Thermodynamic phase transition and quantized vortices in Bose-Einstein condensates

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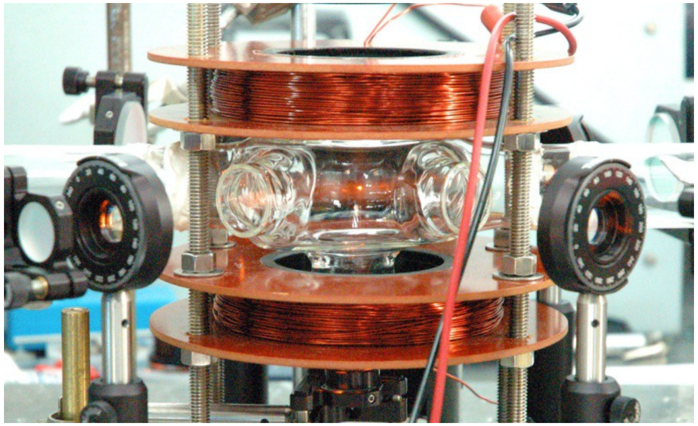
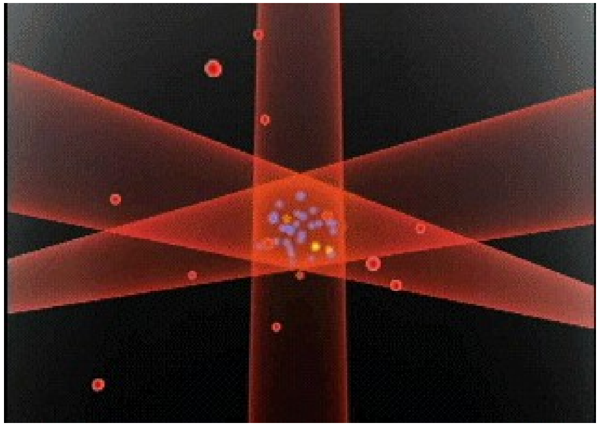
- Bose-Einstein condensates at finite temperatures
- Stochastic Gross-Pitaevskii equation and thermodynamic phase transition
- Geometric transition of quantized vortices
- Phase ordering and quantized vortices in quench dynamics

Jan. 18, 2016 “量子渦と非線形波動2016”

Ultracold atomic Bose gas

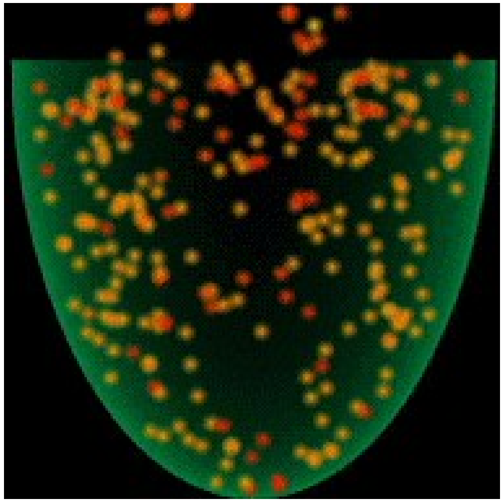


Trapping atoms



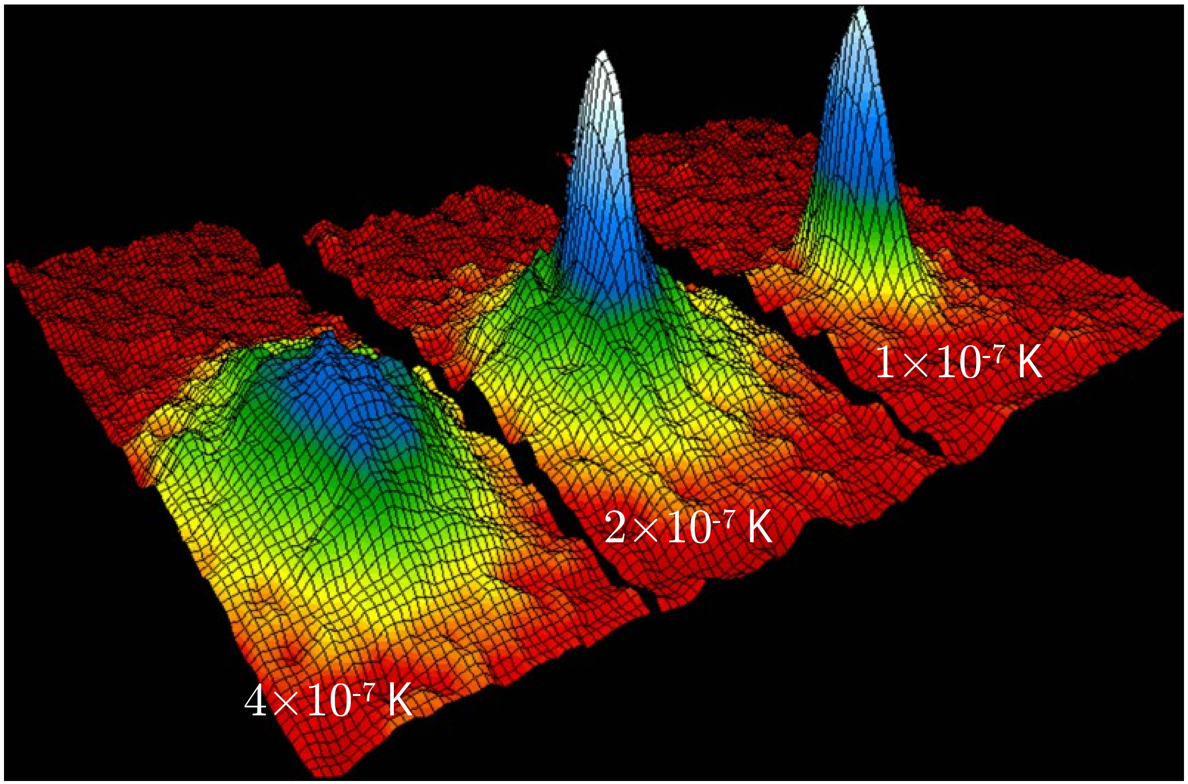
Laser cooling

^{87}Rb, ^{23}Na, ^{7}Li, ^{1}H, ^{85}Rb, ^{41}K, ^{4}He, ^{133}Cs, ^{174}Yb, ^{52}Cr, ^{40}Ca, ^{84}Sr, ^{164}Dy, ^{168}Er

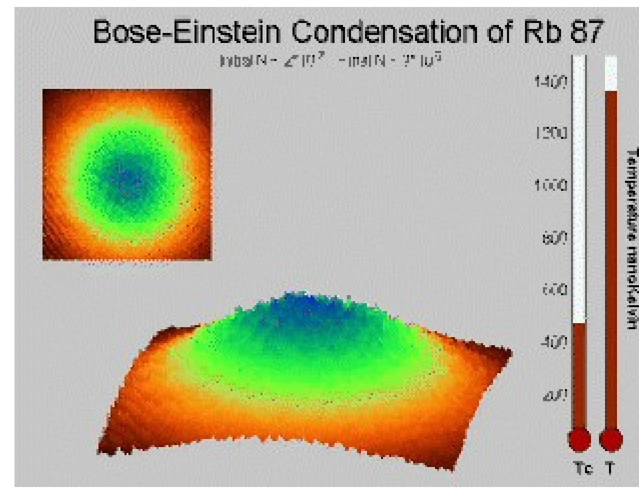


Evaporative cooling

Ultracold atomic Bose gas



Condensation
(not dynamics)



JILA, 1995

Ultracold atomic Bose gas

Phase transition of noninteracting Bose gas

Uniform system

$$T_c = \frac{2\pi\hbar^2}{mk_B}\left\{\frac{n}{\zeta(3/2)}\right\}^{2/3} \quad \text{for 3-dim}$$

$$d_L = 3 \qquad d_U = 4$$

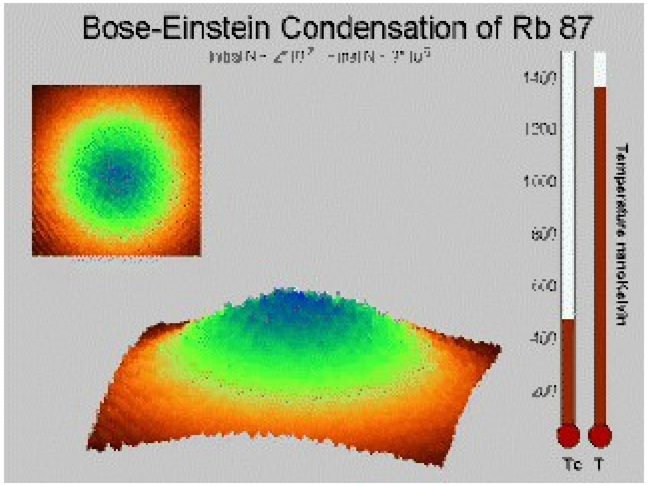
universality class : spherical model

Harmonically trapped system

$$T_c = \frac{\hbar\omega}{k_B}\left\{\frac{N}{\zeta(3)}\right\}^{1/3} \quad \text{for 3-dim}$$

$$d_L = 2 \qquad d_U = 3$$

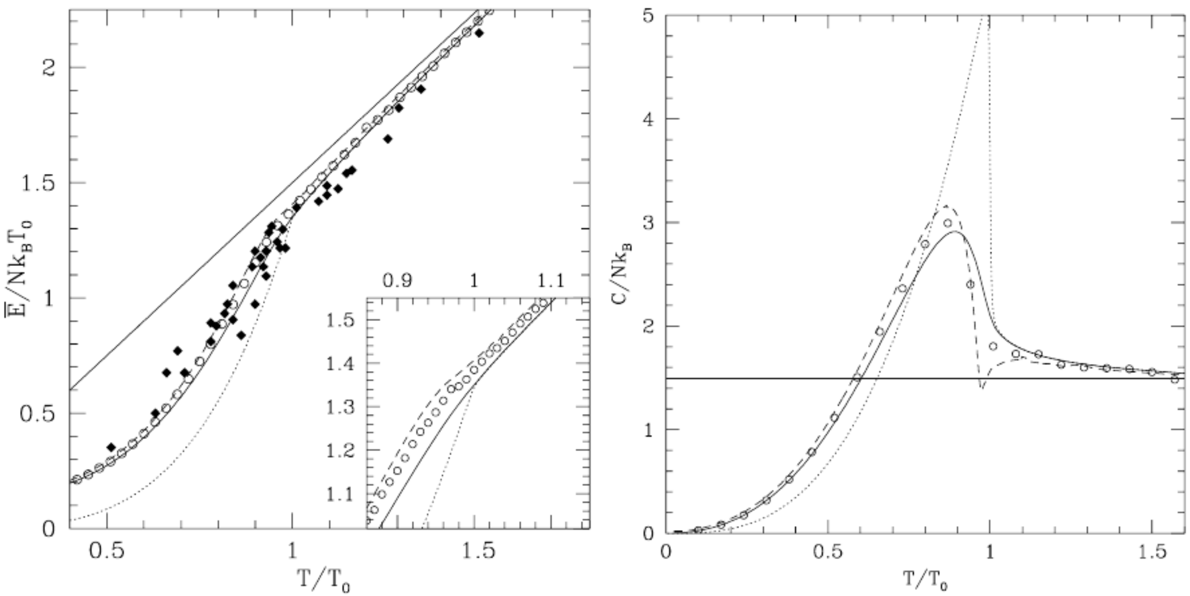
Condensation
(not dynamics)



Bose-Einstein condensates at finite temperatures

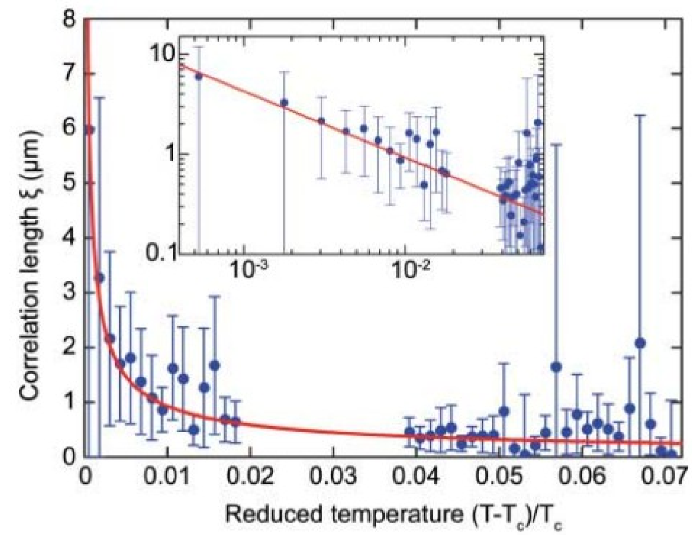
Thermodynamic phase transition

Total energy and specific heat



PRL **77**, 4984 (1996)

Correlation length



Science **315**, 1556 (2007)

Critical behaviors of specific heat and correlation length near the critical temperature

→ 2nd ordered phase transition

Effects of interparticle interaction

$$T_c^{\rm ideal} = \begin{cases} \dfrac{2\pi\hbar^2}{mk_B}\left\{\dfrac{n}{\zeta(3/2)}\right\}^{2/3} & \text{free} \\ \dfrac{\hbar\omega}{k_B}\left\{\dfrac{N}{\zeta(3)}\right\}^{1/3} & \text{trapped} \end{cases}$$

a : s-wave scattering length

$$\frac{\Delta T_c}{T_c^{\rm ideal}} = \begin{cases} c_f (na^3)^{1/3} & \text{free} \quad -1.2 \lesssim c_f \lesssim 2.5 \\ \dfrac{c_t a}{R_{TF}} & \text{trapped} \quad c_f \simeq -1.3 \end{cases}$$

Infinitesimal interaction a changes the universality class for uniform system (a=0 is singular)

→ It is difficult to determine ΔT_c

Theories for BEC at finite T

- Boltzmann & Gross-Pitaevskii（ZNG theory）
- Stochastic Gross-Pitaevskii eq.
- Complex Ginzburg-Landau eq.
- Classical-field Monte Carlo
- Bogoliubov theory
- Projected Gross-Pitaevskii eq.
- Path-integral Monte Carlo
- Trancated Wigner method
- Complex Stochastic Gross-Pitaevskii eq.

•Simple
•Not widely used

SGP equation and thermodynamic phase transition

SGP equation in uniform system

JPhysB **38**, 4259 (2005)

$$(i\hbar-\gamma)\dot{\psi}=-\frac{\hbar^2}{2M}\nabla^2\psi-\mu\psi+g|\psi|^2\psi+\sqrt{\gamma k_{\mathrm{B}}T}\xi$$

$\psi(\boldsymbol{x},t)$: complex field for bosons

γ : dissipation

μ : chemical potential

$g=\dfrac{4\pi\hbar^2 a}{M}$: coupling constant

$\xi=\xi_1+i\xi_2$: Gaussian noise for

$$\langle\xi_a(\boldsymbol{x},t)\rangle=0 \qquad \langle\xi_a(\boldsymbol{x},t)\xi_b(\boldsymbol{x}',t')\rangle=\delta(\boldsymbol{x}-\boldsymbol{x}')\delta(t-t')\delta_{a,b}$$

Unapplicable near the zero temperature due to neglecting the commuation relation $[\psi,\psi^\dagger]=i\delta$ (complexification of ψ is needed)

SGP equation in uniform system

JPhysB **38**, 4259 (2005)

$$(i\hbar - \gamma)\dot{\psi} = -\frac{\hbar^2}{2M}\nabla^2\psi - \mu\psi + g|\psi|^2\psi + \sqrt{\gamma k_{\mathrm{B}} T}\xi$$

$$(i\hbar - \gamma)\dot{\psi} = \lim_{c\to\infty}\frac{\hbar^2}{2M}\left(\frac{\partial_t^2}{c^2} - \nabla^2\right)\psi - \mu\psi + g|\psi|^2\psi + \sqrt{\gamma k_{\mathrm{B}} T}\xi$$

$$\Rightarrow \begin{cases} \phi = \dfrac{\hbar^2}{2Mc^2}\dot{\psi} - i\hbar\psi \\ \dot{\phi} = -\dfrac{\delta E}{\delta\psi^*} - \dfrac{2M\gamma c^2}{\hbar^2}(\phi + i\hbar\psi) + \sqrt{\gamma k_{\mathrm{B}} T}\xi \\ E = \displaystyle\int d\boldsymbol{x}\left(\frac{\hbar^2}{2M}|\nabla\psi|^2 - \mu|\psi|^2 + \frac{g}{2}|\psi|^4\right) \end{cases}$$

SGP equation in uniform system

$$\begin{cases} \phi = \dfrac{\hbar^2}{2Mc^2}\dot{\psi} - i\hbar\psi \\ \dot{\phi} = -\dfrac{\delta E}{\delta\psi^*} - \dfrac{2M\gamma c^2}{\hbar^2}(\phi + i\hbar\psi) + \sqrt{\gamma k_{\mathrm{B}} T}\xi \\ E = \displaystyle\int d\boldsymbol{x} \left(\frac{\hbar^2}{2M}|\nabla\psi|^2 - \mu|\psi|^2 + \frac{g}{2}|\psi|^4 \right) \end{cases}$$

Ito's lemmna

$P = P(\phi, \phi^*, \psi, \psi^*, t)$: probability density functional

$$\frac{\partial P}{\partial t} = \Bigg[-\frac{2Mc^2}{\hbar^2}\left\{ (\phi + i\hbar\psi)\frac{\delta}{\delta\psi} - \gamma \right\} + \left\{ \frac{\delta E}{\delta\psi^*} + \frac{2M\gamma c^2}{\hbar^2}(\phi + i\hbar\psi) \right\}\frac{\delta}{\delta\phi} + \gamma k_{\mathrm{B}} T \frac{\delta^2}{\delta\phi\delta\phi^*} + \mathrm{H.C.} \Bigg] P$$

SGP equation in uniform system

$P = P(\phi, \phi^*, \psi, \psi^*, t)$: probability density functional

$$\frac{\partial P}{\partial t} = \Bigg[-\frac{2Mc^2}{\hbar^2} \left\{ (\phi + i\hbar\psi)\frac{\delta}{\delta\psi} - \gamma \right\}$$

$$+ \left\{ \frac{\delta E}{\delta\psi^*} + \frac{2M\gamma c^2}{\hbar^2}(\phi + i\hbar\psi) \right\} \frac{\delta}{\ldots} \ldots \text{c.c.} \Bigg] P$$

SGP equation gives (at least) equilibrium property with GP energy functional

... : Giving Gibbs measure independent of c

$$\langle f \rangle_{\text{eq}} = \int D\psi^* \, D\psi \, \frac{f e^{-E/k_{\text{B}}T}}{Z} = \lim_{t \to \infty} \frac{1}{t} \int_0^t dt' f(t')$$

: Expectation value in equilibrium

Numerical Simulation of SGP eq.

- rescaled by healing length $\hbar/\sqrt{2M\mu}$
- discretize the space and time

$$(i-\gamma)\Delta\psi_i = \Delta t\left\{\frac{1}{(\Delta x)^2}\sum_{a=x,y,z}(2\psi_i - \psi_{i+a} - \psi_{i-a}) - \mu\psi_i + g|\psi_i|^2\psi_i\right\} + \sqrt{\gamma T \Delta t}\xi_i$$

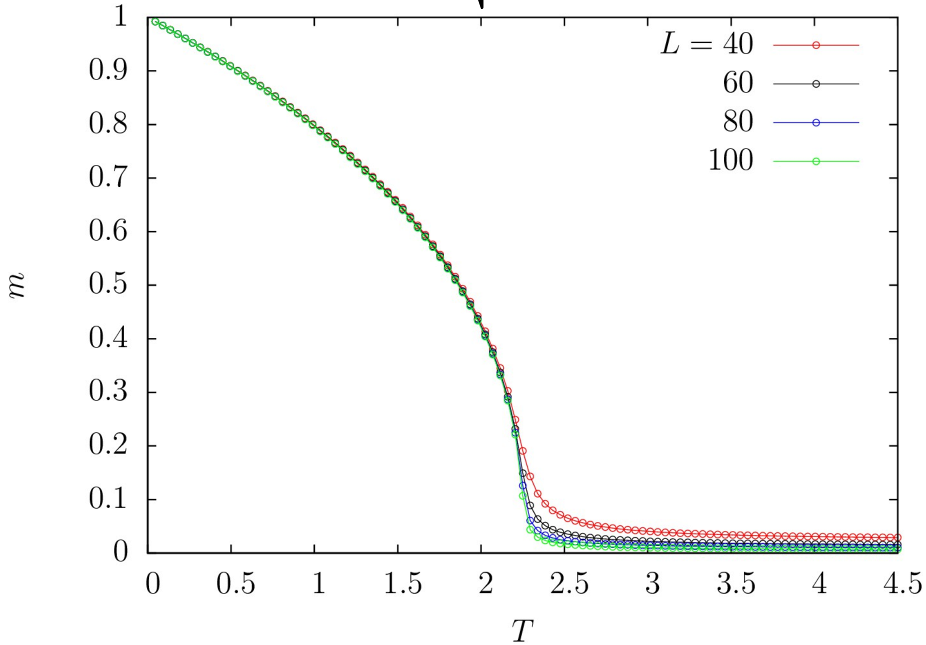
$$\gamma = \mu = g = 1$$

Space : 3-dimensional space with periodic boundary condition

Thermodynamic transition

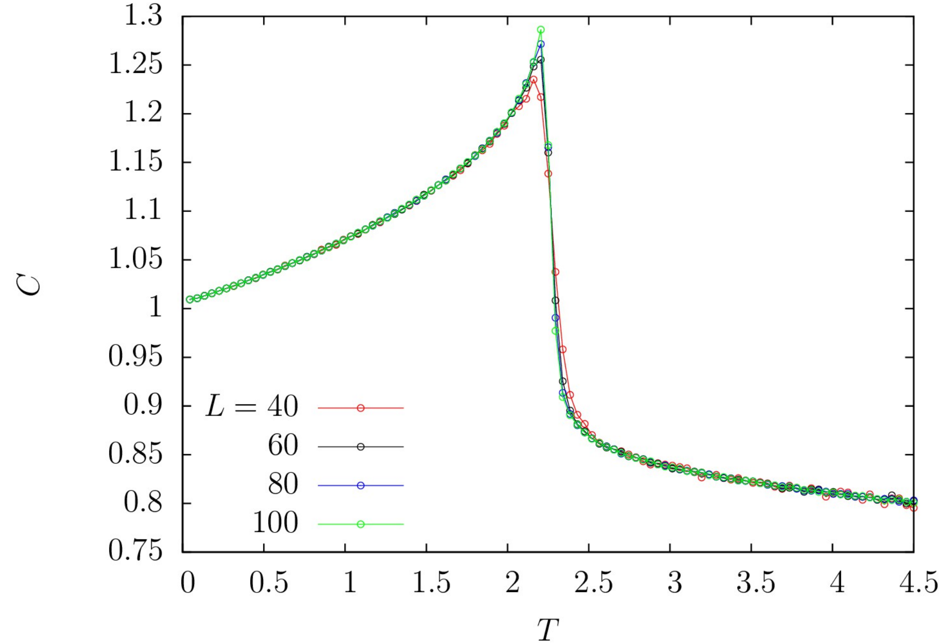
Order parameter

$$m \equiv \frac{1}{L^3}\sqrt{\left\langle \left| \int d\boldsymbol{x}\, \psi \right|^2 \right\rangle}$$



Specific heat

$$C \equiv \frac{\partial \langle E \rangle}{\partial T}$$



Non-analytic behavior emerges at $T \approx 2.26$

Critical exponents and universality class

Nature of thermodynamic transition for interacting Bose gas

→ Symmetry breaking of global $U(1)$ phase shift : $\psi \to \psi\, e^{i\varphi}$

→ Universality class : XY model

Critical exponents and comparison with XY model

		Result	Theory	Free bosons
order parameter	$m \propto (T_c - T)^{\beta}$	0.35	$9/25$	$1/2$
specific heat	$C \propto \lvert T - T_c\rvert^{-\alpha}$	-0.015	- $1/50$	-1
suscestibility	$\chi \propto \lvert T - T_c\rvert^{-\gamma}$	1.32	$121/100$	2
correlation length	$\xi \propto \lvert T - T_c\rvert^{-\nu}$	0.67	$101/150$	1
correlation time	$\tau \propto \lvert T - T_c\rvert^{-\nu z}$	2.1	2.01	2

SGP equation can describe the BEC transition as spontaneous $U(1)$ symmetry breaking

Geometric transition of quantized vortices

Thermodynamic and geometric transitions

Question : Are there geometric transition corresponding to the BEC transition (thermodynamic transition)?

For free bosons : percolation transition of particle worldlines

PRE **63**, 026115 (2001)

$$Z = \int Dx_1(\tau) \cdots Dx_N(\tau) \exp\left(- \int_0^{\beta\hbar} d\tau \sum_i \frac{M\dot{x}_i^2}{2} + \mu N \right)$$

$$= \exp\left(\frac{L^3}{\lambda^3} \sum_w w^{-5/2} e^{\mu w/(k_{\rm B}T)} \right)$$

w : winding number

Thermodynamic and geometric transitions

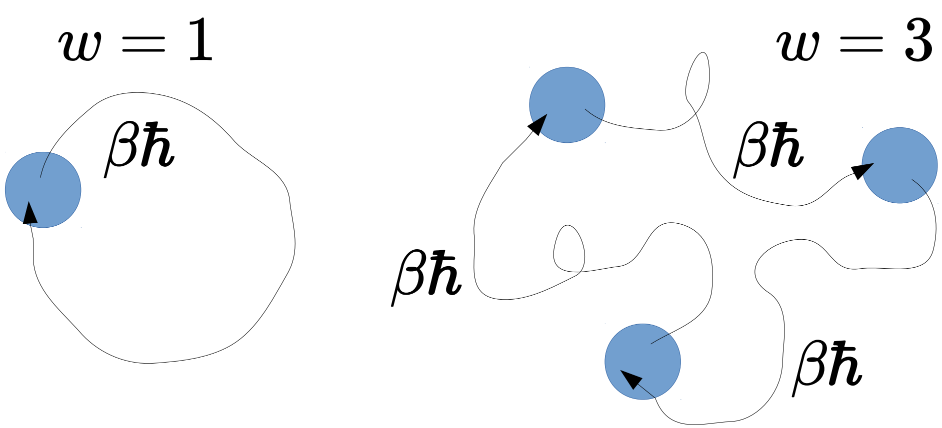
$$Z = \int Dx_1(\tau) \cdots Dx_N(\tau) \exp\left(-\int_0^{\beta\hbar} d\tau \sum_i \frac{M\dot{x}_i^2}{2} + \mu N\right)$$

$$= \exp\left(\frac{L^3}{\lambda^3} \sum_w w^{-5/2} \underline{e^{\mu w/(k_\mathrm{B}T)}}\right)$$

w : winding number

Probability weight for loop w

Example of particle worldlines



For $\mu = 0$ at $T = T_\mathrm{c}$, large worldline loops emerge and worldline percolation occurs (critical exponents are same)

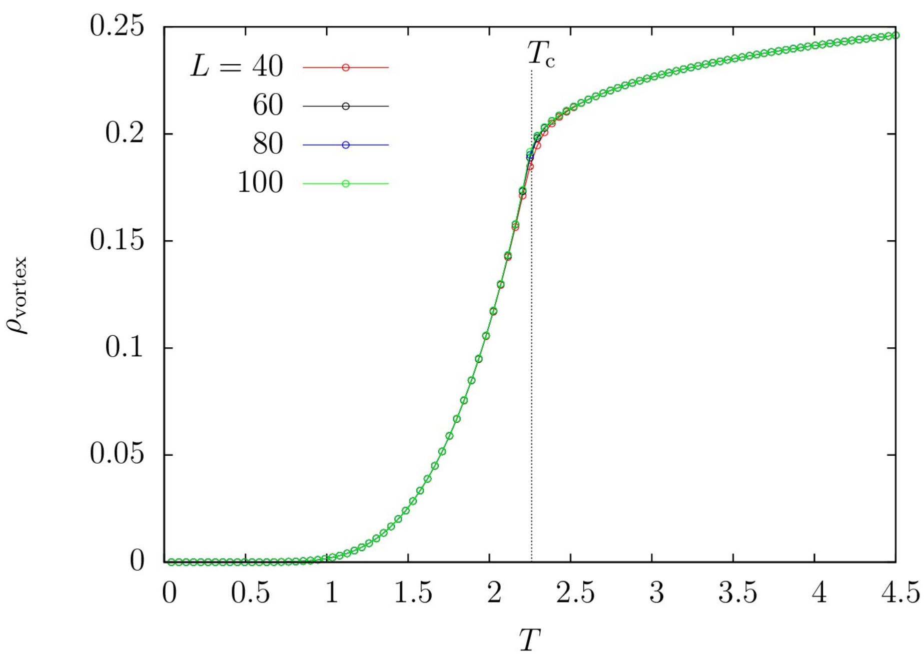
Geometric transition of vortex loops

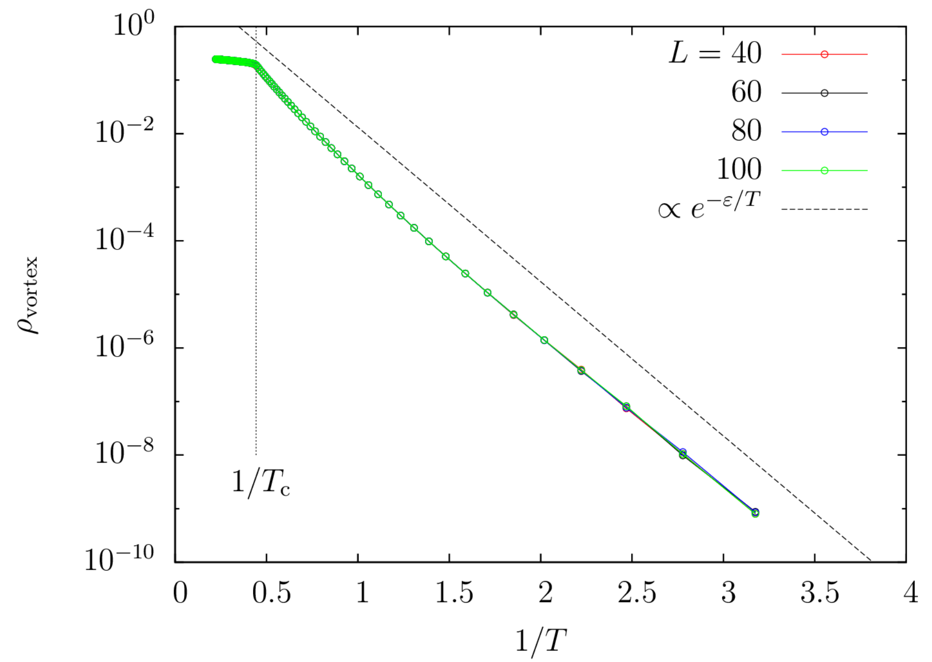
Interacting bosons : discussion of particle worldlines is difficult
(It cannot be discussed within SGP equation)

Can we expect the percolation of vortex loops instead at the thermodynamic transition point?

Vortex line density

$$\rho_{\text{vortex}} \equiv \frac{\text{total length of vortex lines}}{L^3}$$



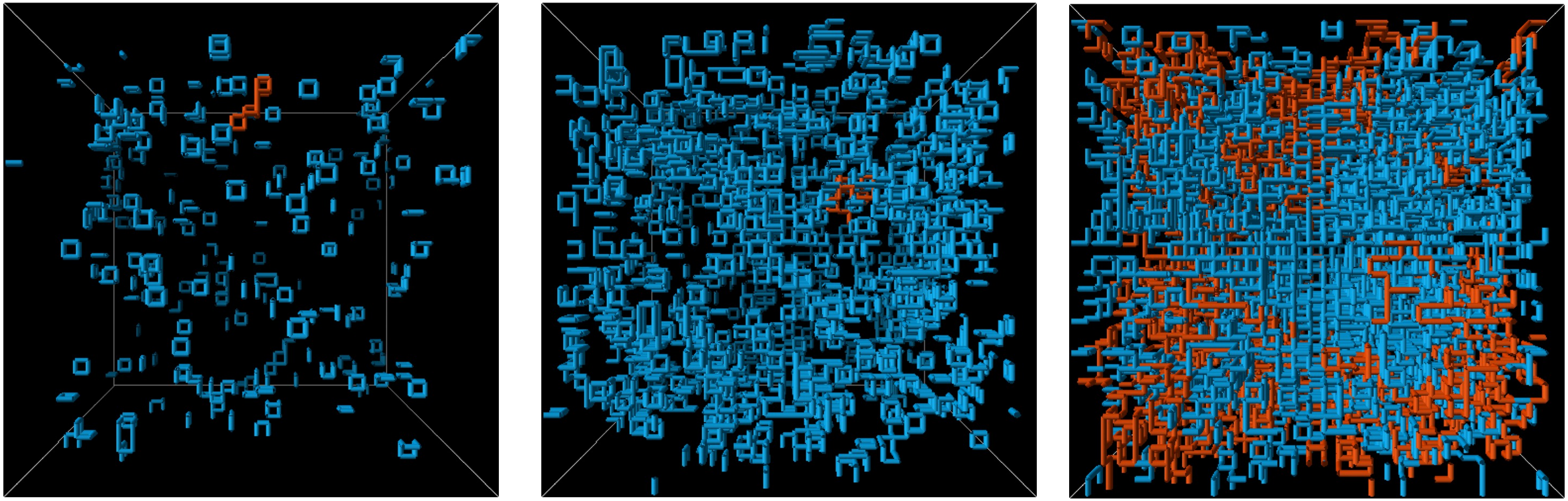


$\rho_{\text{vortex}} \propto e^{-\varepsilon/k_B T}$: for low T

Small loops are generated through the tunneling process

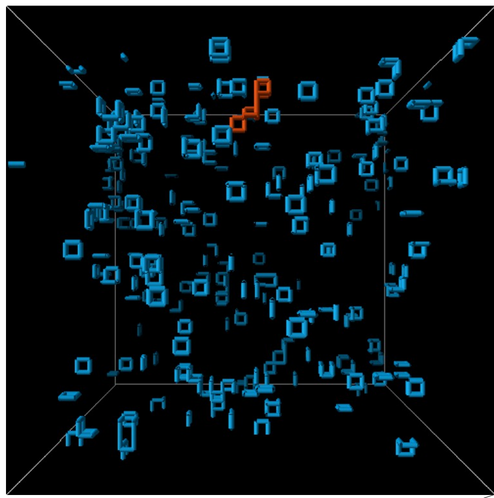
Vortex snapshots (longest loop is highlighted)

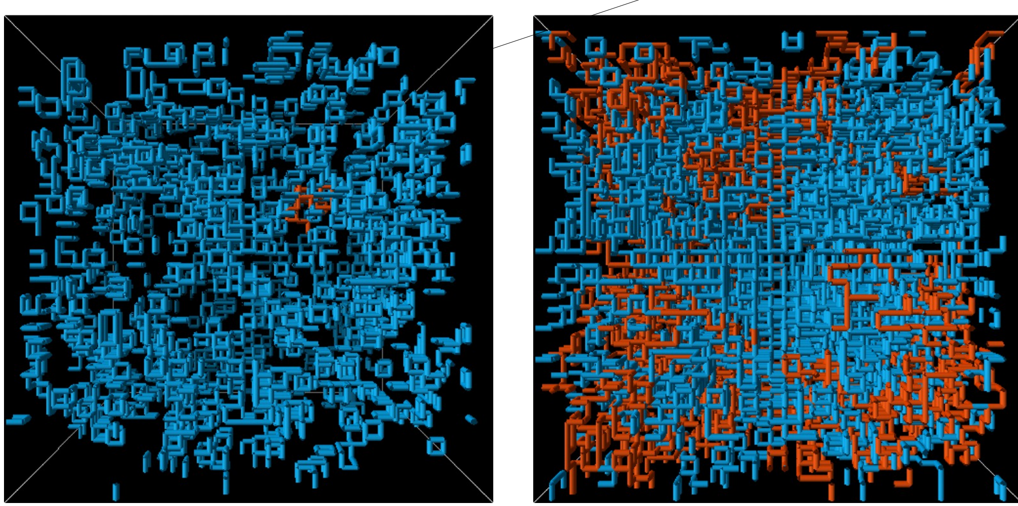
$T = 0.6\ T_c$ $T = 0.8\ T_c$ $T = T_c$

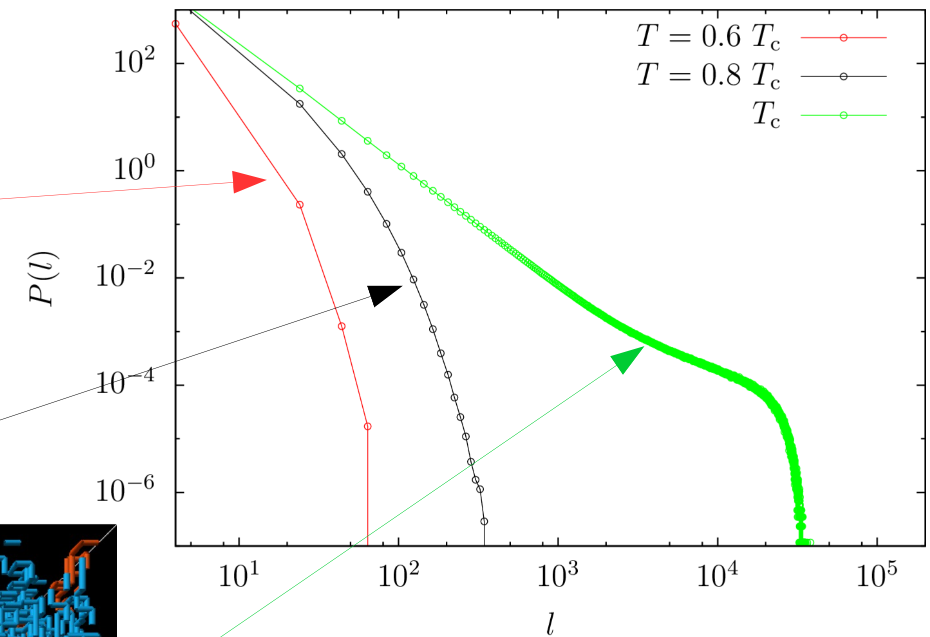


Long loops are generated close to the critical point

Loop length distribution

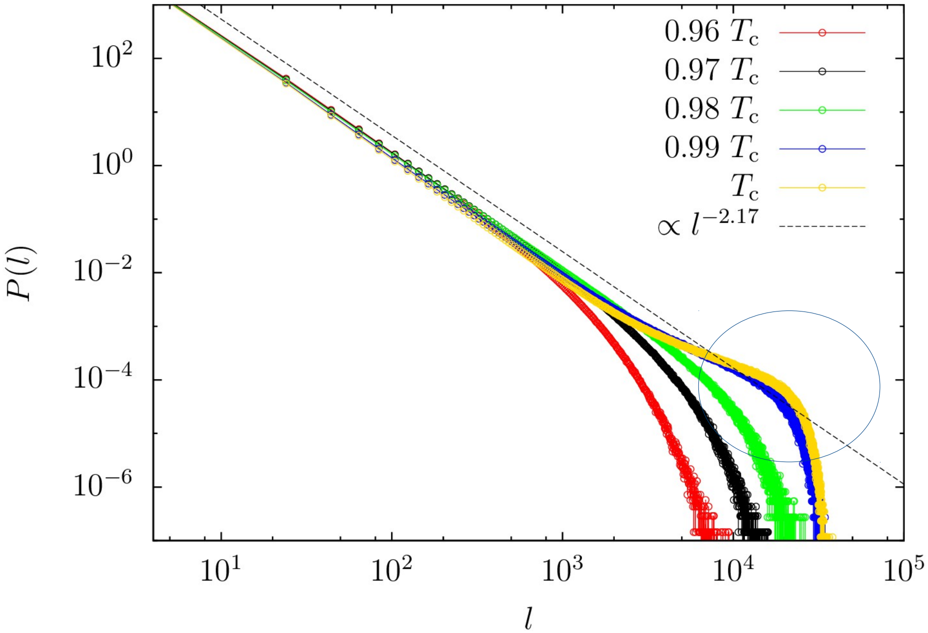




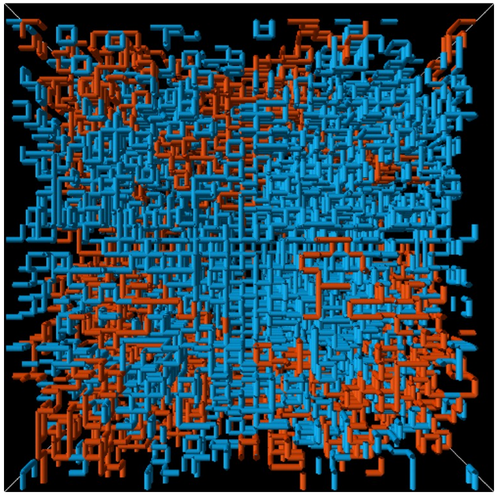


Power-law structure
emerges near T_c
→ Vortex percolation

Loop length distribution



Bump structure at large l for $T=0.99T_c$ and $T=T_c$
→ Percolating loops (finite-size effect)



Power-law fitting $P(l) \propto l^{-\tau}$ is best at $T=0.98T_c$
→ Vortex percolation occurs at $T_p \equiv 0.98T_c$

Discrepancy between T_p (geometric transition) and T_c (thermodynamic transition)

Discrepancy between geometric and thermodynamic transitions

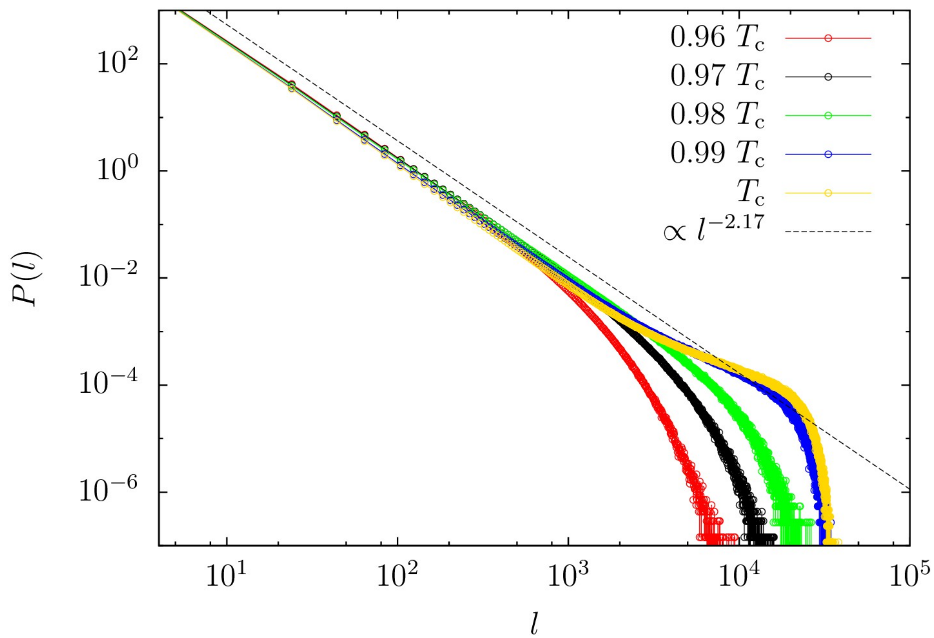
Discrepancy between geometric and thermodynamic transitions are observed in several interacting models

- $SU(2)$ local gauge field model : $T_{\rm p} \approx 0.994\ T_{\rm c}$
- $\mathbb{R}\mathrm{P}^2$ model (nematic liquid crystal) : $T_{\rm p} \approx 0.996\ T_{\rm c}$
- Nonlinear $O(2)$ sigma model : $T_{\rm p} \approx 0.992\ T_{\rm c}$

Phys. Lett. B **482**, 114 (2000)
PRB 72, 094511 (2005)

- Geometric transition of line defects occurs as a precursory phenomenon of thermodynamic transition (both are independent).
- Thermally excited long vortices may be detectable between $T_{\rm c}$ and $T_{\rm p}$

Critical exponents and order parameter



Fisher exponent τ : $P(l) \propto l^{-\tau}$ at T_{p}

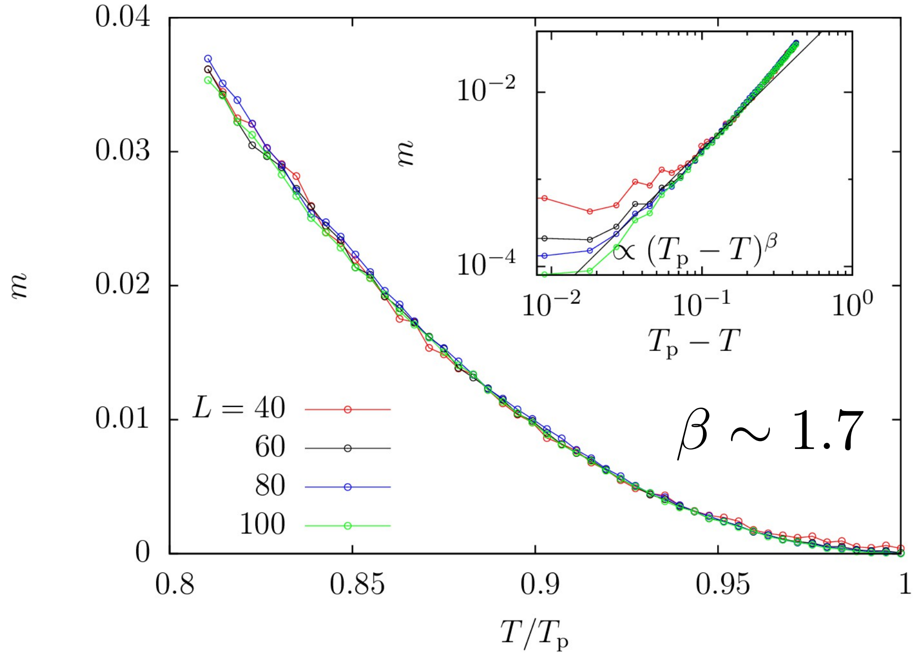
$\tau \sim 2.17$

$\Rightarrow$ Fractal dimension D of vortices :

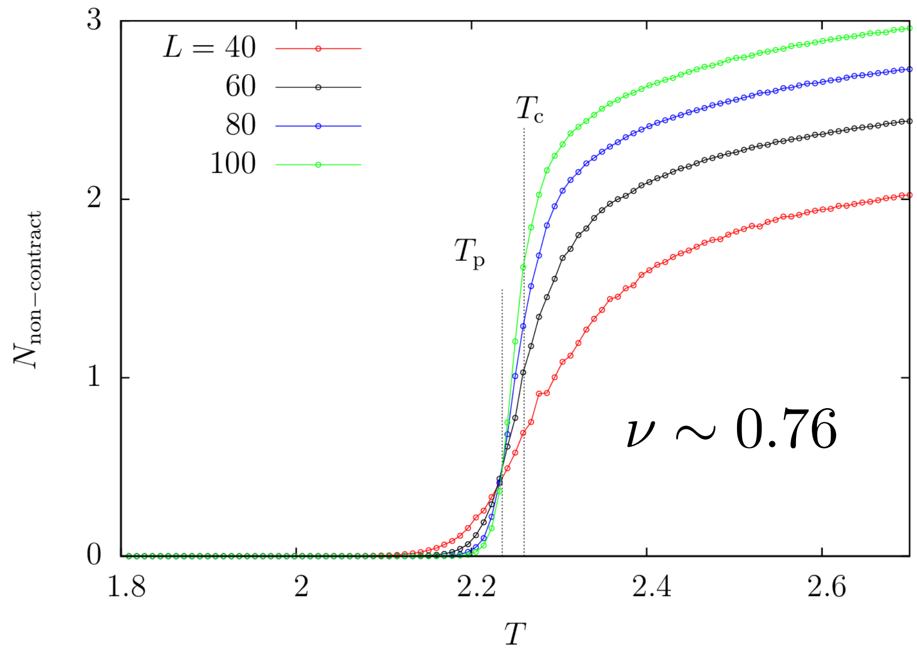
$$D = \frac{3}{\tau - 1} \sim 2.56 \text{ : self-seeking random work}$$

Critical exponents and order parameters

mass parameter : $P(l) \propto l^{-\tau} e^{-lm}$



Number of percolating loops



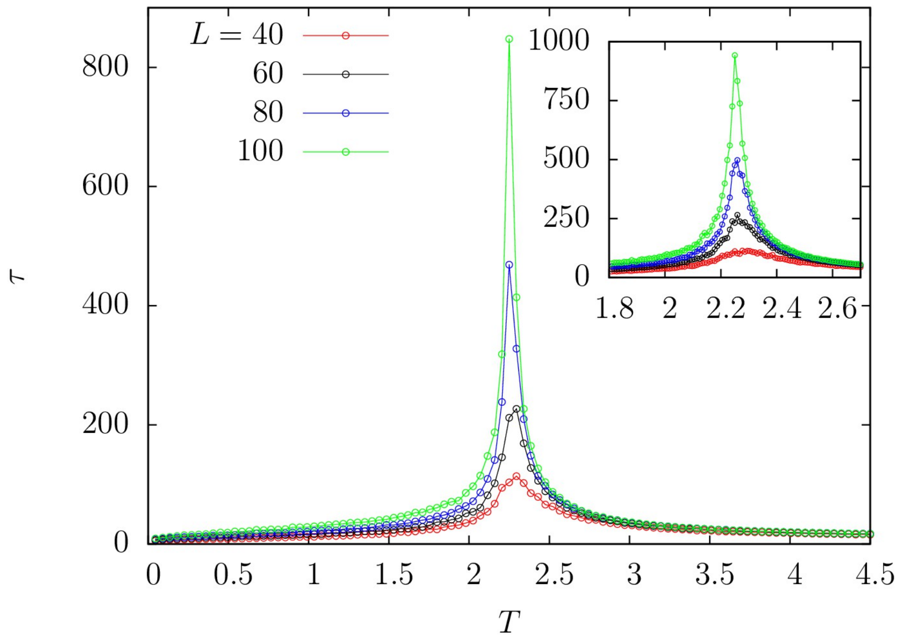
Critical exponents of order parameters are also consistent with universality of self-seeking random work

Phase ordering and quantized vortices in quench dynamics

Melting dynamics

$$(i\hbar - \gamma)\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2M}\nabla^2\psi - \mu\psi + g|\psi|^2\psi + \sqrt{\gamma k_{\mathrm{B}} T}\xi$$

$t = 0$: static solution $\psi = \mu/g$ for $T = 0$

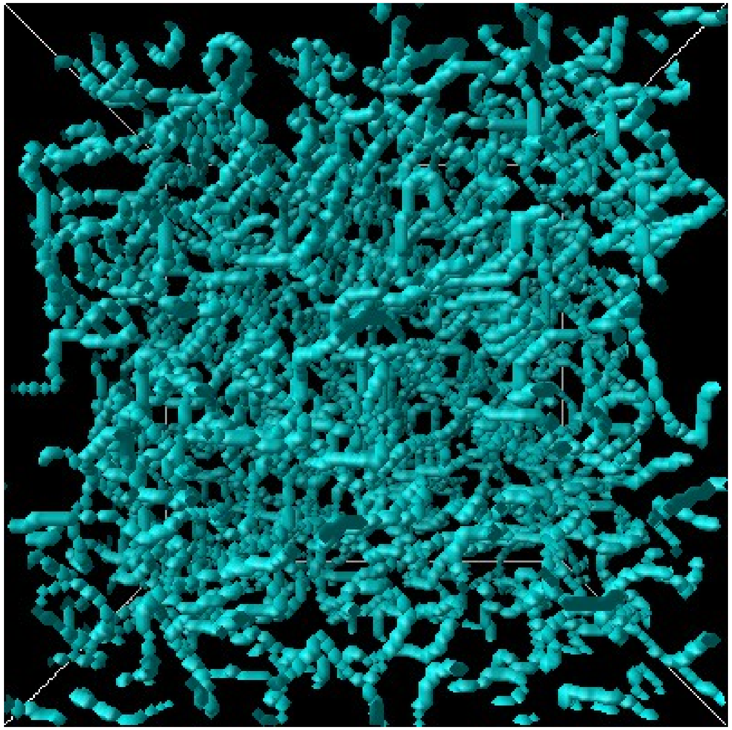


$$m^2 - m_{\mathrm{eq}}^2 \propto e^{-t/\tau}$$

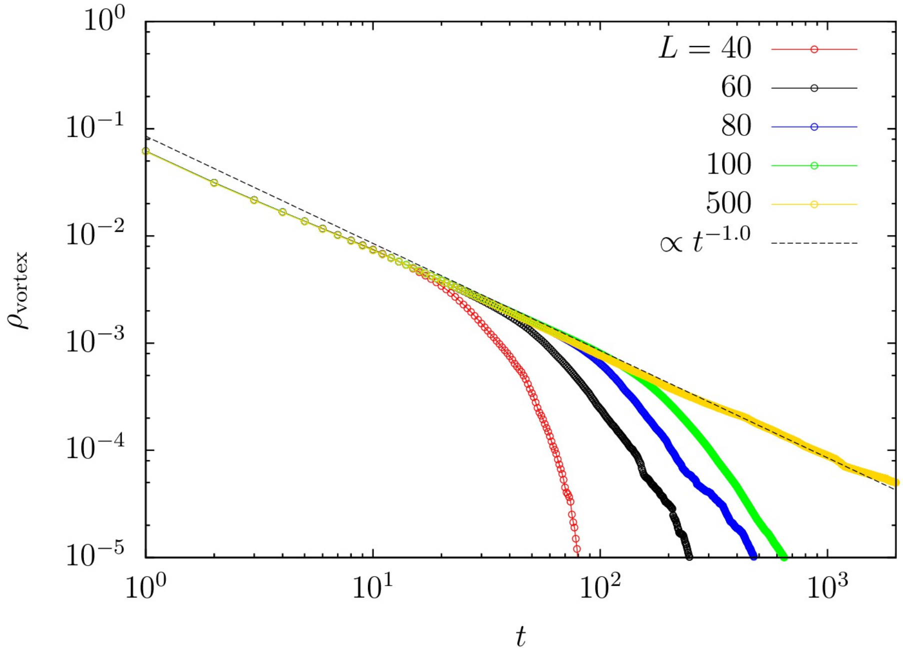
Critical slowing down near the (thermodynamic) critical temperature

Temperature quench dynamics

$$t = 0 : \psi \text{ for } T = 2T_c \qquad t > 0 : T = 0$$



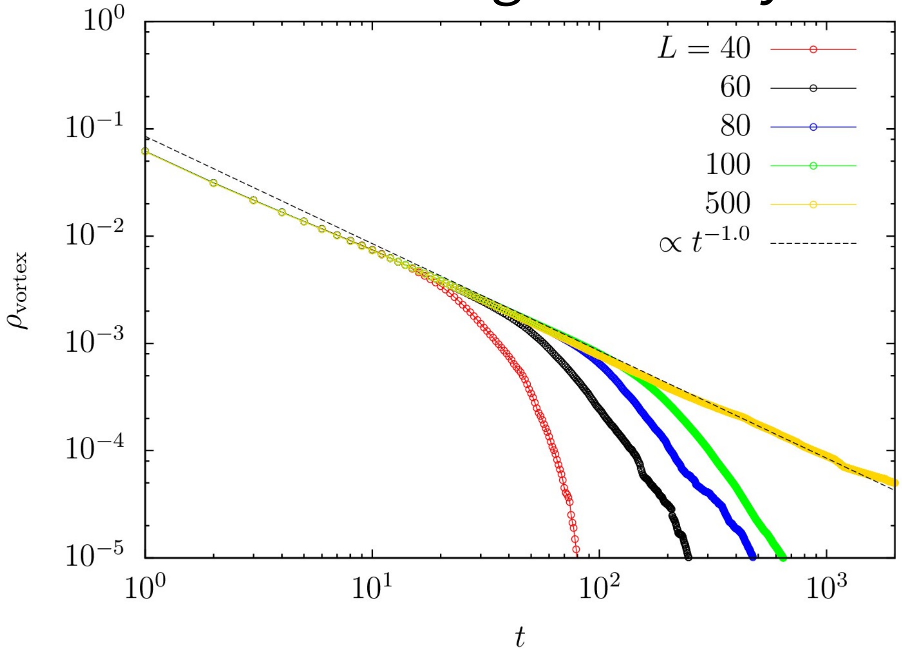
Line length density



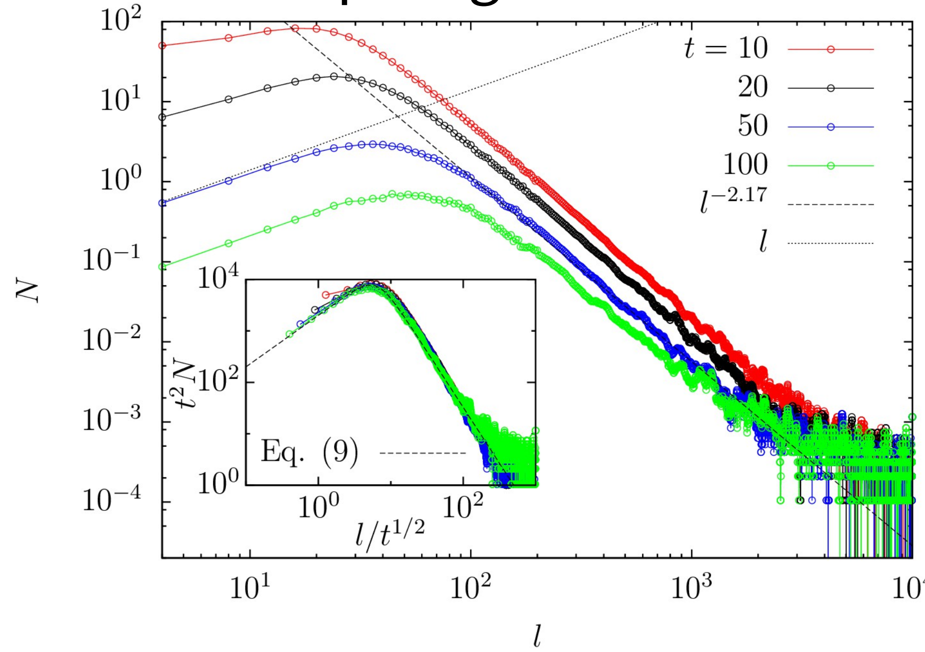
Vortices decays as in power-law : $\propto t^{-1}$

Temperature quench dynamics

Line length density



Loop length distribution



The same critical exponent as that in the equilibrium at T_{p} (not T_{c}) emerges → Spontaneous formation of critical percolating state (not critical thermodynamic state) : dynamics is dominated by vortices!

Summary

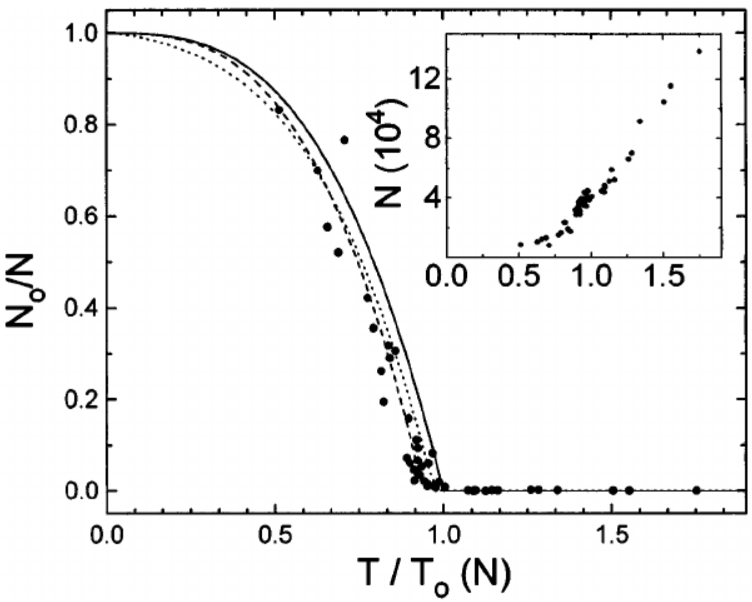
- We consider the statistical properties such as transition of interacting BEC in equilibrium.
- There are two kinds of transitions: well-known thermodynamic transition and geometric transition of quantized vortices and both are independent.
- Universality class:

  XY-model for thermodynamic transition

  Self-forcusing random walk for geometric transition
- Geometric critical state emerges in the quench dynamics.

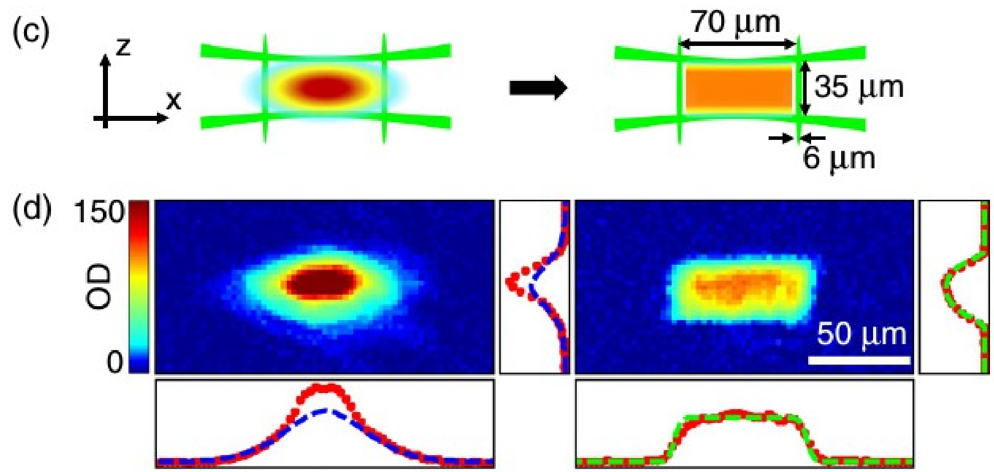
Uniform system vs trapped system

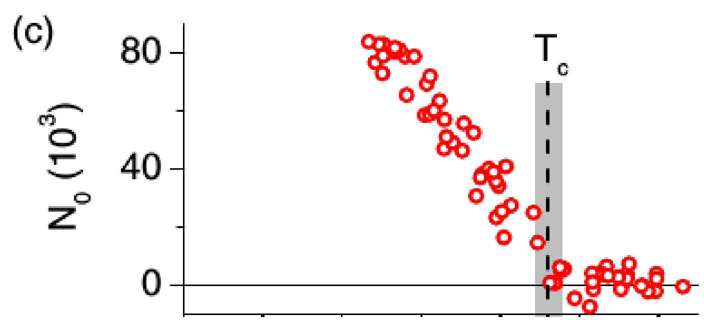
Trapped system



PRL **77**, 4984 (1996)

Toward uniform system





PRL **110**, 200406 (2013)

Zaremba-Nikuni-Griffin theory

JLTP **116**, 277 (1999)

Noncondensate particle : Boltzmann's eq.

$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p} \cdot \nabla f}{M} - 2g\nabla n \cdot \nabla_{\boldsymbol{p}} f = C_{12}(f) + C_{22}(f)$$

Condensate particle : GP eq.

$$\frac{\partial n_{\mathrm{c}}}{\partial t} + \nabla \cdot (n_{\mathrm{c}} \boldsymbol{v}_{\mathrm{c}}) = -\Gamma_{12}(f)$$

Exchange between two components

$$M\left(\frac{\partial}{\partial t} + \boldsymbol{v}_{\mathrm{c}} \cdot \nabla\right)\boldsymbol{v}_{\mathrm{c}} = -g\nabla(n_{\mathrm{c}} + 2\tilde{n})$$

Zaremba-Nikuni-Griffin theory

JLTP **116**, 277 (1999)

Condensate particle : GP eq.

$$\frac{\partial n_{\rm c}}{\partial t} + \nabla\cdot(n_{\rm c}\boldsymbol{v}_{\rm c}) = -\Gamma_{12}(f)$$

Exchange between two components

$$M\left(\frac{\partial}{\partial t} + \boldsymbol{v}_{\rm c}\cdot\nabla\right)\boldsymbol{v}_{\rm c} = -g\nabla(n_{\rm c} + 2\tilde{n})$$

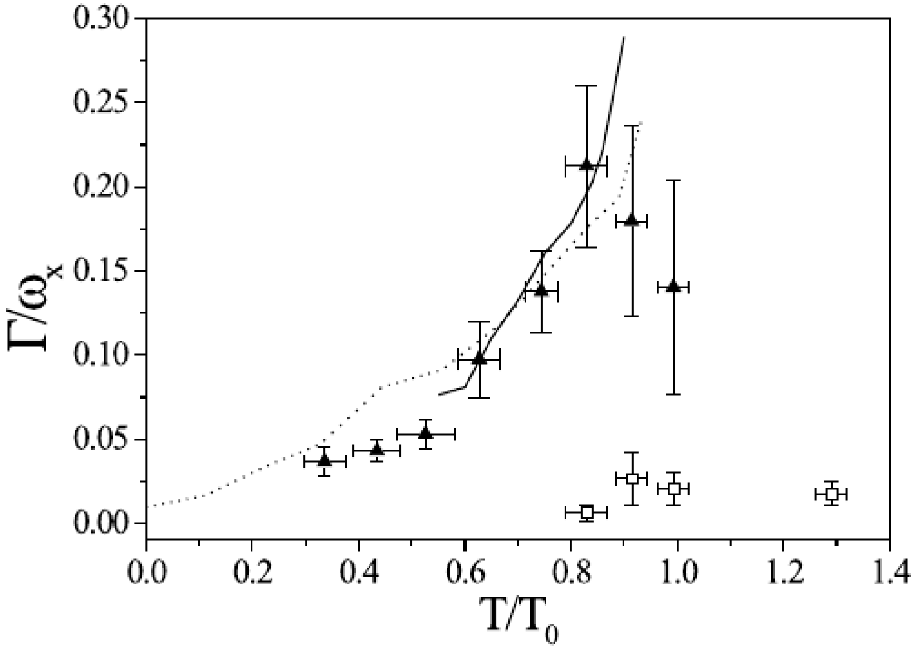
Exchange process : Markov process

$$(i\hbar - \gamma)\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2M}\nabla^2\psi - \mu\psi + g|\psi|^2\psi + \sqrt{\gamma k_{\rm B}T}\xi$$

SGP eq. (discrepancy from Gaussian noise is renormalized into γ)

Estimation of γ

Damping of Scissors mode



PRL **86**, 3938 (2001)

$\gamma \propto (na^3)^{1/3}$ from ZNG theory

Loop length distribution