The XY model, the Bose Einstein Condensation and Superfluidity in 2d (II)

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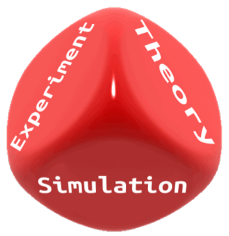
LABORATORY FOR SIMULATION IN PHYSICS



A Guide to Monte Carlo Simulations in Statistical Physics"
by Landau & Binder

Outline

- The planar Rotator and the XY model
- Equations of motion
- Vortices
  - **Dynamics**
- The BKT transition
- Final Remarks

The Planar Rotator

$$\mathcal{H}_{PR} = J\sum_{\langle i,j\rangle} \hat{S}_i \cdot \hat{S}_j = J\sum_{\langle i,j\rangle}\left(S_i^x S_j^x + S_i^y S_j^y\right) = J\sum_{\langle i,j\rangle}\cos(\theta_i - \theta_j)$$

$$\hat{S} = |S|(\cos\theta\,\hat{x} + \sin\theta\,\hat{y})$$

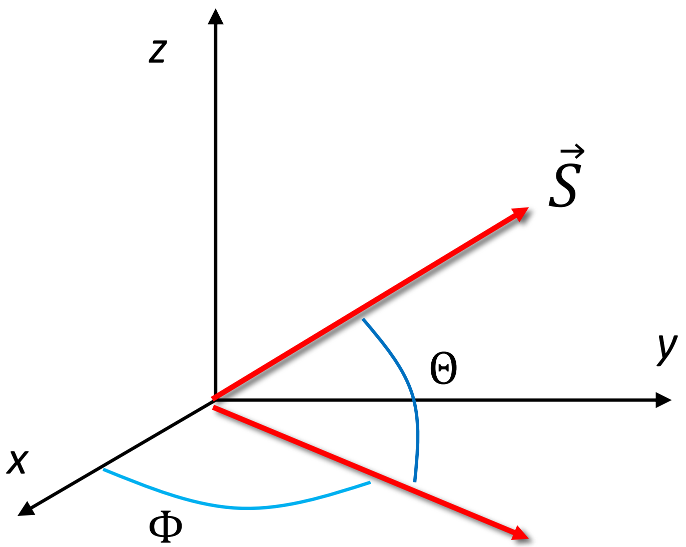
This model has no true dynamics because $S_j^z \equiv 0$

To introduce some dynamics let us consider the Anisotropic Heisenberg model

The XY Model
Anisotropic Heisenberg

$$\mathcal{H}_{XY} = J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j = J \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z \right)$$

$$\hat{S} = |S| (cos\, \Theta\, cos\Phi \hat{x} + cos\Theta \sin \Phi\, \hat{y} + sin\Theta\, \hat{z})$$



Now, we consider:

- Θ is small
- Θ and Φ vary smoothly

The XY Model
Continuum Limit

$$\Theta_{i\pm1,j} = \Theta(x \pm a, y) = \Theta(x,y) \pm a\frac{\partial\Theta}{\partial x} + \frac{a^2}{2}\frac{\partial^2\Theta}{\partial x^2} + O(a^3),$$

$$\Theta_{i,j\pm1} = \Theta(x, y \pm a$$

$$\sin(\Theta_{i\pm1,j}) = \sin\Theta \pm \frac{a}{2}(\sin\Theta \mp 2\cos\Theta)\frac{\partial\Theta}{\partial x} + \frac{a^2}{2}\frac{\partial^2\Theta}{\partial x^2}\cos\Theta + O(a^3),$$

$$\sin(\Theta_{i,j\pm1}) = \sin\Theta \pm \frac{a}{2}(\sin\Theta \mp 2\cos\Theta)\frac{\partial\Theta}{\partial y} + \frac{a^2}{2}\frac{\partial^2\Theta}{\partial y^2}\cos\Theta + O(a^3),$$

$$\cos(\Theta_{i\pm1,j}) = \cos\Theta \pm \frac{a}{2}(\cos\Theta \pm 2\sin\Theta)\frac{\partial\Theta}{\partial x} + \frac{a^2}{2}\frac{\partial^2\Theta}{\partial x^2}\sin\Theta + O(a^3),$$

$$\cos(\Theta_{i,j\pm1}) = \cos\Theta \pm \frac{a}{2}($$

$$\cos(\Phi_{i,j} - \Phi_{i\pm1,j}) = 1 - \frac{1}{2}a^2\left(\frac{\partial^2\Phi}{\partial y^2} + O(a^3)\right)^2,$$

The XY Model and the Plane Rotator

Taking the limit $a \to 0$, and retaining only termos up to $O(2)$ (We use $\lambda = 0$)

$$H_{AH}^{cont} = -2J \int d\,\mu \left[\left(\frac{\partial\, \Phi}{\partial\, x} \right)^2 + \left(\frac{\partial\, \Phi}{\partial\, y} \right)^2 \right].$$

$$Z_{AH} = \int d\mu e^{-J \sum_{\langle i,j \rangle} \cos(\Phi_i - \Phi_j)}, \qquad d\mu \equiv d\Phi_1 d\Phi_2 \ldots d\Phi_n d\Theta_1 d\Theta_2 \ldots d\Theta_n .$$

The integrals over the out-of-plane angle fluctuations, Θ, can readily be done, so that, the averages of in-plane quantities doesn't depends on Θ in a clear indication that it is in the same universality class as the Planar Rotator model.

The XY Model
Equations of Motion

We start written: $\frac{dS_i^\alpha}{dt} = i\hbar[\mathcal{H}_{XY}, S_i^\alpha]$ where $\alpha = x, y, z$

In terms of the spherical angles

$$\dot{\Theta}_n = \frac{\partial H/\partial \Phi_n}{\cos\Theta_n}, \quad \dot{\Phi}_n = \frac{\partial H/\partial \Theta_n}{\cos\Theta_n}.$$

After calculating all commutators and taking the classical continuum limit

$$\dot{\Theta} = 2J[\cos\Phi\nabla^2(\cos\Theta\sin\Phi) - \sin\Phi\nabla^2(\cos\Theta\cos\Phi)]$$

$$-\cos\Theta\dot{\Phi} = 2J\{\lambda\cos\Theta[\sin^2\Phi\nabla^2\sin\Theta + \cos^2\Phi\nabla^2(\sin\Theta\cos\Phi)] - \sin\Theta[\sin\Phi\nabla^2(\cos\Theta\sin\Phi) + \cos\Phi\nabla^2(\cos\Theta\cos\Phi)]\}$$

The XY Model
Equations of Motion

$$\dot{\Theta} = 2J[\cos\Phi\nabla^2(\cos\Theta\sin\Phi) - \sin\Phi\nabla^2(\cos\Theta\cos\Phi)]$$

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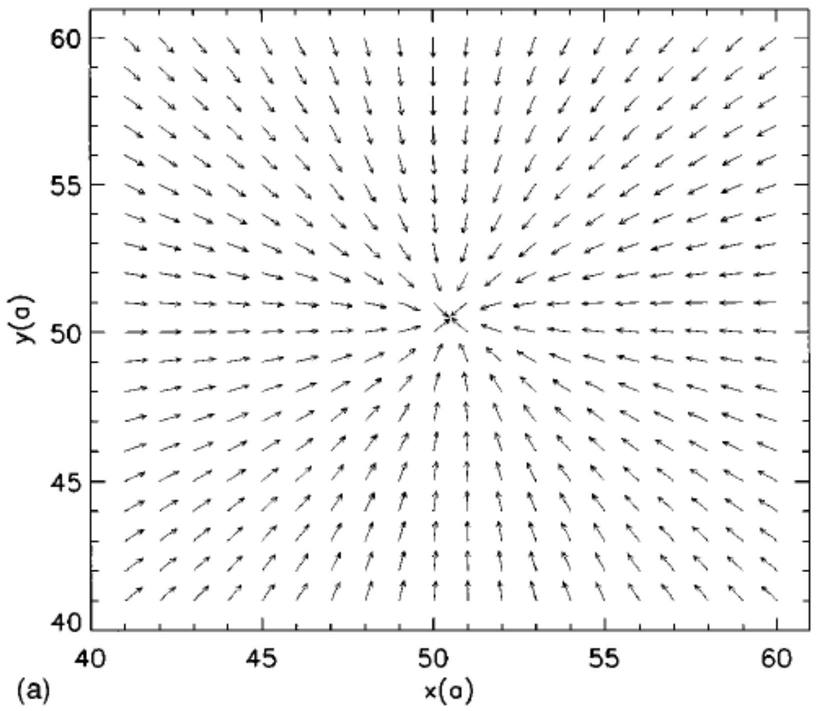
With appropriate boundary conditions we can solve those equations

$$S^\alpha(x,y) = S^\alpha(-x,y), \quad \lim y \to \pm\infty$$

$$S^\alpha(x,y) = S^\alpha(x,-y), \quad \lim x \to \pm\infty$$

$$\Theta_0 = 0 \quad \text{and} \quad \Phi_0 = \arctan\frac{y}{x},$$

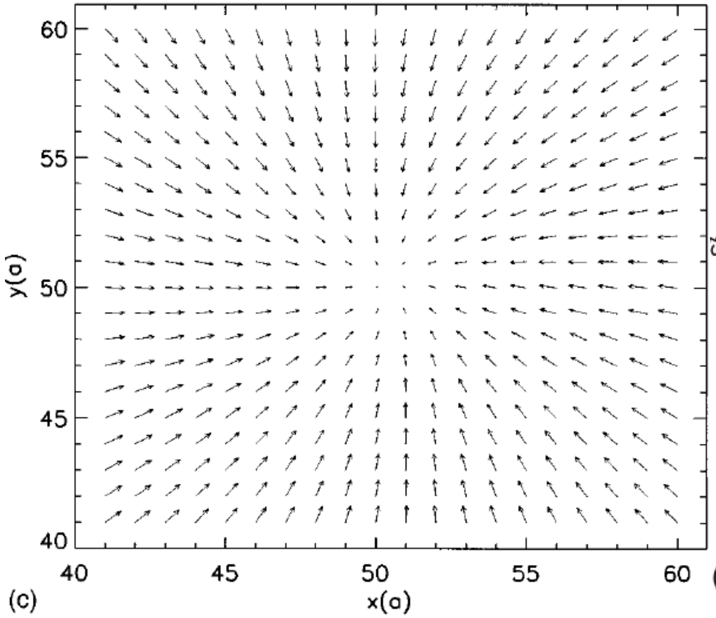


Which describes an in-plane vortex ($\lambda = 0$)

The XY Model
Vortex Solution

$$\dot{\Theta} = 2J[\cos\Phi\,\nabla^2(\cos\Theta\sin\Phi) - \sin\Phi\,\nabla^2(\cos\Theta\cos\Phi)]$$

$$-\cos\Theta\,\dot{\Phi} = 2J\{\lambda\cos\Theta[\sin^2\Phi\,\nabla^2\sin\Theta + \cos^2\Phi\,\nabla^2(\sin\Theta\cos\Phi)] - \sin\Theta[\sin\Phi\,\nabla^2(\cos\Theta\sin\Phi) + \cos\Phi\,\nabla^2(\cos\Theta\cos\Phi)]\}$$



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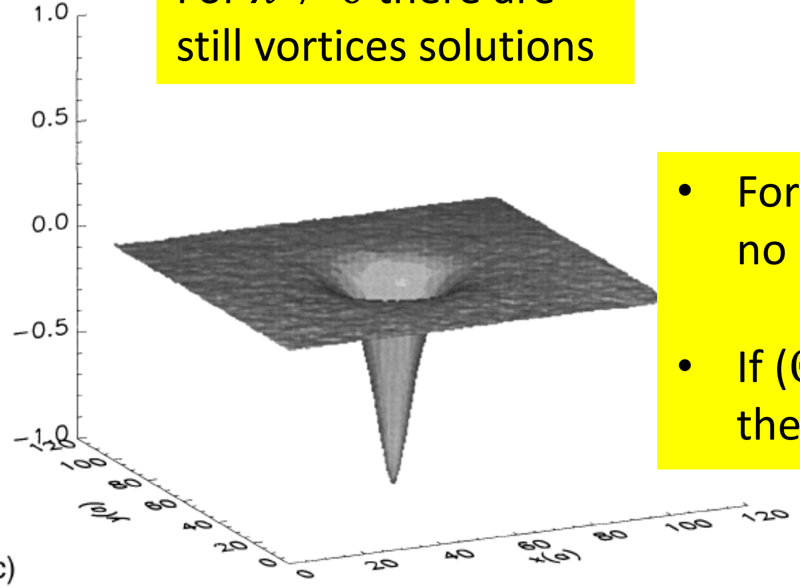
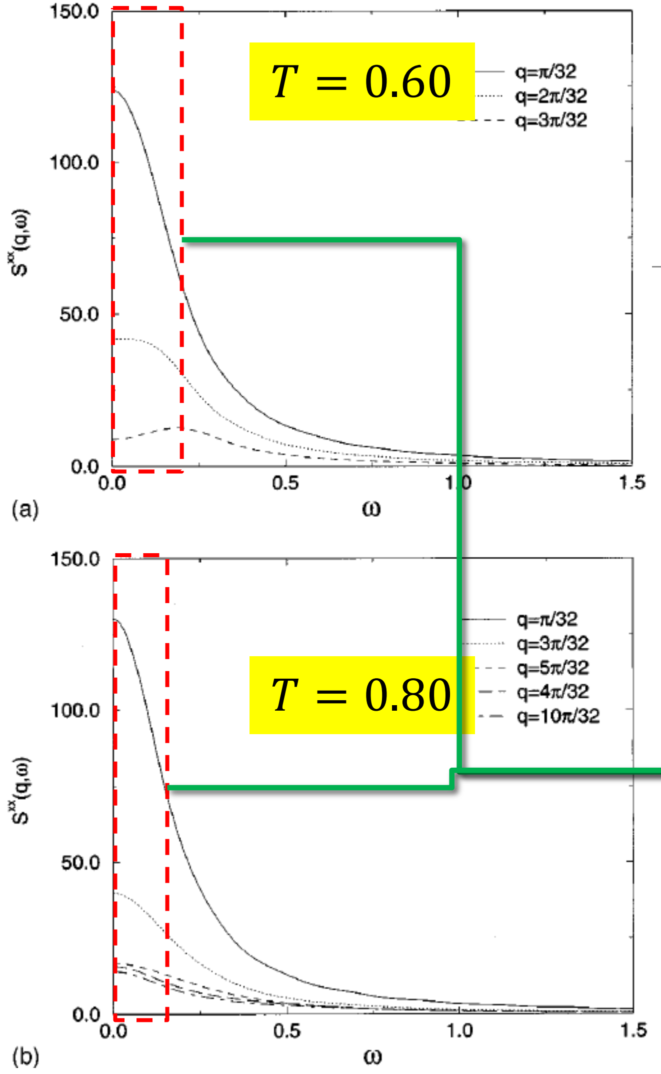


For $\lambda \neq 0$ there are still vortices solutions

- For in-plane vortex ($\Theta = 0$) there is no dynamics.
- If ($\Theta \neq 0$) , $\dot{\Theta}$ *and* $\dot{\Phi} \neq 0$, however, there is no more vortex solution.

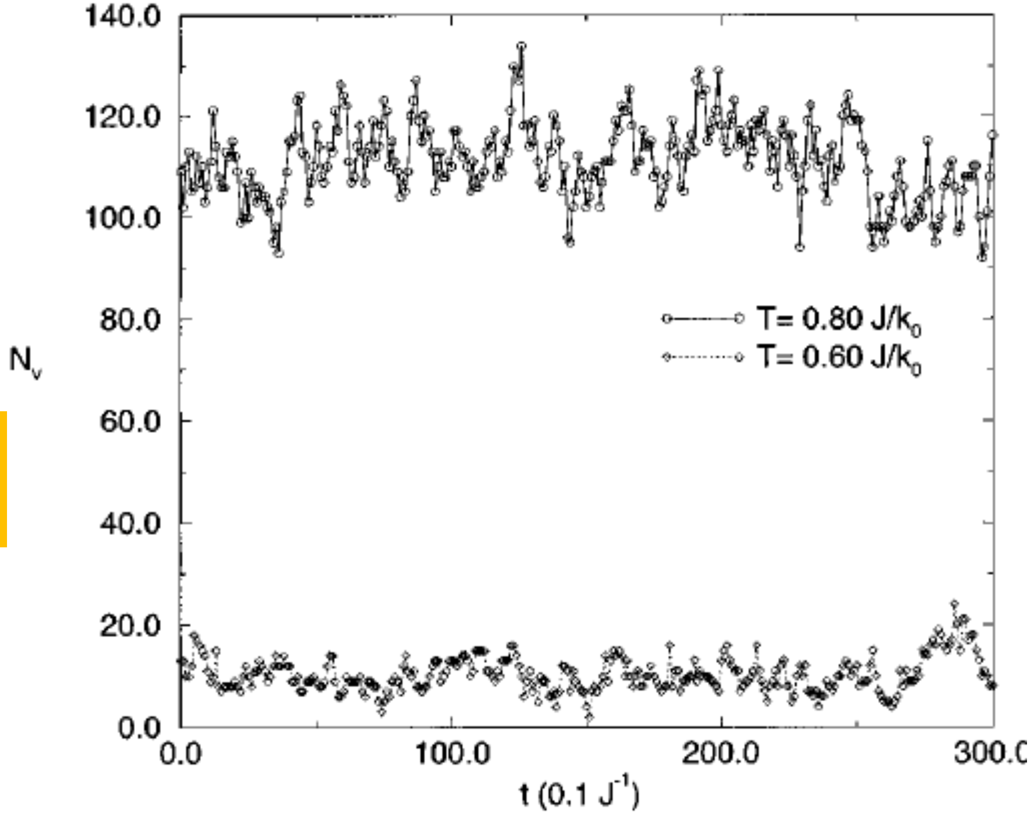
Dynamics (Spin-spin correlation)



$T_{BKT} = 0.7003(3)$

Where do the central peaks come from?

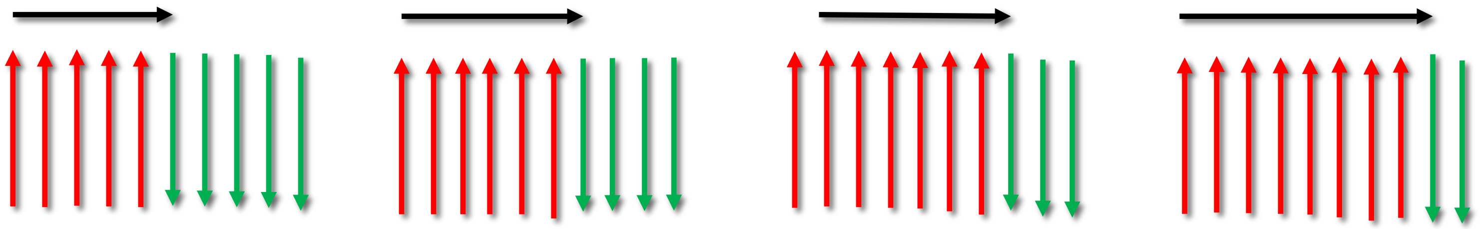
In-plane correlations



Number of vortices as a function of time

Dynamics – Free vortex gas model

Borrowed from an older 1d model (H.J. Mikeska, Journal of Physics C 11 (1978) L29)

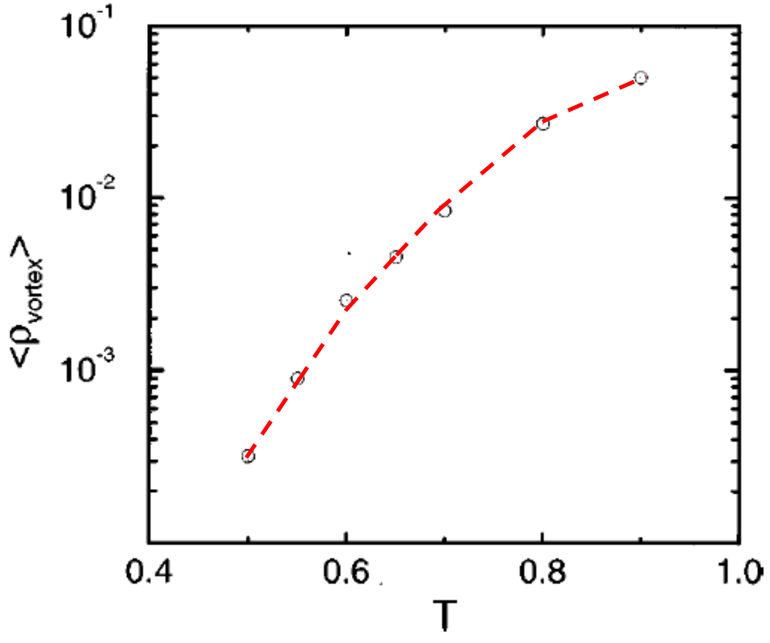


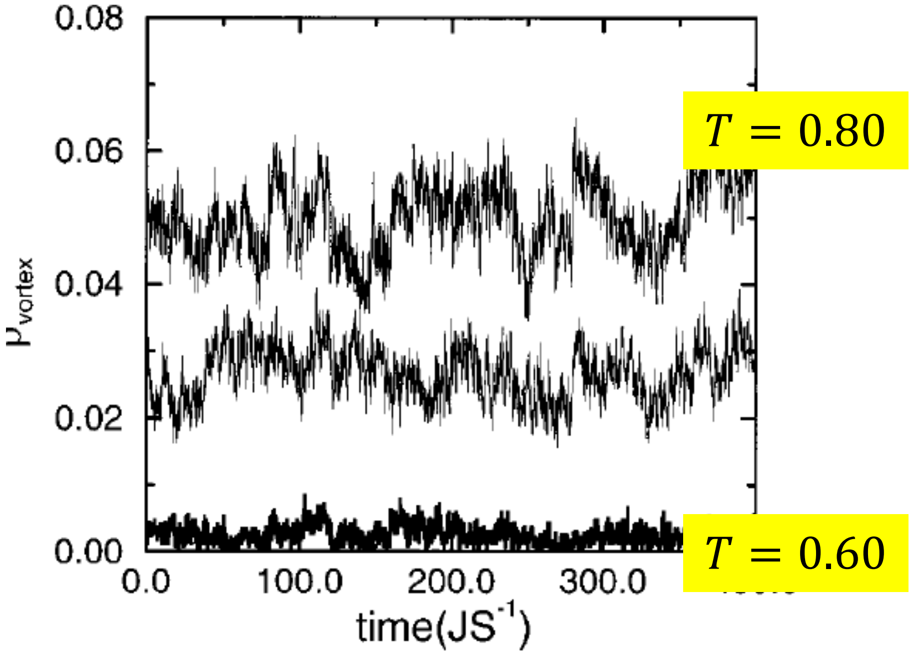
Kinks can freely move
(No energy cost)

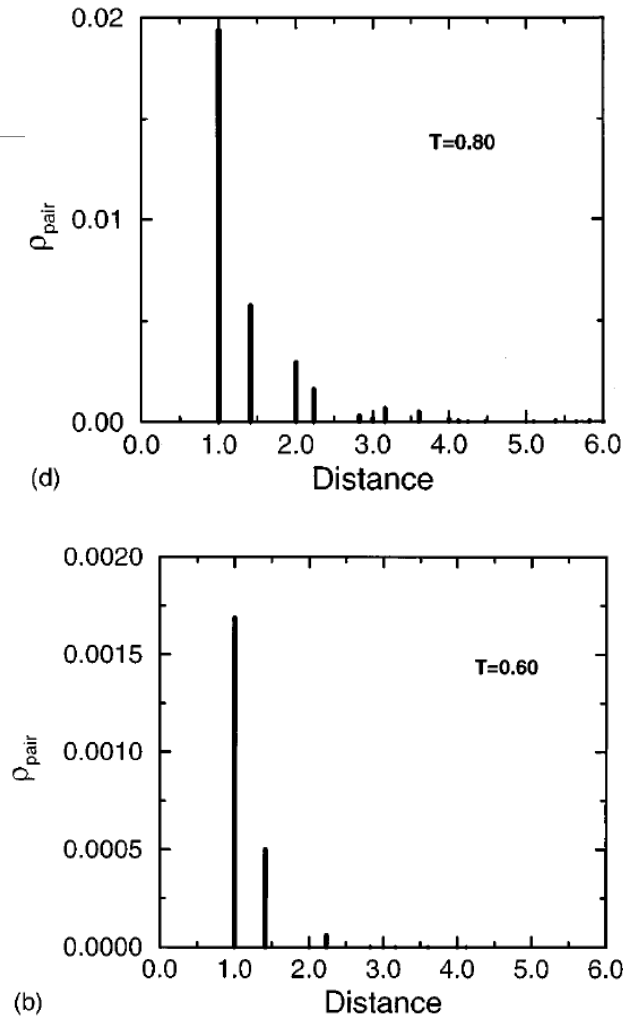
Vortex gas model : F.G. Mertens, A.R. Bishop, G.M. Wysin, C. Kawabata, Physical Review Letters 59 (1987) 117.

Vortices are too large to move. The model doesn't work.

Dynamics
Vortex Behavior

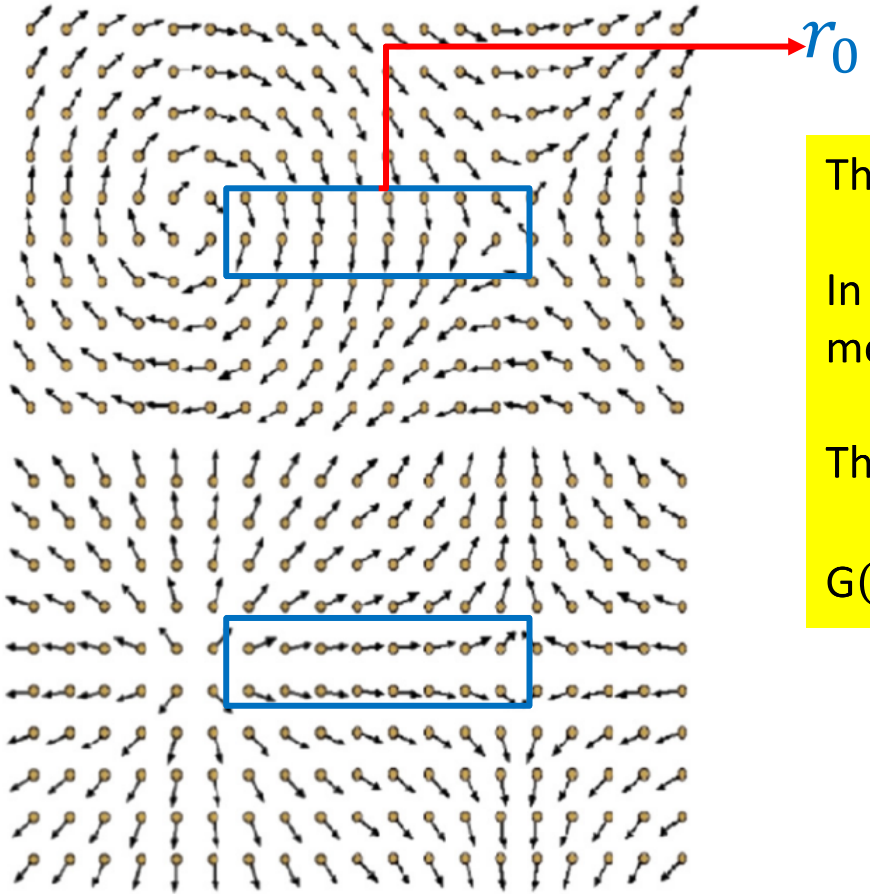






$T_{BKT} = 0.7003(3)$

Dynamics
Vortex-antivortex

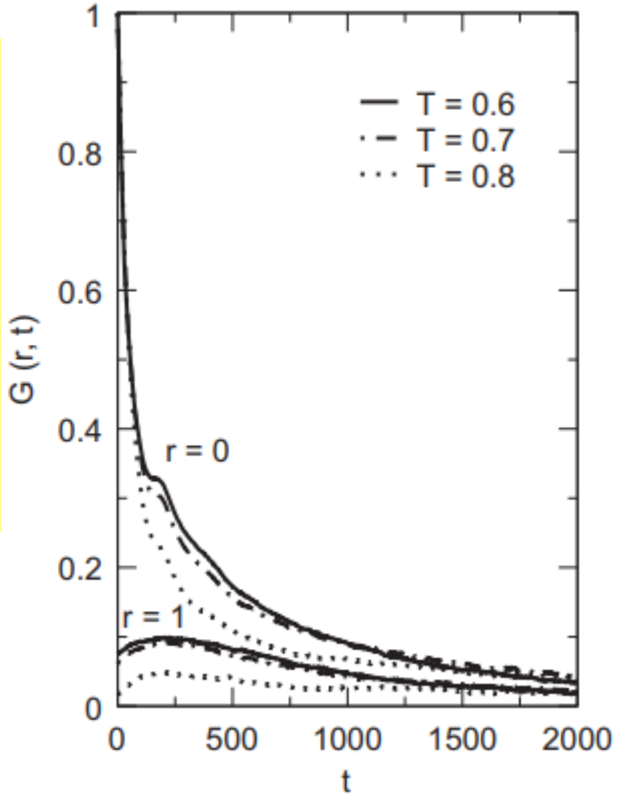


There is a local magnetization $m \propto r_0$

In a neutron scattering experiment we measure the local fluctuations of m

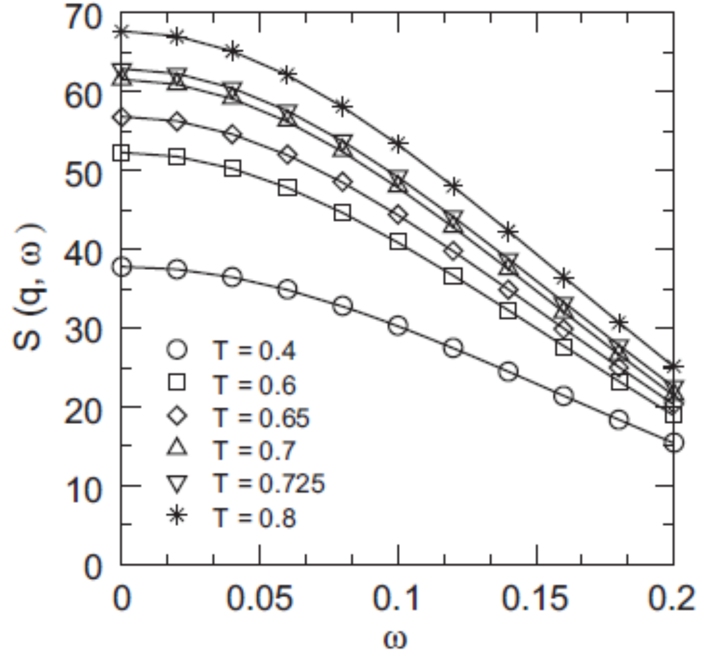
The quantity we want is:

$G(r,t) \sim \langle r_0^2 \rangle \langle \rho_{pair}(0,0) \rho_{pair}(r,t) \rangle$

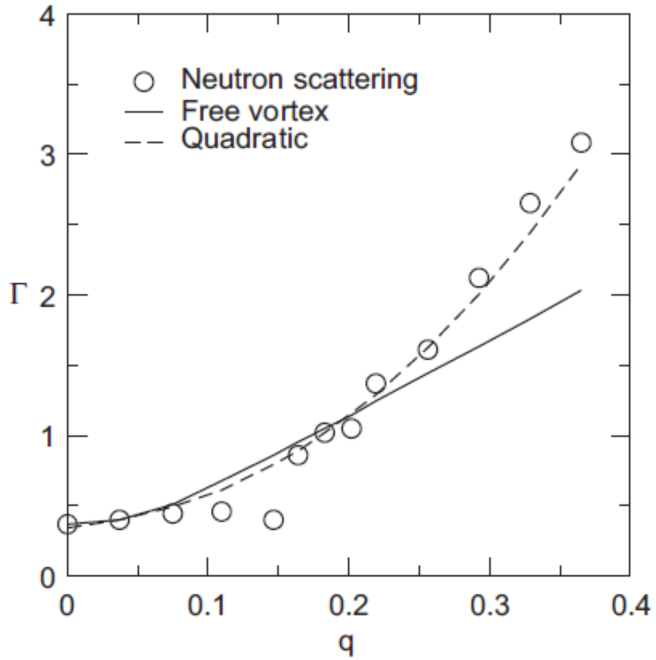


Dynamics Vortex-antivortex

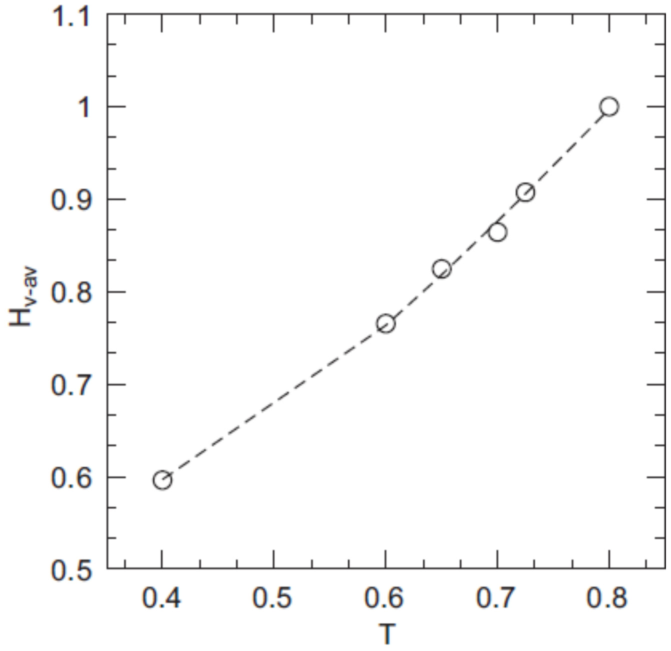
Symbols: Simulation data
Lines: creation-annihilation



Central peak half width



Central peak height



Diffusion due to a pair creation-annihilation process.

$$\tilde{C}^{xx}(q,\omega) \approx 2\pi \langle r_0^2 \rangle N_v^2 \left\{ \pi\delta(\omega)\delta(\vec{q}) - \frac{\gamma\delta(\vec{q})}{4\gamma^2+\omega^2} + \frac{Dq^2+2\gamma}{(Dq^2+2\gamma)^2+\omega^2} \right\}$$

γ : creation-annihilation rate

Dynamics – Magnon-Vortex interaction

(Phase shifts)

$$\dot{\Theta} = 2J[\cos\Phi\,\nabla^2(\cos\Theta\sin\Phi) - \sin\Phi\,\nabla^2(\cos\Theta\cos\Phi)]$$

$$-\cos\Theta\,\dot{\Phi} = 2J\{\lambda\cos\Theta[\sin^2\Phi\,\nabla^2\sin\Theta + \cos^2\Phi\,\nabla^2(\sin\Theta\cos\Phi)] - \sin\Theta[\sin\Phi\,\nabla^2(\cos\Theta\sin\Phi) + \cos\Phi\,\nabla^2(\cos\Theta\cos\Phi)]\}$$

The behavior of small oscillations in presence of a vortex is given by solutions of the eq. of motion of the form $\Theta = \theta \; and \; \Phi = \Phi_0 + \phi$, where $\theta, \phi \ll 1 \; and \; \Phi_0$ is the static vortex solution

Only large wavelengths are relevant.

Dynamics - Conclusion

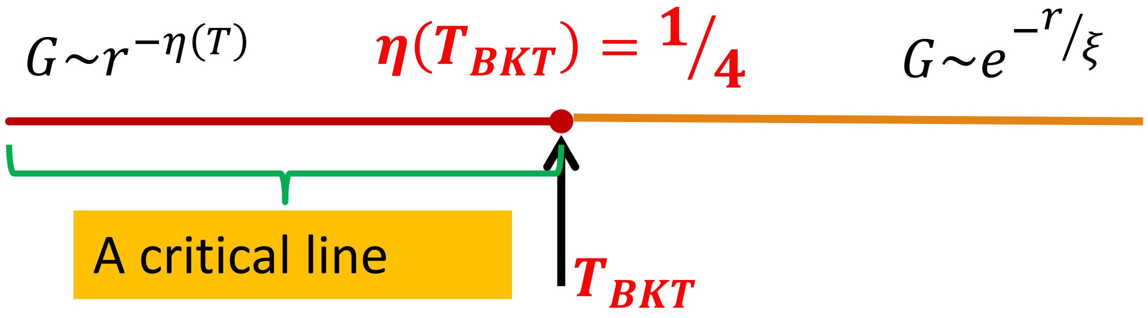
Vortices don’t become “free” at high temperature.

The phase transition occurs when pairs vortices-antivortices are spontaneously created

The central peak is due to a vortex-antivortex creation annihilation process.

The KT Transition

$$G(r) \equiv \langle S(0) \cdot S(r) \rangle$$



Renormalization results

$$\eta(T_{BKT}) = {}^{1}/_{4}$$

$$\xi(T) \approx e^{\left(bt^{-1/2}\right)} \quad ; \quad t = \frac{T - T_{BKT}}{T_{BKT}}$$

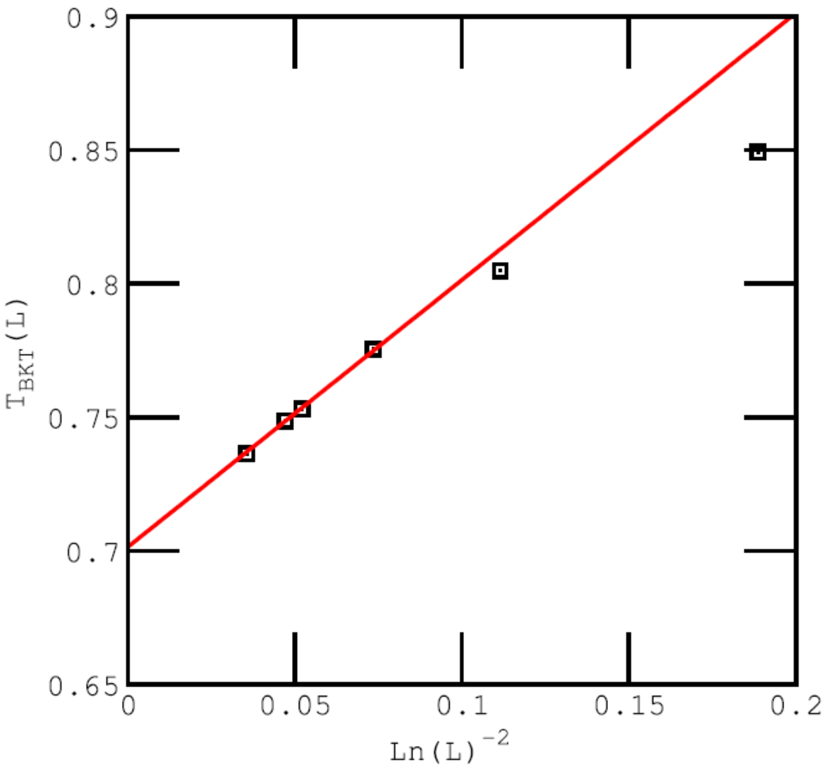
$$m_{XY} \equiv \frac{1}{V} \sum \sqrt{(m_x)^2 + \left(m_y\right)^2} = 0$$

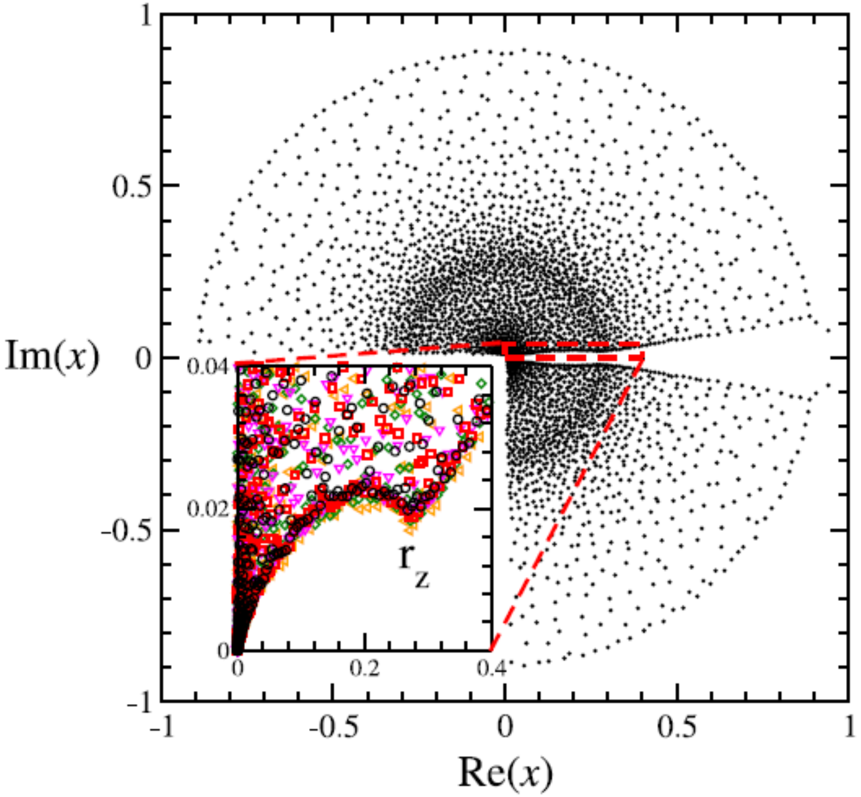
$$\chi_{xy} \equiv \frac{1}{T}\left(m_{xy} - \langle m_{xy} \rangle\right)^2 = \begin{cases} \xi^{2-\eta} & , T > T_{BKT} \\ \infty & , T < T_{BKT} \end{cases}$$

$C_v \equiv \frac{1}{T^2}\left\langle (E - \langle E \rangle)^2 \right\rangle$ ***is finite.***

The free energy is C^{∞}

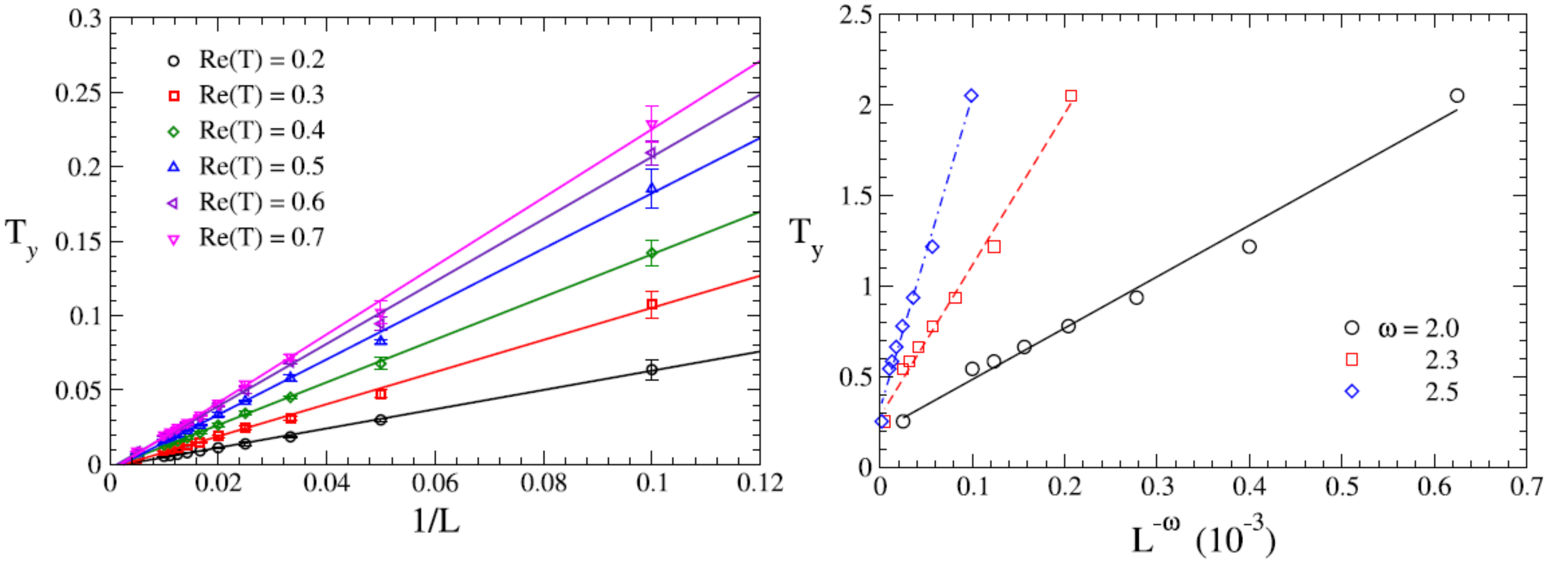
The BKT transition – Fisher Zeros





$$T_{BKT} = 0.7003(3)$$

The BKT transition – Fisher Zeros



Final Remark

As expected from the Mermin-Wagner theorem there is no long-range order in this model

The correlations decay to zero in both sides of T_{BKT}

However, the quasi-long range order at low T is enough to create a quasi-ordered phase

That is the origin of the superfluid transition in Bose fluid films and harmonically-trapped two dimensional ultracold Bose gases.

In other words:

The absence of BEC implies that $\lim_{r\to\infty} G(r) = 0$; however, if phase coherence falls slowly enough this shall turn out to be sufficient to induce superfluidity.

Thank you for your attention

Special thanks for this kind invitation

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