

Ising antiferromagnet on the Archimedean lattices

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Geometric frustration effects were studied systematically with the Ising antiferromagnet on the 11 Archimedean lattices using the Monte Carlo methods. The Wang-Landau algorithm for static properties (specific heat and residual entropy) and the Metropolis algorithm for a freezing order parameter were adopted. The exact residual entropy was also found. Based on the degree of frustration and dynamic properties, ground states of them were determined. The Shastry-Sutherland lattice and the trellis lattice are weakly frustrated and have two- and one-dimensional long-range-ordered ground states, respectively. The bounce, maple-leaf, and star lattices have the spin ice phase. The spin liquid phase appears in the triangular and kagome lattices.

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I. INTRODUCTION

The Ising model [1] has played a crucial role to understand the phase transition and magnetic ordering. There exists a phase transition at finite temperature from a high-temperature disordered phase into a low-temperature ordered phase in a lattice of two and three dimensions, if it is not frustrated [2–5]. With frustration, the Ising model has various ground states such as long-range-ordered phase, spin glass, spin ice, and spin liquid phase [6,7]. Frustration can be induced in two ways: by disorder (spin glass) or by geometry (geometrically frustrated systems) [8]. In this paper, effects of the geometric frustration are investigated systematically for the antiferromagnetic Ising model on the two-dimensional Archimedean lattices.

An Archimedean lattice, also called as a uniform tiling, is a two-dimensional lattice of regular polygons in which all vertices are topologically equivalent. It is known that Kepler proved that there exist only 11 Archimedean lattices [9], which are listed in Fig. 1 and Table I. They are important not only in mathematics but also in materials science, because most of the lattices have corresponding natural material systems [10,11]. Since all vertices are in the same topological environment, they can be labeled by the sequence of the polygons surrounding a vertex [9]. For example, a square and a triangular lattice are represented by (4^4) and (3^6) , respectively. We follow the naming convention of Ref. [10], where homopolygonal lattices (T1, T2, T3) are followed by heteropolygonal lattices (T4, . . . , T11). Due to the simplicity, the Archimedean lattice is a good starting point to study geometric frustration. With the antiferromagnetic nearest-neighbor interaction, four lattices are bipartite and unfrustrated, and the other seven lattices are frustrated.

There have been systematic studies about percolation on the Archimedean lattices [12,13]. As for the magnetic models, the ferromagnetic Ising model [14] and antiferromagnetic quantum Heisenberg model [10,15] were studied. In this paper, we report detailed study of the antiferromagnetic Ising model on the Archimedean lattices. Specific heat, exact residual entropy, and freezing order parameter are obtained to identify

the ground state. Finite temperature phase transitions in weakly frustrated lattices are also discussed.

II. MODEL AND METHOD

The Ising model studied in this work is represented by the following Hamiltonian:

$$H = -J \sum_{\langle i,j \rangle} S_i S_j. \quad (1)$$

The spin at the i th site S_i may take the values of $+1$ or -1 , only. The summation runs for all the nearest-neighbor pairs, excluding double counting. The coupling constant J is set to -1 and $|J|/k_B$ is used as an energy unit, where k_B is the Boltzmann constant. Negative J means an antiferromagnetic interaction.

The calculation was done for parallelepiped lattices with number of sites $N = B \times L \times L$ with the periodic boundary condition. B is the number of sites per unit cell and L is the linear size. Without frustration, the most efficient algorithm for the Ising model is the combination of the Wolff cluster update [17] and the histogram reweighting [18,19]. In the ferromagnetic (antiferromagnetic) case, a cluster is made by adding nearest neighbors of the same (opposite) spin with a probability $P = 1 - \exp(-2/T)$. When a cluster is completed, all spins of the cluster are flipped. The cluster update is not efficient away from the critical temperature, where the cluster size is too small (at high temperature) or too large (at low temperature). Close to the critical temperature, the cluster size is moderate and the critical slowing down can be eliminated. The information of energy and magnetization distribution at a fixed temperature is used by the histogram method to calculate thermodynamic quantities at any temperature near the simulation temperature [20]. With frustration, however, cluster-update methods do not work because the cluster may include the whole lattice and cluster size becomes too large even without a phase transition. Therefore, we used the Wang-Landau algorithm [21] in this study. While conventional Monte Carlo methods such as the Metropolis [22] and the Wolff algorithm [17] perform a simulation within the canonical ensemble at a fixed temperature, the Wang-Landau algorithm calculates the density of states (DOS) as a function of energy $\rho(E)$ directly by the random walk with the transition probability $P(i \rightarrow j) = \min\{1, \rho(E_i)/\rho(E_j)\}$ in the whole energy space.

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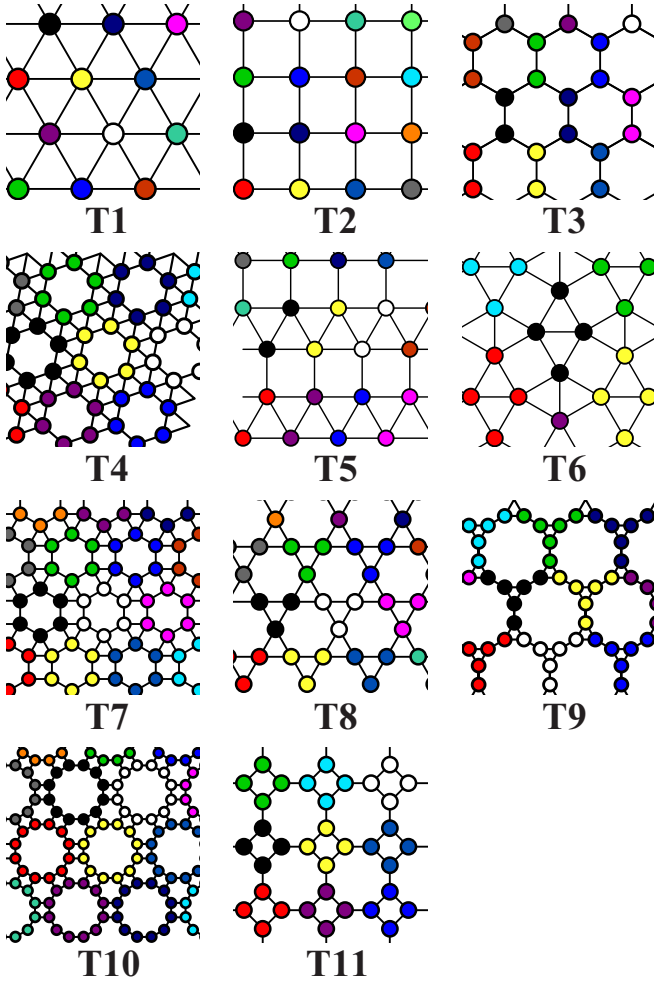


FIG. 1. (Color online) The 11 Archimedean lattices. Lattice points in the same unit cell are represented by circles of the same color (grayscale).

The DOS is adjusted by $\rho(E) \rightarrow f_n \rho(E)$ at each step resulting in a flat histogram in the energy space. The simulation continues until the histogram becomes flat, when its standard deviation is less than 4% of its average. Then, a new iteration is performed with a smaller value of $f_{n+1} = \sqrt{f_n}$. The whole simulation begins with an initial multiplier $f_0 = e$ and stops when f_n becomes close enough to 1: $f_n < \exp(10^{-10})$. The error in DOS depends on many factors, but can be assumed to be the same order as $\ln(f_n)$ if the calculation is proper. Since the random walk is in the whole energy space, it is not stuck to a metastable state and can be applied to any system even with frustration or first-order transition. From the obtained $\rho(E)$, the average energy $\langle E \rangle_T$ and the specific heat $c(T)$ can be calculated easily as a function of temperature T :

$$\langle E \rangle_T = \frac{\sum_i E_i \rho(E_i) e^{-E_i/T}}{\sum_i \rho(E_i) e^{-E_i/T}}, \quad (2)$$

$$\langle E^2 \rangle_T = \frac{\sum_i E_i^2 \rho(E_i) e^{-E_i/T}}{\sum_i \rho(E_i) e^{-E_i/T}}, \quad (3)$$

$$c(T) = \frac{\langle E^2 \rangle_T - \langle E \rangle_T^2}{T^2}. \quad (4)$$

Since the Wang-Landau algorithm can give only static information, we also used the Metropolis algorithm to study fluctuation around an equilibrium state or among equilibrium states.

III. RESULTS AND DISCUSSION

We calculated the specific heat as a function of temperature using the Wang-Landau algorithm, as shown in Fig. 2. The bipartite lattices (T2, T3, T10, and T11) show a phase transition to the antiferromagnetically ordered ground state at the same critical temperatures as their ferromagnetic cases, which are represented by the vertical lines. For strongly frustrated lattices (T1, T4, T7, T8, and T9), the specific heat shows only a broad maximum without a critical feature, implying a disordered

TABLE I. Name, number of lattice points per basis (B), bipartiteness (Bip.), coordination number (z), antiferromagnetic ground state energy per bond (E_g^{AF}), ferromagnetic and antiferromagnetic transition temperatures (T_c), exact residual entropy (S_0), and ground state for each Archimedean lattice. Ferromagnetic transition temperatures are from Ref. [14], where exact values are given. Results of this work is in bold.

Name	B	Bip.	z	E_g^{AF}	T_c^{F}	T_c^{AF}	S_0	Ground state
T2 Square	(4 ⁴)	Y	4	-1	2.2692	$=T_c^{\text{F}}$	ln(2)	Long-range order
T3 Honeycomb	(6 ³)	Y	3	-1	1.5187	$=T_c^{\text{F}}$	ln(2)	Long-range order
T11 CaVO (CaV ₄ O ₉) ^a	(4, 8 ²)	Y	3	-1	1.4387	$=T_c^{\text{F}}$	ln(2)	Long-range order
T10 SHD ^b	(4, 6, 12)	Y	3	-1	1.3898	$=T_c^{\text{F}}$	ln(2)	Long-range order
T6 SSL ^b	(3 ² , 4, 3, 4)	N	5	-0.6	2.9263	1.261(1)	ln(2)	Long-range order
T5 Trellis	(3 ³ , 4 ²)	N	5	-0.6	2.8854	0.19(2)	ln(2)L	Long-range order^c
T7 Bounce	(3, 4, 6, 4)	N	4	-0.6667	2.1433		0.0538N	Spin ice
T4 Maple leaf	(3 ⁴ , 6)	N	5	-0.4667	2.7858		0.0538N	Spin ice
T9 Star ^a	(3, 12 ²)	N	3	-0.5556	1.2315		0.2509N	Spin ice
T1 Triangular	(3 ⁶)	N	6	-0.3333	3.6410		0.3231N	Spin liquid
T8 Kagome	(3, 6, 3, 6)	N	4	-0.3333	2.1433		0.5018N	Spin liquid

^aT11 and T9 are also called bathroom tile and expanded kagome, respectively.

^bSSL and SHD are abbreviations for Shastry-Sutherland lattice [16] and square-hexagonal-dodecagonal, respectively.

^cLong-range order only in one direction.

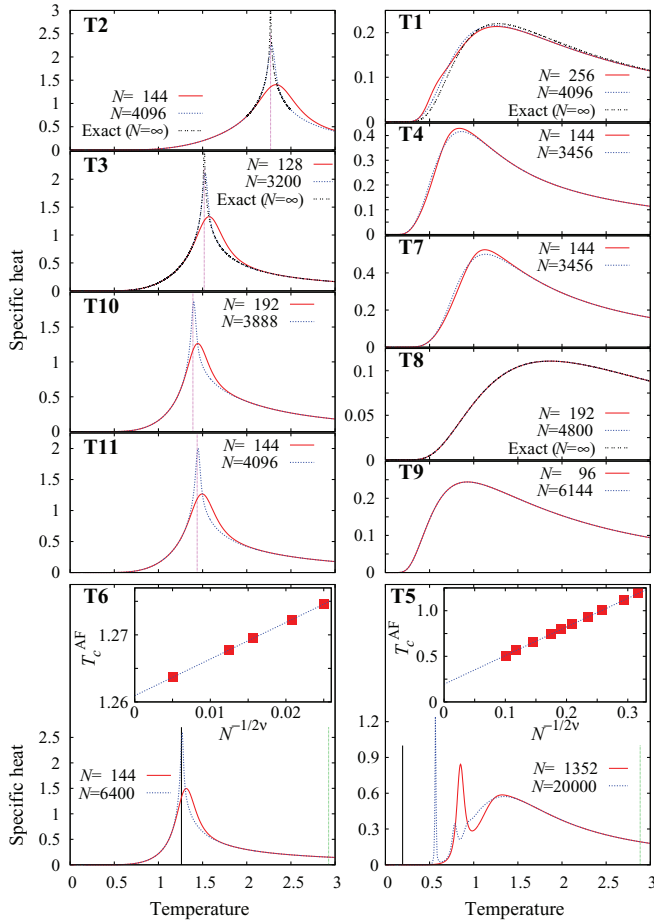


FIG. 2. (Color online) Specific heat as a function of temperature in the Archimedean lattices. Upper left panel is for bipartite lattices (T2, T3, T10, and T11) with long-range-ordered ground states. Vertical dashed lines represent exact $T_c^F = T_c^{AF}$. Upper right panel is for strongly frustrated lattices (T1, T4, T7, T8, and T9). In the case of weakly frustrated lattices (T6 and T5), the antiferromagnetic critical temperatures (T_c^{AF}) were calculated by the finite-size scaling shown in the inset with the critical exponent $\nu = 1$ and $2.3(1)$ for T6 and T5, respectively. They are $T_c^{AF} = 1.261(1)$ for T6 and $T_c^{AF} = 0.19(2)$ for T5. The two vertical lines represent T_c^F (green, right) and T_c^{AF} (black, left). Exact results of the infinite-size lattice are from Refs. [3–5] for the square, triangular, and kagome lattices, respectively.

ground state. Another important feature is very weak size dependence of the specific heat, which can be understood by the absence of the long-range correlation.

In the case of T6 (SSL), the frustration is weak and an ordered ground state is realized. However, the transition temperature $T_c^{AF} = 1.261(1)$ is much lower than its ferromagnetic one ($T_c^F \approx 2.9263$). The transition temperature was obtained by the finite-size scaling of $T_c^{AF}(N) = T_c^{AF} + AN^{-1/2\nu}$ with the critical exponent $\nu = 1$ of the two-dimensional Ising universality class and a lattice-dependent constant A [23]. The trellis lattice (T5) shows both of size-independent broad peak and size-dependent diverging peak. The latter represents a phase transition at $T_c^{AF} = 0.19(2)$ with $\nu = 2.3(1)$. Large value of ν implies the one-dimensional character of the ordering.

To investigate more about the ground state, we investigated the residual entropy S_0 of the Archimedean lattices. It was

calculated directly from the DOS $[\rho(E)]$ obtained by the Wang-Landau algorithm: $S_0 = \ln[\rho(E_0)]$, where E_0 is the lowest energy. The normalization of $\sum_i \rho(E_i) = 2^N$ should be done before the calculation. The residual entropy was confirmed to be $S_0 = \ln(2)$ for the ordered ground states (T2, T3, T10, T11, and T6), as expected. The degeneracy 2 is from the Kramers degeneracy theorem.

As for strongly frustrated lattices (T1, T4, T7, T8, and T9), the residual entropy is proportional to the number of lattice points N , which can be understood by applying Pauling’s method to the ice model [24]. Ice can be considered as a network of corner-sharing tetrahedrons, which are composed of an oxygen atom in the center and four hydrogen atoms at the corners. The hydrogen atom has two possible positions (inside and outside of the tetrahedron), but should follow the ice rule, two-in-two-out for each tetrahedron at zero temperature. Therefore, the residual entropy of ice can be calculated by $S_0^{\text{ice}} = \ln[2^N(6/16)^{N/2}] = (N/2) \ln(3/2)$, where 2^N is the total number of states and $N/2$ is the number of tetrahedra. $(6/16)$ means that only 6 states out of 16 satisfy the ice rule for a tetrahedron. This result is not exact, but only 1.4% lower than recent estimates by the Monte Carlo method [25] and the series expansion [26]. If we apply the same method to the triangular and the kagome lattices, their residual entropies become $S_0^{T1} = \ln[2^N(6/8)^{2N}] \approx 0.11778N$ and $S_0^{T8} = \ln[2^N(6/8)^{2N/3}] \approx 0.50136N$, respectively. Since each triangle should satisfy the 2-1 rule (2 up and 1 down spins or 2 down and 1 up spins) to minimize the energy, only six states out of eight are possible in the ground state. This method is very close to the exact result for the kagome lattice ($S_0^{T8}/N \approx 0.50183$) [5], but fails in the triangular lattice, where the exact result is $S_0^{T1}/N \approx 0.32307$ [4]. Maple-leaf (T4) and bounce (T7) lattices have a unit cell with six points that compose a hexagon, which is arranged in a triangular lattice (see Fig. 1). To minimize energy, each hexagon should have one of the two configurations ($\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$) and ($\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow$). Since energy is lower when the nearest-neighboring hexagons have different kind of configuration, if we define the first kind of hexagon as spin “up” and the second, “down,” the interaction between hexagons is “antiferromagnetic.” Therefore, they can be regarded as a triangular Ising antiferromagnet composed of hexagons, and have the residual entropy of S_0^{T1} per hexagon or $S_0^{T4,T7}/N = S_0^{T1}/6N \approx 0.05384$ per lattice point. As its nickname (expanded kagome lattice) implies, the star lattice (T9) is a kagome lattice of dimers with spin ($\uparrow\downarrow$) or ($\downarrow\uparrow$). Thus, its residual entropy can be obtained by $S_0^{T9}/N = S_0^{T8}/2N \approx 0.250916$. As shown in Fig. 3(a), the Wang-Landau algorithm gives consistent results for the residual entropy of strongly frustrated lattices within 0.2%.

In the case of the trellis lattice, the residual entropy is proportional to the linear size L . This can be understood from its ground state shown in the inset of Fig. 3(b). Spins are antiferromagnetically ordered in each row: ($\uparrow\downarrow\uparrow\downarrow\dots$) or ($\downarrow\uparrow\downarrow\uparrow\dots$). For example, when the first row has a configuration ($\uparrow\downarrow\uparrow\downarrow\dots$), the second row should have the configuration ($\downarrow\uparrow\downarrow\uparrow\dots$). Now the third row may have either configuration ($\uparrow\downarrow\uparrow\downarrow\dots$) or ($\downarrow\uparrow\downarrow\uparrow\dots$). Therefore, there exists degeneracy of two every other rows and the residual entropy becomes $S_0 = \ln(2^L)$. The Wang-Landau simulation supports this conclusion. This one-dimensional long-range

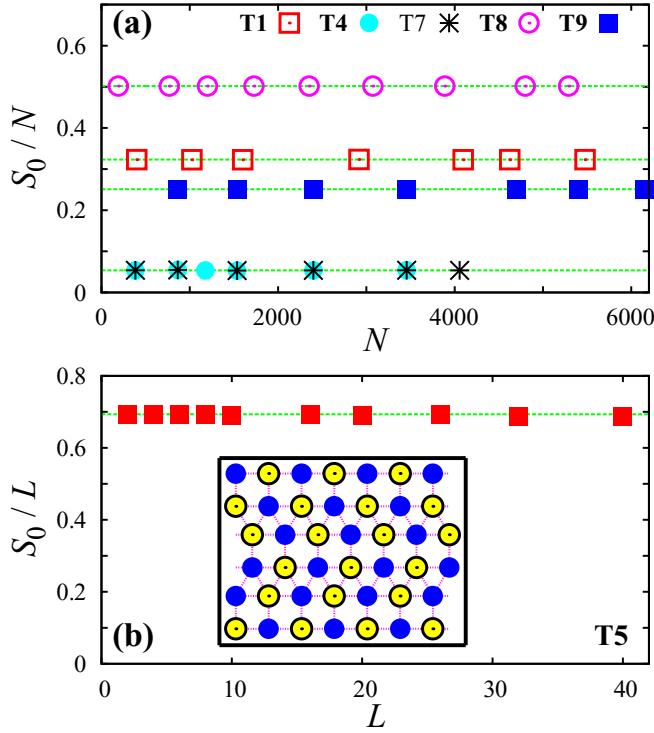


FIG. 3. (Color online) (a) Residual entropy S_0 per lattice point N calculated by the Wang-Landau method for strongly frustrated lattices without long-range-ordered ground state. Lines represent the exact results for each lattice. (b) In the case of the trellis lattice (T5), S_0 is proportional to the linear size L because the long-range order appears only in one direction. One of the ground states is shown in the inset.

ordering is possible because there exist constraints induced by neighboring rows.

Finally, we classified the ground state of the Ising antiferromagnet on the 11 Archimedean lattices. Unfrustrated and weakly frustrated lattices have a long-range-ordered ground state for their residual entropy per site goes to zero. The trellis lattice is a special case where the long-range order is only in one direction. Strongly frustrated lattices have extensive residual entropy and their ground states are disordered even at 0 K. There are three possible phases: spin glass, spin ice, and spin liquid. Since there is no disorder in lattice or magnetic interaction, which is required for the spin glass, they are either spin ice or spin liquid. The difference between spin ice and spin liquid comes from their flexibility or dynamic property: The spin ice is frozen and the spin liquid fluctuates. In order to study the fluctuation behavior, we performed a single-site-update Metropolis simulation with $L = 40$. We calculated the Edwards-Anderson order parameter q_{EA} [27] to measure degree of freezing. It was proposed for the order parameter of spin glasses, but it can be used generally to study freezing phenomena even in ferromagnets and antiferromagnets. It can be defined in a few ways [28–31], which are equivalent to one another. We adopted

$$q_{EA} = \frac{1}{NM} \sum_i^N \left| \sum_t^M S_i(t) \right| \quad (5)$$

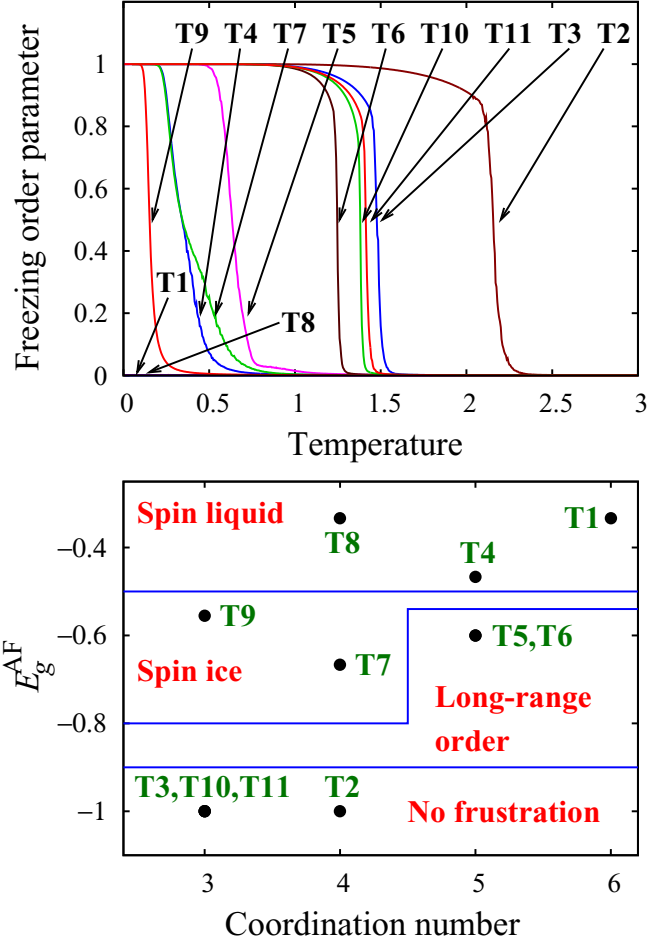


FIG. 4. (Color online) The freezing order parameters vs temperature (upper panel) and the ground state energy per bond (E_g^{AF}) and the coordination number of the 11 Archimedean lattices with their ground states indicated (lower panel). The freezing order parameters were obtained by Eq. (5) with lattice size $L = 40$ and number of measurements $M = 2 \times 10^6$.

from Ref. [30], where M is the number of measurements after equilibration, which is fixed to be $M = 2 \times 10^6$ in this calculation. The spins begin to freeze at the freezing temperature T_f , where the freezing order parameter deviates from zero. q_{EA} does not depend on M for $M \geq 1 \times 10^6$ except very close to the freezing temperature T_f , where larger M makes the freezing sharper. T_f are in the order of T2, T3, T11, T10, T6, T5, T7, T4, and T9. The former four lattices are unfrustrated and the next two are weakly frustrated with long-range-ordered ground states, as expected. The last three lattices can be classified as a spin ice because the spins are frozen without long-range order at zero temperature. As for T1 and T8, the freezing order parameters saturate to very small values, which decrease as $1/\sqrt{M}$. It means spins fluctuate actively even at 0 K and so spin liquid phase.

These results are consistent with the theory about the degree of frustration in Ref. [10]. They proposed two parameters to determine the degree of frustration: ground state energy per bond E_g^{AF} and the coordination number z . $E_g^{AF} = -1$ for unfrustrated lattices and larger E_g^{AF} means more frustration.

Smaller z also strengthen the frustration effect. This is also consistent with the residual entropy: Larger residual entropy implies more frustration. Summarizing all these, the degree of frustration was determined for seven frustrated cases as shown in Fig. 4 and Table I.

IV. CONCLUSIONS

In summary, we studied systematically the frustration effect of the Ising antiferromagnet on the Archimedean lattices. From the results of specific heat, exact residual entropy, and freezing

order parameter we determined ground states of frustrated lattices. They can be listed in the order of degree of frustration: Shastry-Sutherland lattice and the trellis lattice (long-range order); bounce, maple-leaf, and star lattices (spin ice phase); triangular and kagome lattices (spin liquid).

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