Nordita Sept 19 2014

Path integral simulations of bosons with disorder

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- Superfluid transition in a correlated defect network
  Hannes Meier, Mats Wallin, and S. Teitel, PRB 87, 214520 (2013)
- Quantum Critical Dynamics Simulation of Dirty Boson Systems
  Hannes Meier and Mats Wallin PRL 108, 055701 (2012)
- Critical Scaling Properties at the Superfluid Transition of He 4 in Aerogel
  Marios Nikolaou, Mats Wallin, and Hans Weber, PRL 97, 225702 (2006)
- Generalized Anisotropic Scaling Theory and the Transverse Meissner Transition
  Anders Vestergren, Jack Lidmar, and Mats Wallin, PRL 94, 087002 (2005)

Jack Lidmar, Hannes Meier, Anders Vestergren, Marios Nikolaou, Markus Ahlström, KTH
Hans Weber, Luleå Technical University Steve Teitel, University of Rochester

OUTLINE

- Path integrals and quantum matter
- Role of correlated disorder
- Monte Carlo methods
- Finite size scaling
- Examples
  - Boson localization
  - Superfluidity in aerogel
  - Solid Helium

Models

- Path integral formulates quantum problem in d-dimensions as classical problem in d+1 dimensions

$$H = -\lambda \sum_i \nabla_i^2 + \sum_{i<j} V(r_{ij}) \qquad Z = \sum_n e^{-\beta E_n} = \mathrm{Tr}\, e^{-\beta H}$$

$$e^{-\beta H} = \lim_{M\to\infty} \left(e^{-d\tau T} e^{-d\tau V}\right)^M \qquad \rho(r_0, r_M) = \int dr_1 \cdots dr_M \exp(-S)$$

$$S = \frac{dMN}{2} \ln(4\pi d\tau\lambda) + \sum_{i,m} \frac{[r(i,m+1) - r(i,m)]^2}{4\lambda dt} + dt \sum_{j>i,m} V[r(i,m) - r(j,m)]$$

- Extrapolation to *T*=0, exchange, etc is difficult but possible
- Alternatively study coarse grained models on a lattice.
  Will not give all details but useful approximations and insights

Poor mans version: 3DXY and loop lattice models

- 3DXY model in d+1 dimensions $$H = -\sum_{ij} K_{ij} \cos(\theta_i - \theta_j)$$
- Integer current loop model $$H = \sum_{ij} K_{ij} J_{ij}^2$$
- Random coupling constant K_{ij} models random disorder
- Quantum problem means random couplings constant in imaginary time direction: one dimensional correlated random disorder

Monte Carlo methods

- Super efficient new algorithms eliminate severe bottleneck: critical slowing down $\xi \sim (g-g_c)^{-\nu}$, $\tau \sim \xi^z$
- 3DXY Model: **Wolff method**
  Builds and flips clusters of correlated order meter
  U. Wolff, PRL 62, 361 (1989)
- Integer current model: **Worm method**
  Generates current loops as random walks.
  Automatically generates correlation functions and exchange.
  N. Prokof'ev and B. Svistunov, PRL 87, 160601 (2001)
- Fermion minus sign problem unsolved.
  Restricted to systems without minus signs.
- Generate numerical data on small lattice systems and use scaling relations to extract properties

Disordered universality classes and Harris criterion

- Quenched disorder modeled as random coupling constant in XY model for superfluidity with order parameter $\Psi(r) = |\Psi| e^{i\theta(r)}$

$$H = -\sum_{\langle ij \rangle} K_{ij} \cos(\theta_i - \theta_j) \qquad Z = \sum_{\{\theta\}} e^{-H/T} = e^{-F/T}$$

- Harris criterion for irrelevance of quenched disorder

$$\Delta K = \left\langle \left(\frac{1}{\xi^d} \int d^d r\, \delta K(r) \right)^2 \right\rangle^{1/2} = \left(\frac{1}{\xi^{2d}} \int d^d r \int d^d r' \underbrace{\langle \delta K(r) \delta K(r') \rangle}_{=(\delta K)^2 \delta(r-r')} \right)^{1/2} = \delta K \xi^{-d/2} < \Delta T \sim \xi^{-1/\nu}$$

$$\Rightarrow \nu > \frac{2}{d} \qquad \text{or} \qquad \alpha = 2 - d\nu < 0$$

- Must be obeyed at disordered fixed point.

Correlated disorder

- Weinrib, Halperin, Phys. Rev. B 27, 413–427 (1983)

$$C(R)=\left\langle\left(\frac{1}{R^d}\int d^d r\,\delta K(r)\right)^2\right\rangle \sim R^{-a} \qquad \Rightarrow \qquad \nu=\frac{2}{a}$$

- Harris criterion for correlated disorder

$$C(R)=\left\langle\left(\frac{1}{\xi^d}\int d^d r\,\delta K(r)\right)^2\right\rangle=\frac{1}{R^{2d}}\int d^d r\int d^d r'\underbrace{\left\langle\delta K(r)\delta K(r')\right\rangle}_{=(\delta K)^2\,\delta(k(r)-k(r'))}=\left(\delta K\right)^2 R^{-2d}\left\langle\sum_{k=1}^{N} n_k^2\right\rangle=\left(\delta K\right)^2 R^{-2d}\left\langle N\right\rangle\left\langle n^2\right\rangle$$

k(r)=defect number containing site r, N=number of defects, n=number of sites of defect. Applies for disorder potential defined on all sites.

- Can also consider disorder forming correlated curves or planes. In this case the sum runs over lattice sites occupied by defects:

$$C(R)=\left\langle\left(\frac{1}{\xi^d}\int d^d r\,\delta K(r)\right)^2\right\rangle=\left(\Delta K\right)^2 R^{-2d}\left\langle\sum_{k=1}^{N} n_k^2+\sum_{k=1}^{N}\sum_{k\neq l,k=1}^{N} n_k n_l\right\rangle=\left(\Delta K\right)^2 R^{-2d}\left(\left\langle N\right\rangle\left\langle \delta n\right\rangle+\left\langle n\right\rangle^2\left\langle \delta N\right\rangle\right)$$

$\Delta K =$ increment of coupling upon adding a defect

Examples of disordered universality classes for d=3

- I general:

$$C(R) \sim R^{-6} \left\langle N \right\rangle \left\langle n^2 \right\rangle \sim R^{-a} \qquad \nu = \frac{2}{a} \qquad \alpha = 2 - d\nu$$

- Point disorder

$$C(R) \sim R^{-6} \left\langle N \right\rangle \left\langle n^2 \right\rangle \sim R^{-6} \times R^3 \times 1 = R^{-3} \quad a = 3 \quad \nu = \frac{2}{3} \quad (\nu = 0.671 \; , \alpha = -0.015)$$

- Linear disorder

$$C(R) \sim R^{-6} \left\langle n \right\rangle^2 \left\langle \delta N \right\rangle \sim R^{-6} \times R^2 \times R^2 = R^{-2} \qquad a = 2 \qquad \nu = 1 \qquad \alpha = -1$$

- Directed random walk disorder

$$C(R) \sim R^{-6} \left\langle n \right\rangle^2 \left\langle \delta N \right\rangle \sim R^{-6} \times R^2 \times R^2 = R^{-2} \qquad a = 2 \qquad \nu = 1 \qquad \alpha = -1$$

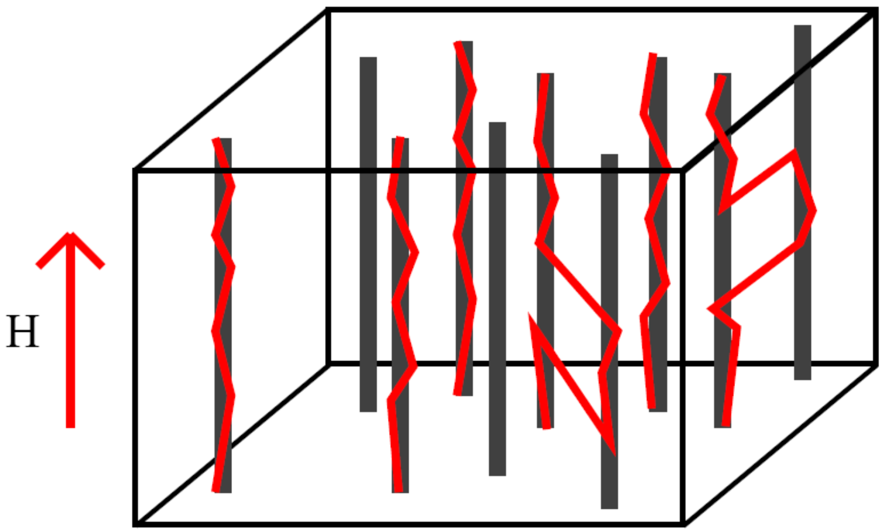
- Random walk disorder

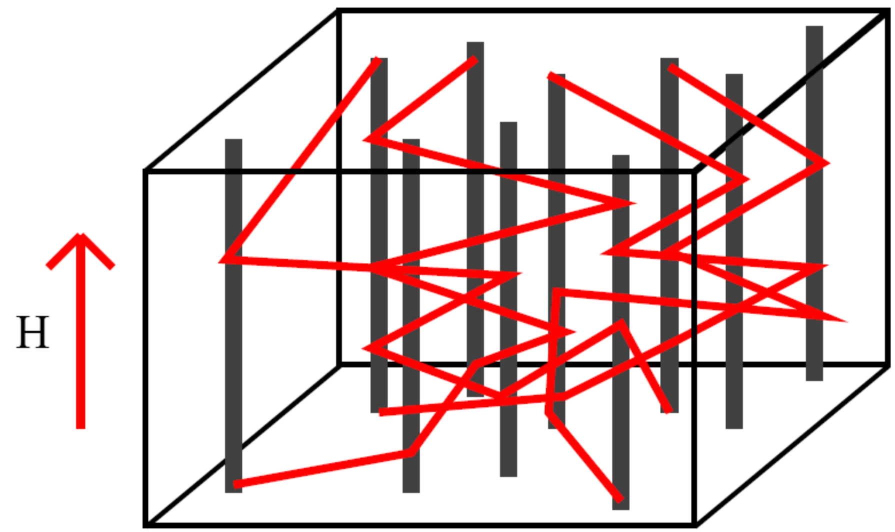
$$C(R) \sim R^{-6} \left\langle n \right\rangle^2 \left\langle \delta N \right\rangle \sim R^{-6} \times R^4 \times R = R^{-1} \qquad a = 1 \qquad \nu = 2 \qquad \alpha = -4$$

- Planar disorder

$$C(R) \sim R^{-6} \left\langle n \right\rangle^2 \left\langle \delta N \right\rangle \sim R^{-6} \times R^4 \times R = R^{-1} \qquad a = 1 \qquad \nu = 2 \qquad \alpha = -4$$

Dirty boson localization quantum phase transition in 2d at T=0
=Superconducting transition with columnar defects in 3d at T>0



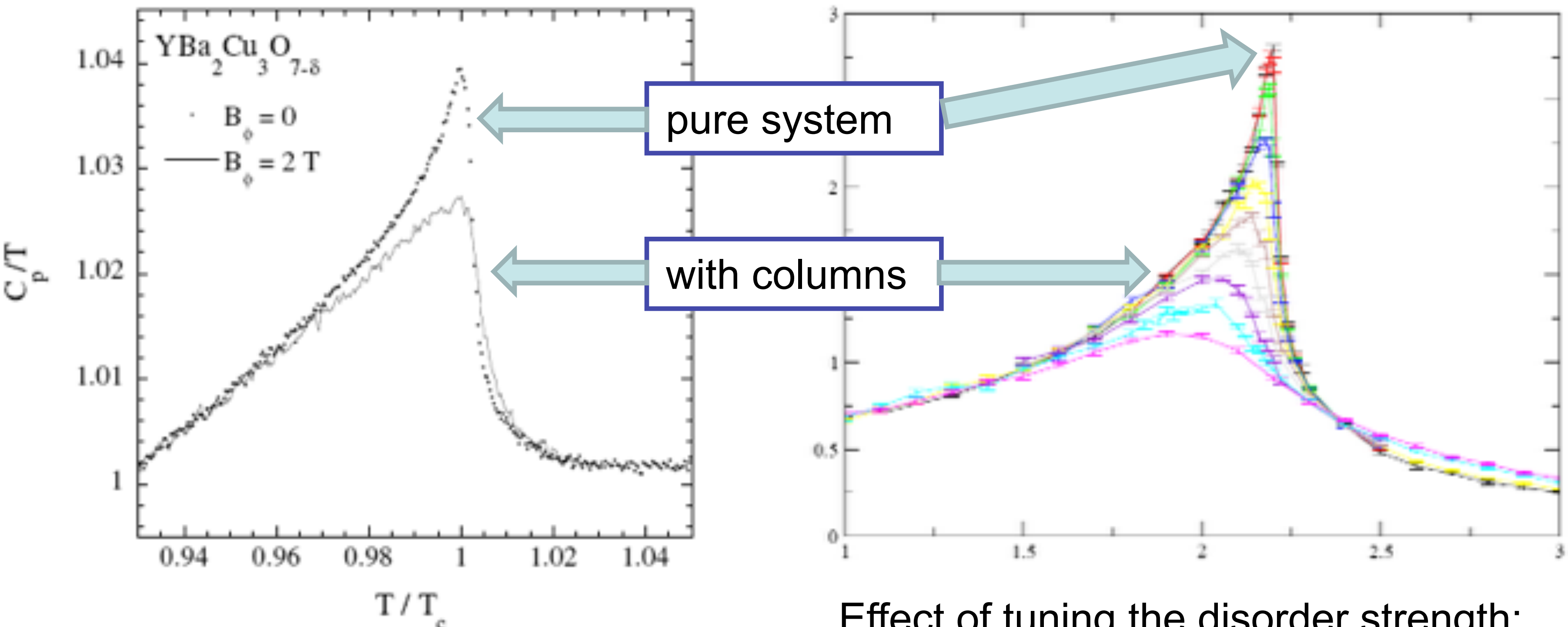


boson insulator phase
vortex insulator=
superconductor
winding number=0

boson superconductor
Vortices delocalized
from defects
winding number nonzero

Data for YBCO in zero field with columnar defects

Experiment: **Simulation:**



Effect of tuning the disorder strength:

$$J_x, J_x = 1 \pm \delta, \delta = 0.1, \ldots, 0.8$$

Result: $\boxed{\alpha \approx -2}$

C. J. van der Beek, Thierry Klein, Rene Brusetti, Christophe Marcenat, Mats Wallin, S. Teitel, and Hans Weber Phys. Rev. B **75**, 100501 (2007)

Worm simulation of dirty bosons

J-current model

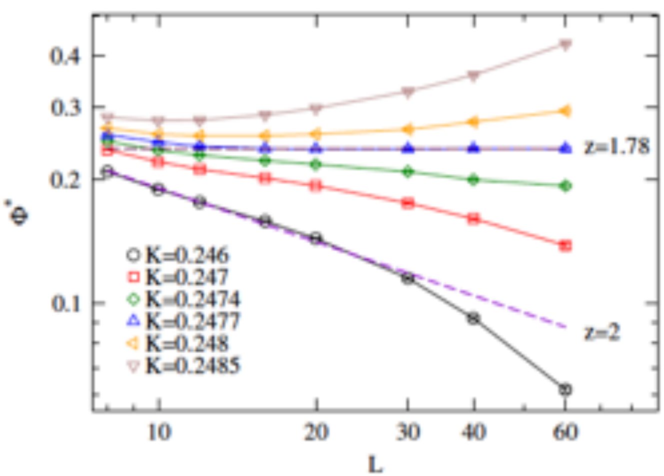
$$H = \frac{1}{K}\left(\sum_{i,\delta}\frac{1}{2}(J_i^\delta)^2 - \sum_i(\mu + v_{\mathbf{r}})J_i^\tau\right)$$

$$W_\delta^2 = \left[\left\langle\left(\frac{1}{L_\delta}\sum_i J_i^\delta\right)^2\right\rangle\right]$$

$$W^2(K, L, L_\tau) = \tilde{W}^2(L^{1/\nu}k, \alpha_\tau) \quad \alpha_\tau = L_\tau/L^z$$

- Test prediction z=d=2 by changing temperature
- Idea: Divide winding number fluctuation by inverse temperature squared and do a scaling analysis. Maximum scales as

$$(W^2/L_\tau^2)^* \sim L^{-2z} \text{ at } K = K_c$$



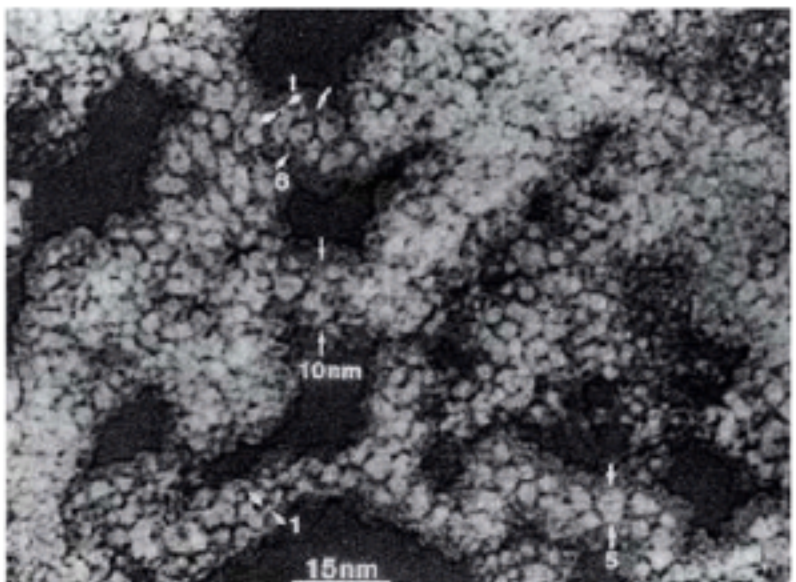
Average each data point over up to 10^5 realizations of random disorder
Simulation results suggest z=1.8
H Meier and MW, PRL 108, 055701 (2012)

Aerogel

- Aerogel is a microporous silica solid (SiO_2) containing up to 99.98 % air.
- 1000 times lighter than window glass, weight as little as 3 times that of air. Typical density of 3 mg/cm^3
- Holds 15 entries in the Guinness Book of Records for material properties, including best insulator and lowest-density solid.
- Melting point of 1200 C
- Refraction index of 1.0-1.04, very low for a solid (air has index 1)
- Recent uses of aerogel: refractive medium in Cerenkov detectors, thermal insulating material, catalysis, gas storage and gas filtering.

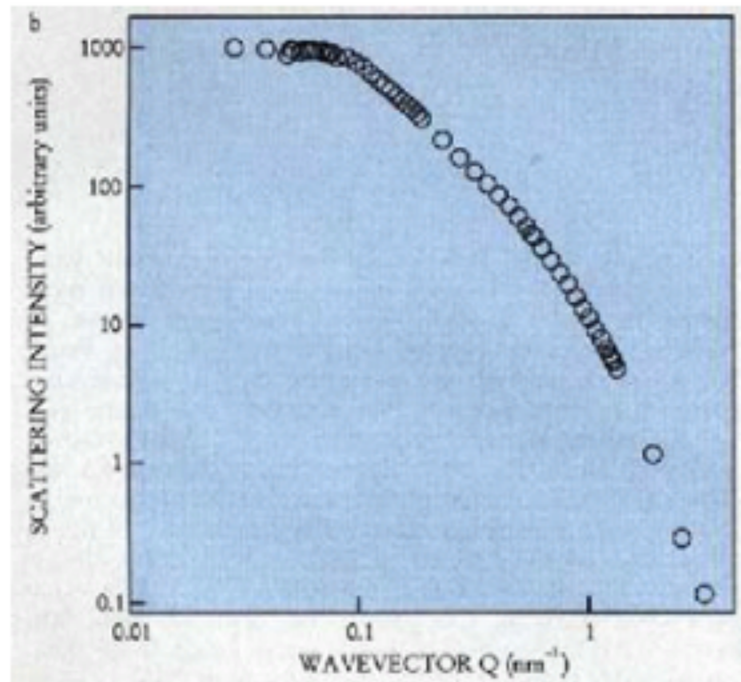
Aerogel structure experiments

Transmission electron micrograph of 98.5% porosity silica aerogel. Silica particles of diameter 1-2 nm aggregate, forming a very open structure made up of strands that interconnect at random sites.



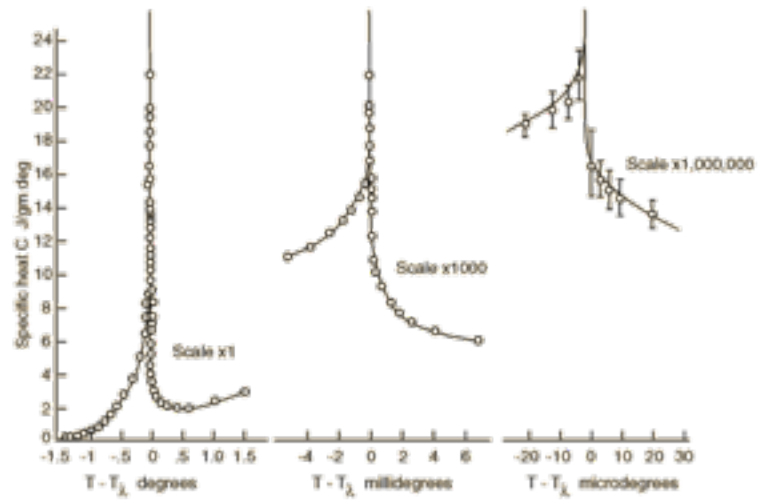
The corresponding small-angle x-ray scattering (SAXS) data shows fractal correlations in the mass distribution up to a length scale of 65 nm.

Fractal dimension $D_F \approx 1.8$



Heat capacity at the lambda transition

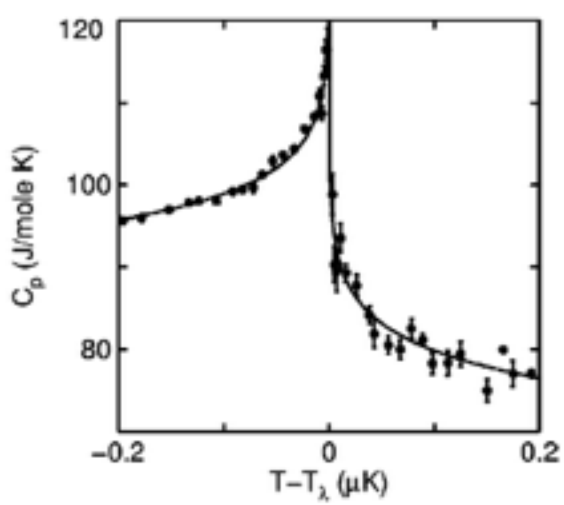
- Buckingham and Fairbank
  "The Nature of the Lambda Transition"
  Progress in Low Temperature Physics III, 1961



- Space shuttle measurements in microgravity
  to eliminate pressure gradient
  J. Lipa et al, PRB 68, 174518 (2003)

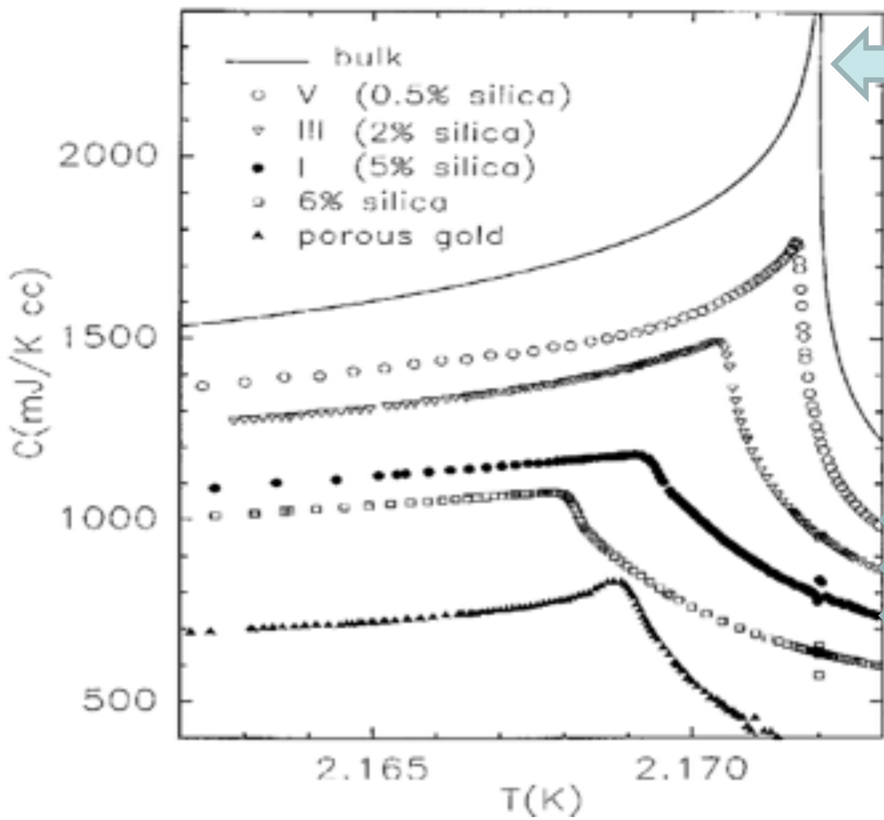
$$C_P = \left(\frac{dQ}{dT}\right)_P = \begin{cases} \frac{A^-}{\alpha} t^{-\alpha}\left(1 + a_C^- t^{\Delta} + b_C^- t^{2\Delta}\right) & T < T_\lambda \\ \frac{A^+}{\alpha} |t|^{-\alpha} + B^- & T > T_\lambda \end{cases}$$

$\alpha = -0.0127 \pm 0.0003 \qquad A^+ / A^- = 1.053 \pm 0.002$



SF transition in bulk and porous media

Experimental heat capacity data from ac heating method
J. Yoon, D. Sergatskov, J. Ma, N. Mulders, and M. H. W. Chan, PRL 80, 80 (1998).



Usual lambda transition in pure He system

He in aerogel porous glass fractal

Lambda transition becomes **rounded** by presence of porous media.
Assumption: pores act as **correlated disorder** for the He.

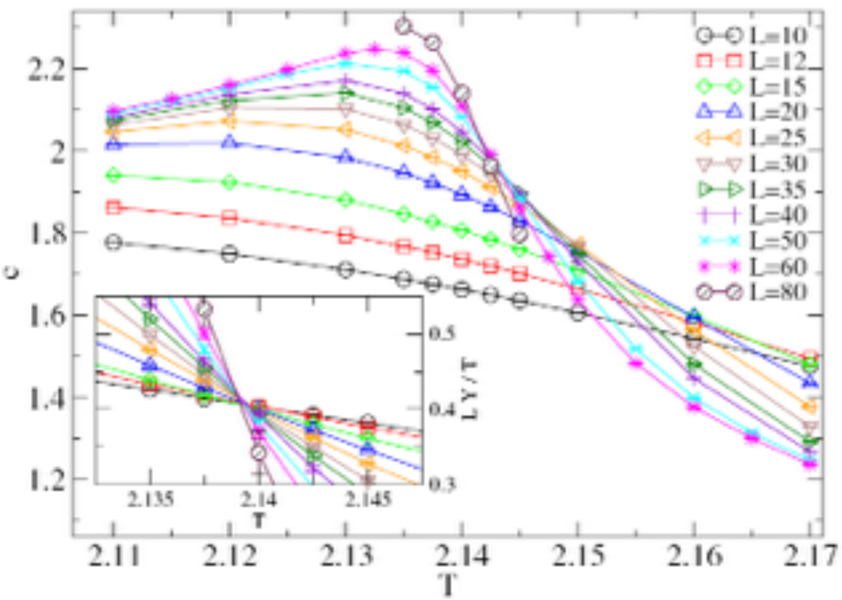
Experimental results

J. Yoon, D. Sergatskov, J. Ma, N. Mulders, and M. H. W. Chan, PRL 80, 80 (1998).

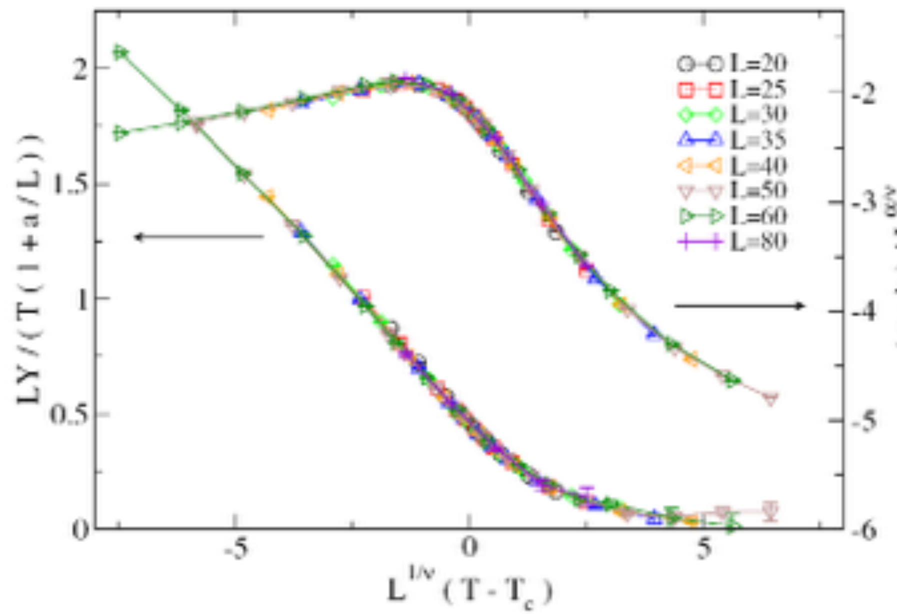
- 5% aerogel: $\rho_s = \rho_0 |t|^\nu$, $t = 1 - T/T_c$, $\nu \approx 0.79$. Significantly bigger than the bulk value $s \approx 0.67$ found in pure ^{4}He.
- The heat capacity has a peak at $T = T_c$ that was fitted to the form $C \sim A_\pm |t|^{-\alpha} + B_0 + B_1 T$, which gives $\alpha \approx -0.57$
- Surprisingly this deviates strongly from the value obtained from the hyperscaling relation: $\alpha = 2 - d\nu \approx -0.37$. **Hyperscaling violation!?**
- For the lightest samples of aerogel, with 0.5% aerogel, the exponents ν, α obtained values in between the exponents for the heavy aerogel samples and the pure bulk exponents.

MC data for SF transition in aerogel

Heat capacity and superfluid density



Finite size scaling data collapses



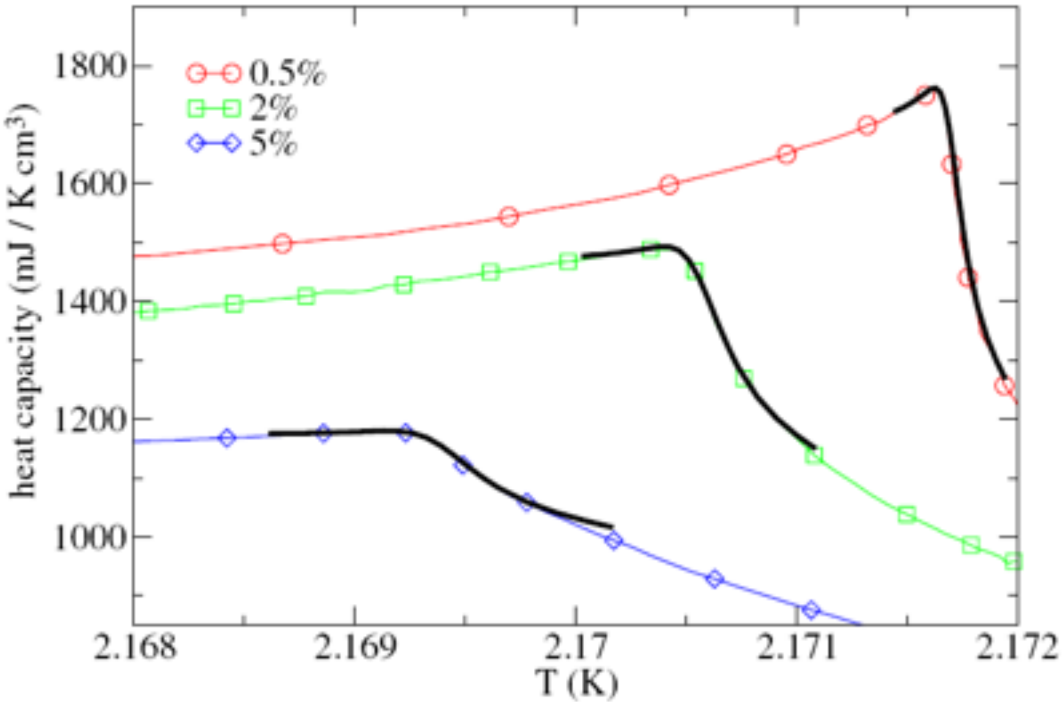
Scaling gives exponents: $\boxed{\nu = 0.73 \pm 0.02 \quad , \quad \alpha = -0.2 \pm 0.05}$

M. Nikolaou, M. Wallin, H. Weber, PRL **97,** 225702 (2006)

Heat capacity scaling at SF transition of ^{4}He in aerogel

- Heat capacity data explained by 3DXY model with DLCA cluster

  M. Nikolaou, M. Wallin, H. Weber, PRL **97** (2006)



- Source of confusion identified: fit to experiments using

$$C(T) = A_{\pm}\left|T - T_c\right|^{-\alpha} + B$$

does not work and indicates scaling violations when $\alpha < 0$

Supersolid

- State which is both solid and superfluid
- Defect carried supersolidity can in principle exist
- Solid order: broken translation symmetry $$n(r) = n(R + r)$$
- Superfluid order: nonzero superfluid density
  Measured by NCRI $$\rho_s = \left.\frac{\partial^2 f}{\partial \Delta\theta^2}\right|_{\Delta\theta=0}$$
- Considerable interest on report by Kim-Chan of supersolidity in He solids: Nature London 427, 225 (2004), Science 305, 1941 (2005)
- Classical shear modulus anomaly explains the NCRI signal.
  J. Day and J. Beamish, Nature (London) 450, 853 (2007).
- No NCRI signal found if mechanical deformations are eliminated.
  Duk Kim and Moses Chan, PRL 109, 155301 (2012)
  Upper limit on the nonclassical rotational inertia or supersolid fraction of 4×10^{-6}. Duk Kim and Moses Chan, PRB 90, 064503 (2014)
- Small superfluid signals seen by Mi and Reppy, PRL 108, 225305 (2012),

Torsion oscillator experiment to measure superfluid density

When part of the helium becomes superfluid it loses its viscosity and remains at rest in the lab frame.
It no longer contributes to the moment of inertia of the oscillator.
The oscillator obtains a non classical rotation inertia (NCRI):

$$I(T) = I_{\text{classical}}\left(1 - \frac{\rho_S(T)}{\rho}\right) \quad \text{or} \quad \frac{\rho_S(T)}{\rho} = \frac{I(T) - I_{\text{classical}}}{I_{\text{classical}}}$$

Suggested by Fritz London, Superfluids Vol II, P144 (1954)
Verified experimentally by Hess, Fairbank, PRL 19, 216 (1967)
Leggett PRL 25, 1543 (1970) proposed similar experiment to detect supersolidity: let solid helium to undergo dc or ac rotation to look for NCRI. Variational estimate of upper limit of the supersolid fraction: $\rho_S(T)/\rho < 10^{-4}$

Resonance period $T = 2\pi\sqrt{\frac{I}{k}}$

I = moment of inertia

k = torsional spring constant

35 year search followed...

Breakthrough in 2004 by Kim and Chan: Torsion oscillator anomaly found in solid He-4 suggesting NCRI and supersolidity

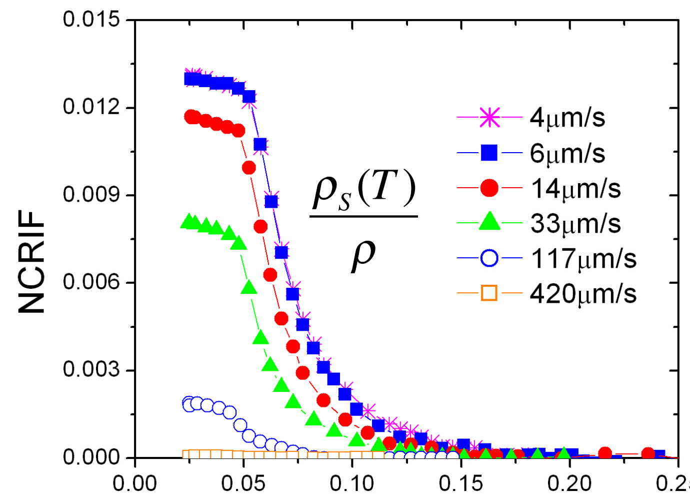
Nature London 427, 225 (2004)
Science 305, 1941 (2005)

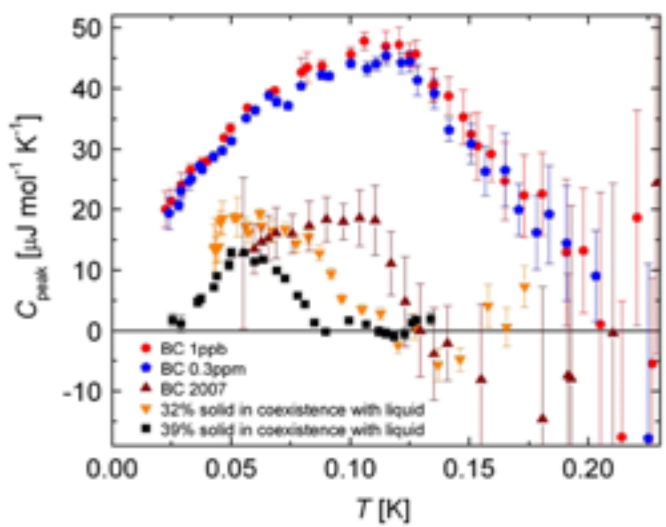
An explosion of activity followed to verify and interpret these results

Similar TO results were verified by other groups

Notably Hallock et al measure superfluid transport in He solids
M.W. Ray, R. B. Hallock
PRL 105, 145301 (2010)
Y. Vekhov, R. B. Hallock, PRL 109, 045303 (2012)

Heat capacity peak observed
X. Lin, A.C. Clark, Z.G Cheng, M.H.W. Chan
PRL 102, 125302 (2009)





What are the properties of a defect supersolid? (assuming that it exists)

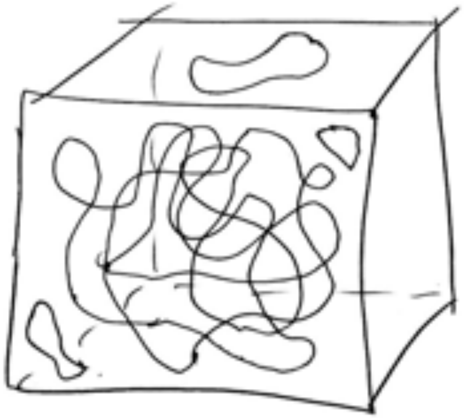
- Numerous theoretical calculations and simulations show the a supersolid should not exist for a pure 4He crystalline state
  N. Prokof'ev, Advances in Physics 56, 381 (2007)
  B. Clark and D. Ceperley, Phys. Rev. Lett. 96, 105302 (2006)
  M. Boninsegni, N. Prokof'ev, and B. Svistunov, Phys. Rev. Lett. 96, 105301 (2006)

- Superfluidity can exist in the cores of crystalline defects
  M. Boninsegni, A. B. Kuklov, L. Pollet, N. V. Prokof'ev, B. V. Svistunov, and M. Troyer, Phys. Rev. Lett. 99, 035301 (2007)

- Superfluid onset given by a 3DXY model with a lambda divergence of the heat capacity due to irrelevance of point disorder at 3DXY transition
  J. Toner, Phys. Rev. Lett. 100, 035302 (2008)
  D. Goswami, K. Dasbiswas, C.-D. Yoo, A. Dorsey, PRB 84, 054523 (2011)

XY model for defect supersolidity

- Study a 3D dislocation network with superflow transport along defects
- Builds in that superfluid density is suppressed upon annealing since the defect free perfect crystal is an insulator
- Model dislocations as correlated quenched line disorder (due to e.g. pinning at He-3 defects) forming 3D interconnected network
- Defects extend in all directions with isotropic distribution

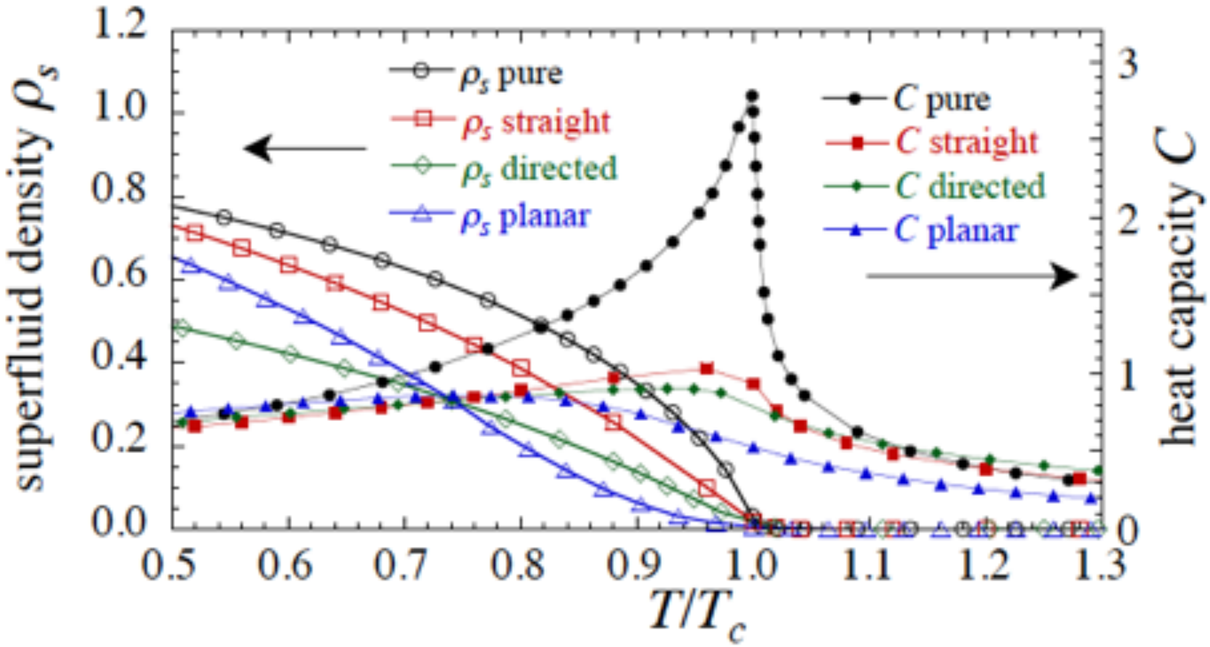


$$H = -\sum_{r,\mu} J_r^\mu \cos(\theta_{r+\mu} - \theta_r) \qquad \text{where } J_r^\mu = \begin{cases} 1 & \text{on defects} \\ 0 & \text{in bulk} \end{cases}$$

- Can study the superfluid onset for a given choice of random defect distribution by Monte Carlo simulations

H. Meier, M. Wallin, S. Teitel, PRB 87, 214520 2013

Here: non-3DXY smooth superfluid onset



- Lambda cusp of heat capacity in pure system replaced by smooth maximum
- Sharp superfluid density onset of pure system replaced by smooth onset
- Experimental dislocation density n~10^6-10^8 cm^{-2}
  Gives superfluid density rho_s/rho~10^{-5} and superfluid onset temperature Tc<1 mK
  Far below Kim-Chan onset at 100 mK
  Rules out superfluidity as source of torsional anomaly in Kim-Chan experiments
- H. Meier, M. Wallin, S. Teitel, PRB 87, 214520 2013

Summary

- Path integral simulation investigations of Bose systems
- Study effects of disorder on phase transitions
- Efficient MC algorithms (Wolff, Worm, hybrids) are crucial
- New insights to dirty boson quantum critical dynamics
- New superfluid universality class in porous aerogel
- New universality class of supersolid transition
  (NOT the physics seen in torsion oscillator experiments on solid Helium)
- Current work:
  tunable disorder correlations from annealing approach