Monte Carlo Simulations of XY Spins on Exotic 2D Lattices

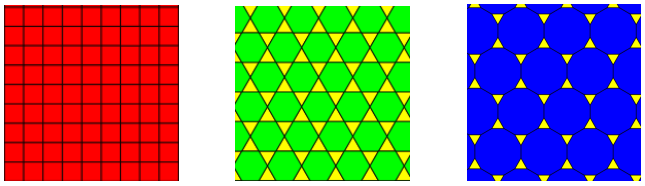
Alexander Lawson[1]

[1] *Undergraduate, Sc.B. Physics, Brown University, Providence, Rhode Island 02912, USA*

INTRODUCTION

The 2D XY Model is a statistical model for spins on a two dimensional lattice, where spins are defined by an angle in the plane, and interact with nearest-neighbors with an energy given by $Jcos(\theta_1 - \theta_2)$. This model is of particular interest in Condensed Matter Physics, as it demonstrates an unusual phase transition, called a Kosterlitz-Thouless transition (KT transition), found in low temperature magnetic systems. This model is particularly useful as it lends itself well to numerical simulations of strongly correlated spin systems, where analytical solutions can be unyielding.

Anti-ferromagnetic spin lattices: lattices where spin-spin coupling favors opposite orientations ($J < 0$), especially those where nearest-neighbor interactions form odd numbered loops, are a critical area of research today. As spins forming odd-numbered loops cannot satisfy their ground state energy with all neighbors, the lattices may exhibit complex phases based on long range entanglement, and evade mean-field approaches. These lattices are considered 'geometrically frustrated'. The 2D 'Kagome' lattice, which is exhibited in real crystals, features nearest-neighbor connections that form triangles (Fig 1), and is known for entering a 'spin-liquid' phase at low temperatures. Though less studied due to its lack of physical analogs, the 'Truncated-Hexagonal' (TH) lattice also features triangular loops (Fig1), and shares structural similarities with the 'Kagome' lattice.



(a) Square (b) Kagome (c) Truncated Hexagonal (TH)

FIG. 1. (a) Square, (b) Kagome and (c) Truncated Hexagonal (TH) tilings. Lattices are constructed by placing a site on every vertex. All share the property that every site appears the same given some rotation. The TH lattice differs in that although every site is the same, not every connection between neighboring sites is the same.

Here, a Simulated Annealing Monte Carlo Algorithm is used to characterize the behavior of anti-ferromagnetic spins on the Kagome and TH lattices comparing results to the non-frustrated Square Lattice.

THEORY

Classical XY Model

The Classical XY model seeks to model the interaction of spins on a two-dimensional lattice by describing each spin as a unit vector in the plane, where interactions are given by:

$$\mathcal{H} = \sum_{\langle ij \rangle} Jcos(\theta_i - \theta_j) + \sum_i Hcos(\theta_i) \tag{1}$$

$\langle ij \rangle$ indicates a sum over all nearest neighbors. H is dependent on the magnitude of an applied field, chosen arbitrarily in the $\hat{x}$ direction. Assuming $H = 0$, when the interaction energy coefficient $J < 0$, the spins tend to align causing the formation of magnetized domains (ferromagnetism (FM)), while $J > 0$ tends toward anti-alignment and no net magnetization in domains (anti-ferromagnetism (AFM)). Though the code fully generalizes to $H \neq 0$, the analysis provided will all be for the case of $H = 0$ and $J = -1$.

Topological Excitation

In these systems, there exists a phase transition around a critical temperature T_c, seen as a sudden change in magnetic susceptibility χ. This transition is related to the formation of vortices and anti-vortices (Fig 2.). I'll present the overview of this transition, called a Kosterlitz-Thouless (KT) transition in terms of a ferromagnetic system ($J < 0$), though similar reasoning holds for a square anti-ferromagnet ($J > 0$).

Neglecting the applied field, for a system at relatively low energy nearest neighbor spins will be close in angle, so $\cos(\theta_i - \theta_j) \approx 1 - \frac{1}{2}(\theta_i - \theta_j)^2$. If we assume the spins form a continuous scalar angle field $\theta_S(\vec{r})$, we can write $(\theta_i - \theta_j) \approx \vec{\nabla}\theta_S(i) \cdot d\vec{l}$, where l is a length between sites. Therefore the difference from the ground state energy can be given as:

$$E_{\text{excitations}} \approx \frac{|J|}{2} \int_A |\vec{\nabla}\theta_S(\vec{r})|^2 dA \tag{2}$$

There is a strong similarity between the energy of this system, and that of a 2D electric field $\vec{\mathcal{E}} = \vec{\nabla}\phi$:

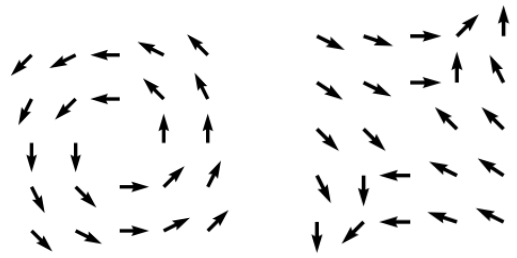
$$E = \frac{\epsilon_0}{2} \int_A |\vec{\nabla}\phi|^2 dA \tag{3}$$

In fact the behavior of this system is quite similar to that of a 2D coulomb gas. Keeping with this analogy, excitations called vortices act much like point charges, and their behavior governs the KT transition.

A vortex of vorticity q can be defined by and asking how the angle rotates as a when walking around a closed loop C.

$$q = \frac{1}{2\pi} \oint_C \vec{\nabla}\theta_S(\vec{r}) \cdot d\vec{r} \tag{4}$$

If the spin rotates in the same direction as a path around the loop, $q = 1$ and the loop is typically called a vortex (Fig.2a), though vortex is often used as a catch-all term for any $q \neq 0$. If the spin rotates in the opposite direction as a path, $q = -1$ and the loop is called an anti-vortex (Fig.2b). Since θ_S is considered continuous,



(a) vortex ($q = 1$) (b) anti-vortex ($q = -1$)

FIG. 2. Isolated vortex (a) and anti-vortex (b) for spins on square lattice.

q must be an integer. Unlike one misaligned spin, where energy can continuously dissipate, the discrete values of q imply that a vortex cannot continuously relax and 'lose its vorticity'. However, a vortex can move through the lattice. This stability and non-locality leads to a characterization of vortices as 'topological' defects. An isolated vortex has an energy and entropy:

$$E \approx \pi |J| q^2 \ln \frac{R}{a} \tag{5}$$

$$S \approx 2k_B \ln \frac{R}{a} \tag{6}$$

where R is the length of the lattice, and a is the number of sites per unit length. Considering only $q = \pm 1$, the critical temperature (where $F = U - T_c S = 0$) is given by:

$$T_c = \frac{\pi |J|}{2k_B} \tag{7}$$

$T < T_c$ does not forbid vortices completely. Like opposing charges in an electric field, total energy is decreased by bringing vortices opposite vortices together, and like vortices apart:

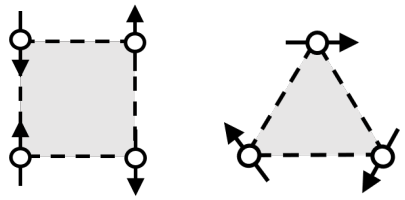
$$E_{\mathrm{vort}_1,\mathrm{vort}_2} = 2\pi |J| q_1 q_2 \ln \frac{|\vec{r}_1 - \vec{r}_2|}{a} \tag{8}$$

For sufficiently close vortex/anti-vortex pairs, the energy in Eq.8 is less than that of Eq.5. Therefore, although for $T < T_c$ single vortices are not thermodynamically favorable, sufficiently close vortex/anti-vortex pairs ($q = 1$ and $q = -1$) are still allowed.

Signatures of this transition can be seen in a spike in Specific Heat C_V and a divergence in magnetic susceptibility χ around T_c.

Geometry and Frustration

Though KT transitions have been understood for over 40 years, more recent research concerns anti-ferromagnetic lattices where nearest-neighbor connections form odd numbered loops. Specifically on triangular loops, the lowest energy configuration for two neighboring spins (opposite directions) cannot be satisfied by connections between all three. Contrasting with the 'alternating' ground state of anti-ferromagnetic (AFM) spins on a square (Fig.3a), AFM spins on a triangle take on a ground state that satisfies the '120 degree rule' (Fig.3b).



(a) a square ground state (b) a triangle ground state

FIG. 3. One of many ground states for XY spins on a (a) square and (b) triangle. Arrows are spins, dashed lines are nearest neighbor connections. In both of these, there is a rotational degeneracy.

One would expect lattices that include triangular loops to have ground states where the 120 degree rule is satisfied. The triangular lattice has only one configuration (barring rotational symmetry of all spins) where all triangles satisfy the rule. For the Kagome lattice, multiple ground states(, not just those permitted by rotational symmetry,) satisfy the '120 degree' rule.

Here, I present another semi-regular lattice, the 'Truncated Hexagonal' (TH) lattice, and compare its thermodynamic qualities with those of the Kagome lattice. As

shown in Fig.1 and Fig.7 an approachable way to think about this lattice is that it can be constructed by taking a Kagome lattice, and pulling apart the triangles such that they no longer share a vertex/site, but instead share a nearest-neighbor connection between vertices. To respect this similarity, simulations of the Kagome and TH lattices had the same number of hexagons and dodecagons respectively. This approximates simulating a Kagome lattice before and after it has been 'stretched out'.

The TH lattice, though to my knowledge not yet studied in this context, also has an exponential number of ground states, largely motivating this comparison. In the Appendix, I present a one class of ground states for the TH lattice where the number of possible ground states scales exponentially with lattice size.

METHODS

A Simulated Annealing Monte Carlo algorithm was used to calculate a possible configuration of the ensemble of spins at each given step. Each lattice site is define by a discrete angle $\theta_i \in \frac{2\pi}{n} * \mathbb{Z}_n$, where n is the resolution, or number of 'ticks' that the angle can access. At each step, every lattice site chooses a new θ_i from a Boltzmann distribution (Eq.4) where E_i is the sum of interaction energies with its nearest neighbors and the applied field (Eq.3).

$$\mathbb{P}(E_i) = \frac{1}{Z} e^{\frac{E_i}{k_B T}}, Z = \sum_i e^{\frac{E_i}{k_B T}} \tag{9}$$

One problem that could occur with updating all spins at each step is that if the spins were updated in a defined order, some spins (those occurring early in the list) would have their Boltzmann probabilities computed using the spins of the previous, 'non-updated' time step, while those occurring later in the list would have Boltzmann probabilities updated based on the spins of the updated step. To avoid this 'preferential treatment' of certain spin sites, all sites are updated using the Boltzmann probabilities calculated from the spins of the previous step. Worth noting is the lack of spin 'inertia' in this method. Since the angle for a given site is only determined based on the configuration of the neighboring spins at the previous time step, there is no direct preference for a spin to maintain its state. There is however an indirect preference for maintaining a spin state, since a spin at a time-step is determined by neighboring spins at the previous time step, which are determined partly by that spin two time steps before. The goal of this is to increase 'mobility' between states for the larger system, though there are likely better update schemes for quickly accessing a larger variety of states.

To access low energy states, Temperature is slowly decreased via:

$$T = T_0 \exp \frac{\text{num steps}}{(\text{total num steps}) \cdot \tau} \tag{10}$$

Total energy is calculated at each time step, and the data is analyzed to extract thermodynamic quantities. Specific heat is then calculated using:

$$C_V = \frac{\text{std}(E)^2}{T^2 k_b} \tag{11}$$

where energies for each time step are binned, and T is the average of the corresponding temperatures for those energies. From this a change in Entropy is calculated using:

$$\Delta S = \int \frac{C_V}{T} dT \tag{12}$$

Torus-like boundary conditions were implemented with lattice sizes (highly limited by computational power) chosen to complement the periodicity of ground states. For example, the ground state presented in the appendix (Fig.7) for the truncated-hexagonal lattice has a periodicity of 27 connections between like sites, taking 7 hours to run for 100,000 steps. Due to the overwhelming computational load, a comparison of thermodynamic quantities between lattice sizes is not presented here.

Included in the code files is an 'interactive' version of the simulation, called `XY_MC_interact.py` where J, T and H can be tweaked to view qualitative behavior. This was done using the python package Tkinter.

RESULTS

First, looking at energy as function of temperature, its clear that the Simulation brings the system down to a low-energy state that agrees with the '120 degree' rule in in the case of both the TH and Kagome lattices. For the Kagome lattice, each site has 4 nearest neighbors, all of which are on triangles, so the total energy per site should be $4J \cos \frac{2\pi}{3} = -2$. Similarly for the TH lattice, each site has 2 nearest neighbors that share a triangle with it, and one nearest neighbor that does not. Therefore the ground state energy per site should be $2J \cos \frac{2\pi}{3} + J = -2$. The Square Kagome and TH lattices reached $\frac{E}{N} = -3.995$, -1.997, and -1.987 respectively. It seems that the simulation was particularly effective on the Square and Kagome lattices, but slightly less effective on the TH lattice, possibly due to the high lattice size chosen to complement the periodic ground state shown in the Appendix.

In the case of specific heat in Fig.5, first looking at the square lattice, the peak at $T = 1.22$ seems somewhat close to the critical temperature predicted by the Kosterlitz-Thouless transition $T_c = \frac{\pi |J|}{2 k_B} \approx 1.57$ for

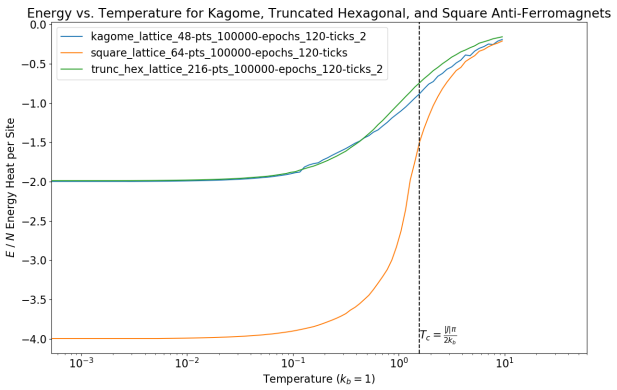


FIG. 4. Energy per site for Kagome, Truncated Hexagonal and Square Lattices

$k_B = 1$. This appears to be close enough to qualify that this peak should be a KT transition. The deviation from the expected value may be from disagreement with approximations made in the derivation of T_c, finite lattice size, or other phenomena like spin wave formation. After returning from that peak, the specific heat levels out around $\frac{C_V}{N} \approx 2.1$, then drops off around $T = 0.004$.

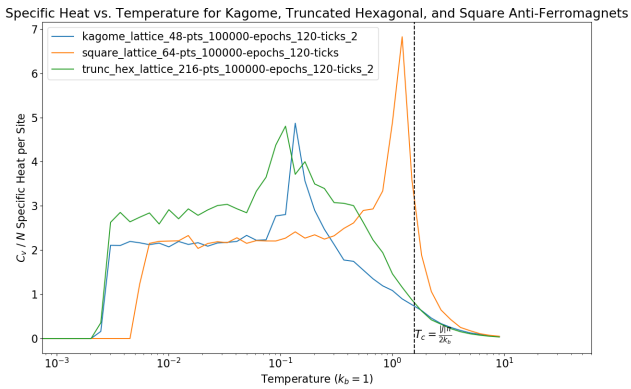


FIG. 5. Specific Heat per site for Kagome, Truncated Hexagonal and Square Lattices

For all three of these lattice site, that drop-off is likely non-physical, since the simulation returns a "dividing by zero message" around that temperature, and the energy of the lattice ceases to fluctuate. This is because the probabilities of all but one state get so close to zero that the computer sets them exactly equal to zero and the motion freezes out abruptly.

The TH and Kagome lattices both share a peak in specific heat around $T \approx 0.12$. Spikes in specific heat are signatures of phase transitions, though it's not clear to me exactly what phase transition this is. Its peak is an order of magnitude different from the KT transition, so I doubt that the same phenomenon is at play. Though, a definition of vortices based on rotating every other spin and using Eq.4 would apply well for a square anti-ferromagnet, a generalization of vorticity for odd-numbered loops seems very hard to define. It may be that an analog of topological excitations like vortices doesn't exist at all for these frustrated lattices. If I had to guess, I would imagine the transition is related to spins aligning on triangles based on the '120 degree rule', and those triangles beginning to act more like composite spin objects. That idea seems more compelling for the TH lattice than Kagome, as triangles are more easily understood as separate from each other in the TH lattice, where they share only a nearest neighbor connection, as apposed to triangles on the Kagome lattice that share a site. It certainly seems that this transition is a signature of geometrical frustration.

There seem to be two notable differences between the Kagome and TH curves. First, the peak is broader for the TH lattice. In highly general terms, I would imagine that the 'non-frustrated' connections between triangular loops have a 'dulling' effect on interactions between those triangular loops. In essence, that connection is one more place to store energy, and 'buffer' the interactions between triangular loops in the Kagome lattice.They would causing a one-step time-delay in an state change moving from triangle to triangle, and add a 'damping'-like effect on the interaction energy between sites. I hope to investigate this in more detail once I better understand the phase transition associated with these peaks in the Kagome lattice.

The Kagome and Truncated Hexagonal lattices also differ in that they level out at $\frac{C_V}{N} \approx 2.1$ and $\frac{C_V}{N} \approx 2.9$ respectively. Strangely, the Kagome Lattice seems to share that behavior with the square lattice, while the TH lattice differs from both of them. This may be a coincidence obscured by numerical imprecision. Qualitatively, as can be seen in `XY_MC_interact.py`, at these particularly low temperatures one can see that the overall state of the system fluctuates much less than the individual spins within it. Though I won't attempt this calculation here, I would guess that the same specific heat per spin could be found in a system comprised of one spin surrounded by nearest neighbors that complement the lattice's ground state. It may also be that this low energy specific heat is a function of the number of neighbors per site (4 for Square and Kagome, and 3 for TH).

Lastly, integrating $\frac{C_V}{T}$,I found that the difference in Entropy of the lowest energy state found from the state at $T = 10$ was actually highest for the truncated hexagonal lattice($\Delta S = -18.9$), followed by the square lattice($\Delta S = -16.0$), and lowest for the Kagome lattice($\Delta S = -14.2$). Since at infinite temperature, spins are completely independent, and $\frac{S}{N} = \log(2)$, This would seem to suggest that the ground state entropy of the Truncated Hexagonal lattice, is lower than that of the square lattice. However, for a number of reasons, this is

probably an non-physical result.

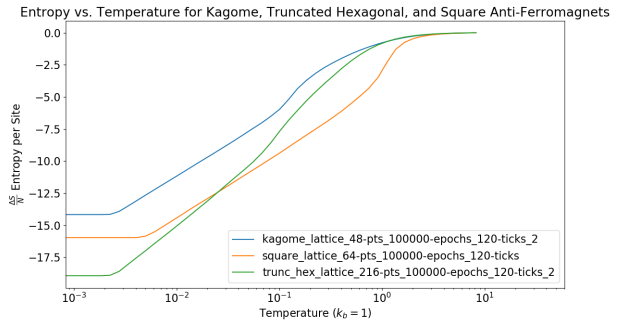


FIG. 6. Change in Entropy per site for Kagome, Truncated Hexagonal and Square Lattices

Firstly $C_V \neq 0$ at $T = 10$ for any of these lattices, so integration from a higher temperature would be necessary to refine this result. Secondly, we know the Kagome and TH lattices actually have exponentially many ground states and therefore at $T = 0$, should have $S \sim N$, while (barring rotations) the square lattice only has one ground state $S = 0$. At sufficiently low temperatures, the simulation method only focuses in on one of these many ground states. Although the degenerate energy of these multiple ground states should mean that they are equally likely, probabilities of states are determined for each spin, not for the lattice as a whole. Because of this, each spin has a tendency to continue to satisfy low energy interactions with its neighbors, and groups of spins have little mobility. Therefore the lattice does not easily transfer between low global energy states.

CONCLUSIONS

The Truncated-Hexagonal lattice, though far less studied than the Kagome lattice due to its lack of physical analogs, shares a number of similarities with the it. They share a similar phase transition, and both have degenerate ground states. For that reason, numerical and theoretical studies of the TH lattice may be useful as a means of separating out what behavior is inherent to only the Kagome Lattice from what behavior is inherent to frustrated spin systems with degenerate ground states.

More advanced measurements in numerical simulations will likely shed more light on why the $T \approx 0.1$ phase transition appears more spread out in the TH lattice, and reflect the true ground state entropies. Similarly, larger simulations with more advanced energy optimization techniques would help to clarify the behavior of these thermodynamic quantities.

Appendices

A ground state for the TH lattice can be constructed as follows:

For any triangular loop, the lowest anti-ferromagnetic energy state possible satisfies the '120 degree' rule, while for a single connection (not on any loop) the lowest possible energy is given by spins in opposite directions. Any class of ground states that satisfies both of these conditions gives the lowest energy ground state of the system.

Lets assume one spin is set fixed, and call it a. let $b = a + \frac{2\pi}{3}$, $c = a - \frac{2\pi}{3}$. So any triangle that contains both a, b, and c is a lowest energy state. We can define: $\bar{a} = a + \pi$, $\bar{b} = b + \pi$, and $\bar{c} = c + \pi$. Any triangle that contains both $\bar{a}$, $\bar{b}$, and $\bar{c}$ is also in a lowest energy state. The lowest energy state for any isolated connection is given by a connecting to $\bar{a}$, b connecting to $\bar{b}$ or c connecting to $\bar{c}$. In the figure below, all defined spin states satisfy these rules. Some dodecagons have all vertices left unlabeled, and are surrounded entirely by alternating $a/\bar{a}$, $b/\bar{b}$ or $c/\bar{c}$. Taking a dodecagon surrounded by $a/\bar{a}$ for example, where $\bar{a}$ is at the top, there are two possible configurations (starting from the top left and going around clockwise): $[b, c, \bar{c}, \bar{b}, b, c, \bar{c}, \bar{b}, b, c, \bar{c}, \bar{b}]$ and $[c, b, \bar{b}, \bar{c}, c, b, \bar{b}, \bar{c}, c, b, \bar{b}, \bar{c}]$. Both of these satisfy the '120 degree' for triangles and the 'opposite spin' rule for isolated connections. This same system generalizes to dodecagons surrounded by $b/\bar{b}$ and $c/\bar{c}$. So for each of these unlabeled dodecagons, there are 2 possible states that still satisfy ground state conditions. So the number of ground states in this class of ground states scales as $2^{\text{number of unlabeled dodecagons}}$ or $2^{\frac{\text{number of sites}}{18}}$.

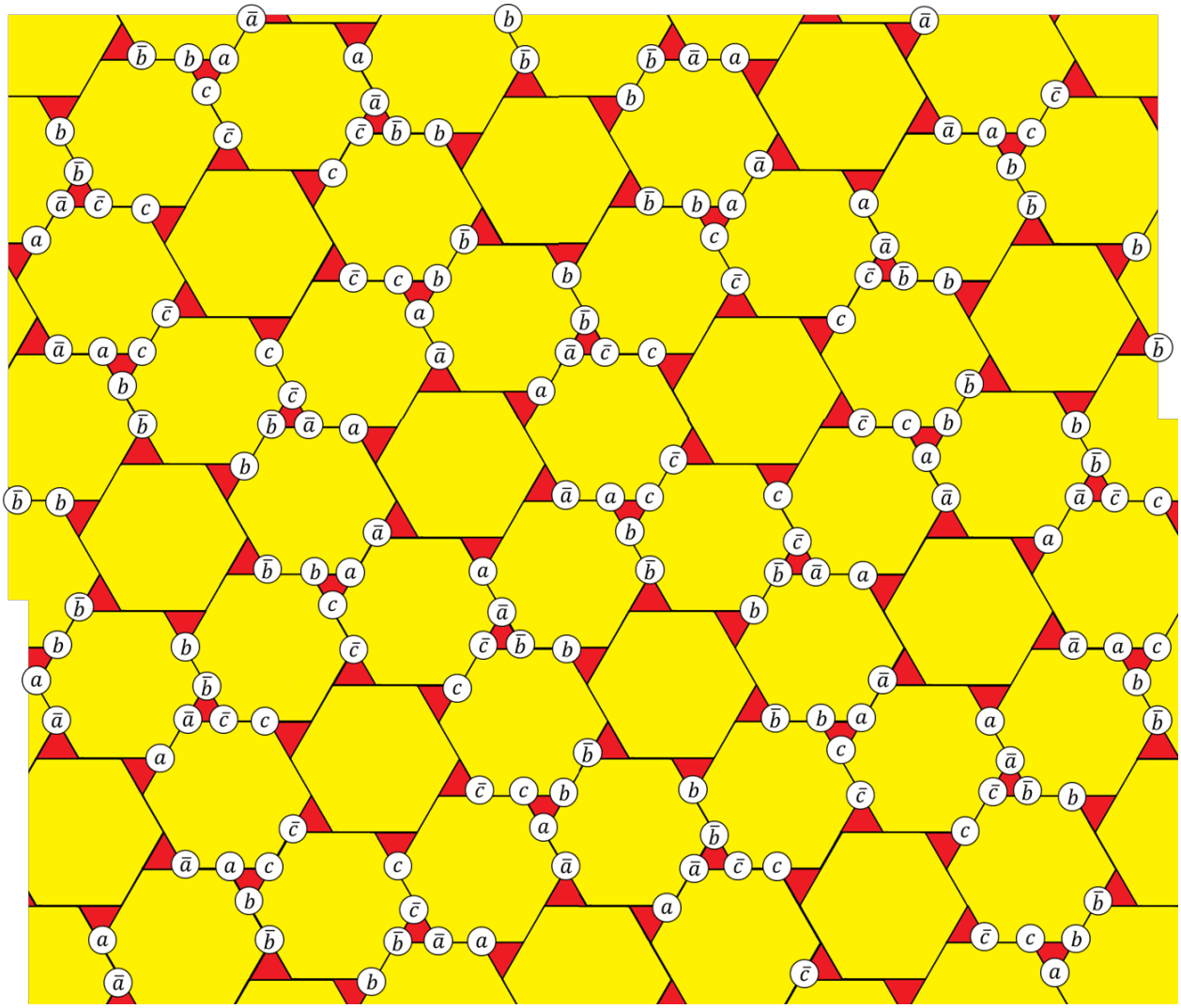


FIG. 7. A class of ground states for the Truncated Hexagonal Lattice