ETH Zürich
Department of Physics

The Berezinskii-Kosterlitz-Thouless Transition

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Computational Statistical Physics (402-0812-00L), Spring 2025

Outline

1. Introduction
2. Theoretical Background
3. Monte Carlo Methods
4. Thermodynamic Observables
5. Estimating $T_{KT}(L)$
6. Implementation Details & Error Analysis
7. Results and Analysis
8. Conclusion

Outline

The 2D XY Model

XY model: classical continuos spins on a 2D lattice, with $O(2)$ symmetry.

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$$

Each spin is a unit vector $\mathbf{S}_i = (\cos\theta_i, \sin\theta_i)$.

- **Mermin-Wagner theorem:** No spontaneous breaking of continuous symmetries at $T > 0$ in $d \leq 2$.
- Yet, the 2D XY model *does* exhibit a phase transition!
- The Berezinskii-Kosterlitz-Thouless (BKT) transition:
  - Topological phase transition
  - Infinite order transition, with no conventional order parameter.

Outline

Order in the 2D XY Model

Hamiltonian Low Temperature expansion:

- Second order Taylor expansion $\cos(\theta_i - \theta_j) \to 1 - \frac{1}{2}(\theta_i - \theta_j)^2$
- Continuum limit $\theta_i \to \theta(r), \quad \theta_i - \theta_j \to \nabla\theta(r)$

$$H \approx E_0 + \frac{J}{2} \int d\mathbf{r} (\nabla \theta(\mathbf{r}))^2$$

Correlation function analysis

$$g(r) = \langle e^{i(\theta(\mathbf{r}) - \theta(0))} \rangle$$

- **Low-T phase (QLRO)** [1]: $g(r) \sim r^{-\eta(T)}$, Algebraic decay of correlations, $\xi = \infty$.
- **High-T phase (Disordered):** $g(r) \sim e^{-r/\xi(T)}$, Exponential decay.

Vortices

Steady states of this Hamiltonian are[1]:

$$\frac{\delta H}{\delta \theta} = 0 \Rightarrow \nabla^2 \theta = 0$$

This Laplace equation has 2 types of solutions

- **Ground state**: $\theta(r) =$ const with Ferromagnetic order, $E = 0$
- **Vortices**: topological defects with winding of $2\pi n$ [1]

$$\oint_{r_0} \nabla\theta \cdot d\mathbf{l} = 2\pi n$$

Energy difference of adding a single vortex is:

$$\Delta E = E_{vort} - E_{no\_vort} = \pi J \int \frac{d\mathbf{r}}{r} = \pi J \ln \frac{L}{a}$$

Entropy of a single vortex:

$$\Delta S = k_B \ln \frac{L^2}{a^2} = 2k_B \ln \frac{L}{a}$$

Identify the Phases

The Free energy of a single vortex is

$$\Delta F = \Delta E - T\Delta S = (\pi J - 2k_B T)\ln\frac{L}{a}$$

It identify 2 different **phases**:

- For $T > \frac{\pi J}{2k_B}$: $\Delta F < 0$ free vortices proliferate ($\Delta F \to -\infty$ as $L \to \infty$)
- For $T < \frac{\pi J}{2k_B}$: $\Delta F > 0$, single vortices are forbidden ($\Delta F \to \infty$ as $L \to \infty$)

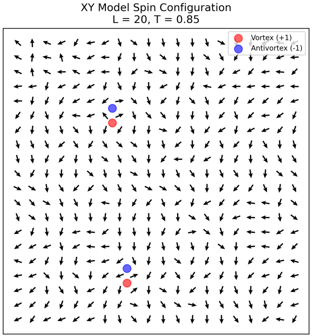
But pairs of a vortex and an antivortex can appear.

$$\Delta F_{pair} = (\pi J - 2k_B T)\ln\frac{r}{a}$$

Pairs are stable because their energy is finite and entropy is insufficient to unbind them.

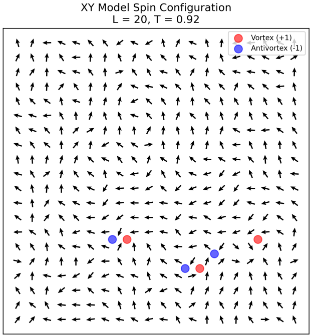
Visualizing Spin Configurations and Vortices

QLRO



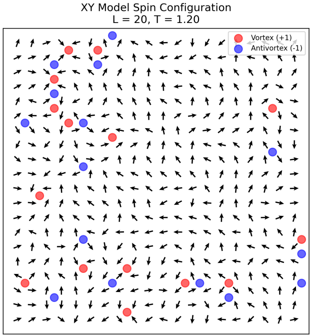
$$T = 0.85 \lesssim T_{KT}$$

Transition



$$T \approx 0.92 \gtrsim T_{KT}$$

Disorder



$$T = 1.20 > T_{KT}$$

Renormalization Group

Understand large-scale behavior by tracking how coupling constants evolve with scale.

- **Mapping** the 2D XY model to a 2D Coulomb gas.

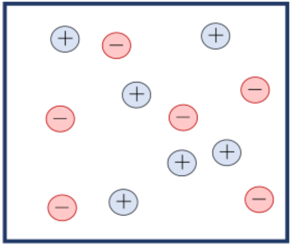
  Topological Hamiltonian:

$$H_v = \sum_i H_{n_i}^{\text{core}} + 2\pi K \sum_{i<j} n_i n_j \ln(|r_i - r_j|)$$

  Fugacity: $y_0 = \exp\left(H_{n_i}^{\text{core}}\right)$ regulates vortex excitation.

- **Screening** modifies the effective interaction:

$$H_{\text{eff}}(r - r') \approx -2\pi K_{\text{eff}} \ln\left(r - r'\right)$$

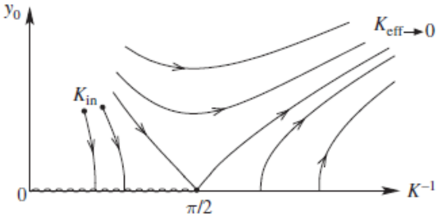


Partition function of XY Model resembles that of a neutral 2D Coulomb gas

Renormalization Group

- RG Flow equations:[1]

$$\begin{cases} \dfrac{dK^{-1}}{dl} = 4\pi^3 y_0^2 + \mathcal{O}(y_0^4), \\ \dfrac{dy_0}{dl} = (2 - \pi K) y_0 + \mathcal{O}(y_0^3) \end{cases}$$



Universal jump:

$$\lim_{l\to\infty} K^{-1}(T_{KT}^-) = \pi/2,$$

$$\lim_{l\to\infty} K^{-1}(T > T_{KT}) = 0$$

- $y_0 = 0$ is a line of fixed points up to $K^{-1} = \pi/2$
- Below T_{KT}: bound vortex pairs (quasi-ordered)
- Above T_{KT}: unbound vortices (disordered)

Outline

Simulating the XY Model

- **Challenges** in simulating BKT transition:
  - Critical slowing down near phase transition
  - Need for large system sizes (finite-size effects)
  - Long correlation times

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  - Energy change for spin flip

$$\Delta E = -J \sum_{\langle i,j \rangle} [\cos\left(\theta_i' - \theta_j\right) - \cos(\theta_i - \theta_j)]$$

  - Accept new state with probability

$$\mathbb{P}_{\text{accept}} = \min(1, e^{-\beta \Delta E})$$

  - **Very inefficient near critical point** due to large correlated regions

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  - **Very inefficient near critical point** due to large correlated regions
- **Wolff cluster algorithm**:
  - Updates entire clusters of spins, **significantly reducing critical slowing down**.

Wolff Cluster Algorithm for the XY Model

Algorithm [1]:

- **Choose a random reflection axis:** Pick an angle $\phi \in [0, 2\pi)$ and define the unit vector $\mathbf{r} = (\cos\phi, \sin\phi)$.
- **Project spins:** For each site i, compute $s_i = \mathbf{S}_i \cdot \mathbf{r} = \cos(\theta_i - \phi)$.
- **Cluster growth:**
  - Pick a random seed site i_0.
  - For each neighbor j of a site i in the cluster, add j to the cluster with probability:

$$\mathbb{P}_{\text{add}} = 1 - \exp\left[\min(0, -2\beta J s_i s_j)\right]$$

  - **Reflect all spins in the cluster:** $\theta_i \to 2\phi - \theta_i \quad \forall i \in$ cluster.

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Remarks

- Non-local updates **reduce autocorrelation times** compared to Metropolis algorithm
- Dramatically **reduces critical slowing down** near T_{KT} by building clusters that scale with correlation length $\xi(T)$

Outline

Thermodynamic Observables

Observable	**Formula**
Energy per spin	$e = \langle H \rangle / N$
Magnetization	$\langle \lvert\mathbf{m}\rvert \rangle$
Specific heat	$c_v = \dfrac{\langle E^2 \rangle - \langle E \rangle^2}{NT^2}$
Susceptibility	$\chi = \dfrac{N}{T} \left(\langle \lvert\mathbf{m}\rvert^2 \rangle - \langle \lvert\mathbf{m}\rvert \rangle^2 \right)$
Spin stiffness (for $J = 1$)	$\rho_s = \dfrac{1}{2N} \left(\left\langle \sum_{\langle i,j \rangle_x} \cos(\Delta\theta_{ij}) \right\rangle - \beta \left\langle \left(\sum_{\langle i,j \rangle_x} \sin(\Delta\theta_{ij}) \right)^2 \right\rangle \right) + (x \leftrightarrow y)$
Vortex density (ω_v)	$\omega_v = \left\langle \dfrac{1}{N} \sum_{\square} \left\lvert \frac{1}{2\pi} \oint_{\square} \mathrm{d}\theta \right\rvert \right\rangle$
Correlation function	$g(r) = \left\langle e^{i(\theta(\mathbf{r}) - \theta(0))} \right\rangle$

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The spin stiffness and correlation function are used to locate T_{KT}

Outline

Estimating $T_{KT}(L)$

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- **Stiffness:** The estimate $T_{KT}^{\rho_s}$ is extracted by intersecting $\rho_s(T)$ with the **Nelson-Kosterlitz Jump** line [5]:

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- **Correlation decay exponent:** The decay exponent η is extracted by fitting the correlation function $g(r) \sim r^{-\eta}$ in the QLRO regime. Intersecting $\eta(T)$ with the **universal value** [3]

$$\eta = 1/4$$

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  yields the estimate $T_{KT}^{\eta}(L)$.
- **Correlation length:** The correlation length ξ is extracted by fitting the correlation function $g(r) \sim e^{-r/\xi(T)}$ in the disordered regime, where for $T \to T_{\mathrm{BKT}}^{+}$, ξ **diverges exponentially** in the thermodynamic limit [1]:

$$\xi(T) \approx a \exp\left[\frac{\pi^2}{8b}\sqrt{\frac{T_{KT}}{T - T_{KT}}}\right]$$

  This fit yields $T_{KT}^{\xi}(L)$.

Outline

Implementation Details

- Simulation structure:
  - **Thermalization**: Ensure equilibrium is reached at each target temperature.
  - **Measurement**: Measure observables over many sweeps in equilibrium.
  - **Analysis**: Calculate averages, estimate $T_{KT}(L)$, perform **finite-size scaling analysis** to extract $T_{KT}(\infty)$

Implementation Details

- Simulation structure:
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  - **Measurement**: Measure observables over many sweeps in equilibrium.
  - **Analysis**: Calculate averages, estimate $T_{KT}(L)$, perform **finite-size scaling analysis** to extract $T_{KT}(\infty)$
- Optimizations:
  - Pre-computation of neighbor indices.
  - Vectorization of NumPy operations.
  - **Just-in-time compilation** (Numba '@njit' [4]) for core simulation loops (Wolff/Metropolis updates, energy calculations, observable measurements).
  - **Parallelization** over (L, T) pairs

Error Analysis: Estimating Statistical Uncertainty

We use the **standard error** for sufficiently decorrelated data, and **Jackknife resampling** otherwise.

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- **Standard Error of the Mean (SEM):**
  - Formula: SE $= s/\sqrt{N_{\text{meas}}}$ (where s is the sample standard deviation).
  - L^2 cluster attempts per Wolff sweep significantly decorrelate direct measurement data
  - Used for: **Energy** and **Magnetization**.

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  - L^2 cluster attempts per Wolff sweep significantly decorrelate direct measurement data
  - Used for: **Energy** and **Magnetization**.
- **Jackknife Resampling:**
  - Recalculate statistics on N_{meas} subsamples obtained in leave-one-out manner

$$\sigma^2_{\text{JK}} = \frac{N_{\text{meas}} - 1}{N_{\text{meas}}} \sum_{i=1}^{N_{\text{meas}}} (\bar{O}_i - \bar{O})^2$$

    where $\bar{O}_i$ is the statistic with the i-th observation removed, and $\bar{O}$ is the average of the $\bar{O}_i$.
  - The variance of the jackknife estimates provides an estimate of the true variance.
  - Convenient for non-linear functions of measured quantities and for correlated data.
  - Used for: **Spin Stiffness**, **Susceptibility**, **Specific Heat**, **Binder Cumulant**, **Vortex Density**, η **exponent**, and **Correlation length** ξ.

Error Analysis

Error Propagation for Derived Critical Temperatures

- To estimate the errors on $T_{KT}(L)$ we
  - directly propagate the errors on the primary observables
  - propagate the covariance matrix of intermediate fits (in the case of $\xi(T)$)

Error Analysis

Error Propagation for Derived Critical Temperatures

- To estimate the errors on $T_{KT}(L)$ we
  - directly propagate the errors on the primary observables
  - propagate the covariance matrix of intermediate fits (in the case of $\xi(T)$)
- Obtain $T_{KT}(\infty)$ by **weighted linear regression** on the scaling form

$$T_{KT}(L) = T_{KT}(\infty) + \frac{a}{(\ln L)^2}$$

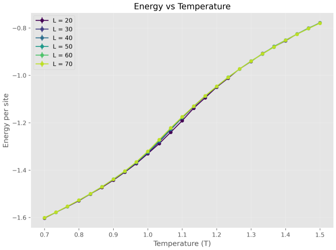
with weights $1/\sigma^2_{T_{KT}(L)}$ (where $\sigma_{T_{KT}(L)}$ is the standard error on each $T_{KT}(L)$).

Outline

Energy and Specific Heat

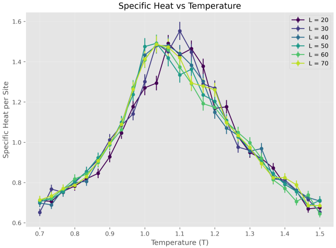
Energy per Spin (e)

- Increases smoothly and monotonically with temperature, no sharp change in slope near the transition.



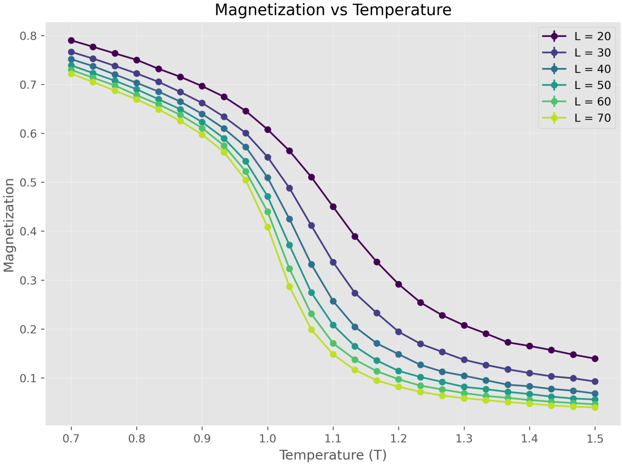
Specific Heat (c_v)

- Exhibits a broad peak around $T \approx 1.1 J/k_B$.
- No divergence at T_{KT}.



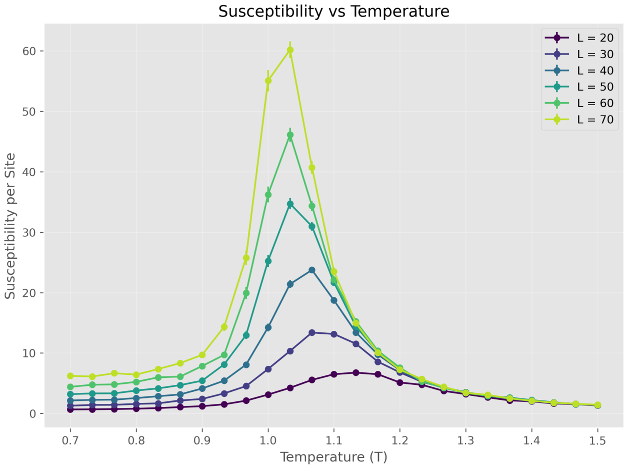
Magnetization ($|\mathbf{m}|$)

- Decreases with L, consistent with the **Mermin–Wagner theorem**.
- Decays slowly with L in the low-temperature phase, consistent with QLRO: $|\mathbf{m}| \sim L^{-\eta(T)/2}$. [2]
- Decays rapidly with L in the high-temperature disordered phase. [2]



Susceptibility (χ)

- Peaks in the range $T \approx 1.0\text{–}1.1\ J/k_B$
- **The peak height increases significantly with L**, as the correlation function decays algebraically in the $T < T_{\mathrm{BKT}}$ phase: $G(r) \sim r^{-\eta(T)}$, leading to a susceptibility that scales as $\chi \sim L^{2-\eta(T)}$ [3].
- χ diverges as $L \to \infty$ for $T \leq T_{KT}$.
- For $T > T_{\mathrm{KT}}$, exponential decay $G(r) \sim e^{-r/\xi}$ implies $\chi \sim \xi^2(T)$, so χ stays finite as $L \to \infty$. [3]

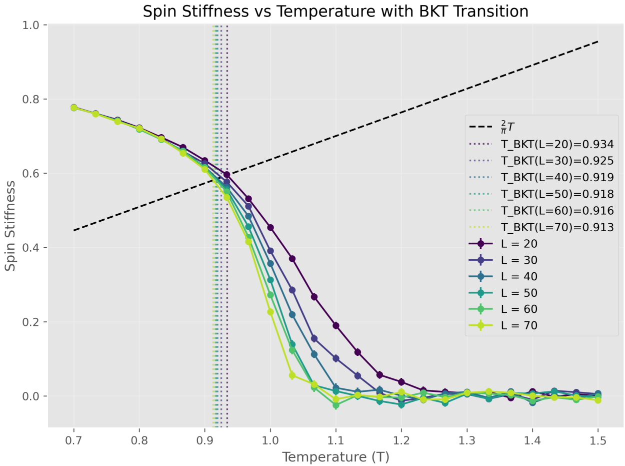


Spin Stiffness (Helicity Modulus ρ_s)

- Smooth curves due to finite sized systems.
- **Universal jump** prediction by Nelson-Kosterlitz:

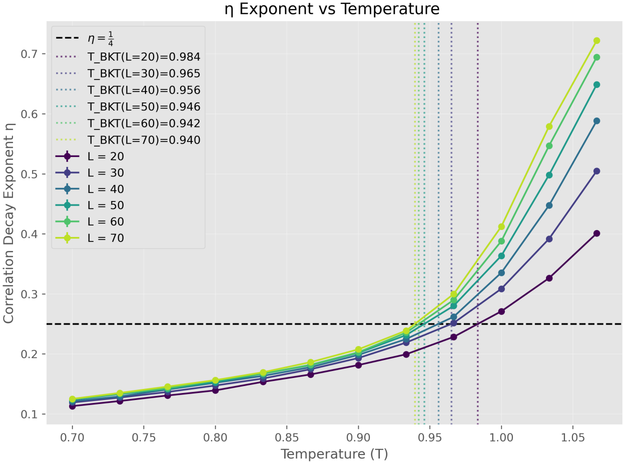
$$\rho_s(T_{KT}^-) = \frac{2k_B T_{KT}}{\pi}$$

- Intersection of $\rho_s(T, L)$ with this line provides an estimate of $T_{KT}(L)$.
- For $L = 70$, our data suggests $T_{KT} \approx 0.913 J/k_B$.



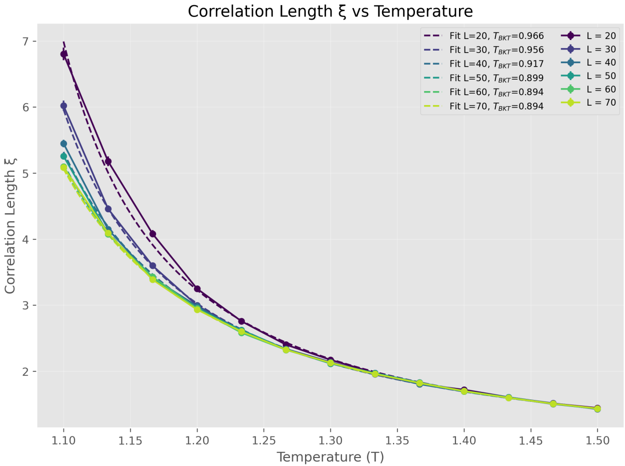
Decay exponent (η)

- The decay exponent η is extracted by fitting the spin–spin correlation function $G(r) \sim r^{-\eta}$.
- The dashed line indicates the BKT transition criterion $\eta = \frac{1}{4}$.
- The crossing points with the dashed line yield the estimates of T_{BKT}.
- For $L = 70$, our data suggests $T_{KT} \approx 0.940 J/k_B$.



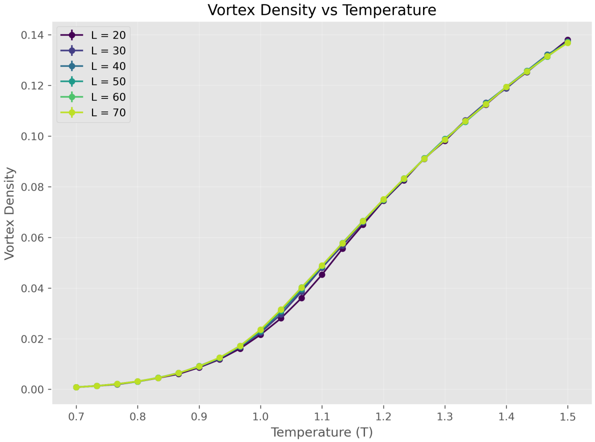
Correlation length (ξ)

- Rapid increase of ξ near the transition.
- As $T \to T_{\mathrm{KT}}^{+}$, ξ diverges exponentially in the thermodynamic limit: $\xi(T) \propto \exp\left[\frac{\pi^2}{8b}\sqrt{\frac{T_{\mathrm{BKT}}}{T-T_{\mathrm{BKT}}}}\right]$, where b is a non-universal constant.
- For $L = 70$, our data suggests $T_{KT} \approx 0.894 J/k_B$.



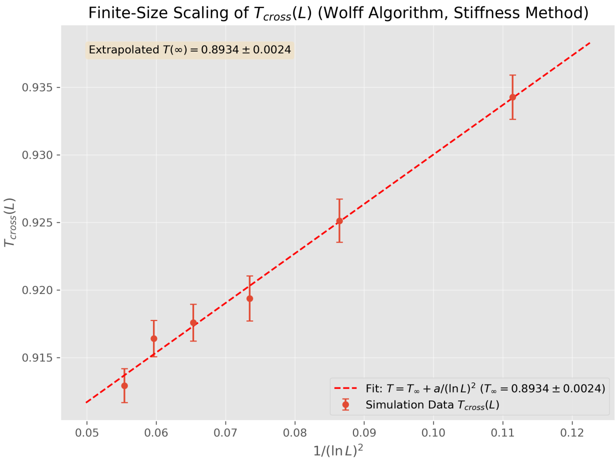
Vortex Density ω_v

- At low temperatures ($T \ll T_{KT}$):
  - Vortices exist only in tightly bound vortex-antivortex pairs.
  - Density is very low.
- Near T_{KT}:
  - Pairs start to unbind.
  - Density increases sharply.
- Above T_{KT}:
  - Proliferation of free vortices/antivortices.
  - Density becomes large, destroying QLRO.



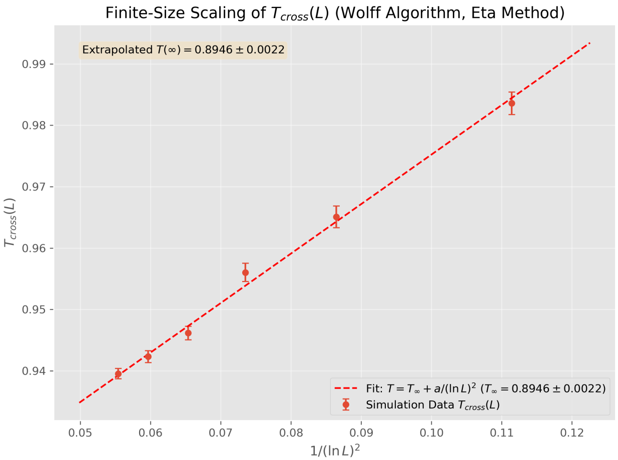
Finite-Size Scaling of $T_{KT}(L)$, Spin Stiffness Method

- Estimate $T_{KT}(L)$ for each size L from the intersection $\rho_s(T, L) = 2k_B T/\pi$.
- $T_{KT}(L) = T_{KT}(\infty) + \frac{a}{(\ln L)^2}$, where a is non-universal constant.
- The y-intercept gives the estimate for $T_{KT}(\infty)$.
- Weighted linear fit yields: $T_{KT}(\infty) \approx 0.8934(24) J/k_B$
- Result is **consistent** with the literature value $T_{KT} \approx 0.89213(10) J/k_B$. [6]



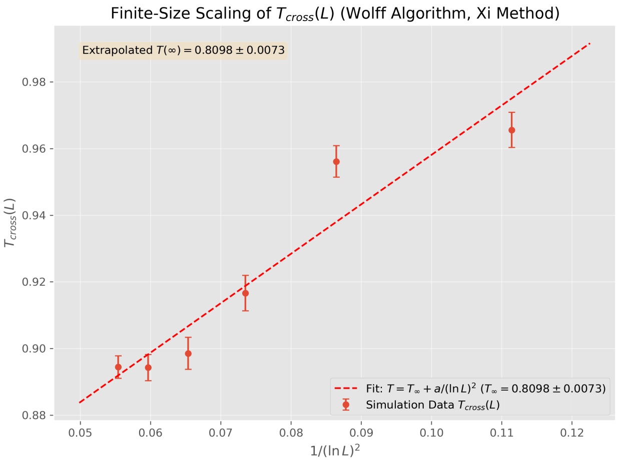
Finite-Size Scaling of $T_{KT}(L)$, η Method

- Estimate $T_{KT}(L)$ for each size L from the intersection $\eta(T, L) = 0.25$.
- $T_{KT}(L) = T_{KT}(\infty) + \frac{a}{(\ln L)^2}$, where a is non-universal constant.
- The y-intercept gives the estimate for $T_{KT}(\infty)$.
- Weighted linear fit yields: $T_{KT}(\infty) \approx 0.8946(22) J/k_B$
- Result is **nearly consistent** with the literature value $T_{KT} \approx 0.89213(10) J/k_B$. [6]



Finite-Size Scaling of $T_{KT}(L)$, ξ Method

- Estimate $T_{KT}(L)$ for each size L using $\xi(T) \propto \exp\left[\frac{\pi^2}{8b}\sqrt{\frac{T_{\mathrm{BKT}}}{T-T_{\mathrm{BKT}}}}\right]$.
- $T_{KT}(L) = T_{KT}(\infty) + \frac{a}{(\ln L)^2}$, where a is non-universal constant.
- The y-intercept gives the estimate for $T_{KT}(\infty)$.
- Weighted linear fit yields: $T_{KT}(\infty) \approx 0.8098(73) J/k_B$
- Result is **not consistent** with the literature value $T_{KT} \approx 0.89213(10) J/k_B$. [6]; possibly due to insufficient number of temperature points to reliably fit the exponential divergence of $\xi(T)$.



Outline

Conclusion

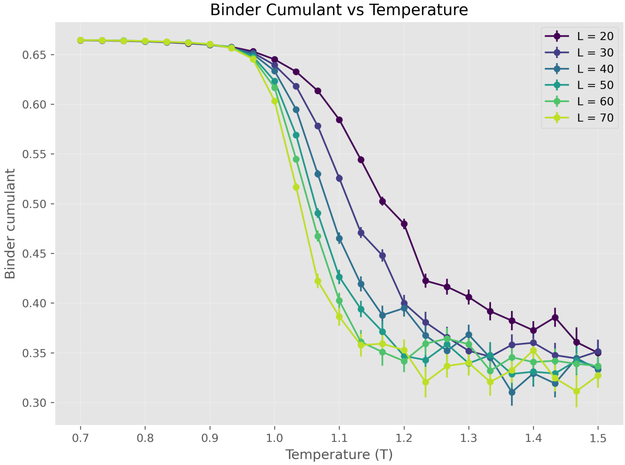
- Implemented the Wolff algorithm
- Measured observables for different system sizes
- Verified BKT transition and estimated $T_{KT} \approx 0.8934(24) J/k_B$

Thank you for your attention!

Back up slide I

Binder Cumulant $|\mathrm{U_L}|$)

- In the low-temperature phase, $|U_L|$ remains high and nearly size-independent.
- Around T_{BKT}, curves for different L start to separate.
- The absence of a common intersection point in the Binder cumulant curves indicates the lack of a conventional second-order phase transition.



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