Cluster Algorithms for Spin Systems

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I. ISING MODEL

The ising model is one of the simplest mathematical models to study phase transitions; for example ferromagnetism. It consists of a configuration of electron spins (σ_i) that can take discrete values ($\pm$). The spins are distributed over a d-dimensional lattice and interact with each other via the exchange interaction as given by the Hamiltonian below.

$$H_{ising} = \sum_{\langle ij \rangle} \sigma_i \sigma_j \tag{1}$$

The transition from a random, disordered state of spins to a ferromagnetic state with all spins aligned in one particular direction occurs at the critical temperature (T_c). In an infinitely large system, thermodynamic quantities like magnetization, specific heat and magnetic susceptibility diverge at T_c. In this article, critical phenomena associated with 2D (square/kagome) and 3D (cubic/pyrochlore) lattices is studied using a variety of algorithms.

II. ORDER PARAMETER, CRITICAL BEHAVIOR AND UNIVERSALITY

Order Parameter is a physical quantity that distinguishes the ordered phase from the disordered phase. In ferromagnetic systems, the order parameter is magnetization (M) which responds to the external variable - temperature (T). Phase transition occurs at T_c where the magnetization takes a non-zero, finite value below T_c and is zero above it. Close to the critical point, thermodynamic quantities display a power law behavior.

$$M \sim (T_c - T)^{\beta} \tag{2}$$

$$\chi \sim |T - T_c|^{-\gamma} \tag{3}$$

$$C_v \sim |T - T_c|^{-\alpha} \tag{4}$$

$$\zeta \sim |T - T_c|^{-\nu} \tag{5}$$

χ, C_v and ζ are magnetic susceptibilty, specific heat and correlation length respectively. α, β, γ and ν are the associated critical exponents. For an infinite system, χ, C_v and ζ diverges. However, since we will be dealing with lattices of finite size, these thermodynamic quantities will produce a peak at T_c. This allows us to calculate the critical exponents which have unique values for a lattice of a given dimension. For example, in 2D, the ising model generates the following critical exponents : $\alpha = 0$, $\beta = 0.125$, $\gamma = 1.75$ and $\nu = 1$.

III. METROPOLIS ALGORITHM

- Initialize the spins of the system by assigning them +1 (spin up) or -1 (spin down) values at random. This is the high temperature phase where all the spins are oriented randomly.
- Select a random spin and flip it. If the change in energy (ΔE) is less than zero, then accept the new configuration otherwise accept it with a probability $p = \exp(-\beta \Delta E)$
- The previous two steps are repeated till all the lattice sites have been probed and the desired configurations are obtained.

An entire sweep of the Metropolis algorithm consists of N trial flips. Since it updates the spins one at a time, it can become quite inefficient at the critical temperature due to large autocorrelation time. There are other problems associated with it which will be discussed later.

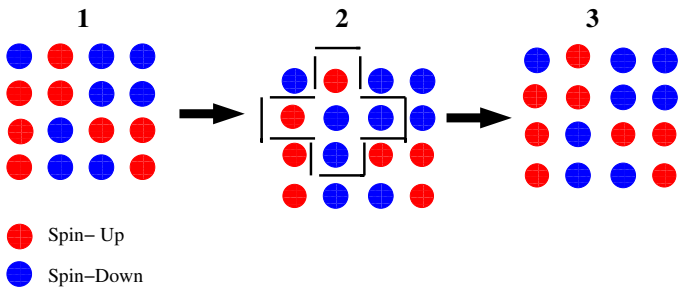

FIG. 1: Step 1 : High temperature phase with a configuration of randomly oriented spins on the square lattice. Step 2 : Flipping a spin and calculating the change in energy of the system. Step 3 : Accept the change to get to a new state. These steps are repeated to move into a perfectly ordered state in the low temperature regime.

IV. SWENDSEN-WANG ALGORITHM

- Initialize the spins on the lattice.
- If the nearest neighbor spins are aligned in the same direction, a bond is assigned to the pair with a probability $p = 1 - \exp(-2\beta)$.
- If two spins are connected by a bond, they belong to the same cluster. Spins without any bonds form a cluster by itself.
- Flip all the spins within each cluster with the probability $p = \frac{1}{2}$.
- The previous two steps are repeated till the desired number of configurations are obtained.

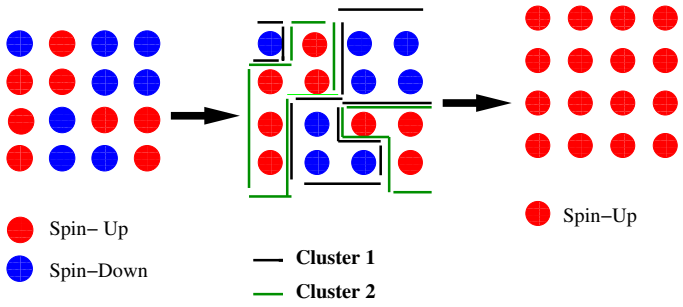

FIG. 2: Swendsen-Wang algorithm incorporates the formation of clusters based on spin distribution on the two dimensional lattice. This is followed by flipping of spins within a cluster with a probability of 0.5. In the low temperature phase, for a sufficiently large number of iterations, one moves into an ordered state.

V. WOLFF ALGORITHM

- Initalize the spins
- Pick a spin at random and establish bonds with its neighbor based on the orientation, i.e., parallel spins have bonds with probability $p = 1 - \exp(-2\beta)$. Spins connected by the same chain of bonds belong to the same cluster.
- Keep repeating the above step for all the aforementioned neighbors and grow the cluster
- After including all the spins in the cluster, flip all the spins within it.
- The above steps are repeated till the desired number of configurations are obtained.

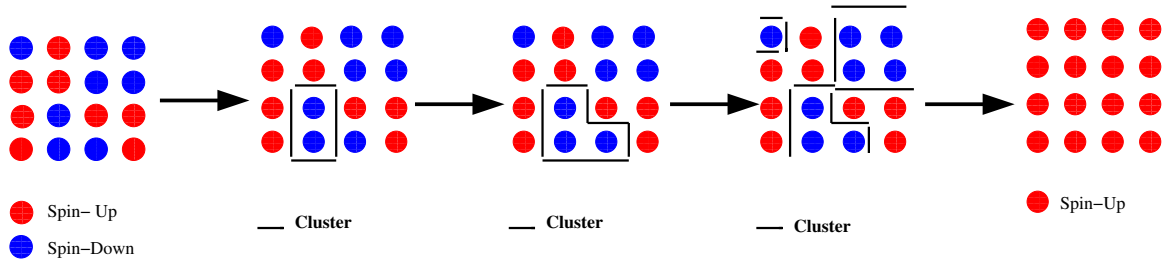

FIG. 3: In the Wolff algorithm, a cluster is generated by picking a spin at random and forming bonds with its neighbors with parallel orientation. New members are added to the cluster by taking the neighbors as the new seeds. Once the cluster is built, all spins within it are flipped.

Both the Swendsen-Wang and the Wolff algorithms are examples of cluster algorithms that incorporate global updating schemes by updating giant clusters at a time. As a result, these algorithms are better at dealing with the problem of critical slowing down that reduces the efficiency of the Metropolis algorithm.

VI. PHASE TRANSITION IN A 2D SQUARE LATTICE - ISING MODEL

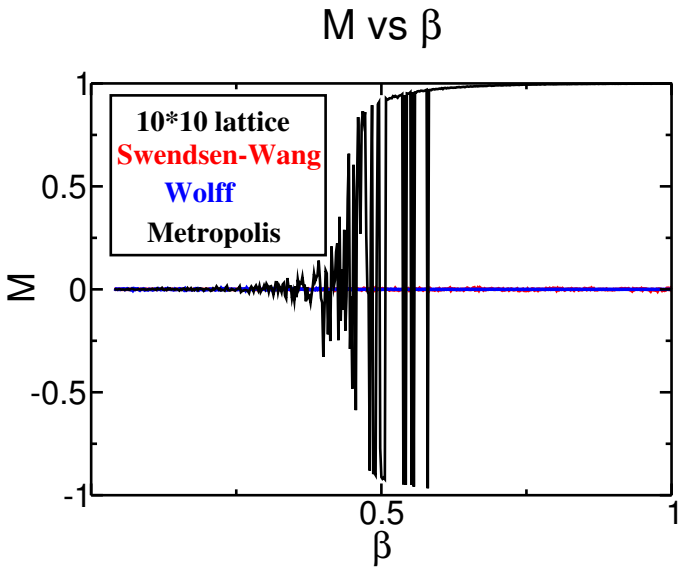

FIG. 4: Average Magnetization (M) versus Inverse of Temperature (β) for Metropolis, Swendsen-Wang and Wolff algorithms on a 2D square lattice. Since there is an equal probability for all the spins to point up or down in the ordered phase, the net magnetization is zero. We need to look at the absolute value of the magnetization instead. This is clearly indicated in the results of the cluster algorithms. The Metropolis algorithm however behaves as if there is an actual transition as indicated by the giant fluctuations close to $\beta = 0.5$. This occurs since close to the critical point, the algorithm gets stuck in a local minima configuration. Due to the relatively small size of the system (10*10 lattice), it is able to cross over from +1 state to -1 state.

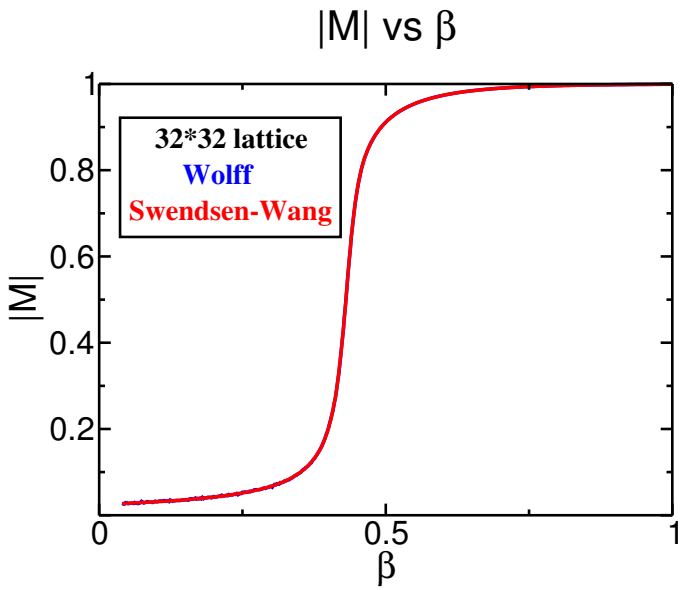

FIG. 5: Absolute value of the average magnetization ($|M|$) versus inverse temperature(β) on a 2D square lattice (32*32) using the cluster algorithms. Phase transition detected close to the critical temperature $T_c = 0.44$.

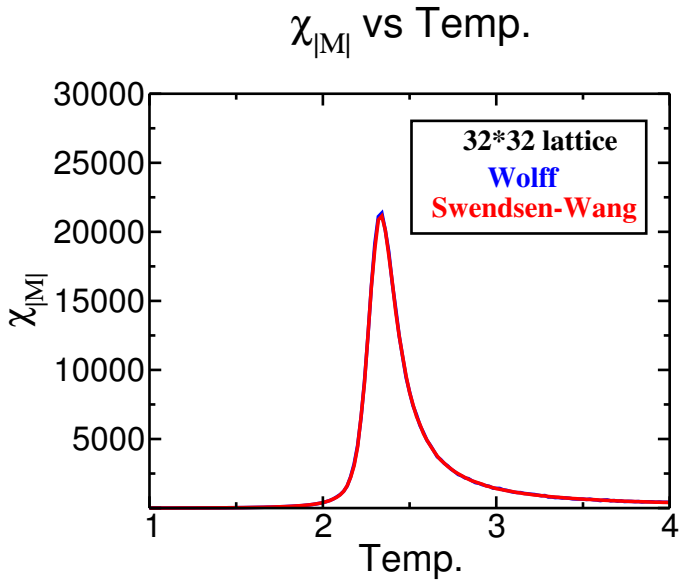

FIG. 6: Absolute value of the magnetic susceptibility ($\chi_{|M|}$) versus inverse temperature(β) on a 32*32 square lattice using the cluster algorithms. $\chi_{|M|} = \beta(\langle M^2 \rangle - \langle M \rangle^2)$.

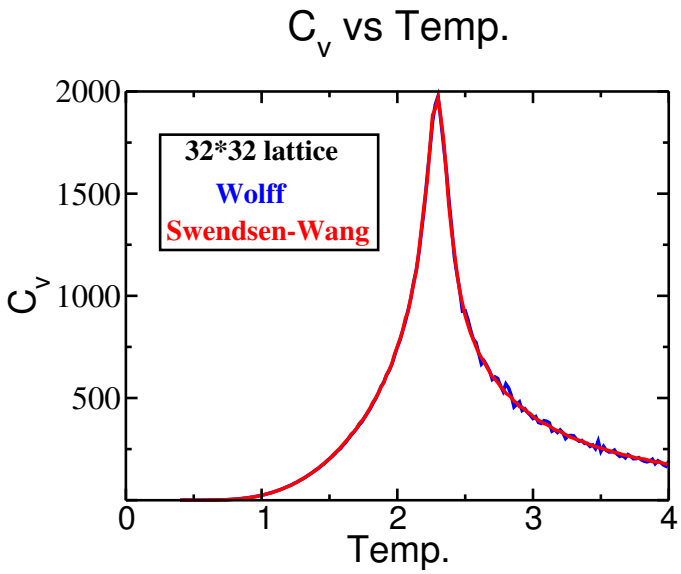

FIG. 7: Absolute value of the specific heat (C_v) versus inverse temperature (β) on a 32*32 square lattice using the cluster algorithms. $C_v = \beta^2(\langle E^{\rangle} - \langle E\rangle^2)$.

A. Critical exponents - Ising model

The critical exponents for the 2D square lattice are reported below using the Swendsen-Wang and Wolff algorithms.

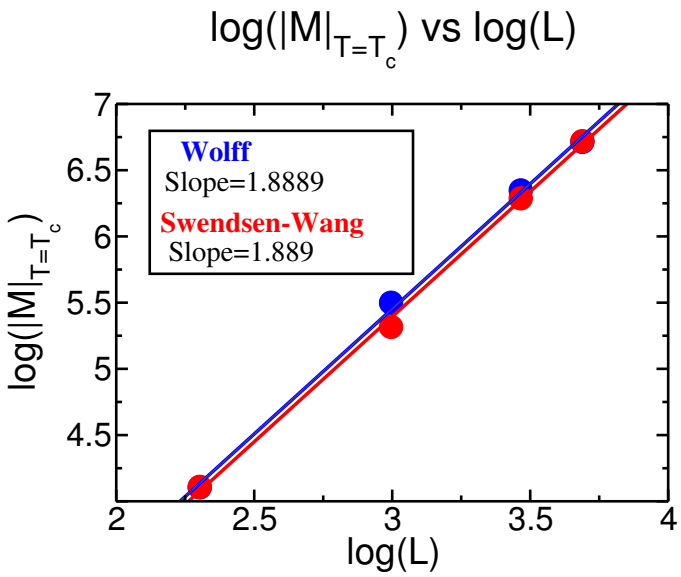

FIG. 8: Critical exponent β is derived from the slope of Log($|M|_{T=T_c}$) versus log(L) plot. The slope is given by the expression $d - \frac{\beta}{\mu}$ where d is the dimension of the system. For $d = 2$, $\frac{\beta}{\mu} = 0.11$ obtained from the cluster algorithms.

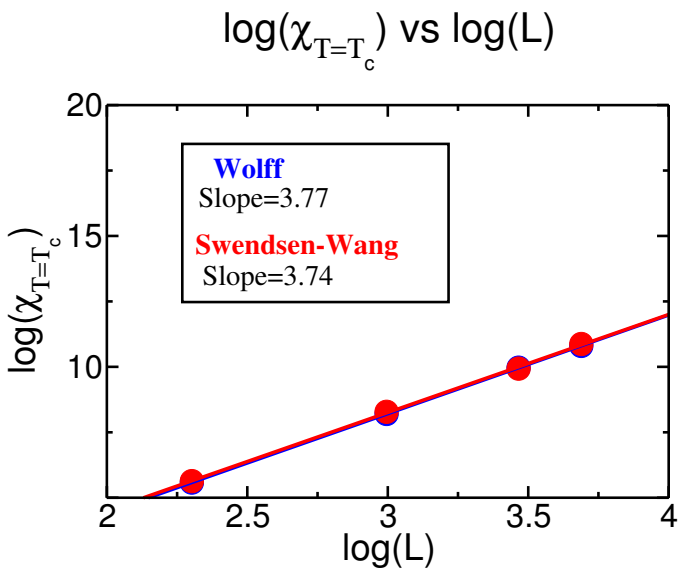

FIG. 9: Critical exponent α is derived from the slope of Log(χ) at the critical point versus log(L) plot. Analytically, *slope* = $\frac{\gamma}{\nu} + d = 3.75$. Hence, for $d = 2$, our calculated $\frac{\gamma}{\nu} = 1.77$ using Wolff algorithm and $\frac{\gamma}{\nu} = 1.74$ using Swendsen-Wang algorithm.

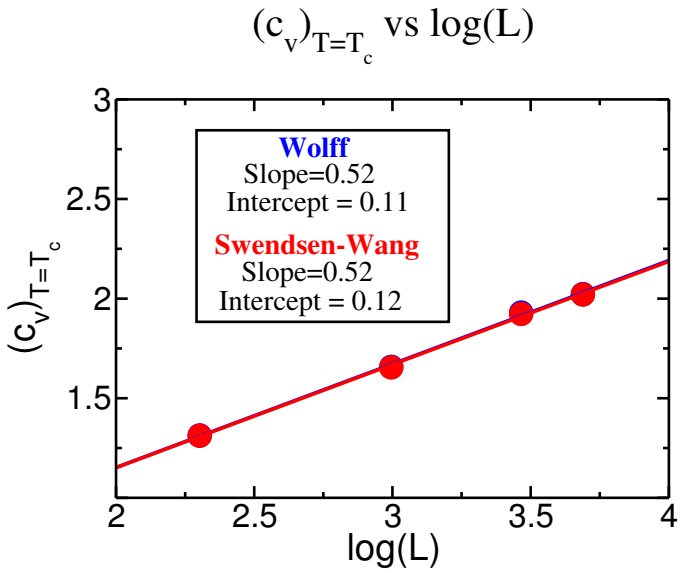

FIG. 10: c_v versus log(L) plot. Since the specific heat capacity per unit volume has a linear relationship with Log(L), one can infer that the critical exponent $\alpha \simeq 0$.

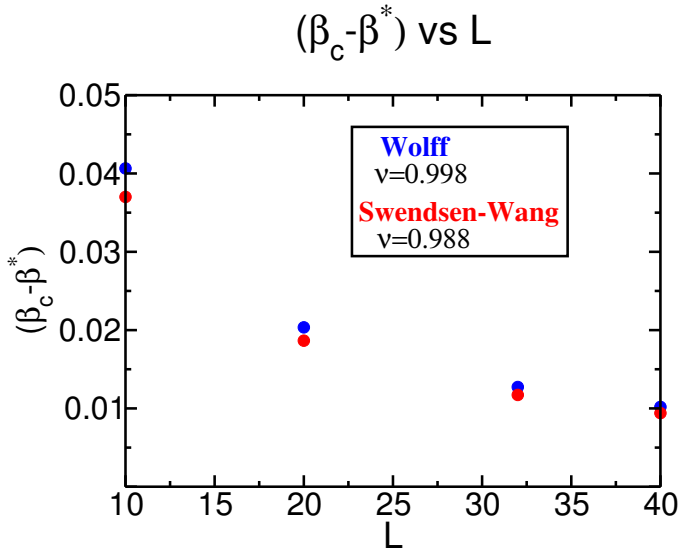

FIG. 11: Obtaining the critical exponent ν. Plot of $\beta_c - \beta^*$ (β^* is the critical temperature of a system of size L and β_c is the critical temperature of the infinite system) versus L. The exact result in 2D is : $\nu = 1$.

The correlation function is given by the following equation :

$$G(r) = \frac{\exp(-\frac{r}{\zeta})}{r^{d-2+\eta}} \tag{6}$$

At the critical temperature, where the correlation length diverges, for $d = 2$, the correlation function $G(r)$ is equal to $r^{-\eta}$.

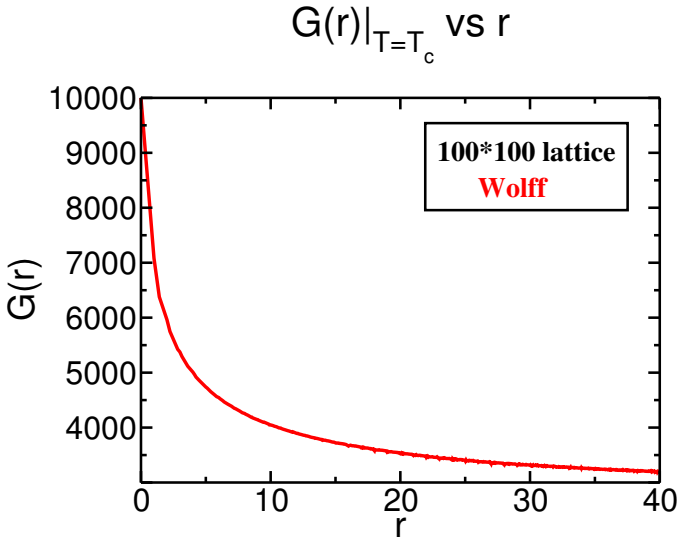

FIG. 12: Plot of correlation function versus the distance between lattice sites for a 100*100 square lattice using the Wolff algorithm.

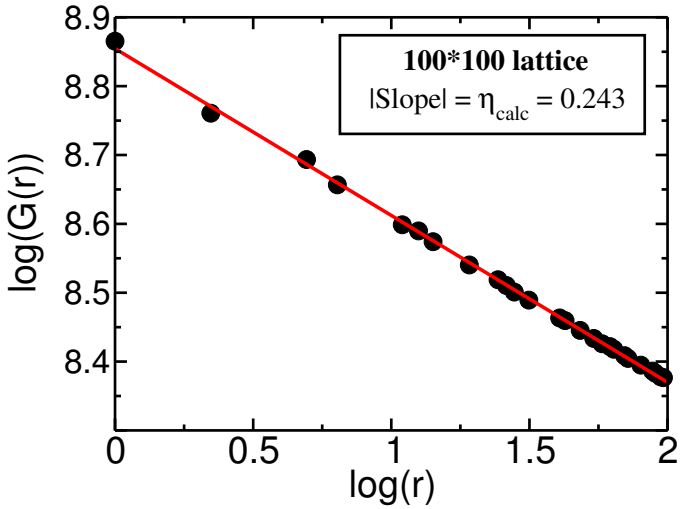

FIG. 13: Critical exponent η is evaluated from the log-log plot of correlation function versus the distance between lattice sites for a 100*100 square lattice using the Wolff algorithm. $\eta_{calculated} = 0.243$ while analytically it should be 0.25.

B. Determining the Critical Temperature

To determine the critical temperature of the 2D square lattice we calcualte the fourth order Binder cumulant which is defined by the equation below

$$U_L = 1 - \frac{\langle s^4 \rangle}{(3\langle s^2 \rangle)^2} \tag{7}$$

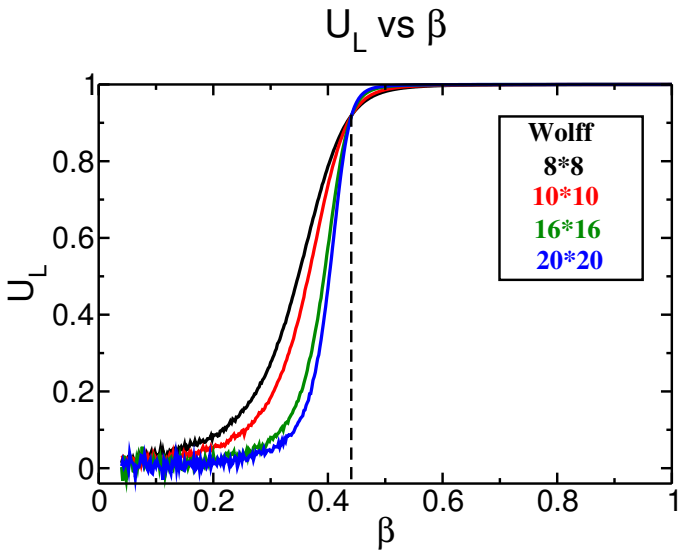

FIG. 14: Plot of the fourth order binder cumulant (U_L) versus the inverse of temperature (β) for 2D square lattices using the Wolff algorithm. Critical temperature occurs at the temperature where the curves for different system sizes intersect.

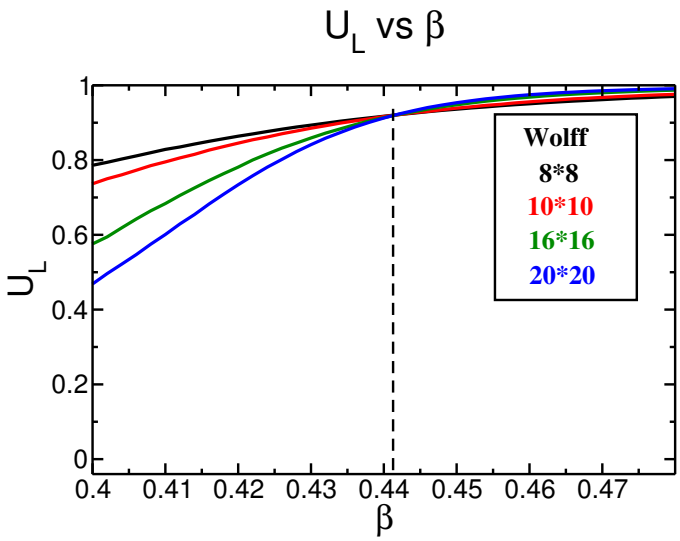

FIG. 15: Magnified plot of U_L versus β. Critical temperature is $\simeq 0.44$.

C. Universality

The critical exponents calculated for a given dimension are universal and different systems with the same critical exponent values fall under the same universality class. As an example, the Wolff algorithm is tested on the two dimensional kagome lattice and the critical exponent β is calculated and compared with the critical exponent calculated above for the 2D square lattice.

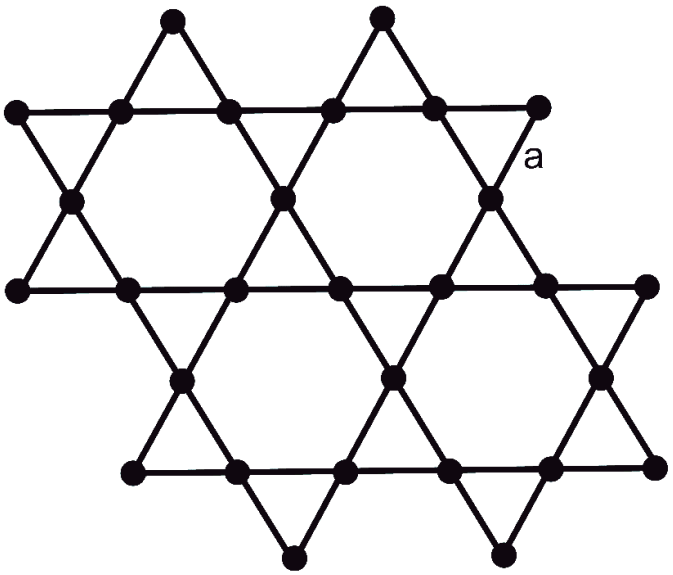

FIG. 16: Image of the two dimensional kagome lattice.

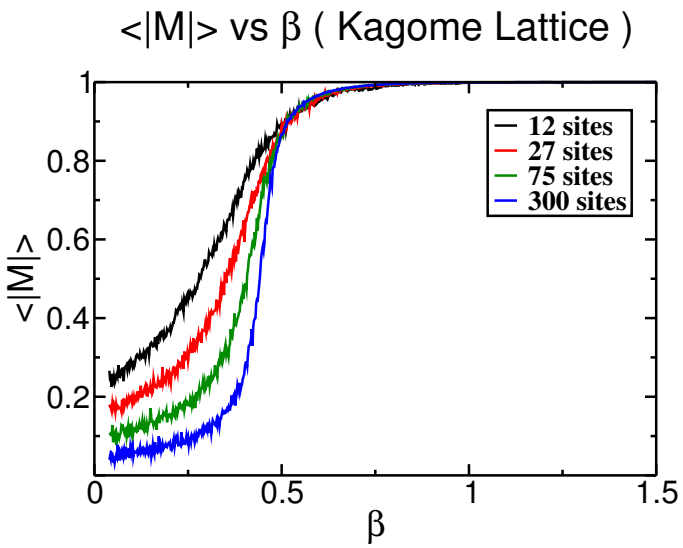

FIG. 17: Phase transition in the kagome lattice.

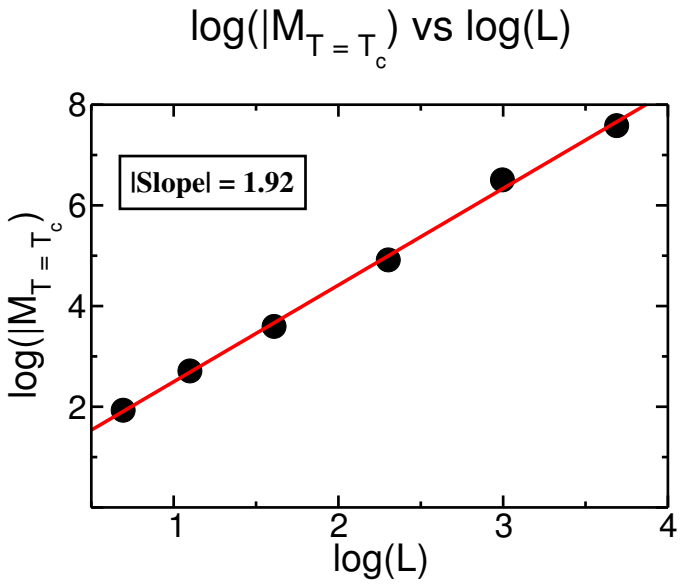

FIG. 18: Log-log plot of the average magnetization versus the size of the kagome lattice. The ratio of the critical exponents β and ν is calculated from the slope. Following the steps outlined in previous section, $\frac{\beta}{\nu} = 0.08$.

VII. PHASE TRANSITION IN A 3D CUBIC LATTICE - ISING MODEL

The Wolff algorithm is extended to the three dimensional cubic lattice.

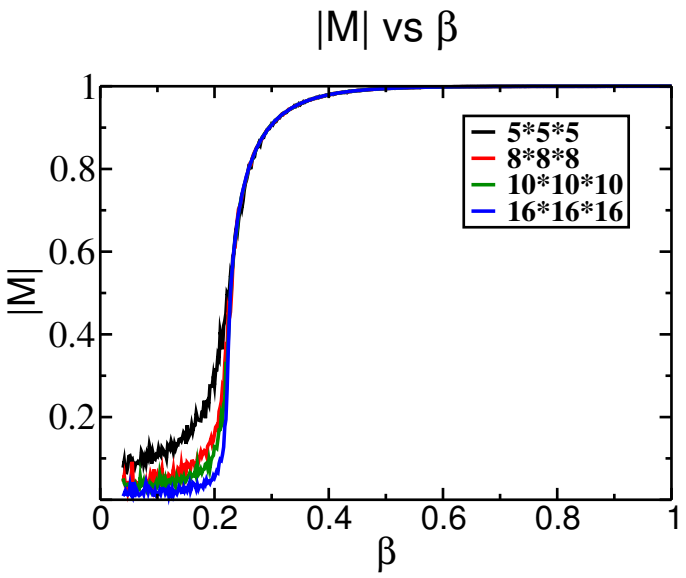

FIG. 19: Phase transition in a 3D cubic lattice given by the plot of M versus β (inverse of temperature). Order Parameter (Average Magnetization) acquires a non-zero value in the low temperature phase. Our calculated value of the inverse of critical temperature is close to 0.22.

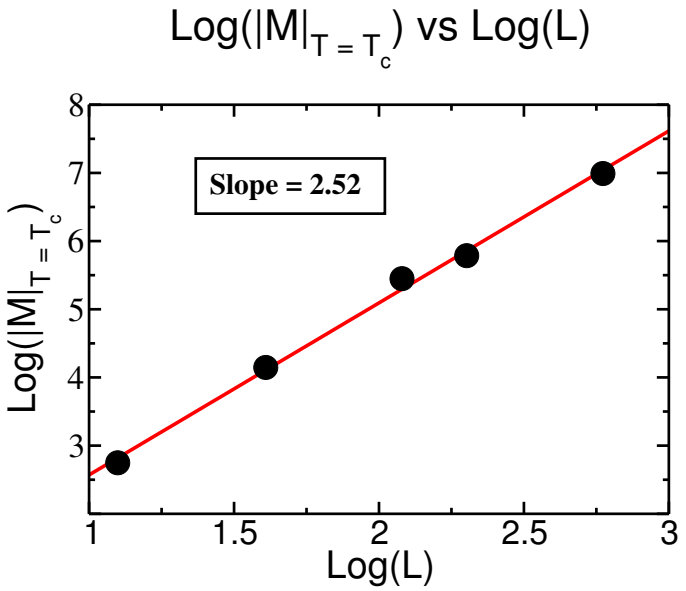

FIG. 20: Log-log plot of the average magnetization versus the size of the lattice. Theoretically, the slope is equal to d - $\frac{\beta}{\nu} = 3 - \frac{0.33}{0.63} = 2.48$

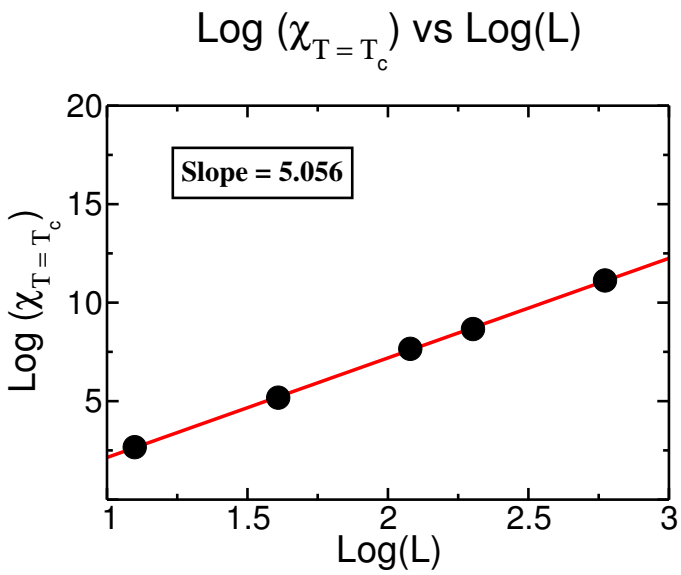

FIG. 21: Log-log plot of the magnetic susceptibilty versus the size of the lattice. Our calculated $\frac{\gamma}{\nu}$ is given by : $\frac{\gamma}{\nu} + d = slope$; $\frac{\gamma}{\nu} = 2.056$. The theoretical value of the ratio is $\simeq 1.963$.

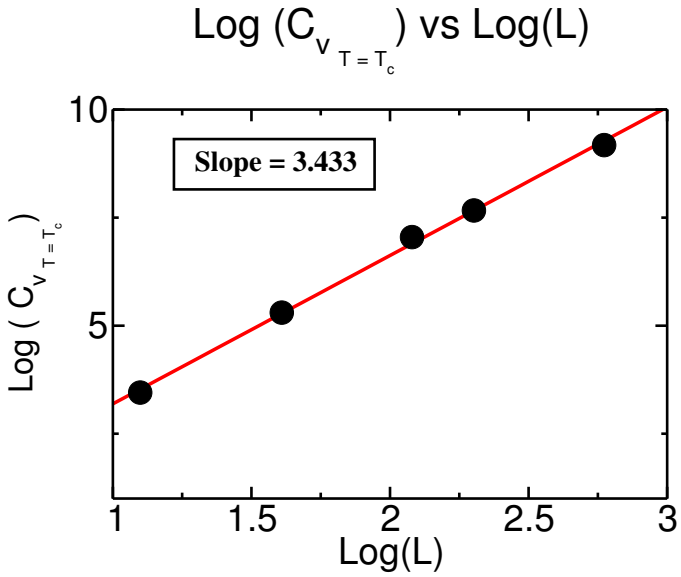

FIG. 22: Log-log plot of the specific heat versus the size of the lattice. Theoretically, the slope of is equal to $\frac{\gamma}{\nu} + d = \frac{0.11}{0.63} + 3 = 3.174$

VIII. PHASE TRANSITION IN THE XY MODEL

The Wolff algorithm can be extended to a general $O(n)$ sigma models. The x-y model will be investigated in this section in two spatial dimensions. This is a peculiar model since magnetization does not undergo a phase transition. This has been shown by the Mermin-Wagner theorem which states that spontaneous symmetry cannot be broken at finite temperatures in systems with short-range interactions with $d < 3$.

$$H_{ising} = \sum_{\langle ij \rangle} \vec{\sigma}_i \vec{\sigma}_j = \sum_{\langle ij \rangle} cos(\theta_i - \theta_j) \tag{8}$$

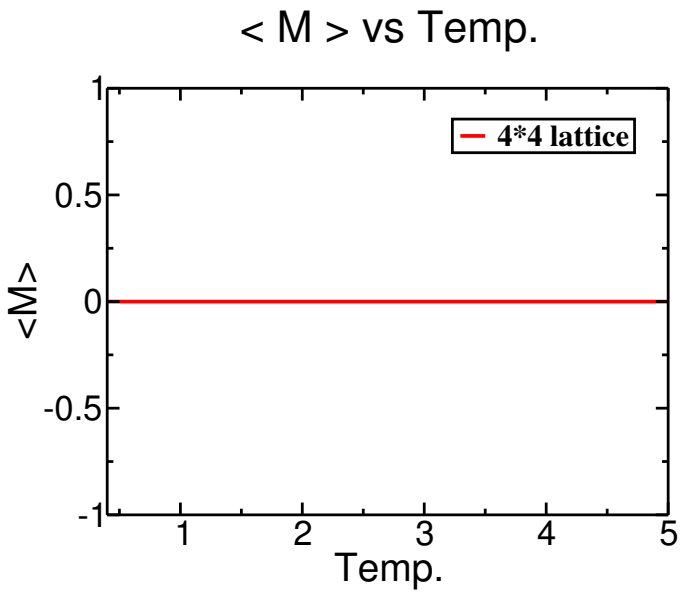

FIG. 23: No observable phase transition as the magnetization of a 2D square lattice in the x-y model remains zero throughout the range of temperature.

Even though the Mermin-Wagner theorem predicts that the order parameter does not change for $d = 2$, there is a different kind of phase transition that occurs in this particular system. Vortices appear beyond a critical temperature T_{KT} which begin to proliferate as the temperature is increased even further. This is known as the Kosterlitz-Thouless transition. Vortices occur in pairs that are bound below T_{KT} and beyond it, they start unbinding. The effect of the unbinding vortex pairs is encapsulated by the spin stiffness ρ which measures the decrease in the gain of free energy.

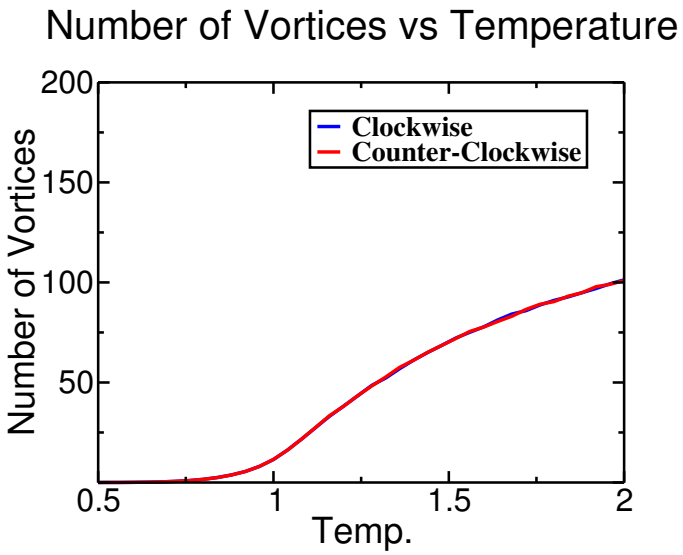

FIG. 24: Topological phase transitions in the x-y model. Appearance of vortex unbinding beyond T_{KT}.

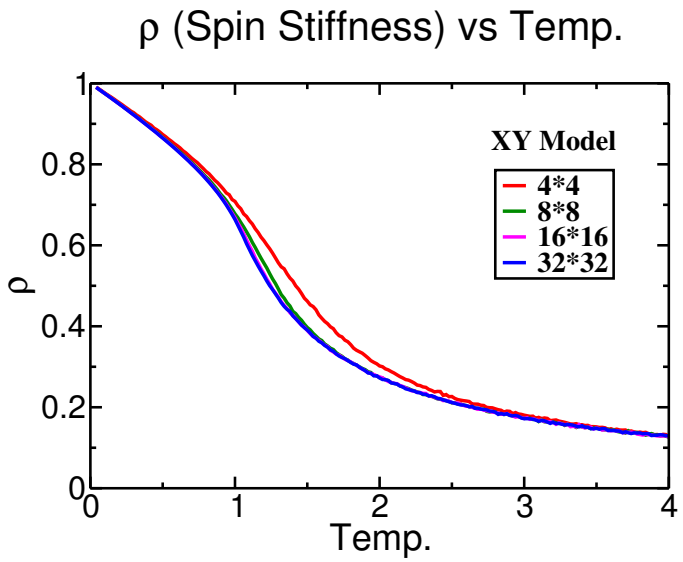

FIG. 25: Phase transition observed in the decrease of spin stiffness ρ beyond the critical temp. T_{KT}.

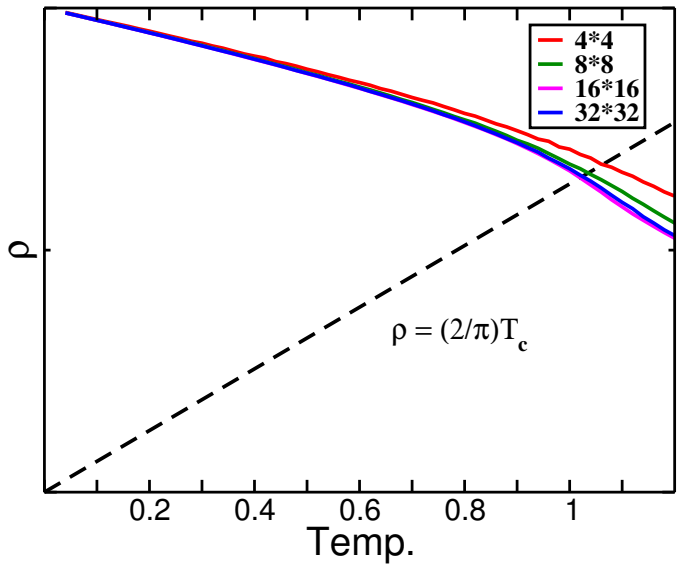

FIG. 26: Critical temperature is determined from the intersection of the spin stiffness plots with the straight line $\rho = \frac{2}{\pi} T_c$.