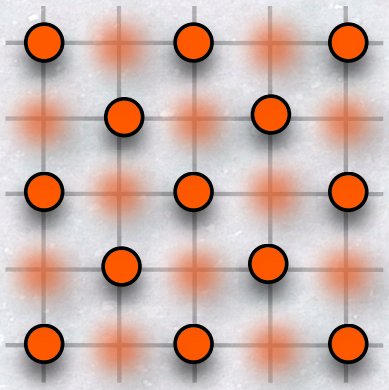
Computer simulations of strongly correlated quantum systems: past successes, current topics, and future challenges

Matthias Troyer (ETH Zürich)



with a guest appearance by
the elusive supersolid

Phases and phase transitions

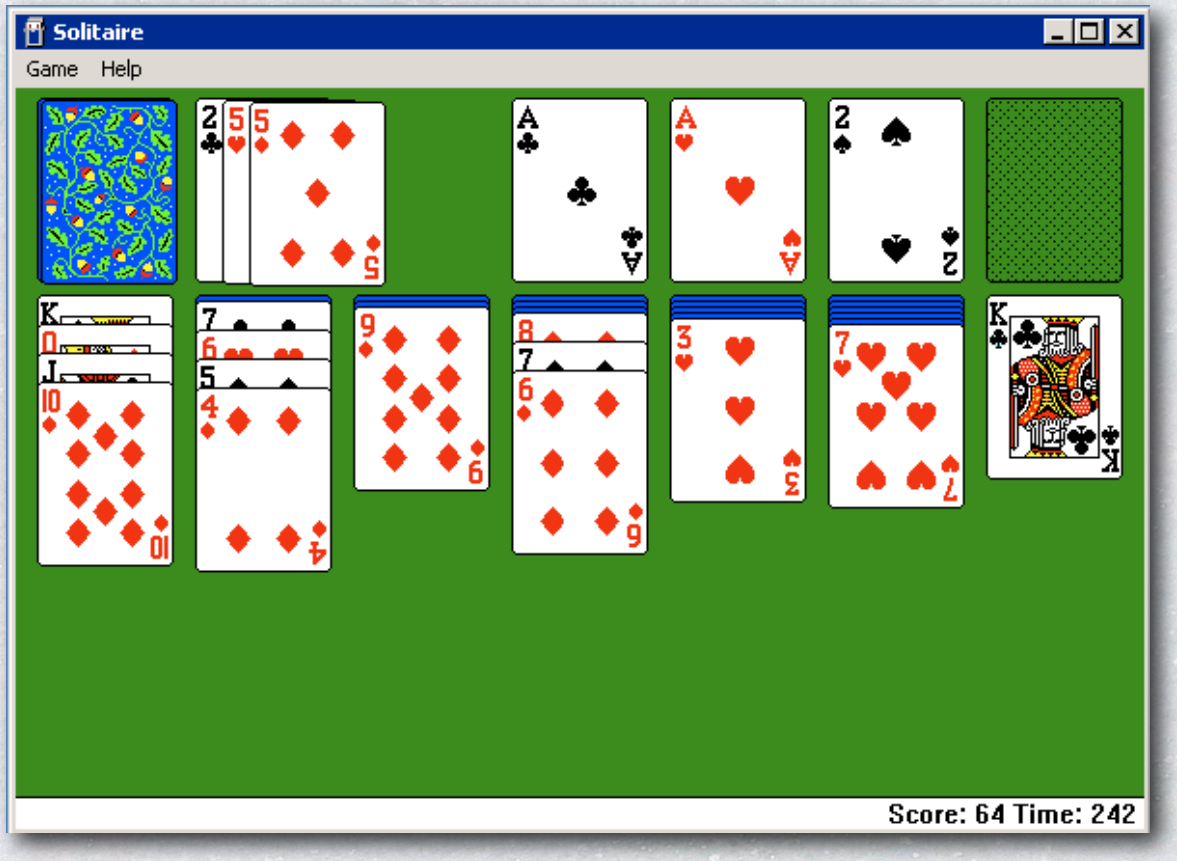
Numerical simulations

- "You let the computer solve the problem for you"

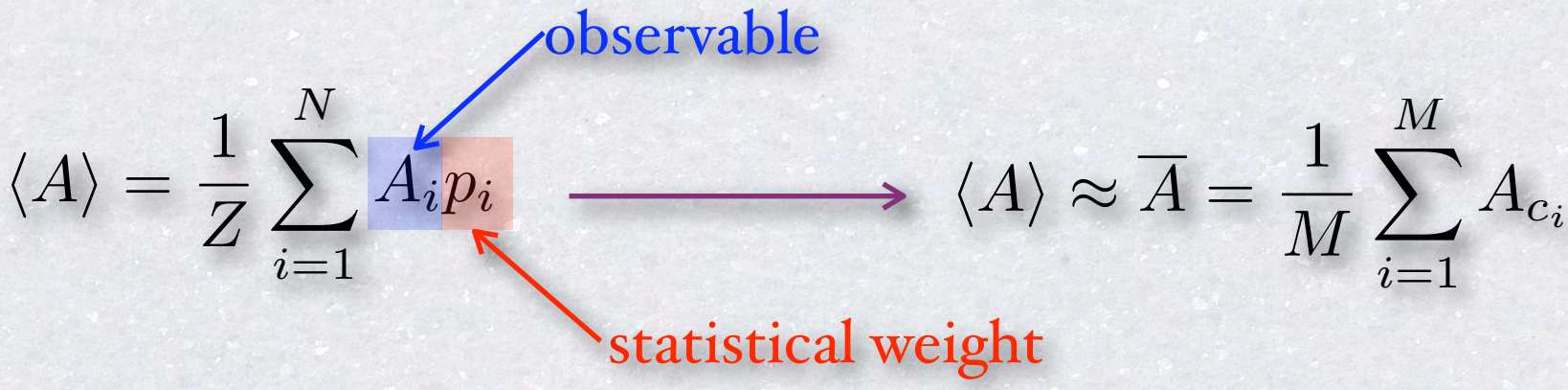
- It's not that easy:
  - Exponentially diverging number of states ✔
  - Critical slowing down of the dynamics at phase transitions ✔
  - negative sign problem for fermions (NP-hard) ✗

Ulam: the Monte Carlo Method

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



The Monte Carlo Method



- Need a representative sample with the correct distribution

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

- fundamental problem of statistical mechanics

GUEST EDITORS' INTRODUCTION

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

computing in SCIENCE & ENGINEERING

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

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.

The Metropolis Algorithm (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 weights

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

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)

Use Metropolis algorithm to update world lines

Autocorrelation effects

- The Metropolis algorithm creates a Markov chain of configurations

$$c_1 \to c_2 \to \ldots \to c_i \to c_{i+1} \to \ldots$$

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

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

- *Critical slowing down* at second order phase transition

$$\tau \propto L^2$$

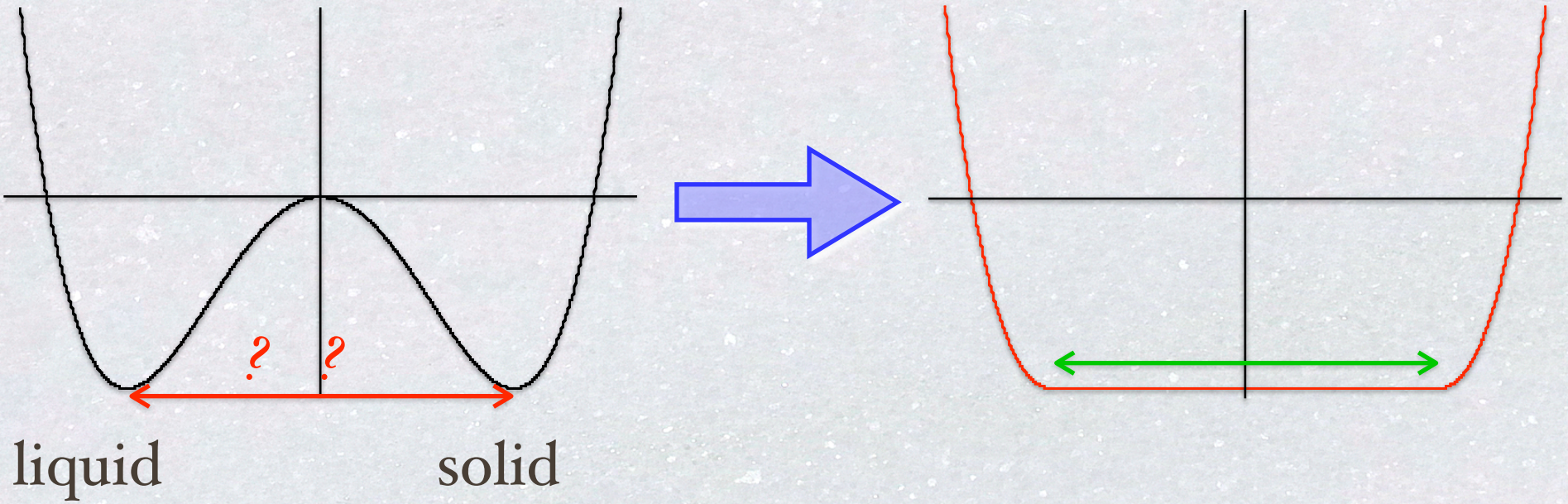
- *Exponential tunneling problem* at first order phase transition

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

Modern algorithms

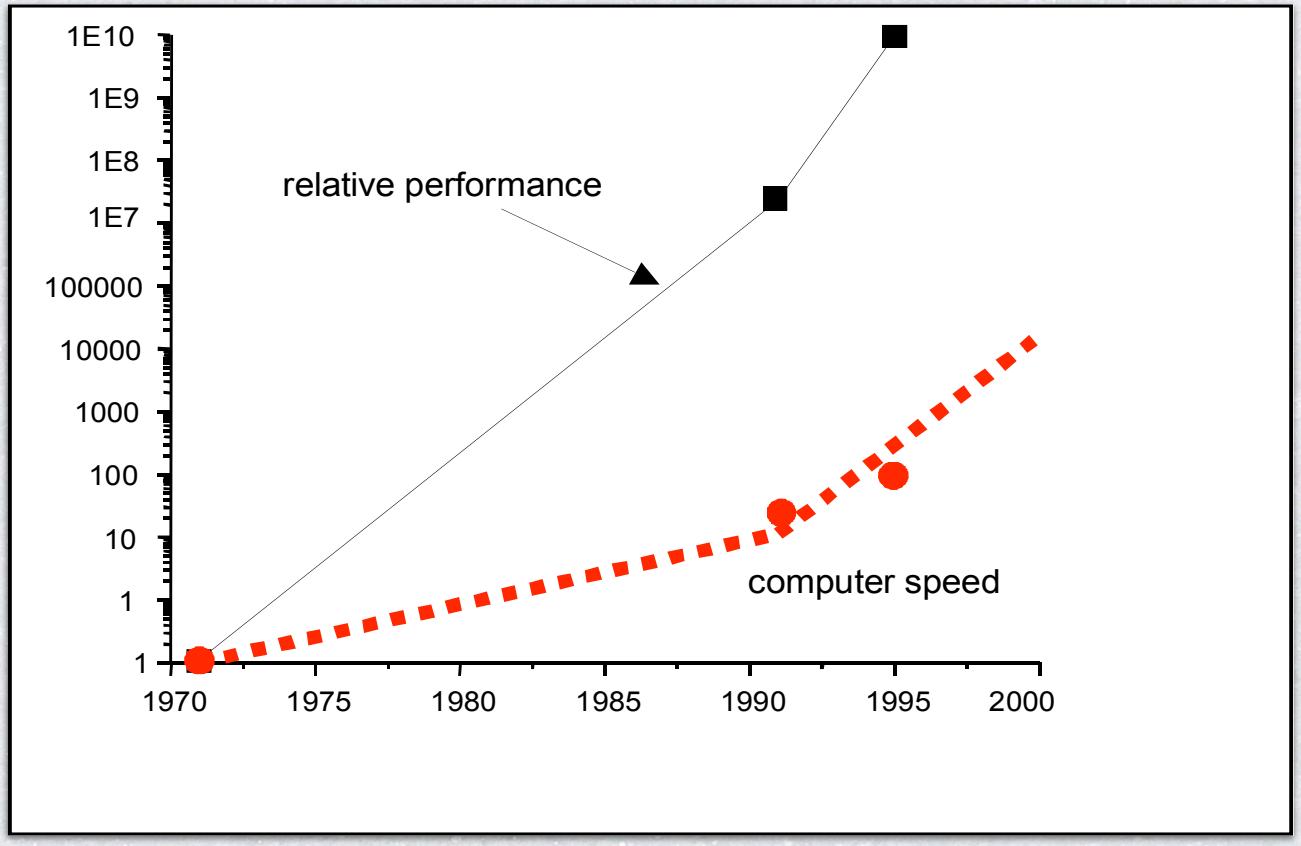
- Critical slowing down at a 2nd order phase transition is solved by *changing the dynamics*: make large global changes
  - Swendsen and Wang, 1987; Evertz *et al*, 1993; Prokof'ev *et al*, 1998 ...

- Tunneling problem at a first order phase transition is solved by *changing the ensemble* to create a flat energy landscape
  - Berg & Neuhaus, 1992; Wang & Landau, 2001; Troyer *et al*, 2003 , ...



Improvements in simulation methods

- 30 years of simulating the Ising model by D.P. Landau
- Today's algorithms on 30 year old computers faster than 30 year old algorithms on today's computers



Modern algorithms for quantum systems

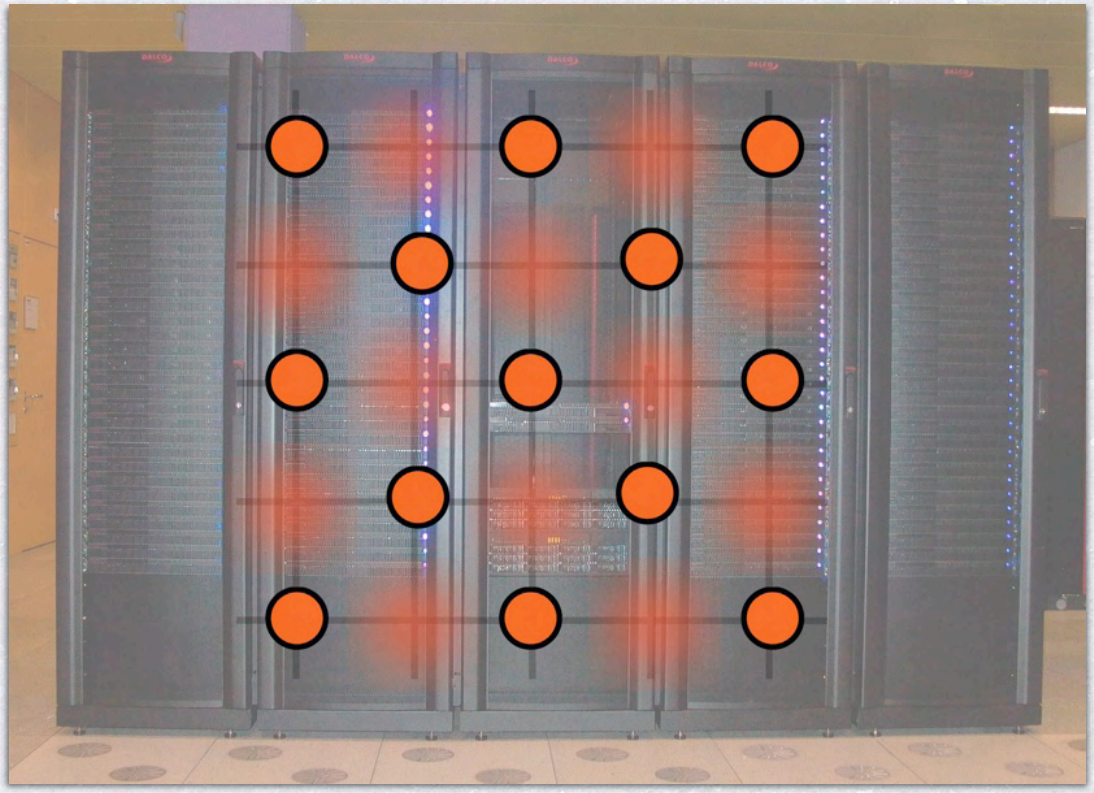
- Larger systems at lower temperature allow accurate simulation of phase transitions in quantum systems

Temperature	Metropolis	Modern algorithms
J	16'000 spins	16'000'000 spins
0.1 J	200 spins	1'000'000 spins
0.005 J	—	50'000 spins
0.1 t	32 lattice bosons	10'000 lattice bosons
50 mK	800 He atoms	8'000 He atoms

Experiments on the computer

- Modern QMC algorithms allow accurate simulation of quantum many body problems: experiments on models

- Example: the search for the supersolid



lattice supersolids

is solid Helium
a supersolid?

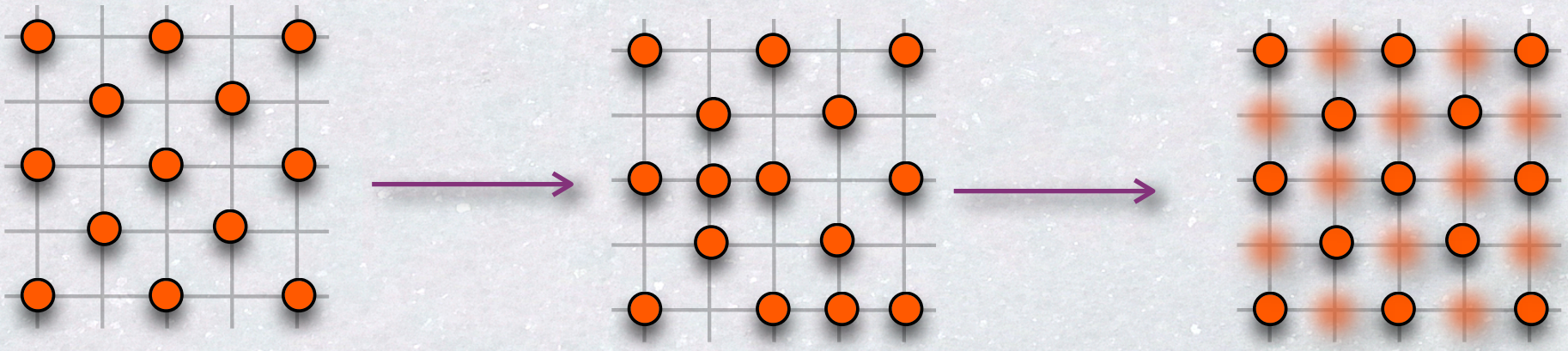
Supersolid

- A supersolid is simultaneously
  - superfluid: broken gauge symmetry
  - solid: broken translational symmetry
- First proposals nearly as old as I am
  - A. F. Andreev and I. M. Lifshitz, Sov. Phys. JETP **29**, 1107 (1969).
  - G. V. Chester, Phys. Rev. A **2**, 256 (1970).
- but not seen in Nature yet

Super solids in lattice boson models

- The simplest proposals are lattice models:
- Square lattice hardcore bosons with repulsion

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



solid (crystal)
caused by large V

doped solid:
interstitials

supersolid:
superfluid interstitials

First simulation results: it exists!

- Batrouni, Scalettar, Zimanyi, Kampf, PRL (1995)
  - evidence for supersolid at 3% doping
  - finite superfluid density and solid structure factor

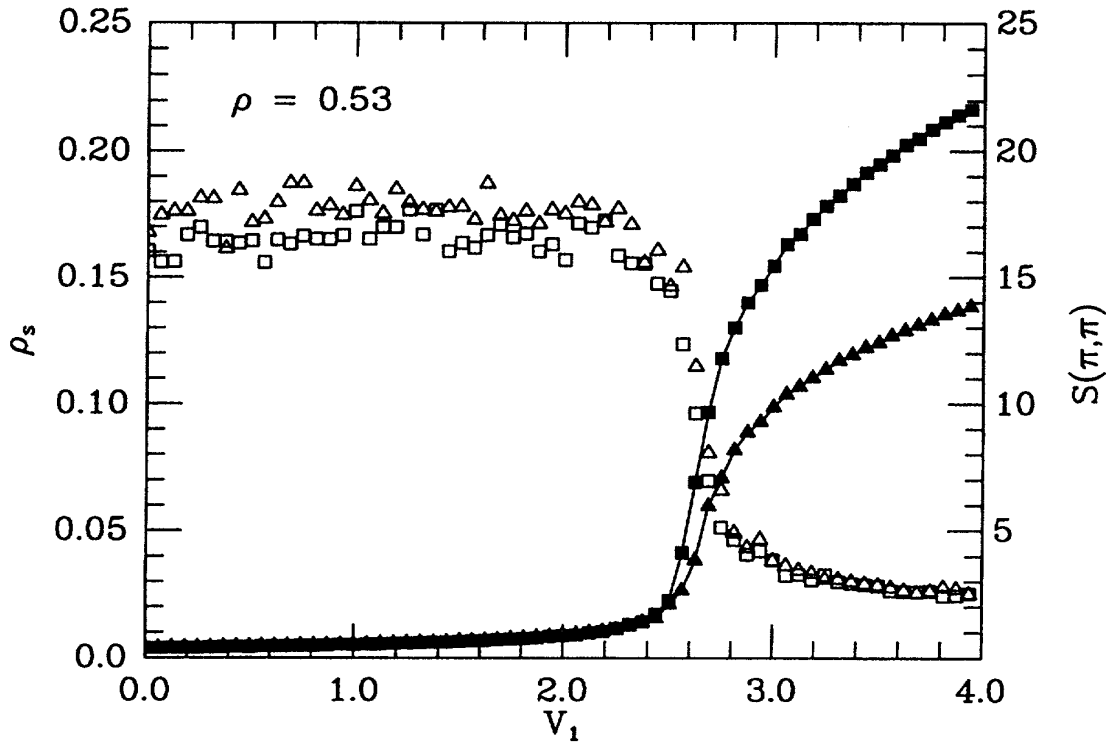
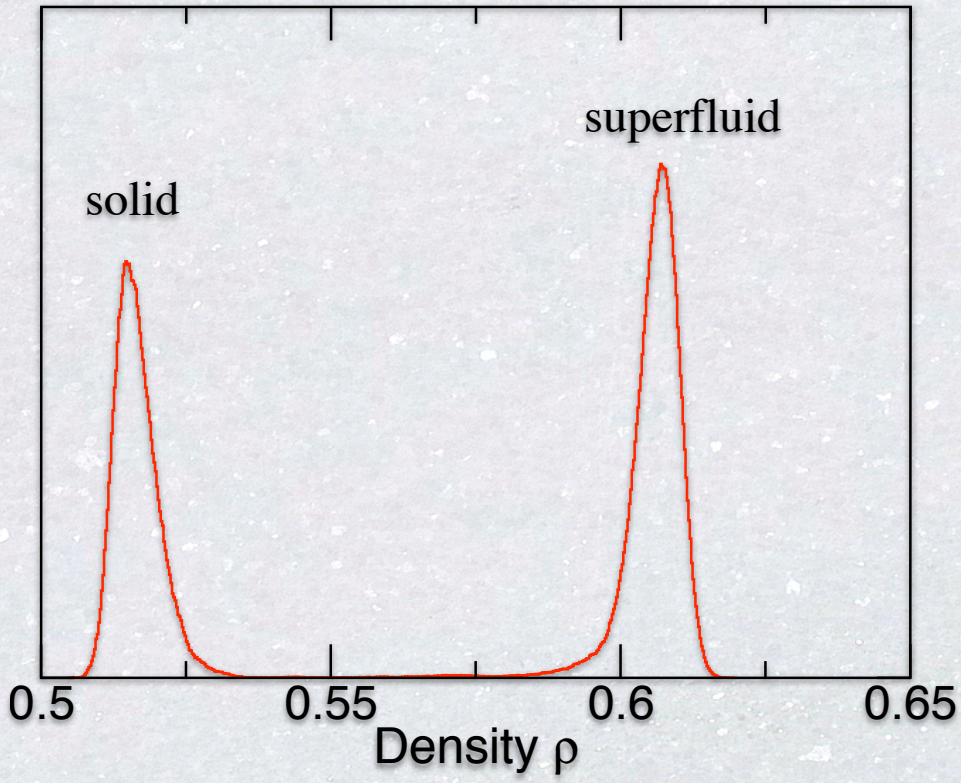
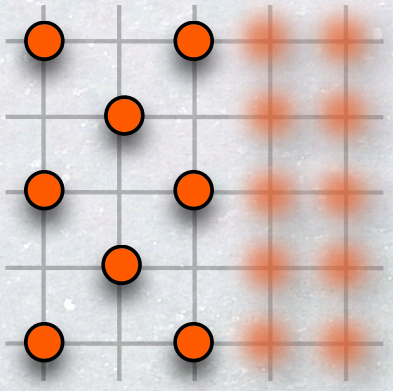


FIG. 2. ρ_s and $S(\pi, \pi)$ are shown at $V_0 = 7.0, V_2 = 0.0$.

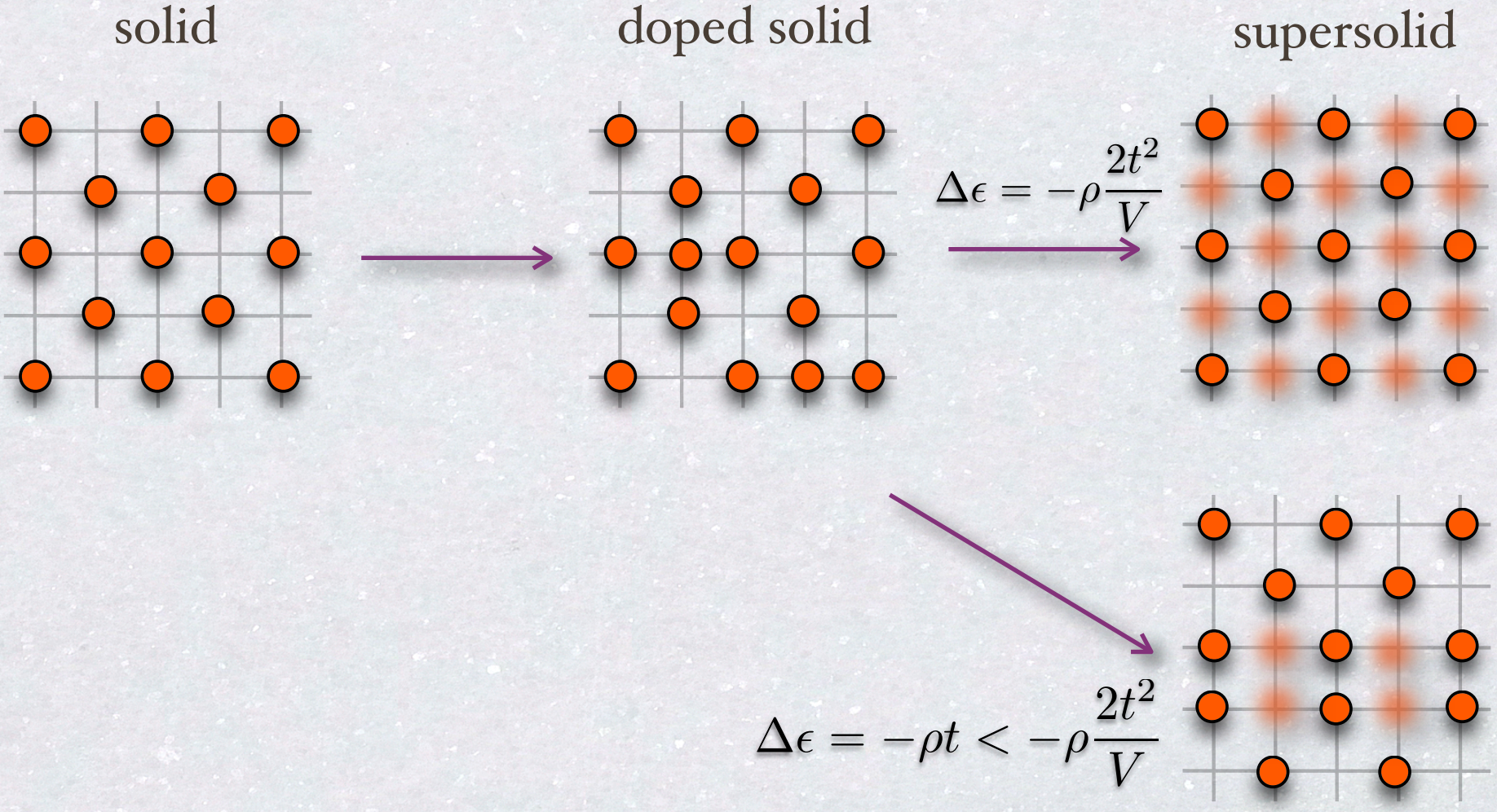
Do lattice supersolids exist?

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





Supersolids versus phase separation

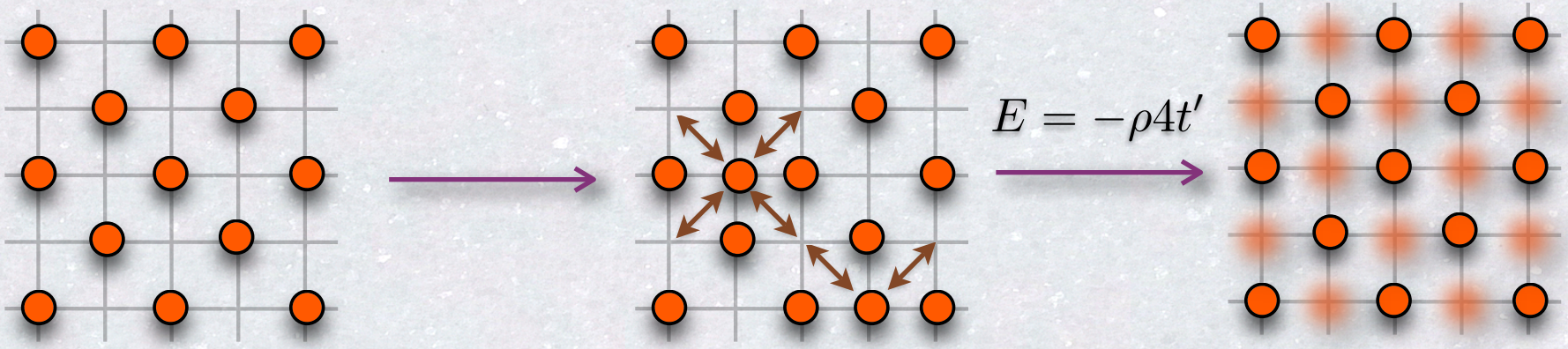


doped particles gain energy
by forming a domain wall

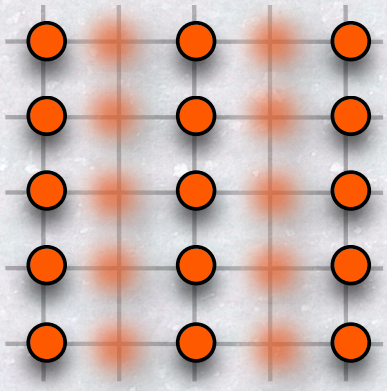
Stabilizing the supersolid

add next nearest neighbor hopping: $\tilde{H} = H - t' \sum_{\langle\langle i,j \rangle\rangle} (a_i^\dagger a_j + a_j^\dagger a_i)$

Sengupta *et al*, PRL 2005

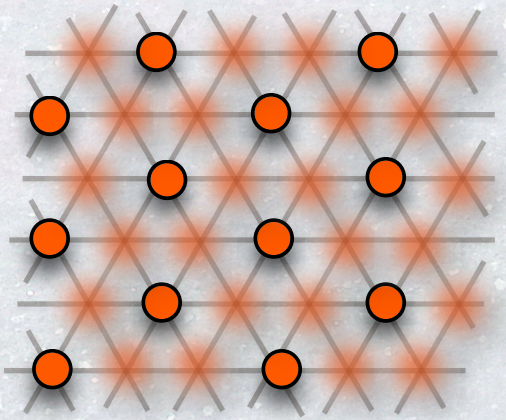


form a striped solid
by longer range repulsion



Batrouni *et al*, PRB 1995
Batrouni and Scalettar, PRL 2000
Hebert *et al*, PRB 2002
Schmid *et al*, PRL 2002
Schmid and Troyer, PRL 2004

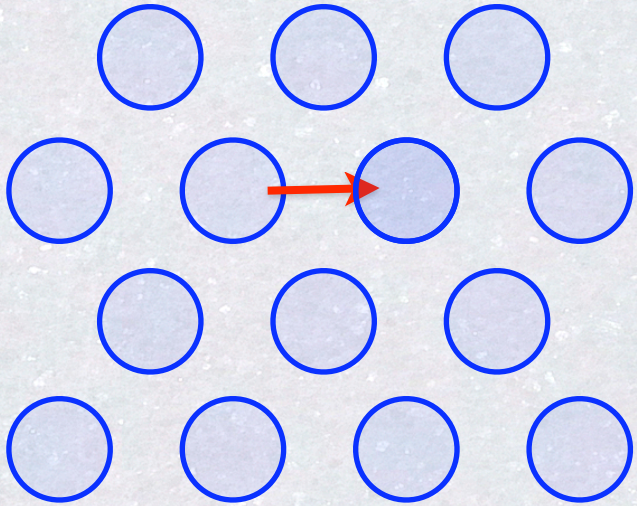
use a triangular lattice



Wessel and Troyer, PRL 2005
Melko *et al*, PRL 2005
Heidarian and Damle, PRL 2005
Boninsegni *et al*, PRL 2005

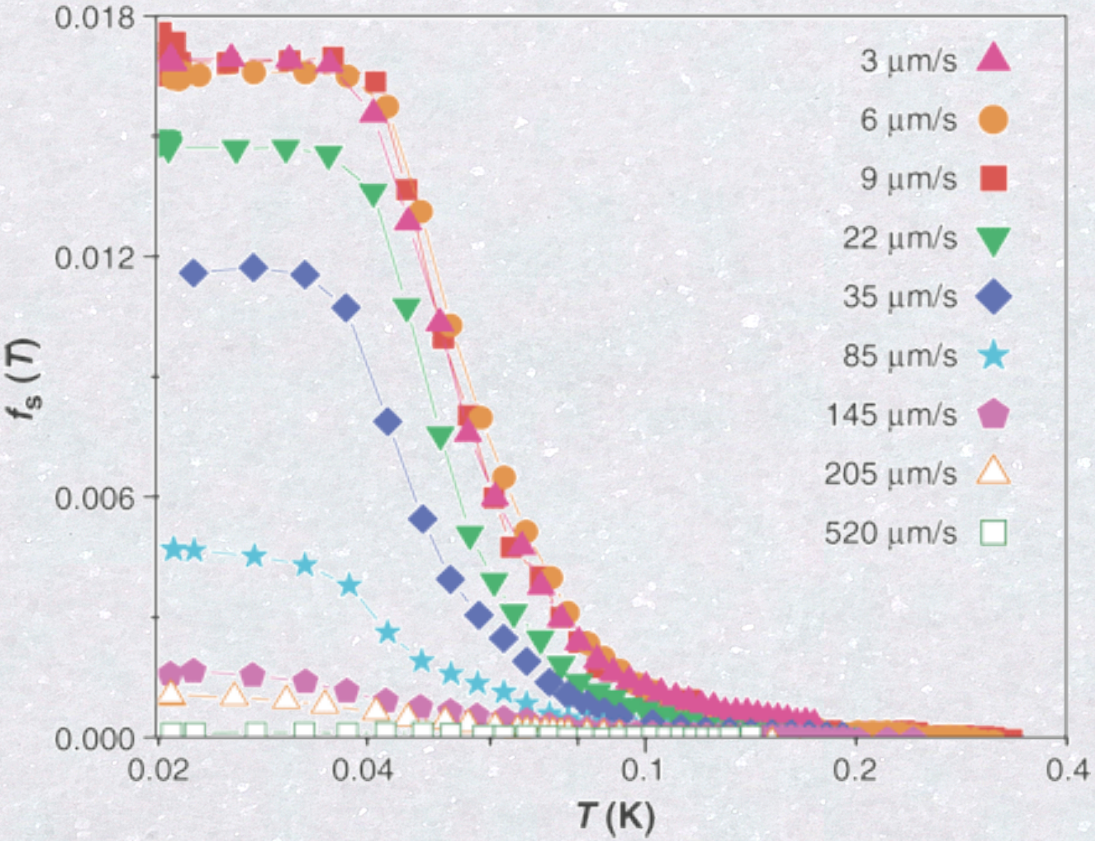
Continuum supersolids

- Supersolidity due to superflow of vacancies in solid
  - A. F. Andreev and I. M. Lifshitz, Sov. Phys. JETP 29, 1107 (1969).
  - G. V. Chester, Phys. Rev. A 2, 256 (1970).

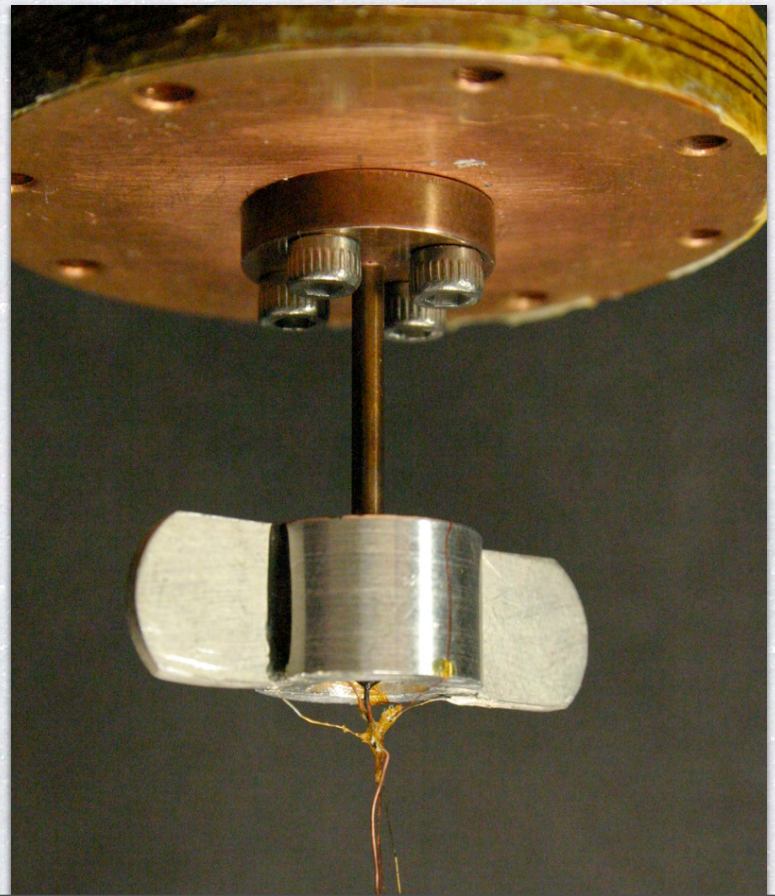


- A related scenario proposed recently by
  - X. Dai, M. Ma, F.-C. Zhang, Phys. Rev. B **72**, 132504 (2005)
  - P.W. Anderson, W.F. Brinkman and D.A. Huse, Science **310**, 1164 (2005).

Experiment by Kim and Chan



E. Kim and M.H.W. Chan
nonclassical moment of inertia
Nature, **427**, 225 (2004)
Science **305**, 1941 (2004)

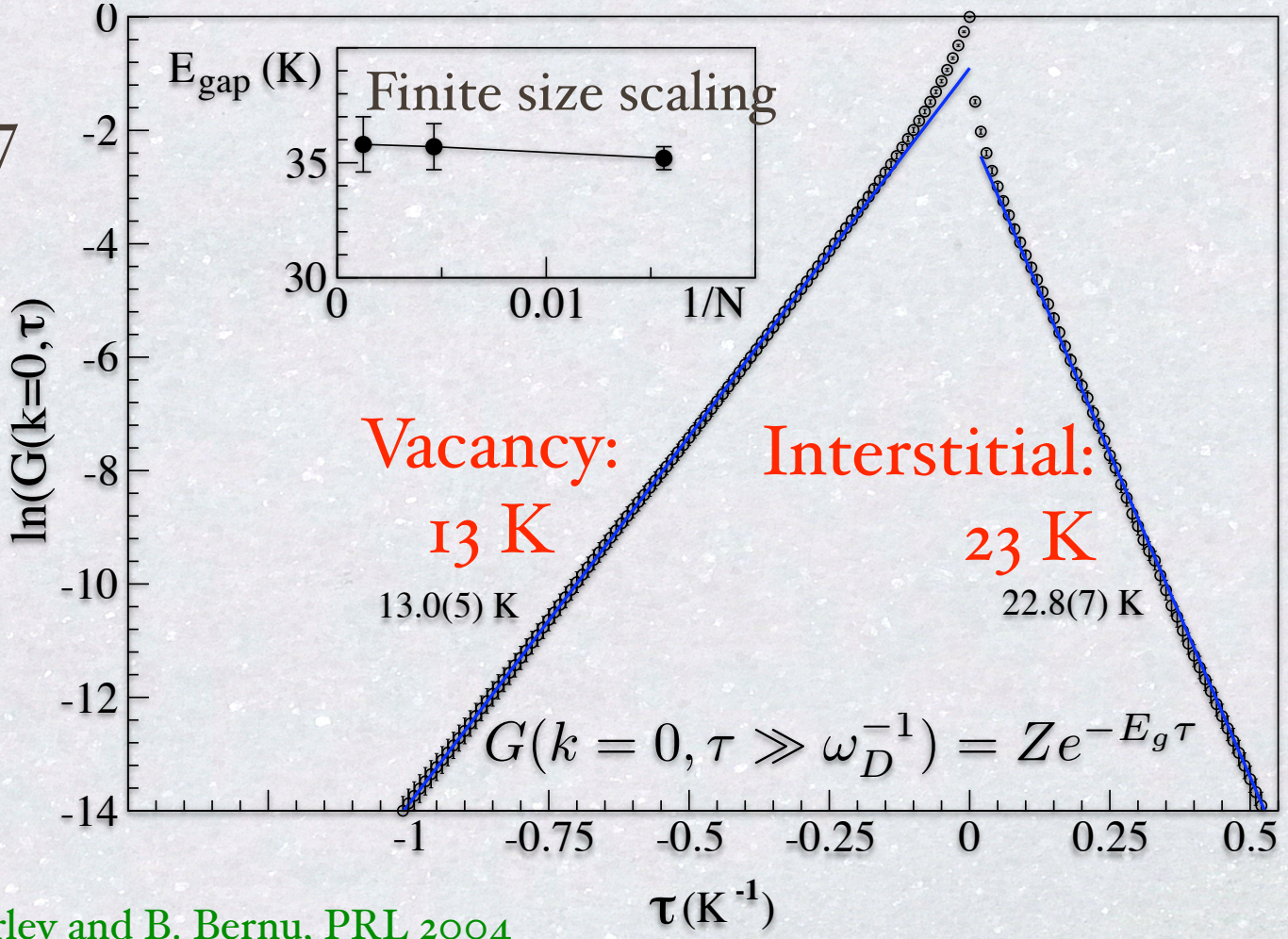


- Reproduced by
  - A. S. Rittner and J. D. Reppy, PRL (2006)
  - M. Kubota *et al.*, unpublished (2006)
  - K. Shirahama *et al.*, unpublished (2006).

Vacancies and interstitials are gapped

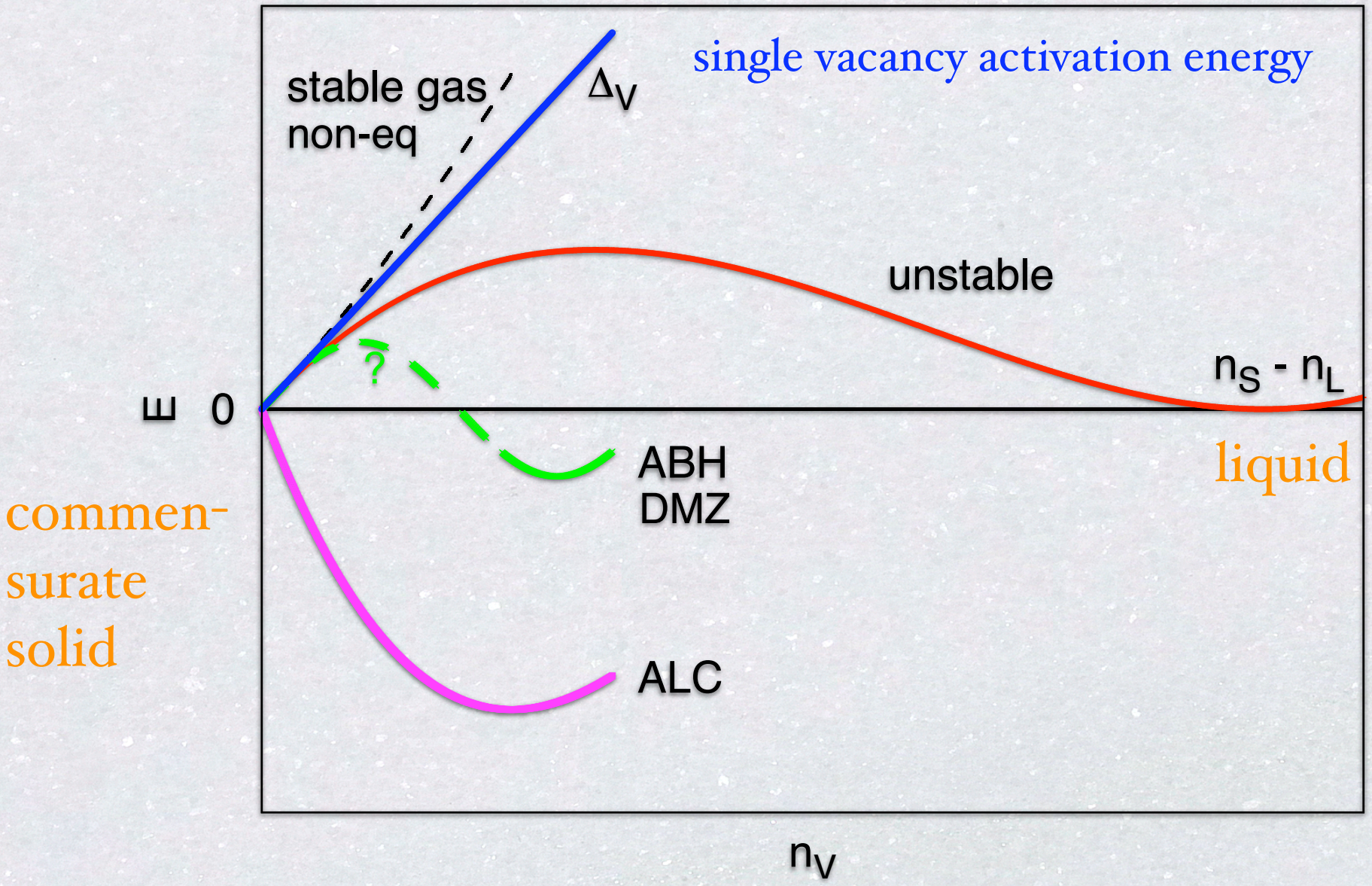
Energy obtained from decay of Green's function

n = 0.0287
T = 0.2 K



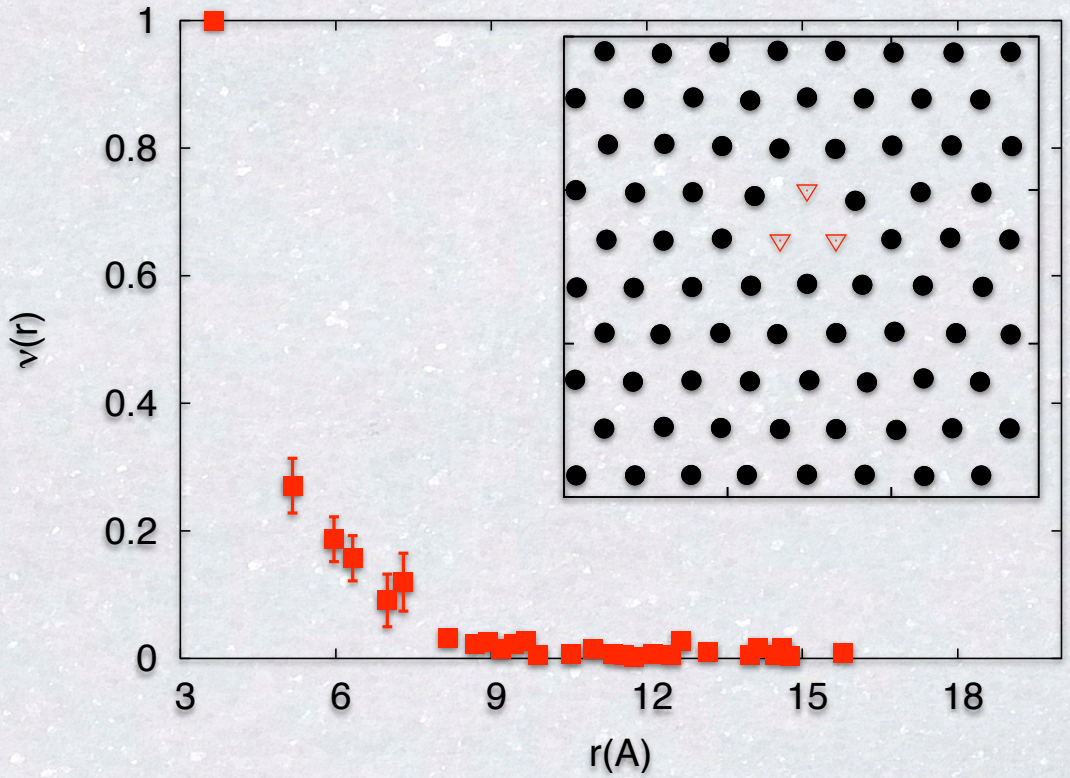
D. M. Ceperley and B. Bernu, PRL 2004
M. Boninsegni, N. V. Prokof'ev and B. V. Svistunov, PRL 2006
B. K. Clark and D. M. Ceperley, PRL 2006
M. Boninsegni, A. Kuklov, L. Pollet, N.V. Prokof'ev, B.V. Svistunov, M. Troyer, PRL 2006

Theories : overview



Phase separation of vacancies

- Strong attraction between vacancies
- Vacancies phase separate: solid Helium is not supersolid



Quantum: M. Boninsegni, A. Kuklov, L. Pollet, N.V. Prokof'ev, B.V. Svistunov, M. Troyer, PRL 2006
Classical: Tama Ma (HKU), L. Pollet and M. Troyer, in preparation

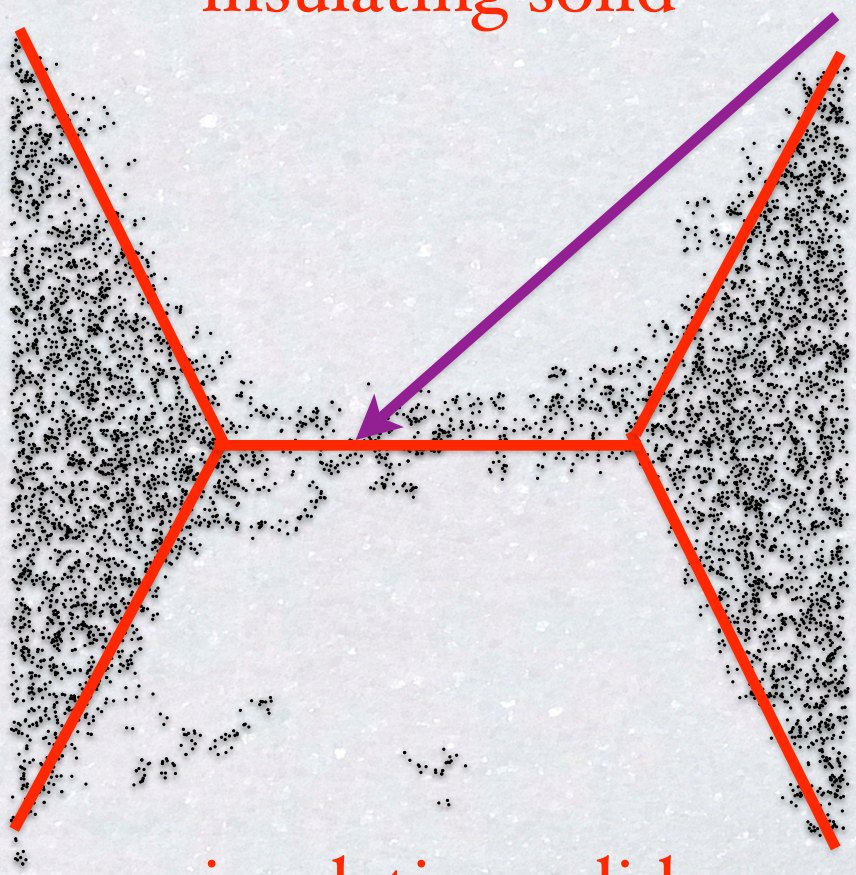
Instability of the supersolid

- Theory of supersolid is based on dilute gas of bosonic vacancies
  - stability of a Bose-Einstein condensate requires repulsive interactions
  - unstable in Helium due to attractive interaction between vacancies

- Future challenges:
  - what is “wrong” with the Helium potential?
  - which potential could give a supersolid?
  - what is seen in the Kim & Chan experiment?
  - maybe due to superflid grain boundaries? (simulation and experiment)

Simulation of grain boundary

- Points on exchange cycles indicate superfluid regions



Future challenges for simulations

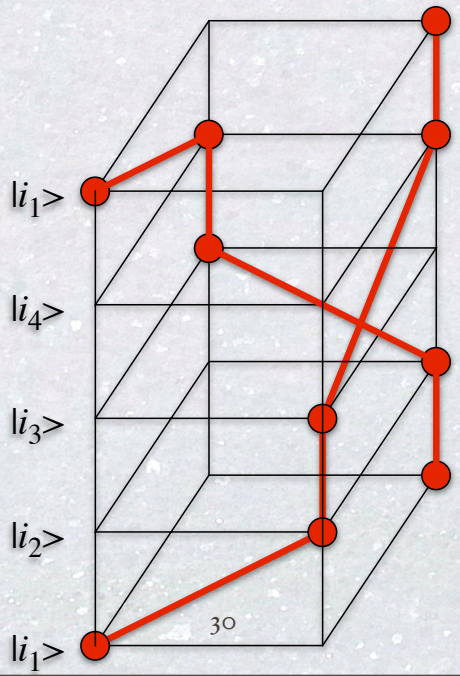
- Dynamics of quantum systems
  - Monte Carlo simulations perfect for static equilibrium properties
  - Dynamic properties and non-equilibrium effects are hard to obtain
- Entropy-driven phase transitions
  - It is hard to form a single crystal from a liquid in experiment
  - Even harder to form a single crystal from a liquid in simulations
- Fermionic simulations
  - The infamous negative sign problem prevents accurate simulations of fermions

The negative sign problem

- In mapping of quantum to classical system

$$Z = \mathrm{Tr} e^{-\beta H} = \sum_i p_i$$

- there is a "sign problem" if some of the $p_i < 0$
  - Appears e.g. in simulation of fermions when two fermions exchange places, since the sign of the wave function changes (Pauli principle)



The negative sign problem

- Sample with respect to absolute values of the weights

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

- Exponentially growing cancellation in the sign

$$\langle sign\rangle = \frac{\sum_i p_i}{\sum_i |p_i|} = Z/Z_{|p|} = e^{-\beta V(f-f_{|p|})}$$

- Exponential growth of errors

$$\frac{\Delta sign}{\langle sign\rangle} = \frac{\sqrt{\langle sign^2\rangle - \langle sign\rangle^2}}{\sqrt{M}\langle sign\rangle} \approx \frac{e^{\beta V(f-f_{|p|})}}{\sqrt{M}}$$

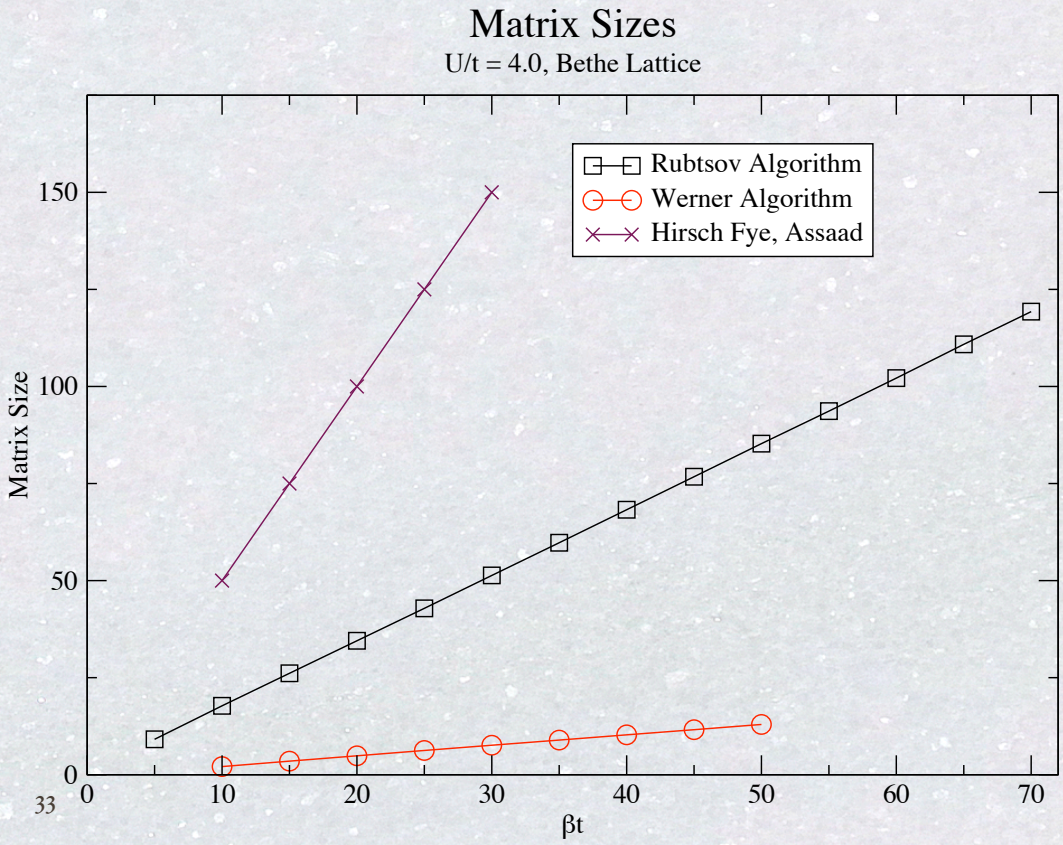
- NP-hard problem (no general solution) [Troyer and Wiese, PRL 2005]

How to overcome the sign problem

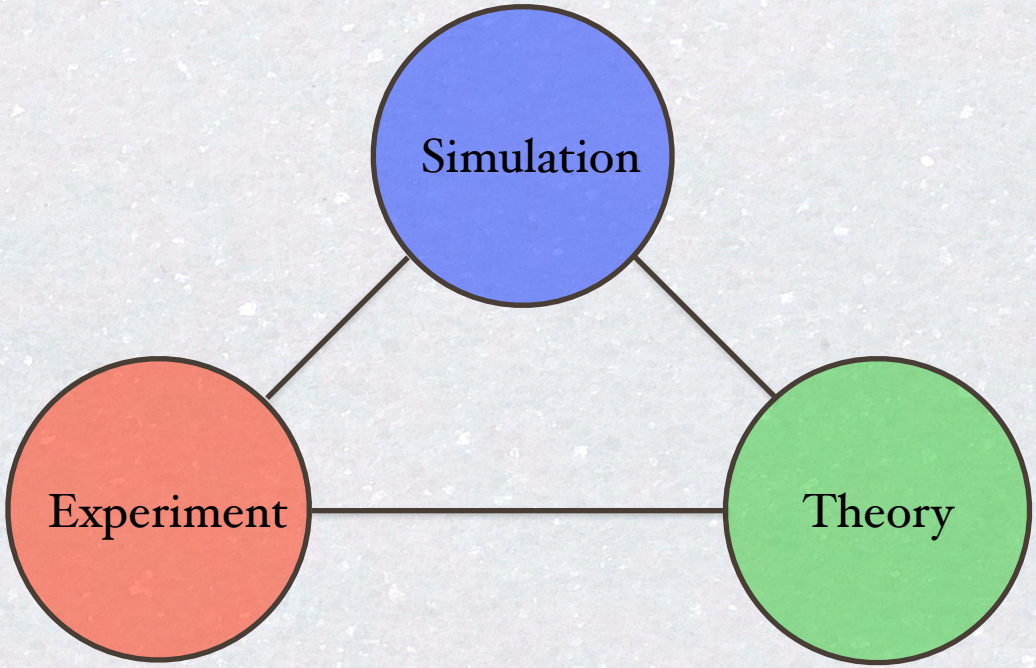
- Full solution is impossible
- Exact solution in one dimension and small clusters
  - exact diagonalization of up to about 30-40 sites
  - density matrix renormalization group method on 1000 sites in 1D
- Approximate solutions in higher dimensions
  - Dynamical mean field theory embeds a small cluster in a self-consistent bath: can model the Mott-transition well
  - Variational Monte Carlo methods, such as fixed-node approximation, can work well but it is hard to unambiguously establish the existence of new exotic phases
- Improved algorithms and new ideas are needed

Example: new DMFT solvers

- Substantial progress is still possible
  - Standard method: Hirsch & Fye, PRL '86
  - New weak coupling expansion: Rubtsov *et al*, PRB '05
  - New hybridizaton expansion: Werner *et al*, PRL '06
- New methods allow
  - 100 x lower temperatures
  - accurate investigation of Mott transition
  - and more to come ...



Computational Physics



Computational Physics has become an important branch of physics, complementary to experiment and theory

Perform "experiments on a model"

Summary

- Modern algorithms allow accurate simulations of phase diagrams and phase transitions of many quantum models
- But substantial challenges remain
  - dynamics
  - entropy-driven phase transitions
  - fermionic simulations
- Example: the search for a supersolid
  - lattice supersolids can be realized using ultracold polar molecules in triangular optical lattices
  - Helium-4 is according to our simulations not a supersolid: defects play an important role in experiments

Thanks to my collaborators

ETHZ
Emanuel Gull
Lode Pollet
Helmut Katzgraber

Universität Stuttgart
Stefan Wessel

Universität Graz
Hans Gerd Evertz

Université de Toulouse
Fabien Alet

Université de Nice
G. George Batrouni
Frederic Hébert

UMass Amherst
Nikolay Prokof'ev
Boris Svistunov

Princeton
David Huse

Columbia University
Philipp Werner
Andy Millis

UC Riverside
Pinaki Sengupta
Leonid Pryadko

Microsoft Station Q
Simon Trebst

ISSP Tokyo
Hirokazu Tsunetsugu
Naoki Kawashima

Kyoto University
Kenji Harada

Hong Kong University
Tama Ma