Accurate simulation of (strongly interacting) quantum systems

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S. Trebst (Microsoft)
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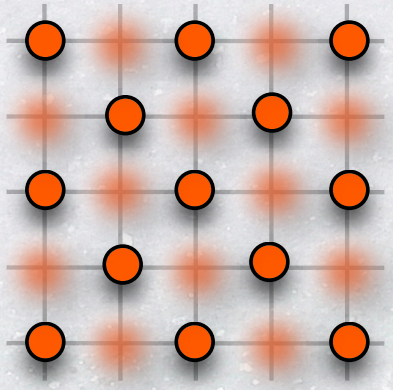
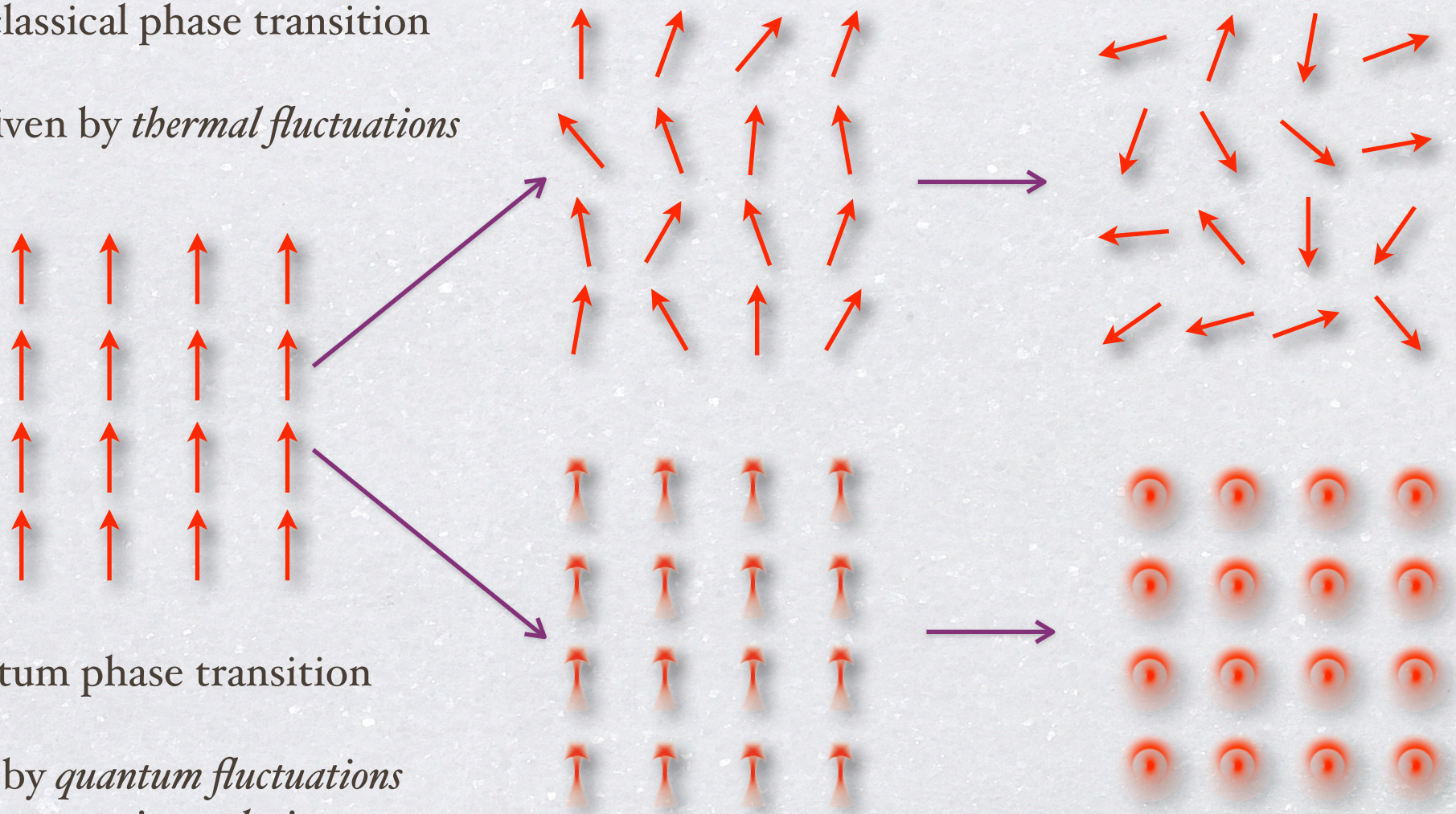


Classical and quantum phase transitions

classical phase transition

driven by *thermal fluctuations*



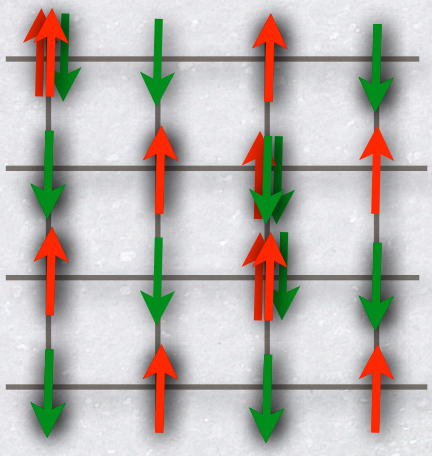
quantum phase transition

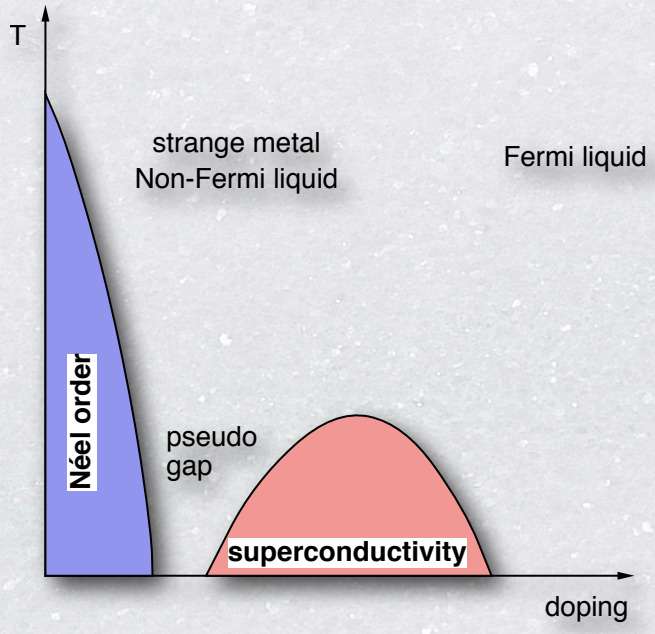
driven by *quantum fluctuations* and *uncertainty relation*

increasing fluctuations

New phases near quantum phase transitions

- Unexpected new physics can happen in strong fluctuation regime near quantum phase transition
  - Doping fermionic Mott-insulator gives high-Tc superconductor
    - Half band filling should be metallic
    - But strong Coulomb repulsion forms a Mott-insulator
    - Doping the Mott insulator gives novel little-understood phases

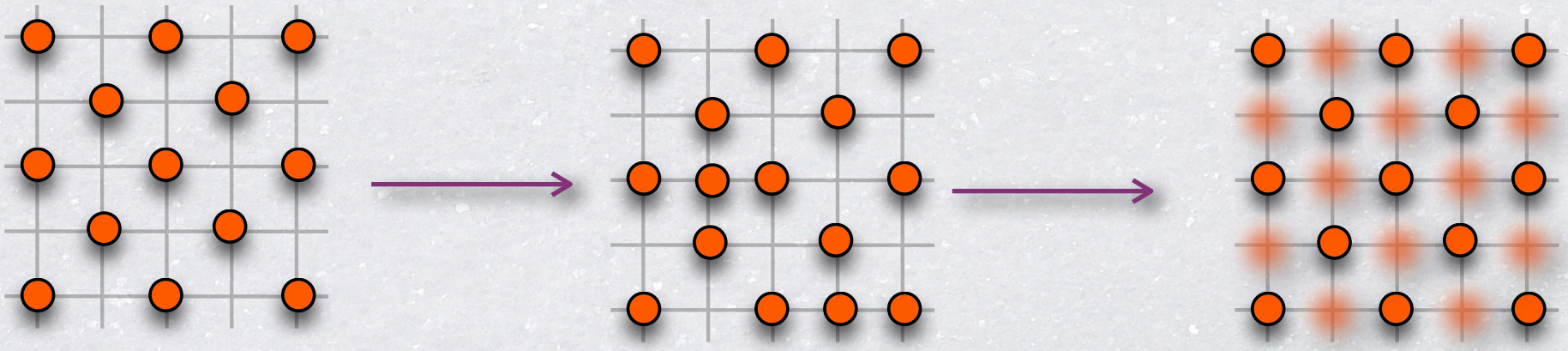




Supersolids in lattice boson models

- A supersolid shows simultaneously superfluidity and solid order
  - proposed in 1969, not observed yet
- Simplest proposal: 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

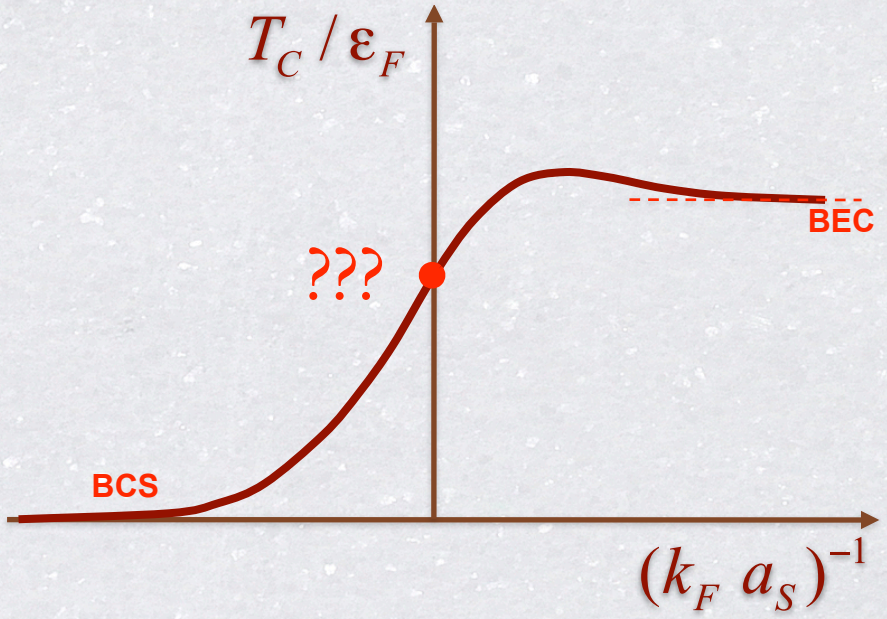
doped solid:
interstitials

supersolid ????
is it stable ???

Critical temperature of the resonant Fermi gas

Phase diagram of dilute Fermi gas

BCS superfluid of Cooper pairs



Bose condensate of strongly bound pairs

Universal behavior at resonance (unitary point)

Previous results for the unitary point

Solving quantum many body problem

- Mean-field approximations
  - work well deep inside ordered phases
  - but fail when fluctuations are strong, close to phase transitions
- Weak-coupling approximations
  - work perfectly in weakly interacting systems
  - but fail when interactions become strong
- Variational methods
  - work well if a good approximation for the true wave function is known
  - but can be very wrong if we guess incorrectly
  - will fail to find novel unexpected phases
- We need unbiased accurate numerical methods

Exact Diagonalization

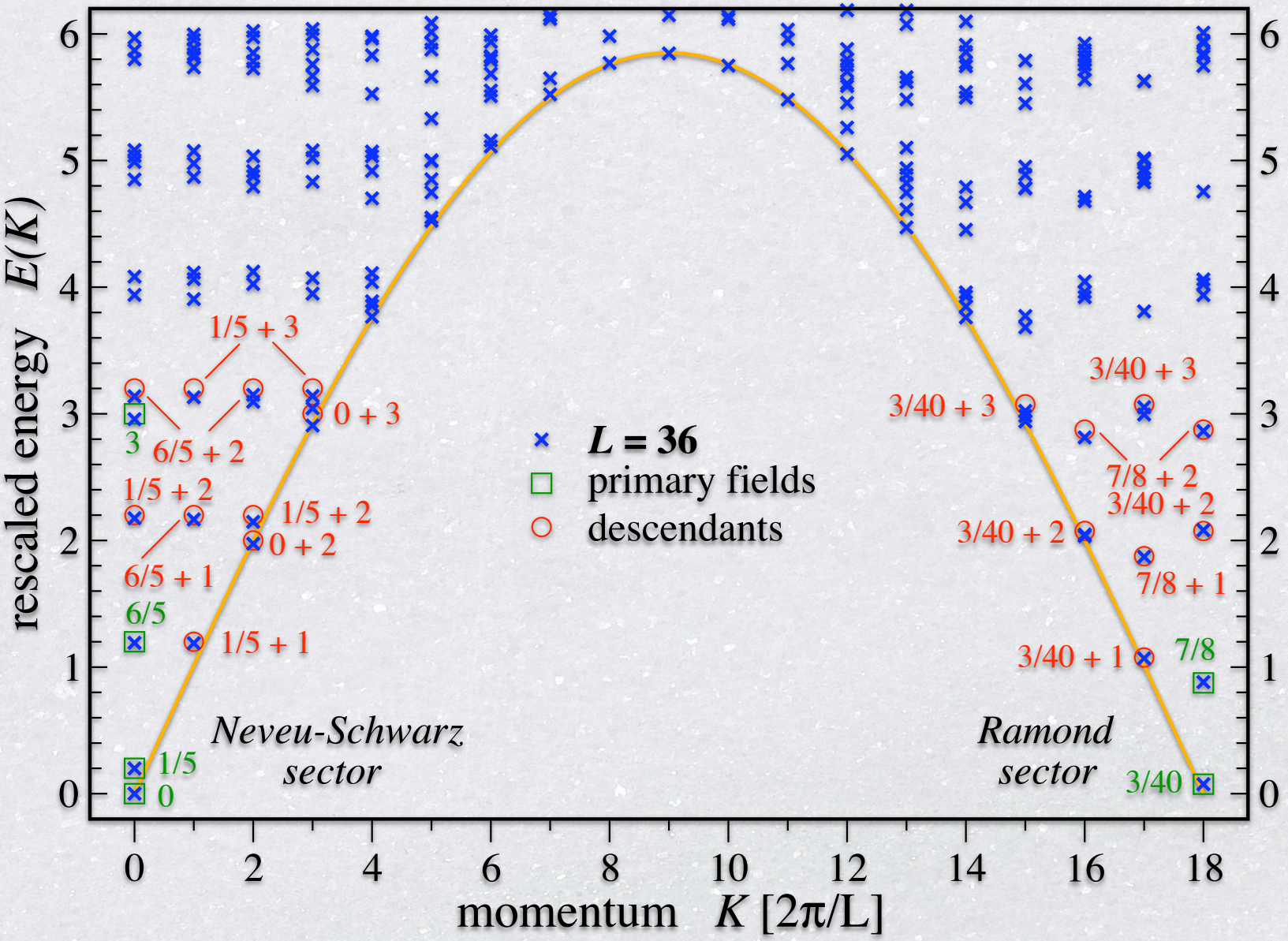
- Construct a basis for the Hilbert space of N-site lattice
  - 2^N states for spin-1/2 model, 4^N states for fermionic Hubbard
  - possible to store up to 10^9 states

- Construct matrix representation of the Hamiltonian
  - using all possible symmetries to reduce the size

- Obtain low-lying eigenvalues and eigenvectors numerically
  - High accuracy, (15 digits)
  - Static and dynamic properties
  - but restricted to small systems of about 20 - 40 sites

Example: spectrum of 1-d anyonic chain

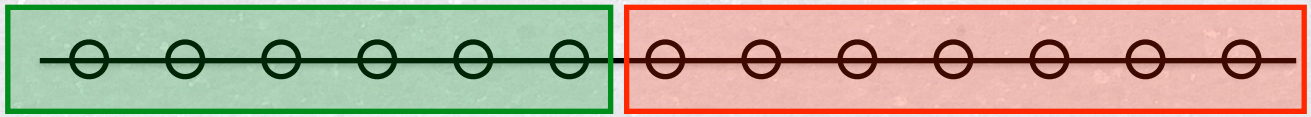
Feiguin, Trebst, Ludwig, Troyer, Kitaev, Wang and Freedman, PRL (2007)



DMRG (Density Matrix Renormalization Group)

S.R. White, PRL 1992

- DMRG cleverly reduces the Hilbert space dimension
- Split the lattice into "system" and "environment"



- Then truncate the Schmid decomposition to m≈ 1000 states

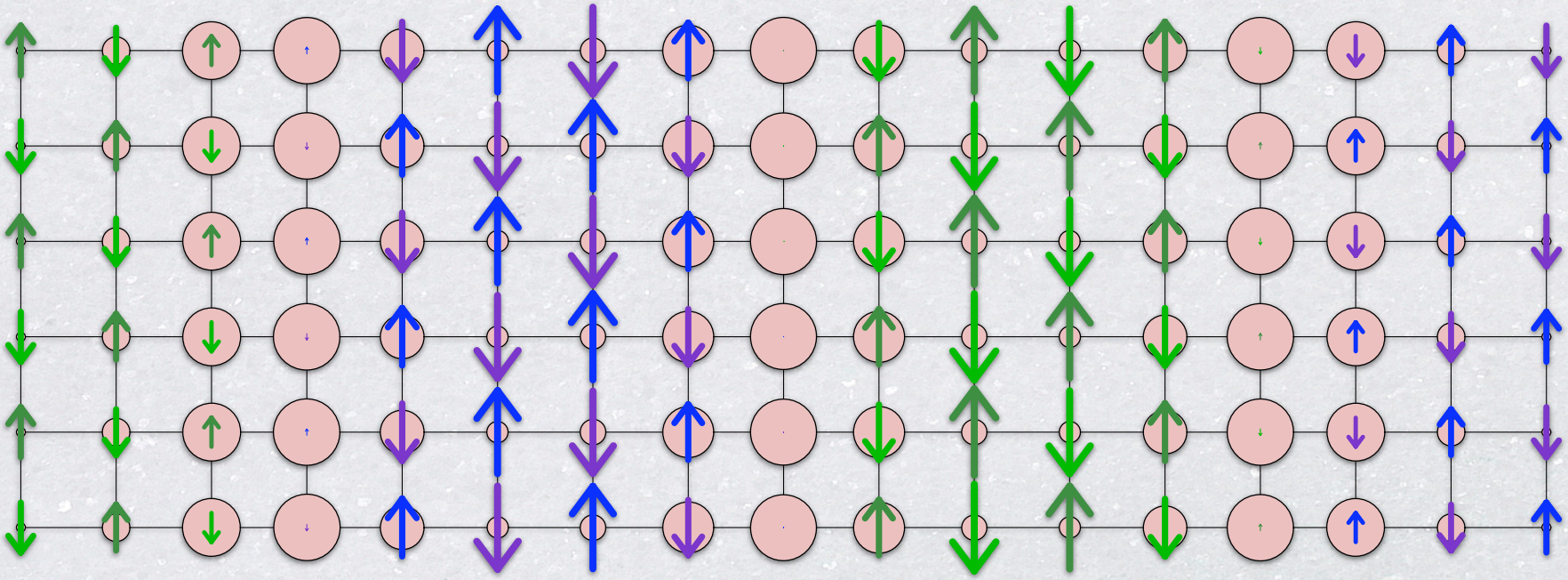
$$|\psi\rangle = \sum_{i=1}^{\dim S} \sum_{i=1}^{\dim E} c_{ij} |i\rangle_S \times |j\rangle_E$$

$$= \sum_{i=1}^{\min(\dim S, \dim E)} \alpha_i |i\rangle_S \times |i\rangle_E \approx \sum_{i=1}^{m} \alpha_i |i\rangle_S \times |i\rangle_E$$

- Works efficiently in quasi-one dimensional systems
  - about 3 - 10 digits accuracy on systems up to 2 x 1000 or 8 x 40

DMRG example: stripe formation

- Stripe (charge density wave) formation in 6-chain fermionic Hubbard ladder
  - S.R. White and D.J. Scalapino (2003)



New developments in DMRG

- Time evolution in non-equilibrium quantum systems
  - G. Vidal, PRL (2003)
  - A. Daley *et al*, JSTAT (2004), S. White and A. Feiguin, PRL (2004)

- Extensions to two dimensions
  - Pairwise entangled product states (PEPS)
  - F. Verstraete and I. Cirac (2004)
  - See talk by G. Vidal later in this session
  - It is still unclear whether the PEPS variational wave function will be as successful in 2D as the DMRG is in 1D

Series expansion methods

- Use the computer to calculate a high (10 - 20) order symbolic series expansion
  - high-temperature series in β=1/T $$f = \sum_n g(n)\beta^n/n!$$
  - or perturbation series in a small coupling constant λ

$$H = H_0 + \lambda V \qquad A(\lambda) = \sum_n c_A(n)\lambda^n/n!$$

  - pioneered by R.R. Singh *et al.* (UC Davis) and J. Oitmaa *et al* (UNSW)
- Works for
  - any lattice model, in any dimension on infinite systems
  - but only high to intermediate temperature or weak to intermediate coupling

The Monte Carlo Method

- Overcome exponential growth of the Hilbert space by stochastic sampling

observable

$$\langle A \rangle = \frac{1}{Z} \sum_{i=1}^{N} A_i p_i \longrightarrow \langle A \rangle \approx \overline{A} = \frac{1}{M} \sum_{i=1}^{M} A_{c_i}$$

statistical weight

- Evaluate phase space average from a representative sample with correct weights

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

- The statistical error is independent of the system size

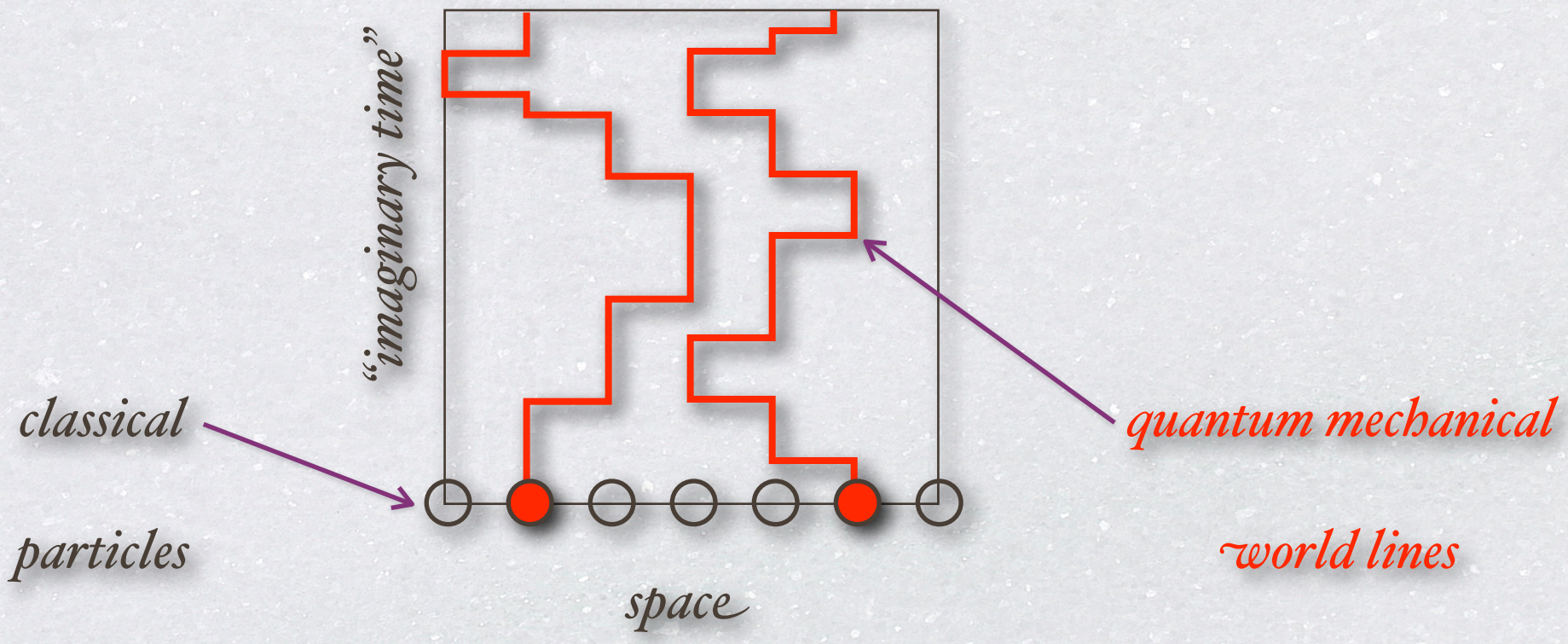
$$\Delta A = \sqrt{\frac{\mathrm{Var}\, A}{M}}$$

Quantum Monte Carlo

- To simulate a quantum system we first need to map it to a classical system

$$\langle A \rangle = \frac{\mathrm{Tr}\, A \exp(-\beta H)}{\mathrm{Tr} \exp(-\beta H)} \longrightarrow \frac{1}{Z} \sum_i A_i p_i \approx \frac{1}{M} \sum_{i=1}^{M} A_{c_i}$$

- Usually done by path integrals or similar diagrammatic expansions



First challenge for QMC: autocorrelations

- A Markov chain is used to get representative sample of configurations

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

- Successive configurations are correlated!

- The development of efficient non-local update schemes with fast decorrelation is an ongoing challenge
  - Cluster updates for quantum magnets (Evertz *et al*, 1993)
  - Worm updates for bosonic systems (Prokof'ev *et al*, 1997)
  - Extended ensembles at first order transitions (Troyer *et al*, 2003)

Modern 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

- Open source codes available at http://alps.comp-phys.org/

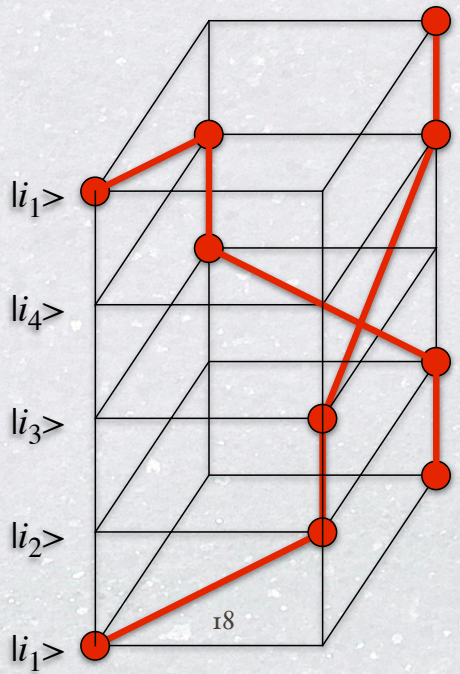
ALPS

Second challenge: the 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

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

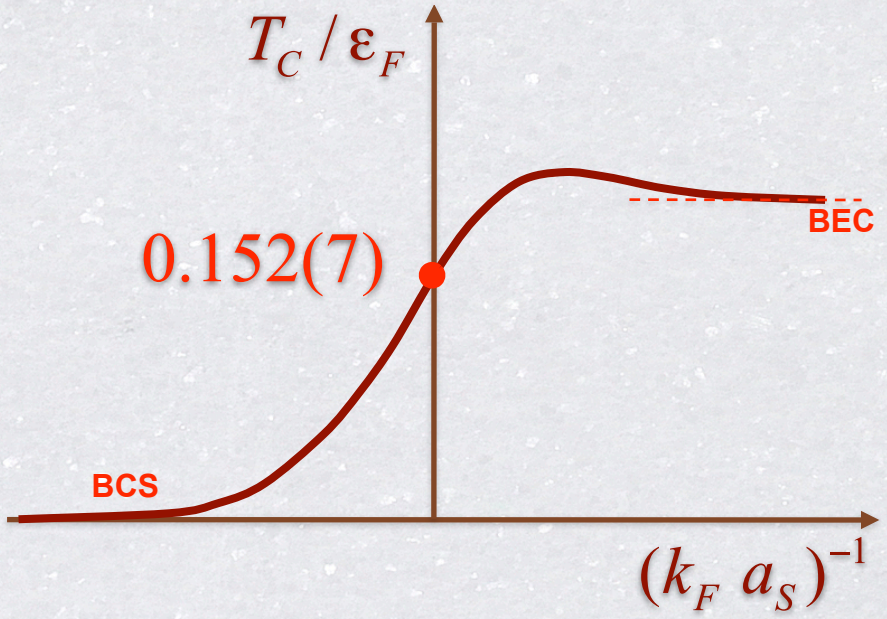
- NP-hard problem (no general solution) [Troyer and Wiese, PRL 2005]

Critical temperature of the resonant Fermi gas

Burovski, Kozik, Prokof'ev, Svistunov, Troyer
PRL (2006), NJP (2006), unpublished(2007)

Phase diagram of dilute Fermi gas

BCS superfluid of Cooper pairs

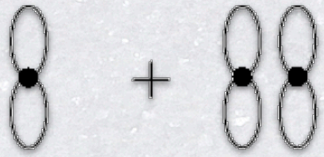


Bose condensate of strongly bound pairs

Universal behavior at resonance
(unitary point)

Diagrammatic QMC

- Sign-problem free diagrammatic QMC method is possible for
  - attractively interacting fermions
  - with balanced population

$Z = 1 +$  $+$

$-$  $-$  $+$  $+ \cdots$

Sign problem!!!

$= 1 +$  $+$  $+ \cdots$

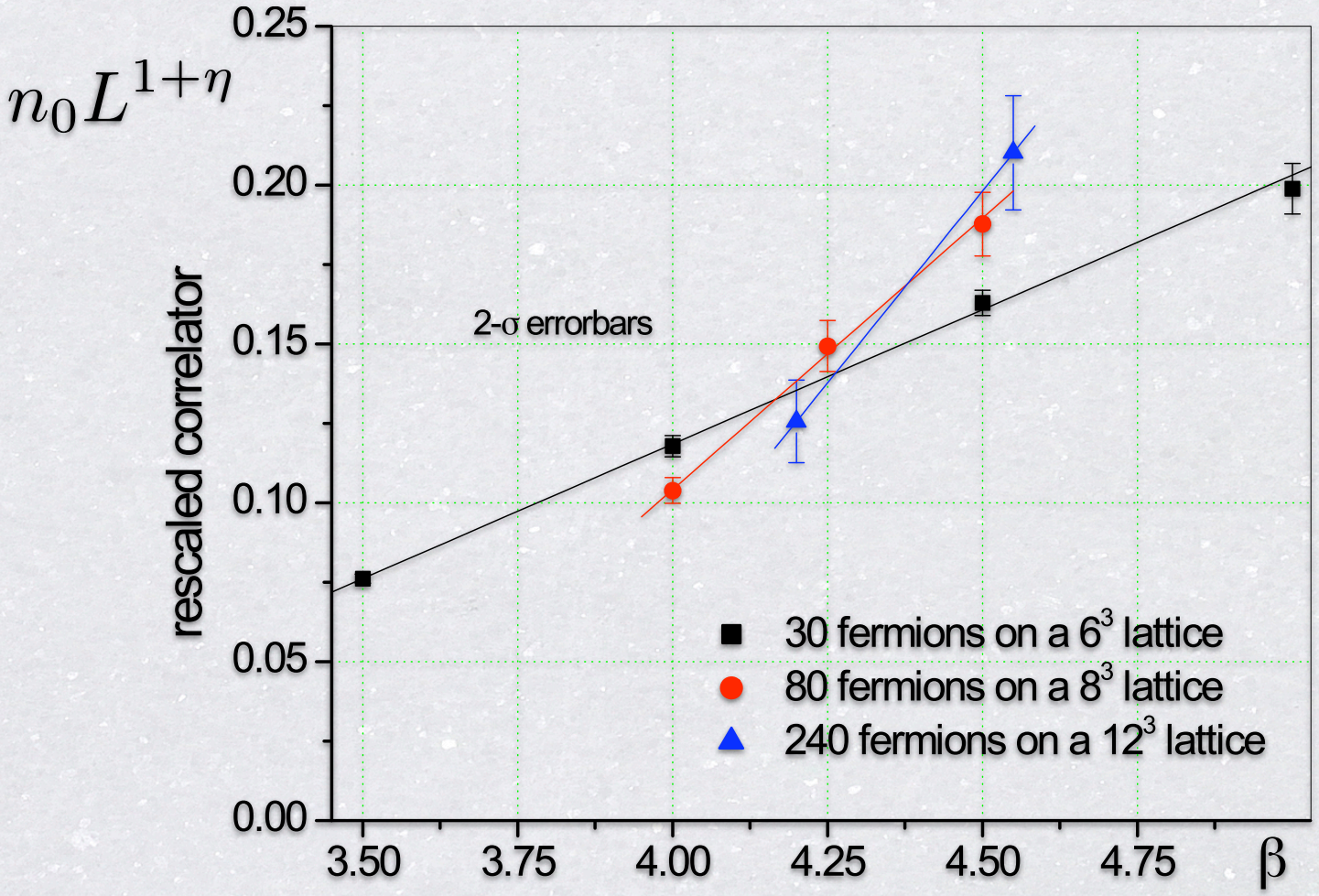
No sign problem, but…
macroscopic determinants

$$\Delta = \det \begin{pmatrix} G_{11} & G_{12} & G_{13} & \cdots & G_{1m} \\ G_{21} & G_{22} & G_{23} & \cdots & G_{2m} \\ G_{31} & G_{32} & G_{33} & \cdots & G_{3m} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ G_{m1} & G_{m2} & G_{m3} & \cdots & G_{mm} \end{pmatrix}$$

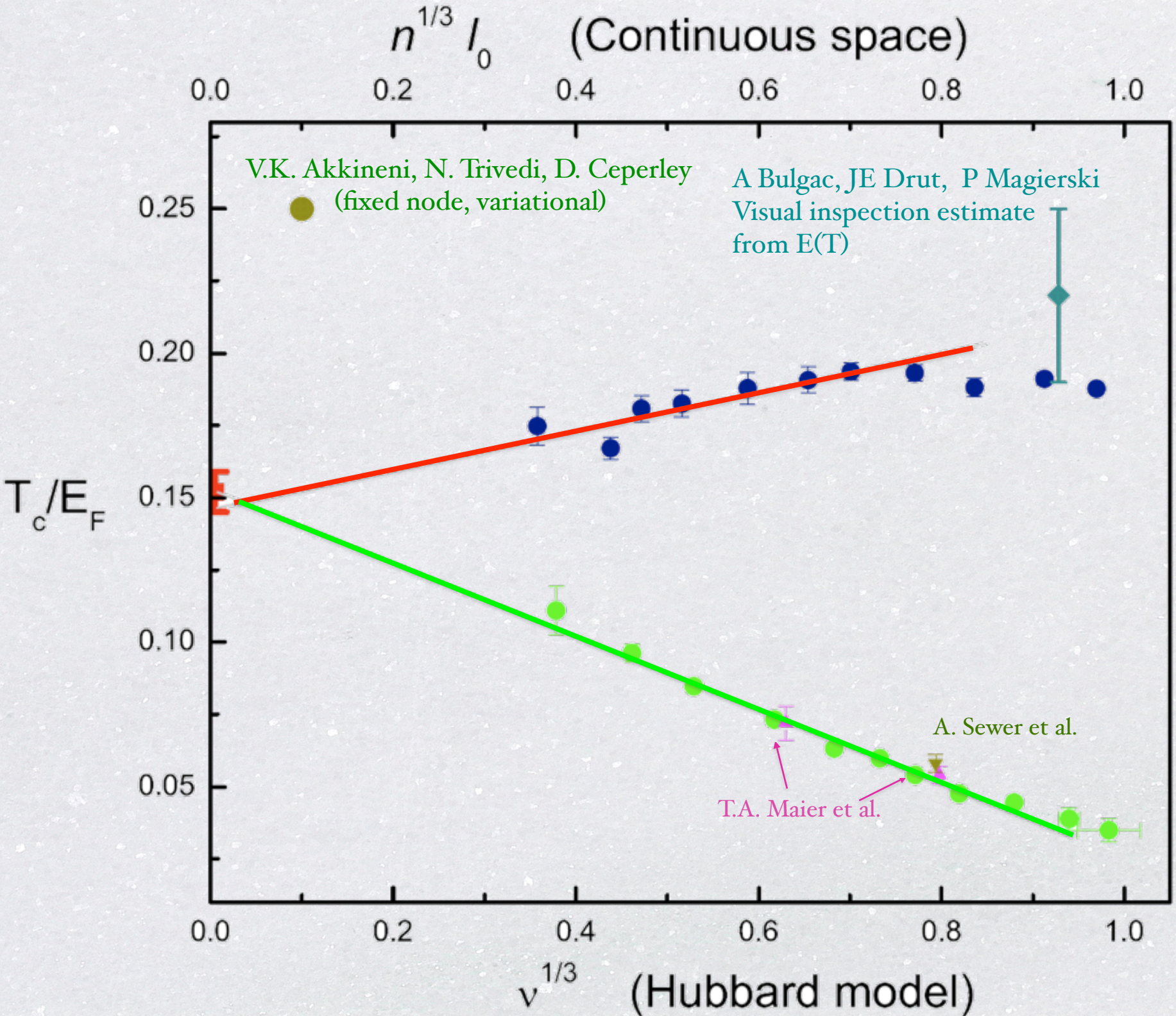
polynomial complexity

$$\mathrm{d}W = (-U)^m \left|\det \Delta_{m\times m}\right|^2 \prod_{j=1}^{m} \mathrm{d}\tau_j$$

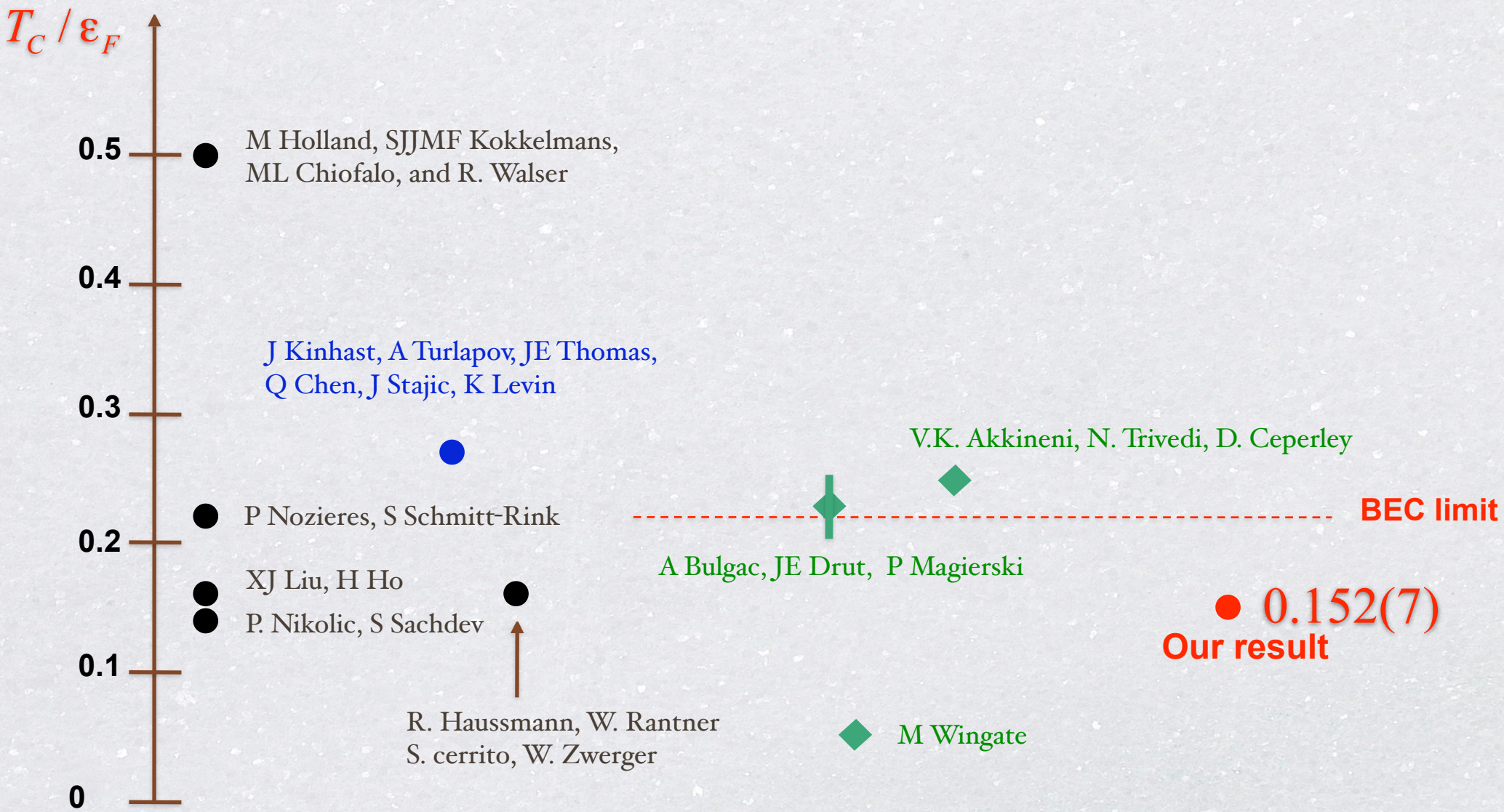
Critical point from finite size scaling



$$T_{\rm cross}(T, \alpha T) = T_C + A/L^{\omega+1/\nu}$$


$n^{1/3} l_0$ (Continuous space)
0.0
0.2
0.4
0.6
0.8
1.0
V.K. Akkineni, N. Trivedi, D. Ceperley
(fixed node, variational)
A Bulgac, JE Drut, P Magierski
Visual inspection estimate
from E(T)
T_c/E_F
0.25
0.20
0.15
0.10
0.05
A. Sewer et al.
T.A. Maier et al.
$\nu^{1/3}$ (Hubbard model)

Previous results for the unitary point



Supersolids in lattice boson models

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  - proposed in 1969, not observed yet
- Simplest example: square lattice hardcore bosons with repulsion

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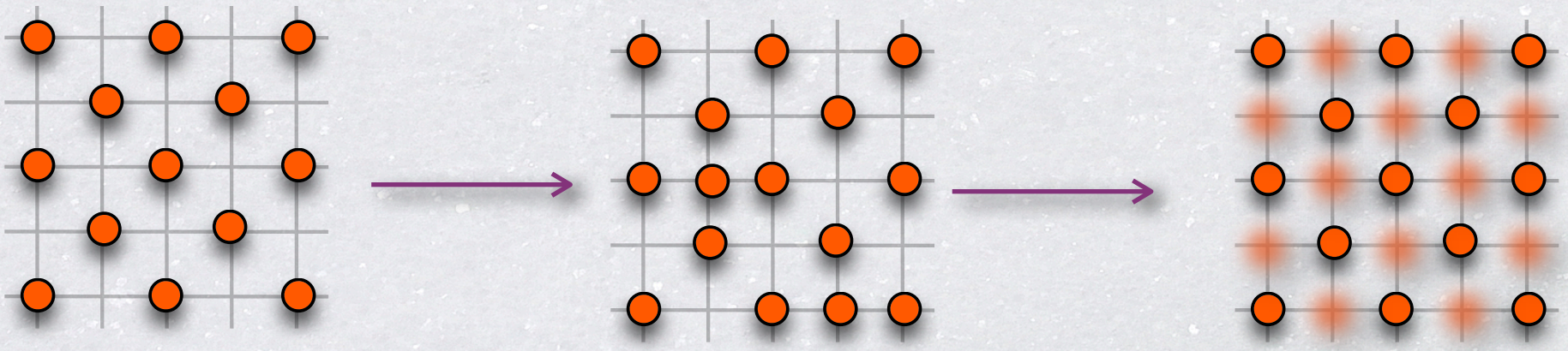


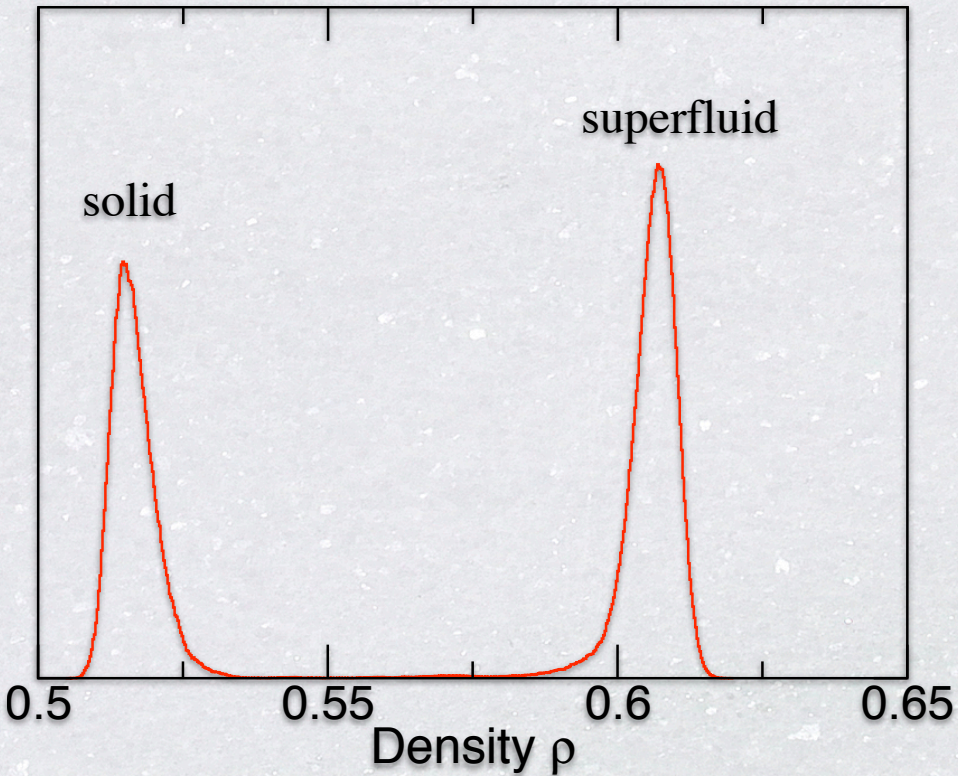
solid (crystal)
caused by large V

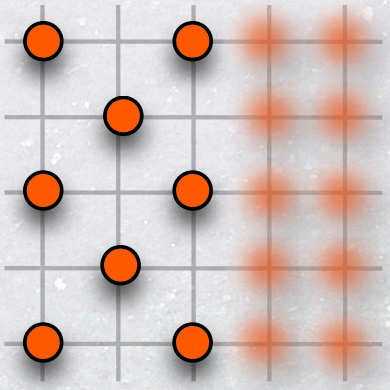
doped solid:
interstitials

supersolid:
superfluid interstitials

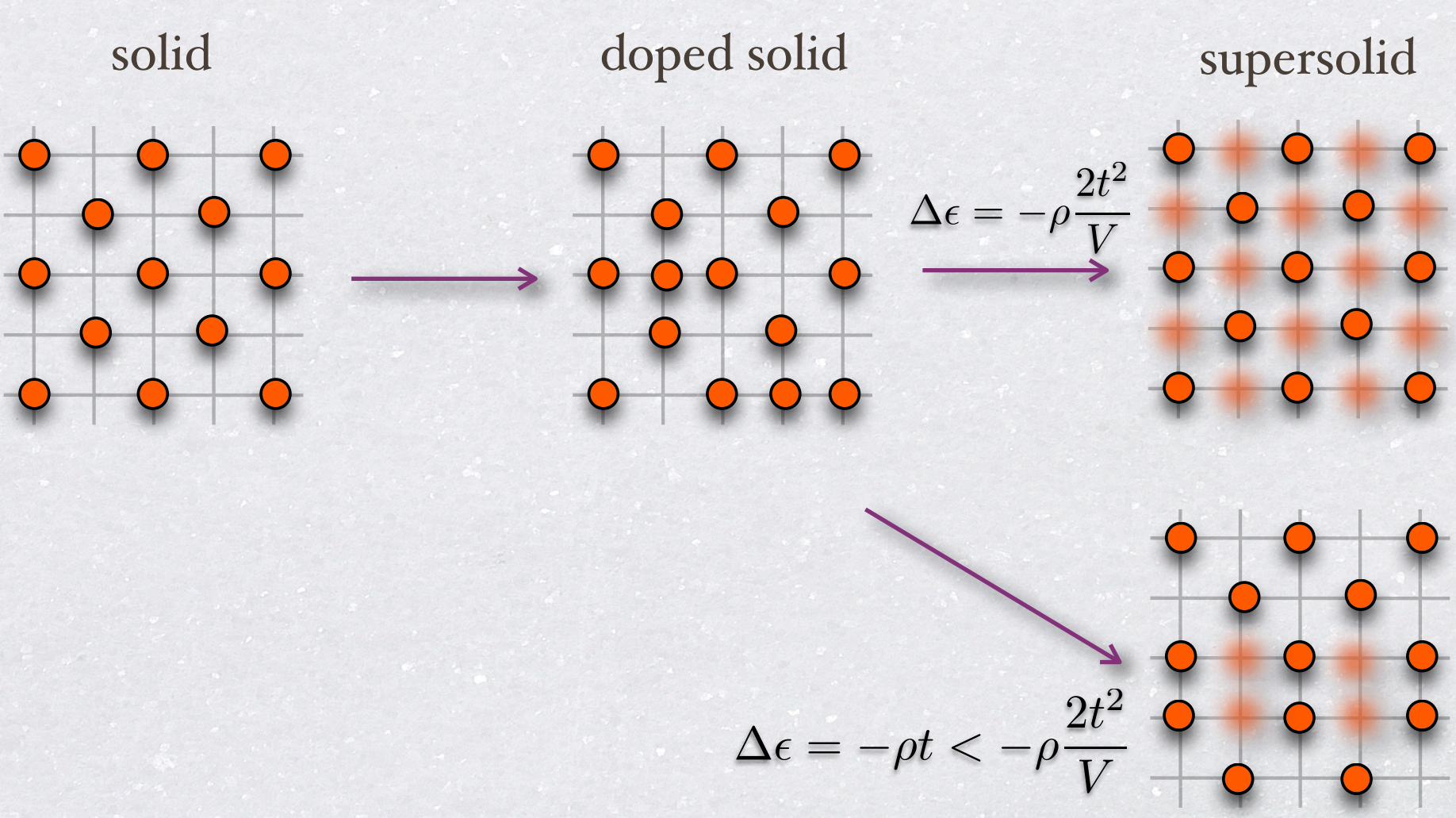
Do lattice supersolids exist?

- 2D Bosons on square lattice with nearest neighbor repulsion
  - mean-field calculations found supersolid
  - variation calculations found supersolid
  - previous simulations on small systems (32 particles) found supersolid
  - new simulations (5000 particles) instead show phase separation and a first order phase transition

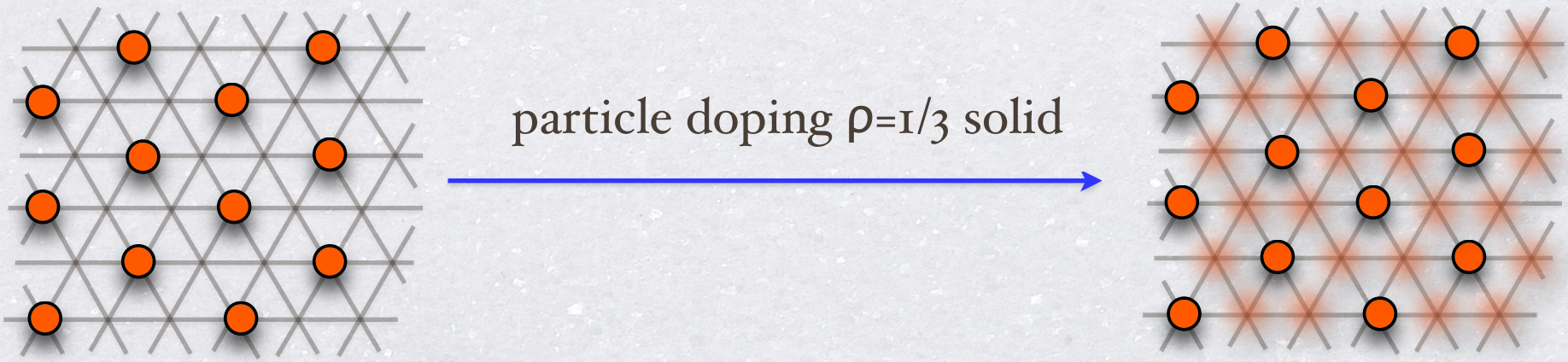




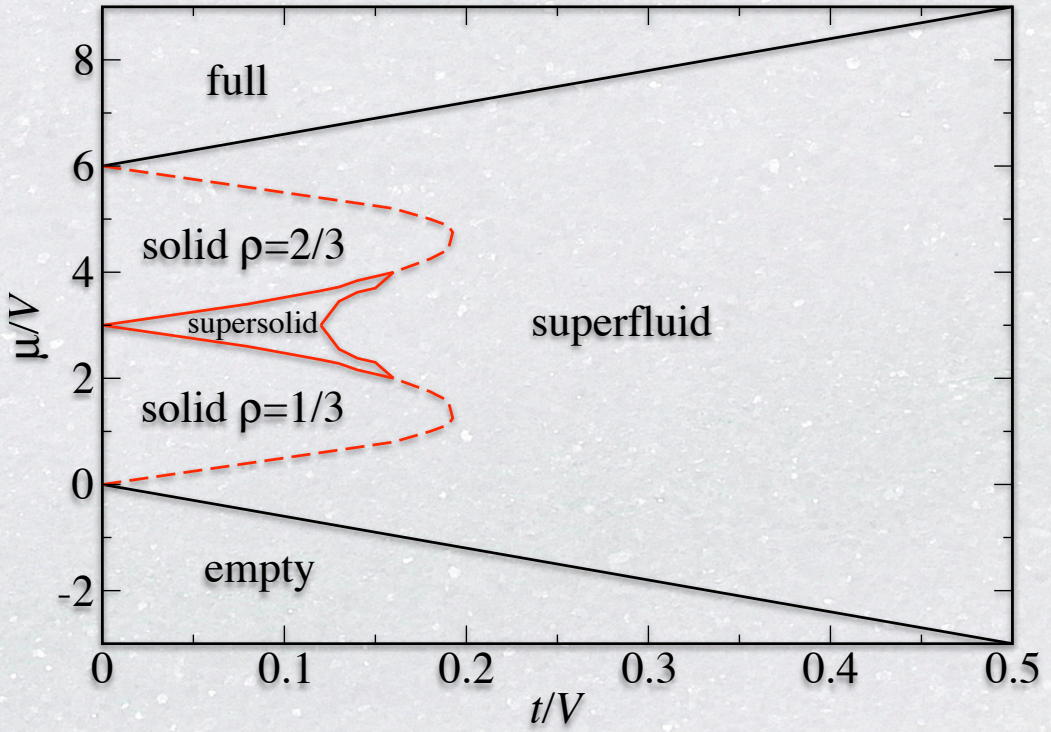
Supersolids versus phase separation



Triangular lattice supersolids



- QMC results confirm supersolid!
- Possible to realize with polar molecules in optical lattices



Summary

- Unbiased numerical simulations are important for strongly interacting quantum systems, such as
  - BCS-BEC crossover in fermions
  - supersolids in lattice bosons
- Powerful algorithms exist for many quantum problems
  - DMRG in 1 dimension
  - QMC for bosons, non-frustrated spins, and some fermion problems
- The fermionic sign problem remains as the biggest challenge
  - some model have no sign problem (attractive Hubbard model)
  - for other models a specialized new method might be found
    e.g. Corney & Drummond's GQMC, see talk by P. Corboz
  - but no general solution possible

Thanks to my collaborators

Methods

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Supersolids

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BCS-BEC

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