The Kitaev-Heisenberg (KH) model and related models on the various lattices have been studied theoretically for the sake of realization of exotic states such as quantum spin liquid and topological orders. On the kagome lattice, in spite of a spin-liquid ground state in the Heisenberg model, the stability of the spin-liquid state has hardly been studied in the presence of the Kitaev interaction. Therefore, we investigate the ground state of the classical and quantum spin systems of the kagome Kitaev-Heisenberg model. In the classical system, we obtain an exact phase diagram that has an eight-fold degenerated canted ferromagnetic phase and a subextensive degenerated Kitaev antiferromagnetic phase. In the quantum system, using the Lanczos-type exact diagonalization and cluster mean-field methods, we obtain two quantum spin-liquid phases, an eight-fold degenerated canted ferromagnetic phase similar to the classical spin system, and an eight-fold degenerated \( q = 0 \) 120° ordered phase induced by quantum fluctuation. These results may provide a crucial clue to recently observed magnetic structures of the rare-earth-based kagome lattice compounds \( A_2RE_3Sb_3O_{14} \) (\( A = \text{Mg, Zn; } RE = \text{Pr, Nd, Gd, Tb, Dy, Ho, Er, Yb} \)).

Concerning spin-liquid phase, the spin-1/2 Heisenberg model on the kagome lattice (KL) is another candidate. The model has been studied for several decades [51–71], and it has theoretically been predicted that the ground state becomes the gapped Z2 spin liquid [53–56] or gapless U(1) spin liquid [57–60]. Moreover, the kagome spin models with strong anisotropy in exchange interactions, such as the kagome ice model, have been studied as well [72–77]. In spite of such intensive studies on the kagome Heisenberg model, the effect of the Kitaev interaction on the spin-liquid state has hardly been studied [11]. Furthermore, the precise phase diagram is not presented.

Recently, the rare-earth-based KL compounds \( A_2RE_3Sb_3O_{14} \) (\( A = \text{Mg, Zn; } RE = \text{Pr, Nd, Gd, Tb, Dy, Ho, Er, Yb} \)) whose space group is \( R\bar{3}m \) have been synthesized [78–83]. The compounds except for \( RE = \text{Gd} \) have an effective spin with \( S = 1/2 \) on the KL because of the Kramers or non-Kramers doublet ground state [83]. The exchange interactions between the nearest-neighbor (NN) spins are expected to be anisotropic [83], that is, magnetic interaction between the NN sites depends on the bond of a triangular unit in the lattice (see Fig. 1). Although these compounds would not have Kitaev-type interactions, the effective Hamiltonian of these compounds must contain the symmetry of \( R\bar{3}m \). Since the kagome KH model contains this symmetry together with bond-dependent anisotropic interactions, there is a possibility that the phase obtained in the KH model are continuously connected with that in the effective models of the compounds. Therefore, the study of this model will contribute to the understanding of \( A_2RE_3Sb_3O_{14} \). Hence, it is necessary to perform a theoretical investigation in order to elucidate its ground-state properties and to find new novel phases.

In this paper, we investigate the ground state of the classical and quantum spin systems of the kagome KH model. In the classical spin system, we obtain an exact phase diagram based on the analytical solution of a three-spin cluster. We confirm two kinds of phases that are an eight-fold degenerated canted ferromagnetic (CFM) and a subextensive degenerated Kitaev antiferromagnetic (KAF). In between CFM and KAF, there are exotic states such as quantum spin liquid and topological orders. On the kagome lattice, in spite of the Kramers or non-Kramers doublet ground state [83]. The black, orange, and purple dashed quadrangles denote the clusters of \( N = 12, 24 \) and 30, respectively, used in ED method with periodic boundary conditions.

![Lattice structure of the KL with three anisotropic exchange interactions, \( J_X, J_Y, \) and \( J_Z \).](image)

The red, green, and blue solid lines denote \( J_X, J_Y, \) and \( J_Z \). The red, green, and blue solid lines denote \( J_X, J_Y, \) and \( J_Z \). The black, orange, and purple dashed quadrangles denote the clusters of \( N = 12, 24 \) and 30, respectively, used in ED method with periodic boundary conditions.
diagonalization (ED) and cluster mean-field (CMF) methods. We find that the spin-liquid state in the kagome Heisenberg model remains even for small Kitaev-type interaction. We also find an eight-fold degenerated CMF phase similar to the classical spin system, and an eight-fold degenerated $q = 0$ 120° ordered phase induced by quantum fluctuations, which corresponds to the subextensive degenerated KAF in the classical spin system. It is interesting that $A_2\text{RE}_2\text{Si}_3\text{O}_{14}$ ($A = \text{Mg}, \text{RE} = \text{Gd, Er}$) and ($A = \text{Mg}, \text{RE} = \text{Nd}$) have the same type of the $q = 0$ 120° order [28] and the CMF [29], respectively.

The Hamiltonian of the KH model on the KL is given by

$$\mathcal{H} = \sum_{\langle i,j \rangle} S_i^T J_{ij} S_j,$$  \hspace{1cm} (1)

where $S_i$ is a classical spin vector $S_i = (S_i^x S_i^y S_i^z)^T \in \mathbb{R}^3$ with $|S_i| = 1$ (a quantum spin operator with $S = 1/2$) at site $i$ for classical (quantum) system. $J_{ij}$ represents the NN interactions as shown in Fig 1 and takes one of the three anisotropic interactions, $J_X = \text{diag}(J + K, J, J)$, $J_Y = \text{diag}(J, J + K, J)$, and $J_Z = \text{diag}(J, J, J + K)$, where $K$ and $J$ correspond to the energy of the Kitaev and Heisenberg interactions, respectively. We note that there is the Klein duality [11] in this model, which transforms $(J, K) \rightarrow (-J, 2J + K)$. We introduce the parametrization $(J, K) = (I \cos \theta, I \sin \theta)$, where $I$ is the energy unit ($I = 1$).

We first determine the exact classical phase diagram. The KL can be divided into three sublattices (three color sites with classical spins, $S_A$, $S_B$, and $S_C$, forming a triangle) as shown in Fig 2. All of the triangles in the KL have the same structure as two triangles shown in the right-hand side of Fig 2. The KH Hamiltonian on a triangle is given by

$$h_\Delta = S_A^T J_Z S_B + S_B^T J_X S_C + S_C^T J_Y S_A.$$  \hspace{1cm} (2)

Then, the Hamiltonian (1) reads $\mathcal{H} = \sum_\Delta h_\Delta$, where the summation is performed for all triangles (not only upward triangles but also downward triangles in Fig 2). A special solution for the ground state of $\mathcal{H}$ can be obtained by covering the KL with the ground-state vectors ($S_A$, $S_B$, $S_C$) of $h_\Delta$, because all triangles on the KL have the lowest energy. The ground-state vectors ($S_A$, $S_B$, $S_C$) and energy $E_{\text{min}_\Delta}$ are given as follows: in $\theta \in [0, \pi - \arctan(2)]$, $S_A = (0, c_\theta c_\theta, c_\theta)$, $S_B = (c_\theta c_\theta, 0, -c_\theta)$, $S_C = (-c_\theta c_\theta, -c_\theta c_\theta, 0)$, and $E_{\text{min}_\Delta} = -\frac{3}{2}(\sin \theta + \cos \theta)$, while in $\theta \in [\pi - \arctan(2), 2\pi]$, $S_A = (c_\theta F(\theta), c_\theta G(\theta), c_\theta G(\theta))$, $S_B = (c_\theta G(\theta), c_\theta F(\theta), c_\theta G(\theta))$, $S_C = (c_\theta G(\theta), c_\theta G(\theta), c_\theta F(\theta))$, and $E_{\text{min}_\Delta} = \frac{2}{3}(\sin \theta + \cos \theta) - \frac{2}{3} \sqrt{\sin^2 2\theta + 4 \cos^2 2\theta + 5}$, where $c_x, c_y, c_z \in \{-1, 1\}$, $F(\theta) = f(\theta)/\sqrt{f(\theta)^2 + 1}$ and $G(\theta) = 1/\sqrt{f(\theta)^2 + 1}$ with $f(\theta) = 4 \cos \theta/(\cos \theta + \sin \theta - \sqrt{\sin^2 2\theta + 4 \cos^2 2\theta + 5})$.

We note that the wave function at the Heisenberg points, i.e., $\theta = 0$ and $\theta = \pi$, and their dual points, i.e., $\theta = \pi - \arctan(2)$ and $\theta = -\arctan(2)$, has the global rotation symmetry.

Figure 3(a) shows the exact classical ground-state phase diagram of the kagome KH model. There are only two phases: one is an eight-fold degenerated CMF phase.
for \( \theta \in [\pi - \arctan(2), 2\pi] \) and the other is a \( 2^{3L} \)-fold degenerated KAF phase for \( \theta \in [0, \pi - \arctan(2)] \), where \( L \) is the linear system size. This \( 2^{3L} \)-fold degeneracy is caused by the absence of one of the three components in \( S_i \), which leads to \( 2^L \) degeneracy for each direction of the three bonds. In between the CFM and KAF phases, there is a macroscopic degenerated CSL state and a dual-CSL state corresponding to the Heisenberg and its dual points, respectively. There is no phase change across the Kitaev ferromagnetic (FM) point, i.e., \( S_i \cdot S_j \rightarrow S_i \cdot \langle S_j \rangle \) with \( \langle S_j \rangle = N^{-1} \sum_{\mu \nu} \langle S_{\mu} \rangle \), where \( \mu \in \{A, B, C\} \) as shown in Fig. 4 and \( i_\mu \) represents a site belonging to \( \mu \) whose total number is \( N_\mu \). Thus, the CMF Hamiltonian reads

\[
\mathcal{H}_{\text{CMF}} = \sum_{(i,j)} S_i^T J_{ij} S_j + \sum_{(i,\mu)} S_i^T J_{i,\mu} \langle S_{\mu} \rangle, \tag{3}
\]

where the first and second terms represent intra-cluster interaction and the mean-field interaction, respectively. \( \langle S_{\mu} \rangle \) is self-consistently determined by applying the ED technique to \( \mathcal{H}_{\text{CMF}} \). The ground state is so obtained as to give the minimum CMF energy. As shown in Fig. 5 we use a three-sublattice structure for both the \( N = 12 \) and 24 clusters. We note that, even if a twelve-sublattice structure was used in the same clusters, the three-sublattice ordered state has the lowest energy. We also note that at the Kitaev points (\( \theta = \pm 0.5\pi \)) the ground state has \( 2^{3L} \) degeneracy with \( L = 2 \) in the twelve-sublattice structure.

The ground-state energies per site, \( \epsilon_{\text{min}} \), and its second derivatives with respect to \( \theta \), \(-d^2 \epsilon_{\text{min}}/d\theta^2\), obtained by the ED and CMF methods are shown in Figs. 5(a) and 5(b). There are two singularities in \(-d^2 \epsilon_{\text{min}}/d\theta^2\) on either side of \( \theta = 0 \) as well as on either side of its Klein duality point \( \theta = \pi - \arctan(2) \) for the \( N = 12 \) and 30
FIG. 6. Quantum ground state energy per site, $e_{\text{min}}$ (a), and its second derivative with respect to $\theta$, $-d^2 e_{\text{min}}/d\theta^2$ (b), obtained by the ED and CMF methods. Normalized magnetization $|M|/M_{\text{sat}}$ (c) and normalized local moment $|\langle S_i \rangle|/S$ (d) for the quantum systems obtained by the CMF method and for the classical system.

ED and $N = 12$ and 24 CMF results. These singularities come from the level crossing of the ground state. In the ED results for $N = 24$, there is no singularity but peak or hump structures are seen near the level crossing points. Furthermore, the separation of the two singular points slightly increases with increasing the system size in the CMF results. Therefore, these results indicate the presence of phase transitions on either side of $\theta = 0$ and its duality point $\theta = \pi - \arctan(2)$. If the level crossing remains in the thermodynamic limit, the phase transition will be the first-order one. We note that the region near $\theta = 0$ corresponds to a gapped quantum spin liquid (QSL) state in our calculation because of the presence of a finite gap between the ground state and the first excited state. If the quantum spin liquid (QSL) at $\theta = 0$ has a finite energy gap in the thermodynamic limit [53–5d], the gapped QSL state will remain near $\theta = 0$ even in the presence of the Kitaev interaction.

Figure 3(b) shows the phase diagram obtained by the $N = 24$ CMF calculation. There is now a solid consensus of the presence of the spin-liquid ground state at the Heisenberg point ($\theta = 0$) [53–5d]. Since there is no anomaly in $d^2 e_{\text{min}}/d\theta^2$ across $\theta = 0$ in Fig. 3(b), the region including the Heisenberg point would be a QSL phase. In this region, the normalized magnetization $|M|/M_{\text{sat}}$, where $M_{\text{sat}}$ is the saturated magnetization, and the normalized local moment $|\langle S_i \rangle|/S$ are zero as shown in Figs. 3(c) and 3(d), as expected from QSL. We note that, in the classical system, $|\langle S_i \rangle|/S = 1$, being independent of $\theta$. The corresponding dual region also shows the same zero value, indicating possible dual QSL state.

The region including the FM and dual FM points is an eight-fold degenerated CFM phase with wave vector $\mathbf{q} = 0$ as is the case of the classical spin system. This is evident from finite value of both $|M|/M_{\text{sat}}$ and $|\langle S_i \rangle|/S$ in Figs. 3(c) and 3(d). On the other hand, we find that the KAF phase in the classical system is replaced by an eight-fold degenerated $\mathbf{q} = 0$ 120° ordered phase due to quantum fluctuation. This order should have zero magnetization, which is clearly seen in Fig. 3(c). A tendency toward the order even in the classical system was discussed above as evidenced by the modulation of the intensity in $S_\mathbf{q}$ shown in Fig. 3(b).

At the Kitaev points ($\theta = \pm 0.5\pi$) in Fig. 3(b), there is neither tendency toward the CFM order nor toward the $\mathbf{q} = 0$ 120° order. This indicates that quantum fluctuation induces the $\mathbf{q} = 0$ orders only when Heisenberg interaction $J$ is present. This tendency is also supported by the previous works [52, 57].

Finally, we compare our results of the KH model on the KL with the experimental results of the rare-earth KL compounds $A_2RE_Sb_2O_4$. The CFM structure in $A = $Mg, $RE = $Nd and the $\mathbf{q} = 0$ 120° ordered structure in $A = $Mg, $RE = $Gd and Er have been observed by the neutron scattering experiments [78, 79]. We note that, although the CFM state can be obtained by introducing the Dzyaloshinsky-Moriya (DM) interactions, the $\mathbf{q} = 0$ 120° ordered structure in Fig. 3(d) cannot be realized even in the presence of the DM interactions [88]. We thus speculate that the latter structure is continuously connected with the $\mathbf{q} = 120°$ order obtained in our KH model. In $A = $Mg and $RE = $Dy, there is a spin ice structure [78, 80], which dose not exist in the KH model. Therefore, we need to add further interactions, for example, so-called $\Gamma$ term [2d] and dipole interactions, to correctly analyze the compound.

In summary, inspired by the recent development of the KH model on various lattices and the discovery of the rare-earth-based KL compounds with anisotropic exchange interactions, we investigated the ground state of the classical and quantum ($S = 1/2$) spin KH model on the KL. In the classical system, we obtained the exact phase diagram with two kinds of phases that are the eight-fold degenerated CFM and the subextensive degenerated KAF. In the quantum system, we found two QSL phases, the eight-fold degenerated CFM phase similar to the classical spin system, and the eight-fold degenerated $\mathbf{q} = 0$ 120° ordered phase induced by quantum fluctuations, which corresponds to the subextensive degenerated KAF in the classical spin system. Moreover, we con-
firmed that the QSL state expected at the Heisenberg limit remains even in the presence of the small Kitaev interaction. \( A_2\text{RE}_3\text{Sb}_2\text{O}_{14} \) for \( A = \text{Mg} \) and \( \text{RE} = \text{Gd}, \text{Er} (A = \text{Mg} \) and \( \text{RE} = \text{Nd} \)) have the \( q = 0 \) \( 120^\circ \) order (the CMF) similar to our results. We hope that our study will motivate further theoretical and experimental investigations on the KL with anisotropic exchange interactions in the future.

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