Chern-Simons theory for magnetization plateaus of the frustrated J_1-J_2 Heisenberg model

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The magnetization curve of the two-dimensional spin-1/2 J_1-J_2 Heisenberg model is investigated by using the Chern-Simons theory under mean-field approximations. We find that the magnetization curve increases monotonically for $J_2/J_1<0.267949$, where the system under zero external field is in the antiferromagnetic Néel phase. For larger ratios of J_2/J_1, various plateaus will appear in the magnetization curve. In particular, in the disordered phase, our results support the existence of the $M/M_{\rm sat}=1/2$ plateau, and predict a plateau at $M/M_{\rm sat}=1/3$. Verification of these interesting results would indicate a strong connection between the frustrated antiferromagnetic system and the quantum Hall system.

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I. INTRODUCTION

Due to quantum and frustration effects, rich physics can appear in frustrated quantum spin systems at zero external field.[1] Exciting behavior was also observed recently in several cases with an external magnetic field. For instance, a recently discovered two-dimensional (2D) $S=1/2$ spin-gap material $SrCu_2(BO_3)_2$, which can be described by the Shastry-Sutherland model,[2] exhibits several plateaus at $M/M_{\rm sat}=1/3$, 1/4, and 1/8 in its magnetization curve, where M ($M_{\rm sat}=1/2$) is the (saturating) magnetization per site.[3] The origin of these plateaus and the nature of the corresponding spin states are under intense debate.[4–7] Recently, by mapping onto spinless fermions carrying one quantum of statistical flux and under mean-field approximations, Misguich *et al.* showed that the original spin model can be related to a generalized Hofstadter problem, where the spin excitation gaps that produce the observed magnetization plateaus arise from some of the Landau level gaps in the integer quantum Hall effect for the fermions on a lattice.[8] For realistic values of the exchange constants, they obtained an excellent quantitative fit to the observed magnetization curve, which demonstrates the success of their approach.

Another prototype of a realistic frustrated two-dimensional system, which was recently realized experimentally in Li_2VOSiO_4 and Li_2VOGeO_4 compounds,[9] is the so-called J_1-J_2 Heisenberg model with the Hamiltonian

$$H=\sum_{\langle i,j\rangle} J_{ij}\vec{S}_i\cdot\vec{S}_j-B\sum_i S_i^z, \qquad (1)$$

where the exchange coupling J_{ij} is equal to J_1 when i and j are nearest neighbors on the square lattice; J_{ij} is equal to J_2 when i and j are connected by a diagonal bond. The external magnetic field B is applied along the z axis. Both couplings are antiferromagnetic, i.e., $J_{1,2}>0$, and the spins $S_i=1/2$. This model has been the object of intense investigation through years.[10–22] At $B=0$, for small J_2/J_1 where the frustration is weak, the system exhibits a Néel ordering described by a wave vector (π,π). When J_2/J_1 is large enough, the ground state is dominated by interactions along the diagonal bonds and has a collinear order described by $(\pi,0)$ or $(0,\pi)$. There is also a general consensus on the disappearance of the magnetic ordering at $0.38<J_2/J_1<0.6$, while the identification of the ground state is still a subject of much controversy.[10–16]

Just like the case of the Shastry-Sutherland model, the plateaus in the magnetization curve are predicted for the J_1-J_2 model,[17–22] while the situation is even more controversial. Strong evidence of a plateau at $M/M_{\rm sat}=1/2$ in the region $0.5\lesssim J_2/J_1\lesssim 0.65$ was recently reported by Honecker and co-workers.[20,21] However, Fledderjohann and Mütter[22] did not find a plateau at $M/M_{\rm sat}=1/2$ in the region of the quantum disorder phase; instead they found some indications of a plateaulike structure at $M/M_{\rm sat}=2/3$. Most previous studies on the plateau were obtained by numerical calculations on small clusters (the typical number of lattice sites in these works is about $6\times6=36$). As discussed in Ref. 22, the plateau structures in the magnetization curve can depend sensitively on the system size. Therefore, these results may be plagued by finite-size effects. For example, some of the predicted plateaus may be an artifact of the special lattice geometry, and the boundary conditions used may frustrate the order which tends to develop. Thus a precise determination of the positions and widths of the plateaus in the frustrated Heisenberg model is indeed a very delicate problem, and a better theoretical understanding of the magnetic order and of the mechanisms which create the plateaus is needed.

To avoid the possible finite-size effects, we apply the Chern-Simons (CS) theory for the magnetization plateaus[8] to the 2D spin-1/2 J_1-J_2 Heisenberg model. Because of its success for the Shastry-Sutherland model, this approach may give reasonable results in the present case. We find that the magnetization curve is monotonically increasing for $J_2/J_1<0.267949$, where the system at zero external field is in the antiferromagnetic Néel phase. In addition, various plateaus will appear in the the magnetization curve for larger ratios of J_2/J_1. In particular, in the disordered phase, our results support the existence of the $M/M_{\rm sat}=1/2$ plateau and predict a plateau at $M/M_{\rm sat}=1/3$.

This paper is organized as follows: In Sec. II we introduce the mean-field approach of Chern-Simons theory. In Sec. III we present our results on the magnetization curves. Section IV is a brief summary.

II. MEAN-FIELD APPROACH OF CHERN-SIMONS THEORY

The Hamiltonian in Eq. (1) can be rewritten as

$$H=H_{xy}+H_z-B\sum_i S_i^z,$$

$$H_{xy}=\frac{1}{2}\sum_{\langle i,j\rangle} J_{ij}(S_i^+S_j^-+S_j^+S_i^-), \tag{2}$$

$$H_z=\sum_{\langle i,j\rangle} J_{ij}S_i^zS_j^z,$$

where H_{xy} and H_z are the spin-flip and Ising parts of the Hamiltonian at zero field. According to Ref. 8, the mean-field Hamiltonian can be reached in the following two-step way. First, the Ising part is approximated by a simple mean-field decoupling,

$$H_z\simeq 2\sum_{\langle i,j\rangle} J_{ij}\, S_i^z\langle S_j^z\rangle-\sum_{\langle i,j\rangle} J_{ij}\langle S_i^z\rangle\langle S_j^z\rangle. \tag{3}$$

Let $\langle S_i^z\rangle=M+\delta M_i$, where M (δM_i) is the uniform (nonuniform) part of the local magnetization and $\Sigma_i\delta M_i=0$. In the subspace where $\Sigma_i S_i^z=MN_s$, with N_s being the number of lattice sites, H_z can be expressed as

$$H_z=\sum_i V_iS_i^z+2(J_1+J_2)M^2N_s-\frac{1}{2}\sum_i\sum_j J_{ij}\delta M_i\delta M_j, \tag{4}$$

where $V_i\equiv\Sigma_j J_{ij}\delta M_j$ serves as a local magnetic field. Second, one can exactly map the spin operators to spinless fermions with an attached flux tube carrying one flux quantum of statistical CS magnetic field,[23–25] where $S_i^z+1/2$ corresponds to the occupation number n_i of site *i*. Therefore, V_i now represents a local electric potential for fermions. Usually, one makes a further approximation such that the flux tube is detached from the fermion on site *i* and is smeared over a nearby plaquette (say the upper right one). Hence the local flux ϕ_i threaded through the *i*th plaquette is then tied to the local density $\langle n_i\rangle$ of fermions and thus to $\langle S_i^z\rangle$:

$$\frac{\phi_i}{2\pi}=\langle n_i\rangle=\langle S_i^z\rangle+\frac{1}{2}. \tag{5}$$

The local statistical flux will give phase factors in the hopping amplitudes of the equivalent system of fermions. Because of this flux, each energy band can split into subbands with a complicated structure. Unlike the conventional spin-wave theory, in this approximation the hard-core constraint is taken into account exactly, although the statistical transmutation from bosonic operators to fermionic ones is treated approximately.

For convenience, we separate ϕ_i and $\langle n_i\rangle$ into uniform and nonuniform parts: $\phi_i\equiv\phi+\delta\phi_i$ and $\langle n_i\rangle\equiv n+\delta n_i$ with $\phi/2\pi=n=M+1/2$ and $\delta\phi_i/2\pi=\delta n_i=\delta M_i$. Therefore,

$$\begin{aligned}H_{xy}+H_z\simeq{}&\frac{1}{2}\sum_{\langle i,j\rangle} J_{ij}[f_i^+\exp(i\theta_{ij})f_j+\text{H.c.}]\\&+\sum_i V_i\left(f_i^+f_i-\frac{1}{2}\right)+2(J_1+J_2)M^2N_s\\&-\frac{1}{2}\sum_i\sum_j J_{ij}\delta M_i\delta M_j,\end{aligned} \tag{6}$$

where $f_i^\dagger$ (f_i) is the fermion creation (annihilation) operator at site *i*, and θ_{ij} is the phase factor defined on the link $\langle i,j\rangle$ with $\Sigma_{\text{plaquette}}\theta_{ij}=\phi_i$. Hence for a uniform mean field with $\delta M_i=0$ and therefore $V_i=0$, the present spin system can be identified as a Hofstadter problem[26] for fermions hopping on a square lattice with nearest-neighbor and next-nearest-neighbor hoppings.[27,28] For δM_i periodic, a modulated magnetic field and a modulated electric potential with the *same* period appear.[25]

III. RESULTS AND DISCUSSION

A. Uniform mean-field calculation

In this subsection, we assume the uniform case. For a given M [or $\phi=2\pi(M+1/2)$], the mean-field ground state is obtained by filling the lowest energy subbands with fermions until their density satisfies $n=\phi/2\pi$. The one-body problem from H_{xy} can be straightforwardly analyzed for rational values of $\phi/2\pi$. For $\phi/2\pi=p/q$ (p and q are mutually prime integers), there are q subbands, and the ground state is the Slater determinant with the lowest p subbands completely filled. The energy of the filled subbands leads to another contribution to the total energy. Hence the total energy per site $E(M)$ as a function of the magnetization becomes

$$E(M)=\frac{1}{N_s}\sum_{\alpha=1,\ldots,p}\sum_{\vec k}\epsilon_{\vec k}^{(\alpha)}+2(J_1+J_2)M^2. \tag{7}$$

Here $\epsilon_{\vec k}^{(\alpha)}$ is the eigenenergy of the αth subband, with the wave vector $\vec k$ being restricted to the first magnetic Brillouin zone. The magnetization can be obtained as a function of *B* by minimizing $E(M)-BM$. It is clear from Eq. (7) that, without the contribution from H_{xy}, the magnetization M will be linearly proportional to *B*, and there is no magnetization plateau. Therefore, the appearance of magnetization plateaus is related to certain features of the Hofstadter spectrum.

The Hofstadter diagrams for $J_2/J_1=0.2$ and 0.3 are shown in Fig. 1, where the lower bold line marks the Fermi level (highest occupied state) and the upper one marks the lowest unoccupied level.[29] A jump of the Fermi energy as a function of M in Fig. 1(b) leads to a discontinuity of the slope of the function $E(M)$. These jumps for various M give rise to plateaus in the magnetization curve. They are closely related to the occurrence of band-crossing when the value of J_2/J_1 is varied. For example, in Fig. 1(a) before the upper

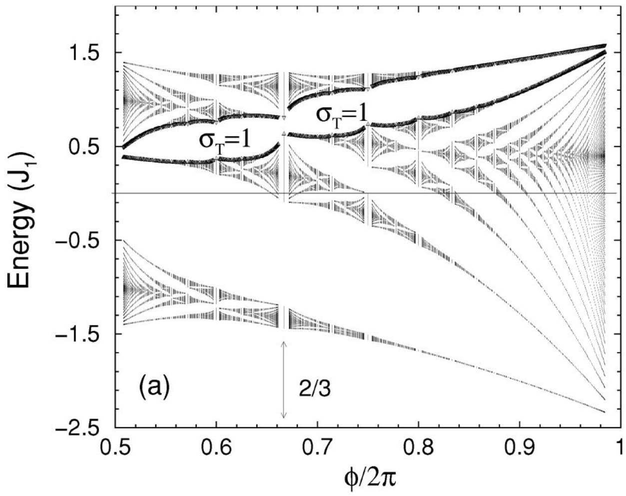

FIG. 1. Hofstadter spectra for a square lattice with nearest-neighbor and next-nearest-neighbor hoppings for $J_2/J_1=0.2$ (a) and 0.3 (b). Vertical lines mark the energy bands as a function of the statistical flux $\phi/2\pi$ per square plaquette. Total Hall conductances σ_T above the Fermi level from $M/M_{\rm sat}=0$ ($\phi/2\pi=1/2$) to $M/M_{\rm sat}=1$ ($\phi/2\pi=1$) are indicated. The Hall conductance at $\phi/2\pi=2/3$ changes from 1 to -2 when the upper two subbands touch at $J_2/J_1=0.267949$ (Refs. 27 and 28).

two subbands at $\phi/2\pi=2/3$ touch at $J_2/J_1=0.267949$,[27,28] the Fermi energy is continuous and there is no magnetization plateau at $M/M_{\rm sat}=1/3$ (see Fig. 2). However, in Fig. 1(b), the "pockets" enclosed by the bold lines are separated at $\phi/2\pi=2/3$. It can be seen that the Fermi level to the right of the contact point is below (above) the band gap before (after) the band crossing. As discussed earlier, the Fermi level marks the position of the pth subband. Therefore, apparently a subband associated with a flux slightly larger than 2/3 is shifted above the energy gap after the band crossing. This shift of a fine subband due to the crossing of the broader subbands at $\phi/2\pi=2/3$ was studied earlier.[28] It is closely related to the jump of the integer-valued Hall conductances of the broader subbands.[28,30] The emergence of the magnetization plateaus for the spin system thus has an interesting connection with the change of the integer-valued Hall conductances induced by band crossing.

To justify the present approach, it is important to check whether the plateau states are robust against fluctuations around the mean-field solutions. It was showed that the Gaussian fluctuations of the CS gauge field are massless only when the Thouless-Kohmoto-Nightingale–den Nijs (TKNN) integer[31] describing the quantized Hall coefficient of the fermions on the frustrated lattice becomes *unity*.[24] In this case, the Gaussian fluctuations induce instabilities for the mean-field ground states. We have computed the TKNN integers numerically (for example, see Fig. 1) and found the Gaussian fluctuations to be massive. Therefore, the plateaus are not destroyed by quantum fluctuations.

Magnetization curves for various J_2/J_1 ratios are shown in Fig. 2. We note that the saturation field $B_{\rm sat}$ can be computed exactly by identifying the energy E_f of the fully polarized state with the (exact) minimum energy $E_{1s}^{\rm min}$ of the states with one spin flipped, $E_f=E_{1s}^{\rm min}$. Thus $B_{\rm sat}/J_1=4$ for $J_2/J_1<1/2$; $B_{\rm sat}/J_1=2+4J_2/J_1$ for $J_2/J_1>1/2$. Our findings agree with these exact results near the saturation.

In the Néel phase, it is expected that the spins cant gradually from the antiparallel configuration toward the parallel configuration until the magnetization saturates at the saturation field $B_{\rm sat}$. The magnetization curve obtained from the present approach is consistent with this expectation: it is featureless all the way to full saturation when J_2/J_1 is small (see the curves for $J_2/J_1=0$ and 0.2 in Fig. 2). Upon increasing J_2/J_1, plateaus emerge and the magnetization curves become more complex. In particular, because of the band crossing at $\phi/2\pi=2/3$ when $J_2/J_1=0.267949$ (see Table I of Ref. 28), a plateau at $M/M_{\rm sat}=1/3$ is found. This is an unexpected result, especially for $0.267949<J_2/J_1\leqslant 0.38$ where the ground state in the absence of an external field is in the Néel phase. In the previous finite-size studies,[17–22] there is no indication of the appearance of this plateau. However, the system sizes and the boundary conditions they used forbid the appearance of the $M/M_{\rm sat}=1/3$ plateau; therefore, the possibility of this plateau cannot be ruled out. Furthermore, when $J_2/J_1=0.382683$, another

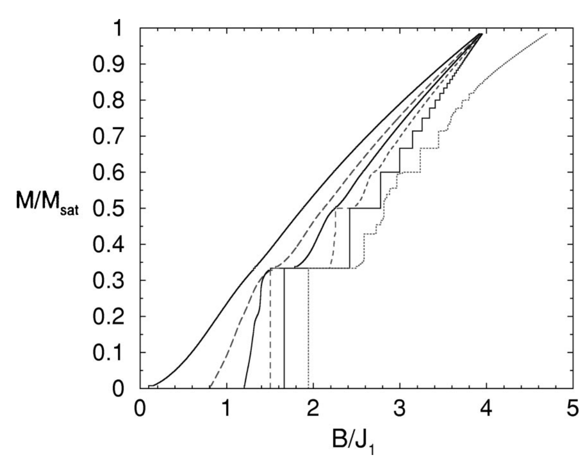

FIG. 2. Magnetization curves for the J_1-J_2 Heisenberg model calculated using a uniform CS mean field. The curves from left to right are for $J_2/J_1=0,0.2,0.3,0.4,0.5$, and 0.7, respectively.

band crossing in the Hofstadter spectrum occurs at $\phi/2\pi = 3/4$ (see Table I of Ref. 28), and a plateau at $M/M_{\rm sat} = 1/2$ ensues. It is interesting to note that the critical value for the appearance of the $M/M_{\rm sat}=1/2$ plateau agrees quite well with the critical point of the quantum phase transition at zero field between the Néel and the quantum disorder phases.[15,16] As mentioned before, while the appearance of a plateau in the quantum disorder phase had been predicted, the value of the plateau is still under debate.[20–22] The controversy may come from the subtle finite-size effects in their investigations. Since the present CS theory is free from the finite-size effects, we give strong support to the existence of the $M/M_{\rm sat}=1/2$ plateau.

More complex structures in the magnetization curves appear when J_2/J_1 is further increased. For example, when $J_2/J_1=0.5$, a series of plateaus at $M/M_{\rm sat}=n/(n+2)$ is found, which corresponds to the band crossing at some magic numbers $\phi/2\pi=(n+1)/(n+2)$. Irregular plateau structures are found for even higher values of J_2/J_1 (see the $J_2/J_1=0.7$ curve in Fig. 2). This behavior is quite similar to the case of the triangular lattice, where many plateaus are predicted under the *uniform* CS mean-field approximation.[8] In the case of the triangular lattice, it is shown that, when the nonuniform mean-field solutions are used, only the main plateau ($M/M_{\rm sat}=1/3$ in that case) survives and other miniplateaus disappear. One may wonder whether the same situation will happen in the present study of the J_1-J_2 model. In Sec. III B we report on a nonuniform extension of the mean field calculation. Unlike the triangular lattice case, our result indicates that the irregular plateau structures in Fig. 2 for large ratios of J_2/J_1 survive under a collinear modulation of the magnetization.

B. One-dimensional periodic mean-field calculation

Here we extend the above discussion to the nonuniform mean-field case. Since the ground state at zero magnetic field for $J_2/J_1>0.6$ is in the collinear phase, it is reasonable to consider a one-dimensional periodic mean-field modulation.

For each $M=(p/q)-\frac{1}{2}$ (or $\phi/2\pi=p/q$), we take $\delta M_i = -\Delta e^{i\vec{\pi}_x\cdot\vec{r}_i}$, where $\vec{\pi}_x=(\pi,0)$ and $\vec{r}_i$ labels the lattice point at the lower left corner of the ith plaquette (the lattice constant is taken to be unity). Thus $\delta\phi_i/2\pi=-\Delta e^{i\vec{\pi}_x\cdot\vec{r}_i}$, $V_i = 4J_2\Delta e^{i\vec{\pi}_x\cdot\vec{r}_i}$, and $\Sigma_i\Sigma_j J_{ij}\delta M_i\delta M_j=-4J_2\Delta^2 N_s$. Thus the present spin system can be identified as a Hofstadter problem for fermions hopping on a square lattice under a modulated magnetic field and a modulated electric potential with the *same* period [see Eq. (6)].[25,32] The modulated Hofstadter problem can then be straightforwardly analyzed for every rational value of $\phi/2\pi$.

The value of Δ is determined self-consistently as follows: for each $M=(p/q-\frac{1}{2}$, one first chooses an initial try of Δ, and then diagonalizes the $Q\times Q$ one-body Hamiltonian matrix in the first magnetic Brillouin zone, $|k_x|\leqslant\pi/Q$ and $|k_y|\leqslant\pi$, where $Q=q$ $(2q)$ for an even (odd) q. By using the normalized eigenvectors $\vec{u}^{(\alpha)}(\vec{k})=[u_1^{(\alpha)}(\vec{k}),\ldots,u_Q^{(\alpha)}(\vec{k})]^T$, where α runs from 1 to Q, one can obtain a new value of Δ by employing the self-consistent equation,

$$2\Delta=\frac{1}{(N_s/Q)}\sum_{\alpha=1,\ldots,P}\sum_{\vec{k}}[|u_1^{(\alpha)}(\vec{k})|^2-|u_2^{(\alpha)}(\vec{k})|^2], \tag{8}$$

where the summation on α is over the lowest P subbands with $P=p$ $(2p)$ for an even (odd) q. This procedure is then repeated until the self-consistency is satisfied. By employing the eigenvalues $\epsilon_{\vec{k}}^{(\alpha)}$ after self-consistency being reached, the total energy per site can be calculated, and it becomes

$$E(M)=\frac{1}{N_s}\sum_{\alpha=1,\ldots,P}\sum_{\vec{k}}\epsilon_{\vec{k}}^{(\alpha)}+2(J_1+J_2)M^2+2J_2\Delta^2. \tag{9}$$

The magnetization is again obtained as a function of B by minimizing $E(M)-BM$.

For ratios of J_2/J_1 smaller than approximately 0.46, we find no difference from the uniform mean field results in Fig. 2, even though nonuniform solutions are allowed. For larger

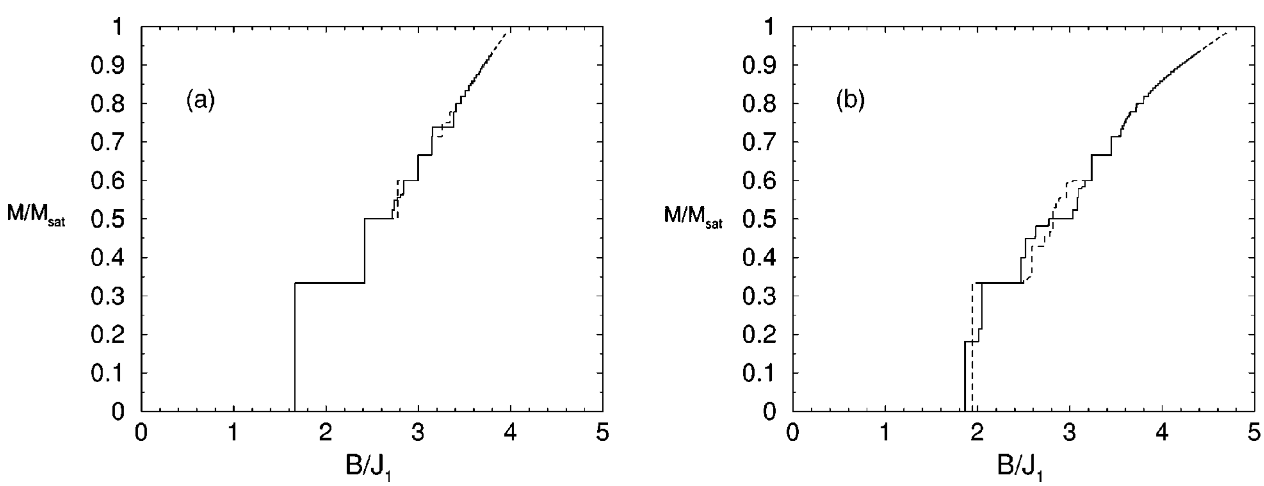

FIG. 3. The magnetization curves for uniform (dotted line) vs nonuniform (solid line) CS mean fields, with the ratios $J_2/J_1=0.5$ (a) and 0.7 (b).

ratios of J_2/J_1, the magnetization curves are visibly shifted, but there is no qualitative change. For comparison, magnetization curves with and without non-uniform modulation for two values of J_2/J_1 are shown in Fig. 3. We find that, for various J_2/J_1 ratios, both calculations always give the same saturation field B_{sat}, and the values of B_{sat} again agree with the exact results near the saturation. However, the non-uniform solution indeed gives some modification at lower magnetic fields. For $J_2/J_1=0.5$, a series of plateaus at $M/M_{sat}=n/(n+2)$, found in the uniform mean-field calculation, is now somewhat modified [see Fig. 3(a)]. Such a modification is even more obvious for $J_2/J_1=0.7$ [see Fig. 3(b)]. Nevertheless, the irregular plateau structures persist within the present CS mean-field approach.

IV. SUMMARY AND OUTLOOK

In conclusion, the magnetization curve of the 2D spin-1/2 J_1-J_2 Heisenberg model is studied by using the Chern-Simons theory under mean-field approximations. In the disordered phase, our result supports the existence of the $M/M_{sat}=1/2$ plateau, and predicts a plateau at $M/M_{sat}=1/3$. Moreover, various plateaus appear in the magnetization curves both in the disordered and collinear phases. There is no major difference between the uniform mean-field calculation and the collinear nonuniform mean-field calculation. We note that it is experimentally accessible to confirm our results. As mentioned before, a 2D spin-1/2 J_1-J_2 Heisenberg model with $J_2/J_1\simeq 1$ was recently realized experimentally in Li_2VOSiO_4 ($J_1+J_2\simeq 8.2$ K) and Li_2VOGeO_4 ($J_1+J_2\simeq 6$ K) compounds.[9] If the g factor is taken to be 2, the corresponding saturation fields will be approximately 18 T for Li_2VOSiO_4 and 13 T for Li_2VOGeO_4. In both cases, these values of the magnetic fields can be reached experimentally. Thus the full magnetization curve could be mapped out to test our results. Verification of these magnetization plateaus would indicate a strong connection between the frustrated antiferromagnetic system and the quantum Hall system.

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