Self-Consistent Spin-Wave Analysis of the 1/3 Magnetization Plateau in the Kagome Antiferromagnet

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We propose a modified spin-wave theory to study the 1/3 magnetization plateau of the antiferromagnetic Heisenberg model on the Kagome lattice. By the self-consistent inclusion of quantum corrections, the 1/3 plateau is stabilized over a broad range of magnetic fields for all spin quantum numbers S. The values of the critical magnetic fields and the widths of the magnetization plateaus are fully consistent with the recent numerical results from exact diagonalization and infinite projected entangled paired states.

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The investigation of low-dimensional frustrated magnetism has become one of the most active frontiers in condensed matter physics. Current frontiers in the field include obtaining full insight into the entanglement structure of quantum many-body wavefunctions for different types of quantum spin liquid[1] and simplex-solid state.[2] Among many different frustrated systems, quantum antiferromagnets on the Kagome lattice may be the most intriguing, due to the fact that the combination of strong geometric frustration and weak constraints maximizes quantum fluctuation effects. The Kagome antiferromagnet has attracted ever-increasing attention over the last two decades, with many different methods applied and resulting in proposals for the nature of the ground state.[3-6] Realizations of the Kagome geometry have now been discovered for many materials, including volborthite (Cu$_3$V$_2$O$_7$(OH)$_2$2H$_2$O),[7] herbertsmithite (ZnCu$_3$(OH)$_6$Cl$_2$),[8] vesignieite (BaCu$_3$(OH)$_6$Cl$_2$),[9] BaNi$_3$(OH)$_2$(VO$_4$)$_2$,[10] KV$_3$Ge$_2$O$_9$,[11] and jarosites of several different metal ions including chromium (KCr$_3$(OH)$_6$(SO$_4$)$_2$).[12]

One of the characteristic features of Kagome antiferromagnets is the appearance of magnetization plateaus in the presence of an external magnetic field. Irrespective of the method applied and the prediction for the zero-field ground state, all theoretical approaches agree that there exists a robust magnetization plateau at $m = 1/3$ for all values of the spin quantum number S. The 1/3 plateau has been investigated theoretically by the real-space perturbation theory (RSPT),[14] exact diagonalization (ED),[15,16] density-matrix renormalization-group methods (DMRG),[17] and infinite projected entangled paired states (iPEPS).[18] The RSPT provides analytical results for the critical magnetic fields and the width of the plateau.[14] However, a qualitative discrepancy has arisen with recent numerical results from ED[15] and iPEPS,[18] not least in that the calculated plateau width increases with increasing S, whereas it decreases within RSPT.

To improve qualitative and quantitative understanding of the 1/3 magnetization plateau in the Kagome antiferromagnet, in this work we employ a self-consistent spin-wave theory to study its properties. The theory contains a single quantum correction parameter, determined self-consistently from the expectation values of the magnon densities. We compute these densities for all S, derive the spin-wave spectrum, and evaluate both the critical magnetic fields and the width of the 1/3 plateau, finding complete consistency with the recent numerical results.

We study the Hamiltonian

$$H = \sum_{\langle i,j \rangle} S_i \cdot S_j - h \sum_i S_i^z,$$

where $S_i$ is the spin-S operator on site i, $\langle i,j \rangle$ denotes the sum over neighboring sites, and J, the nearest-neighbor antiferromagnetic exchange coupling, is set as the energy scale ($J = 1$). Recent numerical studies of the Kagome and Husimi lattices by the method of projected entangled simplex states (PESS)[9] have demonstrated very explicitly[13] that the origin of

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the 1/3-plateau phase is the creation of a semiclassical up-up-down spin configuration on every triangle, as shown in Fig. 1. We stress that this statement holds for all values of $S$, even $S = 1/2$. As a consequence, it is entirely justified to employ a spin-wave description, which we implement by performing a Holstein–Primakoff transformation from spin operators to bosonic degrees of freedom,

$$
S_i^+ = \sqrt{2S - d_i^2} d_i, \quad S_i^z = S - d_i^2, \quad i \in \text{A, B, C},
$$

(2)

$$
S_i^+ = -d_i^1 \sqrt{2S - d_i^2} d_i, \quad S_i^z = d_i^1 d_i - S, \quad i \in \text{C}. \quad (3)
$$

Here we have assumed that spins on the A and B sublattices are oriented along $\hat{z}$, while those on the C sublattice are oriented along $-\hat{z}$. We restrict all of our considerations to zero temperature.

![Fig. 1. The up-up-down spin configuration of the 1/3 magnetization plateau on the kagome lattice. The two primitive lattice vectors are denoted as $a_1 = (1,0)a$ and $a_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)a$, where we set $a = 1$. The unit cell, denoted by the dashed blue lines, contains the three sites (A, B, C). Here $\delta_1$, $\delta_2$, and $\delta_3$ denote the nearest-neighbor lattice vectors.](image-url)

In a conventional linear spin-wave theory ($S \to \infty$), the 1/3 plateau is stable only at $h = 2S$. However, the effects of quantum fluctuations at finite $S$ may be included through the effective mean-field boson densities at each site, $n_i \equiv \langle d_i^\dagger d_i \rangle$, which are determined self-consistently and act to stabilize the magnetization plateau over a finite range of $h$. By introducing the approximation

$$
\sqrt{2S - d_i^2} \approx \sqrt{2S - \langle d_i^\dagger d_i \rangle} = \sqrt{2S - n_i}, \quad (4)
$$

the Hamiltonian (1) can be decoupled in the form

$$
\mathcal{H}_{\text{MF}} = \sum_k \alpha_k \langle \mathcal{H}(k) + \delta h \Lambda \rangle \alpha_k + \mathcal{C}, \quad (5)
$$

where

$$
\alpha_k \equiv (a_k, b_k, c_k^\dagger)^T, \quad a_k, \quad b_k, \quad \text{and} \quad c_k \quad \text{are} \quad \text{the} \quad \text{Fourier} \quad \text{transforms} \quad \text{of} \quad \text{the} \quad \text{operators}, \quad d_i, \quad \text{for} \quad \text{each} \quad \text{of} \quad \text{the} \quad \text{A,} \quad \text{B,} \quad \text{and} \quad \text{C} \quad \text{sublattices}, \quad \delta h = (h - 2S), \quad \Lambda = \text{diag}(1,1,-1), \quad \text{and} \quad \mathcal{C} \quad \text{is} \quad \text{a} \quad \text{constant}.
$$

Here $\mathcal{H}(k)$ specifies the quadratic Hamiltonian at $h = 2S$,

$$
\hat{\mathcal{H}}(k) = \begin{pmatrix}
2S & d_k & f_k \\
d_k & 2S & g_k \\
f_k & g_k & 2S
\end{pmatrix},
$$

where

$$
d_k = \sqrt{(2S - n_A)(2S - n_B)} \cos(k \cdot \delta_1),
$$

$$
f_k = -\sqrt{(2S - n_A)(2S - n_C)} \cos(k \cdot \delta_2),
$$

$$
g_k = -\sqrt{(2S - n_B)(2S - n_C)} \cos(k \cdot \delta_3), \quad (6)
$$

with the bond vectors $\delta_i$ as shown in Fig. 1.

In Eq. (6), $n_A$, $n_B$, and $n_C$ are respectively the expectation values of the magnon densities, $\langle d_i^\dagger d_i \rangle$, on each of the A, B, and C sublattices. From the Holstein–Primakoff transformation, the normalized longitudinal magnetizations on the three sublattices are $m_A = 1 - n_B/S$, $m_B = 1 - n_A/S$, and $m_C = n_B/S - 1$. In the 1/3-plateau phase, by definition $(m_A + m_B + m_C)/3 = 1/3$ and therefore $n_A + n_B = n_C$. Further, in the following we employ the reflection symmetry of the system about a vertical axis through the C sites (Fig. 1), which specifies that $n_A = n_B$ and $n_C = n_B$. Thus the self-consistent spin-wave theory for the 1/3-plateau phase contains only one parameter to be determined, which we denote as $x = n_A = n_B = n_C/2$.

The diagonalization of a general quadratic bosonic Hamiltonian is nontrivial. Here we summarize the procedure[19] to diagonalize the mean-field Hamiltonian (5). In the generalized Bogoliubov transformation

$$
\alpha_k = U_k \beta_k, \quad (7)
$$

the commutation relations of the new bosons, $\beta_k \equiv (\beta_{1,k}, \beta_{2,k}, \beta_{3,k})^T$, will be preserved if $U_k$ satisfies the condition

$$
U_k^\dagger \Lambda U_k = U_k \Lambda U_k^\dagger = \Lambda. \quad (8)
$$

Substituting Eq. (8) into Eq. (5) and making use of the condition (8), one will obtain

$$
\mathcal{H}_{\text{MF}} = \sum_k \beta_k^\dagger \mathcal{H}(k) \beta_k + \delta h \Lambda \beta_k + \mathcal{C}. \quad (9)
$$

To obtain a diagonal form, $U_k$ must satisfy the further condition

$$
U_k^\dagger \mathcal{H}(k) U_k = D_k = \text{diag}(\lambda_1(k), \lambda_2(k), \lambda_3(k)), \quad (10)
$$

where the eigenvalues $\{\lambda_i(k)\}$, which are the spin-wave dispersion relations at $h = 2S$, should be positive definite, i.e., $\lambda_i(k) > 0$. This requires that the matrix $\mathcal{H}(k)$ should also be positively definite[19] in which case there exists a matrix $K$ such that $\mathcal{H}(k) = K^\dagger K$ (Cholesky decomposition or eigen decomposition of $\mathcal{H}(k)$). The diagonalization of $\mathcal{H}(k)$ therefore maps to the diagonalization of $K^\dagger K$, meaning to the exercise of finding a further unitary matrix, $V$, such that $V^\dagger (K^\dagger K) V = L$, with $L$ being diagonal. The solutions satisfying the two conditions (8) and (10) simultaneously are then $D_k = \Lambda L$ and $U_k = K^{-1} V D_k^{1/2}$.
Here $U_k$ may be in fact obtained directly by diagonalizing the matrix $\mathcal{A}\mathcal{H}(k)$, i.e., from the equation $(\mathcal{A}\mathcal{H}(k))U_k = U_k(\mathcal{A}D_k)$.

It is important to note that, due to Eq. (8), the generalized Bogoliubov transformation matrix $U_k$ is independent of the magnetic field $h$. Thus the energies of the spin-wave excitations at fields away from $h = 2S$ are obtained simply by uniform shifts of the three magnon modes at $h = 2S$,

$$\omega_{1,2}(k) = \lambda_{1,2}(k) + \delta h, \quad \omega_3(k) = \lambda_3(k) - \delta h. \quad (11)$$

Thus the mean-field Hamiltonian (5) can be rewritten as

$$\mathcal{H}_{\text{MF}} = \sum_k \sum_{j=1}^3 \omega_j(k) \beta_j^\dagger(k) \beta_j(k) + C. \quad (12)$$

To show the spin-wave dispersion relations $\omega_j(k)$, it is necessary to solve for $x$. However, some preliminary remarks on the nature of the $1/3$-plateau phase are already in order. It is clear from Eq. (11) that modes $\omega_{1,2}(k)$ are pushed up by an increase of the magnetic field while the mode $\omega_3(k)$ is pushed down, and conversely when $h$ decreases. When the lowest mode touches energy zero, the plateau phase becomes unstable. Thus the lower transition point $h_{c1}$, out of the $1/3$-plateau phase is determined by the lower gap of two modes $\lambda_{1,2}(k)$, whereas the upper transition $h_{c2}$, is determined by the gap of $\lambda_3(k)$. Defining $\Delta_j = \min(\lambda_j(k))$ as the energy gaps of the three spin-wave branches at field $h = 2S$,

$$h_{c1} = 2S - \min(\Delta_1, \Delta_2), \quad h_{c2} = 2S + \Delta_3, \quad (13)$$

and the width of the plateau is given by

$$\Delta_w = h_{c2} - h_{c1} = \min(\Delta_1, \Delta_2) + \Delta_3. \quad (14)$$

To determine the magnon-density parameter $x$, we use a numerical iterative method to solve the equation

$$x = \frac{1}{N} \sum_k |U_k(1,3)|^2, \quad (15)$$

where $U_k$ is the Bogoliubov transformation matrix of Eq. (7), which depends in turn on $x$. Due to the fact that $U_k$ does not depend on the magnetic field, $x$ is also independent of $h$ in the $1/3$-plateau phase, although it does depend on $S$. As the above noted, we need therefore solve Eq. (15) only at $h = 2S$ to obtain the spin-wave spectra, $\{\omega_j(k)\}$, and hence the critical fields $h_{c1}$ and $h_{c2}$ in Eq. (13).

The spin-wave spectra for the $S = 1/2$ case at field $h = 2S$ are shown in Fig. 2. The minima of the two lower modes, $j = 1$ and $3$, are both located at the $\Gamma$ point ($k = 0$). There are two trivial level-crossings between these modes, occurring at the points marked $P_1$ and $P_2$ in Fig. 2 while actually forming a circle in the Brillouin zone, which changes size with $\delta h$. However, the crossing between modes $j = 1$ and $2$, which have the same $\delta h$-dependence, occurs at a single point, $P_3$, along the line $\Gamma - X$. This nontrivial exact crossing is a consequence of the reflection symmetry through the $\gamma$-axis and leads to a Dirac-type spectrum between the eigenmodes $j = 1$ and $2$. In more detail, the magnon spectra along $\Gamma - X$ can be found analytically by diagonalizing the matrix $\mathcal{A}\mathcal{H}(k = (k_x, 0))$ to obtain

$$\lambda_1(k_x) = \left\{ \begin{array}{l} 2S - (2S - x) \cos(k_x/2), \quad k_x \leq k_c, \\ \frac{1}{2} \sqrt{k_x + (2S - x) \cos(k_x/2)}, \quad k_x > k_c, \end{array} \right. \quad (16)$$

$$\lambda_2(k_x) = \left\{ \begin{array}{l} \frac{1}{2} \sqrt{k_x + (2S - x) \cos(k_x/2)}, \quad k_x \leq k_c, \\ 2S - (2S - x) \cos(k_x/2), \quad k_x > k_c, \end{array} \right. \quad (17)$$

where $\gamma_k = [(2S - x) \cos(k_x/2) + 4x^2]^{1/2} + 24x(S - x)$. The crossing point is therefore located at momentum $k_x = k_c = 2 \cos^{-1} \left( \frac{3 + x/2 - \sqrt{1 + 18(x/2)^2 - 3(x/2)^4}}{4 - 2(x/2)^2} \right)$. In the classical limit, $S \to \infty$, the position of crossing is $k_c = 2\pi/3$. The gaps of modes 1 and 3 are

$$\Delta_1 = x, \quad \Delta_3 = \frac{x}{2} - S + \sqrt{S^2 + 9Sx - \frac{15}{4} x^2}, \quad (18)$$

and hence the normalized critical magnetic fields and the width of the $1/3$ plateau are

$$\frac{h_{c1}}{S} = 2 - \frac{x}{S}, \quad (19)$$

$$\frac{h_{c2}}{S} = 2 - (1 - \frac{x}{2S}) + \sqrt{1 + 9 \left( \frac{x}{S} \right)^2 - \frac{15}{4} \left( \frac{x}{S} \right)^2}, \quad (20)$$

$$\frac{\Delta_w}{S} = \frac{3}{2} \left( \frac{x}{S} \right) - 1 + \sqrt{1 + 9 \left( \frac{x}{S} \right)^2 - \frac{15}{4} \left( \frac{x}{S} \right)^2}. \quad (21)$$
Concerning the form of the magnon-density function \( x(S) \) in Fig. 3 we show the quantity \( x/S \) determined numerically by solving the self-consistent equation (15). It is clear that \( x/S \) grows sub-linearly from zero, and similarly that \( m_A = m_B = 1 - x/S \) (inset of Fig. 3) falls monotonically from full polarization in the classical limit. We propose the power-law form

\[
m_A = m_B = \frac{1}{1 + \mu (1/S)^n}, \tag{21}
\]

for the sublattice magnetization and thus

\[
x/S = \frac{\mu (1/S)^n}{1 + \mu (1/S)^n} = \frac{1}{1 + \mu^{-1} S^n}, \tag{22}
\]

for the magnon density. We find that this two-parameter fit, with prefactor \( \mu = 0.206(1) \) and exponent \( n = 0.690(1) \), offers an excellent account of the data over the entire range of \( S \), i.e., not only where \( 1/S \) is small while even when \( S = 1/2 \) (last point). We comment that significantly better statistics still can be obtained by generalizing this type of power-law fit to two exponents.

Returning to Eqs. (18)–(20), the nonzero boson-density expectation values on all sites \( n_A = n_B = n_C/2 = x \) lead to finite energy gaps (Eq. (17)), which stabilize the 1/3 plateau over a broad range of magnetic fields, as shown in Fig. 4 for all values of \( S \). In the self-consistent spin-wave treatment, all of these quantities increase with the spin quantum number \( S \), although their normalized values decrease towards the expected limits (Figs. 3 and 4). This type of behavior is completely consistent with the numerical results obtained from ED\(^{[13]}\) and iPEPS\(^{[18]}\), which are shown for comparison in Fig. 4. The 1/3 dependence of both critical fields \( h_{c1} \) and \( h_{c2} \), and of the plateau width \( \Delta_w \), predicted by the self-consistent spin-wave theory have the correct qualitative trends, and in fact close quantitative agreement with the numerical calculations. It is striking that our analytical results are accurate at a semi-quantitative level even for the extreme quantum case \( S = 1/2 \). These results demonstrate that the self-consistent spin-wave theory captures properly the nature of the 1/3 magnetization plateau in the kagome antiferromagnet.

By contrast, in the RSPT approach\(^{[14]}\) one performs an expansion in powers of \( 1/S \) to obtain the plateau properties in the form

\[
h_{c1} = 2 - \frac{1}{8S} - \frac{1}{4S^2}, \tag{23}
\]

\[
h_{c2} = 2 + \frac{3}{8S} + \frac{1}{4S^2}, \tag{24}
\]

\[
\Delta_w = \frac{1}{2S} + \frac{1}{2S^2}, \tag{25}
\]

to order \((1/S)^2\). However, not only is this form fated to diverge in the most quantum systems, as \( 1/S \to 1 \), but there is also a qualitative discrepancy with our analytical results and with the recent numerical results: the RSPT predictions for \( h_{c1} \) and \( h_{c2} \) are concave up as a function of \( 1/S \) where they should be concave down, and conversely, while the non-normalized
plateau width trends in the wrong direction. Thus only in the extreme classical limit do the considerations of RSPT appear to be valid.

In summary, we have investigated the 1/3 magnetization plateau of the kagome antiferromagnet using a straightforward modified spin-wave theory, which contains only one self-consistent parameter. We have shown that the quantum corrections contained in this magnon-density parameter open finite energy gaps, which stabilize the 1/3-plateau phase over a broad range of magnetic fields. The qualitative and quantitative behavior of the critical fields and plateau widths is in excellent agreement with the recent numerical results for the same quantities obtained by exact diagonalization[15] and by tensor-network methods.[18] These results indicate that the self-consistent spin-wave theory provides an accurate description of the properties of the magnetization plateau in the kagome antiferromagnet. We suggest that the same type of theory should also be applied to describe the properties of magnetization plateaus in a number of other frustrated systems, including the extended square and honeycomb geometries as well as the triangular,[26] checkerboard, Shastry–Sutherland, and Husimi antiferromagnets.[13]

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