

Influence of quantum fluctuations on the spin-flop transition in hematite

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Magnetic phase transitions between ordered phases are often understood on the basis of semiclassical spin models. Deviations from the classical description due to the quantum nature of the atomic spins as well as quantum fluctuations are usually treated as negligible if long-range order is preserved, and are rarely quantified for actual materials. Here, we demonstrate that a fully quantum-mechanical framework is required for a quantitatively correct description of the spin-flop transition in the insulating altermagnet hematite between the collinear antiferromagnetic and the weakly ferromagnetic spin-flop phase at low temperature. By applying both exact diagonalization and density-matrix renormalization group theory to the quantum Heisenberg Hamiltonian, we show how a quantum-mechanical treatment of an *ab initio* parametrized spin model can significantly improve the predicted low-temperature spin-flop field over a classical description when compared to measurements. Our results imply that quantum fluctuations have a measurable influence on selecting the ground state of a system out of competing ordered magnetic phases at low temperature.

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Magnetic ordering is inherently a quantum-mechanical phenomenon, which relies on concepts like the spin angular momentum and the Pauli exclusion principle. However, ordered phases are characterized by a finite local expectation value of the spin operator, and this local magnetization vector may also be described by the methods of classical statistical mechanics or field theory. Common approaches for treating such systems include classical generalized Heisenberg models on the atomic level and continuum micromagnetic models on the mesoscopic scale. Density-functional theory also utilizes the local magnetization density; thus, it is particularly well suited for parametrizing such classical models [1–6]. The frequencies of magnetic excitations may be determined within the classical approach, enabling the comparison with (anti)ferromagnetic resonance [7,8] or neutron scattering measurements [9], which provide an alternative way of fitting the parameters of the model. The numerical solution of these models using stochastic atomistic spin dynamics [10] or micromagnetic simulations [11,12] has proven immensely successful in uncovering and interpreting exotic magnetic textures and dynamical phenomena in the field of spintronics.

However, the classical approach cannot reproduce certain phenomena connected to the quantum nature of the magnetic excitations, or magnons, in these ordered phases. The

Bose-Einstein statistics of magnons results in the magnetization of ferromagnets scaling as $T^{\frac{3}{2}}$ at low temperature [13], in contrast to the linear temperature dependence predicted by the classical theory [14]. In antiferromagnets, quantum fluctuations of the magnons lead to a reduction in the sublattice magnetizations compared to the saturation value [15], and these fluctuations also split the degeneracy via an order-by-disorder mechanism between states that classically have the same energy [16]. Recent efforts endeavored to correct these shortcomings of classical simulations by applying a quantum thermostat [17,18] or via rescaling the temperature [19].

Recently, it was suggested that quantum fluctuations are also responsible for the discrepancy in the spin-flop fields between experiments and classical atomistic spin simulations in the insulating iron oxide hematite (α -Fe₂O₃) [6]. At low temperature, hematite assumes a collinear antiferromagnetic order with spins of all four sublattices aligned along the z axis of threefold rotational symmetry, as depicted in Fig. 1(a).

If an external field is applied along the z axis, the spin system undergoes a first-order transition into the spin-flop phase depicted in Fig. 1(b) [20]. In addition to the magnetization along the field direction, the system acquires a small in-plane magnetization due to canting between the sublattices induced by the Dzyaloshinskii-Moriya interaction (DMI) [21–23]. For high enough (experimentally unachievable) fields, the system would become completely polarized along the field direction in a second-order transition [Fig. 1(c)]. The ground state also transforms into the spin-flop or weak ferromagnetic state with DMI-induced canting when the temperature is raised above the Morin temperature $T_M \approx 250$ K [24] in the field-free case.

The classical atomistic spin dynamics simulations based on an *ab initio* parametrized spin model in Ref. [6] reproduced

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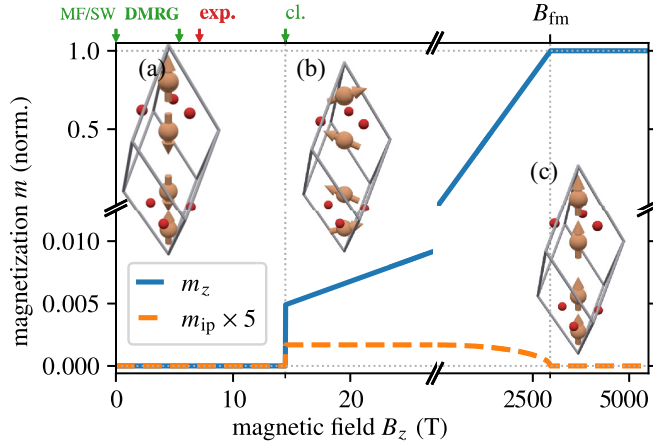


FIG. 1. Out-of-plane (m_z) and in-plane (m_{ip}) magnetization of hematite as a function of a magnetic field applied along the z axis, calculated analytically at $T = 0$ within classical theory. The insets show the corresponding spin configurations within the primitive unit cell: (a) antiferromagnetic ground state, (b) spin-flop phase, and (c) ferromagnetically polarized phase. The green arrows show the spin-flop field in the classical theory compared to mean-field (MF) and spin-wave theory (SW) calculations and DMRG results presented below. The red arrow shows the experimentally observed value.

the experimentally observed Morin and Néel temperatures accurately, but overestimated the spin-flop field at zero temperature (cf. Fig. 1). This is caused by a qualitative difference in the low-temperature behavior: Below 160 K, the spin-flop field increases approximately linearly as the temperature is decreased in classical simulations, reaching 14.5 T at $T = 0$, while in experiments it stays approximately constant around 7 T [6,20]. It was demonstrated in Ref. [6] that a mean-field description of a quantum instead of a classical spin model can qualitatively reproduce the weak temperature dependence of the spin-flop field observed in the experiments. However, the mean-field model proved to be quantitatively inaccurate in its prediction of the critical temperatures or fields. Determining the spin-flop field of quantum magnets quantitatively is challenging from the theoretical point of view: In two-sublattice antiferromagnets without DMI, predictions exist based on spin-wave theory at zero temperature [25], but this has proven difficult to extend to finite temperatures [26]. In the presence of DMI, calculations have been mainly restricted to mean-field theory [27].

Here, we present a quantum spin model for hematite based on the material-specific description of Ref. [6]. We transform the parameters of the classical model to the quantum one while keeping the spin-wave frequencies constant. Within linear spin-wave theory, this model does not reproduce the correct ground state, but we will show that a more accurate treatment of quantum fluctuations in exact diagonalization (ED) and density-matrix renormalization group (DMRG) theory restores the collinear antiferromagnetic ground state and predicts a spin-flop field at zero temperature that compares favorably with the experimental value (see Fig. 1).

The magnetic properties of hematite can be understood on the basis of an extended Heisenberg model with the Hamilto-

nian [6]

$$\mathcal{H} = -\frac{1}{2} \sum_{i \neq j} \mathbf{S}_i^T \mathcal{J}_{ij} \mathbf{S}_j - \sum_i [d_2 S_{i,z}^2 + d_4 S_{i,z}^4 + \mu \mathbf{B} \cdot \mathbf{S}_i]. \quad (1)$$

The $\mathcal{J}_{ij}$ represent tensorial exchange interactions, incorporating the isotropic exchange, DMI, and easy-plane two-ion anisotropies. The latter lead to the Morin transition in competition with the easy-axis on-site anisotropy energies d_2 and d_4 . The fourth-order term creates an additional energy barrier between the collinear and the canted states and needs to be included to correctly represent the nature of the Morin and spin-flop transitions as first-order phase transitions. The last term is the Zeeman energy with the atomic magnetic moment μ and the external magnetic field $\mathbf{B}$.

Classically, the $\mathbf{S}_i$ are seen as vectors on the unit sphere. For the quantum-mechanical treatment, we have to replace them with angular momentum operators $\hat{\mathbf{S}}_i = (\hat{S}_{i,x}, \hat{S}_{i,y}, \hat{S}_{i,z})^T$. To express the Hamiltonian in matrix form, we replace the x and y components of the spin operators with the ladder operators $\hat{S}_i^\pm = \hat{S}_i^x \pm i\hat{S}_i^y$, which yields

$$\begin{aligned} \hat{\mathcal{H}} = & -\frac{1}{2} \sum_{i \neq j} \left[\left(\frac{1}{4} J_{ij}^{xx} - \frac{i}{4} J_{ij}^{xy} - \frac{i}{4} J_{ij}^{yx} - \frac{1}{4} J_{ij}^{yy} \right) \hat{S}_i^+ \hat{S}_j^+ \right. \\ & + \left(\frac{1}{4} J_{ij}^{xx} + \frac{i}{4} J_{ij}^{xy} - \frac{i}{4} J_{ij}^{yx} + \frac{1}{4} J_{ij}^{yy} \right) \hat{S}_i^+ \hat{S}_j^- \\ & + \left(\frac{1}{4} J_{ij}^{xx} - \frac{i}{4} J_{ij}^{xy} + \frac{i}{4} J_{ij}^{yx} + \frac{1}{4} J_{ij}^{yy} \right) \hat{S}_i^- \hat{S}_j^+ \\ & + \left(\frac{1}{4} J_{ij}^{xx} + \frac{i}{4} J_{ij}^{xy} + \frac{i}{4} J_{ij}^{yx} - \frac{1}{4} J_{ij}^{yy} \right) \hat{S}_i^- \hat{S}_j^- \\ & + \left(\frac{1}{2} J_{ij}^{xz} - \frac{i}{2} J_{ij}^{yz} \right) \hat{S}_i^+ \hat{S}_j^z + \left(\frac{1}{2} J_{ij}^{xz} + \frac{i}{2} J_{ij}^{yz} \right) \hat{S}_i^- \hat{S}_j^z \\ & + \left(\frac{1}{2} J_{ij}^{zx} - \frac{i}{2} J_{ij}^{zy} \right) \hat{S}_i^z \hat{S}_j^+ + \left(\frac{1}{2} J_{ij}^{zx} + \frac{i}{2} J_{ij}^{zy} \right) \hat{S}_i^z \hat{S}_j^- \\ & \left. + (J_{ij}^{zz}) \hat{S}_i^z \hat{S}_j^z \right] - \sum_i [d_2 (\hat{S}_i^z)^2 + d_4 (\hat{S}_i^z)^4 + \mu \mathbf{B}^z \hat{S}_i^z]. \end{aligned} \quad (2)$$

We represent this operator in the basis of product states described below to obtain the matrix form, which is a very sparse matrix, since the Hamiltonian is limited to two-spin interactions, making the use of matrix-free methods such as the Arnoldi algorithm very efficient.

The classical model is obtained in the $S \rightarrow \infty$ limit of the quantum description, where the components of the vector operator $\hat{\mathbf{S}}_i/S$ assume infinitely many eigenvalues between -1 and 1 , and the three components together map the whole unit sphere. To establish a correspondence between the classical and quantum Hamiltonians, we rescale terms that are of second order in spin operators by a factor of S^2 and fourth-order terms by S^4 :

$$\mathcal{J}_{ij}^q(S) = \frac{\mathcal{J}_{ij}^c}{S^2}, \quad d_2^q(S) = \frac{d_2^c}{S^2}, \quad d_4^q(S) = \frac{d_4^c}{S^4}, \quad (3)$$

where the q and c superscripts denote the coefficients in the quantum and the classical models, respectively. With this

approach, the spin-wave frequencies calculated from performing a linearized Holstein-Primakoff transformation on the quantum Hamiltonian and from the linearization of the classical Landau-Lifshitz-Gilbert equation will be identical. This rescaling was used in Ref. [18], where the spin-wave spectrum was compared to previous experimental results.

The atomic magnetic moments in hematite appear due to the $3d^5$ electron configuration of the Fe^{3+} ions. As free ions, these should have a quantum number of $S = \frac{5}{2}$ according to Hund's rules, corresponding to a magnetic moment of approximately $5\mu_B$. For the oxygen-ligated ions in hematite, however, density functional theory calculations have shown that delocalization of the $3d$ electrons leads to a reduction of the atomic moment toward $4\mu_B$ (4.11 – $4.24\mu_B$) [2,5,6], which is confirmed by experimental measurements [28]. This would suggest an alternative quantum number of $S = 2$. In the following, we will therefore present results with both of those values, $S = 2$ and $S = \frac{5}{2}$.

To determine the ground state of the quantum spin Hamiltonian exactly, we express it in matrix form using the basis of products of S_i^z eigenstates with projection quantum numbers $m_i = -S, \dots, S$ for each spin $i \in \{1, \dots, n\}$. For n spins, this basis consists of $N = (2S + 1)^n$ states. Since the primitive magnetic unit cell contains four spins, the total number n of spins in the system should be a multiple of 4. To have the same number of neighbors regardless of the system size, we apply periodic boundary conditions. To find the ground state, i.e., the lowest-energy eigenstate of $\hat{\mathcal{H}}$, we use the Arnoldi method (as implemented in the ARPACK package [29]), which is a matrix-free iterative method that can compute the lowest eigenvalue and corresponding eigenvector with a run-time complexity of $\mathcal{O}(N^2)$. To investigate the spin-flop transition, we apply an external magnetic field $\mathbf{B} = (0, 0, B_z)$, determine the resulting ground-state vector $\psi_0(B_z)$ and calculate the expectation value of the normalized magnetization in z direction, which is given by

$$m_z(B_z) = \frac{1}{\hbar S n} \sum_{i=1}^n \psi_0^\dagger \hat{S}_i^z \psi_0. \quad (4)$$

Since at the spin-flop field m_z displays a step in the thermodynamic limit (cf. Fig. 1), we identify the spin-flop field in a finite-sized system with the position of the first such step in m_z . To keep the atomic magnetic moment consistent with the classical case, we set $\mu_q S = \mu_{cl}$ in the Zeeman term for each S value, where $\mu_{cl} = 4.2313\mu_B$ is the magnetic moment per iron atom from the *ab initio* calculations [6]. An example of the resulting magnetization curves, here for the quantum number $S = \frac{1}{2}$, is shown in Fig. 2 for magnetic fields from zero to above 3000 T, at which point the system becomes fully polarized.

Below the transition into this ferromagneticlike state, we see that the magnetization of the quantum-mechanical system consistently remains below the classical magnetization curve, suggesting that quantum fluctuations reduce the polarization in the spin-flop phase. This is consistent with the observation that the classical system reaches its saturation magnetization at a slightly smaller critical field than the quantum model (the difference is less than 2 T and therefore not visible in the figure).

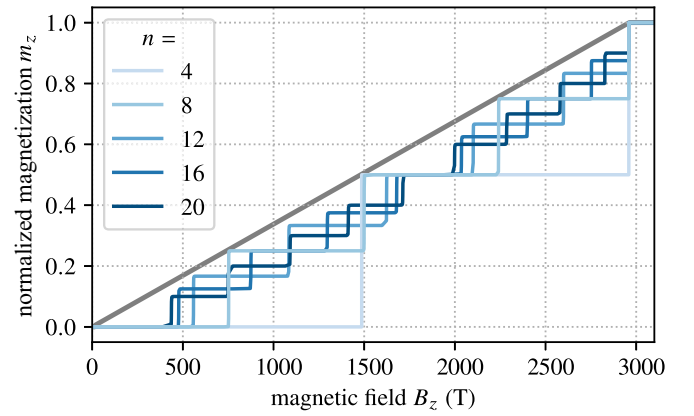


FIG. 2. Magnetization curve for a system of n spins with a quantum number $S = \frac{1}{2}$ computed with ED. The thicker gray line indicates the classical magnetization curve.

Since the terms in the Hamiltonian that do not conserve the total spin $S^z = \frac{1}{N} \sum_i S_i^z$ are small, m_z is almost a conserved quantity and it increases in steps. The position of the first step, identified with the spin-flop field, is very large in very small systems and slowly converges toward the bulk value for increasing system sizes, as illustrated in Fig. 2. Following Ref. [30], we expect this finite-size correction to be proportional to the inverse volume n^{-1} , which we use to extrapolate to the corresponding bulk value.

Since the computational effort of ED scales with $(2S + 1)^{2n}$, these calculations are limited to very small clusters, even with further optimizations. Due to the long-range interactions in hematite, the memory requirements are also significant, limiting our ED calculations to systems of eight spins for the relevant quantum numbers of $S = 2$ and $\frac{5}{2}$. The spin-flop fields obtained for these small systems are shown as black crosses in Fig. 3. While two data points would suffice for a

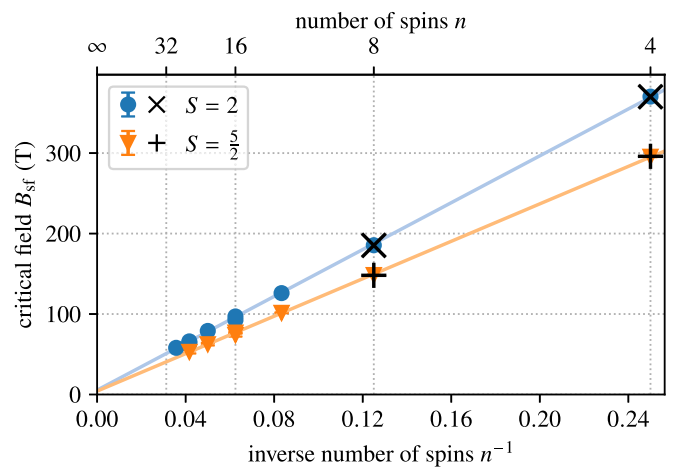


FIG. 3. Spin-flop field computed by ED and DMRG for clusters of different sizes n and quantum numbers S . The colored points are DMRG results and the black crosses mark the corresponding ED results for the two smallest clusters. Uncertainty ranges for the DMRG results were also calculated but are smaller than the symbol size. The two lines are linear fits to the chainlike clusters used to extrapolate the critical field in the bulk limit.

linear extrapolation, it does not allow us to quantify the statistical uncertainty of the extrapolated values. We therefore turn to DMRG theory to scale our calculations to larger clusters and obtain more data points.

The DMRG algorithm [31–35] is a variational technique, which relies on the assumption that the many-body wave function can be represented faithfully in a matrix-product-state form. The accuracy of the ansatz is controlled by the bond dimension (size of the matrices), which is gradually increased during the local DMRG updates. We used the single-site variant of the DMRG algorithm with subspace expansion [36]. The large sizes of the local Hilbert space for $S = 2$ and $S = \frac{5}{2}$ and the lack of spin symmetries of the Hamiltonian severely impact the achievable system sizes in DMRG. Accordingly, the largest bond dimension is restricted to $\chi = 2500$, since we have to work with full dense complex matrices. Nevertheless, this was sufficient to obtain converged results for clusters containing up to seven unit cells (28 spins). We then determined the spin-flop transition in the same fashion as for the ED.

The DMRG results are also shown in Fig. 3. Reassuringly, the ED and DMRG results agree almost perfectly. For some system sizes, differently shaped clusters with the same number of spins are possible to simulate using DMRG; for example, with six unit cells, we considered both the shapes $1 \times 1 \times 6$ and $1 \times 2 \times 3$. As can be seen in Fig. 3, the differences in the resulting spin-flop field between differently shaped clusters are relatively small (5% for $n = 16$ and 3% for $n = 24$). For the extrapolation to the bulk case, we limit ourselves to the linear (chainlike) clusters of shape $1 \times 1 \times n$. Linear extrapolation with these clusters results in the bulk spin-flop fields $B_{sf}(S = 2) = 5.4(7)$ T and $B_{sf}(S = \frac{5}{2}) = 4.2(5)$ T. The uncertainty ranges here are the standard deviation errors of the unweighted least-squares regression. However, as detailed in Appendix B: *Bulk spin-flop field extrapolation*, the values can vary slightly more (between 5 and 7.2 T for $S = 2$ and between 4.2 and 5.3 T for $S = \frac{5}{2}$) depending on the minimum cluster size included in the fit (see the lighter data points in Fig. 4). These extrapolated bulk spin-flop fields are all significantly reduced compared to the value of 14.5 T predicted by the classical model and in the same range or slightly lower than the low-temperature experimental value of approximately 7 T [6], suggesting that a quantum-mechanical treatment of the same spin model can indeed resolve the quantitative overestimation of the zero-temperature spin-flop field produced by semiclassical simulations.

To estimate the importance of the quantum fluctuations captured by DMRG, we compare the obtained spin-flop fields to semianalytical methods, which are closer to the classical description, namely, mean-field theory and linear spin-wave theory (further details in Appendix C: *Mean-field theory* and Appendix D: *Spin-wave theory*).

In a completely mean-field approach, the way we scaled the parameters leads to a constant spin-flop field independent of the quantum number (blue points in Fig. 4), coinciding with the classical case. However, a correct description of the Morin transition requires a slightly modified approach [6], where the on-site anisotropy terms are not included in the mean field. This allows for quantum fluctuations in the spin-flop phase, which lowers its energy and therefore reduces the spin-flop

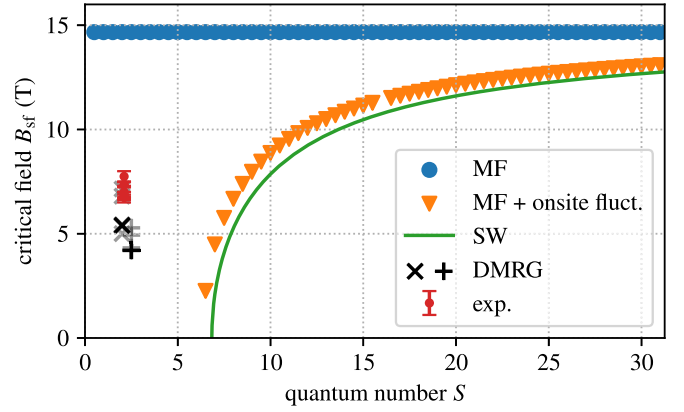


FIG. 4. Spin-flop field for different quantum numbers calculated from mean-field theory, both without and including on-site fluctuations, as well as spin-wave theory, compared to the values extrapolated from the DMRG calculations and to experimental observations [6]. The lighter DMRG data points show the extrapolation results for different cluster size cutoffs.

field significantly (orange points in Fig. 4). For $S \leq 6$, the spin-flop field vanishes, and the flop state becomes the field-free ground state.

Linear spin-wave theory is based on an expansion around the classical ground state of the system, but by performing the Bogoliubov transformation it also includes zero-point quantum fluctuations of magnons, which reduce the energy of the system. These fluctuations are correlated between the sites, unlike the mean-field approach extended by on-site fluctuations discussed above; therefore, spin-wave theory is expected to approximate the quantum-mechanical ground state better.

Considering the correlations described by the zero-point fluctuations results in a slight decrease of the spin-flop field (green line in Fig. 4), compared to the mean-field result including on-site fluctuations. Comparing the results for different quantum numbers, we find that zero-point quantum fluctuations stabilize the spin-flop phase over the antiferromagnetic state in linear spin-wave theory. This may be connected to the fact that the magnon spectrum in the spin-flop phase contains a Goldstone mode due to the rotational freedom of the state around the field direction, while the spectrum in the collinear antiferromagnetic state is gapped by the anisotropy terms (the very small triaxial in-plane anisotropy is neglected in the model). The magnon states closer to zero energy in the spin-flop phase contribute strongly to the ground-state quantum fluctuations, thereby decreasing the energy of this state relative to the collinear phase. As in mean-field theory, the spin-flop field vanishes for small spin quantum numbers. This underscores the need for more exact methods such as ED and DMRG, which can more accurately treat spin fluctuations, resulting in a reduced but finite spin-flop field for $S = 2$ and $\frac{5}{2}$.

To summarize, we have shown that the highly accurate description of quantum fluctuations provided by ED and DMRG calculations is required to quantitatively determine the spin-flop field of hematite at low temperature. A classical spin model with *ab initio* parameters can correctly describe the

spin-flop field and the Morin transition above $T = 160$ K, but it overestimates the spin-flop field at low temperatures compared to the measured value [6]. Transforming the parameters to a quantum model, we found that the spin-flop field vanishes at low temperature in mean-field theory and linear spin-wave theory, which only limitedly account for quantum fluctuations. In contrast, the DMRG calculations result in a finite spin-flop field by correctly describing the fluctuations that stabilize the collinear antiferromagnetic phase. Extrapolating the calculated spin-flop field to the thermodynamic limit results in a value that compares favorably to the measurements [6]. The validity of the DMRG results is supported by the fact that they are in perfect agreement with ED at the system sizes that are achievable with the latter.

Our results demonstrate that quantum fluctuations play an important role for the quantitatively correct description of phase transitions, not only in hematite, but most likely in other insulating magnets as well. This is observed in spite of the transition happening between two long-range-ordered phases and the not particularly small ($S = 2$ or $S = \frac{5}{2}$) spin magnetic moment of the ferrous ions in hematite, both of which are conventional arguments for supporting a semiclassical treatment of the spin model. This implies that it may be necessary to go beyond the semiclassical description when parametrizing spin models based on first-principles calculations for the quantitative interpretation of low-temperature measurements, particularly in insulating magnets with even smaller quantum numbers.

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Data availability. The data that support the findings of this article are openly available [37].

Appendix A: Scaling procedures. As discussed in the main text, a rescaling of the classical parameters according to Eq. (3) leaves the spin-wave frequencies and the magnetic moment invariant. Since a quantum model differs in many aspects from a classical one, the way that the model parameters should be scaled for different quantum numbers is a matter of choice,

and in the following we want to consider some alternative approaches.

Another common ansatz (cf., e.g., Ref. [38]) is to rescale spins with the corresponding spin length, $S \rightarrow S/\sqrt{S(S+1)}$, which means to scale the parameters as

$$\begin{aligned}\mathcal{J}_{ij}^q(S) &= \frac{\mathcal{J}_{ij}^c}{S(S+1)}, \\ d_2^q(S) &= \frac{d_2^c}{S(S+1)}, \\ d_4^q(S) &= \frac{d_4^c}{[S(S+1)]^2}.\end{aligned}\quad (\text{A1})$$

This leaves the mean-field Néel temperature [39]

$$k_B T_N = \frac{1}{3} J S(S+1), \quad (\text{A2})$$

with the Boltzmann constant k_B and the sum of the isotropic exchange constants J , invariant. This rescaling was used in Ref. [40] to study the deviations in the critical temperature from the mean-field critical temperature using a high-temperature expansion.

However, the critical temperature of three-dimensional magnets depends weakly on the anisotropy, which means that choosing a different rescaling for the anisotropy would not considerably modify the critical temperature. A different rescaling is also motivated by the fact that the on-site anisotropy becomes meaningless for $S = \frac{1}{2}$; for this reason, it was proposed in Ref. [25] to rescale the exchange terms by S^2 and the anisotropy by $S(S - \frac{1}{2})$. We also investigate the approach where we rescale the exchange interactions with $S(S+1)$ to retain the same critical temperature in mean-field theory, while keeping the scaling from Eq. (3) for the other parameters:

$$\mathcal{J}_{ij}^q(S) = \frac{\mathcal{J}_{ij}^c}{S(S+1)}, \quad d_2^q(S) = \frac{d_2^c}{S^2}, \quad d_4^q(S) = \frac{d_4^c}{S^4}. \quad (\text{A3})$$

This approach is similar to Ref. [25] in the sense that the anisotropy coefficients are rescaled by a smaller factor than the exchange term.

Appendix B: Bulk spin-flop field extrapolation. The values for the bulk spin-flop field that are given in the main text were extrapolated by fitting a linear function to the DMRG-calculated finite-size spin-flop fields for clusters of shape $1 \times 1 \times N$. Fitting to clusters of the shape $1 \times 2 \times N$ instead results in an extrapolated spin-flop field of 7 T for $S = 2$, which is closer to the experimental value but does not allow for statistical uncertainty quantification because we only have two data points available (and only one for $S = \frac{5}{2}$).

For the chainlike clusters, we have enough data points to estimate the statistical uncertainty from the linear regression. In Fig. 5, we plot the fit results for different minimum cluster sizes to see how much the choice of the cutoff point changes the result.

These extrapolation results are also shown as lighter gray data points in Fig. 4. Taking only large clusters into account should improve the fit because these points are closer to the bulk case, but fewer data points also reduce the quality of the fit due to the uncertainty of the individual data points. Taking the linear extrapolation with all data points but weighted by

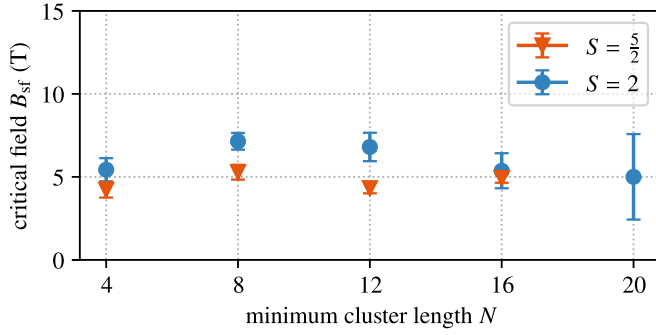


FIG. 5. Extrapolated bulk spin-flop fields for clusters of shape $1 \times 1 \times N$ when including only clusters of minimum size N .

cluster size leads to $B_{\text{sf}}(S = 2) = 6.2(5)$ T and $B_{\text{sf}}(S = \frac{5}{2}) = 4.6(3)$ T. With either weighting, it seems that the spin-flop field for $S = 2$ is larger than for $S = \frac{5}{2}$ (although that cannot be determined definitively) and both are significantly lower than the classical spin-flop field.

The magnetization curves from Fig. 2 can also be used to extrapolate a spin-flop field for $S = \frac{1}{2}$, resulting in 105(38) T, but this is not a very reliable extrapolation because the range of fields that were accessible with ED are very far from the bulk value (between roughly 400 and 1500 T).

Appendix C: Mean-field theory. Here, we discuss the two approaches to mean-field theory discussed in Fig. 4. Following Ref. [6], we replace the quantum version of Eq. (1) by the mean-field Hamiltonian

$$\hat{\mathcal{H}}_{\text{MF}} = \frac{1}{2} \sum_{i \neq j} \langle \hat{\mathbf{S}}_i^T \rangle \mathcal{J}_{ij} \langle \hat{\mathbf{S}}_j \rangle - \sum_i [d_2 S_{i,z}^2 + d_4 S_{i,z}^4 + \mu \mathbf{B}_{\text{MF}} \cdot \mathbf{S}_i], \quad (\text{C1})$$

with the mean field

$$\mathbf{B}_{\text{MF}} = \frac{1}{\mu} \sum_j \mathcal{J}_{ij} \langle \hat{\mathbf{S}}_j \rangle + \mathbf{B}. \quad (\text{C2})$$

Note that while this approach results in a single-site problem where the parameters $\langle \hat{\mathbf{S}}_i \rangle$ can be determined, the single-ion anisotropy terms are not included in the mean field. This has important implications for the low-temperature behavior. In the antiferromagnetic state, the mean field is pointing along the z direction, meaning that the spins being maximally polarized along the positive or negative z axis are eigenstates of the Hamiltonian including the anisotropy terms, meaning that quantum fluctuations are absent in this state. However, in the weak ferromagnetic or spin-flop state the mean field has an in-plane component, and the mean-field term does not commute with the anisotropy terms. This means that the lowest-energy state will typically not be a maximally polarized spin eigenstate that would have a classical analog; i.e., this approach takes on-site quantum fluctuations into account in the spin-flop phase.

In Fig. 6, we compare the behavior of the mean-field spin-flop transition as a function of the quantum number for different parameter scaling methods. We used the rescaling $\mu_q = \mu_{\text{cl}}/S$ in each approach to keep the atomic magnetic

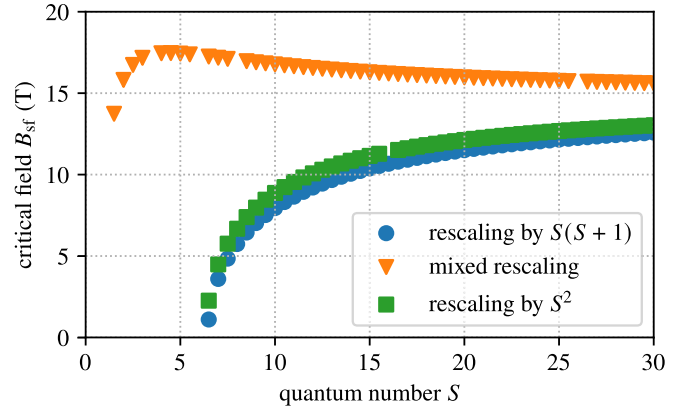


FIG. 6. Mean-field calculated spin-flop field as a function of the quantum number for different scaling methods: blue circles, Eq. (A1); orange triangles, Eq. (A3); green squares, Eq. (3).

moment constant regardless of the spin quantum number; this appears to be the most consistent choice for ensuring a finite magnetic moment as $S \rightarrow \infty$ in the classical limit.

For large quantum numbers S , the relative differences between all three scaling methods become arbitrarily small and approach the classical spin-flop field. For $S = \frac{1}{2}$, all three result in a spin-flop ground state, since the on-site anisotropy terms d_2 and d_4 stabilizing the antiferromagnetic state are not functional in this limit. In between, the critical field depends on the scaling method. When both the exchange and anisotropy parameters are scaled the same way [Eq. (3) or (A1)], we find a very similar behavior in both cases, with only slightly lower critical fields when the parameters are reduced more. With a mixed scaling according to Eq. (A3), we can keep the mean-field Néel temperature constant, while the critical spin-flop energy remains almost constant as well.

We use the latter scaling method to analyze the mean-field temperature dependence of the spin-flop field for $S = 2$.

Figure 7 shows the difference in free energy between the antiferromagnetic phase (blue) and the spin-flop phase (red) for both the classical and the $S = 2$ quantum case. The free energy is calculated according to the procedure described in Ref. [6]. White color indicates a vanishing free-energy difference, which shows the boundary between the two phases at low temperature, and the paramagnetic phase at high temperature, where the expectation values $\langle \hat{\mathbf{S}}_j \rangle$ are low. While the general shape of the phase boundary agrees very well with measurements in the quantum case and with atomistic spin dynamics simulations in the classical case, the actual values of the critical fields and temperatures are substantially different, with the exception of the classical spin-flop field at zero temperature, where the mean-field approximation becomes exact, and even an analytical solution can be derived.

Finally, we comment on the completely mean-field approach, where also the anisotropy terms in Eq. (C1) are incorporated in the mean field. In this case, the lowest-energy configuration will be a maximally polarized spin eigenstate at zero temperature in both the antiferromagnetic and the weak ferromagnetic phases, meaning that quantum fluctuations are

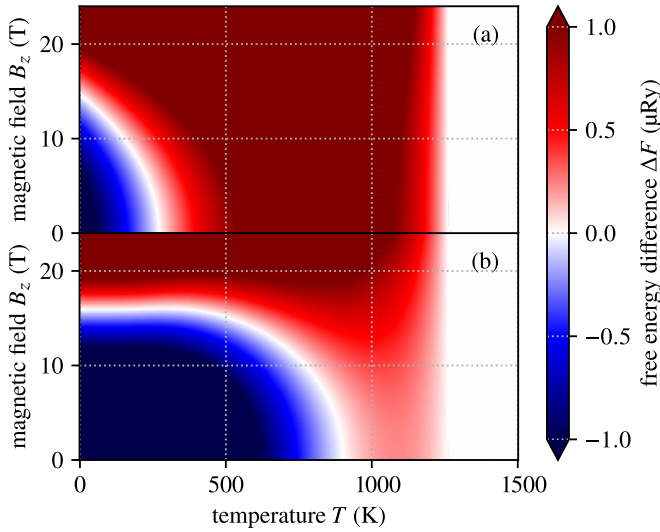


FIG. 7. Calculated free-energy difference between the collinear antiferromagnetic and the flop phases, $F_{\text{afm}} - F_{\text{flop}}$, in the (a) classical and (b) quantum ($S = 2$) mean-field model with parameters scaled according to Eq. (A3).

completely absent. This results in a spin-flop field equal to its classical value for all quantum numbers S when the rescaling in Eq. (3) is used. However, this does not lead to a qualitatively correct description at finite temperatures: The spin-flop field does not decrease linearly with the temperature in the classical case, and the Morin transition is usually absent. This implies that the fluctuations in the on-site anisotropy terms captured by Eq. (C1) are necessary for the qualitatively correct description of the temperature dependence mentioned above.

Appendix D: Spin-wave theory. To derive the spin-wave approximation, we rewrite the anisotropy terms in the spin Hamiltonian in Eq. (2) in tensorial form as

$$\hat{\mathcal{H}} = -\frac{1}{2} \sum_{i,j} \hat{\mathbf{S}}_i^T \mathcal{J}_{ij} \hat{\mathbf{S}}_j - \sum_i \hat{\mathbf{S}}_i^T \mathcal{K}_i \hat{\mathbf{S}}_i - \sum_{i,\alpha,\beta,\gamma,\delta} \mathcal{K}_{i,4}^{\alpha\beta\gamma\delta} S_i^\alpha S_i^\beta S_i^\gamma S_i^\delta - \mu \sum_i \mathbf{B}^T \hat{\mathbf{S}}_i. \quad (\text{D1})$$

First, we determine the classical ground state of the Hamiltonian by finding the unit vectors $\mathbf{S}_i^{(0)}$ satisfying

$$\mathbf{S}_i^{(0)} \times \frac{\partial \mathcal{H}}{\partial \mathbf{S}_i^{(0)}} = 0 \quad (\text{D2})$$

at each lattice site, where $\mathcal{H}$ is the classical Hamiltonian (1). An approximate quantum ground state may be obtained by determining the low-energy excitations around this classical ground state within linear spin-wave theory. For this, we introduce a right-handed orthonormal basis $\{\mathbf{e}_{i,1}, \mathbf{e}_{i,2}, \mathbf{e}_{i,3} = \mathbf{S}_i^{(0)}\}$ at each lattice site, express the components of the spin operators in this basis, $\hat{S}_{i,\alpha} = \hat{\mathbf{S}}_i \cdot \mathbf{e}_{i,\alpha}$, and apply the linearized Holstein-Primakoff transformation [41],

$$\begin{aligned} \hat{S}_{i,1} &= \sqrt{\frac{S}{2}} (\hat{a}_i + \hat{a}_i^\dagger), \\ \hat{S}_{i,2} &= -i\sqrt{\frac{S}{2}} (\hat{a}_i - \hat{a}_i^\dagger), \\ \hat{S}_{i,3} &= S - \hat{a}_i^\dagger \hat{a}_i, \end{aligned} \quad (\text{D3})$$

where S is the spin quantum number and $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$ are bosonic creation and annihilation operators. We define the rotation matrix $\mathbf{R}_i$ at site i as $\mathbf{R}_i \tilde{\mathbf{S}}_i^{(0)} = \mathbf{S}_i^{(0)}$, where $\tilde{\mathbf{S}}_i^{(0)}$ points along the z axis in the local coordinate system. We introduce the exchange tensor, single-site anisotropy tensor and magnetic field in the local coordinate system as

$$\begin{aligned} \tilde{\mathbf{B}}_i^T &= \mathbf{B}_i^T \mathbf{R}_i, \quad \tilde{\mathcal{J}}_{i,j} = \mathbf{R}_i^T \mathcal{J}_{i,j} \mathbf{R}_j, \quad \tilde{\mathcal{K}}_i = \mathbf{R}_i^T \mathcal{K}_i \mathbf{R}_i, \\ \tilde{\mathcal{K}}_{i,4}^{\alpha\beta\gamma\delta} &= \sum_{\alpha',\beta',\gamma',\delta'} \mathcal{K}_{i,4}^{\alpha'\beta'\gamma'\delta'} \mathbf{R}_i^{\alpha'\alpha} \mathbf{R}_i^{\beta'\beta} \mathbf{R}_i^{\gamma'\gamma} \mathbf{R}_i^{\delta'\delta}. \end{aligned} \quad (\text{D4})$$

The spin-wave Hamiltonian up to second-order terms in the creation and annihilation operators may be written as

$$\hat{\mathcal{H}} = E_0 + \hat{\mathcal{H}}_{\text{SW}}, \quad (\text{D5})$$

where

$$\begin{aligned} E_0 &= -\frac{1}{2} \sum_{i,j} \tilde{\mathcal{J}}_{ij}^{zz} S(S+1) - \sum_i \tilde{\mathcal{K}}_i^{zz} S(S+1) \\ &\quad - \sum_i \tilde{\mathcal{K}}_{i,4}^{zzzz} S^3(S+2) - \mu \sum_i \tilde{B}_i^z \left(S + \frac{1}{2}\right) \end{aligned} \quad (\text{D6})$$

and

$$\begin{aligned} \hat{\mathcal{H}}_{\text{SW}} &= \frac{1}{2} \sum_{i,j} [\hat{a}_i^\dagger \quad \hat{a}_i] \\ &\quad \times \begin{bmatrix} D_{0,i,j} + D_{\text{nr},i,j} & D_{\text{a},i,j} \\ D_{\text{a},j,i}^* & D_{0,i,j} - D_{\text{nr},i,j} \end{bmatrix} \begin{bmatrix} \hat{a}_j \\ \hat{a}_j^\dagger \end{bmatrix} \end{aligned} \quad (\text{D7})$$

is the harmonic spin-wave Hamiltonian containing the coefficients

$$D_{0,i,j} = -\frac{S}{2} \left[\tilde{\mathcal{J}}_{ij}^{xx} + \tilde{\mathcal{J}}_{ij}^{yy} + \delta_{ij} 2 \left(\tilde{\mathcal{K}}_i^{xx} + \tilde{\mathcal{K}}_i^{yy} + 6\tilde{\mathcal{K}}_{i,4}^{xxzz} S^2 + 6\tilde{\mathcal{K}}_{i,4}^{yyzz} S^2 - \sum_k \tilde{\mathcal{J}}_{ik}^{zz} - 2\tilde{\mathcal{K}}_i^{zz} - 4\tilde{\mathcal{K}}_{i,4}^{zzzz} S^2 - \mu \tilde{B}_i^z / S \right) \right], \quad (\text{D8})$$

$$D_{\text{nr},i,j} = -\frac{S}{2} [\tilde{\mathcal{J}}_{ij}^{yx} - \tilde{\mathcal{J}}_{ij}^{xy} + \delta_{ij} 2 (\tilde{\mathcal{K}}_i^{yx} - \tilde{\mathcal{K}}_i^{xy} + 6\tilde{\mathcal{K}}_{i,4}^{yxzz} S^2 - 6\tilde{\mathcal{K}}_{i,4}^{xyzz} S^2)], \quad (\text{D9})$$

$$\begin{aligned} D_{\text{a},i,j} &= -\frac{S}{2} [\tilde{\mathcal{J}}_{ij}^{xx} - \tilde{\mathcal{J}}_{ij}^{yy} + i(\tilde{\mathcal{J}}_{ij}^{yx} + \tilde{\mathcal{J}}_{ij}^{xy}) + \delta_{ij} 2 [\tilde{\mathcal{K}}_i^{xx} - \tilde{\mathcal{K}}_i^{yy} \\ &\quad + 6\tilde{\mathcal{K}}_{i,4}^{xxzz} S^2 - 6\tilde{\mathcal{K}}_{i,4}^{yyzz} S^2 + i(\tilde{\mathcal{K}}_i^{yx} + \tilde{\mathcal{K}}_i^{xy} + 6\tilde{\mathcal{K}}_{i,4}^{yxzz} S^2 + 6\tilde{\mathcal{K}}_{i,4}^{xyzz} S^2)]]. \end{aligned} \quad (\text{D10})$$

The energy in the uncorrelated state, defined as the vacuum of the bosonic operators $a_i|0\rangle = 0 \forall i$, is

$$\langle 0|\hat{\mathcal{H}}|0\rangle = E_0 + \frac{1}{2}\text{tr}(\mathbf{D}_0 - \mathbf{D}_{\text{nr}}). \quad (\text{D11})$$

Note that $\text{tr}\mathbf{D}_{\text{nr}} = 0$ since the nonreciprocal part of the matrix is antisymmetric. This coincides with the ground-state energy of the mean-field Hamiltonian (C1) in the collinear antiferromagnetic state. However, it differs from the mean-field energy in the weak ferromagnetic phase due to the noncommuting nature of the different terms in the Hamiltonian mentioned above.

A better approximation for the ground-state energy may be obtained in spin-wave theory from solving the equations of motion,

$$\partial_t \begin{bmatrix} \hat{a}_i \\ \hat{a}_i^\dagger \end{bmatrix} = -\frac{i}{\hbar} \sum_j \sigma^z \begin{bmatrix} D_{0,i,j} + D_{\text{nr},i,j} & D_{\text{a},i,j} \\ D_{\text{a},j,i}^* & D_{0,i,j} - D_{\text{nr},i,j} \end{bmatrix} \times \begin{bmatrix} \hat{a}_j \\ \hat{a}_j^\dagger \end{bmatrix}, \quad (\text{D12})$$

where $\sigma^z = \text{diag}(1, -1)$ is a Pauli matrix. This can be diagonalized via the Bogoliubov transformation,

$$\begin{bmatrix} \hat{\alpha}_q \\ \hat{\alpha}_q^\dagger \end{bmatrix} = \sum_j \begin{bmatrix} V_{qj} & W_{qj} \\ W_{qj}^* & V_{qj} \end{bmatrix} \begin{bmatrix} \hat{a}_j \\ \hat{a}_j^\dagger \end{bmatrix}, \quad (\text{D13})$$

resulting in $i\partial_t \hat{\alpha}_q = \omega_q \hat{\alpha}_q$. Substituting the Bogoliubov transformation back into the Hamiltonian leads to

$$\hat{\mathcal{H}} = E_0 + \frac{1}{2} \sum_q \hbar \omega_q (\hat{\alpha}_q^\dagger \hat{\alpha}_q + \hat{\alpha}_q \hat{\alpha}_q^\dagger). \quad (\text{D14})$$

The vacuum of the transformed operators, $\hat{\alpha}_q|0'\rangle = 0 \forall k$, is an eigenvector of the Hamiltonian, and it has the energy

$$\langle 0'|\hat{\mathcal{H}}|0'\rangle = E_0 + \frac{1}{2}\text{tr}\hbar\omega, \quad (\text{D15})$$

which is lower by $\frac{1}{2}[\text{tr}(\hbar\omega) - \text{tr}(\mathbf{D}_0 - \mathbf{D}_{\text{nr}})]$ than the uncorrelated energy calculated above. However, as shown in Fig. 4, even the zero-point fluctuations are insufficient for a quantitatively correct description of the spin-flop field for $S = 2$ or $S = \frac{5}{2}$.

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