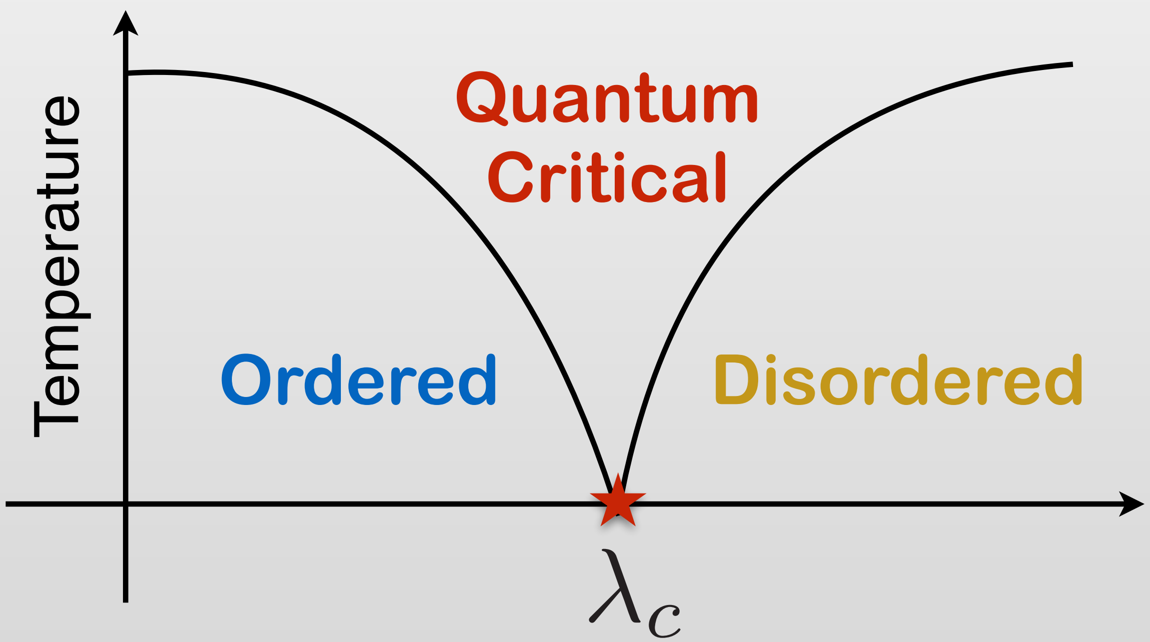
Recent Surprises in the Simulation of Quantum Phase Transitions

Lei Wang, ETH Zürich

Cologne 2015.04

Quantum Phase Transitions

$$\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{H}_1$$



- Where is the QCP ?
- What are the phases ?
- What is the universality class ?
- What are the experimental signatures ?

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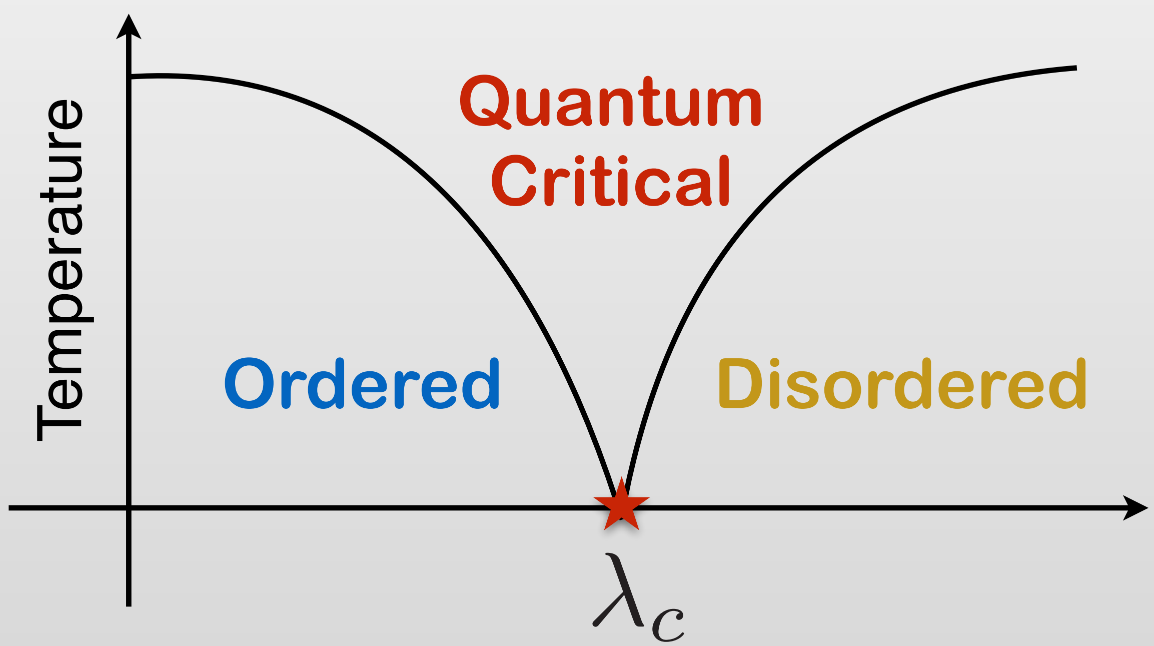

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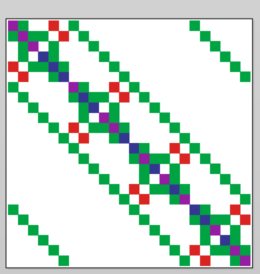
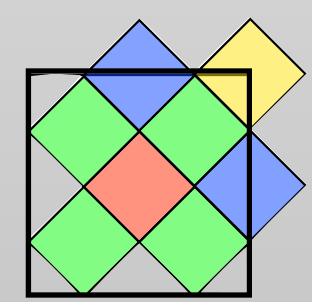
Algorithms for quantum many body systems



exact diagonalization

quantum Monte Carlo

tensor network states



dynamical mean field theories

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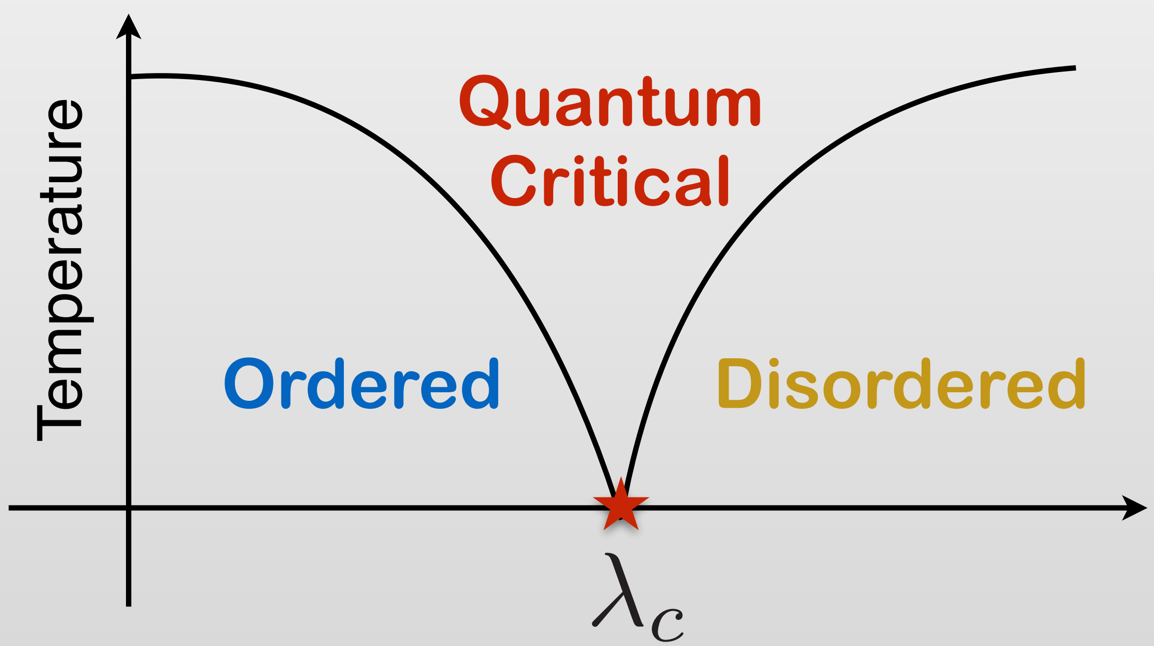

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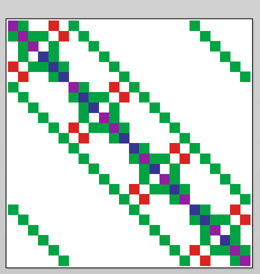

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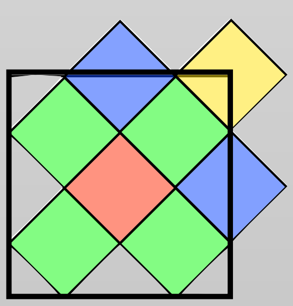
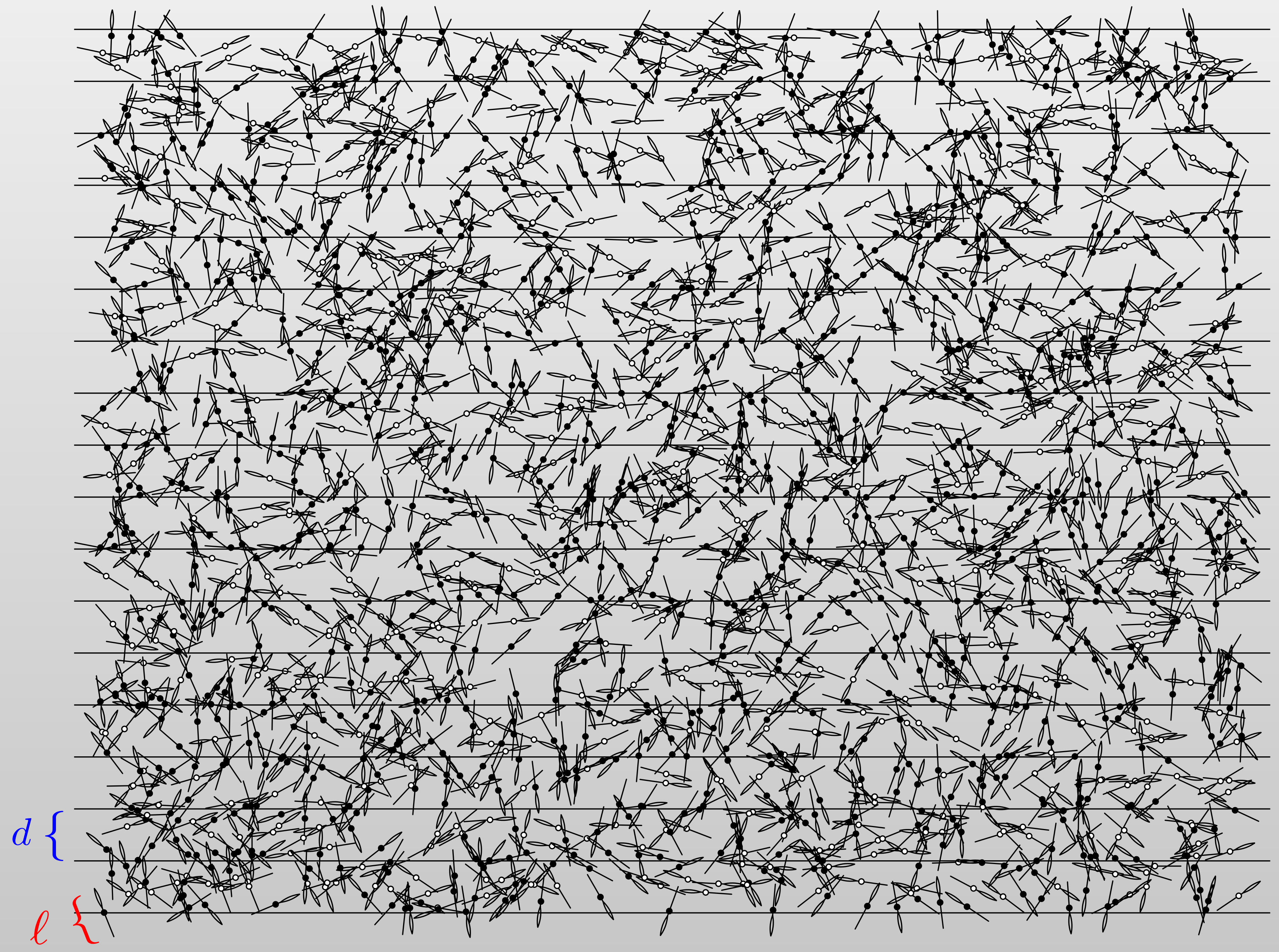
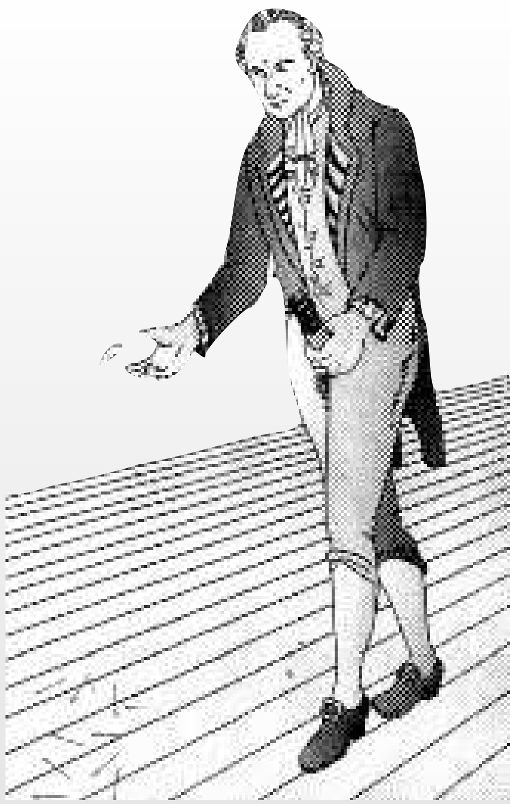


dynamical mean field theories

Monte Carlo Method

$$\langle N_{\text{hits}} \rangle = \frac{2}{\pi} \frac{\ell}{d}$$





Buffon 1777

Statistical Mechanics:
Algorithms and Computations
Werner Krauth

The first recorded Monte Carlo simulation

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)

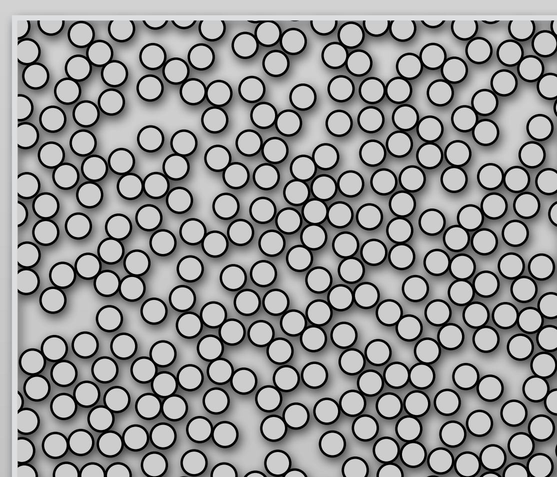
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional 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.

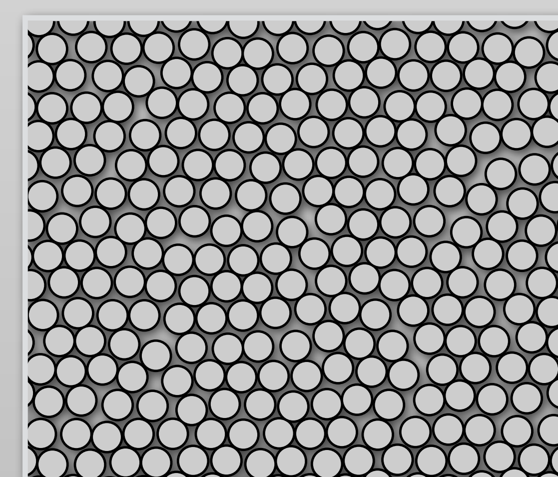
I. INTRODUCTION

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-





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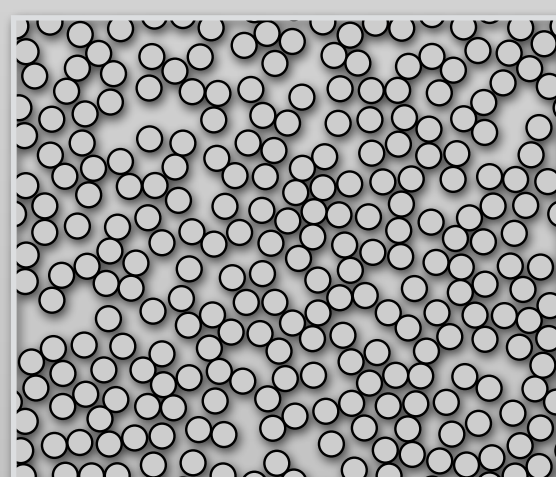
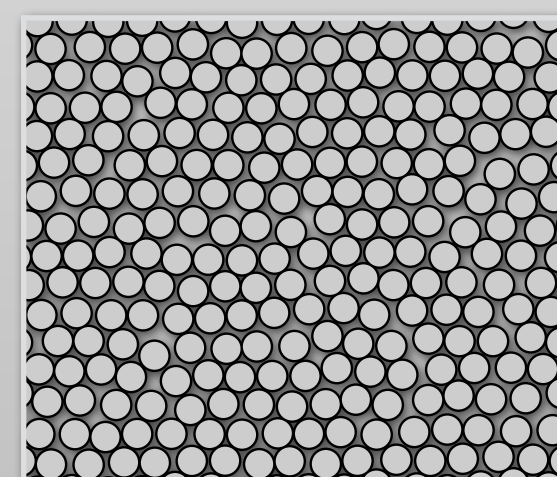


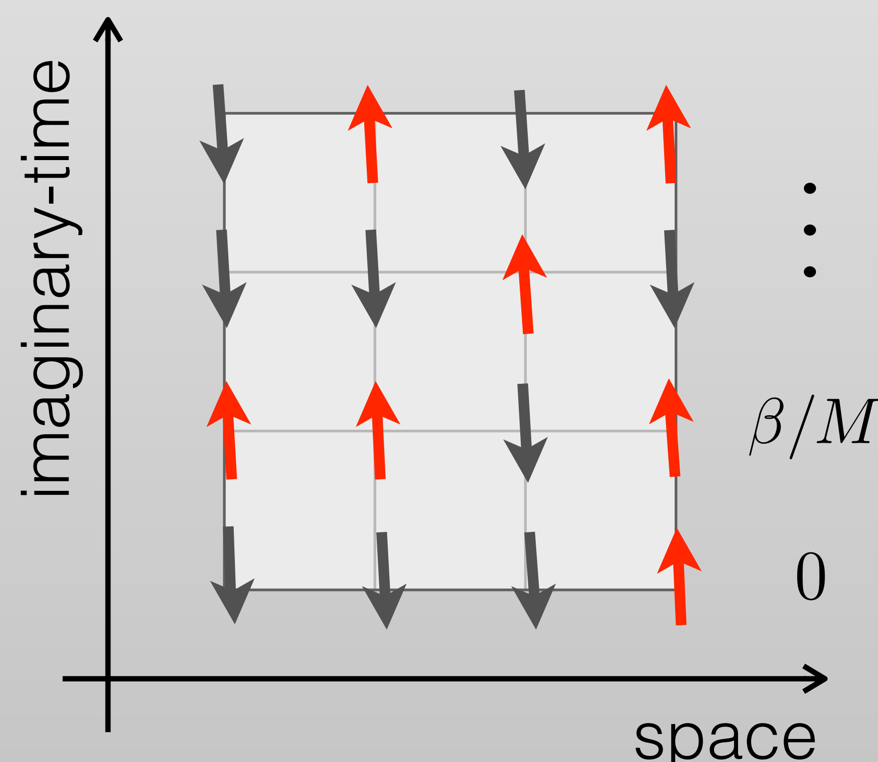


Quantum to Classical Mapping

$$Z = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right) \qquad \hat{H} = \hat{H}_0 + \lambda \hat{H}_1$$

Traditional approach

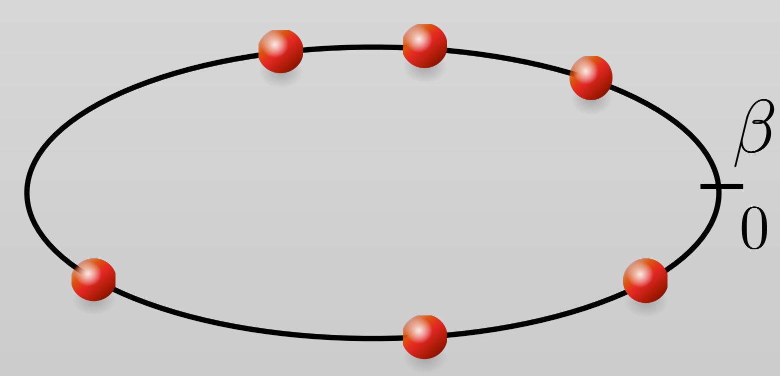
$$Z = \mathrm{Tr}\left(e^{-\frac{\beta}{M}\hat{H}} \dots e^{-\frac{\beta}{M}\hat{H}}\right)$$



Modern approach

$$Z = \sum_{k=0}^{\infty} \lambda^k \int_0^{\beta} d\tau_1 \dots \int_{\tau_{k-1}}^{\beta} d\tau_k \times$$

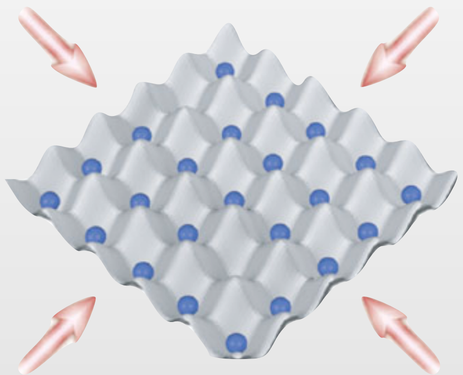
$$\mathrm{Tr}\left[(-1)^k e^{-(\beta-\tau_k)\hat{H}_0} \hat{H}_1 \dots \hat{H}_1 e^{-\tau_1 \hat{H}_0}\right]$$

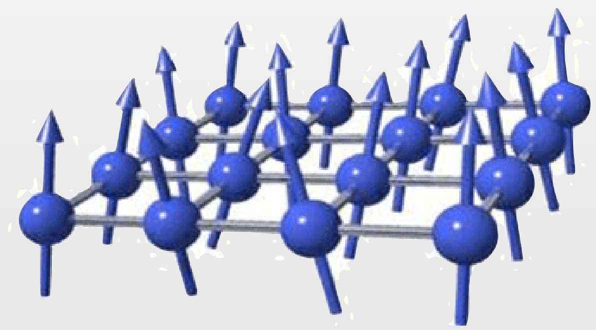


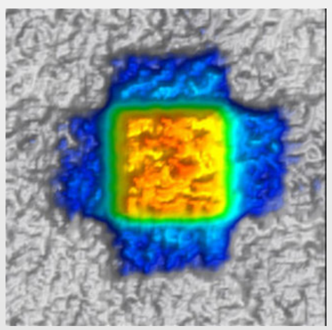
imaginary-time axis

Beard and Wiese, 1996
Prokof'ev et al, 1996

Modern QMC Methods







bosons

World-line Approach

N. V. Prokof'ev et al, JETP, **87**, 310 (1998)

quantum spins

Stochastic Series Expansion

A. W. Sandvik et al, PRB, **43**, 5950 (1991)

fermions

Determinantal Methods

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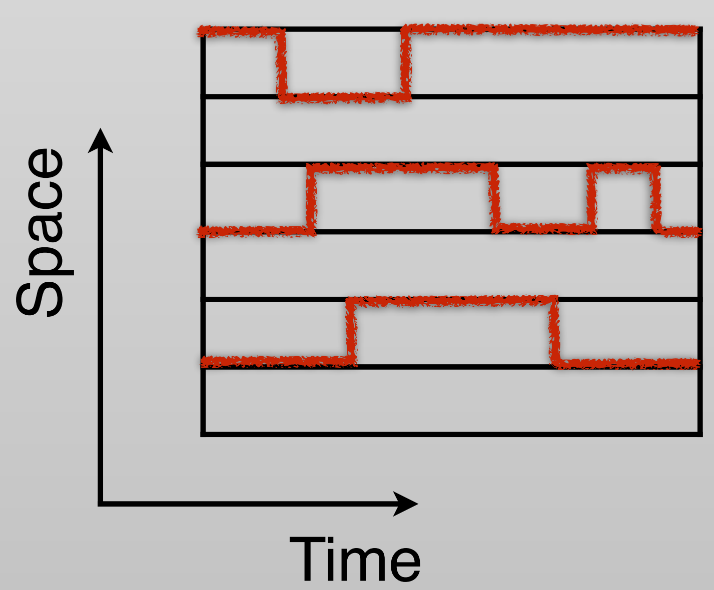

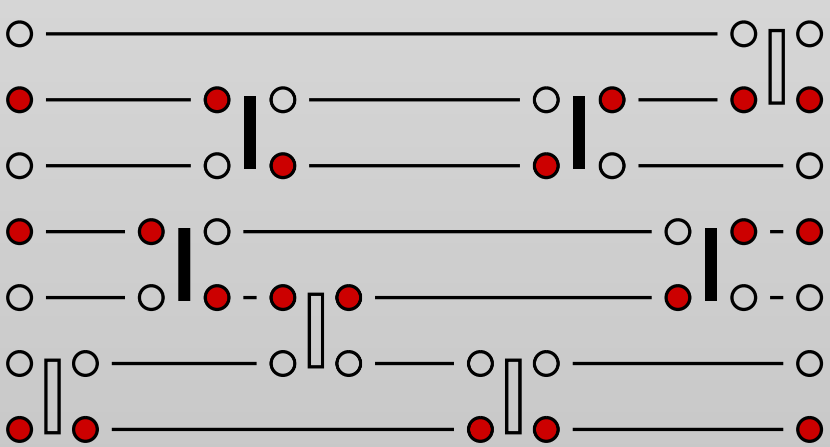

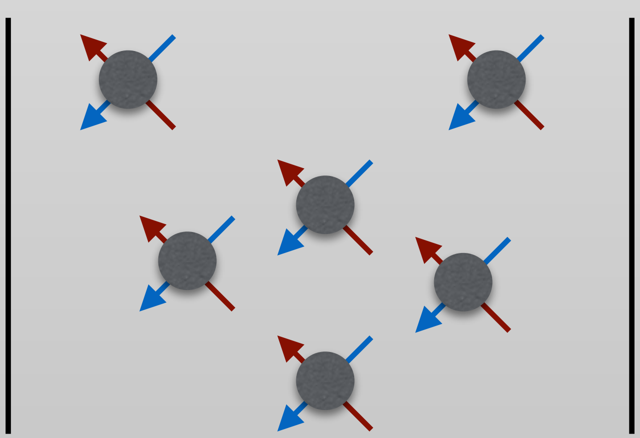

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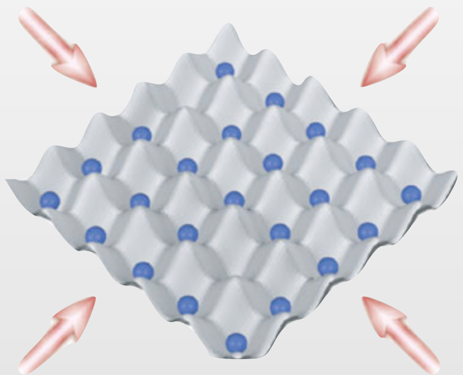

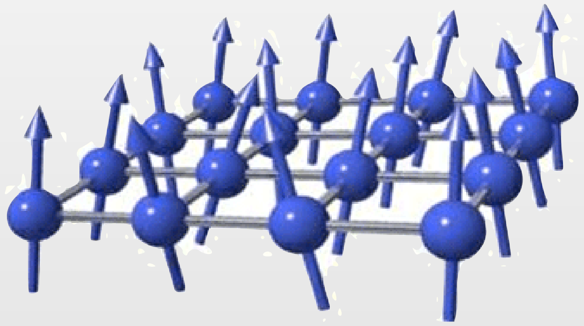

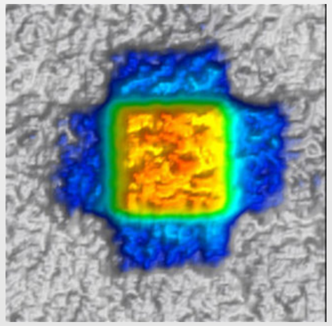

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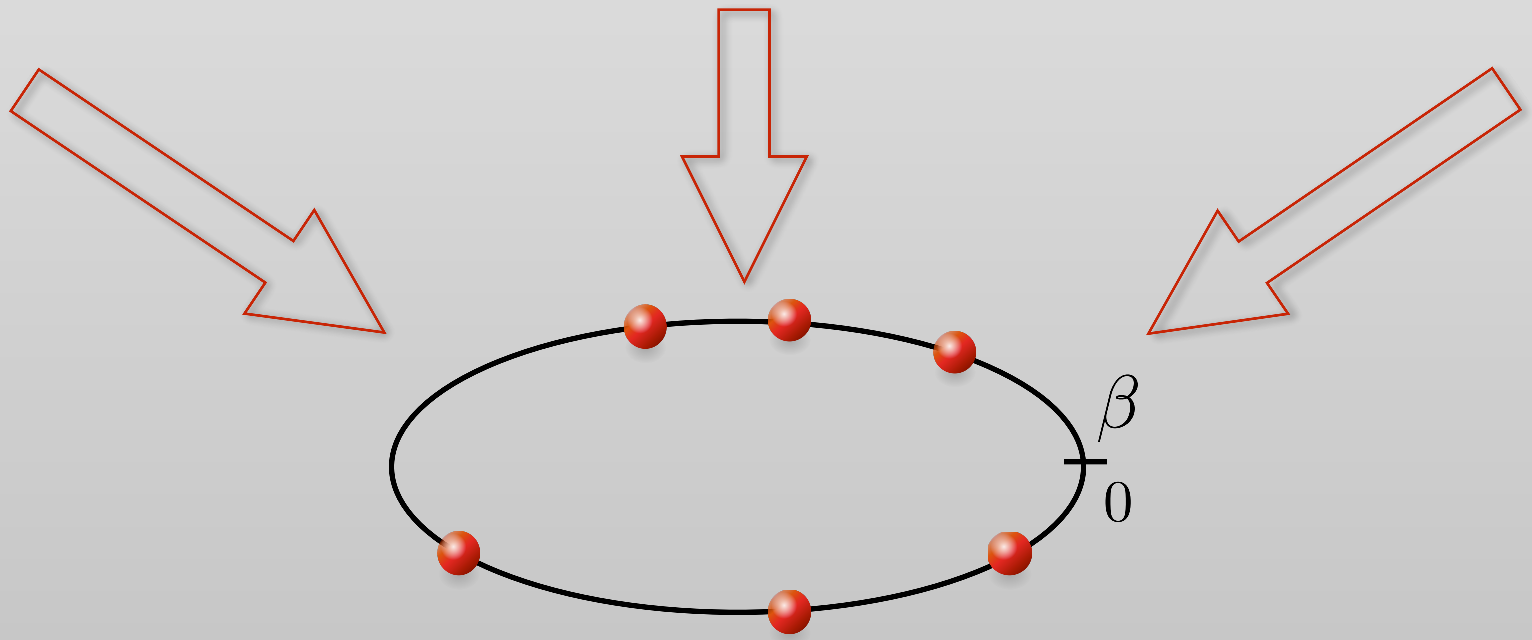


Challenges

Sign problem

What about a negative probability ?

General solution implies P=NP Troyer and Wiese, 2005

But, do we need a general solution ?

There has always been surprise...

Berg et al, Science, 2012

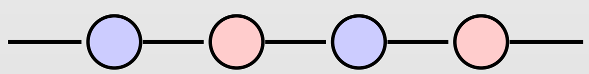
"designer" Hamiltonian

Huffman and Chandrasekharan, PRB, 2014

new solution to the sign problem

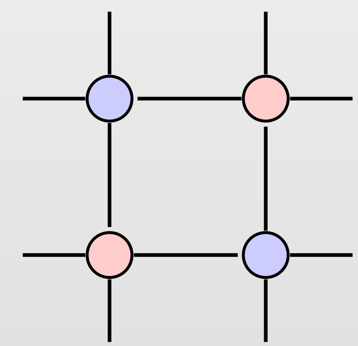
Spinless t-V Model

$$\hat{H} = -t \sum_{\langle i,j \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right) + V \sum_{\langle i,j \rangle} \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_j - \frac{1}{2} \right)$$

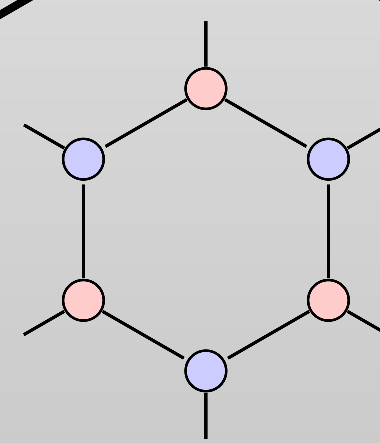


Maps to an XXZ model

$V_c/t = 2$



Orders at infinitesimal V due to Fermi surface nesting



?

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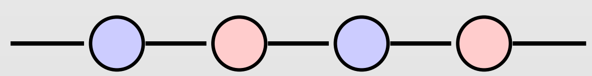

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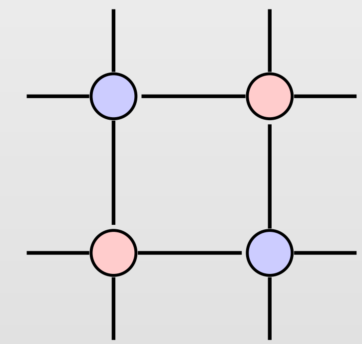
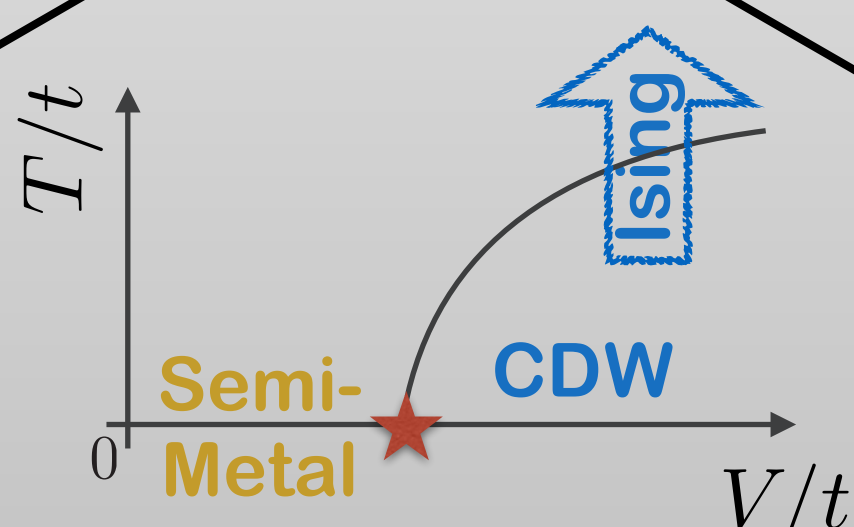


Orders at infinitesimal V due to Fermi surface nesting



Spinless t-V Model

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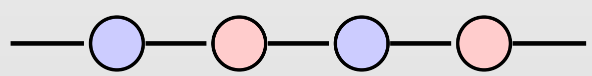

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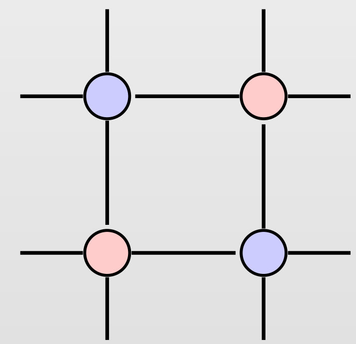

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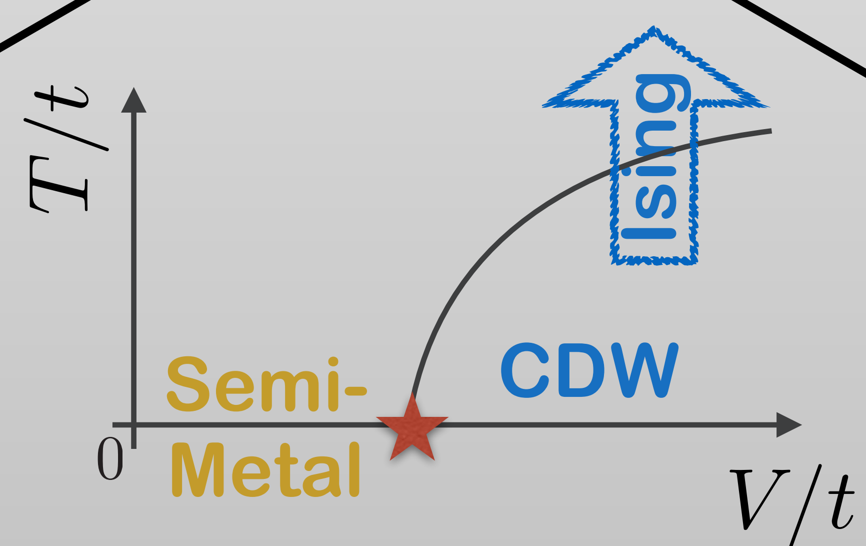


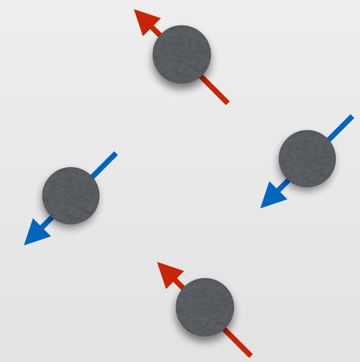
Critical point ? Universality class ? C

A 30 years old sign problem

No sign problem

model at

$$w(\mathcal{C}) = \det M_{\uparrow} \times \det M_{\downarrow}$$
$$= |\det M_{\uparrow}|^2 \geq 0$$

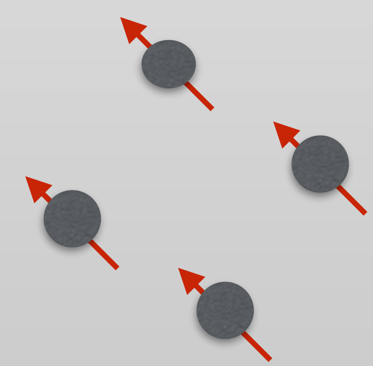


Kramers pairs

Wu et al, PRB, 2005

But, h

$$w(\mathcal{C}) = \det M$$



e.g. spinless t-V model

Scalapino et al, PRB, 1984 Gubernatis et al, PRB, 1985

up to 8*8 square lattice and T≥

Meron cluster approach, Chandrasekharan and Wiese, PRL, 1999

solves sign problem only for V ≥ 2t

Determinant = Pfaffian²

For real skew-symmetric

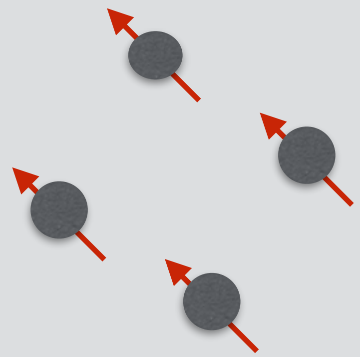
Huffman and Chandrasekharan, PRB, 2014

$$\boxed{M^T = -M}$$

$$\det M = (\mathrm{pf}\, M)^2 \geq 0$$

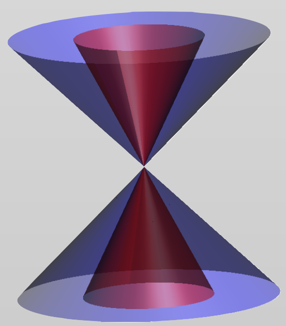
Appears naturally in modern CT-QMC

Small idea solves big problems!

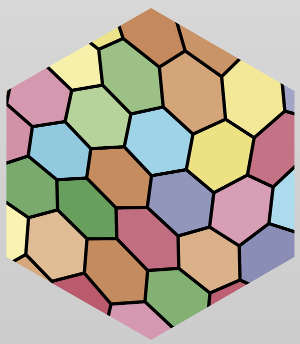


spinless fermions

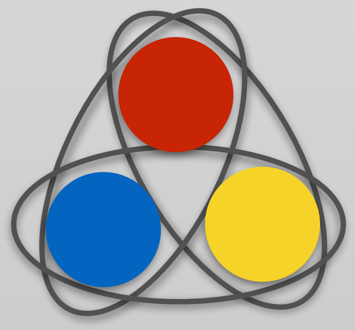
LW and Troyer, PRL 2014
LW, Corboz, Troyer, NJP 2014 (IOPselect)
LW, Iazzi, Corboz, Troyer, 1501.00986, PRB in press (Editors' Suggestion)



split Dirac cone



strain

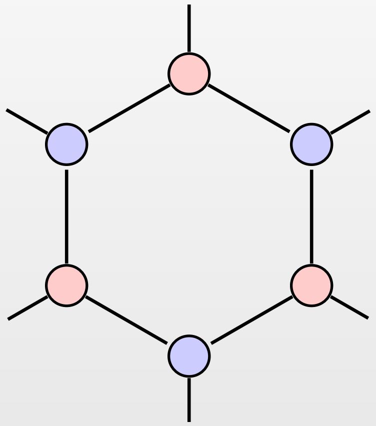


SU(3)

Observables & Scaling Ansatz

± 1 for A(B) sublattice

$$M_2 = \frac{1}{N^2} \sum_{i,j} \eta_i \eta_j \left\langle \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_j - \frac{1}{2} \right) \right\rangle$$

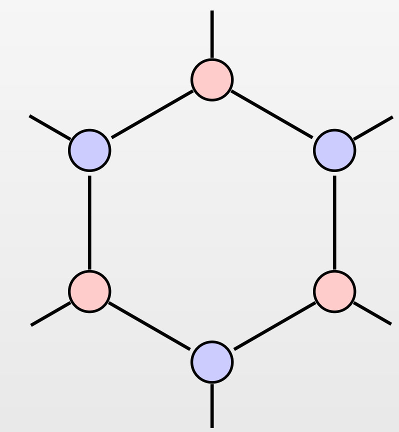


$$M_4 = \frac{1}{N^4} \sum_{i,j,k,l} \eta_i \eta_j \eta_k \eta_l \left\langle \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_j - \frac{1}{2} \right) \left(\hat{n}_k - \frac{1}{2} \right) \left(\hat{n}_l - \frac{1}{2} \right) \right\rangle$$

$2L^2$ up to 450 sites

Observables & Scaling Ansatz

± 1 for A(B) sublattice



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$2L^2$ up to 450 sites

Scalings ansatz close to the QCP

$$M_2 = L^{-z-\eta} \mathcal{F}[L^{1/\nu}(V - V_c), L^z/\beta]$$

$$M_4 = L^{-2z-2\eta} \mathcal{G}[L^{1/\nu}(V - V_c), L^z/\beta]$$

Observables & Scaling Ansatz

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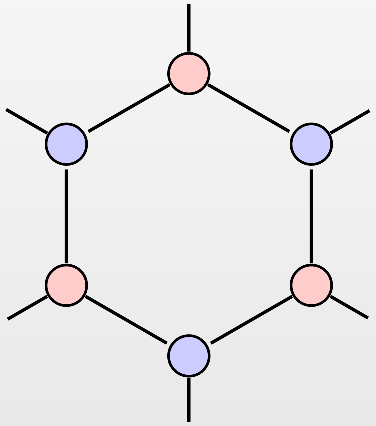

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$2L^2$ up to 450 sites

relativistic invariance

$z = 1$

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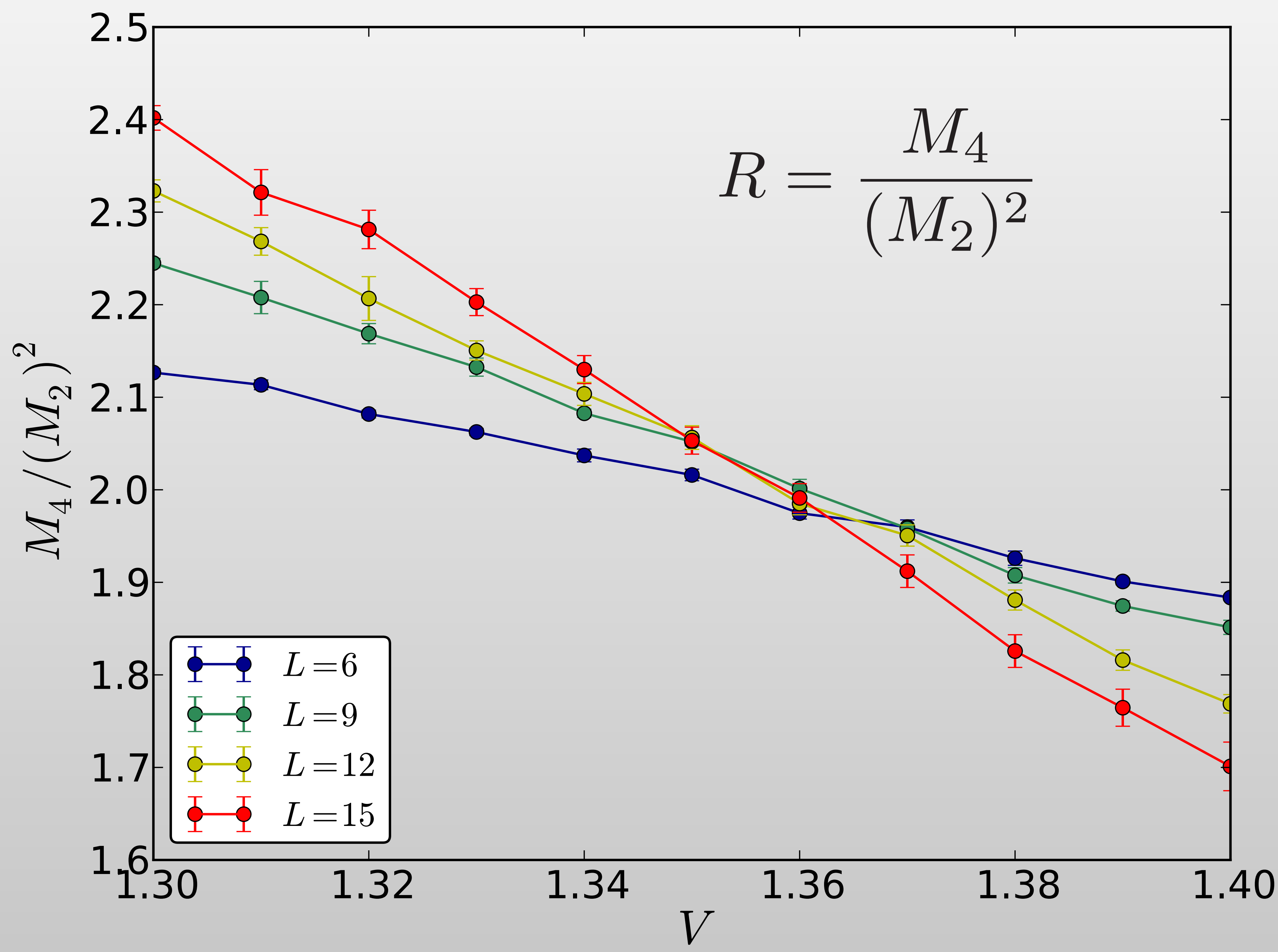
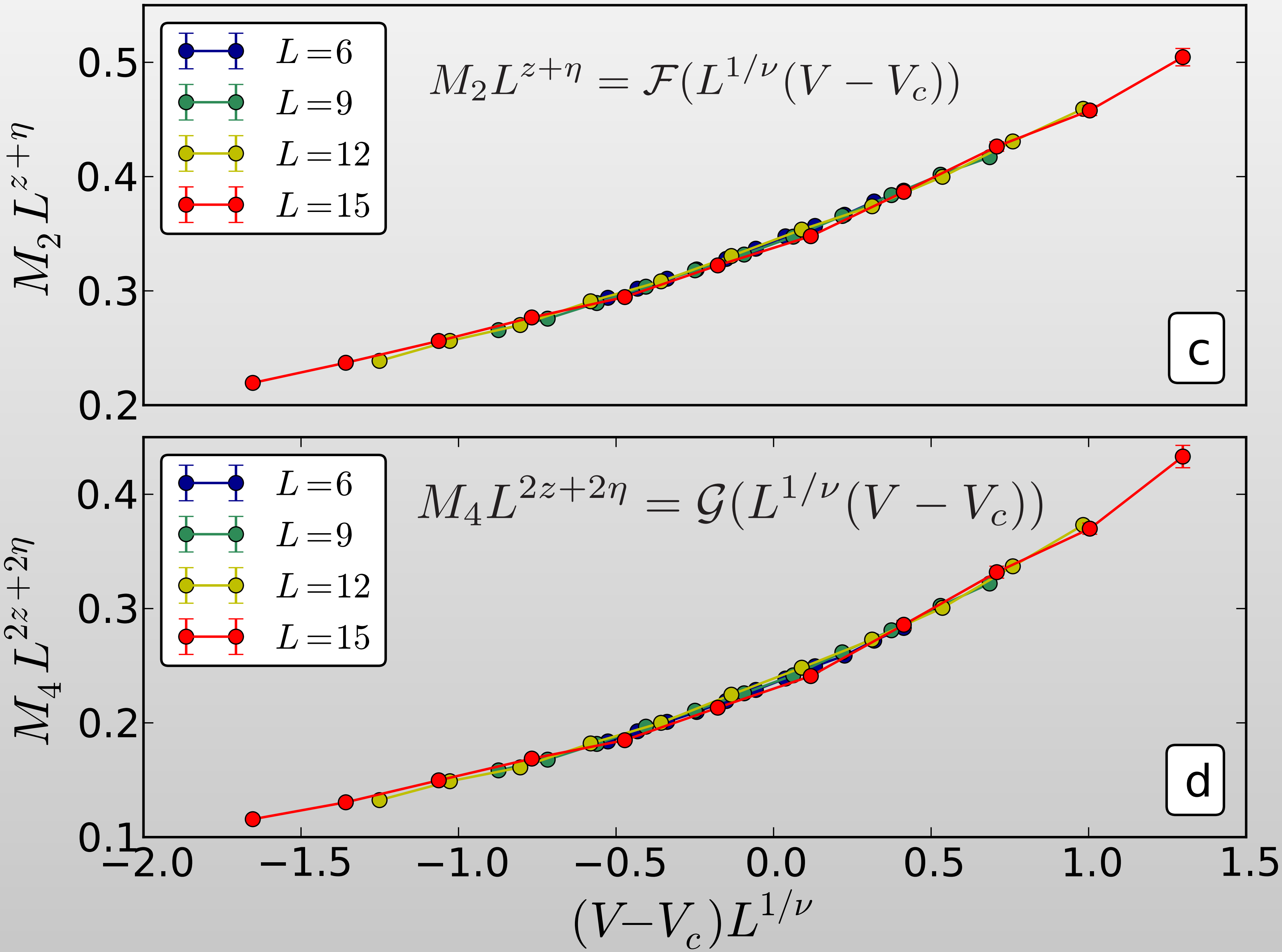
Binder Ratio

LW, Corboz, Troyer, NJP **16**, 103008 (2014)



Data Collapse

LW, Corboz, Troyer, NJP **16**, 103008 (2014)



$V_c/t = 1.356(1)$

$\nu = 0.80(3)$

$\eta = 0.302(7)$

* Errorbars $\chi^2 + 1$

Gross-Neveu-Yukawa Theory

- ε Rosenstein et al, PLB, 1993

$$\nu = 0.797 \qquad \eta = 0.502$$

- functional renormalization group Rosa et al, PRL,2001 Höfling et al, PRB, 2002

$$\nu = 0.738 \sim 0.927 \quad \eta = 0.525 \sim 0.635$$

Honeycomb

$$\nu = 0.80(3)$$

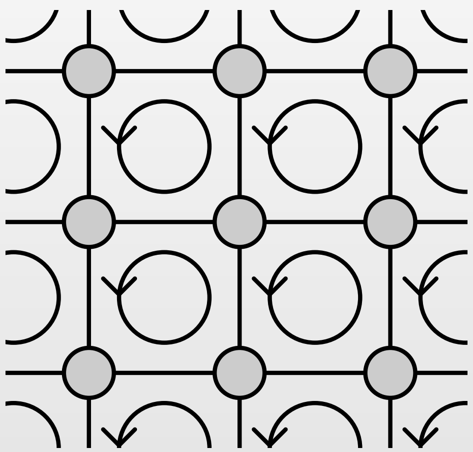
$$\eta = 0.302(7)$$

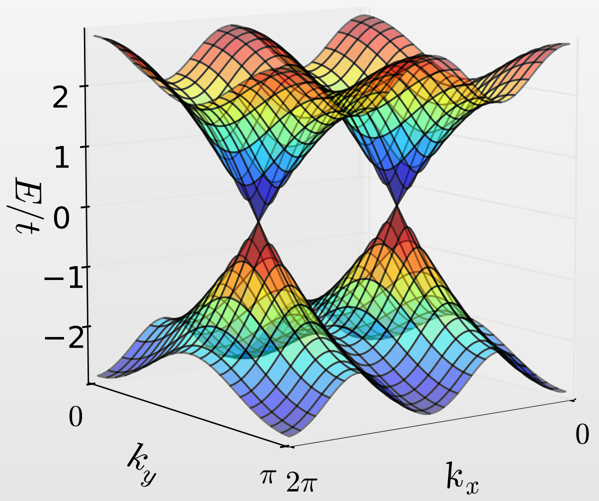
ν

η

* Field theory calculations are based on 2-flavors of 2-component Dirac fermions with the

Check-I: π-flux square lattice





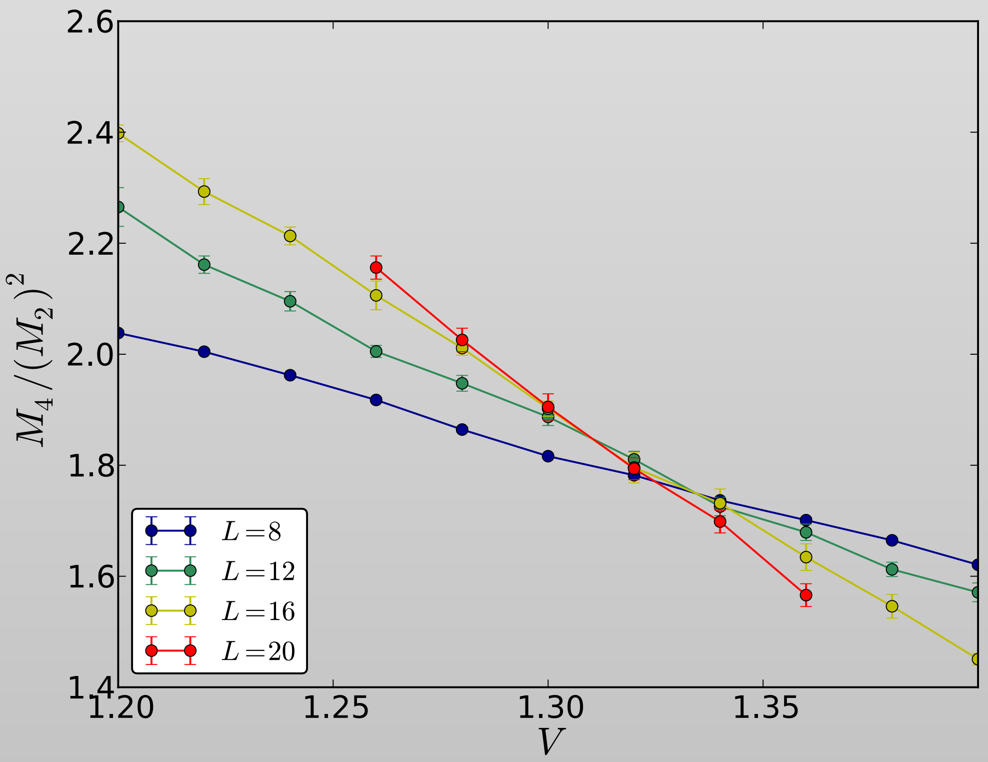
also features two Dirac points

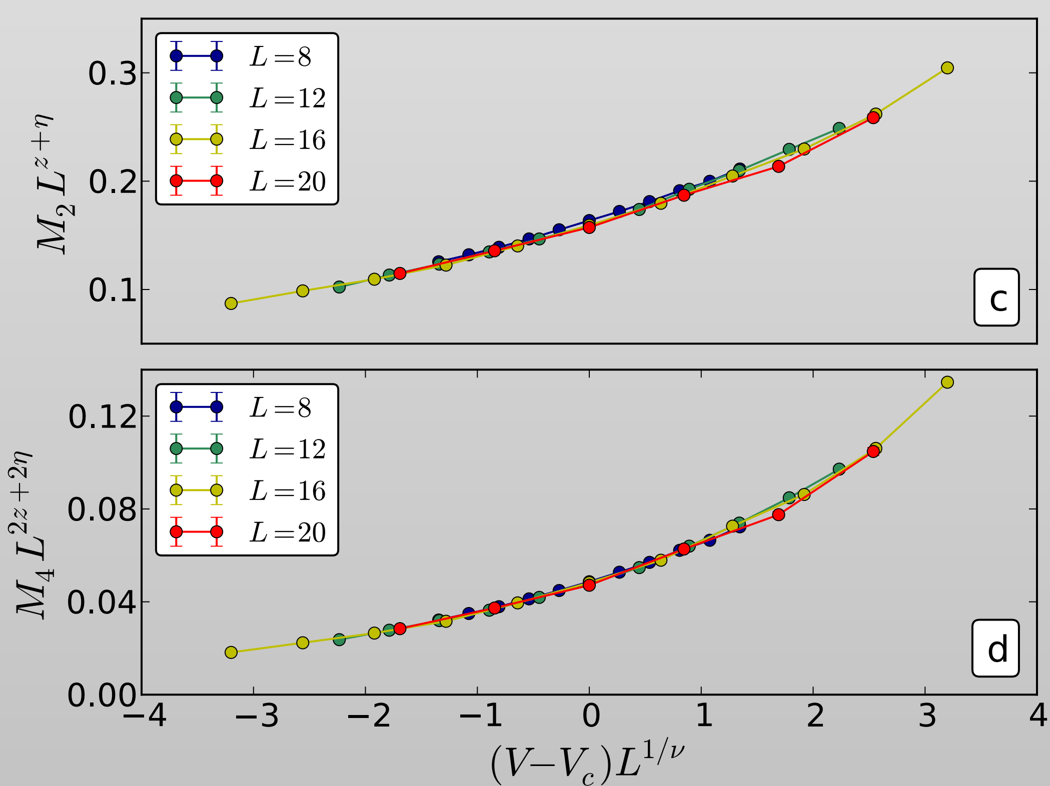
π-flux lattice

$$V_c/t = 1.304(2)$$

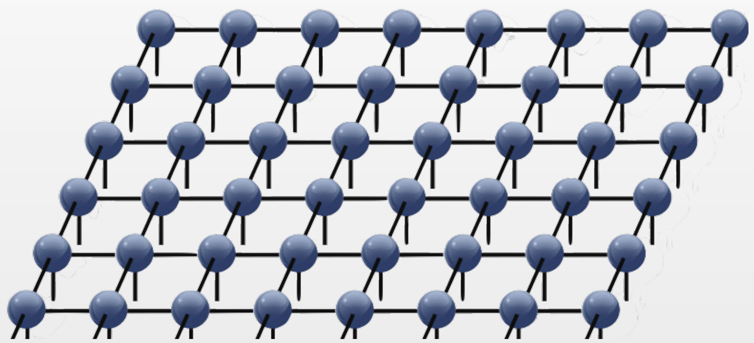
$$\nu = 0.80(6)$$

$$\eta = 0.318(8)$$

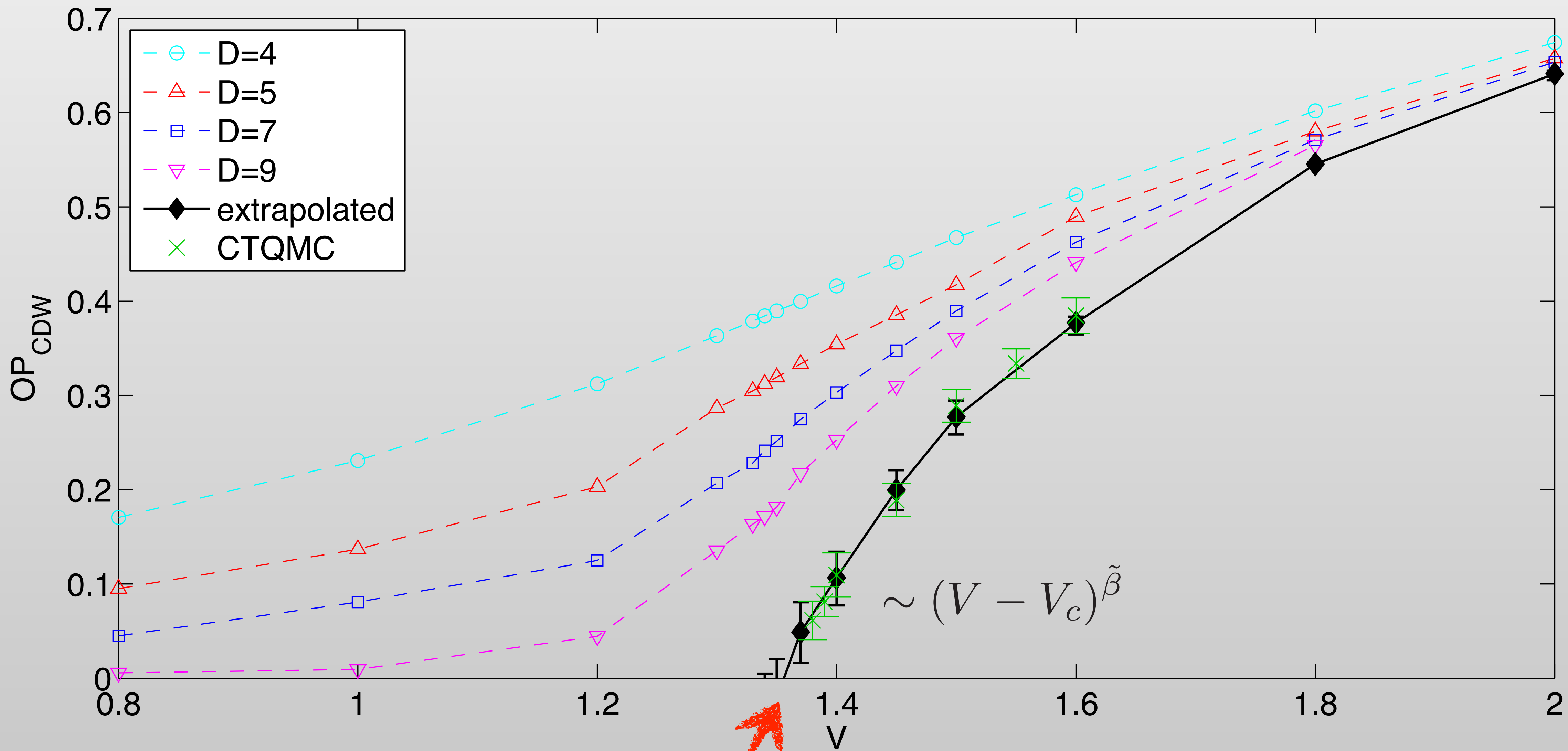




Check-II: iPEPS

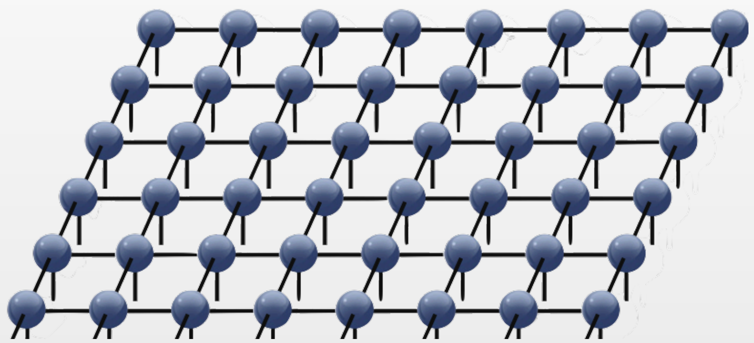


Philippe Corboz
Amsterdam



$$V_c = 1.36(3)$$

Check-II: iPEPS



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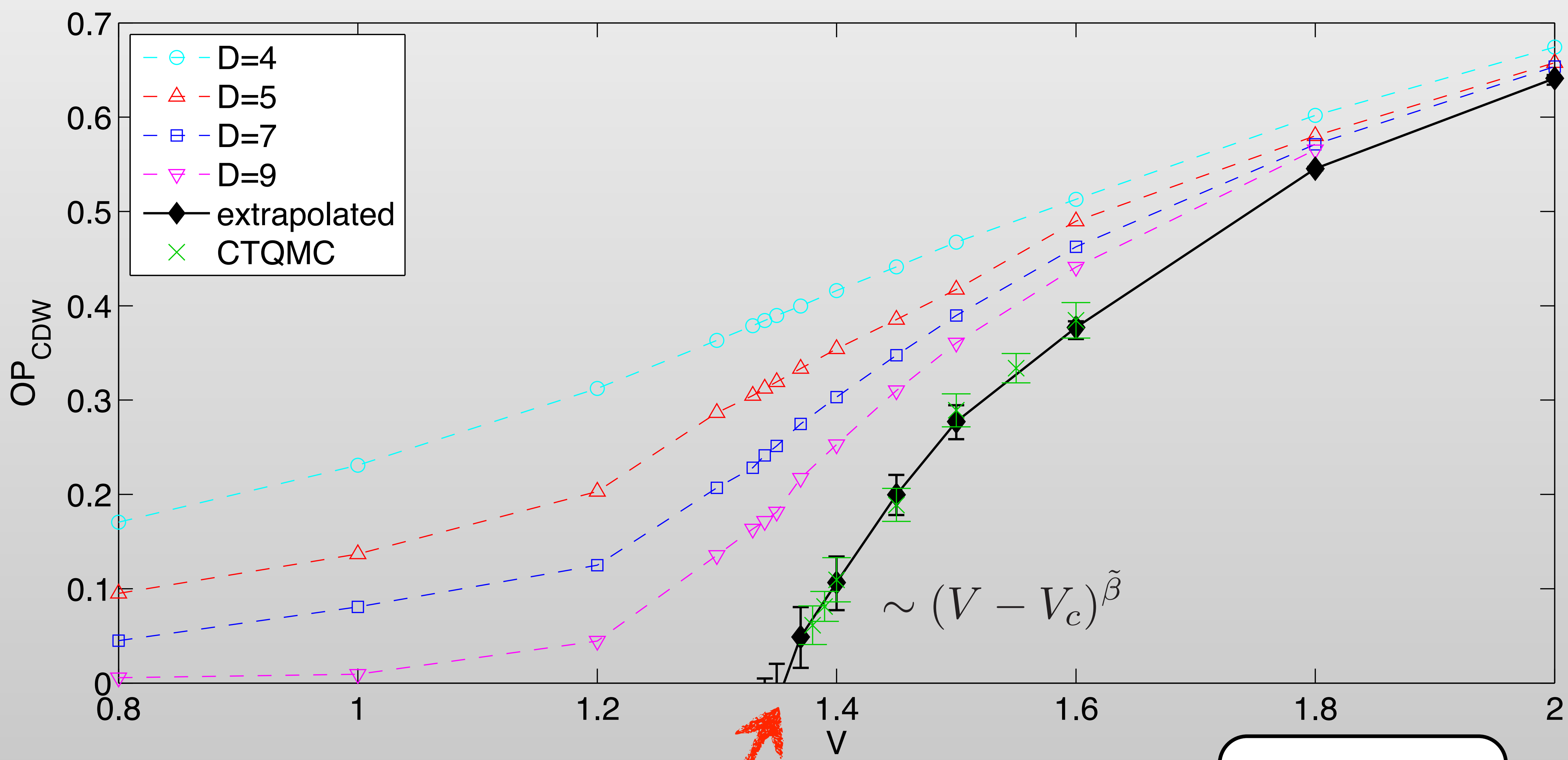


$V_c = 1.36(3)$

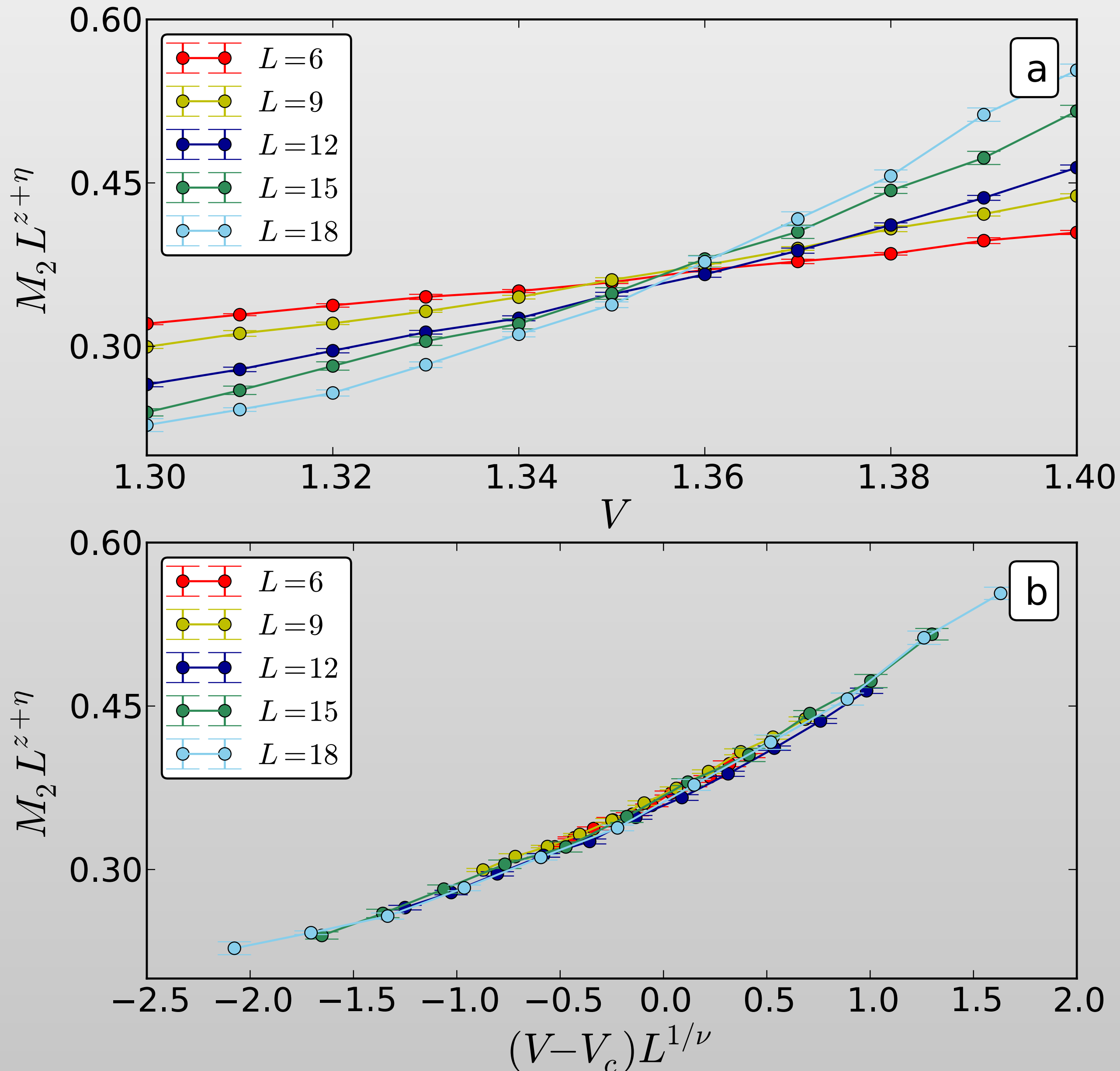
CTQMC

$$\tilde{\beta} = \frac{\nu}{2}(z + \eta) = 0.52(3)$$

Updates: results at T=0

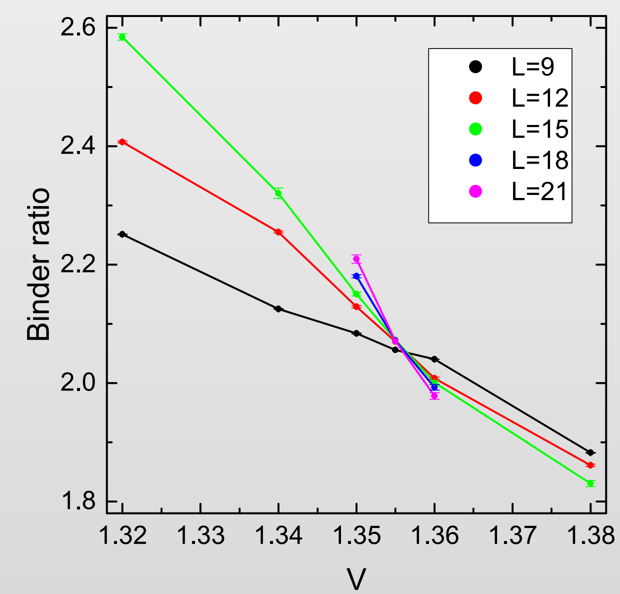
L

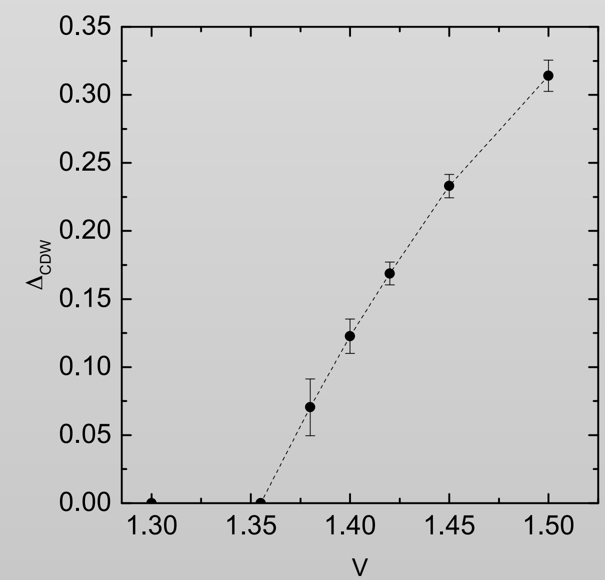
Iazzi, Troyer, 1411.0683
LW, Iazzi, Corboz, Troyer, 1501.00986



Majorana

Li, Jiang and Yao, 1408.2269
Li, Jiang and Yao, 1411.7383





Consistent with finite-T results

$V_c/t = 1.355(1)$ $\nu = 0.77(3)$ $\eta = 0.45(2)$

Summary-I

The new solution
old problem about spinless fermions

Critical point ? Universality class ? C

There are still some discrepancies, to resolve them

- Compare
- Make sure to compare with the
- Larger systems

CTQMC

$$V_c/t = 1.356(1)$$

$$\nu = 0.80(3)$$

$$\eta = 0.302(7)$$

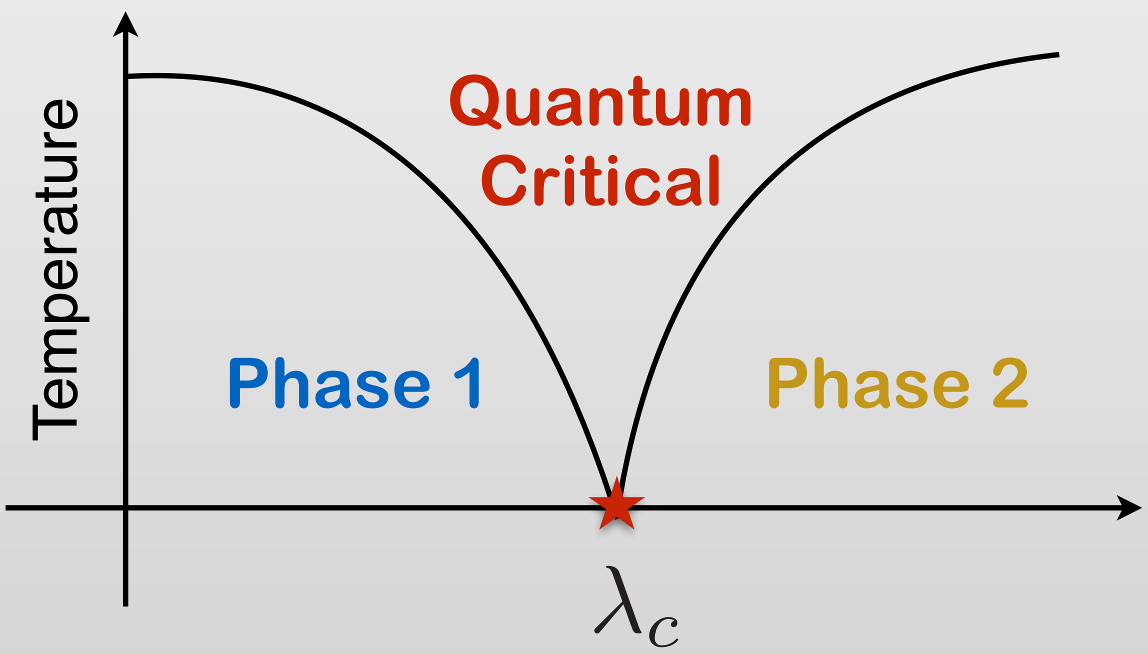
A very recent surprise to us

Fidelity Susceptibility

What's that ? Why should I care ?

$$\boxed{\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{H}_1}$$

You, Li, and Gu, 2007
Campos Venuti et al, 2007



Fidelity $F(\lambda, \epsilon) = |\langle \Psi(\lambda) | \Psi(\lambda + \epsilon) \rangle|$

$$= 1 - \frac{\chi_F}{2}\epsilon^2 + \dots$$

Fidelity Susceptibility

What's that ? Why should I care ?

$$\hat{H}(\lambda) = \hat{H}_0 + \lambda \hat{H}_1$$

You, Li, and Gu, 2007
Campos Venuti et al, 2007

A general indicator of quantum phase transitions
No need for local order parameter e.g. Kitaev model, Abasto et al 2008, Yang et al 2008

Fulfills scaling law around QCP Gu et al 2009, Albuquerque et al 2010

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No need for local order parameter e.g. Kitaev model, Abasto et al 2008, Yang et al 2008

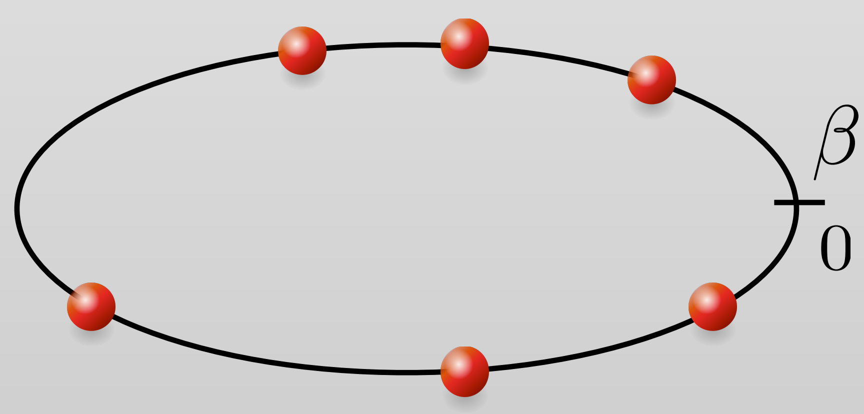
Fulfills scaling law around QCP Gu et al 2009, Albuquerque et al 2010

However, very hard to compute, only a few limited tools

Fidelity Susceptibility Made Simple !

LW, Liu, Imriška, Ma and Troyer, 1502.06969

$$\chi_F = \frac{\langle k_L k_R \rangle - \langle k_L \rangle \langle k_R \rangle}{2\lambda^2}$$



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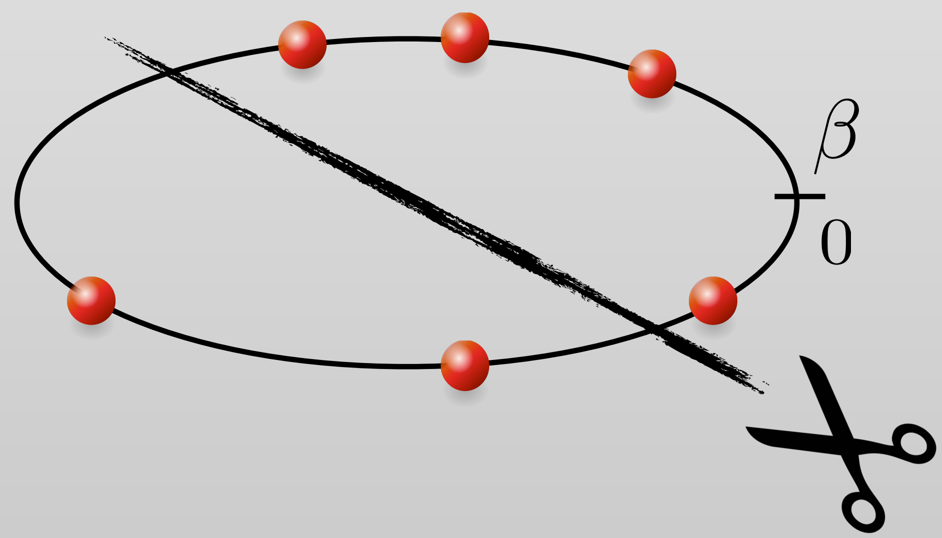

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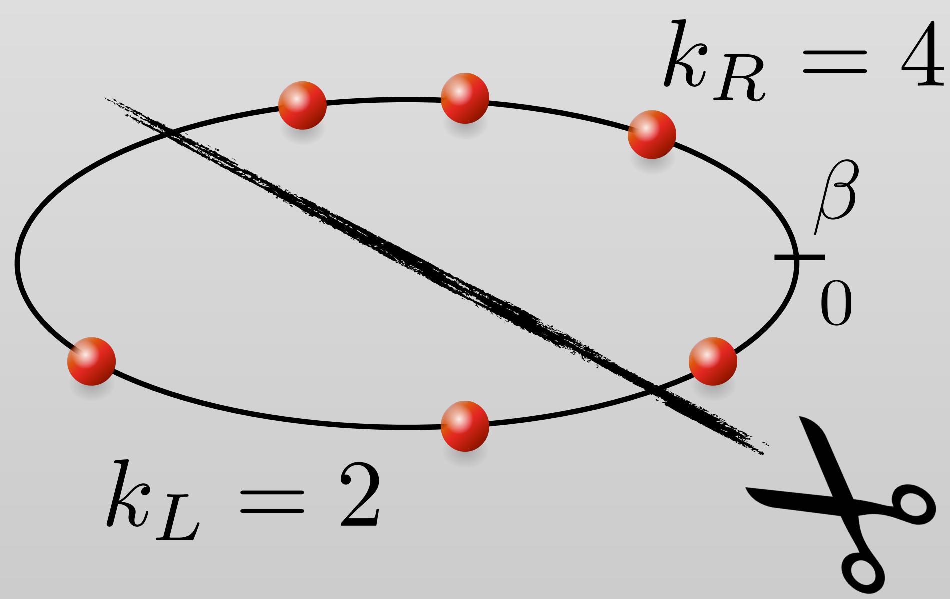


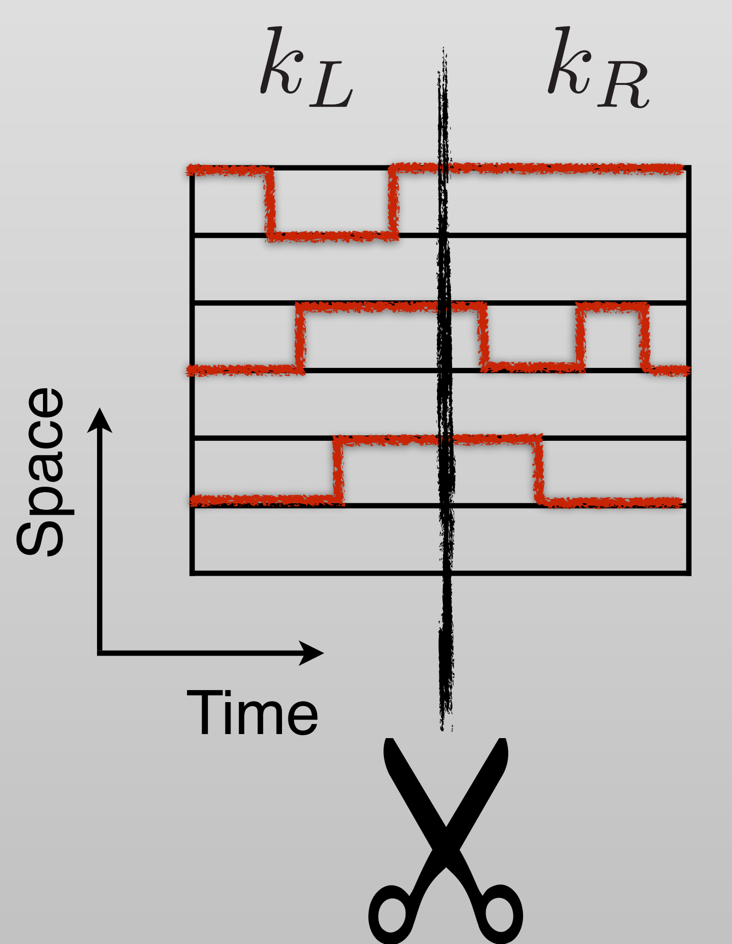
Fidelity Susceptibility Made Simple !

LW, Liu, Imriška, Ma and Troyer, 1502.06969

$$\chi_F = \frac{\langle k_L k_R \rangle - \langle k_L \rangle \langle k_R \rangle}{2\lambda^2}$$

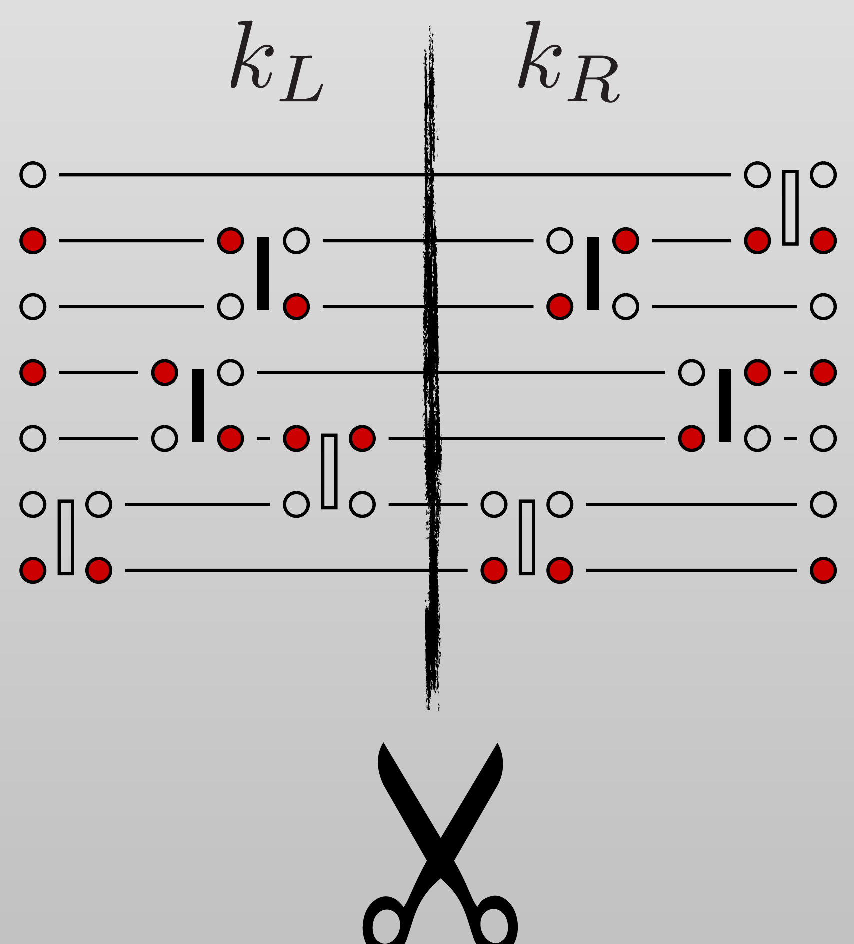
Worldline Algorithms

(bosons)



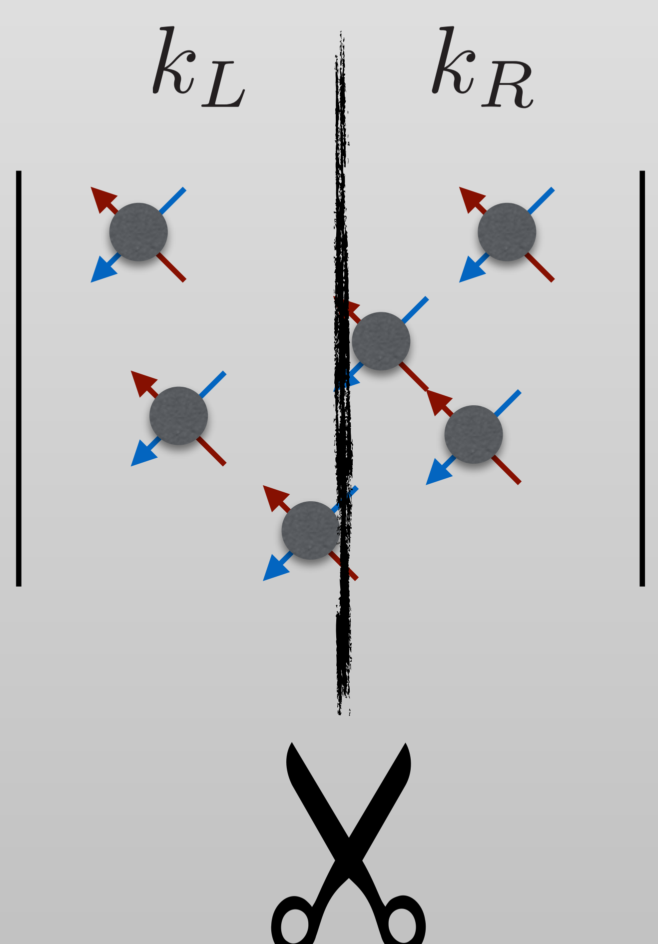
Stochastic Series Expansion

(quantum spins)



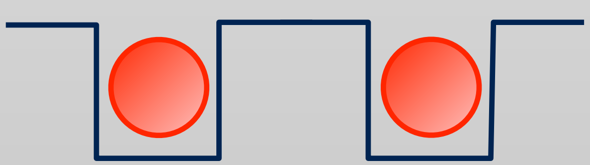
Determinantal Methods

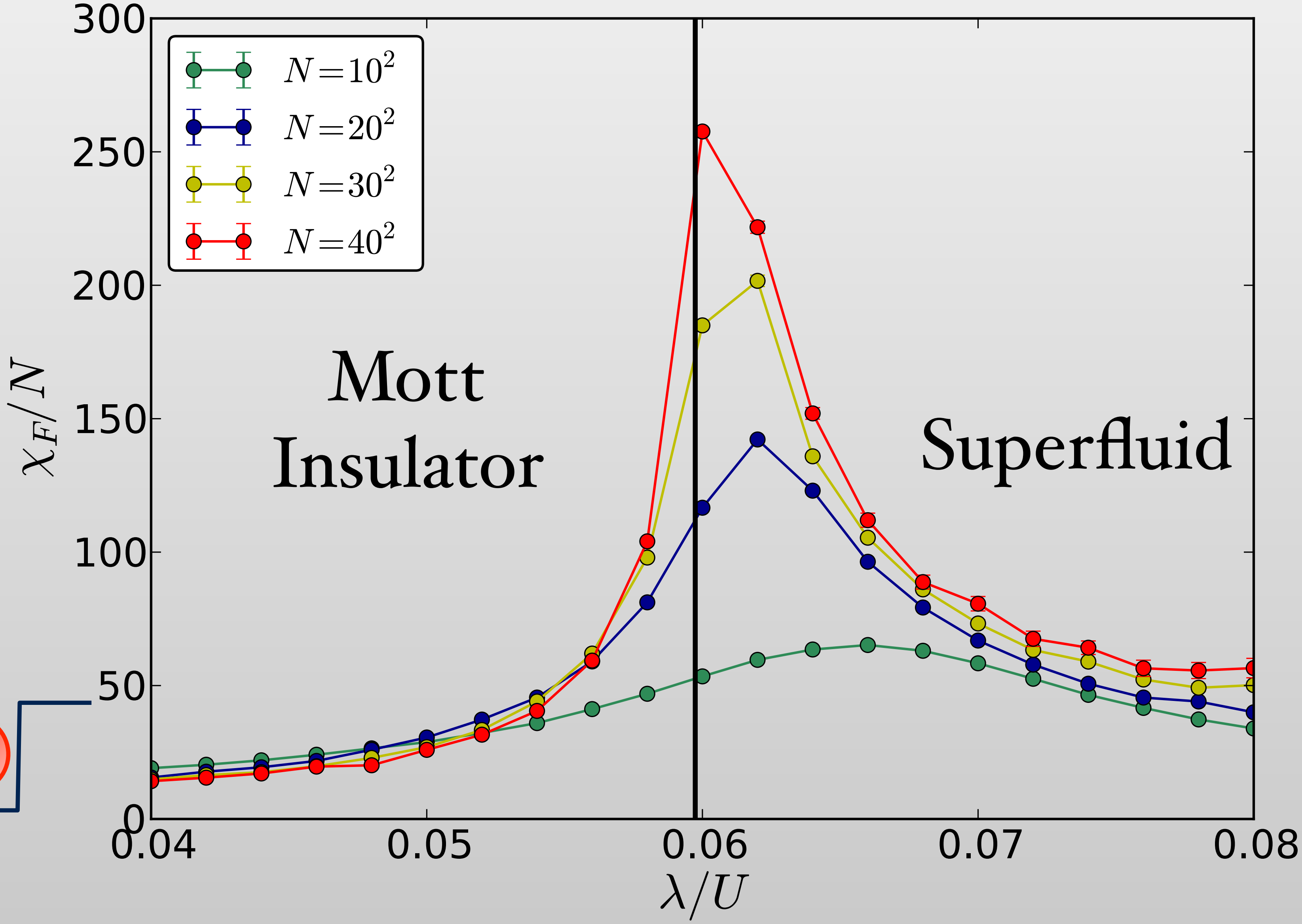
(fermions)

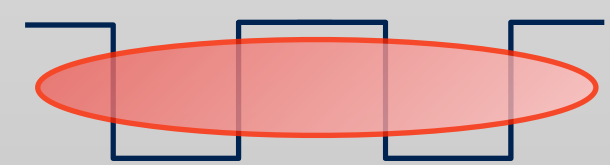


Bose-Hubbard Model

$$\hat{H} = \frac{U}{2} \sum_i \hat{n}_i \left(\hat{n}_i - 1 \right) - \lambda \sum_{\langle i,j \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i \right)$$





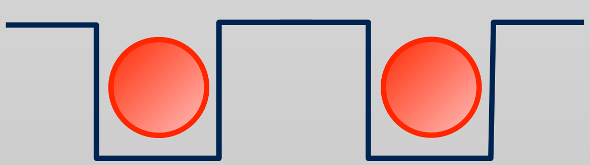


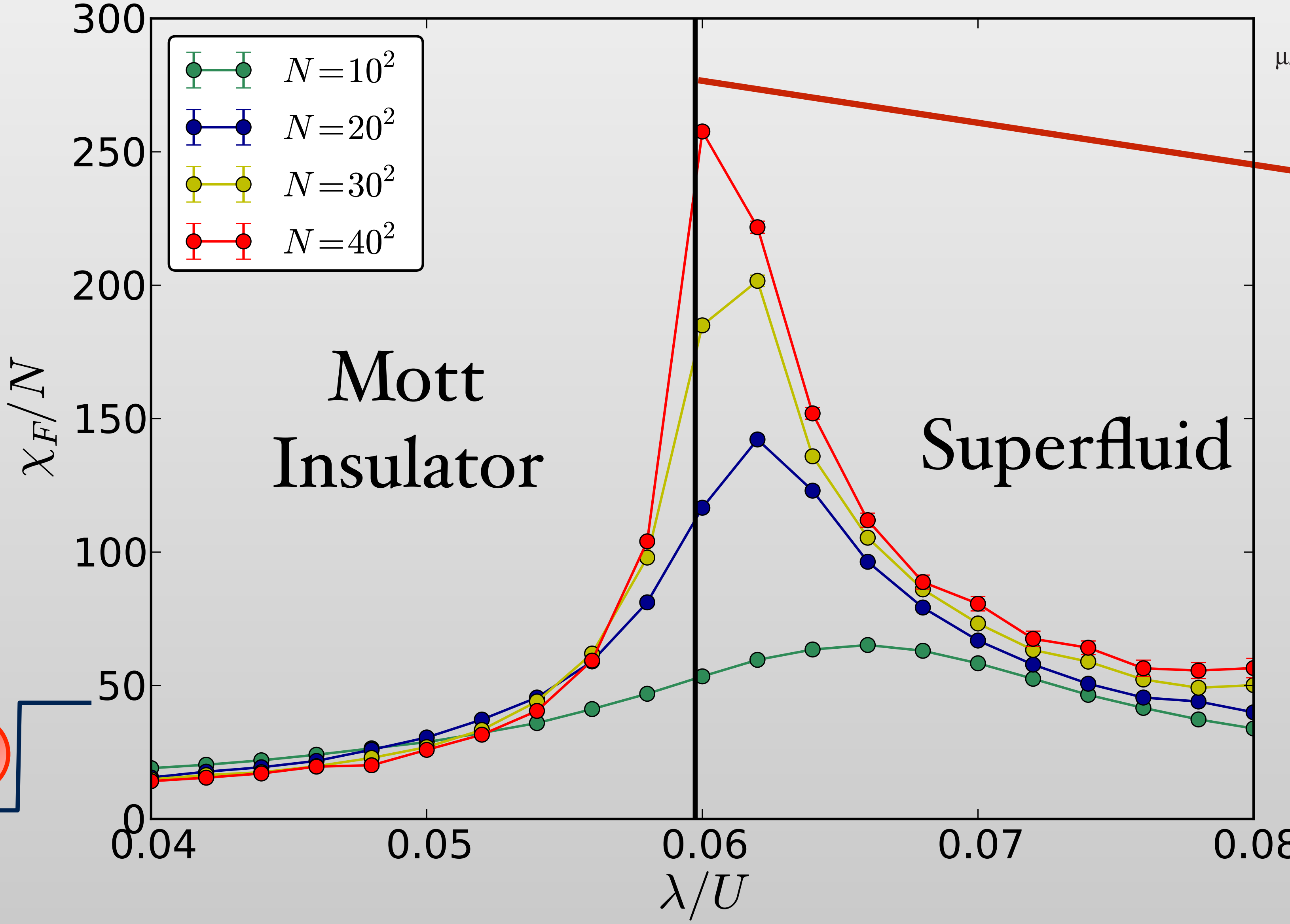
Divergence of fidelity susceptibility

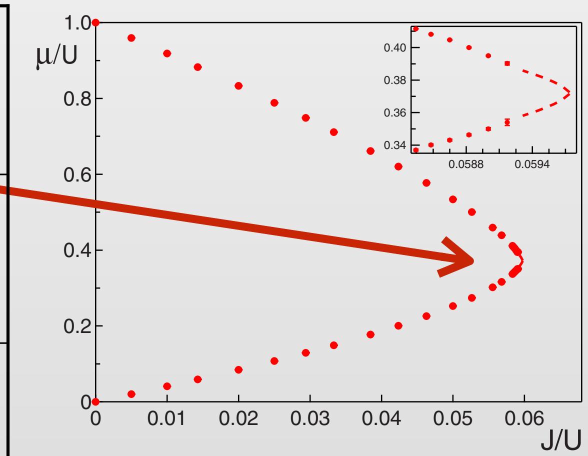
correctly single out the quantum critical point

Bose-Hubbard Model

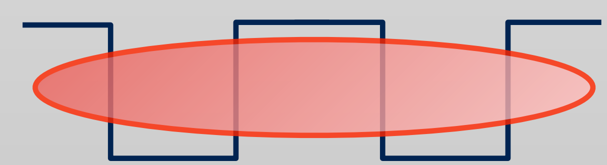
$$\hat{H} = \frac{U}{2}\sum_i \hat{n}_i\left(\hat{n}_i - 1\right) - \lambda \sum_{\langle i,j\rangle}\left(\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i\right)$$







Capogrosso-Sansone, et al., PRA, **77**, 015602 (2008)

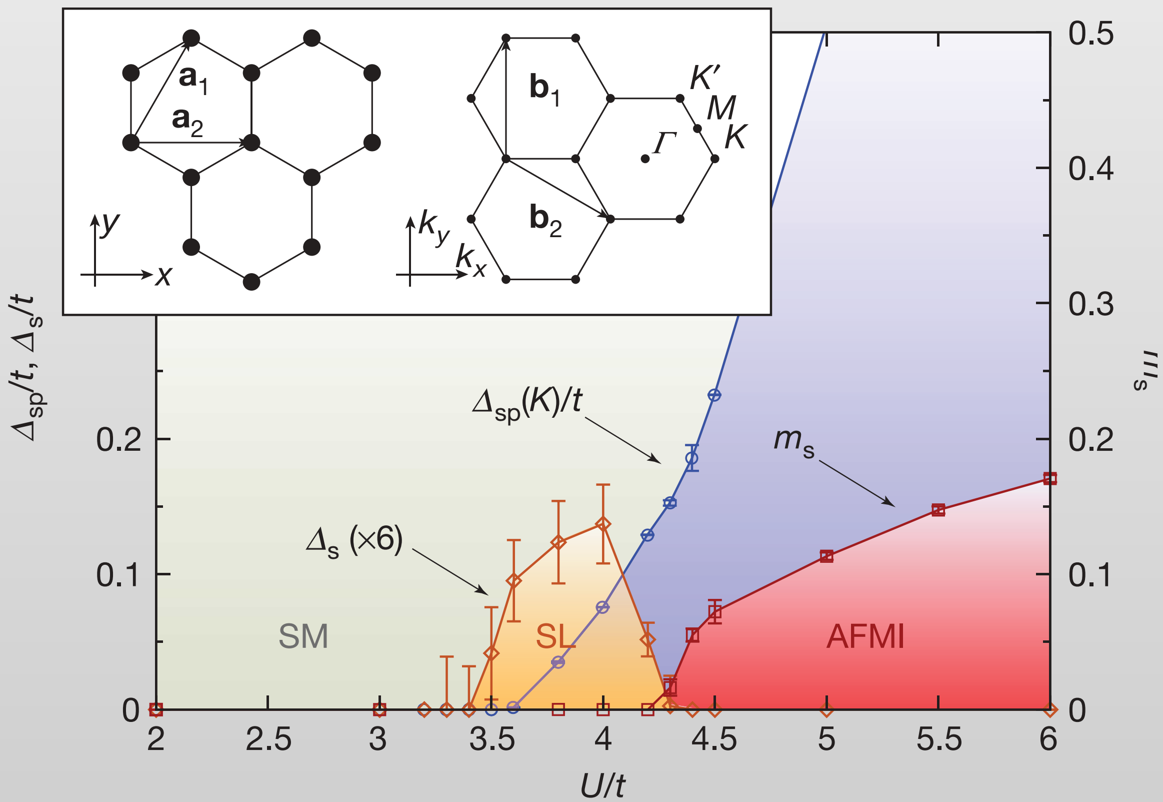


Divergence of fidelity susceptibility correctly single out the quantum critical point

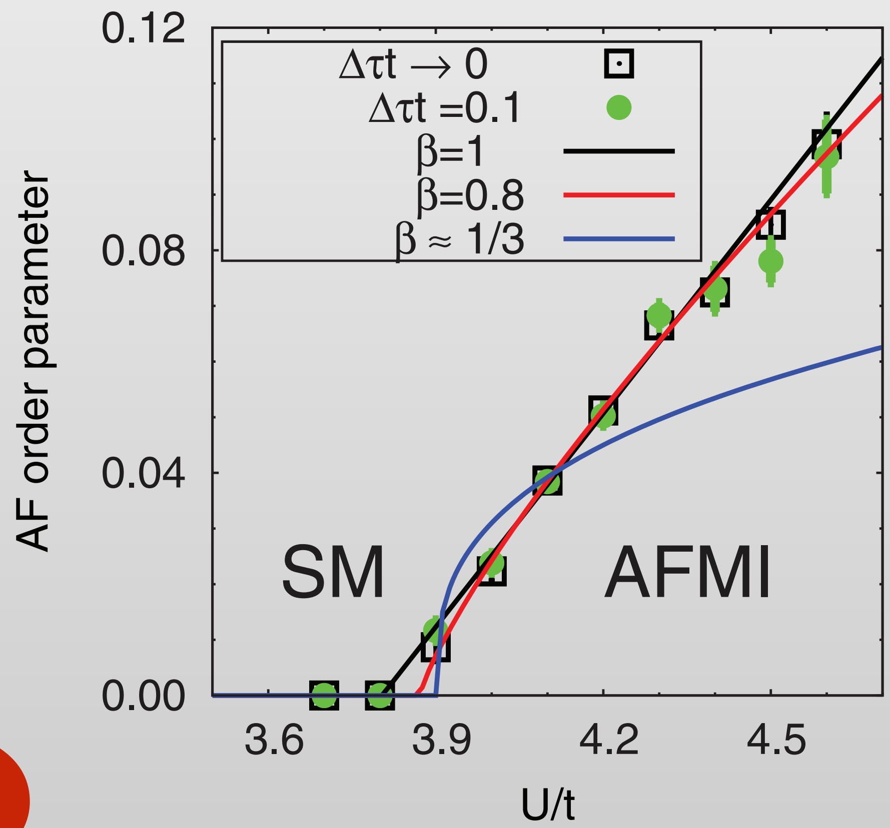
Honeycomb Hubbard Model

$$\hat{H} = -t \sum_{\langle i,j \rangle} \sum_{\sigma = \{\uparrow,\downarrow\}} \left(\hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^\dagger_{j\sigma} \hat{c}_{i\sigma} \right) + \lambda \sum_i \left(\hat{n}_{i\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i\downarrow} - \frac{1}{2} \right)$$

Meng et al, Nature 2010



Sorella et al, Sci.Rep 2012



?

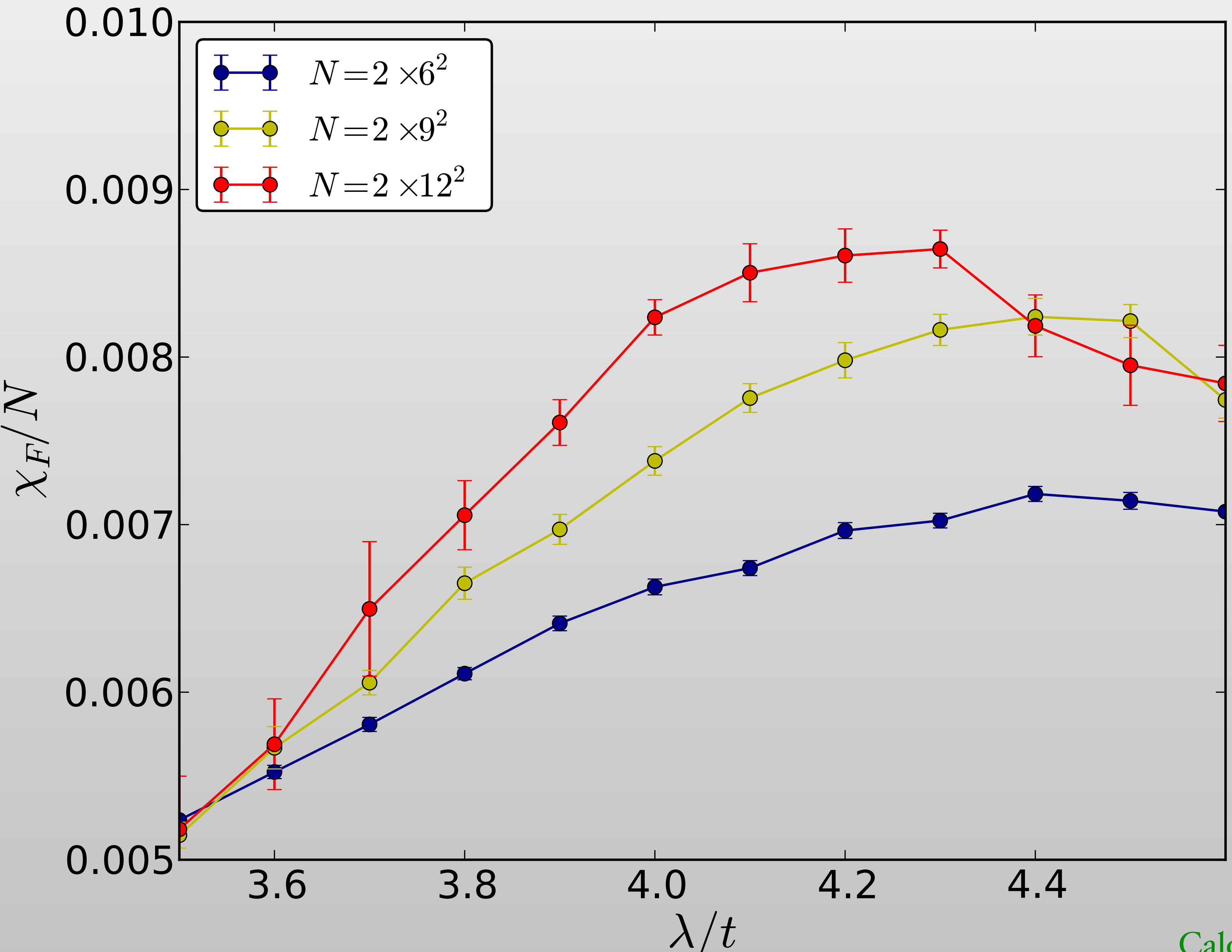
cf. Assaad et al, PRX 2013
Toldin et al, PRB 2015

A hotly debated problem in recent years

There is only one peak !

Suggesting a single transition,

i.e. no intermediate phase



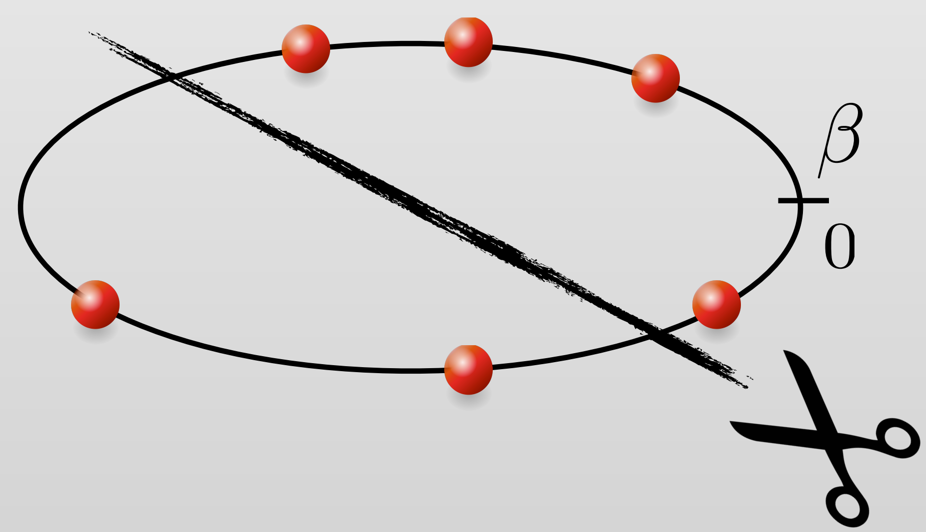
Calculated using LCT-INT
cf. 1411.0683 & 1501.00986

Why it works ?

$$\chi_F = \frac{\langle k_L k_R \rangle - \langle k_L \rangle \langle k_R \rangle}{2\lambda^2}$$

$$Z = \sum_{k=0}^{\infty} \lambda^k \int_0^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^{\beta} d\tau_k \times \mathrm{Tr}\left[(-1)^k e^{-(\beta-\tau_k)\hat{H}_0} \hat{H}_1 \ldots \hat{H}_1 e^{-\tau_1 \hat{H}_0}\right]$$

fugacity



Quantum Phase Transition

Classical Particle Condensation

cf. Anderson and Yuval, 1969

Maps the Kondo model to a classical Coulomb gas

Summary-II

Fidelity Susceptibility: A general purpose indicator of quantum phase transition

Thanks to my collaborators !

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Ping Nang Ma

Matthias Troyer

Summary-II

Fidelity Susceptibility: A general purpose
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Thank You !