Exact ground state of the Shastry-Sutherland lattice with classical Heisenberg spins

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An exact analytical solution of the ground state problem of the isotropic classical Heisenberg model on the Shastry-Sutherland lattice in external magnetic field $H$ is found for arbitrary ratio of diagonal and edge exchange constants $J_2/J_1$. The phase diagram of this model in the $(J_2/J_1, H/J_1)$ plane is presented. It includes spin-flop, spin-flip and umbrella phases. The magnetization curves are found to be linear until saturation. It is shown numerically that the inclusion of the easy-axis anisotropy into the model leads to the appearance of the 1/3 magnetization plateau, corresponding to the collinear up-up-down spin structure. This explains the appearance of the 1/3 magnetization plateau in rare earth tetraborides RB$_4$. In particular, magnetization curve of the compound HoB$_4$ is explained.

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I. INTRODUCTION

Shastry-Sutherland lattice (SSL) was first introduced in the work of Shastry and Sutherland$^1$ as a purely theoretical example of a two-dimensional frustrated spin system. SSL is a square lattice with classical Heisenberg, quantum Heisenberg, or Ising spin $S_i$ at every lattice site $i$, with antiferromagnetic (AFM) exchange $J_1$ along the edges, and AFM exchange $J_2$ along certain diagonals, as shown in Fig. 1. Its Hamiltonian (in the presence of the external field $H$ directed along the $z$-axis) is

$$\mathcal{H} = J_1 \sum_{\text{edges}} S_i \cdot S_j + J_2 \sum_{\text{diagonal}} S_i \cdot S_j - H \sum_i S_i^z, \quad (1)$$

and the Hamiltonian normalized by $J_1$ is

$$\tilde{\mathcal{H}} = \frac{\mathcal{H}}{J_1} = \sum_{\text{edges}} S_i \cdot S_j + \rho \sum_{\text{diagonal}} S_i \cdot S_j - h \sum_i S_i^z, \quad (2)$$

where we have introduced the notations

$$\rho \equiv \frac{J_2}{J_1}, \quad h \equiv \frac{H}{J_1}. \quad (3)$$

Surprisingly, ten years after the work of Shastry and Sutherland, SSL has been experimentally realized in SrCu$_2$(BO$_3$)$_2$, which has a layered structure, with each Cu$^{2+}$ ion carrying spin $S = 1/2$. If exchange interactions with only two spheres of nearest neighbors are included, the magnetic lattice of SrCu$_2$(BO$_3$)$_2$ is equivalent to SSL. At low temperatures SrCu$_2$(BO$_3$)$_2$ exhibits a sequence of magnetization plateaus at fractional values of the saturation magnetization $M_s$$^{3–5}$. A number of theories of this phenomenon has been proposed$^6–8$.

Similar fractional magnetization plateaus have been observed recently in rare earth tetraborides$^9–12$ RB$_4$, where R=Tm, Er or Ho, where the rare earth ions also form layered structure equivalent to SSL. The important difference is that while Cu$^{2+}$ ions in SrCu$_2$(BO$_3$)$_2$ have spins $s = 1/2$, the rare earth ions in RB$_4$ systems have large spins, which can be treated as classical ones. These compounds also possess a strong easy-axis magnetocrystalline anisotropy.

The discovery of magnetization plateaus in RB$_4$ compounds led to a number of theoretical and computational studies of SSL with classical Heisenberg$^{13–16}$ and Ising$^{17–22}$ spins. Deep understanding of these two models is vital for explaining the peculiar magnetization curves of RB$_4$ systems, as they can serve as the foundation stones on which more complicated models with additional interactions can be built. A major breakthrough for Ising SSL in external magnetic field came very recently as its exact ground state has been found analytically$^{20}$. This model gives a single $M/M_s = 1/3$ magnetization plateau, which corresponds to the so-called up-up-down (UUD) phase (Fig. 2, lower left). On the other hand, a Monte Carlo simulation for the classical Heisenberg SSL$^{13}$ found magnetization curves with no steps. However, when the easy-axis anisotropy was included in the

![FIG. 1. (Color online) Shastry-Sutherland lattice. The red (gray) triangle marks the elementary cluster of the SSL.](image-url)
model\textsuperscript{14–16}, the \(1/3\) UUD plateau appeared for a certain range of \(J_2/J_1\). Magnetization steps other than \(1/3\) do not appear for either Ising or Heisenberg SSL. Additional exchange or dipolar interactions\textsuperscript{16,17,20,22} or lattice disorder\textsuperscript{14} were employed to account for those plateaus, in particular the large \(1/2\) plateau found in TmB\(_3\) (Ref. 16). If these additional interactions are included, Ising model on SSL essentially succeeds in explaining the appearance of fractional magnetization plateaus in RB\(_3\). A typical zero-temperature magnetization curve \(M(H)\) of the Ising SSL has the "staircase" shape, namely it consists of horizontal magnetization steps (including the \(M = 0\) and \(M = M_s\) ones) separated by first-order phase transitions (vertical segments of the \(M(H)\) curve). This is very similar to the experimental \(M(H)\) curve of TmB\(_3\) (Ref. 11). Anisotropic Heisenberg SSL\textsuperscript{14–16}, on the other hand, gives smoother \(M(H)\) curves with inclined regions, which were experimentally observed for HoB\(_4\) (Ref. 12) and possibly ErB\(_4\) (Ref. 9). Of course, the latter model can be applied to TmB\(_3\) as well\textsuperscript{16}, provided that the anisotropy constant is large enough.

While the exact ground state of the Ising SSL in magnetic field has been found, the complete understanding of the classical Heisenberg SSL is still lacking. In particular, its exact ground state has not been determined, except for special cases \(H = 0\) (Ref. 1) and \(J_2/J_1 = 2\) (Ref. 13). The Monte Carlo simulations\textsuperscript{13–16} mainly focused on the special point \(J_2/J_1 = 2\) or its vicinity, while the phase diagram in the \((J_2/J_1, H/J_1)\) plane has never been published. The present paper is an attempt to clarify these issues. Its goal is to study in detail the ground-state problem of the isotropic classical Heisenberg SSL and to determine the phase diagram of this model in the \((\rho, h)\) plane. The very interesting problem of the classical Heisenberg SSL with easy-axis anisotropy is also addressed briefly in the present paper.

The paper is organized as follows. Section II introduces different possible magnetic structures of the SSL and presents its phase diagram in the \((\rho, h)\) plane. In section III the exact ground state of the SSL is calculated and it is proven that the three phases of the previous section are indeed the ground state spin structures. Section IV checks the exact result with numerical simulation and examines the effect of the uniaxial anisotropy on the magnetization curves. The experimental magnetization curve of HoB\(_4\) is also analyzed in this section. It is followed by a conclusion.

II. MAGNETIC STRUCTURES AND THE PHASE DIAGRAM

In this and the following sections we consider the problem of the ground state of the SSL as the function of two parameters: \(h \equiv H/J_1\) and \(\rho \equiv J_2/J_1\). In the absence of external magnetic field \((h = 0)\) the problem has been solved in Ref. 1. For \(\rho < 1\) (\(J_2 < J_1\)) the ground state is the regular Neel AFM state (Fig. 2, upper left) with the energy per lattice site

\[
\epsilon_{\text{Neel}} = -2 + \frac{\rho}{2}.
\]

The Neel state satisfies all \(J_1\) exchange interactions, but not \(J_2\) ones. For \(\rho > 1\) (\(J_2 > J_1\)) the ground state is the so-called spiral state. The angle between neighboring spins is \(\pi - \Delta \phi\) along the edges, and \(2\Delta \phi\) along the diagonals, where \(\Delta \phi = \cos^{-1}(1/\rho) = \cos^{-1}(J_1/J_2)\). The energy of this structure is

\[
\epsilon_{\text{Spiral}} = -\frac{1}{\rho} - \frac{\rho}{2}.
\]

Such configuration can be constructed in different ways, leading to a degeneracy\textsuperscript{1,13}. In general, it is incommensurate with the crystal lattice, but for chosen values of \(\rho\), namely for \(\cos^{-1}(1/\rho) = \pi m/n\) with integer \(m, n\), periodic spirals can be realized. One possible spiral configuration for \(\rho = 2\) is presented in Fig. 2, lower right.

The special case \(\rho = 2\) (\(J_2/J_1 = 2\)) for \(h > 0\) has been solved in Ref. 13. In this case the Hamiltonian (1) possesses an additional degeneracy, and there is an infinite number of spin structures which share both total energy and the magnetization with the umbrella structure introduced below. The generic case \(h > 0\) is a bit more complicated. First we introduce several candidate spin structures which correspond to the local extrema of the total energy and present the phase diagram of the SSL in the \((\rho, h)\) plane. In the next section we prove rigorously

FIG. 2. (Color online) Neel, spin-flip, UUD and spiral (for \(J_2/J_1 = 2\)) spin structures. Black and white circles denote spins pointing up and down respectively. Red, green and blue circles denote three different directions of the spiral structure, with angle 120° between each two directions. The magnetic unit cells are shown with purple (gray) rectangles.
that the three structures considered (spin-flop, spin-flip and umbrella) are indeed the lowest-energy structures in the respective regions of the \((p, h)\) plane.

UUD structure, shown in Fig. 2, has energy and magnetization per site:

\[
\epsilon_{UUD} = -\frac{2}{3} - \frac{\rho}{6} - \frac{h}{3}, \quad M_{UUD} = 1/3. \tag{6}
\]

Here and in the following we define \(M\) as the magnetization per lattice site, so that \(M_s = 1\). The first term in Eq. (6) is calculated by including 16 edges \((J_1\) bonds\) within the unit cell of the UUD structure with factor 1, and 16 edges which cross the unit cell boundary with factor 1/2. The total contribution of these terms to the unit cell energy is equal to \(-8\), which gives per site contribution of \(-2/3\) when divided by the number of sites.

In the dimer structure every \(J_2\) bond connects two oppositely aligned spins (e.g. \(+z\) and \(-z\)). This can be done in an infinite number of ways as each dimer can be oriented independently from all others. This structure satisfies all \(J_2\) bonds and its energy is

\[
\epsilon_{\text{Dimer}} = -\frac{\rho}{2}, \quad M_{\text{Dimer}} = 0. \tag{7}
\]

As we will see below, the dimer structure is never a ground state of the isotropic classical Heisenberg SSL, except in the limit \(J_1 = 0\) \((\rho = \infty)\). It is important for the anisotropic Heisenberg and Ising SSL, however, and it is also realized for finite values of \(\rho\) in a quantum Heisenberg SSL.

The spin-flop structure is the Neel structure with all spins tilted by the angle \(\theta^* = \pi/2 - \theta = \sin^{-1}(h/8)\) out of the \(xy\) plane. This solution exists for \(h < 8\), and its energy and magnetization are given by

\[
\epsilon_{\text{Flop}} = -2 + \frac{\rho}{2} - \frac{h^2}{16}, \quad M_{\text{Flop}} = \cos(\theta) = \frac{h}{8}. \tag{8}
\]

The spin-flip (ferromagnetic) structure (Fig. 2, upper right) has all spins aligned along the magnetic field. It’s energy is

\[
\epsilon_{\text{Flip}} = 2 + \frac{\rho}{2} - h, \quad M_{\text{Flip}} = 1. \tag{9}
\]

At \(h = 8\) the spin-flop structure turns into the spin-flip structure in a continuous fashion. Since \(M(h)\) is continuous at the point \(h = 8\), but \(\partial M(h)/\partial h\) is not, this is a second-order phase transition.

Another possible structure is the umbrella structure, proposed in Ref. 13. It is essentially a tilted spiral structure. In the umbrella structure the spherical angles \(\theta_i\) of all spins are equal, and the angles \(\phi_i\) are distributed like in the spiral structure above. The energy for given \(\theta, \Delta \phi\) is

\[
\epsilon(\theta, \Delta \phi) = 2 \left(-\sin^2 \theta \cos(\Delta \phi) + \cos^2 \theta\right) + \frac{\rho}{2} \left(\sin^2 \theta \cos(2 \Delta \phi) + \cos^2 \theta\right) - h \cos \theta. \tag{10}
\]

\[
M_{\text{Umb}} = \cos \theta = \frac{h \rho}{2 (\rho + 1)^2}. \tag{11}
\]

\[
\epsilon_{\text{Umb}} = -\frac{1}{\rho} - \frac{\rho}{2} - \frac{h^2 \rho}{4 (\rho + 1)^2}. \tag{12}
\]

The umbrella structure exists for \(\rho > 1\) and \(h < h_{\text{max}} = 2 (\rho + 1)^2 / \rho\), has energy lower than the spin-flop one, and turns into the spin-flip structure at \(\rho = 1\). At \(h = h_{\text{max}}\) it becomes the spin-flip structure. Both phase transitions are of the second order. In Fig. 3 and Fig. 4 numerically calculated umbrella structures for \((\rho, h) = (1.5, 3)\) and \((1.2, 3)\) respectively are presented (see section IV below for details).

The phase diagram of the classical isotropic SSL is shown in Fig. 5. The solid lines mark the lines of the second order phase transitions. For \(\rho < 1\) SSL behaves exactly like a regular Neel antiferromagnet, while for \(\rho > 1\) the spin-flop phase is replaced by the umbrella phase. The dotted line denotes the special degenerate case \(\rho = 2\). Magnetization curve \(M(h)\) is linear until saturation, and there is no magnetization plateaus for the isotropic Heisenberg SSL. Note that the 1/3 pseudo-plateau observed in Ref. 13 was a finite-temperature effect. The phase diagram in Fig. 5 has been constructed by comparing energies of different spin structures introduced in this section and selecting the one with the lowest
FIG. 4. (Color online) Umbrella structure for $\rho = 1.2$, $h = 3$ calculated numerically on the $12 \times 12$ lattice with periodic boundary conditions. The arrows show the $xy$ components of spins. The red (gray) circles show the $z$ components of spins (all equal in this case).

III. EXACT GROUND STATE

In order to prove that the three spin structures introduced in the previous section (spin-flop, spin-flip and umbrella) are indeed the ground state structures for respective $(\rho, h)$ we use the method of decomposing the Hamiltonian into overlapping elementary clusters, which has been used previously in, e.g., Refs. 1, 13, and 20

$$\hat{H} = \sum_{\triangle} H_{\triangle}.$$ (13)

For SSL such elementary cluster has the shape of the right triangle, highlighted in red in Fig. 1. Each triangle includes one spin $S_0$ at the right angle, two spins ($S_1$ and $S_2$) at the 45° angles; two $J_1$ bonds, and one $J_2$ bond shared by two triangles. The number of triangles on the lattice is the same as the number of lattice sites, as each triangle includes 3 spins and each spin $S_i$ is a part of 3 triangles, acting the roles of $S_0$, $S_1$ and $S_2$ in turn. The Hamiltonian of a triangle is

$$H_{\triangle} = \beta S_0 (S_1 + S_2) + \frac{\rho S_1 \cdot S_2 - h}{2} \left[ \alpha S_0 + \frac{1 - \alpha}{2} (S_1 + S_2) \right],$$ (14)

where $\alpha$ is an arbitrary real number. It corresponds to an arbitrary way in which the term $-h \cdot S_i$ of the original Hamiltonian can be divided between three different triangles which include the site $S_i$. While the triangle Hamiltonian $H_{\triangle}$ depends on $\alpha$, the lattice Hamiltonian $\hat{H}$ does not, as all $\alpha$-dependent terms cancel each other upon summation in Eq. (13).

The triangle Hamiltonian is invariant under three basic symmetry operations: simultaneous rotation of all spins around $z$-axis, reflection of all spins in the $xz$ plane, and interchange $S_1 \leftrightarrow S_2$, where $z$-axis is parallel to $h$, and $x$-axis is an arbitrary axis perpendicular to $z$-axis. These operations generate a symmetry group, which also includes such operations as reflection in the $yz$ plane (or any other plane containing $z$-axis) and inversion of the $xy$ components of all spins $S_i^x \rightarrow -S_i^x$, $S_i^y \rightarrow -S_i^y$ ($i = 0, 1, 2$). This symmetry leads to the degeneracy of most energy levels $\epsilon(\alpha, S_0, S_1, S_2)$, as the only configurations invariant under the symmetry group of $H_{\triangle}$ are collinear ones with $S_0 = \pm z$ and $S_1 = S_2 = \pm z$. At the special point $\rho = 2$ there is an additional symmetry operation $S_0 \leftrightarrow S_1$ (or $S_0 \leftrightarrow S_2$).

The triangle Hamiltonian has an $\alpha$-dependent ground state energy $\epsilon_\alpha(\alpha)$, thus for every possible configuration of three unit vectors $S_0$, $S_1$, and $S_2$ the inequality

$$\epsilon_{\triangle}(S_0, S_1, S_2, \alpha) \geq \epsilon_0(\alpha)$$ (15)

holds true. The equality is achieved for a possibly degenerate ground state configuration of the triangle Hamiltonian. There is also an inequality for the lattice energy, which holds true for all values of $\alpha$

$$N \epsilon \{ S_i \} = \sum_{\triangle} \epsilon_{\triangle} \geq \sum_{\triangle} \epsilon_0(\alpha) = N \epsilon_0(\alpha),$$ (16)
or $\epsilon \{S_i\} \geq \epsilon_0(\alpha)$, where $N$ is the number of lattice sites, and $\epsilon \{S_i\}$ is the energy per site. The equality here is possible only for a spin structure $\{S_i\}$ that minimizes the energy of each triangle simultaneously. Here and in the following we use the word "structure" for spin structures $\{S_i\}$ on the lattice, and the word "configuration" for configurations $S_0, S_1, S_2$ of the three spins of a triangle. According to (16), for every other spin structure $\{S'_i\}$ one can write an inequality $\epsilon \{S'_i\} \geq \epsilon(\alpha) = \epsilon \{S_i\}$, which proves that the structure $\{S_i\}$ is indeed the ground state of the lattice Hamiltonian (2), or, in general, one of the degenerate ground state structures. In other words, in order to find the ground state of the lattice Hamiltonian (2) for a given $(\rho, h)$, we have to construct a lattice spin structure $\{S_i\}$ from the ground state configuration $(S_0, S_1, S_2)$ of a triangle (let us call it "brick"), or from a set of such bricks in case of degeneracy. In case of a degenerate ground state, it is important to note that any possible lattice structure constructed from bricks is a ground state structure, and, vice versa, any possible ground state structure can be constructed from bricks (which can be seen from the fact that for any ground state structure the energy of each triangle is equal to $\epsilon_0$).

The question is whether it is possible to construct a lattice structure from a given set of bricks, which includes all possible realization of the degenerate ground state of $\mathcal{H}_\Delta$, spawned by the symmetry group of $\mathcal{H}_\Delta$. The problem is not trivial, since each spin is a part of three different triangles, so the bricks must match each other perfectly. This is obviously not possible for arbitrary $\alpha$, however, as we are going to see below, such construction can indeed be performed for the right choice of $\alpha$. The required values are $\alpha = 1/2$ for $\rho \leq 1$, and $\alpha = 1/(\rho + 1)$ for $\rho > 1$, respectively. For these values of $\alpha$ we can construct the spin-flop, spin-flip and umbrella structures from the ground state configurations of $\epsilon_\Delta$, and confirm the phase diagram of Fig. 5. Contrary to the case of the Ising SSL, the phase diagram of the classical Heisenberg SSL does not have the convexity property, so the search for ground state must be performed for arbitrary $(\rho, h)$, rather than for a finite number of special points.

For simplicity we assume that $h > 0$, so that the field $h$ provides a fixed direction $z$. The rather trivial case $h = 0$ (solved in Ref. 1 by the same method) has been discussed in the previous section. Let us find all possible steady states (energy extrema) of the triangle Hamiltonian (14) and their energies (listed in Table I). They can be found from the system of three vector equations

$$\frac{\partial}{\partial S_j} \left( \mathcal{H}_\Delta - \frac{1}{2} \sum_i \xi_i S_i \cdot S_i \right) = 0,$$
for the three unit vectors $S_0, S_1, S_2$:

$$\frac{\partial \mathcal{H}_\Delta}{\partial S_1} = S_0 + \frac{\rho}{2} S_2 - \frac{1 - \alpha}{2} h = \xi_1 S_1,$$

$$\frac{\partial \mathcal{H}_\Delta}{\partial S_2} = S_0 + \frac{\rho}{2} S_1 - \frac{1 - \alpha}{2} h = \xi_2 S_2,$$

$$\frac{\partial \mathcal{H}_\Delta}{\partial S_0} = S_1 + S_2 - \alpha h = \xi_3 S_0,$$

where $\xi_i$ are the three real Lagrange multipliers used to enforce the conditions $S_i \cdot S_i = 1$. They are nonpositive for local energy minima, and nonnegative for local maxima.

First, let us consider collinear $(S_i = \pm z)$ solutions of Eqs. (18)–(20). Any collinear configuration is a solution. The energies of two spin-flip-like configuration $(S_i = \pm z)$ are $\epsilon_{F\text{lip}1,2} = 2 + \rho/2 \mp h$ and do not depend on $\alpha$. The two Neel-like configurations $(S_1 = S_2 = S_0 = \pm z)$ have energies $\epsilon_{N\text{e}1,2} = -2 + \rho/2 \mp h(1 - 2\alpha)$. Finally, the two dimer-like configurations $(S_1 = -S_2 = S_0 = \pm z)$ have energies $\epsilon_{D\text{em}1,2} = -\rho/2 \mp h\alpha$. Now let us find all noncollinear solutions of Eqs. (18)–(20). Subtracting first two equations gives

$$S_1 \left( \frac{\xi_1 + \rho}{2} \right) = S_2 \left( \frac{\xi_2 + \rho}{2} \right).$$

(21)

It means that either $S_1$ and $S_2$ are collinear, or that both expressions in parentheses are equal to zero. There are 3 possible cases

Case 1: $\xi_1 = \xi_2 = -\rho/2$,

Case 2: $S_1 = -S_2$,

Case 3: $S_1 = S_2$.

Below we shall consider all 3 cases in detail.

Case 1: $\xi_1 = \xi_2 = -\rho/2$. We introduce a new variable $S = (S_1 + S_2)/2$, and note that $0 \leq |S| \leq 1$, but $|S_0| = 1$. The equations (18)–(20) become

$$S_0 + \rho S = h(1 - \alpha)/2,$$

$$2S - \alpha h = \epsilon_0 S_0,$$

(22)

(23)
Excluding \( S_0 \) gives

\[
S (2 + \xi \rho) = h \left[ \alpha + \xi (1 - \alpha)/2 \right]. \tag{24}
\]

There are again two possible cases.

**Case 1.1:** \( 2 + \xi \rho = \alpha + \xi (1 - \alpha)/2 = 0 \). This is only possible for \( \alpha = 1/(\rho + 1) \) (for \( \alpha = 1/2, \rho < 1 \) there are no solutions of this kind), which shows that it is indeed the correct value of \( \alpha \) for \( \rho > 1 \), since no other value of \( \alpha \) can produce the umbrella phase. For this value of \( \alpha \) there is an entire family of the degenerate ”umbrella-like” solutions of the form

\[
S_0 + \rho S = \frac{\rho h}{2(\rho + 1)} \tag{25}
\]

for \( h < h_{\text{max}} = 2(\rho + 1)^2/\rho \) with the energy

\[
\epsilon_{Umb} = -\frac{1}{\rho} - \frac{\rho}{2} - \frac{h^2 \rho}{4(\rho + 1)^2}. \tag{26}
\]

This energy is found from Eqs. (14), (25) using the identities

\[
S_1, S_2 = 2S^2 - 1, \tag{27}
\]

\[
2S_0 \cdot S + \rho S^2 = \frac{1}{\rho} \left[ (S_0 + \rho S)^2 - 1 \right], \tag{28}
\]

and also the fact that

\[
\left[ \alpha S_0 + \frac{1 - \alpha}{2} (S_1 + S_2) \right] = \frac{1}{\rho + 1} \left( S_0 + \rho S \right) \tag{29}
\]

for \( \alpha = 1/(\rho + 1) \).

Any structure constructed from umbrella-like bricks has magnetization given by Eq. (11). This can be seen by averaging Eq. (25) over all triangles and using \( \langle S_0 \rangle = \langle S \rangle = M \). For case \( \rho = 2 \), the degeneracy of the umbrella-like brick is fully preserved at the lattice level, namely, every configuration with \( S_0 + S_1 + S_2 = h/3 \) can form a lattice structure consisting of three types of sites (for example, ordered as in Fig. 2, lower right), since \( S_0, S_1, \) and \( S_2 \) can be interchanged freely. In particular, the UUD structure can be realized at a single point \((\rho, h) = (2, 3)\) (large dot in Fig. 5). For \( \rho \neq 2 \) the requirement of bricks matching each other partly lifts the degeneracy. The umbrella structure introduced above, for which \( S_1 \cdot h \cos \theta \) is equal for all spins, is a possible way to match bricks on the lattice. In our numerical simulations (see the next section) we found no other structures degenerate with the umbrella one for \( \rho \neq 2 \), but we were not able to prove their absence rigorously.

**Case 1.2:** \( S, S_0 \) and \( h \) are collinear (but \( S_1,2 \) and \( h \) are not). This gives up to two Y-like configurations, with \( S \parallel z \) and \( S_0 = \pm z \). The \( Y_1 \) configuration with \( S_0 = -z \) has the energy

\[
\epsilon_{Y_1}(\alpha) = -\frac{1}{\rho} - \frac{\rho}{2} + h \left( \alpha - \frac{1}{\rho} - \frac{(1 - \alpha)^2 h^2}{4\rho} \right) \tag{30}
\]

and it exists for \( h < 2(\rho - 1)/(1 - \alpha) \). The \( Y_2 \) configuration with \( S_0 = +z \) has the energy

\[
\epsilon_{Y_2}(\alpha) = -\frac{1}{\rho} - \frac{\rho}{2} - h \left( \alpha - \frac{1}{\rho} - \frac{(1 - \alpha)^2 h^2}{4\rho} \right) \tag{31}
\]

and it exists for \( 1 - \rho < (1 - \alpha)h/2 < 1 + \rho \).

For \( \alpha = 1/(\rho + 1), \rho > 1 \) the \( Y_{1,2} \) solutions are just two special cases of the umbrella-like solution introduced above. For \( \alpha = 1/2, \rho < 1 \) there is a single \( Y_2 \) solution with the energy

\[
\epsilon_{Y_2} = -\frac{1}{\rho} - \frac{\rho}{2} - h(\rho - 1)/2 - \frac{h^2}{4\rho}. \tag{32}
\]

**Case 2:** \( S_1 = -S_2 \). The dimer-like collinear solutions belong to this case, but there are no noncollinear solutions.

**Case 3:** \( S_1 = S_2 = S \) and \( \xi_1 = \xi_2 = \xi \). The equations (18)–(20) take the form

\[
S_0 + \left( \frac{\rho}{2} - \xi \right) S = \frac{1 - \alpha}{2} h \tag{33}
\]

\[
2S - \alpha h = \xi_0 S_0, \tag{34}
\]

or, after excluding \( S_0 \),

\[
h \left[ \alpha + \frac{\xi_0 (1 - \alpha)}{2} \right] = S \left[ 2 - \xi_0 \left( \xi - \frac{\rho}{2} \right) \right]. \tag{35}
\]

As before, it can mean either that \( S \) is collinear with \( h \) (which leads to collinear spin-flip and Neel-like solutions), or that both expressions in the square brackets are equal to zero, which leads to

\[
\xi_0 = -\frac{2\alpha}{1 - \alpha}, \quad \xi = \frac{\rho}{2} - \frac{1 - \alpha}{\alpha}, \tag{36}
\]

and

\[
S + S_0 = \frac{\alpha}{1 - \alpha} = \frac{\alpha}{2} h, \tag{37}
\]

which is the spin-flop-like solution with the energy

\[
\epsilon_{\text{Fl}}(\alpha) = \frac{\rho}{2} - \frac{\alpha (1 - \alpha)}{4} h^2 - \frac{1 - \alpha}{\alpha} - \frac{\alpha}{1 - \alpha}. \tag{38}
\]

It exists for \( h < 2/\alpha (1 - \alpha) \). For \( \alpha = 1/(\rho + 1), \rho > 1 \) this is again a special case of the umbrella-like solution. For \( \alpha = 1/2, \rho \leq 1 \) this is the spin-flip solution \( (S + S_0 = h/4) \) with the energy \( \epsilon_{\text{Fl}} = -2 + \rho/2 - h^2/16 \). The spin-flip bricks only match if \( S \cdot h = S_0 \cdot h \), i.e. that all spins are tilted by the same angle \( \theta' \) relative to the \( xy \)-plane. This condition gives \( \alpha = 1/2 \) as the only value of \( \alpha \) for which the construction of the spin-flip lattice structure is possible.

Some of the configurations corresponding to the energy extrema of \( H_{\Delta} \) do not match and thus cannot form a spin structure on the lattice. The ones that do are: spin-flop
and Neel (for $\alpha = 1/2$), umbrella-like (for $\alpha = 1/(\rho + 1)$), dimer (for $\alpha = 0$), and spin-flip (for any $\alpha$). The direct comparison of their energies (listed in Table I) for respective values of $\alpha$ shows that spin-flop, umbrella-like and spin-flip solutions indeed minimize the triangle Hamiltonian (14) in the three respective regions of Fig. 5. The Neel structure is only realized for $h = 0$, $\rho \leq 1$. The dimer structure does not exist for the isotropic classical Heisenberg SSL. This confirms the phase diagram shown in Fig. 5.

IV. NUMERICAL SIMULATIONS AND THE EFFECT OF ANISOTROPY

In order to give an independent check of our exact results we performed a series of numerical simulations, calculating the ground state of lattice Hamiltonian $\mathcal{H}$ for different values of $\rho$, $h$. We have also examined the effect of uniaxial anisotropy by adding the term

$$\mathcal{H}_A = \frac{B}{2} \sum_i (1 - (S_z^i)^2)$$

(39)

to the Hamiltonian $\mathcal{H}$, or, equivalently, adding the term

$$\tilde{\mathcal{H}}_A = \frac{\beta}{2} \sum_i (1 - (S_z^i)^2)$$

(40)

to $\tilde{\mathcal{H}}$, where $\beta \equiv B / J_1$ is the anisotropy constant.

The minimum of $\mathcal{H}$ was found by a discrete micromagnetic simulation with only the Gilbert damping term included. We considered the system of equations

$$\frac{dS_i}{dt} = -\lambda \left[ \frac{\partial \tilde{\mathcal{H}}}{\partial S_i} - S_i \left( S_i \cdot \frac{\partial \tilde{\mathcal{H}}}{\partial S_i} \right) \right],$$

(41)

where $\lambda > 0$ is the damping parameter, for each spin $S_i$ of the lattice; and solved it using the first-order Runge–Kutta method in spherical coordinates with our own computer code. This method decreases the energy of the system on each step (provided that $\lambda$ is small enough) eventually finding a (local) minimum. It can be viewed as a variation of the steepest descend method. Unlike previously used Monte Carlo methods, our method looks for the ground state of the system avoiding any finite-temperature effects. We have used square cells of different size (usually 6 x 6, 12 x 12, or 24 x 24) with periodic boundary conditions. In order to minimize the probability of finding a local energy minimum instead of the ground state, each simulations was performed 50 times with different random initial conditions, and the result with the lowest energy was chosen.

A number of simulations for different values of $\rho$, $h$ have been performed. Our results fully confirm the phase diagram of Fig. 5, in particular, the second order phase transitions and the additional degeneracy for $\rho = 2$ are clearly seen in our calculations. We have also applied the same method to the triangle Hamiltonian $\mathcal{H}_\triangle$ and checked numerically the validity of the results of the previous section. Two typical magnetization curves $M(h)$ are presented in Fig. 6 (upper panel) for $\rho = 0.5$ and $\rho = 2.5$. The numerical results are plotted as circles in this figure, while the analytical formulae (4)–(11) are presented as lines. For $\rho = 0.5$ the system goes through the sequence of the Neel–spin-flop–spin-flip structures, all of them being periodic with 4 atoms per unit cell, exactly as predicted by our analytical treatment above. The $M(h)$ curves in fact do not depend on $\rho$ at all as long as $\rho \leq 1$. For $\rho > 1$ the ground state is the umbrella structure, which is in general incommensurate with the lattice. The numerical calculations with a finite lattice size cannot reproduce this structure exactly, of course. Two examples of the calculated umbrella structures with periodicity forced by the lattice size are presented in Fig. 3 and Fig. 4 for $(\rho, h) = (1.5, 3)$ and (1.2, 3) respectively.
In order to analyze the dependence of the calculated magnetization and energy of the umbrella structure on the lattice size, we have calculated the $M(h)$ and $E(h)$ curves for $\rho = 2.5$ using $n \times n$ square lattices for different values of $n$ and compared them to the exact results. The relative magnetization difference $\Delta M(h) = (M_{\text{calc}}(h) - M_{\text{exact}}(h))/M_{\text{exact}}(h)$ and the absolute energy difference $\Delta E(h) = (E_{\text{calc}}(h) - E_{\text{exact}}(h))/J_1$ are presented in Fig. 6, middle and lower panels respectively, for $n$ ranging from 6 to 24. The results for $n = 6$ and $n = 12$ are identical, as are the ones for $n = 10$ and $n = 20$. The general trend of the convergence of the calculated $M$ and $E$ to the exact values upon the increase of $n$ is clearly seen, although the process of the convergence is far from steady. The best results are obtained for the 16 x 16 and 22 x 22 lattices, while the results for the 8 x 8 and 14 x 14 lattices are the worst. This stems from the fact that the elementary angle $\Delta \phi = \cos^{-1}(1/\rho)$ of the umbrella phase is approximated on a $n \times n$ lattice by $\pi/n \cdot 360^\circ$, with integer $m$. For $\rho = 2.5$ this angle is $\Delta \phi \approx 66.22^\circ$ and it is close to $\pi/3 \cdot 360^\circ$ and $\pi/2 \cdot 360^\circ$. The worst results are generally obtained when $\Delta \phi$ is close to $(m+1/2)/n \cdot 360^\circ$, as is the case for $n = 8$ and $n = 14$. With the increase of $n$ the rational approximations $\pi/n \cdot 360^\circ$ converge to the exact $\Delta \phi$. As long as the lattice size is 6 x 6 or larger, the differences $\Delta M$ and $\Delta E$ are smaller or of the order of $10^{-2}$, a difference too small to be seen in the scale of Fig. 6 (upper panel). For $n = 6$, $\Delta M$ is of the order of $9 \cdot 10^{-4}$. For $n = 24$ the calculated $M$ is actually worse compared to $n = 6$ for very small $h$, however, for larger values of $h$, the calculated magnetization is better for $n = 24$; and, more importantly, the calculated energy for $n = 24$ is lower and therefore $\Delta E$ is smaller compared to $n = 6$ for all values of $h$. We have also calculated the $M(h)$ and $E(h)$ curves for the $n \times 2$ lattices, where $n = 6, 8, \ldots, 24$. The results (not shown) are identical to the ones obtained for the $n \times n$ lattices. The reason for this is that the typical umbrella structure (see e.g. Fig. 3 and Fig. 4) has period 2 in one of the directions ($x$ or $y$).

If the magnetic anisotropy $\beta$ is switched on, the single UUD point $(\rho, h) = (2, 3)$ (large dot in Fig. 5) expands into a finite region of the UUD phase. The $M(h)$ curves for $\rho \neq 2$ first get a noticeable kink at around $M = 1/3$ (Fig. 6, upper panel, dashed blue curve), which eventually turns into the $M = 1/3$ UUD plateau when the anisotropy constant is increased (Fig. 6, upper panel, dashed-dot red curve). For $\rho = 2$ the $M = 1/3$ step appears for any finite value of $\beta$. Our $M(h)$ curves are very similar to the $M(h)$ curves of Ref. 14, which were obtained using Monte Carlo method for $\rho = 2$. However, we observed the onset of the 1/3 plateau at a finite value of $\beta$, which was not seen in Ref. 14 due to the choice of a non-arbitrary point $\rho = 2$. No fractional plateaus other than 1/3 appear in our calculations. Apart from the UUD structure, the anisotropy also stabilizes other collinear structures. The stabilization of the spin-flip structure leads to the decrease of the saturation field with increasing $\beta$. A region of the Neel phase appears in the ($\rho, h$) plane, leading to the $M = 0$ plateau in the $M(h)$ curve and the spin-flop transition at a final $h$. For $\rho \leq 1$ this step appears for any finite $\beta$, while for $1 < \rho < 2$ it appears for $\beta$ above a certain threshold. For $\rho > 2$ and large enough $\beta$ the dimer structure is the ground state at small $h$, which also leads to a $M = 0$ plateau (Fig. 6, upper panel, dash-dot-dot green curve). The $M = 0$ plateau cannot exist for $\rho = 2$, not even in the Ising model. Further examples of the $M(h)$ curves with the $M = 0$ plateau can be seen in Fig. 7, see the discussion below.

Let us compare our results to the experimental $M(H)$ curve of HoB$_4$ (Ref. 12), which contains a single 1/3 fractional plateau and inclined segments. Note that this curve has a large $M = 0$ plateau, which would require strong anisotropy and $\rho \neq 2$ to explain it within our model. Also note that transition from $M = 0$ (Neel or dimer structure) to $M = 1/3$ (UUD structure) is rather sharp in the experiment, while there is a wide inclined segment between the 1/3 plateau and the saturation. From the experimental data we can roughly estimate the position of three most important points in the $M(h)$ curve: the transition between $M = 0$ and $M = 1/3$ ($H_1 = 1.79$ T), end of the $M = 1/3$ step ($H_2 = 2.6$ T), and saturation ($H_3 = H_{sat} = 3.2$ T). In Fig. 7 the experimental magnetization curve $M(H/H_{sat})$ of HoB$_4$ (solid black curve) is compared to the magnetization curves of Ising (dotted green line) and Heisenberg SSL (red circles and dashed blue line). The latter ones have been calculated using our code on the 6 x 2 lattice (the results were found to coincide with the ones obtained on the 6 x 6 and 12 x 12 lattices for the values of $\rho$ used). Ising

![Diagram](image)
model can account for the sharp Neel/dimer–UUD transition, but it necessarily predicts a sharp UUD–Spin Flip transition as well, which contradicts the experiment. Using the exact solution of the Ising SSL\textsuperscript{20}, we find that the desired ratio $H_1/H_3$ is achieved for $\rho = 0.6886$, or, alternatively, for $\rho = 9.617$ (dotted green line in Fig. 7). The $M = 0$ plateau corresponds to Neel and dimer structure for these two cases respectively. With the two parameters $\rho$, $\beta$ of the anisotropic Heisenberg SSL it is possible to reproduce the correct values of both ratios $H_1/H_3$ and $H_2/H_3$. It is achieved either for $\rho = 0.4997$, $\beta = 2.6359$, $H_{\text{sat}} = 5.3641J_1$ (red circles in Fig. 7), or for $\rho = 14.0$, $\beta = 10.69$, $H_{\text{sat}} = 21.453J_1$ (dashed blue line in Fig. 7). The first set of values provides better overall agreement with the experiment, as it gives a sharp first order Neel-UUD transition. In fact, all main features of the experimental magnetization curve of HoB\textsubscript{4} are reproduced. Note that both possible values of $\rho$ are quite far from the special point $\rho = 2$. It is important to stress that the values $\rho = 0.4997$, $\beta = 2.6359$ were obtained within the anisotropic SSL as effective parameters which give a best fit to the experimental curve $M(H/H_{\text{sat}})$ of HoB\textsubscript{4}. In real HoB\textsubscript{4} the ratios $J_2/J_1$ and $B/J_1$ might have slightly different values, as this material is likely to possess additional long-range exchange and dipolar interactions which were ignored in our model.

It is interesting to compare the different physics of Ising and classical Heisenberg SSL (the difference between these two models has also been discussed recently in Ref. 16). The Ising SSL allows for collinear structures only, and its zero-temperature $M(h)$ curves consist of vertical and horizontal segments only (plateaus and first order phase transition). In contrast, magnetization curves for isotropic Heisenberg SSL are linear until saturation thanks to noncollinear spin-flop and umbrella structures. The anisotropic Heisenberg SSL combines features of both Ising and Heisenberg models. Its magnetization curve $M(h)$ can include both horizontal steps (corresponding to collinear spin structures) and inclined regions (corresponding to noncollinear structures). While the Ising approach might be sufficient for TmB\textsubscript{4}, both types of regions are clearly seen experimentally in HoB\textsubscript{4}. The next logical step in the study of classical Heisenberg SSL would be determining the phase diagram of the classical Heisenberg SSL with easy-axis anisotropy. This problem is, however, beyond the scope of the present paper and will be addressed in our future research.

V. CONCLUSION

We have found analytically the exact ground state of the classical Heisenberg SSL in the external field $h$ and presented the phase diagram of this model in the $(\rho, h)$ plane. The phase diagram includes the spin-flop phase for $\rho \leq 1$, the umbrella phase for $\rho > 1$, and the spin-flip phase for sufficiently large $h$. The phase transitions between these three phases are of the second order. The zero-temperature magnetization curves $M(h)$ are linear until saturation with no features. For $\rho = 2$ there is an additional degeneracy and an infinite number of spin structures which share the energy and magnetization with the umbrella one. In particular, UUD structure can be realized at a single point $(\rho, h) = (2, 3)$.

The effect of the easy-axis uniaxial anisotropy on $M(h)$ curves has been examined by numerical micromagnetic simulation. The anisotropy leads to the onset of the $M = 1/3$ UUD plateau at a certain finite value of the anisotropy constant $\beta$ for $\rho \neq 2$ (and at $\beta = 0$ for $\rho = 2$). Our results demonstrate the existence of both collinear (steps of the $M(h)$ curve) and noncollinear (inclined parts of the $M(h)$ curve) spin structures for anisotropic Heisenberg SSL. The results explain the magnetization curve of HoB\textsubscript{4}, while the $M(h)$ curves of TmB\textsubscript{4} are more Ising-like in nature, and cannot be explained without introducing additional long-range interactions into the model.

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