Quantum criticality of dipolar spin chains

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We show that a chain of Heisenberg spins interacting with long-range dipolar forces in a magnetic field $h$ perpendicular to the chain exhibits a quantum critical point belonging to the two-dimensional Ising universality class. Within linear spin-wave theory the magnon dispersion for small momenta $k$ is $[\Delta^2 + \nu_k^2 k^2]^{1/2}$, where $\Delta^2 \propto |h - h_c|$ and $\nu_k^2 \propto |\ln k|$. For fields close to $h_c$ linear spin-wave theory breaks down and we investigate the system using density-matrix and functional renormalization group methods. The Ginzburg regime where non-Gaussian fluctuations are important is found to be rather narrow on the ordered side of the transition, and very broad on the disordered side.

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\section{I. INTRODUCTION}

The long-range nature and spatial anisotropy of the dipole-dipole interaction in quantum many-body systems can give rise to unconventional effects such as exotic ordered phases and excitation spectra. The experimental study of these phases is now possible due to substantial progress in controlling the parameters of trapped ultracold atoms. While both bosonic and fermionic dipolar quantum gases have been realized, it remains a challenge to design purely dipolar spin systems by localizing ultracold atoms or molecules with permanent magnetic or electric moments on an optical lattice. A promising strategy to obtain experimental realizations of dipolar magnets with localized spins uses trapped ions, which were recently employed to design spin Hamiltonians with tunable interactions between the spins.

Heisenberg magnets with dipole-dipole interactions in two and three dimensions have been investigated theoretically for more than half a century, but one-dimensional dipolar spin chains have not received much attention. This may be due the fact that in condensed matter systems the exchange interaction is usually much larger than the dipole-dipole interaction, so that it has not been possible to realize experimentally purely dipolar spin chains before the emergence of the field of ultracold atoms. Recently several authors pointed out that tunable spin chains with dipole-dipole interactions can be derived from two-component dipolar gases as effective models for the spin degrees of freedom. The investigations presented in this work are motivated by the expectation that in the near future it will be possible to design purely dipolar spin chains using trapped atoms or ions at ultra-low temperatures.

In a previous study of dipolar spin chains, the long-range dipole-dipole interaction was truncated at the next-nearest neighbor, which misses the logarithmic correction to the spin-wave velocity discussed below. Moreover, the spin-wave calculations of Ref. did not take into account the tilted geometry of the classical ground state in the low-field phase, thus missing the quantum critical point which separates the tilted phase from the high-field phase where all spins align with the magnetic field.

\section{II. CLASSICAL GROUND STATE AND SPIN-WAVE EXPANSION}

We consider a chain of quantum spins $S_i$ of spin $S$ in an external magnetic field $h$ perpendicular to the chain which are coupled by both dipolar and exchange interactions. Choosing our coordinate system such that the chain lies along the $x$-axis and the external magnetic field $h = h \hat{z}$ points in the $z$-direction, our Hamiltonian reads

\begin{equation}
\mathcal{H} = -\frac{1}{2} \sum_{ij, i \neq j} \frac{\mu^2}{|x_i - x_j|^3} [3S_i^x S_j^x - S_i \cdot S_j] - \frac{1}{2} \sum_{ij} J_{ij} S_i \cdot S_j - h \sum_{i} S_i^z, \tag{1}
\end{equation}

where sums are over the $N$ sites $x_i$ of a one-dimensional lattice with spacing $a$. The long-range dipolar interaction is characterized by an effective magnetic moment $\mu = g \mu_B \hat{\mu}$, where $g$ is the effective gyromagnetic factor and $\mu_B$ is the Bohr magneton. We assume that the spins are also coupled by nearest-neighbor ferromagnetic exchange interactions, i.e., $J_{ij} = J > 0$ if $|x_i - x_j| = a$ and $J_{ij} = 0$ otherwise. Due to the competition between the Zeeman energy, which favors alignment of the spins along the $z$-axis, and the dipolar interaction, which favors spin alignment along the $x$-axis, the spins align with a finite tilt angle $\vartheta$ relative to the field direction below a certain critical field $h_c$, as shown in Fig. The magnetization points then in the direction of the unit vector $\vec{m} = \sin \vartheta \hat{x} + \cos \vartheta \hat{z}$. The tilt angle $\vartheta$ in the classical ground state ($S \to \infty$) can be determined by replacing the spin operators $S_i$ in Eq. (1) by classical vectors $\vec{S}_i$ of length $S$, which yields the classical ground state energy per site

\begin{equation}
\mathcal{H}_0/N = -JS^2 - hS \cos \vartheta - D_0 S(3\sin^2 \vartheta - 1)/6, \tag{2}
\end{equation}
where $D_0$ is controlled by the dipole-dipole interaction,

$$D_0 = 3S \sum_{i,j \neq j} |x_i - x_j|^3 = 6\zeta(3)\frac{S\mu^2}{a^3}. \quad (3)$$

Minimizing $\mathcal{H}_0$ with respect to the tilt angle $\vartheta$ we find $\cos \vartheta = h/D_0$ for $h \leq D_0$, and $\vartheta = 0$ for $h > D_0$. In this work we show that at the critical magnetic field $h_c$ where the tilt angle $\vartheta$ vanishes the system undergoes a continuous quantum phase transition. Classically the critical field is $h_c = D_0$, but for small $S$ the value of $h_c$ is substantially smaller than $D_0$ due to quantum fluctuations. Since Hamiltonian (1) has no continuous spin symmetry, and the $Z_2$ symmetry $S^z \rightarrow -S^z$ is spontaneously broken in the tilted phase, we expect that the quantum phase transition belongs to the universality class of the two-dimensional Ising model.

To calculate the spin-wave spectrum, we expand the spin operators in the tilted basis $\{e_1, e_2, \hat{m}\}$ shown in Fig. 1. Introducing spherical basis vectors $e^p = e_1 + ip e_2$ with $p = \pm$, we write $S_i = S_i^{||} \hat{m} + S_i^\bot$ and $S_i^\bot = \frac{1}{2} \sum_{\nu = \pm} S_{-i}^\nu e^\nu$. We then express the spin components in terms of canonical boson operators $b_i$ using the Holstein-Primakoff transformation, $S_i^{||} = S - b_i^\dagger b_i$, $S_i^\bot = (S_i^\bot)^\dagger = [2S - b_i^\dagger b_i]^{1/2} b_i$. Retaining only quadratic terms in the bosons and Fourier transforming, $b_i = \frac{1}{\sqrt{2\pi}} \sum k e^{ikx} b_k$, our bosonized spin Hamiltonian is approximated by

$$\mathcal{H} \approx \mathcal{H}_0 + \sum_k \left[ A_k b_k^\dagger b_k + B_k \left( b_k^\dagger b_{-k} + b_{-k}^\dagger b_k \right) \right] \quad (4)$$

with

$$A_k = \left[ \frac{D_0}{3} + \frac{D_k}{6} \right] (3\sin^2 \vartheta - 1) + J_0 - J_k + h \cos \vartheta \quad (5)$$

and

$$B_k = -\frac{D_k}{2} \cos^2 \vartheta, \quad J_k = 2JS \cos(ka)$$

and

$$D_k = \frac{D_0}{\zeta(3)} \sum_{n=1}^{\infty} \frac{\cos(nka)}{n^3}. \quad (6)$$

The infinite series $\sum_{n=1}^{\infty} \frac{\cos(nka)}{n^3}$ represents the so-called Clausen function $\text{Cl}_3(ka) = \text{Re} \text{Li}_3(e^{ika})$, where $\text{Li}_3(z)$ is the polylogarithm. From the known series expansion of $\text{Li}_3(e^n)$ we obtain for $|ka| \ll 1$,

$$D_k/D_0 = 1 - \frac{3}{2} (ka)^2 \ln(d_2/|ka|) + \mathcal{O}((ka)^3). \quad (7)$$

where $d_1 = 1/[3\zeta(3)]$ and $d_2 = e^{3/2}$. Using a Bogoliubov transformation to diagonalize the Hamiltonian (1), we obtain the magnon dispersion $E_k = \sqrt{A_k^2 - |B_k|^2}$, which is shown graphically in Fig. 2. For simplicity we set $J = 0$ from now on. For $|ka| \ll 1$ and $|h - D_0| \ll D_0$ the magnon dispersion is then approximated by $E_k \approx \sqrt{\Delta^2 + v_k^2 k^2}$, where the square of the gap is $\Delta^2 = D_0(h-D_0)$ for $h > D_0$, and $\Delta^2 = 2D_0(D_0-h)$ for $h < D_0$. The squared velocity $v_k^2$ exhibits a logarithmic divergence for small wave vectors, $v_k^2 = v_0^2 \ln(1/|ka|) + c_0^2$, with $v_0^2 = (D_0a)^2d_1$ and $c_0^2 = \frac{3}{2} v_0^2$. The logarithmic divergence of $v_k$ is a unique signature of the $1/|x|^3$-decay of the dipolar interaction in one dimension. Indeed, logarithmic corrections to the dispersion are characteristic of one-dimensional systems with long-range interactions decaying as $1/|x|^\beta$ with odd $\beta$ (see Refs. [16] and [17] for the case of the Coulomb interaction, $\beta = 1$, and Ref. [18] for the case of an arbitrary $\beta$).

Despite the unusual logarithmic correction to the dispersion in Gaussian approximation, it seems at first glance that our spin-wave approach remains valid for all values of the magnetic field. This is not the case, however, because in a narrow range of magnetic fields close to $D_0$ the leading quantum correction to the magnetic moment $m$ per site completely overwhelms the classical result $m \approx S$. Retaining the leading $1/S$ quantum correction to $m$, we obtain

$$m = \frac{1}{N} \sum_i S^{||}_i = S + \frac{1}{2} - \frac{1}{N} \sum_k \frac{A_k}{2E_k}. \quad (8)$$

Because $E_{k=0}$ vanishes for $h \rightarrow D_0$ while $A_{k=0}$ remains finite for sufficiently small $|h-D_0|$, the last term in Eq. (8) becomes arbitrarily large, which is also evident from the numerical evaluation of Eq. (8) shown in Fig. 3 (a).

Obviously, for any $S < \infty$ there is a range of magnetic fields where the tilt angle is small and the leading quantum correction to the magnetization is larger than the classical result $m \approx S$. In this regime our simple spin-wave approach breaks down and we need more sophisticated methods to investigate the behavior of the system. We have studied the quantum critical regime $|h-h_c| \lesssim h_c$ using both the numerical density-matrix renormalization group (DMRG) and the analytical functional renormalization group (FRG) methods.

### III. DMRG APPROACH

Using the DMRG, we have calculated the ground state and its magnetization for systems of up to $N = 128$ sites and a varying bulk magnetic field $h$ in the $z$-direction. In the simulations, we kept up to 320 density-matrix eigenvalues, leading to a maximum discarded weight of $10^{-12}$. It should be noted that DMRG simulations of the dipolar spin chains are numerically demanding for several reasons. First, the long-range nature of the interaction leads to increased correlations between different parts of the system that have to be encoded in the
increase the efficiency of the DMRG, is not possible. Finally, for \( h < h_c \) the ground state is two-fold degenerate due to the \( Z_2 \) symmetry \( S_+^z \rightarrow -S_+^z \). Accordingly, it is crucial that we mix two states into the density matrix and target both states of the ground-state doublet. In the \( h/h_c \rightarrow 0 \) limit, the system is fully polarized in either the +\( x \)- or the −\( x \)-direction, but while the \( Z_2 \) symmetry is spontaneously broken in the infinite chain, the variational DMRG ground state, which always describes a finite system, is an arbitrary linear combination of two states with opposite polarization directions. Since the mixing angle is not fixed, the measured magnetization in the \( x \)-direction is random. We have found that we can obtain reliable results by adding a small local magnetic field \( h_x = 10^{-10}\mu^2/a^3 \) on the end sites. This field explicitly breaks the \( Z_2 \) symmetry and, consequently, leads to a unique ground state while generating an energy difference of the order \( 10^{-10}\mu^2/a^3 \) in the formerly degenerate doublet states.

In finite systems, the correlation length \( \xi \) is bounded by the system size \( L \). Therefore, phase transitions are strictly possible only in infinite systems; the inverse size \( 1/L \) plays the role of an additional parameter that moves the system away from the critical point. To determine the critical parameters in the thermodynamic limit, the dependence of thermodynamic quantities on the system size can be investigated with finite-size scaling theory. In this context, one uses the notion of a pseudo-critical field \( h_c(L) \) associated with indications of critical behavior in a finite system of size \( L \). Note that, for a given system, multiple definitions of \( h_c(L) \) that result in the correct value of \( h_c \) in the limit \( L \rightarrow \infty \) are possible. In general, one finds that the pseudo-critical field \( h_c(L) \) scales as \( L^{-1/\nu} \), where \( \nu \) is the correlation-length critical exponent and \( \xi \propto |h-h_c|^{-\nu} \). The order parameter scales as \( m(L) \propto L^{-\beta/\nu} \), with \( \beta \) the order-parameter critical exponent. For the two-dimensional Ising universality class, the relevant critical exponents have the values \( \nu = 1 \) and \( \beta = 1/8 \).

In Fig. 3(b) we show our numerical result for the total magnetic moment

\[
m = \sqrt{m_x^2 + m_y^2 + m_z^2}, \quad m_\alpha = \frac{1}{N} \sum_i (S_i^\alpha) \quad (9)
\]
the two-dimensional Ising model versus \(N\) magnetization \(h/D\). The inset shows the raw data as a function of \(m\) for different numbers of sites \(N\). We ascribe the imperfect collapse of the \(N=48\) data to the fact that the dipolar interaction is long-range so that sufficiently large systems have to be treated before the true critical behavior manifests itself.

IV. FRG APPROACH

To investigate our model for general \(S\) and to verify that the RG flow in the vicinity of the critical point indeed is consistent with the Ising universality class, we have studied the effect of spin-wave interactions using the functional renormalization group. Since we are interested in the critical fluctuations, we may simplify the calculations using the hermitian field parametrization of the spin-wave interactions in which we express the Holstein-Primakoff bosons \(b_k\) in terms of two canonically conjugate hermitian field operators, \(b_k = [\phi_k \sqrt{n_k} + i \Pi_k / \sqrt{n_k}] / \sqrt{2}\), where \(h_k = A_k + |B_k|\). Since the fluctuations of the canonical momentum \(\Pi_k\) remain gapped at the quantum critical point, we may integrate over the field \(\Pi_k\) in Gaussian approximation and obtain an effective Euclidean action \(S_{\text{eff}}[\phi]\) for the field \(\phi_k\) describing the critical fluctuations. The Gaussian propagator of the \(\phi\)-field is then \(G_0(K) = |\omega^2 + E_k^2|^{-1}\), where \(K = (k, \omega)\) denotes both momentum and frequency, and the effective action \(S_{\text{eff}}[\phi]\) of the critical fluctuations can be expanded as

\[
S_{\text{eff}}[\phi] = \frac{1}{2T} \sum_K G_0^{-1}(K) \phi_K \phi_K + \frac{1}{T} \sum_{n=0}^{\infty} \frac{1}{n! N^{1/2}} \times \sum_{K_1 \cdots K_n} \delta_{K_1 + \ldots + K_n, 0} \Gamma^{(n)}_0(k_1 \ldots k_n) \phi_{K_1} \cdots \phi_{K_n}, \tag{10}
\]

with \(T\) the temperature. The interaction vertices \(\Gamma^{(n)}_0(k_1 \ldots k_n)\) can be expressed in terms of the Fourier transform \(D_k\) of the dipole-dipole interaction by expanding the spin operators in powers of the Holstein-Primakoff bosons \(b_k\) and then setting \(b_k \rightarrow \phi_k \sqrt{n_k}/2\). For vanishing external momenta, the interaction vertices have finite limits \(\Gamma^{(n)}_0 \propto S^{-1/2}\), and in the symmetric phase \((h > h_c)\) the odd vertices vanish.

The magnon spectrum can be obtained from the poles of the true propagator \(G(K) = [G_0^{-1} + \Sigma(K)]^{-1}\), where \(\Sigma(K)\) is the irreducible self-energy of the effective field theory defined in Eq. (10). Since the higher order vertices involve increasing powers of \(1/S\) for large \(S\), one could calculate \(\Sigma(K)\) perturbatively. However, the corrections become arbitrarily large for \(h \rightarrow h_c\), which is not surprising because all higher order vertices of our \(1 + 1\)-dimensional field theory are relevant at the Gaussian fixed point, with canonical dimension +2. To regulate the infrared singularities, we replace the inverse Gaussian propagator by \(G_\lambda^{-1}(K) = G_0^{-1}(K) + R_A(k)\), using the regulator function \(R_A(k)\) proposed by Litim.

In the limit of vanishing flow parameter \(\Lambda\), the regulator vanishes, so that we recover our original model.

We use a simple truncation of the formally exact hierarchy of FRG flow equation for scalar field theories of the type (10) to re-sum the perturbation series, expand-
ing the flowing self-energy as

\[ \Sigma_A(K) = \Sigma_A(0) + Y_A k^2 + (Z_A^{-1} - 1) \omega^2 + \mathcal{O}(k^3, \omega^3), \]  

(11)

with flowing coupling constants \( \Sigma_A(0) \), \( Y_A \), and \( Z_A \). The scale-dependent long-wavelength magnon spectrum is then

\[ E_{\Delta A}^2 = \Delta A^2 + [v_A^2 \ln(1/|k|a)] + c_A^2 k^2, \]

(12)

where the renormalized squared gap is \( \Delta A^2 = Z_A[\Delta^2 + \Sigma_A(0)] \), and the renormalized magnon velocities are given by \( v_A^2 = Z_A v_0^2 \) and \( c_A^2 = Z_A[c_0^2 + Y_A] \). Note that in general the low energy expansion of the self-energy can also contain terms proportional to \( k^2 \ln(1/|k|a) \) and \( \omega^2 \ln(1/|k|a) \), which are of the same order as the terms retained in Eq. (11). However, we find that the flowing self-energy \( \Sigma_A(K) \) is analytic in \( K = 0 \) for any finite \( \Lambda \), due to the presence of the regulator function \( R_A(k) \), so that these terms do not appear in our FRG approach. Moreover, in our truncation we retain only the momentum and frequency-independent parts \( f_A^{(3)} \) and \( f_A^{(4)} \) of the three-point and four-point vertices. This truncation is then not sufficient to calculate the critical exponent \( \eta \) for the anomalous dimension, which is determined by the frequency-dependent part of the four-point vertex.

Analyzing the structure of the FRG flow equations in the vicinity of the quantum critical point, corresponding to a non-Gaussian fixed point of the flow equations, we find that the FRG confirms the Ising universality class expected from the general symmetry arguments and numerically derived within the DMRG analysis. For \( h = h_c \) the wave function renormalization factor \( Z_A \) and the rescaled three-point vertex \( \gamma_A^{(3)} \propto Z_A^{3/2} \Gamma_A^{(3)}/(\Lambda a)^2 \) flow to zero in the limit \( \Lambda \to 0 \), while the rescaled four-point vertex \( \gamma_A^{(4)} \propto Z_A^{2} \Gamma_A^{(4)}/(\Lambda a)^2 \) approaches a finite fixed-point value. In particular, the three-point vertex is marginally irrelevant at the fixed point, flowing asymptotically as \( \gamma_A^{(3)} \sim [\ln(\Lambda_0/\Lambda)]^{-1/2} \) in the limit \( \Lambda \to 0 \). (Here \( \Lambda_0 \sim 1/a \) is the initial RG scale, corresponding to an ultraviolet cutoff.) Importantly, we also find that the logarithmic correction to the spin-wave velocity becomes marginally irrelevant at the fixed point, namely \( v_A^2 \sim [\ln(\Lambda_0/\Lambda)]^{-r} \) for \( \Lambda \to 0 \), with \( r \approx 0.017 \), while \( c_A^2 \) remains finite. This signals that scale invariance is eventually restored at the critical point, strengthening the confidence in the finite-size scaling analysis of the DMRG results.

Besides investigating the behavior of the RG flow in the vicinity of the non-Gaussian fixed point, we may also use the FRG approach to estimate the critical field \( h_c^{(S)} \) for different values of the spin \( S \). For a given magnetic field \( h < h_c \), we fine-tune the tilt angle \( \vartheta(h) \) so that the linear vertex \( \Gamma_A^{(1)} \) vanishes for \( \Lambda \to 0 \) and fix the value of the critical field \( h_c \) where the magnetization \( m \) drops more steeply, corresponding to the limit \( \vartheta(h_c) \to 0 \). For \( S = 1/2 \) we obtain \( h_c^{(1/2)} \approx 0.72D_0 \), which is significantly smaller than the classical result \( h_c = D_0 \). However, the DMRG result \( h_c \approx 0.51D_0 \) is even smaller, showing that our FRG truncation probably still misses some sizable effects of quantum fluctuations. In Fig. 5 we plot our FRG results for higher values of the spin.

V. CONCLUSIONS

In this work, we have calculated the magnon spectrum and the magnetization curve of dipolar spin chains in a transverse magnetic field using spin-wave theory and renormalization group methods. We have shown that at a critical field \( h = h_c \) the system exhibits a quantum critical point belonging to the two-dimensional Ising universality class. Outside the critical regime, where the excitation spectrum is well described by linear spin-wave theory, the magnon velocity exhibits a logarithmic dependence on the wave vector, which might be useful to characterize dipolar interactions in experimental realizations of spin chains. Using the numerical density-matrix renormalization group method, we have presented quantitatively accurate results for the magnetization curve and the location of the critical point for the case of spin \( S = 1/2 \), finding a strong reduction in the value of \( h_c \) in comparison to the classical limit (\( S \to \infty \)). Finally, analyzing an effective low-energy field theory for our model by means of the functional renormalization group method, we have pointed out the emergence of a scale-invariant excitation spectrum in the vicinity of the critical point, where the logarithmic correction to the magnon velocity becomes an irrelevant perturbation, thus confirming the consistency of our numerical DMRG results with the expected universality class.

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