Monte Carlo Study of the Phase Transition of the *XY* Model on a Diamond Lattice

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We study the phase transition of the classical *XY* model on a diamond lattice by Monte Carlo simulations using the Wolff cluster algorithm. Finite-size scaling (FSS) analysis of the Binder cumulant and the second-moment correlation length ratio $\xi_{2\mathrm{nd}}/L$ yields $T_c = 1.30036(1)$ and $\nu = 0.671(6)$. Data collapse of both quantities confirms the three-dimensional *XY* universality class.

The classical *XY* model—a system of two-component unit vectors with nearest-neighbor interaction—is one of the most fundamental models in statistical mechanics, exhibiting the Berezinskii–Kosterlitz–Thouless transition in two dimensions and a continuous transition to long-range order in three dimensions (3D). While the critical behavior of the 3D transition has been extensively studied on cubic lattices, investigations on other lattice geometries remain scarce. The *XY* model on a diamond lattice has recently attracted interest in the context of multipolar order in Pr-based 1-2-20 compounds[1)] and as the dual representation of the $S = 1$ pyrochlore spin ice in the monopole-free limit.[2)] Hattori and Tsunetsugu studied this model with Z_3 single-ion anisotropy, finding a continuous 3D *XY* transition,[1)] but a precise value of the critical temperature T_c of the isotropic *XY* model is still lacking, apart from an early high-temperature series expansion study.[3)] This Note provides a precise determination of T_c for the isotropic case and confirms the 3D *XY* universality class.

Model and method.— We consider the classical ferromagnetic *XY* model on the diamond

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lattice,

$$H = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j), \tag{1}$$

with $J = 1$, where $\theta_i \in [0, 2\pi)$ and the sum is over nearest-neighbor pairs. Since the diamond lattice is bipartite, a spin rotation by π on one sublattice maps this model exactly onto the antiferromagnetic one, so the two cases share the same critical behavior.

The diamond lattice is a face-centered-cubic Bravais lattice with a two-atom basis. We place it in an L^3 simulation box using the standard 8-site conventional cubic cell, which contains four A sites at the face-centered-cubic positions and four B sites displaced by $\frac{1}{4}(1, 1, 1)$, giving $N = 8L^3$ sites with periodic boundary conditions. Each A site has $z = 4$ nearest neighbors on the B sublattice with bond vectors $\boldsymbol{\delta}_k \in \frac{1}{4}\{(1, 1, 1), (1, \bar{1}, \bar{1}), (\bar{1}, 1, \bar{1}), (\bar{1}, \bar{1}, 1)\}$ ($\bar{1} \equiv -1$). The tetrahedral symmetry yields $\sum_k \boldsymbol{\delta}_k = \mathbf{0}$ and $\sum_k \delta_{k,\alpha}\delta_{k,\beta} \propto \delta_{\alpha\beta}$, ensuring that the acoustic-mode dispersion is isotropic and the effective continuum geometry of the simulation box is cubic—a prerequisite for the dimensionless finite-size scaling (FSS) ratios to converge to the known cubic universal values.[4)]

We simulate the model using the Wolff single-cluster algorithm.[5)] A random reflection axis $\alpha \in [0, \pi)$ is drawn, and neighboring spins are added to the cluster with probability

$$p_{ij} = \max(0,\ 1 - e^{-2\beta J \sin(\theta_i - \alpha)\sin(\theta_j - \alpha)}), \tag{2}$$

where $\beta = 1/T$; all cluster spins are then reflected across α. This algorithm practically eliminates critical slowing down, keeping the integrated autocorrelation time $\tau_{\mathrm{int}} \approx 1$ Wolff sweep for all system sizes.

Simulations were carried out for fourteen system sizes from $L = 4$ to 56 (N from 512 to 1,404,928) on a 21-point temperature grid $T \in [1.290, 1.310]$ with step $\Delta T = 0.001$. For the FSS collapse analysis, additional "wing" temperatures extending to $|T - T_c| \lesssim 0.1$ were computed for $L = 10$–16. The number of measurements per temperature point was graded from $n_{\mathrm{meas}} = 25{,}000$ at $L = 4$ to approximately 925,000 at $L = 56$. All configurations were initialized via sequential cooling from $T = 1.45$ with 300 Wolff sweeps per temperature, followed by an additional thermalization of $\max(2000, 500L)$ Wolff sweeps before measurement.[6)] Statistical errors were estimated by the jackknife method with 50 bins.

The primary observables are the Binder cumulant[7)]

$$B = 1 - \frac{\langle Q^4 \rangle}{2\langle Q^2 \rangle^2}, \tag{3}$$

where $Q = |\boldsymbol{Q}|$ with $\boldsymbol{Q} = N^{-1} \sum_i \boldsymbol{S}_i$ the magnetization and $\boldsymbol{S}_i = (\cos\theta_i, \sin\theta_i)$, and the second-

moment correlation length ratio $\xi_{2\mathrm{nd}}/L$, where

$$\xi_{2\mathrm{nd}} = \frac{1}{2\sin(\pi/L)}\sqrt{\frac{S(\mathbf{0})}{S(\boldsymbol{q}_{\min})} - 1} \tag{4}$$

with $S(\boldsymbol{q}) = N^{-1}\langle\left|\sum_i \boldsymbol{S}_i\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}_i}\right|^2\rangle$ the structure factor and $\boldsymbol{q}_{\min} = (2\pi/L, 0, 0)$; the ratio $\xi_{2\mathrm{nd}}/L$ is averaged over the three Cartesian directions. Both B and $\xi_{2\mathrm{nd}}/L$ are dimensionless and approach universal L-independent values at T_c in the thermodynamic limit.

Numerical results.— Figure 1(a) shows the Binder cumulant B versus T for all fourteen system sizes. The curves from different system sizes cross near $T \approx 1.3$, signaling a continuous phase transition. A polynomial FSS fit of B against the scaling variable $x = (T - T_c)\, L^{1/\nu}$ for $L \geq 12$ in the range $T \in [1.297, 1.303]$ yields $T_c \approx 1.3004$ and $\nu \approx 0.69$, with the reduced chi-squared $\chi^2_{\mathrm{red}} = 2.0$, consistent with the 3D XY value $\nu = 0.6717(1)$.[4] However, the ratio $\langle Q^4\rangle/\langle Q^2\rangle^2$ in B amplifies statistical noise in the disordered phase where $\langle Q^2\rangle$ becomes small, limiting the achievable precision.

To refine the critical temperature, we analyze $\xi_{2\mathrm{nd}}/L$ [Fig. 1(b)], which does not suffer from this noise amplification. The size-doubling ($b = 2$) crossing temperatures for the seven largest pairs ($L_1 = 10$–28) cluster tightly within 1.3001–1.3005, indicating rapid convergence. A polynomial FSS fit $\xi_{2\mathrm{nd}}/L = \sum_{n=0}^{5} a_n x^n$ with $x = (T - T_c)\, L^{1/\nu}$ to the data for $L \geq 12$ in the range $T \in [1.297, 1.303]$ [inset of Fig. 1(b)] yields

$$T_c = 1.30036 \pm 0.00001, \quad \nu = 0.671 \pm 0.006, \tag{5}$$

with $\chi^2_{\mathrm{red}} = 1.32$ (70 data points, 8 parameters). The improvement over the Binder analysis is reflected in both the smaller uncertainties and the lower χ^2_{red}. Fixing $\nu = 0.6717$ gives $T_c = 1.30036(1)$ with $\chi^2_{\mathrm{red}} = 1.30$; the 3D XY value lies within the 1σ region of the joint (T_c, ν) confidence contour.

Corrections to scaling affect ν but not T_c. A pure-scaling collapse gives an effective ν drifting from ≈ 0.66 to ≈ 0.68 as the smallest fitted size is raised; including a leading correction $(1 + c\, L^{-\omega})$ with $\omega = 0.789$[4] stabilizes $\nu = 0.670(6)$, while fixing $(\xi_{2\mathrm{nd}}/L)^* = 0.5927$ returns $T_c = 1.30036(1)$ independently of the fit range.

The crossing values $(\xi_{2\mathrm{nd}}/L)^*$ from the seven largest pairs lie in the range 0.577–0.601, within 1–3% of the 3D XY cubic universal value $(\xi_{2\mathrm{nd}}/L)^* = 0.5927$,[4] with the residual deviation attributable to corrections to scaling ($\omega = 0.789$).[4] The clean data collapse of both B and $\xi_{2\mathrm{nd}}/L$ [insets of Fig. 1(a) and (b)] confirms the 3D XY universality class.

To extract other critical exponents, we analyze finite-size power-law behavior at T_c. Physical quantities at T_c are obtained by cubic-spline interpolation of the temperature-grid data to

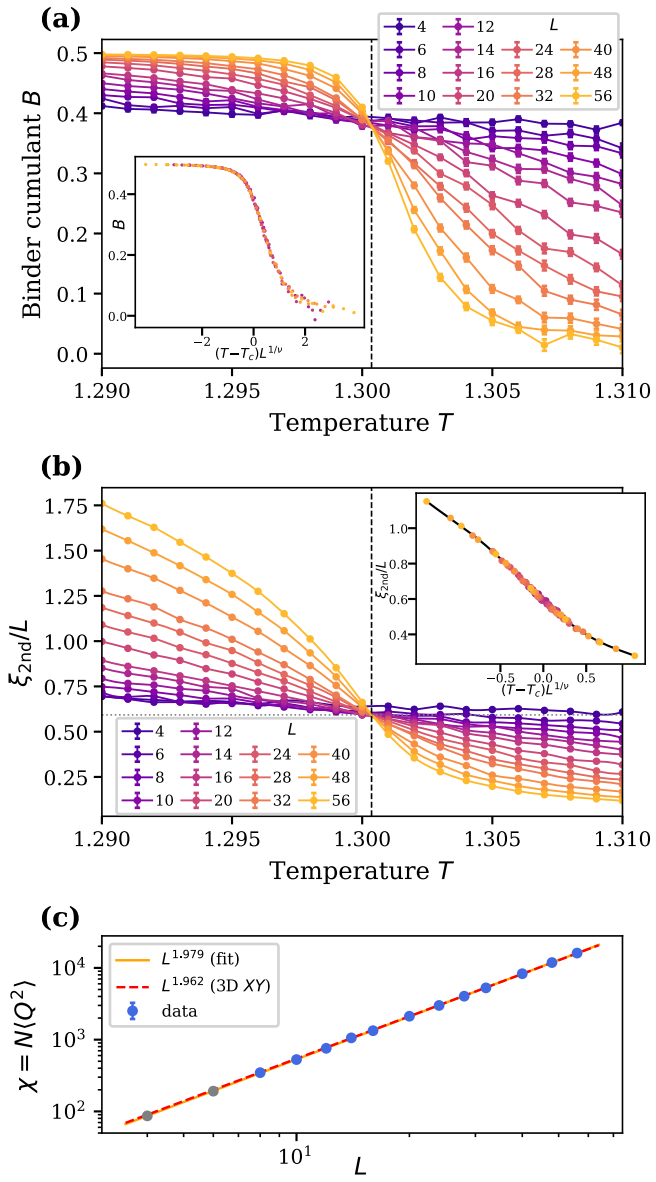

Fig. 1. (Color online) (a) Binder cumulant B vs T for $L = 4$–56. Inset: FSS collapse of B for $L = 14$–56. (b) $\xi_{2\mathrm{nd}}/L$ vs T for $L = 4$–56. Inset: FSS data collapse of $\xi_{2\mathrm{nd}}/L$ for $L = 12$–56, $T \in [1.297, 1.303]$, with the polynomial fit (solid curve). Vertical dashed lines in (a), (b): $T_c = 1.30036$; horizontal dotted line in (b): 3D XY universal value $(\xi_{2\mathrm{nd}}/L)^* = 0.5927$. (c) Susceptibility $\chi = N\langle Q^2\rangle$ vs L at $T_c = 1.30036$ (cubic-spline interpolation). Solid line: power-law fit ($\gamma/\nu = 1.98$); dashed line: accepted 3D XY slope ($\gamma/\nu = 1.962$). Gray points ($L < 8$) are excluded from the fit.

$T_c = 1.30036$; this eliminates the systematic bias that would arise from evaluating observables at the nearest grid point $T = 1.300$, where the finite scaling variable $x = (T - T_c)L^{1/\nu} \approx -0.06$ for $L = 32$ shifts the effective exponents appreciably. We fit the susceptibility

$$\chi = N\langle Q^2\rangle \sim L^{\gamma/\nu} \tag{6}$$

for $L = 8$–56 [Fig. 1(c)]. Since $\chi = 8L^3\langle Q^2\rangle$, the order-parameter exponent ratio $2\beta/\nu = d - \gamma/\nu$ follows identically from the same data and is not an independent fit. Naïve log-log fits give effective exponents $\gamma/\nu \approx 1.98$ and $2\beta/\nu \approx 1.02$, in good agreement with the 3D XY values $\gamma/\nu = 1.962$ and $2\beta/\nu = 1.038$.[4,8] The residual $\sim 1\%$ deviation is attributable to corrections to scaling of order $L^{-\omega}$ with $\omega = 0.789$;[4] the dashed line in Fig. 1(c) shows the accepted 3D XY slope $\gamma/\nu = 1.962$ for comparison.

Conclusion.— Using the Wolff cluster algorithm on system sizes up to $L = 56$ ($N = 1{,}404{,}928$), we have precisely determined the critical temperature of the isotropic XY model on the diamond lattice: $T_c = 1.30036(1)$, approximately 2.4% above the anisotropic value $T_c \approx 1.2695(3)$ obtained with Z_3 single-ion anisotropy.[1] The reduction of T_c by the Z_3 anisotropy can be understood by noting that, under the sublattice rotation that maps the antiferromagnet onto a ferromagnet, a uniform single-ion anisotropy becomes sublattice-dependent and frustrates uniform ordering, thereby lowering T_c. FSS analysis of both the Binder cumulant and the correlation length ratio $\xi_{2\mathrm{nd}}/L$ yields the critical exponent $\nu = 0.671(6)$, consistent with the 3D XY value $\nu = 0.6717(1)$,[4] and the data collapse of both quantities confirms the 3D XY universality class. Power-law fits of the susceptibility at T_c yield $\gamma/\nu = 1.98$ and $2\beta/\nu = 1.02$, consistent with the 3D XY values to within $\sim 1\%$. These results agree with, and substantially sharpen, the early tenth-order high-temperature series estimates of Lambeth *et al.*[3] for the planar model on the diamond lattice: $\gamma = 1.34(2)$ and $2\nu + \gamma = 2.70(5)$ give $\gamma/\nu \approx 1.97$ and $\nu \approx 0.68$, and their critical coupling, 1.540(5) times the mean-field value, corresponds—after rescaling the $|\boldsymbol{S}_i|^2 = 2$ normalization to unit spins—to $T_c = 1.299(4)$. This precise reference value provides quantitative grounding for dual theories of quantum spin liquids and multipolar ordered materials where the isotropic diamond-lattice XY model serves as the effective description.[2]

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