Bachelor Thesis Defense

Berezinskii-Kosterlitz-Thouless phase transition in 2D XY model

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Motivation

PHYSICAL REVIEW B **75**, 132506 (2007)

Using inhomogeneity to raise the superconducting critical temperature in a two-dimensional *XY* model

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Superconductors with low superfluid density are often dominated by phase fluctuations of the order parameter. In this regime, their physics may be described by *XY* models. The transition temperature T_c of such models is of the same order as the zero-temperature phase stiffness (helicity modulus), a long-wavelength property of the system: $T_c = A\Upsilon(0)$. However, the constant A is a nonuniversal number, depending on dimensionality and the degree of inhomogeneity. In this Brief Report, we discuss strategies for maximizing A for two-dimensional *XY* models; that is, how to maximize the transition temperature with respect to the zero-temperature, long-wavelength properties. We find that a framework type of inhomogeneity can increase the transition temperature significantly. For comparison, we present similar results for Ising models.

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Outline

- Quanlitative Berezinskii-Kosterlitz-Thouless phase transition.
- Markov chain Monte Carlo methods.
- Non-equilibrium dynamics.
- Quantitative Berezinskii-Kosterlitz-Thouless phase transition.

Quanlitative Berezinskii-Kosterlitz-Thouless

2D XY the model

- The model is a square lattice of linear dimension L, lattice spacing a of $N = L \times L$ sites, at each site a unit vector historically called spin is located.
- The spin can rotate in the lattice's plane and is represented by a spin phase angle θ.
- The Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij,lm \rangle} J_{ijlm} \mathbf{s}_{ij}^{T} \mathbf{s}_{lm} - \mathbf{H}\mathbf{M} = -\sum_{\langle ij,lm \rangle} J_{ijlm} \cos\left(\theta_{ij} - \theta_{lm}\right) \qquad (1)$$

where the circumstance has $J_{ijlm} = 1, \mathbf{H} = 0$.

Rough approximation

Bloch spin wave

The spinwave low temperature approximation for a configuration of a single vortex or anti-vortex:

- The energy of a single vortex, $n = 1$,

$$\mathcal{H}_{vor} = n^2 \pi \ln(L/r_0) = \pi \ln(L/r_0) \quad (2)$$

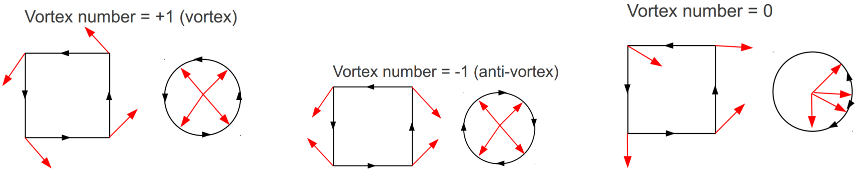
  where the smallest length scale $r_0 \gg a$.[1]
- The change of entropy introduced by the presence of a single vortex is $\Delta\mathcal{S}_{vor} = k_B T \ln (L/r_0)^2$.
- The change of Helmholtz free energy

$$\Delta F = \mathcal{H}_{vor} - T\Delta\mathcal{S}_{vor} = (\pi - 2k_B T) \ln(L/r_0) \quad (3)$$

- $T < \pi/2 \, (J/k_B)$.
- $T > \pi/2 \, (J/k_B)$.

[1] Theory wants $r_0 \gg a$ for integration. Practice realizes $r_0 \sim a$.

Phenomenological demonstration



[2]

- Vortex number is specified by $\oint_{\mathcal{P}} d\mathbf{l}\nabla\theta\left(\mathbf{r}\right)$ where $\mathcal{P}$ is a closed path connecting four corners of a primitive spin cell. $dE \in [-\pi : \pi]$.
- The number of vortices equal the number of anti-vortices with periodic boundary condition.
- Stokes' theorem[3]:

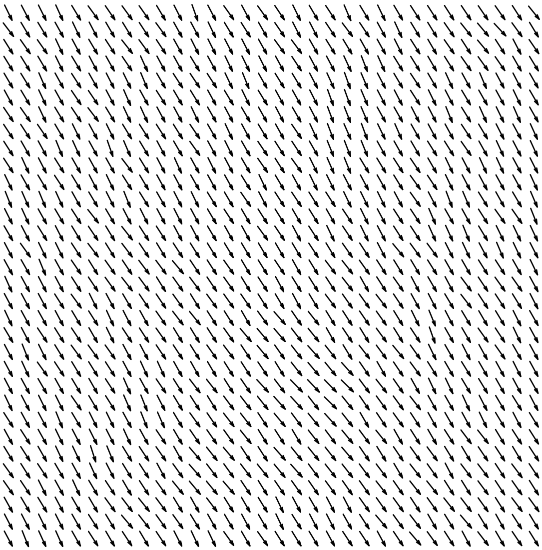
$$\oint_{\mathcal{P}} d\mathbf{l}\nabla\theta\left(\mathbf{r}\right) = \int_{\mathcal{S}} \left[\nabla \times \nabla\theta\left(\mathbf{r}\right)\right] \cdot d\mathbf{a} = 0 \tag{4}$$

- Physics: $\mathcal{H}_{vor} = \pi \ln(L/r_0)$, $\mathcal{H}_{\text{pair}} \sim \ln\left|d\mathbf{r}/r_0\right|$. No isolated vortex.

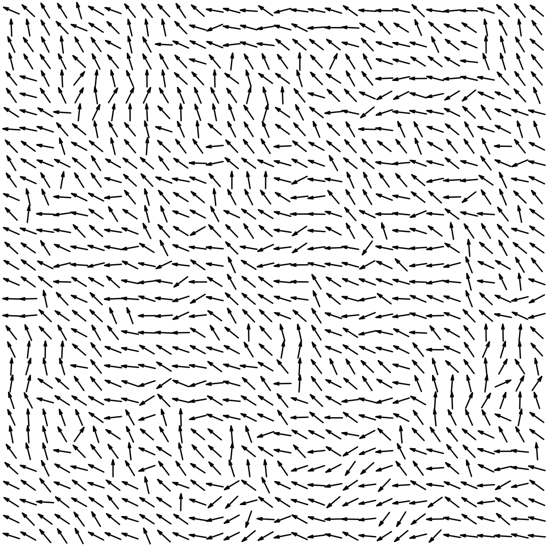
[2] Urs Gerber, et al. Feb. 2014 @ arXiv:1402.2341v1 [hep-lat]

[3] Curl of gradient is zero, said the Electrodynamics professor Anh-Tuan Nguyen.

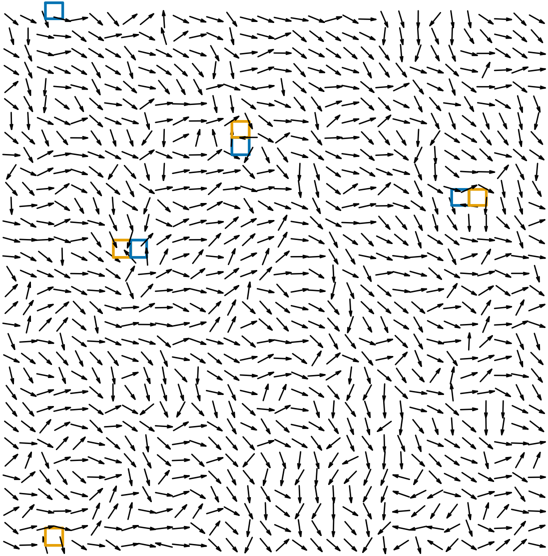
Temperature $T = 0.01\,(J/k_B)$



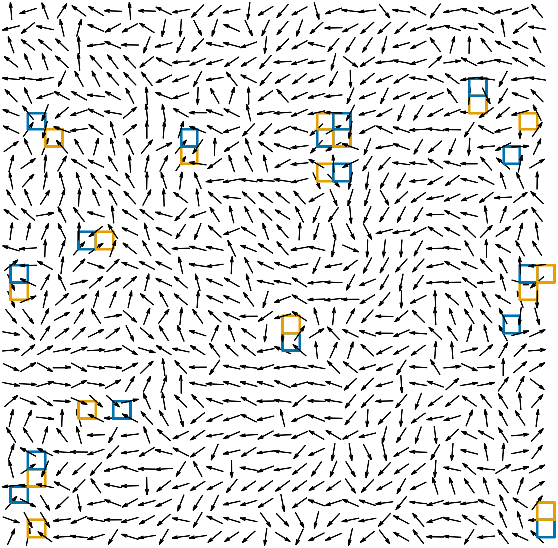
Temperature $T = 0.50\,(J/k_B)$



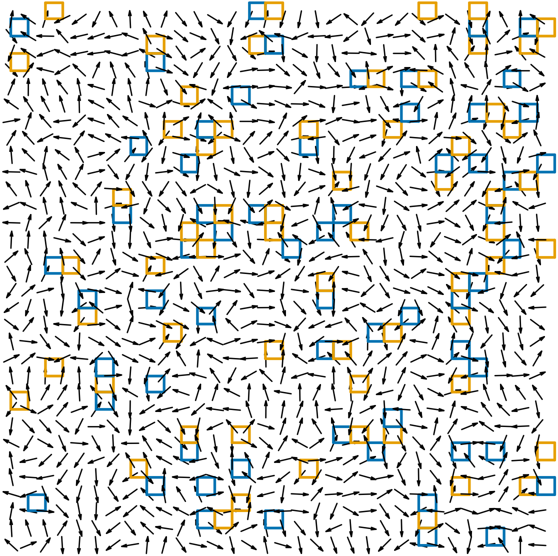
Temperature $T = 0.85\,(J/k_B)$



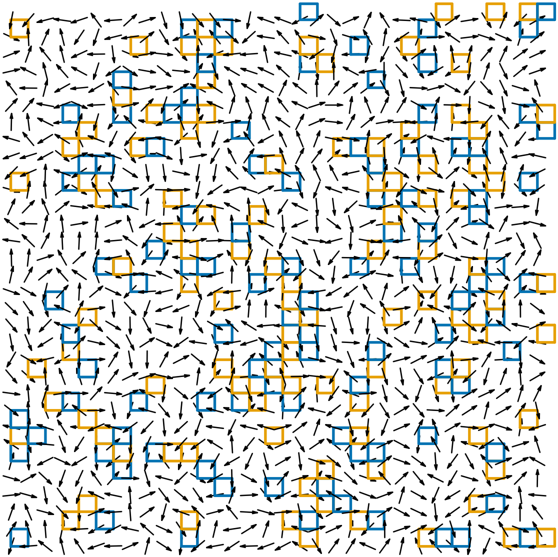
Temperature $T = 1.00\,(J/k_B)$



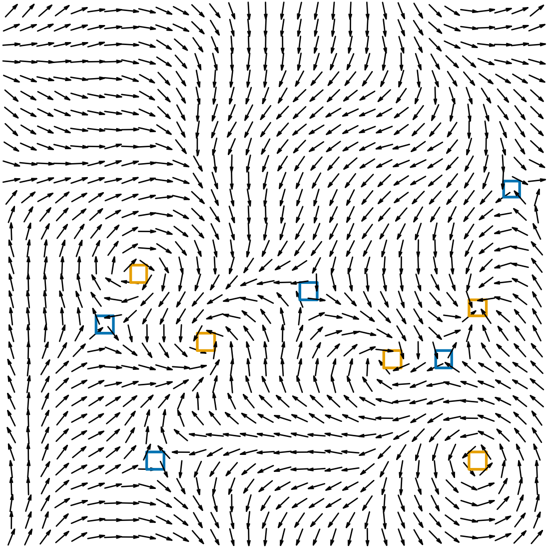
Temperature $T = 1.50\,(J/k_B)$



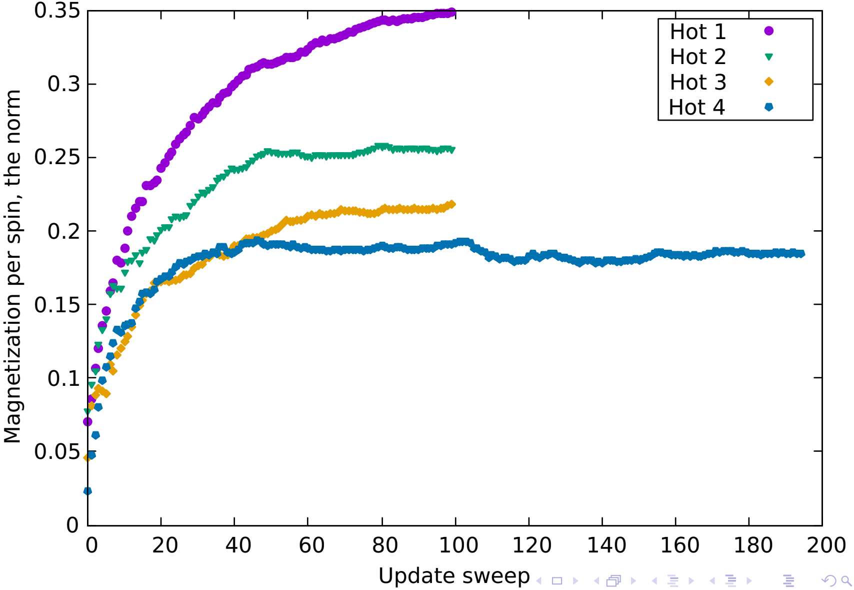
Temperature $T = 2.00\,(J/k_B)$



Metastability — $L = 32$, $T = 0.01\,(J/k_B)$



Metastability — $L = 32$, $T = 0.01\,(J/k_B)$



Markov chain Monte Carlo methods

Markov chain

A stochastic process is termed a Markov chain requires

- Markovian.
- Conservation of transition probability.
- Ergodicity: irreducibility and/ or aperiodicity.
- Existence of a stationary distribution $\boldsymbol{\nu}$.
  - Detailed balance.
  - Global balance.
  - Master equation.

Metropolis random proposal

The transition process:

- Satisfactory of detailed balance $\frac{p_{xy}}{p_{yx}} = \frac{P(y)}{P(x)}$.
- Transition probability $p_{xy} = \rho(x, y)\alpha(x, y)$.
- Proposal probability $\rho(x, y) = 1/N$.
- Acceptance probability

$$\alpha(x, y) = \min\{1, P(y)/P(x)\} = \min\{1, \exp(-\Delta\mathcal{H}/k_B T)\} \tag{5}$$

- $P(x)$ the stationary distribution. In the circumstance it's the Boltzmann distribution.
- Checker board proposal satisfies the global balance.

Wolff dynamics

$\boxed{\text{A cluster of spins}}$ is flipped with a common axis $\mathbf{r}$ chosen randomly in the spin state space according to the generalized spin flip operation

$$\mathbf{R}(\mathbf{r})\mathbf{s}_{ij} = \mathbf{s}_{ij} - 2\left(\mathbf{s}_{ij} \cdot \mathbf{r}\right)\mathbf{r} \tag{6}$$

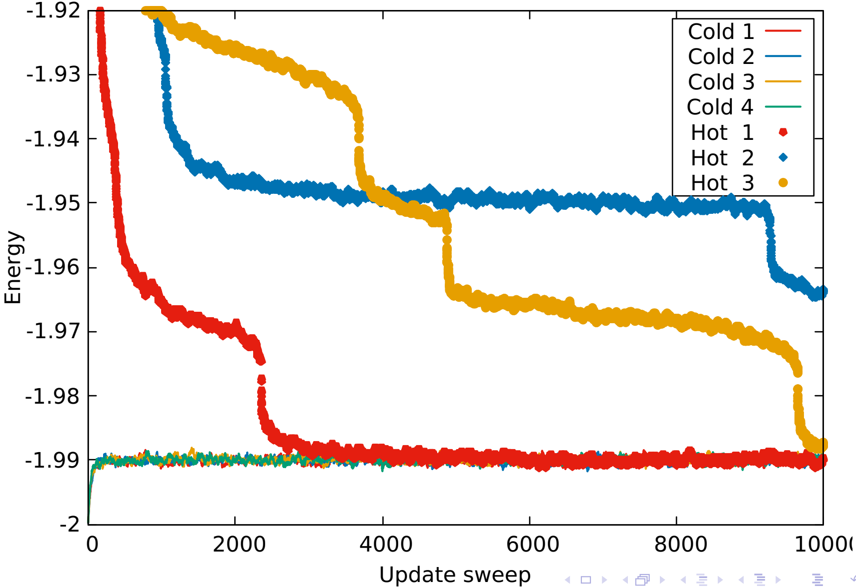
- Computational form $\theta'_{ij} = 2r - \theta_{ij} + \pi$.
- Transition probability $p_{xy} = \rho(x, y)\alpha(x, y)\beta\left(x, y\right)$.
  - Proposal probability is symmetric.
  - Acceptance probability is unity.
  - Bonding probability $\beta(x, y) = \mathcal{P}(x, y) \quad \vee \quad 1 - \mathcal{P}(x, y)$.
  - Bond activation probability is symmetric for any pair of spins in a single cluster $\mathcal{P}\left(\mathbf{s}_{ij}, \mathbf{s}_{lm}\right) =$

$$1 - \exp\left(\min\left\{0, -J_{ijlm}\left[\mathbf{s}_{ij}^{T}\left(\mathbf{R}\mathbf{s}_{lm}\right) - \mathbf{s}_{ij}^{T}\mathbf{s}_{lm}\right]/k_B T\right\}\right) \tag{7}$$

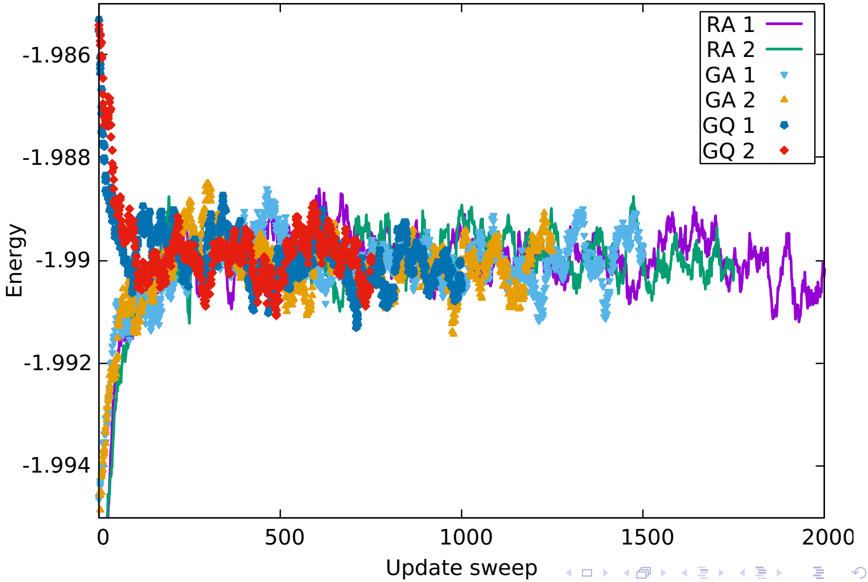
  - $\mathcal{P}\left(\mathbf{s}_{ij}, \mathbf{s}_{lm}\right)$ is not symmetric for a spin inside and a spin outside the cluster. Forming a cluster requires non-activated bonds $1 - \mathcal{P}\left(x, y\right)$ at the boundary.
  - Satisfactory of detailed balance.

Non-equilibrium dynamics

Practical ergodicity, $L = 32$, $T = 0.02\,(J/k_B)$ on GPGPU



Solution, $L = 32$, $T = 0.02\,(J/k_B)$



Quanlitative Berezinskii-Kosterlitz-Thouless phase transition

Statistics

- $L = 16, 32$ with Wolff dynamics on CPU were equilibrated with 2000 and 4000 update sweeps respectively.
- $L = 32, 64, 128$ with CUDA API were equilibrated correspondingly with 2048, 4096 and 8192 update sweeps.
- All measurements taken on 131072 samples, except otherwise stated.
- Estimations with the binning analysis and Jackknife resampling methods.

Physical observables

The measured quantities:

- Spin-spin correlation function $\vartheta(r,t)$.
- Spin-spin correlation length ξ.
- Norm of magnetization per spin m.
- Empirical magnetization per spin M.
- Magnetic susceptibility χ.
- Reduced susceptibility $k_B T \chi$ and square of magnetization per spin $\mathbf{m}^2$.
- Vortex density.
- Energy per spin E.
- Specific heat C_v.
- Helicity modulus or spin stiffness Υ.

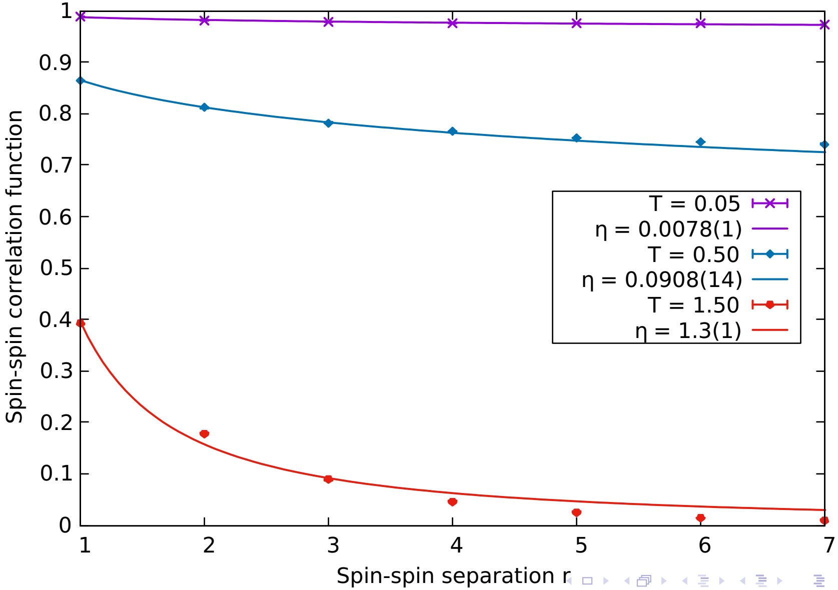
Spin-spin correlation function

$$\vartheta(r,t) = \langle \mathbf{s}_{ij}(t)\mathbf{s}_{lm}(r,t)\rangle - \mathbf{m}^2(t) \tag{8}$$
$$= \langle \mathbf{s}_{ij}(t)\mathbf{s}_{lm}(r,t)\rangle = \langle \cos\left[\theta_{ij}(t) - \theta_{lm}(r,t)\right]\rangle \tag{9}$$

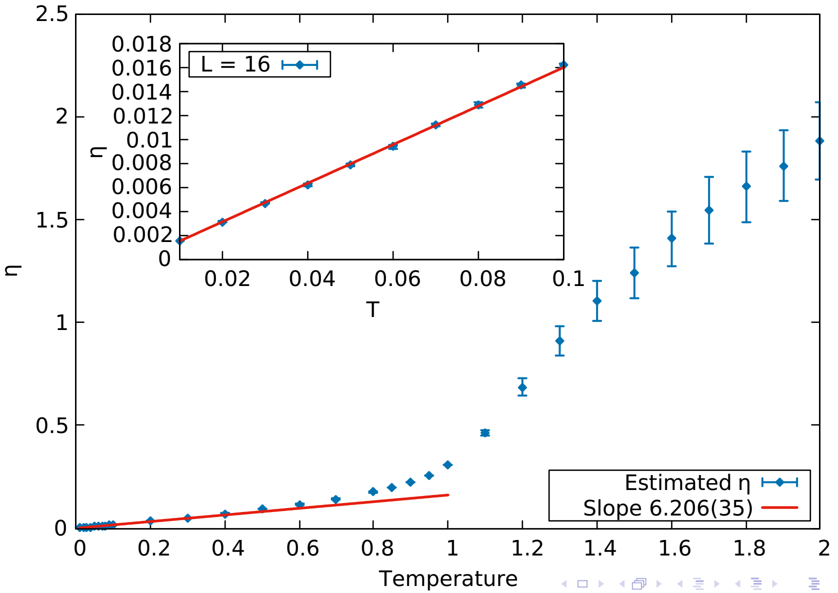
where $\mathbf{m}(t)$ the magnetization per spin is set to be zero.

- At low temperatures, the decay in power law $\vartheta(r,t) \sim r^{-\eta}$ where $\eta = k_B T/2\pi J$ by spin wave theory.
- In high temperature phase, the decay is exponential $\vartheta(r,t) \sim \exp(-r/\xi)$.
- The correlation length diverges at low temperatures as $\xi \sim a \exp\left(bt^{-1/2}\right)$ where $t = \left|T - T_{BKT}\right| / T_{BKT}$ the reduced temperature, T_{BKT} the critial temperature of BKT phase transition, and a, b are non universal constants.

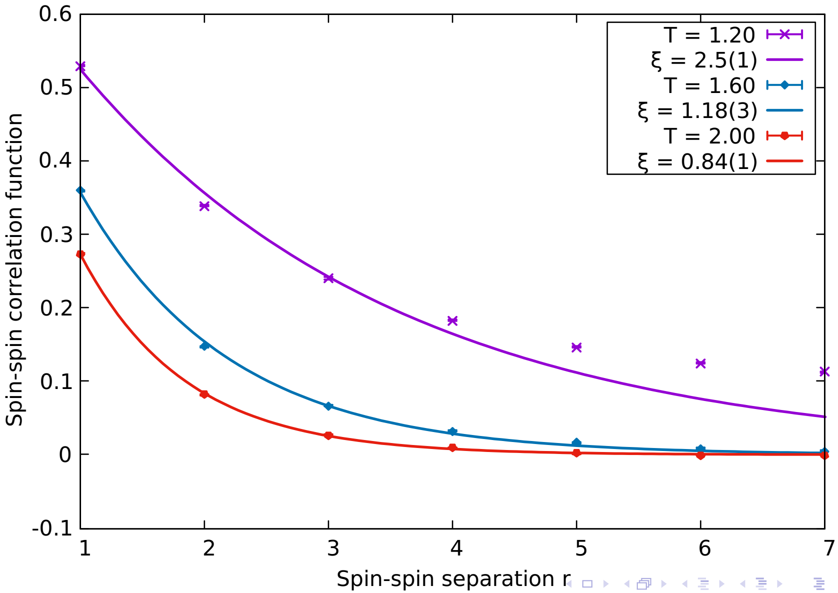
$\vartheta(r,t) \sim r^{-\eta}$ at $T < T_{BKT}$ — $L = 16$



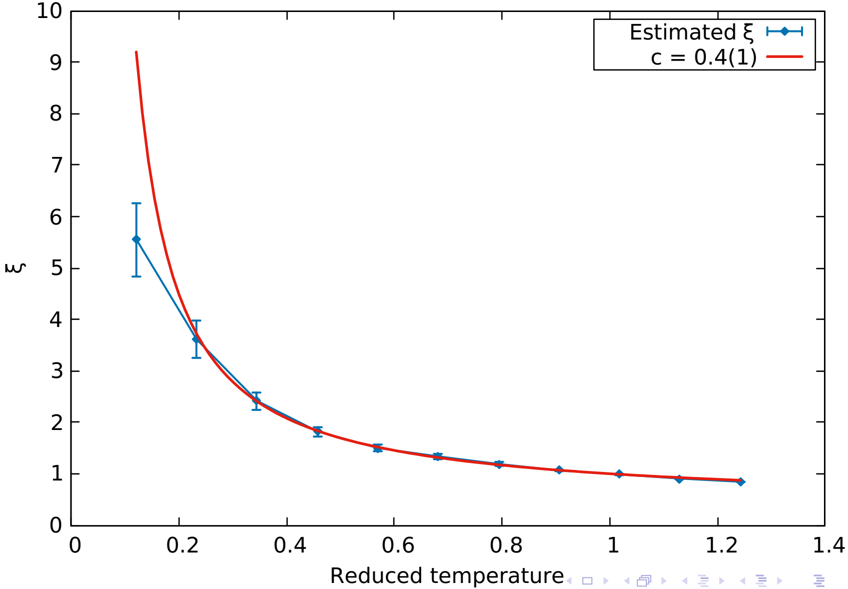
$\eta = k_B T/2\pi J$ — Slope 6.206(35) vs $2\pi \approx 6.283...$



$\vartheta(r,t) \sim \exp(-r/\xi)$ at $T > T_{BKT}$ — $L = 16$



$\xi \sim a \exp\left(bt^{-1/2}\right)$ — $c = 0.416454 \pm 0.1863$ — $L = 16$



Norm of magnetization

Norm of magnetization per spin m is computed by

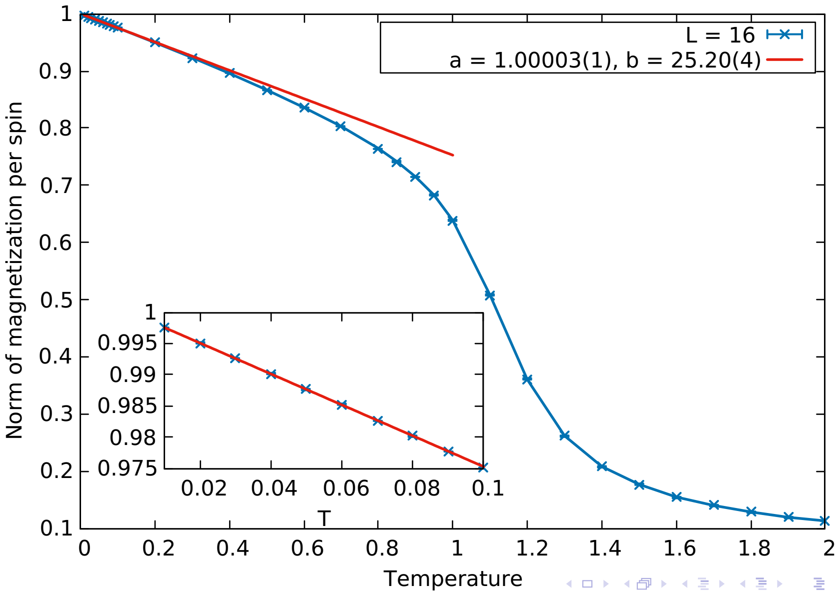
$$m^2 = \left(\sum_{ij} \cos\theta_{ij}\right)^2 + \left(\sum_{ij} \sin\theta_{ij}\right)^2 / N^2 \qquad (10)$$

at low temperatures the relation $m = 1 - T\left(\ln N + \ln 2\right)/8\pi$ holds.

Table 1: Fit results at low temperatures from $T = 0.01$ to $T = 0.10$. $8\pi \approx 25.132...$

Type	PRNG	Lattice	$\bar{a}$	σ_a	$\bar{b}$	σ_b
Wolff	MT	16	1.00003	0.00001456	25.2058	0.04578
Wolff	MT	32	1.00005	0.00001345	25.1389	0.03407
CUDA	XORWow	32	1.00008	0.00006787	25.1368	0.1839
CUDA	XORWow	64	1.00011	0.00007479	25.1891	0.179
CUDA	XORWow	128	1.00004	0.0001228	25.8772	0.3432

$m = 1 - T\left(\ln N + \ln 2\right)/8\pi$



Magnetization empirical consistency

The exponent β for magnetization the first derivative of free energy with respect to an external field is defined by

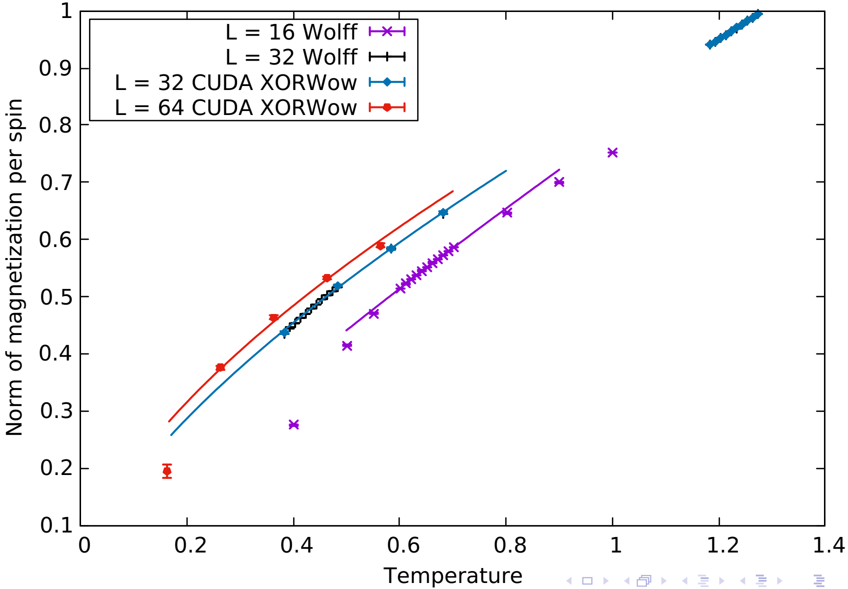
$$\beta = \frac{\partial \ln M}{\partial \ln(t)}, \; M = t^{\beta} \tag{11}$$

where $t = T_C - T, \; T_C(L) = T_{BKT} + \pi^2/c\,(\ln L)^2$, and $c \approx 2.1$ a constant.

- In a Ref., the author's simulation measured $\beta = 0.231...$ consistent with experiment of some compounds, e.g. $\mathrm{BaNi_2\,(PO_4)_2}$, $\mathrm{Rb_2CrCl_4}$.
- The author introduced a correction to the simulation results on the order of magnitude of $\beta/\ln\left(L^2\right)$.

Type	L	T_C	Fit range	$\langle\beta\rangle$	σ_β	Correction
Wolff	16	1.503	$0.80 \div 0.90$	0.419824	0.00423	0.075709
Wolff	32	1.283	$0.80 \div 0.90$	0.368365	0.003955	0.053143
CUDA	32	1.283	$0.60 \div 0.90$	0.33249	0.01043	0.047968
CUDA	64	1.164	$0.60 \div 1.00$	0.309588	0.02828	0.037220
CUDA	128	1.092	wait	wait	wait	wait

$M \sim t^{\beta}$, choose $T_{BKT} = 0.892$

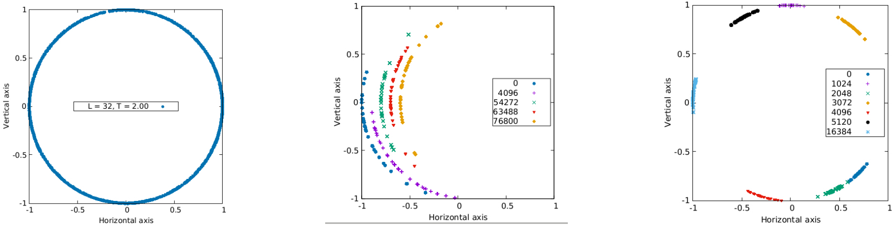


Susceptibility

The second derivative of free energy with respect to an externally applied field

$$\chi = N \left[\left\langle \mathbf{m}^2 \right\rangle_{T,\mathbf{H}} - \langle \mathbf{m} \rangle^2_{T,\mathbf{H}} \right] / k_B T \tag{12}$$

where $\mathbf{m} = 0$ confirmed by Mermin-Wagner theorem.



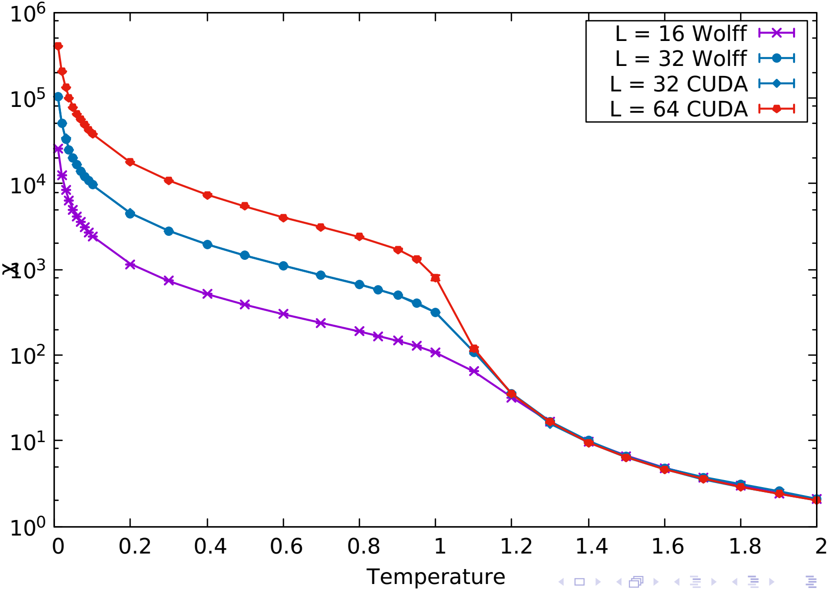
(d) $T = 2.00$. Metropolis.

(e) $T = 0.20$. Metropolis.

(f) $T = 0.01$. Wolff.

Figure 1: $L = 32$. Spin phase angle on unit circles. Mid: the horizontal coordinates are shifted for clarity, and the key numbers are the number of MCS.

Susceptibility



Reduced susceptibility and square of magnetization

At low temperature[4]

$$k_B T \chi \approx N \left\langle \mathbf{m}^2 \right\rangle = N N^{-T/4\pi} = N^{1-T/4\pi} \tag{13}$$

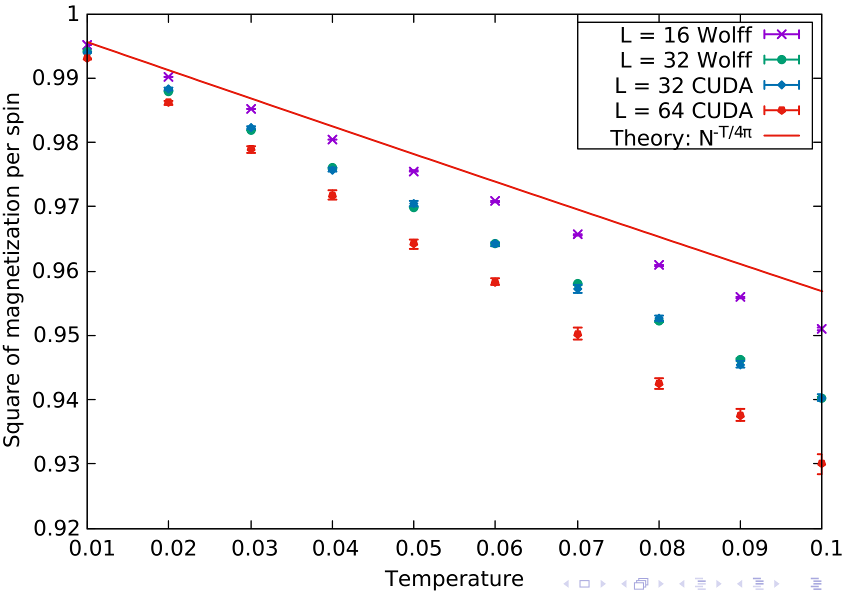
Table 2: Results of fitting parameters for the relation (13) of form $f(x) = aN^{-x/b}$ at low temperatures from $T = 0.01$ to $T = 0.10$.

Type	Lattice	$\bar{a}$	σ_a	$\bar{b}$	σ_b
Wolff	16	1.00013	0.00004234	11.0872	0.02923
Wolff	32	1.00019	0.00004081	11.2788	0.02316
CUDA	32	1.00027	0.0001508	11.278	0.09137
CUDA	64	1.00033	0.0001588	11.4594	0.08544

b checked with $4\pi \approx 12.566...$ Inconsistent.

[4] Phys. Rev. B, 20:3761–3769, Nov 1979.

$k_B T \chi$, the theoretical line for $L = 16$



Logarithmic correction

Our failure of consistency check with the paper in 1979 is correct, since in Ref. J. Phys. A, 38(26):5869, 2005, the author mentioned about logarithmic correction.

- First correction

$$k_B T\chi \sim N^{-T/4\pi} (\ln L)^{-2r} \tag{14}$$

- Second correction

$$k_B T\chi \sim N^{-T/4\pi} (\ln L + C)^{-2r} \tag{15}$$

Unfortunately our Levenberg–Marquardt non-linear fit program as well as the built-in fit function in GNUplot failed to perform the two corrected functions that we stopped to pursuit further.

Vortex density

The number of vortices or anti-vortices per unit volume, at low temperatures, obeys

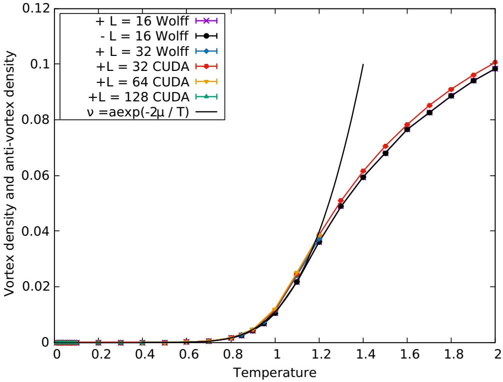
$$\nu \sim \exp\left(-2\mu/T\right) \tag{16}$$

where $2\mu = 10.2$ is the asymptotic energy for a vortex pair to occur.

Type	L	Fit range	$\bar{a}$	σ_a	$\bar{b}$	σ_b
Wolff	16	$0.40 \div 1.10$	25.6938	2.731	7.81554	0.1002
Wolff	32	$0.40 \div 1.10$	30.5109	3.829	7.91173	0.1162
CUDA	32	$0.40 \div 1.10$	27.7669	4.071	7.78041	0.1303
CUDA	64	$0.40 \div 1.10$	29.6065	4.641	7.82637	0.1402

The results are not consistent with the theoretical prediciton of BKT theory, $2\mu = 10.2$, however our results, e.g. with the case $L = 32$ with Wolff, $2\mu = 7.91173 \pm 0.1162$ whose upper bound within three sigma is not very much inconsistent with the lower bound of three sigma also of 9.4 ± 0.3 in a Ref. [**?**].

Vortex / anti-vortex density and $\nu \sim \exp\left(-2\mu/T\right)$



For $L = 16, 32, 64$ non-zero vorticity first occurs at $T = 0.40$ while for $L = 128$ with CUDA, it is $T = 0.30$. Note that the data for CUDA are approximately the same that is separated from the data for Wolff in CPU. This should be not enough statistics.

Energy

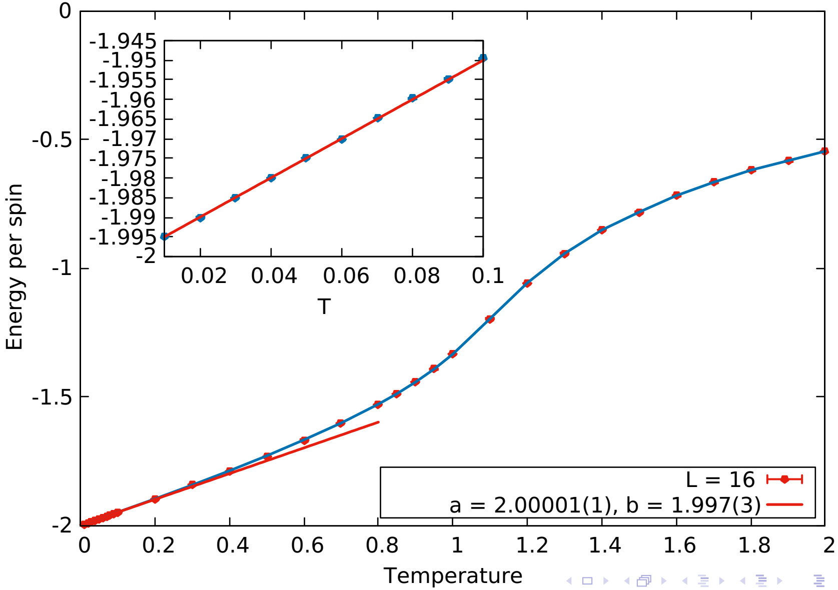
At low temperature $E = -2 + T/2$.

Table 3: Results of fitting parameters for $f(x) = -a + x/b$ at low temperatures.

Type	L	Fit range	$\bar{a}$	σ_a	$\bar{b}$	σ_b
Wolff	16	$0.01 \div 0.06$	2.000015	0.000019	1.997105	0.003023
Wolff	32	$0.01 \div 0.04$	2.000015	0.000014	1.992407	0.002845
CUDA	32	$0.01 \div 0.03$	2.000014	0.000012	1.993617	0.002768
CUDA	64	$0.01 \div 0.03$	2.000025	0.000006	1.989055	0.001497
CUDA	128	$0.01 \div 0.03$	2.000023	0.000003	1.989176	0.000684

The results mostly consistent in 3 sigma with fit range reduced, however, the data for CUDA simulation doesn't appear to be consistent. Argue with aid of specific heat.

Energy

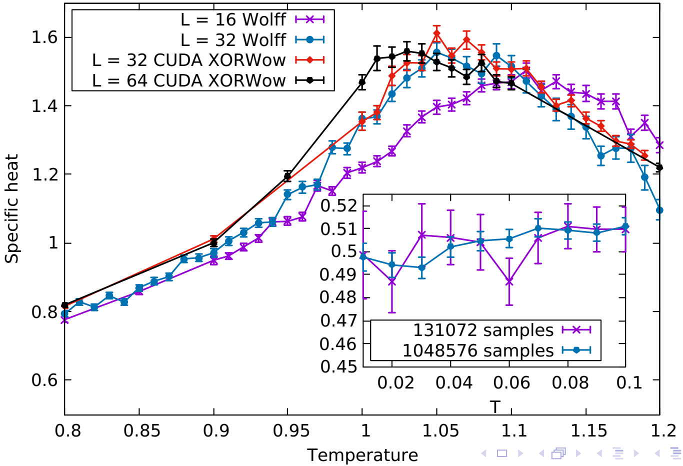


Energy per spin
Temperature
0
-0.5
-1
-1.5
-2
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
-1.945
-1.95
-1.955
-1.96
-1.965
-1.97
-1.975
-1.98
-1.985
-1.99
-1.995
-2
0.02
0.04
0.06
0.08
0.1
T
L = 16
a = 2.00001(1), b = 1.997(3)

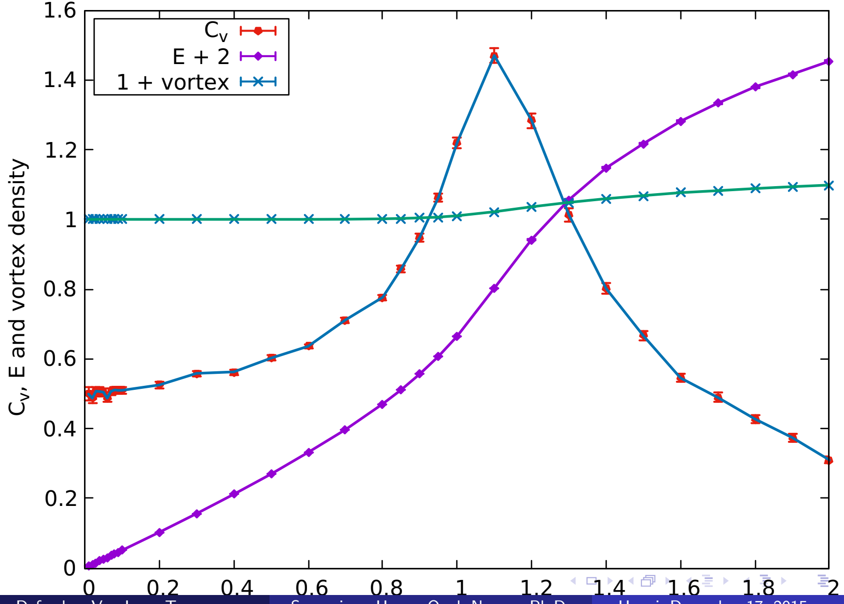
Specific heat

The second derivative of Helmholtz free energy w.r.t T

$$\mathcal{C}_v = N\left[\left\langle E^2\right\rangle_{T,\mathbf{H}} - \langle E\rangle^2_{T,\mathbf{H}}\right]/k_B T^2 \qquad (17)$$



The peak of specific heat



Helicity modulus

A twist of phase angle α applied on either directions of the boundaries introduces the helicity modulus or spin stiffness

$$\Upsilon = \frac{\partial^2}{\partial \alpha^2} F(\alpha)\Big|_{\alpha=0} \tag{18}$$

and some author derives a computational form

$$\Upsilon = -\frac{1}{2}\langle E\rangle - \frac{J}{k_B TN}\left\langle \left\{ \sum_{ij} \left[\sin\left(\theta_{ij} - \theta_{lmr}\right) - \sin\left(\theta_{ij} - \theta_{lml}\right)\right] \right\}^2 \right\rangle \tag{19}$$

$$= \left\langle -\frac{1}{2}E - \frac{J}{k_B TN}\left\{ \sum_{ij} \left[\sin\left(\theta_{ij} - \theta_{lmr}\right) - \sin\left(\theta_{ij} - \theta_{lml}\right)\right] \right\}^2 \right\rangle \tag{20}$$

Helicity modulus (cont)

- At low temperature $\Upsilon \approx \langle E \rangle /2 = 1 - T/4$.
- Nelson-Kosterlitz universal jump

$$\lim_{\substack{T \to T_{BKT},\\ N \to \infty}} \Upsilon(T)/k_B T = \frac{2}{\pi} \tag{21}$$

- Renormalization group extrapolation to $N = \infty$

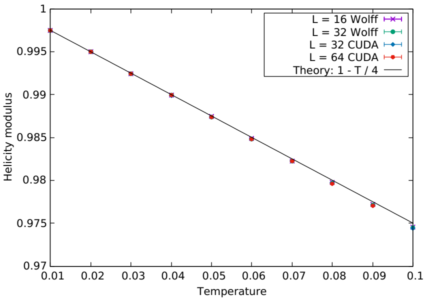
$$\Upsilon(N) = \Upsilon_\infty \left[1 + \frac{1}{2} \frac{1}{\ln(N) + C} \right] \tag{22}$$

where C is some free parameter.

- With (21)

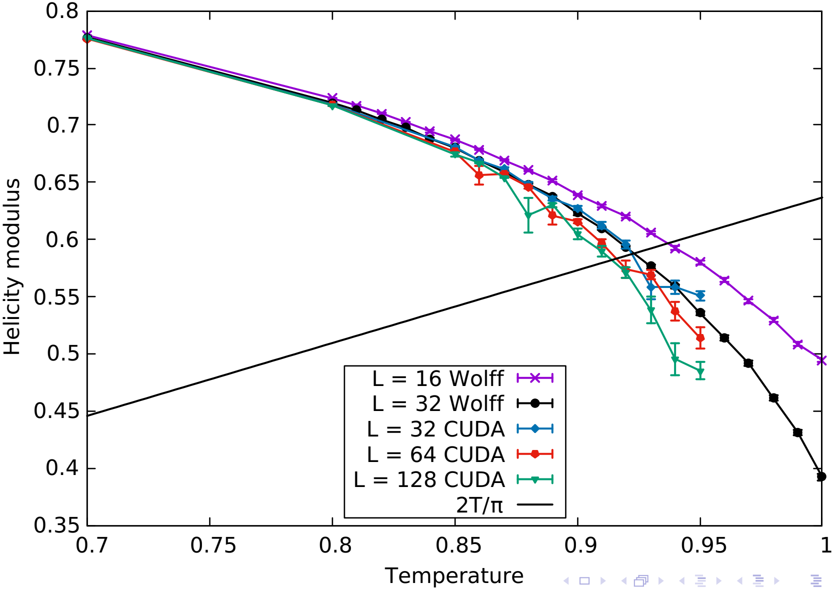
$$\Upsilon(N) = \frac{2}{\pi} T \left[1 + \frac{1}{2} \frac{1}{\ln(N) + C} \right] \tag{23}$$

$\Upsilon \approx 1 - T/4$ at $T < T_{BKT}$

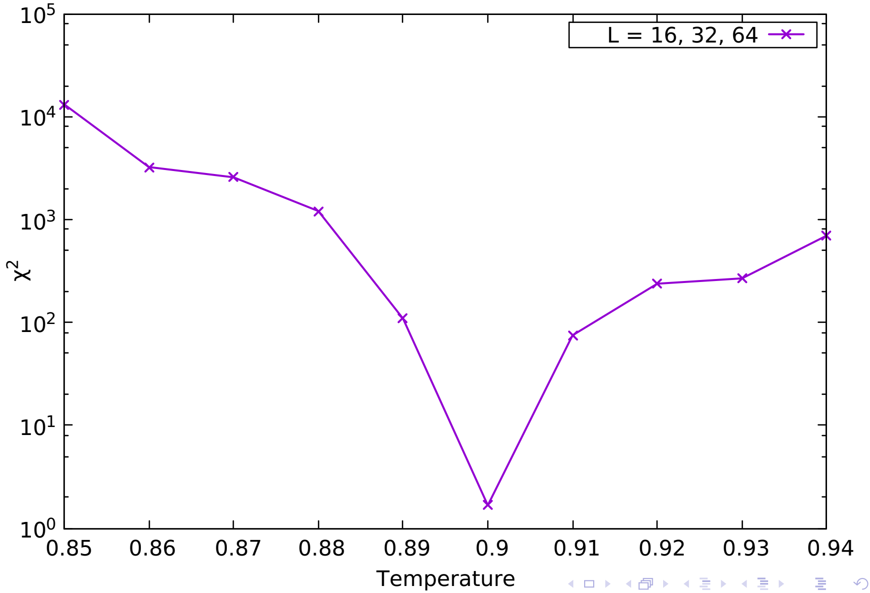


Type	L	$\bar{a}$	σ_a	$\bar{b}$	σ_b
Wolff	16	1.000044	0.000008	3.951209	0.004068
Wolff	32	1.000053	0.000005	3.933712	0.002263
CUDA	32	1.000056	0.000004	3.931145	0.001775
CUDA	64	1.000054	0.000002	3.929123	0.000837
CUDA	128	1.000018	0.000001	3.965626	0.001386
CUDA	256	1.000016	0.000001	3.967394	0.000619

Helicity modulus(cont)



Smallest chi square value, $T_{BKT} = 0.90(1)$



Conclusion

Conclusions

- The Berezinskii-Kosterlitz-Thouless phase transition is between two phase:
  - One with no free vortex at sufficiently low temperatures together with the quasi-long range order of power law decay of spin-spin correlation function, and a bit higher temperature still below T_{BKT}, with tightly bound vortex-anti-vortex pairs.
  - At T_{BKT}, these pairs dissociate and the system transits to the high temperature phase in which the spin-spin correlation function decays exponentially.
- The exponent β of magnetization is best found to be 0.30(6) consistent with experiment and theoretical approximation.
- The temperature at which the vortex density is non-zero for the first time is $T_0 = 0.4(1)$ in finite system.
- The transition temprature $T_{BKT} = 0.90(1)$.