Magnetization plateau and supersolid phases in the spin-1/2 antiferromagnetic Heisenberg model on a tetragonally distorted face center cubic lattice

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Highly frustrated strongly correlated systems have been studied for decades because of a good playground to find exotic quantum states [1–3]. One of the playgrounds is the magnetization process of frustrated quantum spin systems, where magnetization plateaus induced by quantum fluctuations have been studied both theoretically and experimentally [4–33]. For example, a 1/3 magnetization plateau has been observed in the triangular lattice (TL) compound Ba$_{1/3}$ magnetization plateau has been observed in the triangular lattices, where magnetization plateaus induced by quantum fluctuations has been proposed theoretically [20, 34]. The FCCL compounds exhibit lattice distortions [45–47]. The FCCL compounds exhibit lattice distortions [45–47]. It is interesting that in the same XXZ model on the TL but with large easy-plane anisotropy, a nonclassical coplanar state induced by quantum fluctuations has been proposed theoretically [20, 34]. The coplanar state in this case is called supersolid (SS) phase.

In condensed matter physics, studies finding SS phases have been carried out repeatedly [36, 37]. In quantum spin systems, a solid state can be defined as a state with a diagonal long-range order such as an up-up-down state corresponding to the 1/3 magnetization plateau in the TL [20, 34]. On the other hand, a superfluid (SF) state is defined as a state with an off-diagonal long-range order that breaks $U(1)$ symmetry. Accordingly a SS state is defined as a state having both the orders of the solid and the SF phases [36]. The search for SS phases has extensively been performed in recent years [37–44]. For example, the SS phases have been observed in SrCu$_2$(BO$_3$)$_2$ with spin-1/2 Shastry-Sutherland lattice [41, 42] and Cr spinel compounds with spin-3/2 pyrochlore lattice [43, 44].

Finding new SS phases is an important issue for fully understanding frustrated quantum spin systems. One of unexploited systems is the Heisenberg model on a face center cubic lattice (FCCL), which is a typical three-dimensional frustrated spin system expected to have magnetization plateaus and SS phases. There are model compounds for the FCCL, which are $A_2$CoTeO$_6$ ($A =$ Ca, Sr, Pb) with the double perovskite structure [45–47]. The FCCL compounds exhibit lattice distortions that may induce new phases due to strong frustration. Therefore, it is necessary to investigate theoretically the ground state of the distorted FCCL for the sake of finding new phases such as SS phases and to provide helpful hints for forthcoming experiments.

In this Letter, we investigate the ground states of the spin-1/2 Heisenberg model on a tetragonally distorted FCCL (TDFCCL) at zero temperature in a magnetic field using a large-size cluster mean-field (CMF) method. We find five supersolid phases. The solid phase has up-up-up-down structure corresponding to a 1/2 magnetization plateau. One of the SS states at high magnetic field is similar to the nonclassical coplanar state obtained in the XXZ model on the triangular lattice.
The Hamiltonian of a tetrahedron, \( H \), is given by integrating the magnetization \( M \) with respect to \( h \):

\[
M/M_{\text{sat}} = \frac{1}{\mathcal{Z}} \int M(h) \, dh',
\]

where \( h_s \) is the magnetic field giving rise to the saturated magnetization \( M_{\text{sat}} \) and \( E(h_s) \) is easily obtained.

We first show the magnetization curve at \( J = J' \), which is shown in Fig. 3. Since there is little difference of the magnetization curve between \( N = 16 \) and \( N = 28 \), the finite size effect is expected to be small. We obtain four phases except for the full moment (saturated magnetization) phase. The arrows and the symbols in Fig. 3 represent schematic magnetic structures in the four sublattices and the broken symmetry in each phase, respectively. The symmetry \( Z_4 \) (\( Z_3 \)) corresponds to the degrees of freedom choosing one from four (three) spins, and the \( U(1) \) corresponds to the rotation symmetry in the direction of the magnetic field. All magnetic structures become coplanar or collinear structure generated by so-called “order-by-disorder” mechanism. Judging from the broken symmetry and magnetic structure, we can assign each phase as SF, SS, solid, and SS phases from small to large \( h \).
FIG. 4. Phase diagram of the TDFCCL at zero temperature in a magnetic field using the CMF method with (a) \( N = 16 \) and (b) \( N = 28 \) clusters. The blue dots denote the phase transition points determined by the CMF method. The solid gray and thin black lines denote first-order and second-order phase boundaries, respectively. The number from I to VIII represent different phases. (c) Schematic magnetic structures in the I–VIII phases, where the upward direction corresponds to the direction of the magnetic field. The colors of the arrows correspond to those of the spheres shown in Fig. 2. The characters under the arrows indicate the broken symmetry in each phase. The I and II phases are SF, the VI phase (the 1/2 plateau phase) is solid, and the III, IV, V, VII, and VIII phases are SS.

The broken symmetry in each phase is shown as the symbols below the arrows in Fig. 4(c). The \( Z_4 \) in the III–VII phases corresponds to the degree of freedom choosing a downward or leftward spin [colored by orange in Fig. 4(c)] from four spins. The \( Z_4 \) in the VIII phase corresponds to the degree of freedom exchanging the green spin for gray spin. The \( Z_4 \) in the VIII phase corresponds to the degree of freedom exchanging the green and gray spin pair for orange and purple spin pair. The \( U(1) \) corresponds to the rotation symmetry in the direction of the magnetic field. The I and II phases belong to SF, which is defined as the state with magnetic order in a plane perpendicular to the \( z \) direction and with uniform local magnetization (\( S_z^\ast \)). The VI phase being the 1/2 plateau phase with up-up-up-down structure belongs to solid, which has a magnetic order in parallel to the \( z \) direction. The III, IV, V, VII, and VIII phases belong to SS having features of both SF and solid.

We compare our results on the TDFCCL with the known results of the XXZ model with large easy-plane anisotropy on the TL [20, 34]. The magnetic structure in the VIII phase, i.e., the SS phase, is similar to the structure of the nonclassical coplanar (so-called \( \pi \)-coplanar or \( \Psi \)) state obtained on the TL [20, 34]. In fact, the \( \pi \)-coplanar structure is obtained by removing either green or gray spin in the VIII phase [see Fig. 4(c)]. We should emphasize that the VIII phase is obtained in the Heisenberg model without strong anisotropy in contrast to the \( \pi \)-coplanar phase. Therefore, our finding of the SS phases in the TDFCCL may encourage efforts to observe the SS states in spin-1/2 systems.

As seen in Fig. 4(c), the green and gray spins in the spin structure of the VIII phase align completely their direction to the magnetic field. This alignment is continuously achieved from the spin structure of the VII phase when \( h \) increases. This means that the VII \( \rightarrow \) VIII phase transition is a continuous one, i.e., second-order transition. Experimentally, a phase transition similar to the VII \( \rightarrow \) VIII phase transition has been observed in Cr spinel compounds with the spin-3/2 pyrochlore lattice at the high magnetic field, i.e., \( \text{ZnCr}_2\text{O}_4 \) at 350 T [41] and \( \text{HgCr}_2\text{O}_4 \) at 36 T [54], although the magnetic structure of the phases have not been specified. As for the present the VII \( \rightarrow \) VIII phase transition, the phase transition in the Cr spinel compounds cannot be explained by the analysis of a classical spin system [53, 56]. Although there are differences in spin size and lattice geometry between the

transition in Fig. 8 are the same as those reported previously [58]. These agreements encourage the use of the CMF method for the analysis of the TDFCCL.
Cr spinel lattice and our TDFCCL, there are similarities each other in terms of three-dimensional frustrated lattice and four sublattice structure. Therefore, we believe that the VII $\rightarrow$ VIII transition at the high magnetic field obtained in our TDFCCL might be related to the phase transitions of the Cr spinel compounds and the phases at higher magnetic field might have the same characteristic of the VIII phase.

In summary, inspired by the recent understanding of the SS phase in frustrated quantum spin systems and the presence of highly frustrated FCCL compounds, we investigated the ground state of the spin-1/2 Heisenberg model on the TDFCCL in the magnetic field using the large-size CMF method. We obtained phase diagrams at zero temperature and found five SS phases. The magnetic structure in one of these phases is similar to the $\pi$-coplanar state induced by quantum fluctuation in the TL with large easy-plane anisotropy. We believe that our results are closely related to the phase transition that cannot be explained by the classical spin system observed with Cr spinel compounds. Our study will motivate new experimental investigations on FCCL compounds in the future.

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