlations at the three-sublattice wavevector $\mathbf{Q}$.

A transverse field $\Gamma$ that couples to $\sigma^x$ induces quantum fluctuations of the Ising spins $\sigma^z$, and would ordinarily be expected to further reduce any residual ordering tendency of the Ising spins. However, in reality, these quantum fluctuations immediately stabilize a ground-state with long-range three-sublattice order of $\sigma^z$ for any nonzero $\Gamma$. In contrast to the ferromagnetic three-sublattice order exhibited by the classical Ising antiferromagnet with ferromagnetic further neighbour coupling\textsuperscript{3}, the $\Gamma > 0$ ground state is characterized by antiferromagnetic three-sublattice order\textsuperscript{7} i.e., the modulation of $\langle \sigma^z \rangle$ at wavevector $\mathbf{Q}$ is not accompanied by any net ferromagnetic moment. At $T = 0$, this three-sublattice ordered persists up to a critical value $\Gamma_c \approx 1.7$\textsuperscript{12} (in units of $J_1$), beyond which the system becomes a quantum paramagnet in which the spins are polarized in the $\hat{x}$ direction\textsuperscript{12,13} When the system is heated to nonzero temperatures above this three-sublattice ordered ground state, the three-sublattice order melts via an intermediate-temperature phase characterized by power-law order: $\langle \sigma^z(\mathbf{R})\sigma^z(0) \rangle \sim \cos(\mathbf{Q} \cdot \mathbf{R})/|\mathbf{R}|^{\eta(T)}$ for $T \in (T_1, T_2)$, with a temperature-dependent power-law exponent $\eta(T)$ that is expected\textsuperscript{13} to increase from $\eta(T_1) = 1/9$ to $\eta(T_2) = 1/4$\textsuperscript{12}.

A recent field-theoretical analysis\textsuperscript{13} predicts that the ferromagnetic easy-axis susceptibility $\chi_u(B)$ to the uniform longitudinal field $B$ along the easy-axis diverges at small $B$ in a large portion of such power-law ordered phases associated with the two-step melting of three-sublattice order in frustrated easy-axis antiferromagnets with triangular lattice symmetry: $\chi_u(B) \sim |B|^{-\frac{4-18\eta}{1-9\eta}}$ for $\eta(T) \in (1/9,2/9)$. For the specific case of the transverse field Ising antiferromagnet on the triangular lattice, this is a rather counter-intuitive prediction: The Ising spins in Eq. (1) have no ferromagnetic couplings, and
ferromagnetic correlations remain short-ranged in the low-temperature phase with long-range three-sublattice ordered phase. Yet, the prediction is for the uniform easy-axis susceptibility to start diverging once this three-sublattice order melts partially due to thermal fluctuations.

Our goal here is to test this general prediction using the test-bed provided by the transverse field Ising antiferromagnet (Eq. 11) on the triangular lattice. In order to do this, we need to obtain an accurate characterization of the long-distance form of the correlations of the easy-axis magnetization density as well as correlations of the three-sublattice order parameter for this model. These can be used to obtain the finite-size easy-axis susceptibility to start diverging once this three-sublattice ordered phase. If the easy-axis susceptibility is indeed singular as predicted, then standard finite-size scaling arguments imply that \( \chi_u(L) \sim L^{-2+\eta} \) for \( \eta(T) \in (1/9, 2/9) \) in the power-law ordered phase. In this paper, we test this form of the prediction using a newly developed quantum-cluster algorithm\(^{11}\) that provides an efficient tool for performing Quantum Monte Carlo simulations of frustrated transverse field Ising models within the Stochastic Series Expansion\(^{12-13}\) framework.

The rest of this paper is organized as follows: In Section II, we discuss the antiferromagnetic nature of the three-sublattice order induced by the transverse field and contrast it with the ferrimagnetic three-sublattice ordered phase established by additional ferromagnetic couplings. We also review the standard Landau theory framework used for describing this kind of low-range order, and use it to discuss the possible theoretical scenarios for the phase transition between these two phases. In Section III, we provide a brief sketch of the actual computational method used to obtain our numerical results. In Section IV, we summarize our results for the uniform magnetization density as well as the three-sublattice order parameter and compare them with the field-theoretical predictions alluded to earlier.

II. PHASES AND TRANSITIONS

The antiferromagnetic (with no net easy-axis magnetic moment) three-sublattice order exhibited by the \( \Gamma > 0 \) ground state of \( H_{\text{Ising}} \) can be thought of in terms of the following useful caricature: Ising spins on one spontaneously chosen sublattice (out of the three sublattices corresponding to the natural tripartite decomposition of the triangular lattice) freeze into the \( |\sigma^x = +1\rangle \) state. Equivalently, one may think of them as fluctuating freely between the \( |\sigma^z = +1\rangle \) and \( |\sigma^x = -1\rangle \) states due to the effects of quantum fluctuations. On the other two sublattices of the triangular lattice, the system orders antiferromagnetically, with spins on one sublattice pointing up along the \( \hat{z} \) axis, and spins on the other sublattice pointing down. This is also the picture for the long-range ordered phase that persists up to the lower-critical temperature \( T_1(\Gamma) \) that marks the onset of the power-law ordered intermediate phase associated with the two-step melting of three-sublattice order.

On incorporating an additional next-neighbour ferromagnetic coupling \( J_2 < 0 \), the antiferromagnetic three-sublattice order of the low-temperature phase gives way to ferrimagnetic (with net easy axis moment) three-sublattice order beyond a non-zero threshold value \( J_2^c \). This is because the classical \( (\Gamma = 0) \) model with \( J_2 < 0 \) is known to develop ferrimagnetic three-sublattice order beyond a \( T = 0 \) threshold at which \( \sigma^z \) have power-law correlations \( \langle \sigma^z(\vec{R})\sigma^z(0) \rangle \sim \cos(\vec{Q} \cdot \vec{R})/|\vec{R}|^\eta \) with \( \eta = 1/9 \). This ferrimagnetic three-sublattice order can be understood in terms of the following caricature: The system spontaneously chooses one sublattice on which the spins all point along the \(+\hat{z}\) direction (\(-\hat{z}\) direction), while the spins on the other two sublattices all point along the \(-\hat{z}\) direction (\(+\hat{z}\) direction).

With this picture of the low temperature phases in mind, we focus our attention on the uniform easy axis magnetization \( m \) and the complex three-sublattice order parameter \( \psi \), defined as

\[ m = \frac{1}{L^2} \sum_{\vec{R}} \sigma^z_{\vec{R}} \quad (2) \]

\[ \psi = \frac{1}{L^2} \sum_{\vec{R}} \sigma^z_{\vec{R}} \exp(i\vec{Q} \cdot \vec{R}) \quad (3) \]

where \( \vec{Q} \) is the three-sublattice ordering wave vector \( ((2\pi/3, 2\pi/3) \text{ in the standard basis}) \) and \( \vec{R} \) represents the coordinates of triangular lattice sites. In the standard Landau-Ginzburg approach\(^{15-17}\) to thermal (nonzero temperature) phase transitions involving such three-sublattice ordered states, the physics of three-sublattice ordering is represented in terms of a classical order parameter field \( \psi_{cl} \), which may be identified with the static (Matsubara frequency \( \omega_n = 0 \)) part of the \( \psi \) operator defined above:

\[ \psi_{cl} = \frac{1}{\beta} \int_0^\beta d\tau \psi(\tau) \quad (4) \]

Here, we used the usual notation for the imaginary-time analog of Heisenberg operators, \( \mathcal{O}(\tau) = e^{\tau H_{\text{TFIM}}} \mathcal{O} e^{-\tau H_{\text{TFIM}}} \), corresponding to any Schrödinger operator \( \mathcal{O} \).

In this Landau-Ginzburg framework, the free energy is written as an integral over a coarse-grained free-energy density \( \mathcal{F}(\psi_{cl}) \) that admits an expansion in powers and gradients of a coarse-grained order-parameter field \( \psi_{cl}(\vec{r}) \) which may be thought of as a local version of the order parameter defined in Eq. 4. Keeping various low-order terms consistent with the action of various symmetries
of the microscopic Hamiltonian, one writes:
\[
\mathcal{F}(\psi_{cl}) = \kappa |\nabla \psi_{cl}|^2 + r |\psi_{cl}|^2 + u_4 |\psi_{cl}|^4 + u_5 |\psi_{cl}|^6 + \lambda_6 |\psi_{cl}|^6 \cos(6\theta) + \lambda_{12} |\psi_{cl}|^{12} \cos(12\theta) + \ldots
\]
where, \(\theta(\vec{r})\) is the phase of the complex order parameter field \(\psi_{cl}(\vec{r})\). As usual, one assumes that the coefficients of various terms in this phenomenological free-energy are smooth functions of microscopic parameters. In this approach, three-sublattice ordering corresponds to \(r < 0\). The sign of \(\lambda_6\) determines the nature of three-sublattice ordering: \(\lambda_6 > 0\) favors antiferromagnetic ordering with the phase \(\theta\) pinned at \((2n + 1)\pi/6\) \((n = 0, 1, \ldots, 5)\), while \(\lambda_6 < 0\) favors ferrimagnetic ordering with the phase pinned at \((2n)\pi/6\) \((n = 0, 1, \ldots, 5)\). The \(\lambda_{12}\) term is not expected to be important except when \(\lambda_6\) is driven to the vicinity of zero by the competition between first-neighbour ferromagnetic couplings (in the microscopic Hamiltonian) that favour ferrimagnetic three-sublattice ordering, and other effects (such as quantum fluctuations induced by a transverse field) that favour antiferromagnetic three-sublattice ordering.

If fluctuations of \(\theta\), the phase of the order parameter, play a dominant role in driving the transition to a para-magnetic high-temperature state, one expects a phase-only description to capture the long-wavelength properties near such a transition. In other words, one then expects that \(|\psi_{cl}|\), the amplitude of the order parameter, remains nonzero near the transition (corresponding to \(r < 0\)), and the physics of the transition is controlled by the interplay between the effective phase-stiffness \(\kappa |\psi_{cl}|^2\) and the six-fold anisotropy \(\lambda_6\). This gives rise to the expectation\(^{15}\) of critical behaviour in the universality class of the six-state clock model\(^{14,15}\) of statistical mechanics.

As is well-known, two-dimensional six-state clock models represent an unusual example of a system which can display a variety of critical behaviours, each of which is a generic possibility that can be realized for a range of microscopic parameters\(^{15}\). Of particular interest in the present context is the possibility of a two-step melting transition, whereby the low-temperature phase with long-range order in \(\exp(i\theta)\) is separated from a high-temperature paramagnetic phase by an intermediate phase with power-law order in \(\exp(i\theta)\). As is well known, this power-law ordered phase is controlled by a line of Gaussian fixed point\(^{15}\) with effective free-energy density \(\frac{1}{2\pi g} \int d^2 r (\nabla \theta)^2\). For \(g \in (1/9, 1/4)\), the six-fold anisotropy \(\lambda_6\) and the vorticity in the \(xy\) field \(\theta\) are both irrelevant perturbations of this fixed-point free-energy density, which controls the long-wavelength behaviour of order parameter correlations in the intermediate power-law ordered phase. The continuously varying power-law exponent \(\eta(T)\) for order parameter correlations, which serves as a “universal coordinate” that locates a given microscopic system within this power-law ordered phase, is set by the coupling constant \(g\) via the relation \(\eta(T) = g(T)\).

The Landau-Ginzburg theory also sheds light on the nature of the low temperature transition between the two kinds of three-sublattice ordered phases, modeled by \(\lambda_6\) going through zero smoothly and changing sign. Since both phases have long-range three-sublattice order, fluctuations of \(|\psi_{cl}|\) may again be neglected in the vicinity of this transition. With the amplitude \(|\psi_{cl}|\) remaining essentially constant across this transition, the physics of the transition is again controlled by the phase \(\theta\) of the three-sublattice order parameter. Minimizing the free-energy density \(\mathcal{F}\) yields a spatially uniform configuration with a particular optimal value \(\theta^*\) for this phase variable. When \(\lambda_{12} < 0\), \(\theta^*\) takes on the values \((2n + 1)\pi/6\) \((2n)\pi/6\) \((n = 0, 1, \ldots, 5)\) when \(\lambda_6 > 0\) \((\lambda_6 < 0)\). When \(\lambda_6 = 0\), all values \(\theta^* = m\pi/6\) \((m = 0, 1, \ldots, 11)\) minimize the free-energy. Clearly, this corresponds to a first-order transition between ferrimagnetic and antiferromagnetic three-sublattice ordered states, with both kinds of three-sublattice order coexisting at the transition point.

If, on the other hand, \(\lambda_{12} > 0\), we obtain
\[
\theta^* = \begin{cases} 
\frac{2\pi n}{6} & \text{if } \lambda_6 < -4\lambda_{12} |\psi_{cl}|^6 \\
\frac{2\pi n}{6} + \frac{1}{6} \arccos(-\lambda_6/4\lambda_{12} |\psi_{cl}|^6) & \text{if } |\lambda_6| < \lambda_{12} |\psi_{cl}|^6 \\
\frac{2\pi n}{6} - \frac{1}{6} \arccos(\lambda_6/4\lambda_{12} |\psi_{cl}|^6) & \text{if } \lambda_6 > 4\lambda_{12} |\psi_{cl}|^6 
\end{cases}
\]
where \(n = 0, 1, \ldots, 5\) represents the six-fold degeneracy of the minima in each case. In this case, as \(|\lambda_6|\) becomes small and \(\lambda_6\) goes through zero, \(\theta^*\) switches continuously from the antiferromagnetic phase to the ferrimagnetic phase via an intermediate mixed phase that is established for \(|\lambda_6| < 4\lambda_{12} |\psi_{cl}|^6\). In what follows, we will confront these two quite different scenarios with data obtained in the vicinity of the transition between antiferromagnetic and ferrimagnetic three-sublattice order in the low-temperature state of \(H_{\text{Ising}}\) with an additional ferromagnetic second-neighbour coupling \(J_2\) between the Ising spins.

### III. METHODS

Our numerical work uses the Stochastic Series Expansion (SSE) framework\(^{12,13,20,22}\) to compute equilibrium averages \(\langle \ldots \rangle\) for transverse field Ising models at nonzero temperature. For models with geometric frustration, which results in a macroscopic degeneracy of minimally frustrated classical configurations (with minimum Ising-exchange energy), it is important that the computational method correctly captures the interplay between this macroscopic degeneracy, and the disordering effects of classical and quantum fluctuations. In the present case, this interplay is expected to be crucial to the establishment of antiferromagnetic three-sublattice order in the low temperature phase, as well as its two-step melting\(^{21,23}\).
Therefore, to obtain reliable results, we use the recently developed quantum cluster algorithm\cite{newref} that works within the SSE framework to provide an efficient way of sampling the partition function for such frustrated transverse field Ising models. In this cluster algorithm, which facilitates the construction of “space-time clusters” with a broad distribution of cluster sizes, allowing the algorithm to efficiently sample the configuration space of SSE operator strings at low temperature.

Using this approach, we study $H_{\text{Ising}}$ on $L \times L$ triangular lattices with periodic boundary conditions, with $L$ ranging from $L = 24$ to 96. We compute the static susceptibilities corresponding to the order parameters defined in Eq. [2]. These susceptibilities are defined as

$$\chi_u = \frac{L^2}{\beta} \langle |\int_0^\beta d\tau m(\tau)|^2 \rangle$$

and

$$\chi_Q = \frac{L^2}{\beta} \langle |\int_0^\beta d\tau \psi(\tau)|^2 \rangle$$

Additionally, we compute the static susceptibility $\chi_{Q}^x$ to a transverse field (along $\hat{x}$) oscillating at wavevector $Q$, defined as

$$\chi_{Q}^x = \frac{L^2}{\beta} \langle |\int_0^\beta d\tau \sigma_Q^x(\tau)|^2 \rangle$$

These calculations confirm the algorithm local information that is set to unity. Furthermore, to fit reasonably well to the single parameter form $kL^{-2}$ with $k = 15.18(8)$ for the largest four sizes studied here. This analysis also confirms that the low-temperature phase of $H_{\text{Ising}}$ is indeed antiferromagnetic, i.e., with no net easy-axis moment. All other temperature and energy scales are measured in units of $J_1$ which is set to unity.
where $\sigma_{Q}^2$ is given by

$$
\sigma_{Q}^2 = \frac{1}{L^2} \sum_{\vec{R}} \sigma_{\vec{R}}^2 \exp(i\vec{Q} \cdot \vec{R})
$$

(10)

IV. RESULTS

We begin by revisiting the phase diagram obtained in previous work\[7\] for the case with no next-nearest-neighbour coupling ($J_2 = 0$). From their results, we note that the low temperature order persists up to the highest temperature at $\Gamma = 0.8$. Therefore, we set the transverse field to this value in most of our work and study the three-sublattice ordering of the low temperature phase, as well as its two-step melting.

As expected, we find that the order parameter susceptibility $\chi_{Q}$ scales with the volume of the system at low enough temperature, confirming the presence of long-range three-sublattice order in the low temperature phase. Since this is entirely consistent with earlier results,\[7\] we do not display this explicitly here. Since our focus in what follows will be an unusual singular behaviour in the ferromagnetic susceptibility $\chi_{u}$ to a uniform field along the easy-axis, we find it useful to first study the same quantity deep in the low-temperature ordered state. From Fig. 1 and Fig. 2, which display the $L$ dependence of $\chi_{u}$ and $\chi_{u}/L^2$ deep in the low-temperature ordered state, we see that the three-sublattice ordering in the low temperature phase is not accompanied by any net moment along the easy-axis.

This confirms earlier results\[7\] that have identified the antiferromagnetic nature of the three-sublattice ordering at low temperature. However, the approach to the thermodynamic limit is seen to involve a slow crossover, suggesting the presence of a proximate phase with a net easy-axis moment. This is consistent with the fact that a relatively small value of second-neighbour ferromagnetic exchange $J_2 < 0$ is sufficient to access a nearby state with ferrimagnetic three-sublattice ordering at low temperature.\[11\]

In the power-law ordered phase associated with the two-step melting of three-sublattice order, the static susceptibility $\chi_{Q}$, defined in Eq. (8) for a finite size $L \times L$ system, is expected to scale as

$$
\chi_{Q} \sim L^{2-\eta(T)}
$$

(11)

From the renormalization group picture (summarized in the previous section) of this power-law ordered phase, it is also clear that $\eta(T)$ ranges from $\eta(T_1) = 1/9$ at the lower phase boundary $T_1(\Gamma)$ of the power-law phase, to $\eta(T_2) = 1/4$ at the upper phase boundary $T_2(\Gamma)$.

To locate these upper and lower transition temperatures for $\Gamma = 0.8$, we plot $\chi_{Q} L^{\frac{1}{2}-2}$ and $\chi_{Q} L^{\frac{1}{2}-2}$ for various sizes $L$ as a function of temperature and identify the temperature at which curves corresponding to the different sizes all cross. This is shown in Fig. 3. The location of transitions obtained in this way are consistent with those obtained earlier in Ref. [7].

Since the upper (lower) transitions out of the power-law ordered phase correspond to vorticity (six-fold anisotropy) in $\theta$ becoming relevant, we expect these transitions to be of the Kosterlitz-Thouless (inverted Kosterlitz-Thouless) type. To confirm that this is indeed the case, we perform fits of our Quantum Monte Carlo data in the vicinity of the upper phase boundary to the finite-size scaling form predicted by Kosterlitz-Thouless theory.\[19\] This scaling form follows from the following argument: Above $T_2(\Gamma)$, order parameter correlations decay exponentially, with a correlation length $\xi$ given by\[23\]

$$
\xi \sim \exp(at^{-1/2})
$$

(12)

where $t = (T - T_2)/T_2$ is the reduced temperature. This Kosterlitz-Thouless form of the correlation length, Eq. (12), in conjunction with the standard finite size scaling ansatz $\chi_{Q}(t, L) = L^{2-\eta} f(\xi/L)$ gives the finite-size scaling form\[19\]

$$
\chi_{Q}(t, L)L^{\frac{1}{2}-2} = f(L^{-1}\exp(at^{-1/2}))
$$

(13)

where we have used $\eta_2 = 1/4$, and $f$ is the finite-size scaling function that we expect our data to collapse onto. In practice, we use $T_2$ obtained from Fig. 3 and attempt a finite-size scaling collapse with a single adjustable parameter $a$. This is shown in Fig. 4.

When ferromagnetic second-neighbour interactions $J_2 < 0$ of sufficient magnitude are present, one expects the ground state ordering pattern to change to ferrimagnetic three-sublattice order.\[13\] In recent work, the
threshold value of $J_2$ corresponding to this onset of ferrimagnetism was estimated to be roughly $J_2^c \approx -0.03$. With a view towards comparing the melting behaviour of this ferrimagnetic three-sublattice order with the two-step melting of antiferromagnetic three-sublattice order, we also study the effect of thermal fluctuations at $J_2 = -0.1$, i.e., deep in this ferrimagnetic three-sublattice ordered state. We find that long-range order is again lost via a two-step melting process, with an intermediate power-law ordered phase. The locations of the upper and lower transitions that demarcate the extent of the power-law ordered phase are obtained as before. This is displayed in Fig. 5. Above $T_2$, the static order parameter susceptibility again collapses quite convincingly onto the Kosterlitz-Thouless finite-size scaling form. This is shown in Fig. 6.

With these preliminaries out of the way, we are now in a position to study in a unified way the behaviour of the uniform easy-axis susceptibility $\chi_u$ in the power-law ordered phase associated with the two-step melting of antiferromagnetic three-sublattice order as well as ferrimagnetic three-sublattice order. As mentioned earlier, our goal is to test a recent prediction\(^{10}\) that $\chi_u$ provides a thermodynamic signature of two step melting due to the presence of a singular $B$ dependence: $\chi_u(B) \sim |B|^{-\frac{2-\eta}{2-\eta_2}}$ for $\eta(T) \in (1/9, 2/9)$.

Here, we test this via the equivalent prediction\(^{10}\) for the finite-size susceptibility $\chi_u(L)$ of an $L \times L$ sample when $B = 0$: $\chi_u(L) \sim L^{2-\eta \eta_2}$ for $\eta(T) \in (1/9, 2/9)$. In Landau theory terms, this singularity in $\chi_u$ is a direct consequence of a symmetry-allowed coupling of the form $m_{cl}^3 |\psi_{cl}|^3 \cos(3\theta)$ between the static component $m_{cl}(\vec{r})$ of the uniform magnetization density and the order parameter field $\psi_{cl}$. In the power-law ordered phase, this coupling is predicted\(^{10}\) to cause $m_{cl}$ to have the same power-law correlations as $\cos(3\theta)$, leading to a singular $\chi_u$ independent of whether the low temperature ordered state is ferrimagnetic or antiferromagnetic. Thus, while the predicted effect is particularly counter-intuitive for the antiferromagnetic case, i.e., with $J_2 = 0$ for the system under

\(\Gamma = 0.8, J_1 = 1.0, J_2 = -0.1\)

\(\Gamma = 0.8, J_1 = 1.0, J_2 = -0.1\)

\(\Gamma = 0.8, J_1 = 1.0, J_2 = -0.1\)
FIG. 8. $\chi_Q$ and $\chi_u$ fit rather well to power-law forms $k_1 L^{2-\eta}$ and $k_2 L^{2-3\eta}$ respectively for three different values of temperature in the intermediate power-law ordered phase associated with the melting of ferrimagnetic three-sublattice order when $J_2 = -0.1$, $\Gamma = 0.8$. All other temperature and energy scales are measured in units of $J_1$ which is set to unity.

$\Gamma = 0.8, J_1 = 1.0, J_2 = 0.0$  $\Gamma = 0.8, J_1 = 1.0, J_2 = -0.1$

$\eta = 0.129, T = 0.50$  $\eta = 0.129, T = 0.50$  $\eta = 0.160, T = 0.60$  $\eta = 0.160, T = 0.60$  $\eta = 0.200, T = 0.75$  $\eta = 0.200, T = 0.75$

FIG. 9. $\chi_{xx}^Q$ fits the power-law form $k_3 L^{2-4\eta}$ for three different values of temperature in the intermediate power-law ordered phase associated with the melting of antiferromagnetic as well as ferrimagnetic three-sublattice order. All other temperature and energy scales are measured in units of $J_1$ which is set to unity.

$\Gamma = 0.8, J_1 = 1.0, J_2 = 0.0$  $\Gamma = 0.8, J_1 = 1.0, J_2 = -0.1$

$\eta = 0.129, T = 0.21$  $\eta = 0.117, T = 0.31$  $\eta = 0.187, T = 0.33$

FIG. 10. Histograms of $\chi_u/L^2$ show a characteristic two-peak structure suggestive of a first order transition. All other temperature and energy scales are measured in units of $J_1$ which is set to unity.

$T = 0.1, J_1 = 1.0, \Gamma = 0.8, L = 96$

$J_2 = -0.0280$  $J_2 = -0.0320$  $J_2 = -0.0350$  $J_2 = -0.0400$

As is clear from Fig. 9, our data for $\chi_{xx}$, which is set to unity.

A similar argument, which identifies $\beta^{-1} \int_0^\beta \sigma_Q^2(\tau)$ with $\psi_0^2$ on symmetry grounds, immediately predicts that $\chi_{xx}^Q \sim L^{2-4\eta}$ throughout the power-law ordered phase. As is clear from Fig. 9, our data for $\chi_{xx}^Q$ is seen to be completely consistent with this prediction as well.

Finally, we comment on the nature of the transition between the antiferromagnetic and ferrimagnetic three-sublattice ordered states. In previous work which studied relatively small samples at moderately low temperatures in the vicinity of this transition, the phase of the estimator for the three-sublattice order parameter, as measured in the Quantum Monte Carlo simulations, was seen to be distributed more or less uniformly in the interval $(0, 2\pi)$. If this behaviour were to persist to larger sizes, it would be indicative of a power-law ordered phase that interpolates between the antiferromagnetic and ferrimagnetic three-sublattice ordered phases at nonzero temperature. However, from the Landau theory considerations of Sec. II, we see that the two generic possibilities for this phase transition are first-order behaviour, or an intermediate mixed-phase. An intervening power-law ordered phase can, in this picture, only arise in the fine-tuned limiting case where $\lambda_{12}$ and higher order anisotropies are all absent. With this in mind, we measure the histogram of the estimator for $\chi_u/L^2$ to look for signals of phase coexistence in the transition region. These histograms are shown in Fig. 10. The two-peak nature of these histograms suggests that the transition is in fact of a weakly first-order type. This is consistent with the fact that the $L$-dependence of $\chi_Q$ is certainly not a power-law, and the fact that Binder ratios of the estimator of $\chi_Q$ also do not show a clear crossing (indicative of a second-order
Thus, we have obtained fairly convincing evidence for a singular uniform easy-axis susceptibility $\chi_u(B)$ in the power-law ordered phase associated with the two-step melting of antiferromagnetic three-sublattice order in triangular lattice transverse-field Ising antiferromagnets. This (at-first-sight) counter-intuitive thermodynamic signature of two-step melting is already of some general interest, since the transverse-field Ising antiferromagnet on the triangular lattice is a paradigmatic example of the interplay between quantum fluctuations and frustrated classical interactions. Of course, this thermodynamic signature of two-step melting would be of much greater interest and direct experimental relevance if the model Hamiltonian $H_{\text{Ising}}$ were to emerge as a good description of magnetic exchange interactions in some frustrated magnet.

In this context, it should be noted that a closely related model Hamiltonian, the one-dimensional transverse field Ising chain, does serve as a good starting point for the theoretical description of an interest-

V. DISCUSSION

Thus, we have obtained fairly convincing evidence for a singular uniform easy-axis susceptibility $\chi_u(B)$ in the power-law ordered phase associated with the two-step melting of antiferromagnetic three-sublattice order in triangular lattice transverse-field Ising antiferromagnets. This (at-first-sight) counter-intuitive thermodynamic signature of two-step melting is already of some general interest, since the transverse-field Ising antiferromagnet on the triangular lattice is a paradigmatic example of the interplay between quantum fluctuations and frustrated classical interactions. Of course, this thermodynamic signature of two-step melting would be of much greater interest and direct experimental relevance if the model Hamiltonian $H_{\text{Ising}}$ were to emerge as a good description of magnetic exchange interactions in some frustrated magnet.

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