

Numerical Simulation of Strongly Correlated Systems

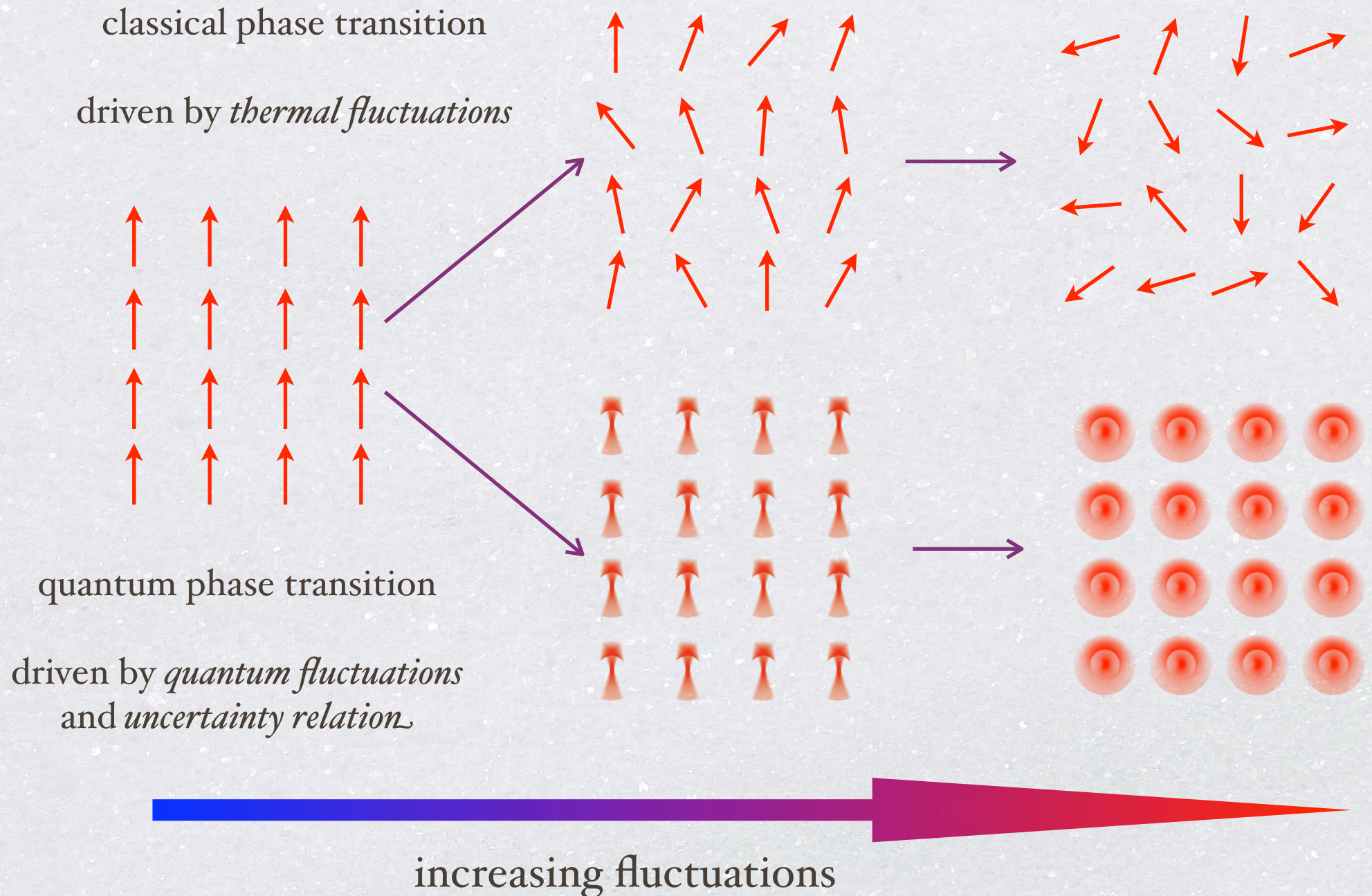
Part II: QMC for spins and bosons

Matthias Troyer (ETH)




Phases and phase transitions



Classical and quantum phase transitions

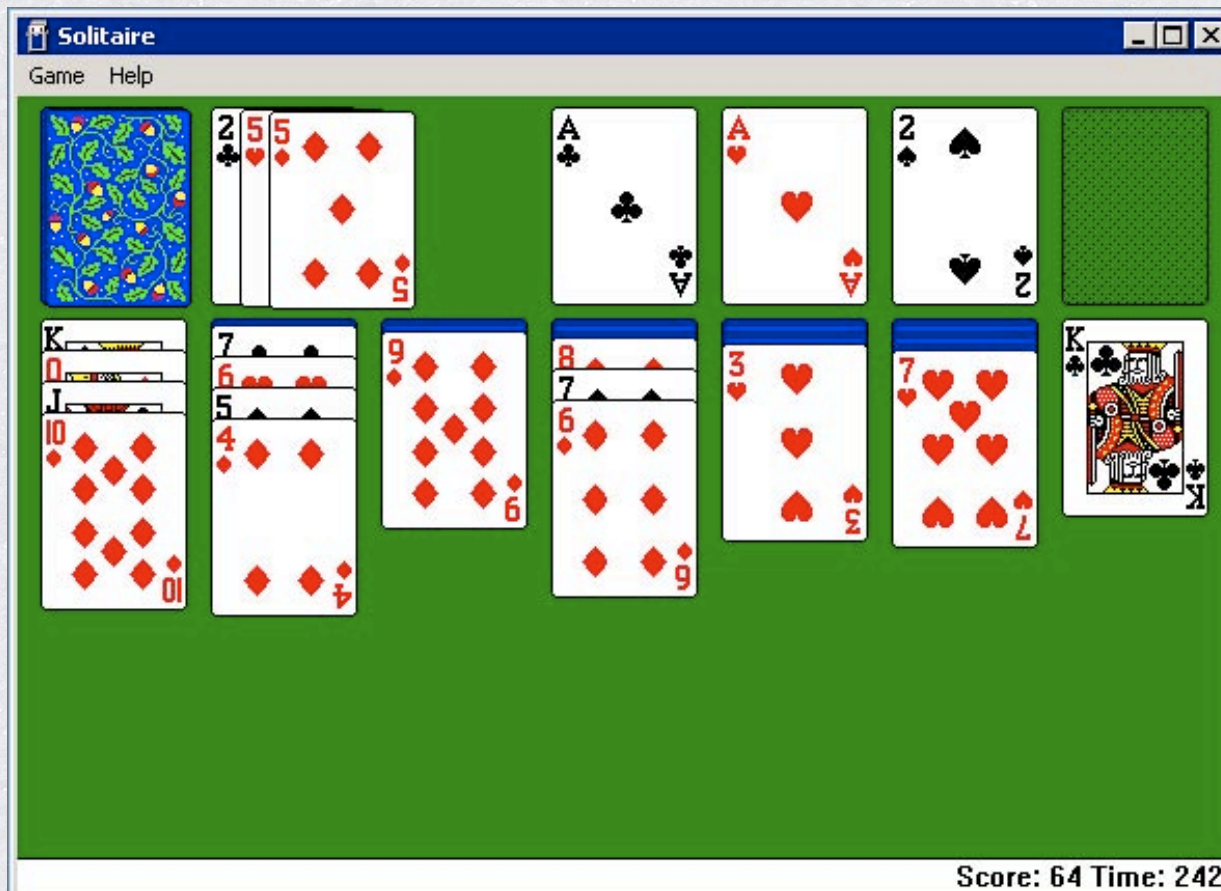


Numerical simulations

- “You let the computer solve the problem for you”
- It’s not that easy:
 - Exponentially diverging number of states 
 - 1 site: q states
 - N sites: q^N states
 - Critical slowing down of the dynamics at phase transitions 
 - negative sign problem for fermions (NP-hard) 

Ulam: the Monte Carlo Method



- What is the probability to win in Solitaire?
- answer play it 100 times, count the number of wins and you have a pretty good estimate



The Monte Carlo Method

- Estimate an average by a statistical sample

-
-
-
-
-
-

$\langle A \rangle = \frac{1}{Z} \sum_{i=1}^N$   $\rightarrow \langle A \rangle \approx \bar{A} = \frac{1}{M} \sum_{i=1}^M A_{c_i}$

observable

probability

- Need a representative sample with the correct distribution

$$P[c_i] = \frac{p_{c_i}}{Z}$$

- How can this be achieved?
 - fundamental problem of statistical mechanics

the Top 10 Algorithms



- Metropolis Algorithm for Monte Carlo
- Simplex Method for Linear Programming
- Krylov Subspace Iteration Methods
- The Decompositional Approach to Matrix Computations
- The Fortran Optimizing Compiler
- QR Algorithm for Computing Eigenvalues
- Quicksort Algorithm for Sorting
- Fast Fourier Transform
- Integer Relation Detection
- Fast Multipole Method

The Metropolis algorithm (1953)

THE JOURNAL OF CHEMICAL PHYSICS

VOLUME 21, NUMBER 6

JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

I. INTRODUCTION

THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed,

II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number N may be as high as several hundred. Our system consists of a square† con-

I. INTRODUCTION

[REDACTED] suitable for fast electronic computing machines, [REDACTED] which may be considered as composed of interacting individual molecules.

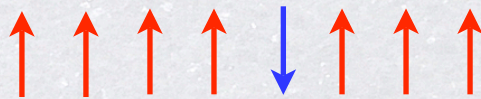
The Metropolis algorithmus (1953)

- creates a representative sample for any system

start with a configuration i



propose a small change to a configuration j



calculate the ratio of probabilities

$$\frac{p_j}{p_i}$$

accept the new configuration with probability

$$P = \min \left(1, \frac{p_j}{p_i} \right)$$

Quantum Monte Carlo

- Feynman (1953) lays foundation for quantum Monte Carlo
- Map quantum system to classical world lines

THE PHYSICAL REVIEW

A journal of experimental and theoretical physics established by E. L. Nichols in 1893

SECOND SERIES, VOL. 91, No. 6

SEPTEMBER 15, 1953

Atomic Theory of the λ Transition in Helium

R. P. FEYNMAN

California Institute of Technology, Pasadena, California

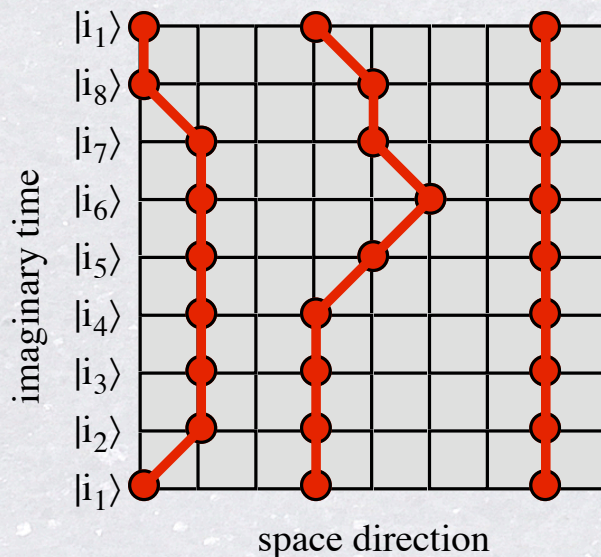
(Received May 15, 1953)

Discrete time path integrals

- An expansion of the partition function

$$\begin{aligned} Z &= \text{Tr} e^{-\beta H} = \text{Tr} e^{-M\Delta\tau H} = \text{Tr} (e^{-\Delta\tau H})^M = \text{Tr} (1 - \Delta\tau H)^M + O(\beta\Delta\tau) \\ &= \sum_{\{(i_1 \dots i_M)\}} \langle i_1 | 1 - \Delta\tau H | i_2 \rangle \langle i_2 | 1 - \Delta\tau H | i_3 \rangle \cdots \langle i_M | 1 - \Delta\tau H | i_1 \rangle \end{aligned}$$

- gives a mapping to a $(d+1)$ -dimensional classical model



place particles (spins)

for Hamiltonians conserving
particle number (magnetization)
we get world lines

- partition function of quantum system is sum over classical world lines

Monte Carlo updates

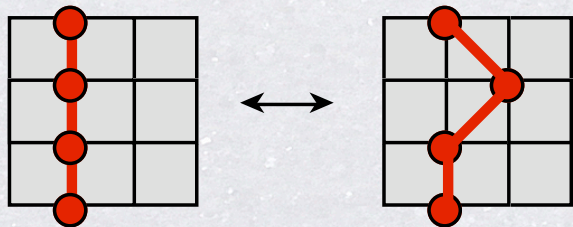
□ just move the world lines locally

□ probabilities given by matrix element of Hamiltonian

□ example: tight binding model

$$H = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i)$$

introduce or remove two kinks:



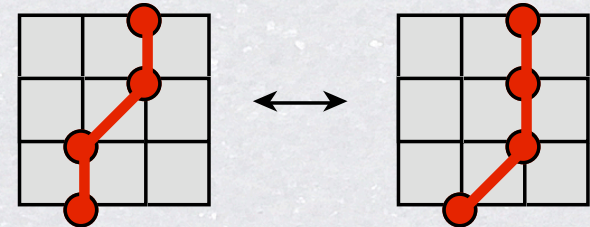
$$P = 1$$

$$P = (\Delta\tau t)^2$$

$$P_{\rightarrow} = \min[1, (\Delta\tau t)^2]$$

$$P_{\leftarrow} = \min[1, 1/(\Delta\tau t)^2]$$

shift a kink:

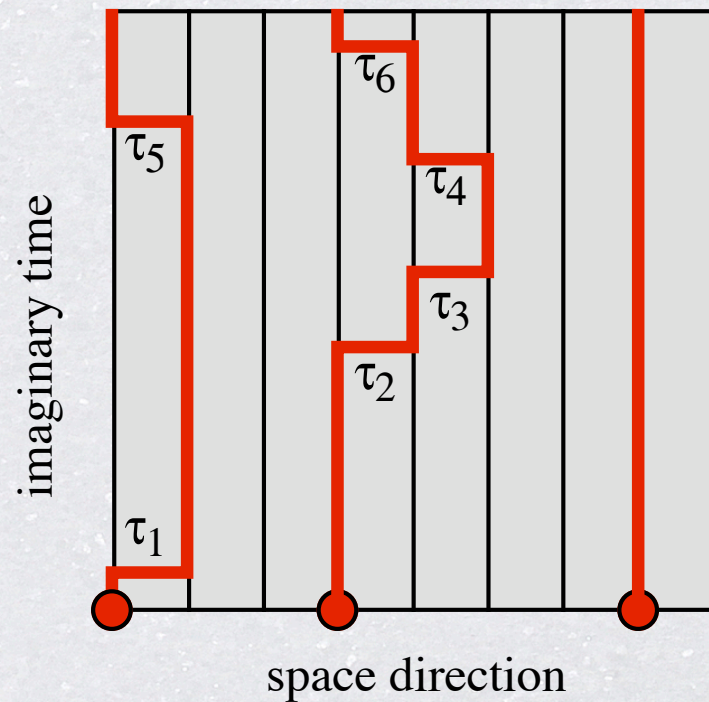
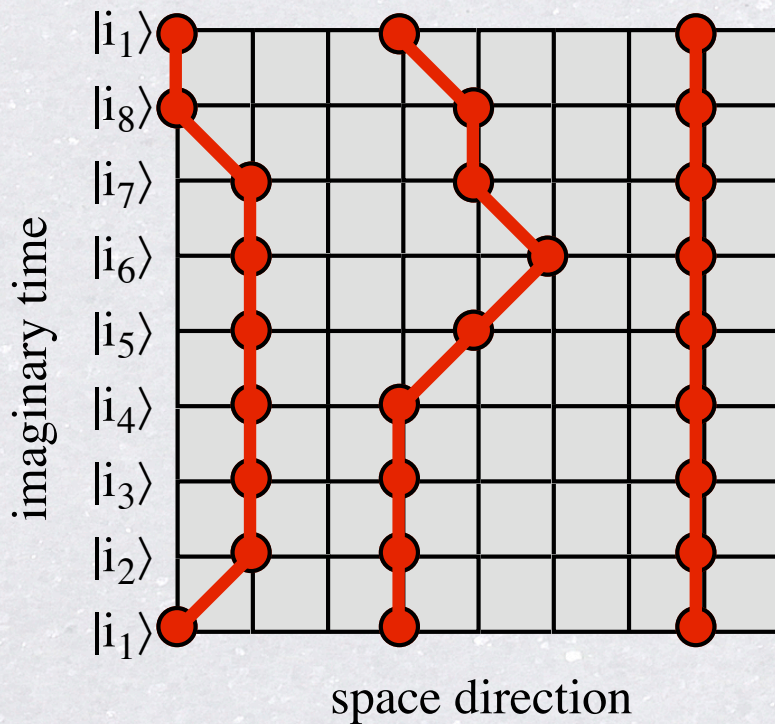


$$P = \Delta\tau t$$

$$P_{\rightarrow} = P_{\leftarrow} = 1$$

The continuous time limit

- the limit $\Delta\tau \rightarrow 0$ can be taken in the construction of the algorithm [Prokof'ev *et al.*, Pis'ma v Zh.Eks. Teor. Fiz. **64**, 853 (1996)]



- discrete time: store configuration at all time steps
- continuous time: store times at which configuration changes

Path Integral Formulation

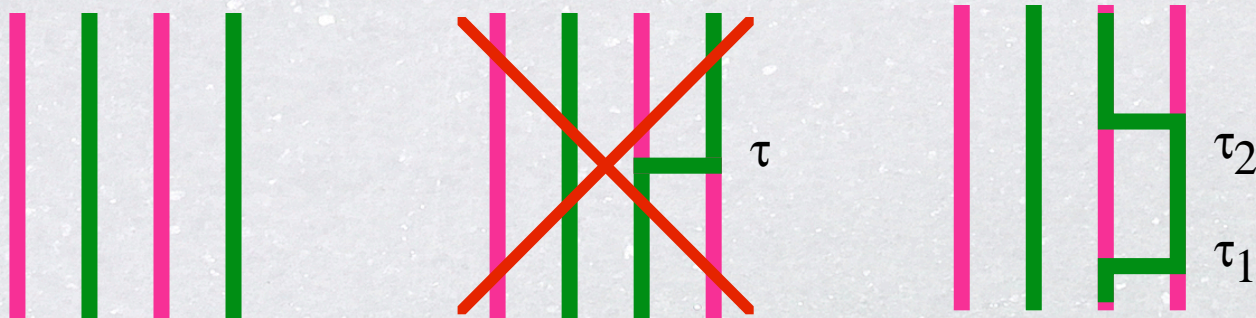
- interaction representation

$$H = H_0 + V, \quad H_0 = \sum_{\langle i,j \rangle} J_{ij}^z S_i^z S_j^z - \sum_i h S_i^z, \quad V = \sum_{\langle i,j \rangle} J_{ij}^{xy} (S_i^x S_j^x + S_i^y S_j^y)$$

$$Z = \text{Tr}(e^{-\beta H}) = \text{Tr}(e^{-\beta H_0} \mathcal{T} e^{-\int_0^\beta d\tau V(\tau)})$$

$$Z = \text{Tr}(e^{-\beta H_0} (1 - \int_0^\beta d\tau V(\tau) + \int_0^\beta d\tau_1 \int_{\tau_1}^\beta d\tau_2 V(\tau_1) V(\tau_2) + \dots))$$

- each term is represented by a world line configuration



Stochastic Series Expansion (SSE)

- based on high temperature expansion, developed by A. Sandvik

$$\begin{aligned} Z &= \text{Tr}(e^{-\beta H}) = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \text{Tr} \left[(-H)^n \right] \\ &= \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \sum_{\alpha_1, \dots, \alpha_n} \langle \alpha_1 | -H | \alpha_2 \rangle \langle \alpha_2 | -H | \alpha_3 \rangle \cdots \langle \alpha_n | -H | \alpha_1 \rangle \end{aligned}$$

- also has a graphical representation in terms of world lines



- Advantage: easier algorithms since no times associated with operators
- Disadvantage: perturbation in all terms of the Hamiltonian

The negative sign problem

- In mapping of quantum to classical system

- $$\langle A \rangle = \text{Tr}[A \exp(-\beta H)] / \text{Tr}[\exp(-\beta H)] = \sum_i A_i p_i / \sum_i p_i$$

- there is a “sign problem” if some of the $p_i < 0$

- Appears e.g. in simulation of electrons (Pauli principle)

$$\langle A \rangle = \sum_i A_i p_i / \sum_i p_i = \frac{\sum_i A_i \text{sgn } p_i |p_i| / \sum_i |p_i|}{\sum_i \text{sgn } p_i |p_i| / \sum_i |p_i|} \equiv \frac{\langle A \cdot \text{sign} \rangle_{|p|}}{\langle \text{sign} \rangle_{|p|}}$$

- Exponentially growing cancellation in the sign

$$\langle A \cdot \text{sign} \rangle_{|p|} \approx \langle \text{sign} \rangle_{|p|} \approx \exp(-c\beta N) \Rightarrow \Delta A \approx \exp(+c\beta N)$$

Autocorrelation effects

- The Metropolis algorithm creates a Markov chain of configurations

$$c_1 \rightarrow c_2 \rightarrow \dots \rightarrow c_i \rightarrow c_{i+1} \rightarrow \dots$$

- successive configurations are correlated, leading to an increased statistical error

$$\Delta A = \sqrt{\left\langle \left(\bar{A} - \langle A \rangle \right)^2 \right\rangle} = \sqrt{\frac{\text{Var } A}{M} (1 + 2\tau_A)}$$

- *Critical slowing down* at second order phase transition

$$\tau \propto L^2$$

- *Exponential tunneling problem* at first order phase transition

$$\tau \propto \exp(L^{d-1})$$

Solving slowing down at phase transitions

- **Changing the dynamics** solves critical slowing down at second order phase transitions: make large, global, changes instead of local ones
 - Cluster updates for classical spins (Swendsen and Wang, 1987)
 - Loop algorithm for quantum spins (Evertz *et al*, 1993)
 - Worm algorithm (Prokof'ev *et al*, 1998)
- **Changing the ensemble** solves tunneling problem at first order phase transitions: remove the energy barriers
 - Multicanonical sampling (Berg & Neuhaus, 1991)
 - Wang-Landau sampling (F. Wang & D.P. Landau, 2001)
 - Flat histogram methods for quantum systems (Troyer *et al*, PRL 2003)

Cluster algorithms for quantum systems

- Which system sizes can be studied?

temperature	Metropolis	modern algorithms
1	16'000 spins	16'000'000 spins
0.1	200 spins	1'000'000 spins
0.1	32 bosons	10'000 bosons
0.005	—	50'000 spins

- Modern algorithms allow to accurately study quantum phase transitions

ALPS project: <http://alps.comp-phys.org/>

Open source software for quantum lattice models

Workshop and tutorials

Lugano, Switzerland, September 27 - October 1, 2004



Hands-on tutorials

Classical Monte Carlo
Spin Dynamics
Quantum Monte Carlo
Exact diagonalization
DMRG

Speakers (preliminary)

H.G. Evertz (TU Graz)
A. Läuchli (Toulouse)
R. Noack (Marburg)
U. Schollwöck (RWTH)

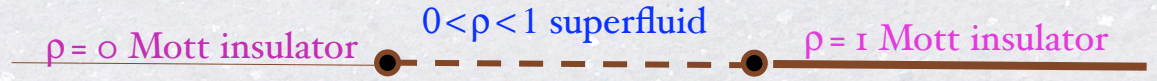
T. Schulthess (ORNL)
S. Todo (Tokyo)
Shan-Ho Tsai (UGA)
M. Troyer (ETH)

Hard-core bosons

Two-dimensional hard-core boson model

- Seems trivial, but actually strongly interacting system (infinite repulsion)

- $$H = -t \sum_{\langle i,j \rangle} (a_i^\dagger a_j + a_j^\dagger a_i) - \mu \sum_i n_i$$



- equivalent to XY model in a perpendicular magnetic field

$$H = J_{xy} \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_j^y S_i^y) - h \sum_i S_i^z$$

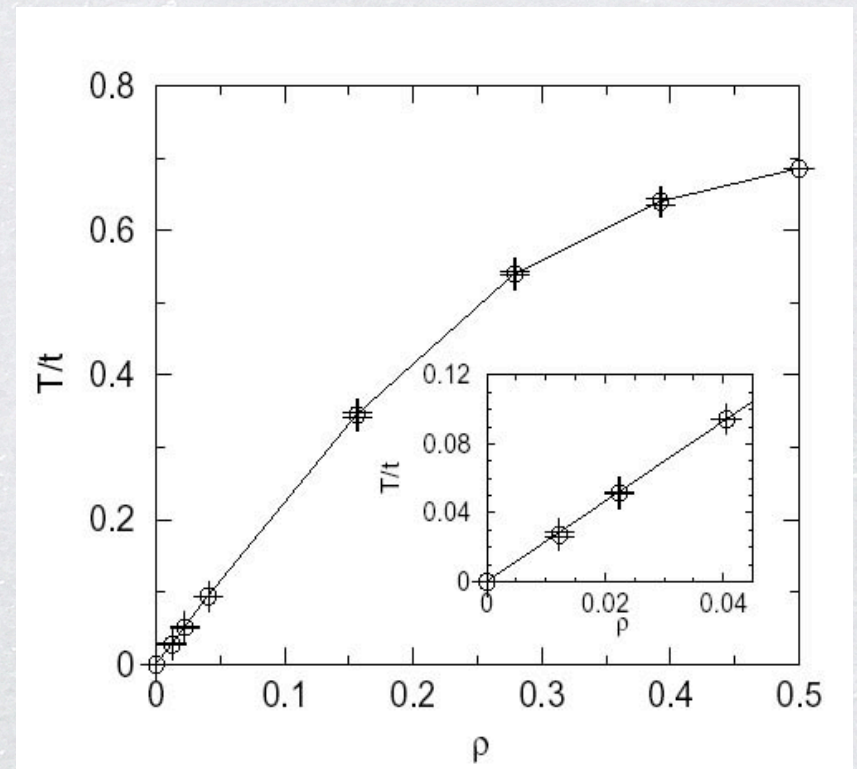
Approximately **linear** T_c at low doping

$$T_c = \frac{\pi}{2m} \rho_s(T_c) \text{ with } \rho_s(T_c) \approx 0.74 \rho$$

Agrees well with experiments on ^4He films

G. Agnolet, et al. PRB '89

P.S. Ebey, et al., J. Low Temp. Phys. '98



Fisher - Hohenberg theory

- For bosons at low doping [D. Fisher and P. Hohenberg, PRB '88]

$$~~T_c = \frac{\pi}{2m} \frac{4\rho}{-\ln \ln a^2 \rho}~~$$

But we also know

$$T_c = \frac{\pi}{2m} \rho_s \quad \begin{array}{l} \rho_s(T_c) \leq \rho \\ \rho_s(T_c) \approx 0.74\rho \end{array}$$

Fisher-Hohenberg formula only valid when $\rho < a^{-2} e^{e^6} \approx 10^{-90} a^{-2}$

With $a=10^{-15}$ m we need less than 10^{-18} bosons in visible universe

Irrelevant for experiments, better use our result

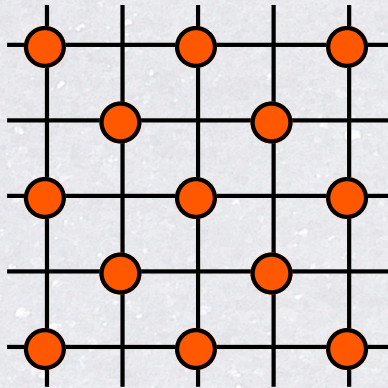
$$T_c = 0.75 \frac{\pi}{2m} \rho$$

Simple limits with longer range repulsion

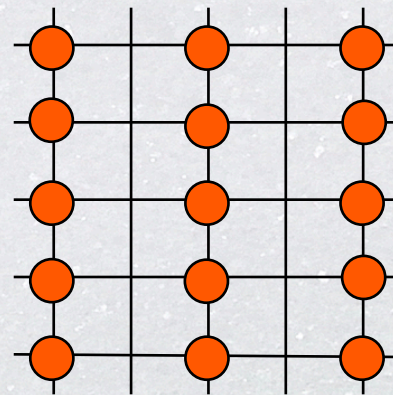
$$H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + U \sum_i n_i(n_i - 1)/2 + V_1 \sum_{\langle i,j \rangle} n_i n_j + V_2 \sum_{\langle\langle i,j \rangle\rangle} n_i n_j$$

- $t \rightarrow \infty$: superfluid phase
- $U = \infty$ at half filling: solid phases at large V_1 or V_2

$V_1 \rightarrow \infty$
checkerboard solid

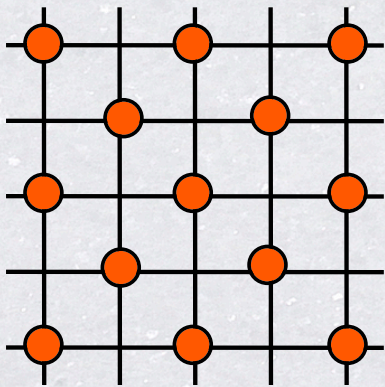


$V_2 \rightarrow \infty$
striped solid

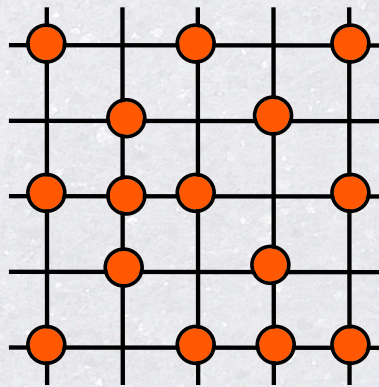


Super solids

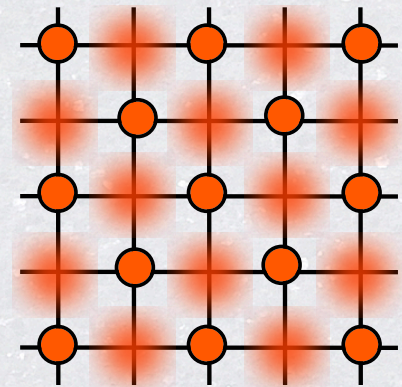
- A super solid shows simultaneously **solid order** (crystalline) and **superfluidity**



solid (crystal)



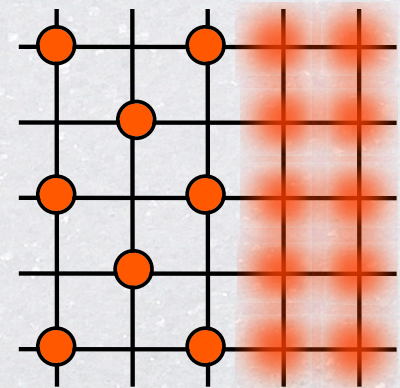
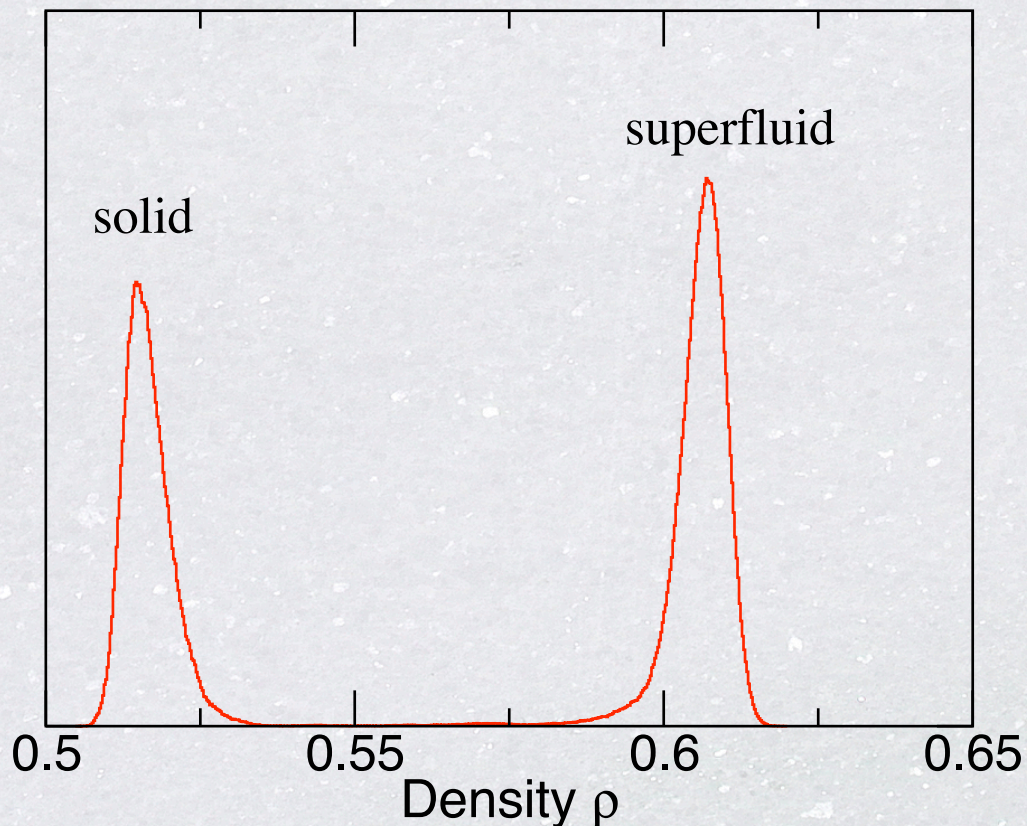
doped solid:
interstitials



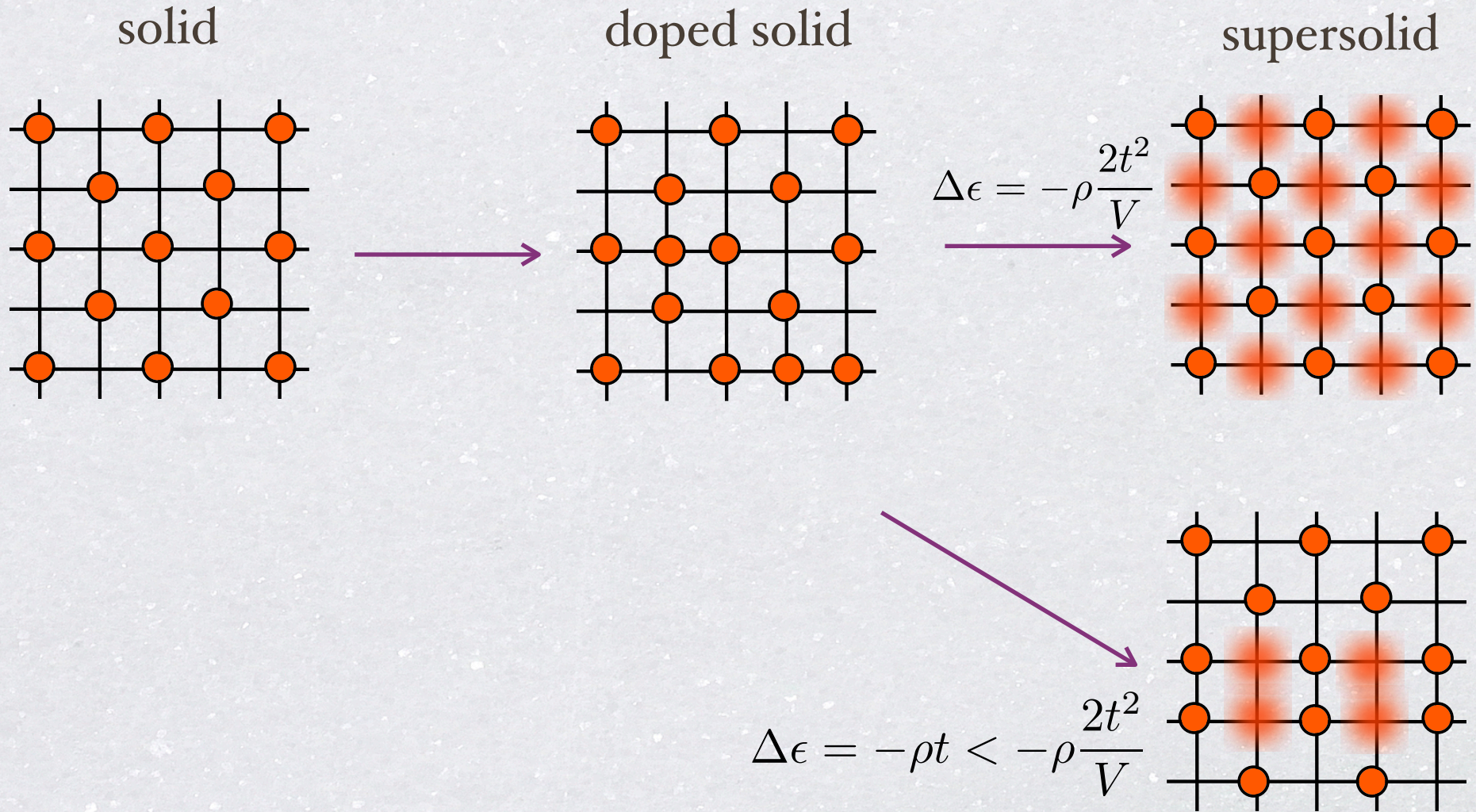
supersolid:
superfluid interstitials

Do supersolids exist?

- 2D Bosons with nearest neighbor repulsion
 - previous simulations (32 particles) found **supersolid**
 - new simulations (5000 particles) instead show phase separation at **first order phase transition**

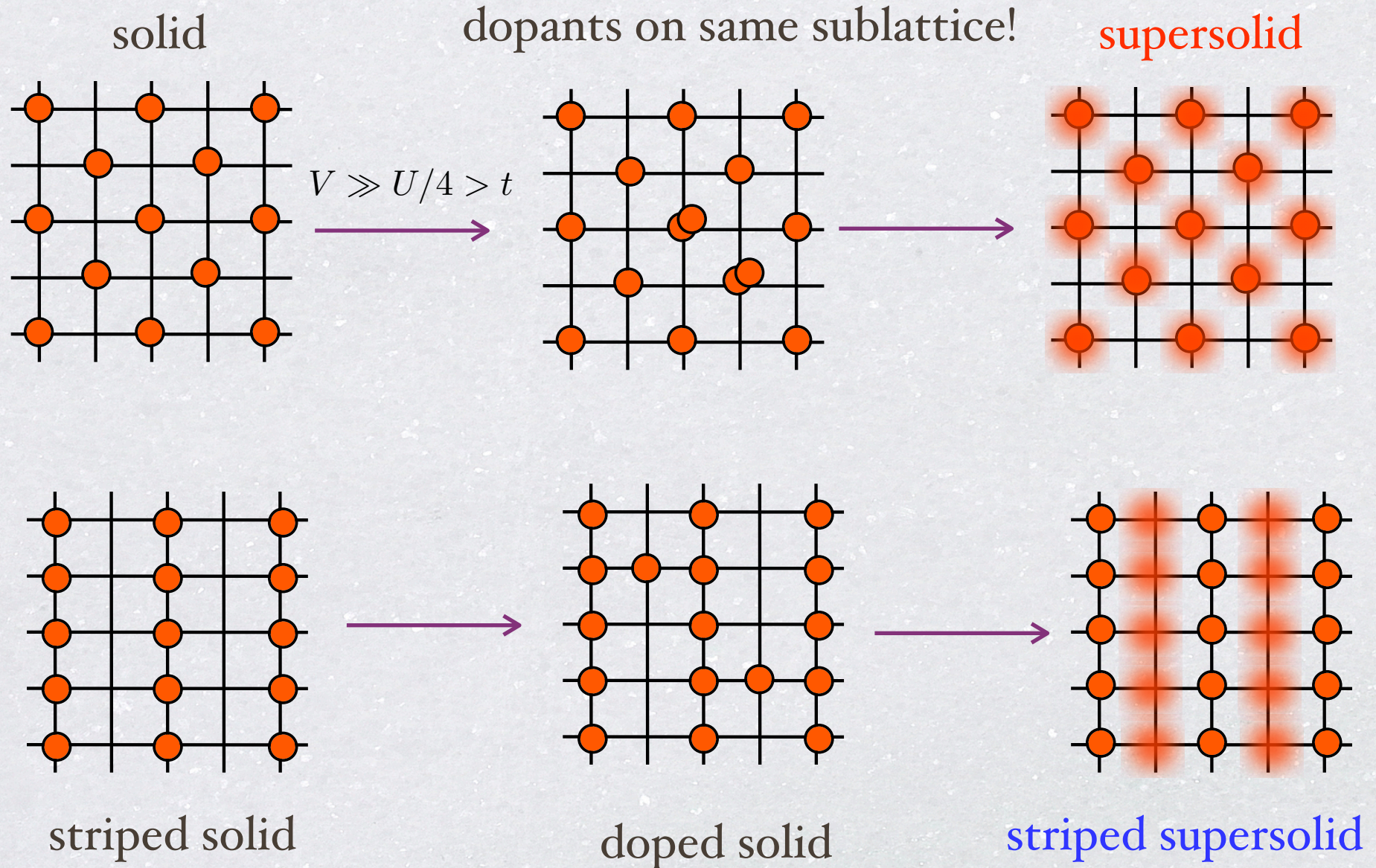


Supersolids versus phase separation



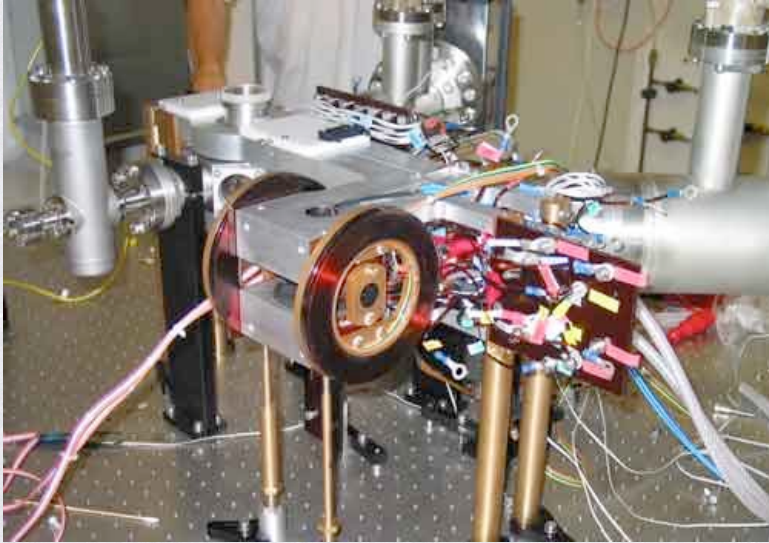
doped particles gain energy
by forming a domain wall

Two routes to supersolids

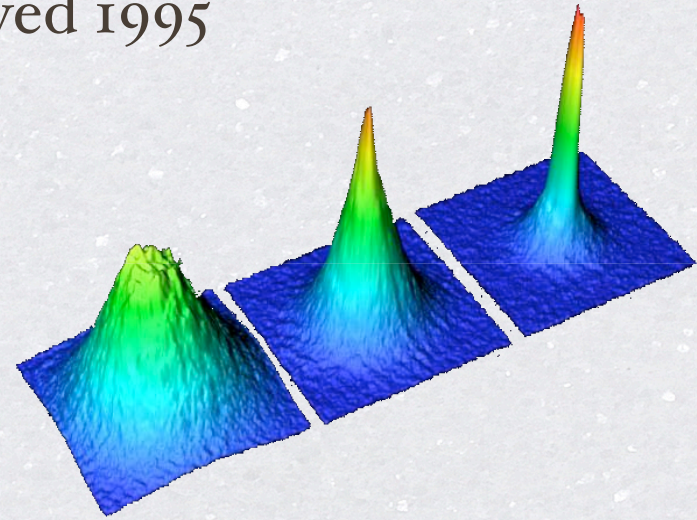


Trapped bosonic atoms

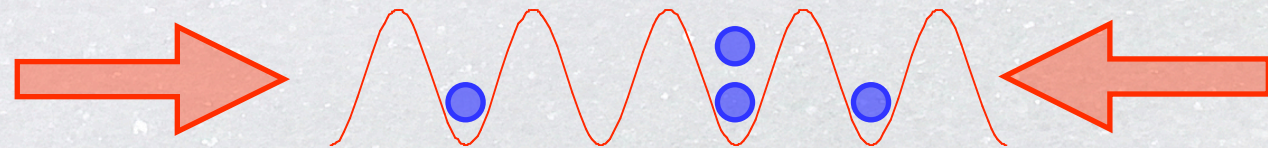
BEC in cold bosonic atoms



Ultra-cold trapped ^{87}Rb atoms form BEC first observed 1995

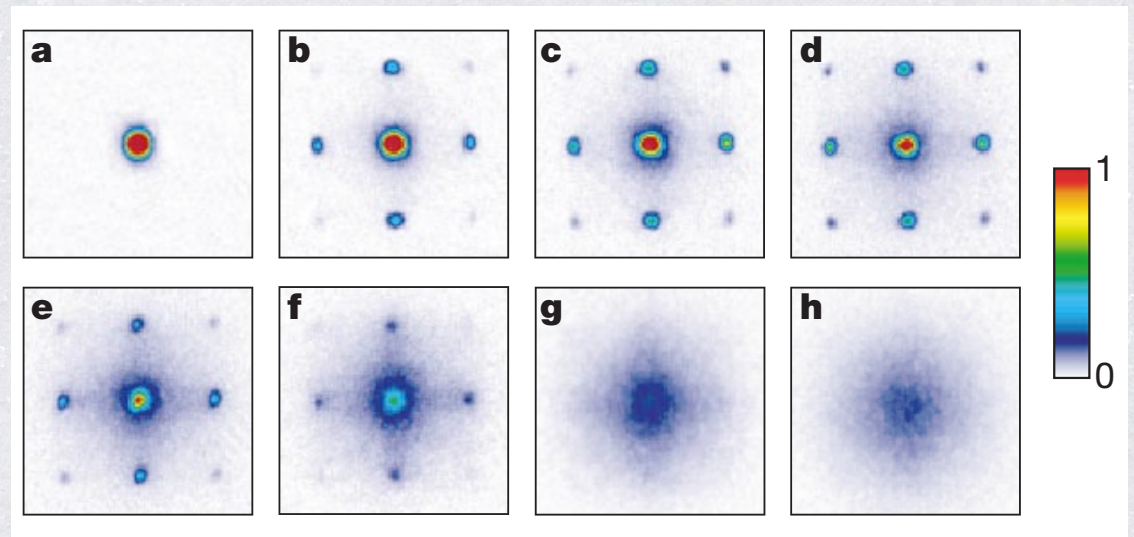
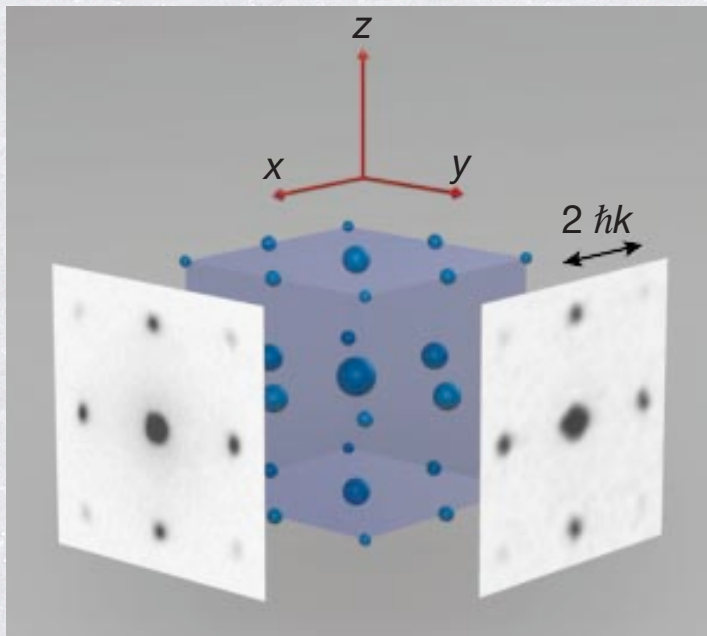


Standing waves from laser superimpose an optical lattice (2002)



Experiments on trapped atoms

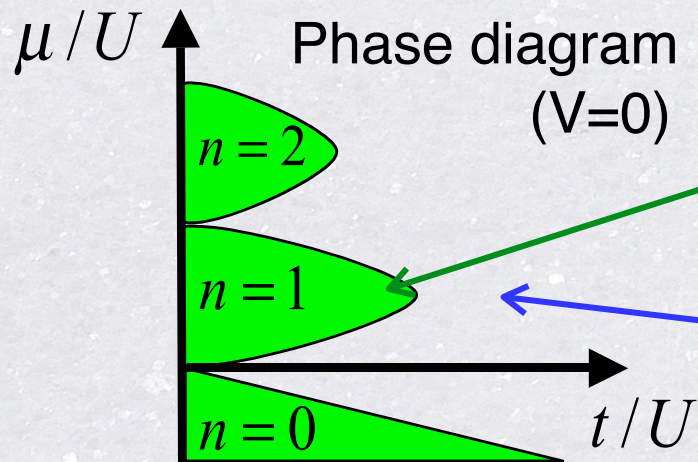
- Trapped atoms in an optical lattice
- Quantum phase transition as lattice depth is increased
 - Greiner *et al*, Nature (2002)
 - detected by measuring the **momentum distribution function**



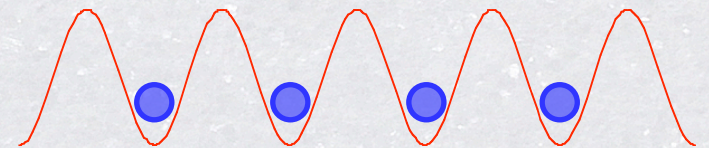
Boson-Hubbard model

- describes bosonic atoms in optical lattice
- well understood without the trap: Fisher *et al*, PRB 1989

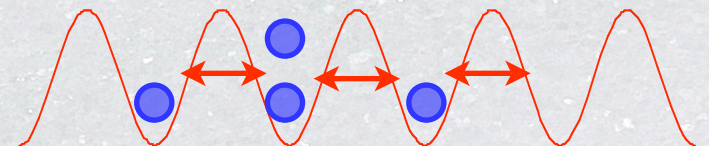
$$H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + U \sum_i n_i(n_i - 1)/2 - \mu \sum_i n_i$$



Incompressible Mott-insulator
Integer filling



superfluid

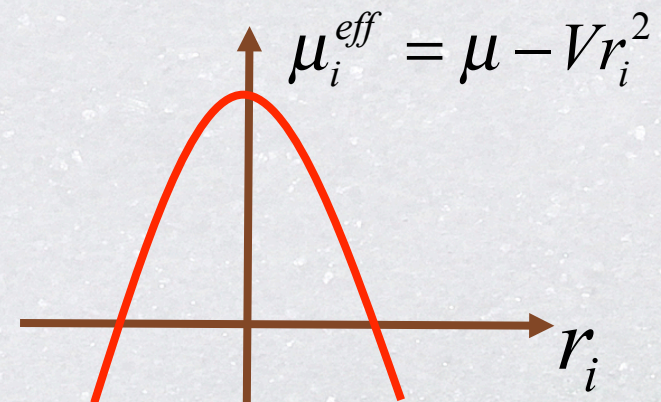
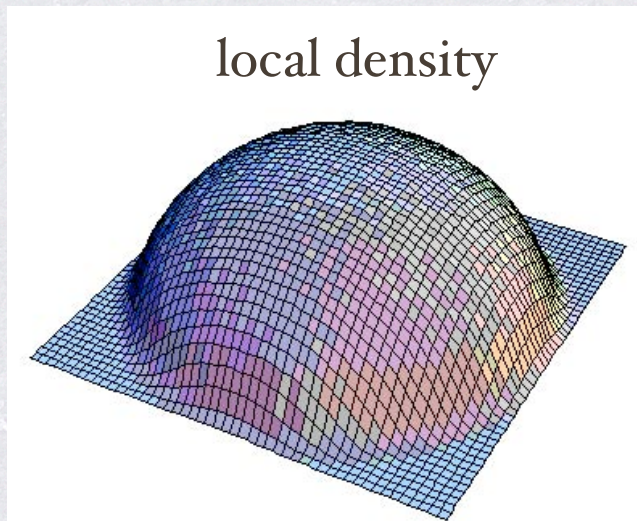


Boson-Hubbard model in a trap

- trap introduces a site-dependent chemical potential
 - results in inhomogeneous system

$$H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + U \sum_i n_i(n_i - 1)/2 - \mu \sum_i n_i + V \sum_i r_i^2 n_i$$

$$H = -t \sum_{\langle i,j \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + U \sum_i n_i(n_i - 1)/2 - \sum_i \mu_i^{eff} n_i$$



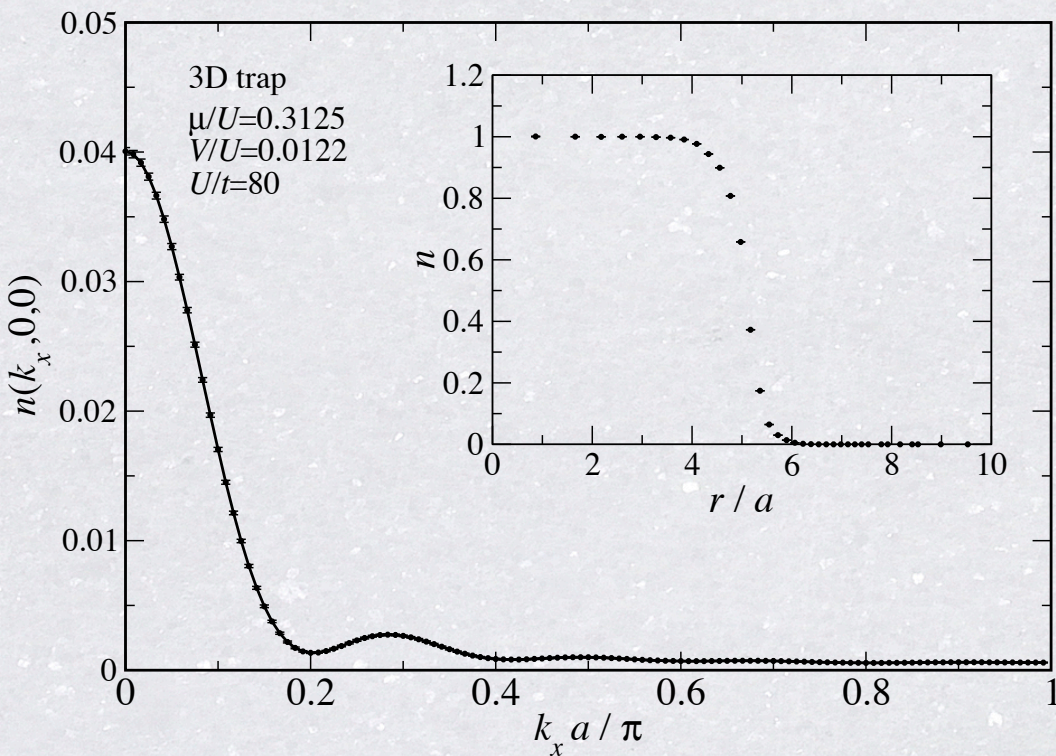
increasing repulsion U/t

forms Mott insulator in center of trap, surrounded by superfluid shell

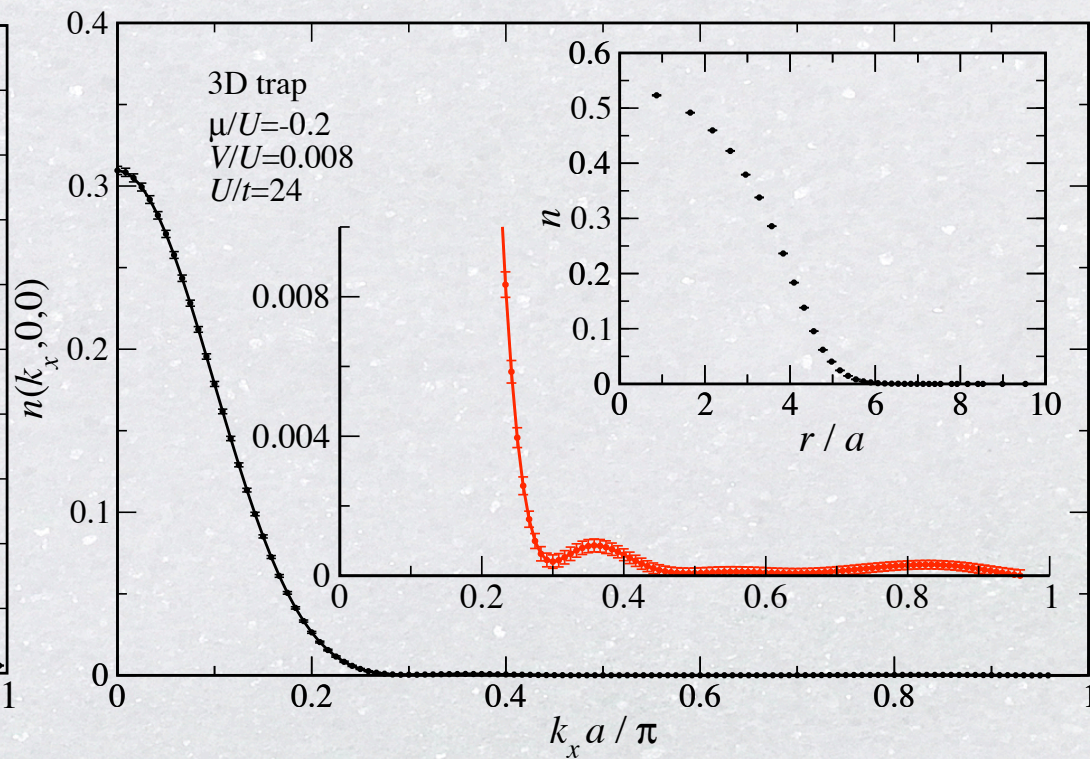
Detecting the quantum phase transition (I)

- Original proposal by Prokof'ev and Svistunov
 - look for fine structure in momentum distribution

secondary peak in Mott insulator



no such peak in superfluid

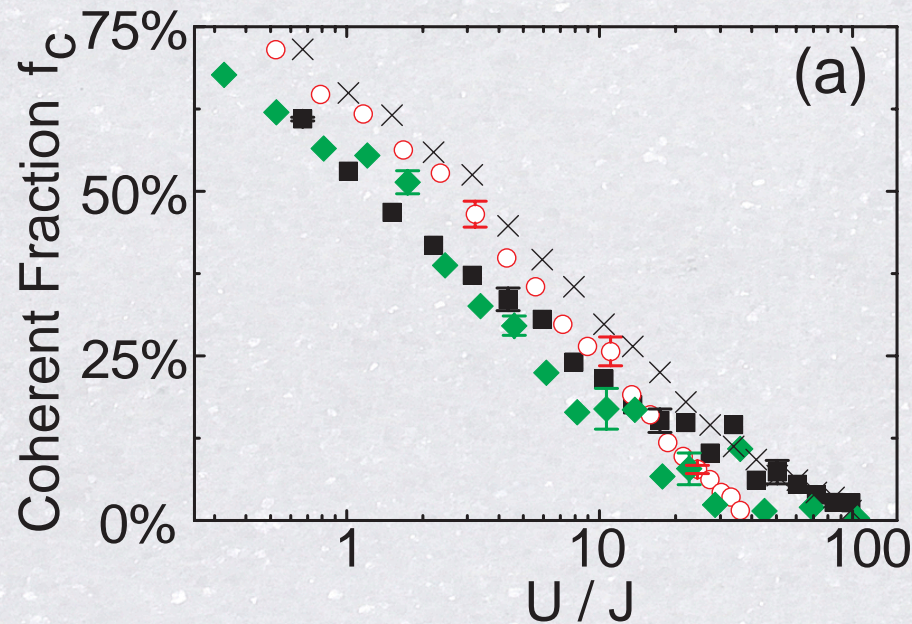


a closer look reveals that this is wrong

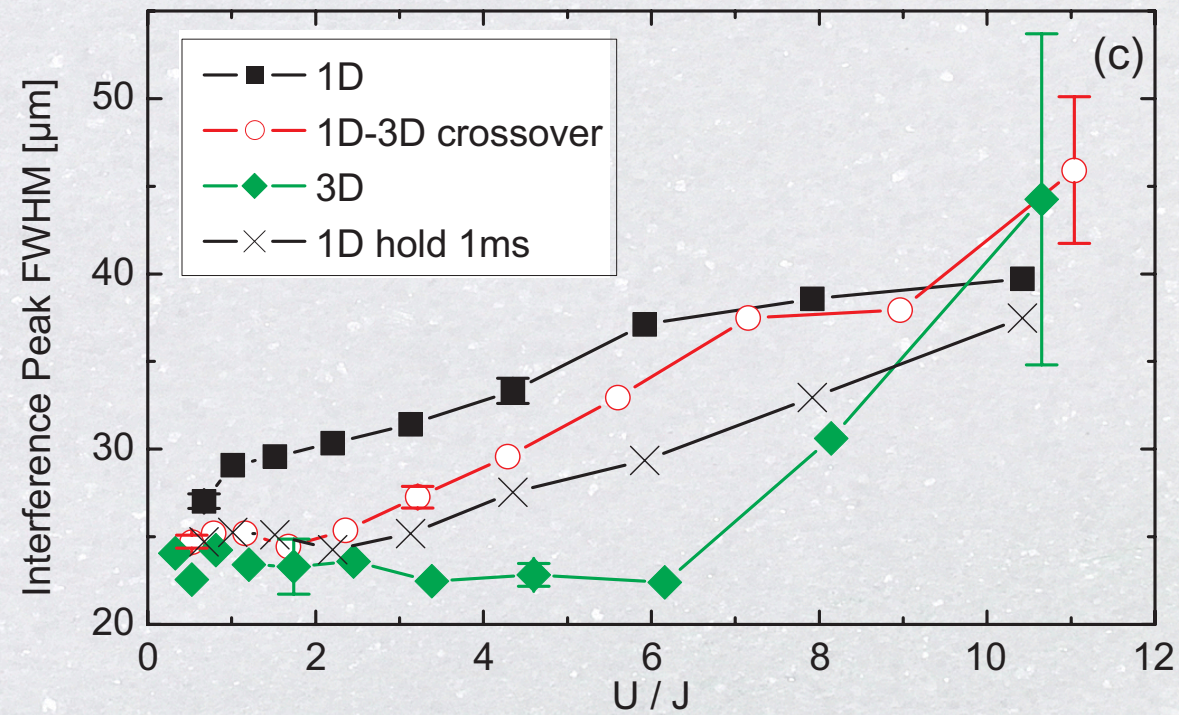
Detecting the quantum phase transition (2)

Measurements at ETH by Stöferle *et al* [PRL, 2004]

peak height
(coherence fraction)



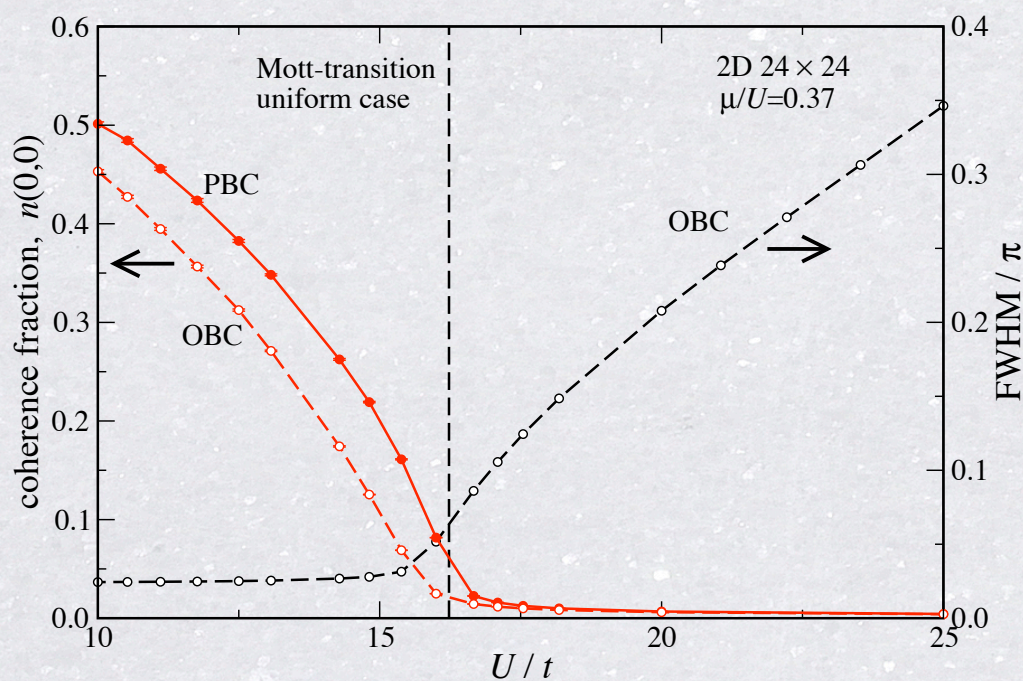
peak width
(FWHM)



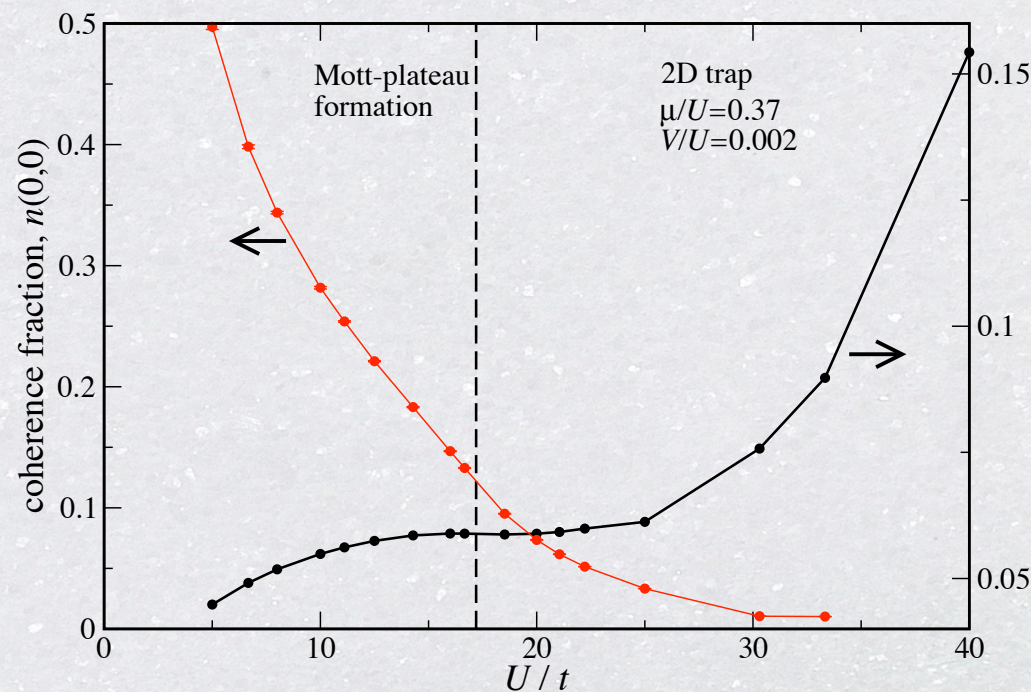
can this be used to detect quantum phase transition?

Detecting the quantum phase transition (3)

- Numerical simulations to check whether the QPT can be detected from peak width and height



uniform system (flat trap)
easy to detect QPT

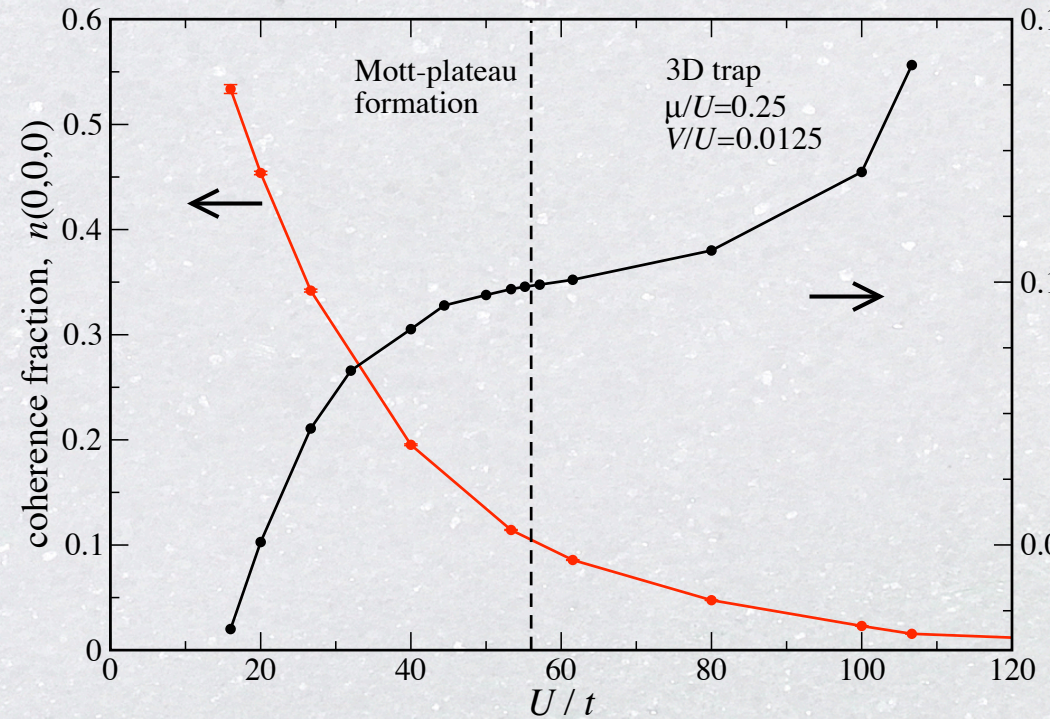
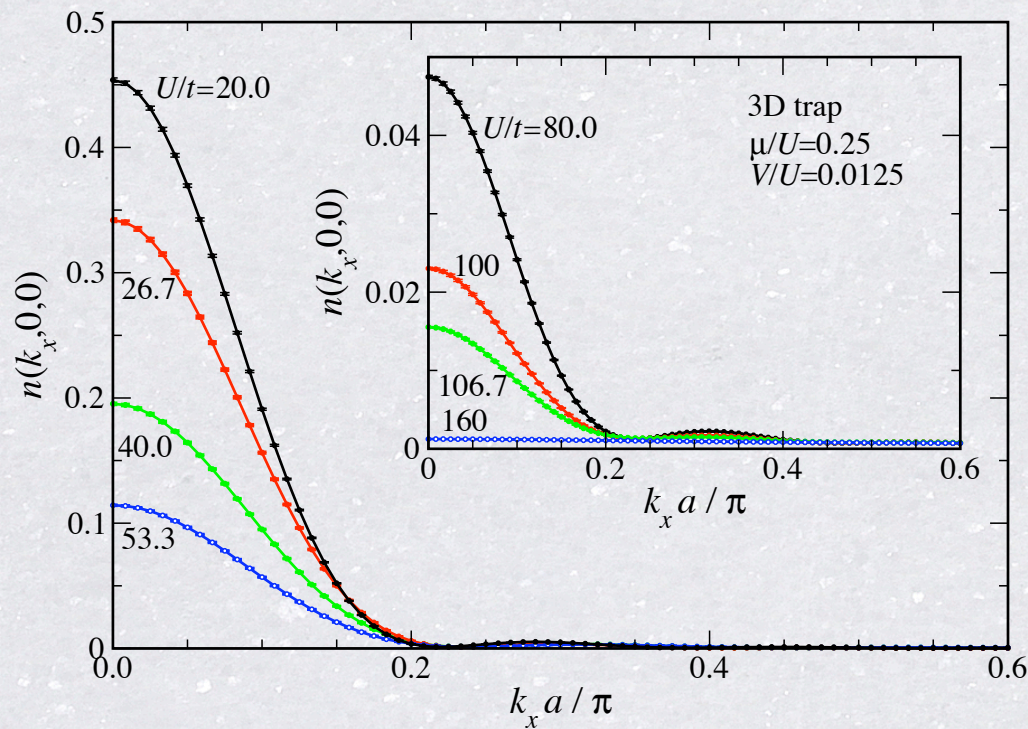


parabolic trap
comparison to simulation needed

a flat trap would be preferred!

Other dimensions

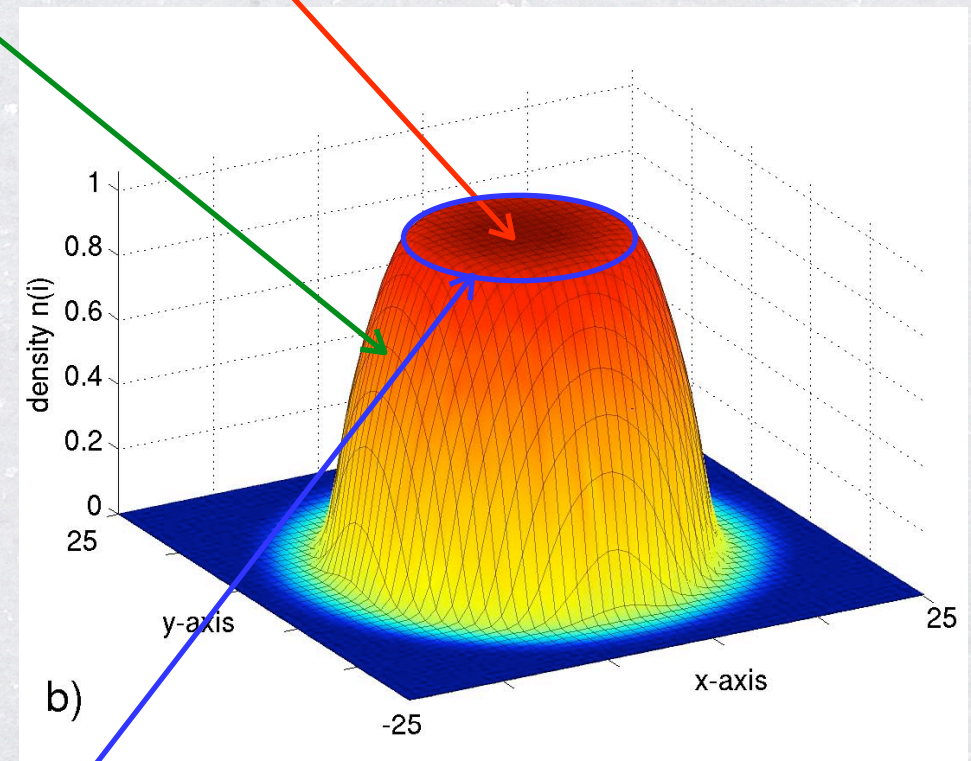
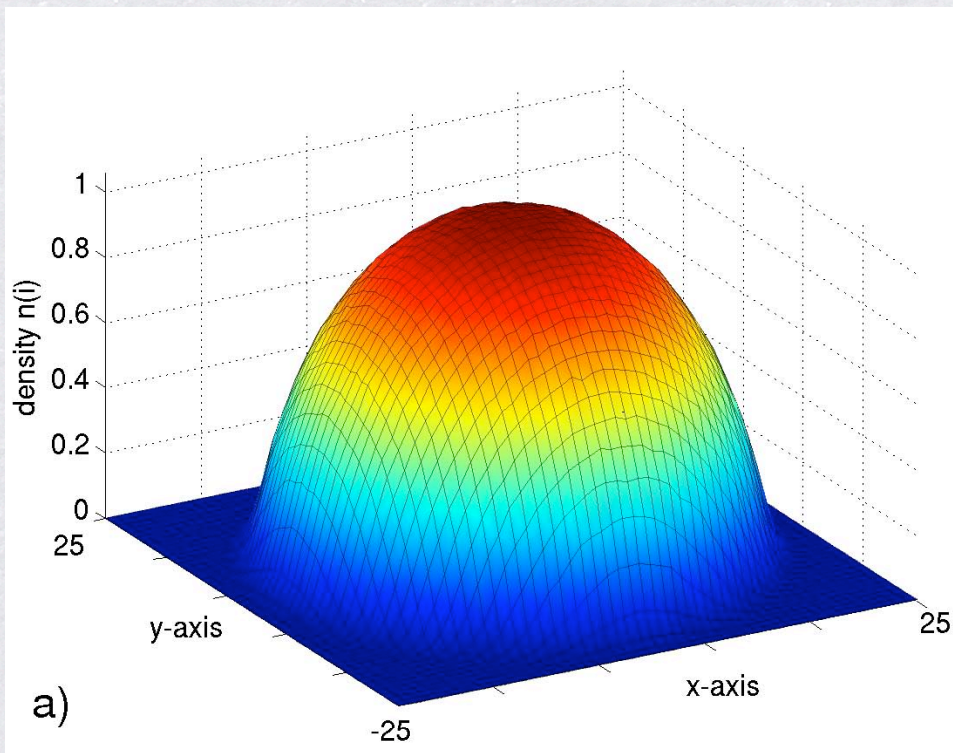
- 1D results by C. Kollath *et al* [PRA, 2004]
- Our 3D results are very similar to 2D



Quantum criticality in trapped bosonic atoms

Describing the phases

- How shall we *quantitatively* understand the phases?
 - A Mott-insulating core forms in the center of the trap
 - surrounded by superfluid (*1D or 2D?*)



quantum criticality at interface?

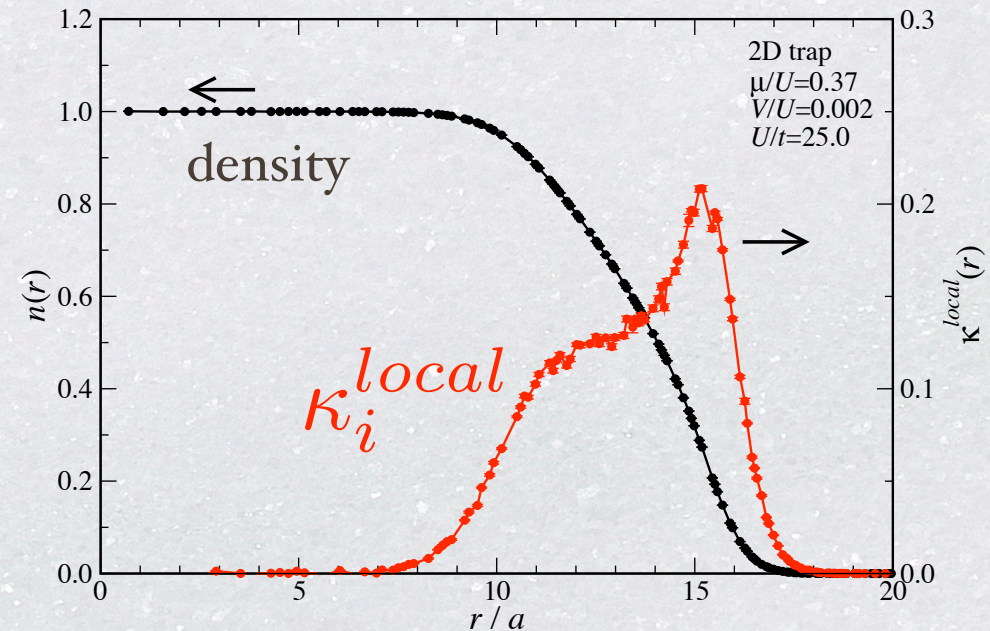
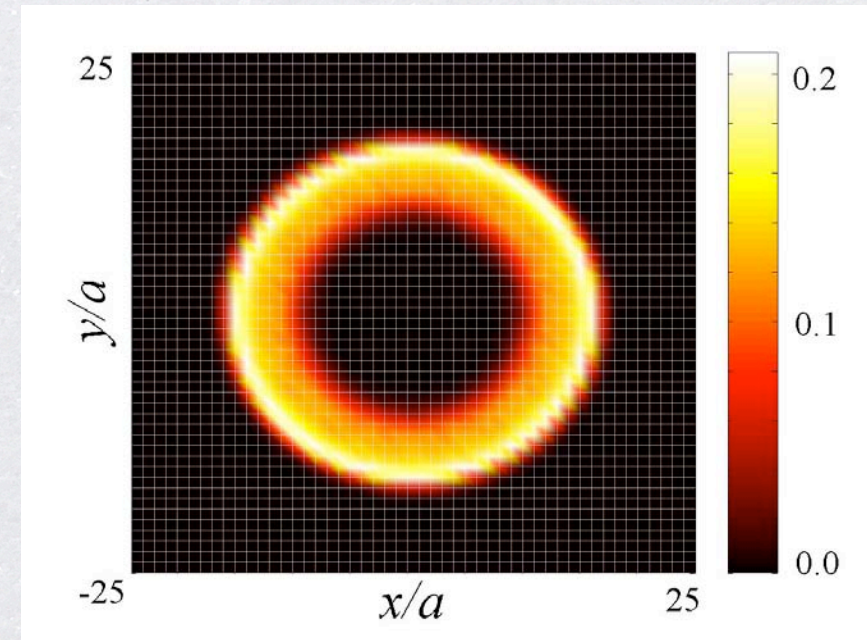
Identifying the local phases

- Measure local compressibility

$$\kappa_i^{local} = \frac{\partial n}{\partial \mu_i^{eff}} = \frac{\partial n_i}{\partial \mu} = \beta (\langle n_i n \rangle - \langle n_i \rangle \langle n \rangle)$$

- Superfluid remains compressible
- Mott-insulator incompressible

- Increased fluctuations near the edge of the superfluid

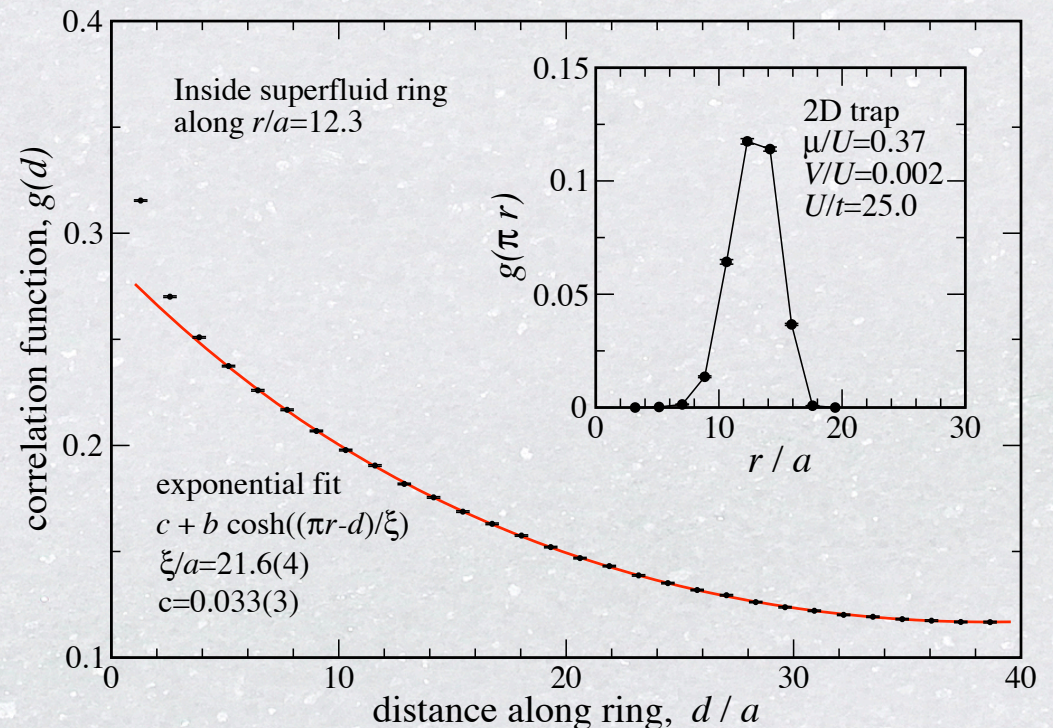
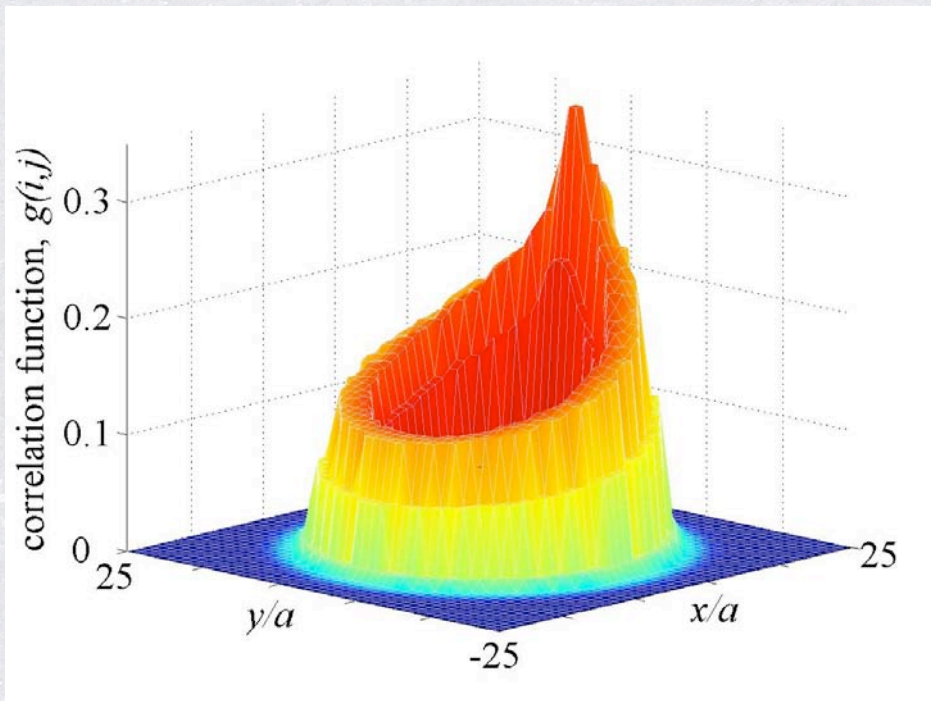


Coherence within the superfluid ring

Equal-time Green's function $\langle b_i^+ b_j \rangle$ along the superfluid ring

better described by 2D behavior $g(d) = \langle b^\dagger(0)b(d) \rangle = c + a \cosh\left(\frac{\pi r - d}{\xi}\right)$

than by 1D behavior $g(d) = \langle b^\dagger(0)b(d) \rangle \propto [d^{-\kappa} + (2\pi r - d)^{-\kappa}]$



Absence of quantum criticality

Local potential approximation

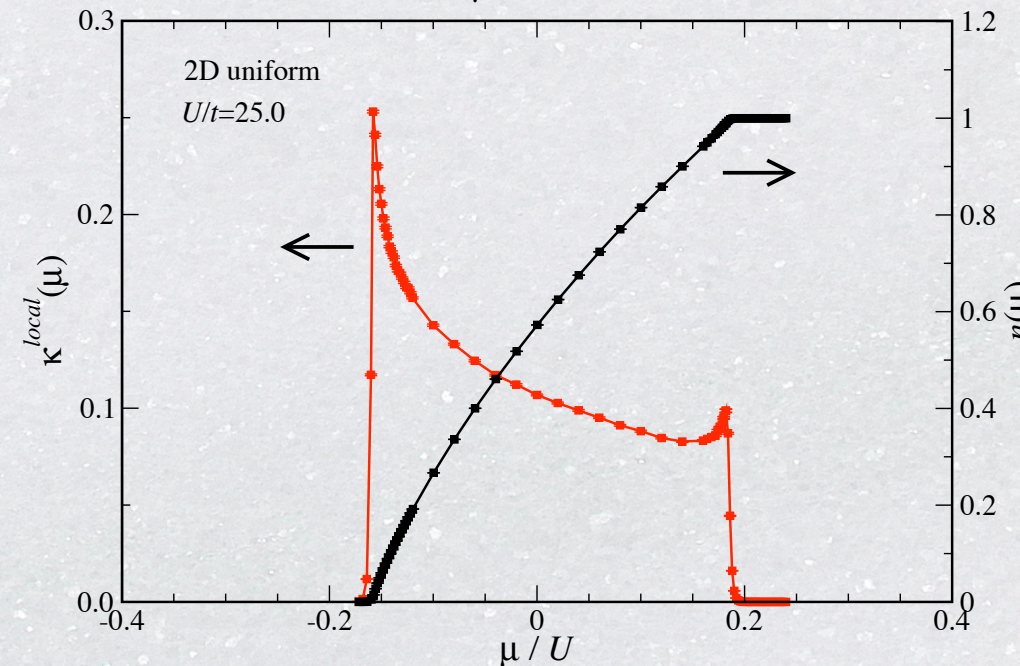
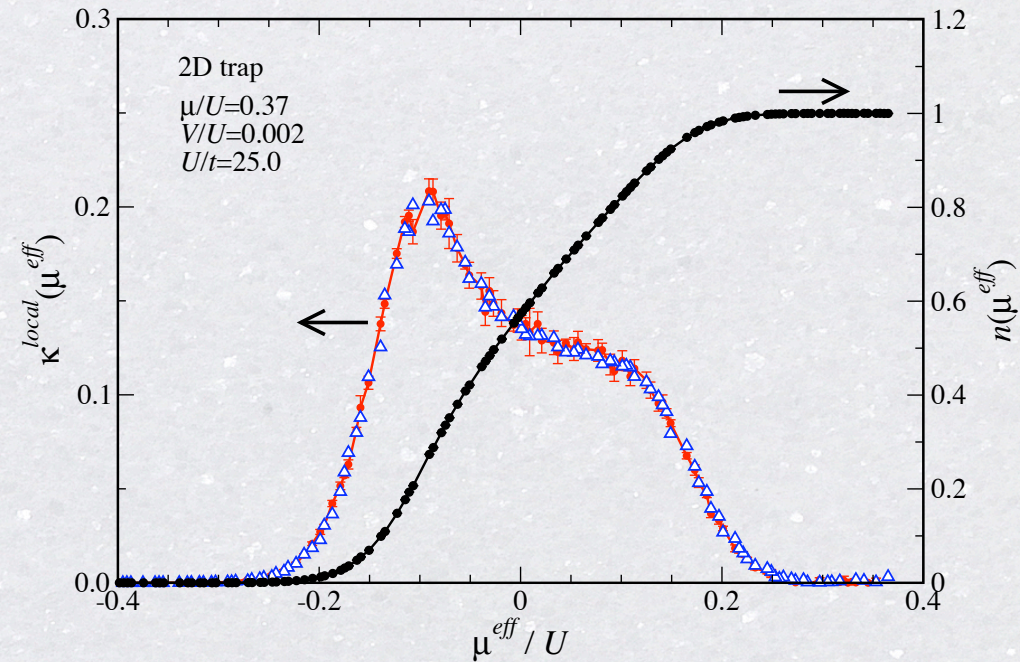
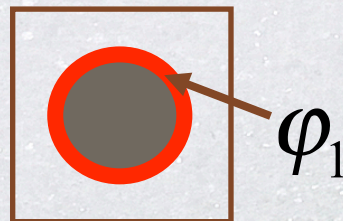
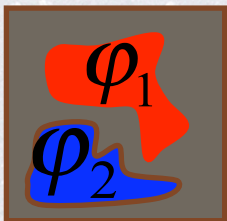
- Data collapses onto a single curve
- This curve varies from trap to trap
- Not reducible to homogenous case

Absence of cusps and singularities

- A singularity emerges in uniform 2D
- Even qualitatively different in trap

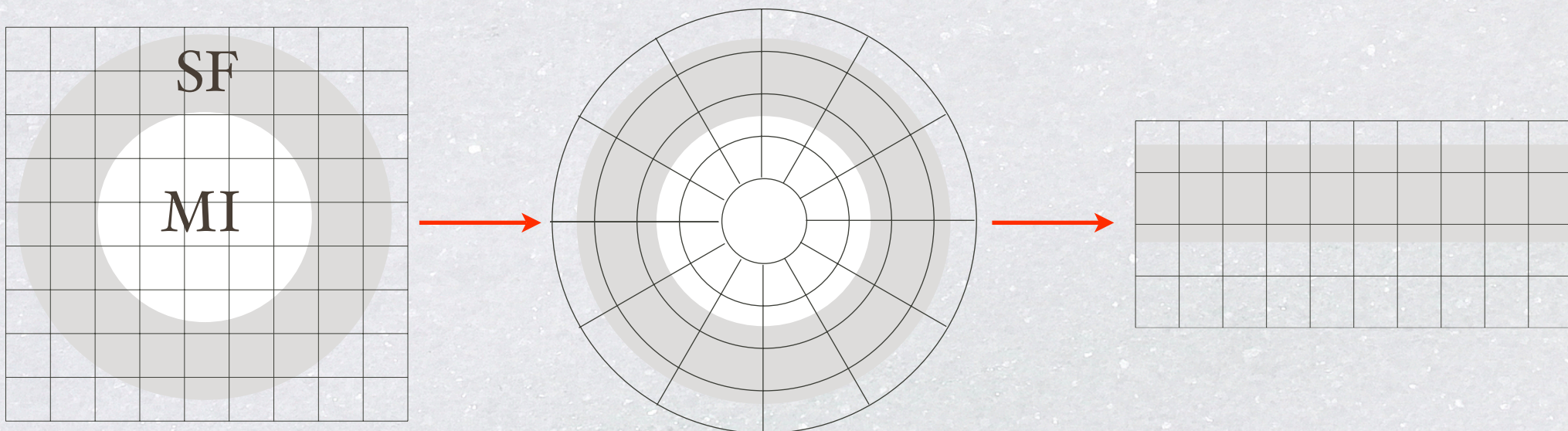
No signature of quantum criticality

- Single domain formation
- No critical slowing down



Effective Ladder model

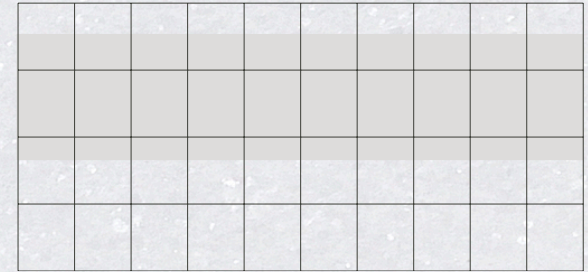
- What causes the absence of quantum criticality?
 - finite size effect?
 - effect of potential gradient?
 - structural quenching?
- Structural disorder removed by considering a ladder model



Effective Ladder model

- Describe the critical region by an inhomogeneous ladder

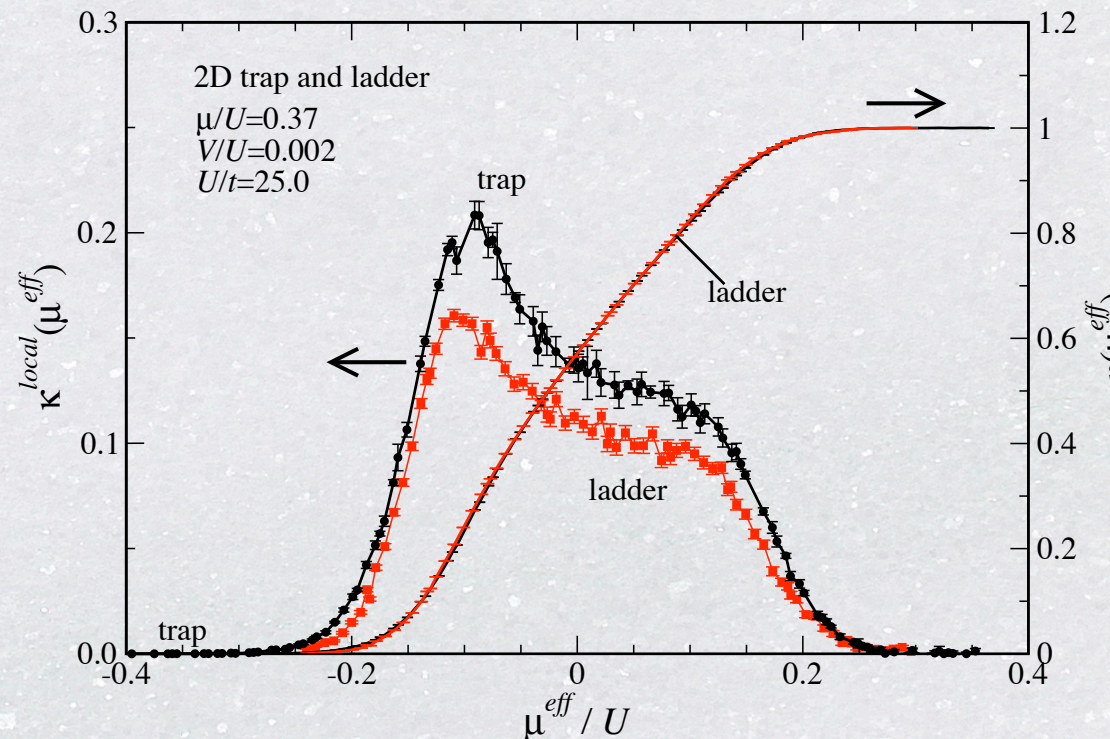
$$H = -t \sum_{i,j} \left(b_{i,j}^\dagger b_{i+1,j} + b_{i,j}^\dagger b_{i,j+1} + H.c. \right) + \frac{U}{2} \sum_{i,j} n_{i,j} (n_{i,j} - 1) - \sum_{j=1}^W \mu(j) \sum_{i=1}^L n_{i,j}$$



- in a linearized potential

$$\mu(\text{leg } i) = \mu_0 + i\Delta\mu$$

Quantitative agreement
with 2D trap



Thermodynamic limits

Usual thermodynamic limit in the trap

$$N_{\text{bosons}} \rightarrow \infty, \quad N_{\text{bosons}} \sqrt{V/t} = \text{const.}$$

- Changes curvature
- Recover critical behavior of d -dimensional system
- but not what describes experiments

What happens for a finite gradient?

- Is there a critical chain in the ladder?
- Increasing length of the ladder
 - No divergence
 - No sign of quantum criticality

Absence of quantum criticality due to

- Inhomogeneity
- Coupling to the rest of the system

