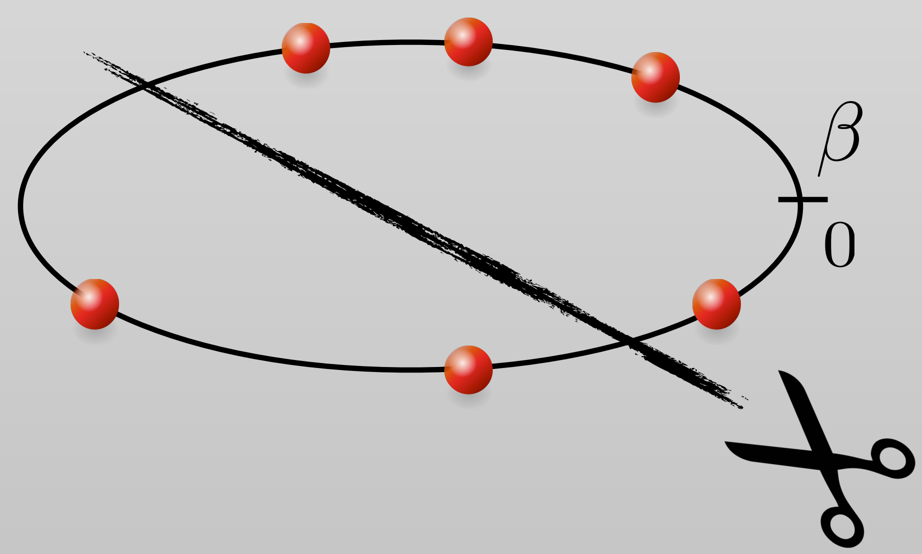
From Fidelity Susceptibility to Recommender Engines

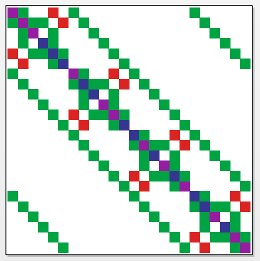
Lei Wang

Institute of Physics, CAS



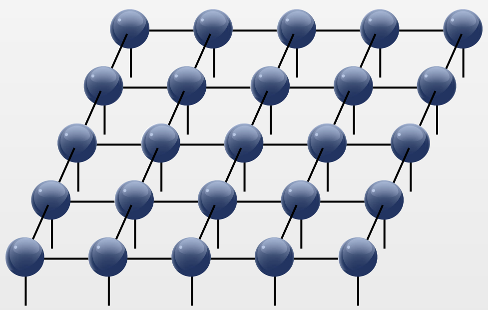
http://wangleiphy.github.io/

Algorithms for quantum many-body systems

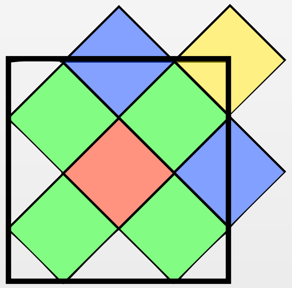


exact diagonalization

quantum Monte Carlo

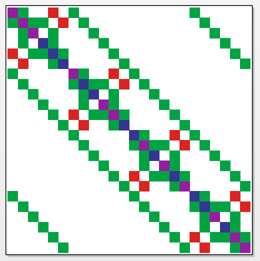


tensor network states



dynamical mean field theories

Algorithms for quantum many-body systems



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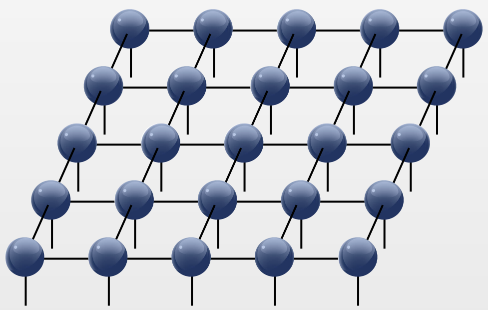

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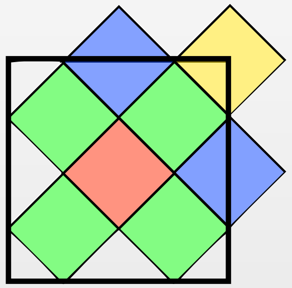
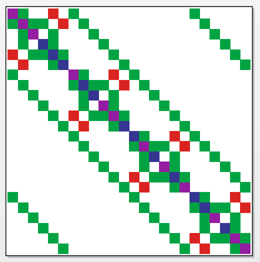


dynamical mean field theories

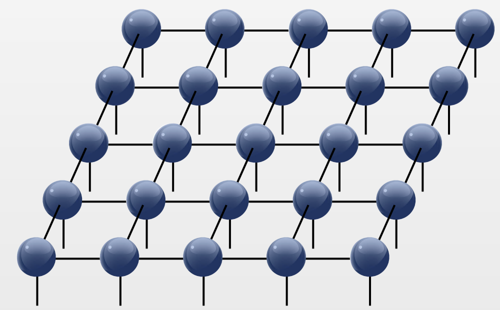
Algorithmic improvement in past 20 years outperformed Moore’s law

Algorithms for quantum many-body systems

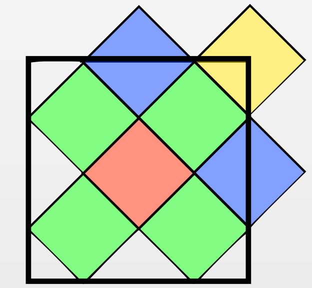


exact diagonalization

quantum Monte Carlo



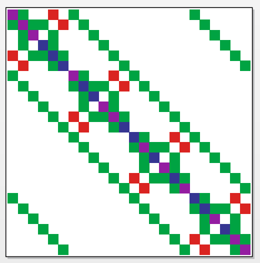
tensor network states



dynamical mean field theories

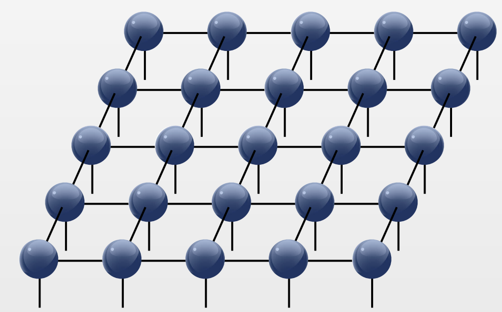
is faster than

Algorithms for quantum many-body systems

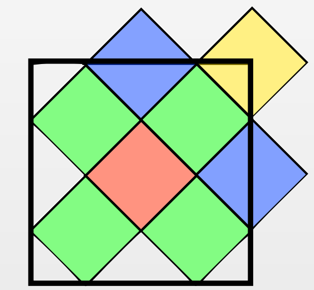


exact
diagonalization

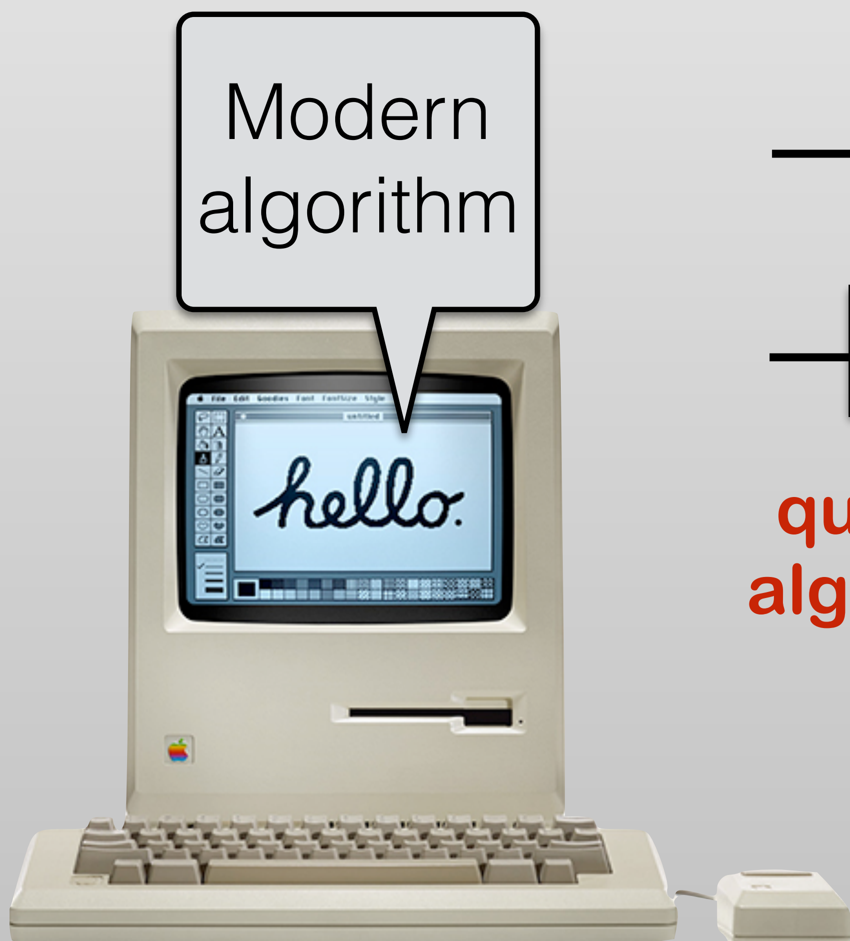
quantum
Monte Carlo

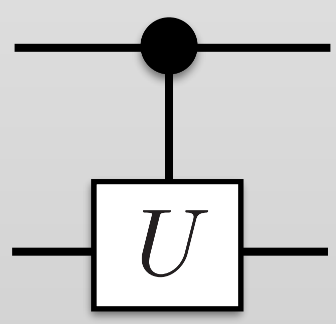


tensor network
states

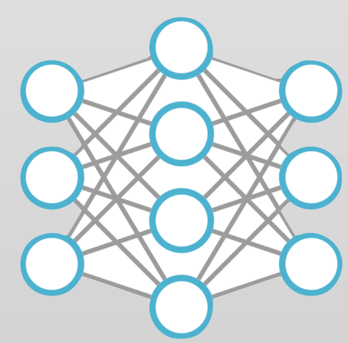


dynamical mean
field theories

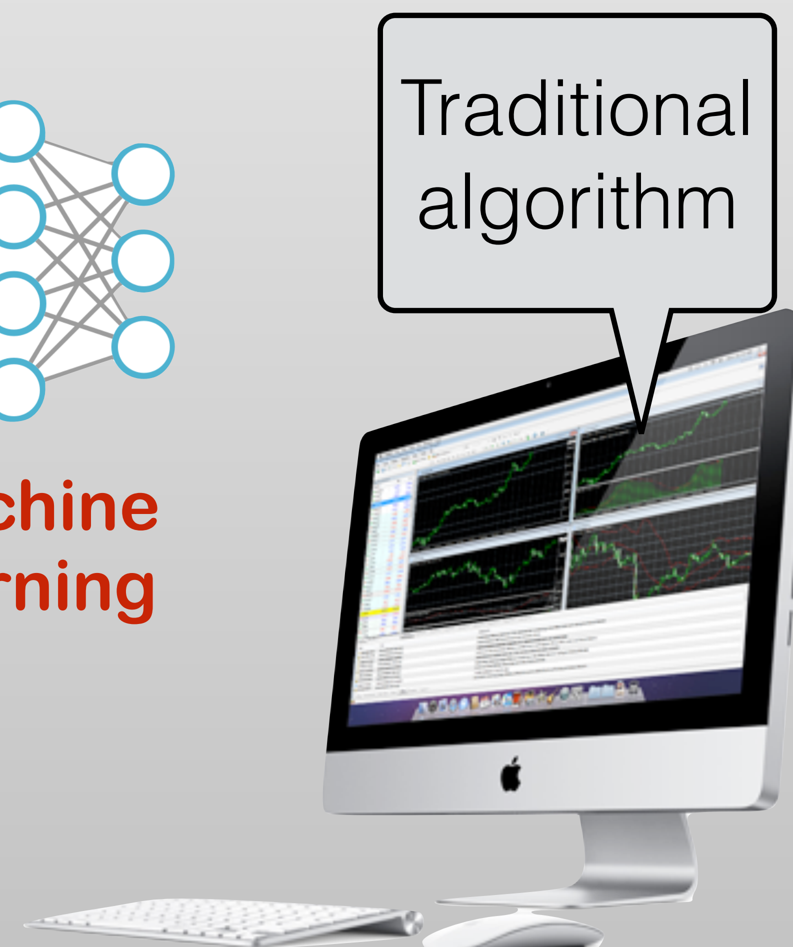


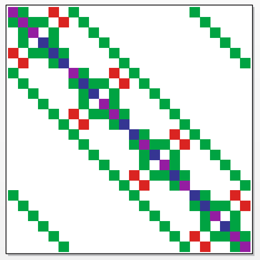


quantum
algorithms



machine
learning





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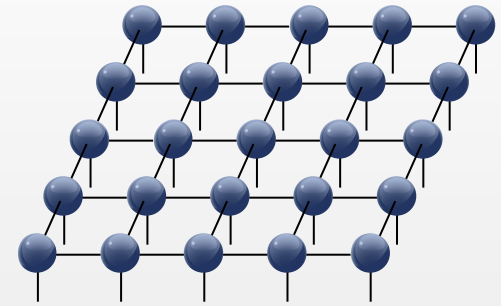
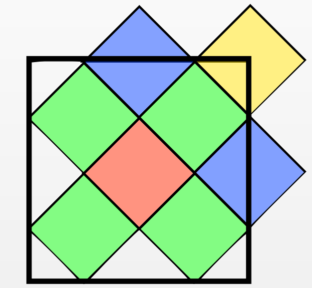


tensor network states



dynamical mean field theories

better scaling

Iazzi and Troyer, PRB 2015

LW, Iazzi, Corboz and Troyer, PRB 2015

Liu and LW, PRB 2015

LW, Liu and Troyer, PRB 2016

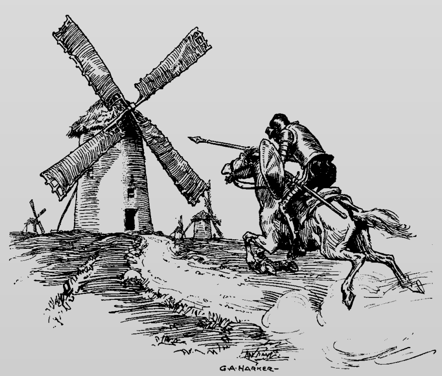
entanglement & fidelity

LW and Troyer, PRL 2014

LW, Liu, Imriška, Ma and Troyer, PRX 2015

LW, Shinaoka and Troyer, PRL 2015

Huang, Wang, LW and Werner, arXiv 2016



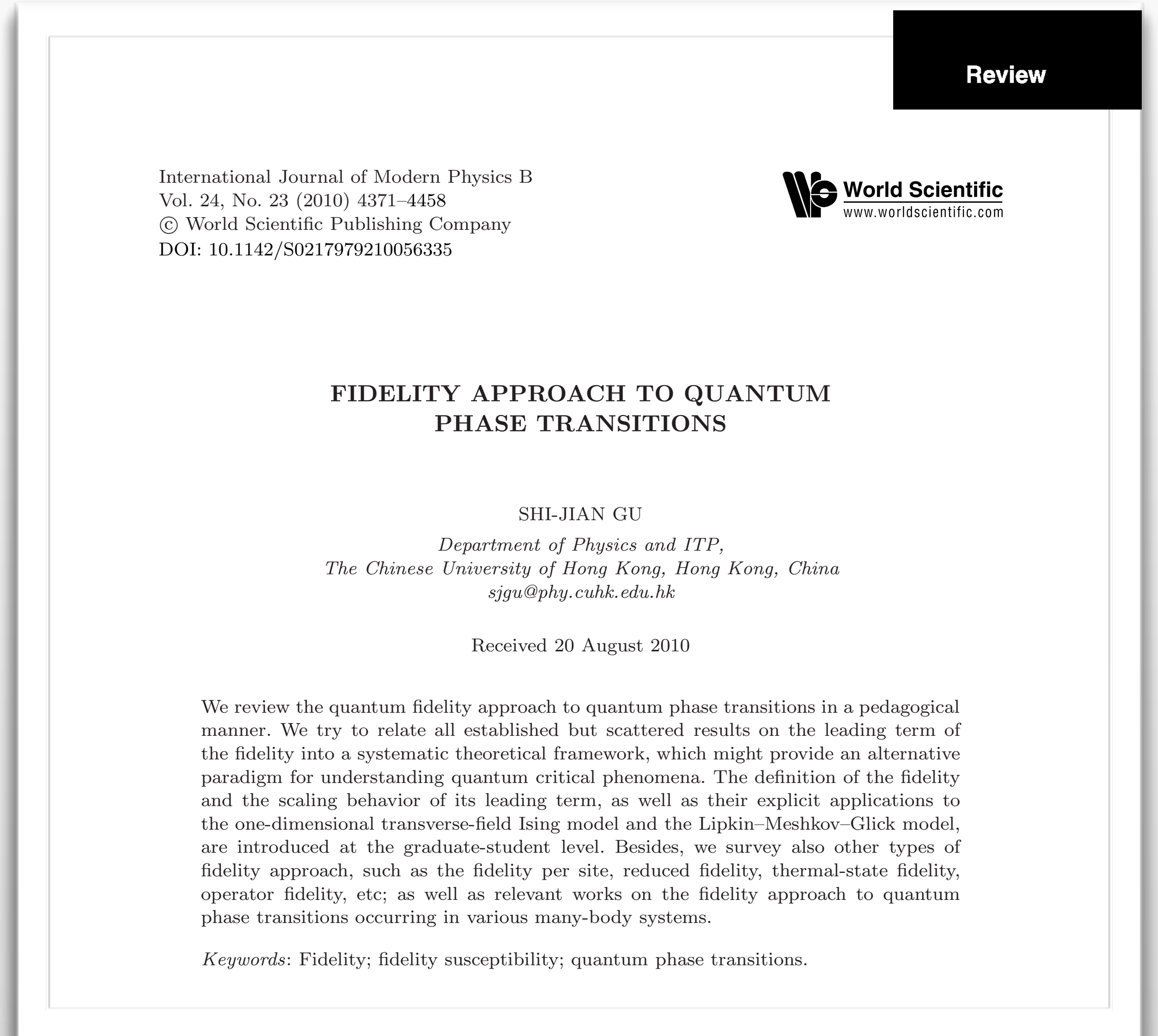
sign problem

Huffman and Chandrasekharan, PRB 2014

Li, Jiang and Yao, PRB 2015

LW, Liu, Iazzi, Troyer and Harcos, PRL 2015

Wei, Wu, Li, Zhang and Xiang, PRL 2016


Review

International Journal of Modern Physics B
Vol. 24, No. 23 (2010) 4371–4458

DOI: 10.1142/S0217979210056335

World Scientific
www.worldscientific.com

FIDELITY APPROACH TO QUANTUM PHASE TRANSITIONS

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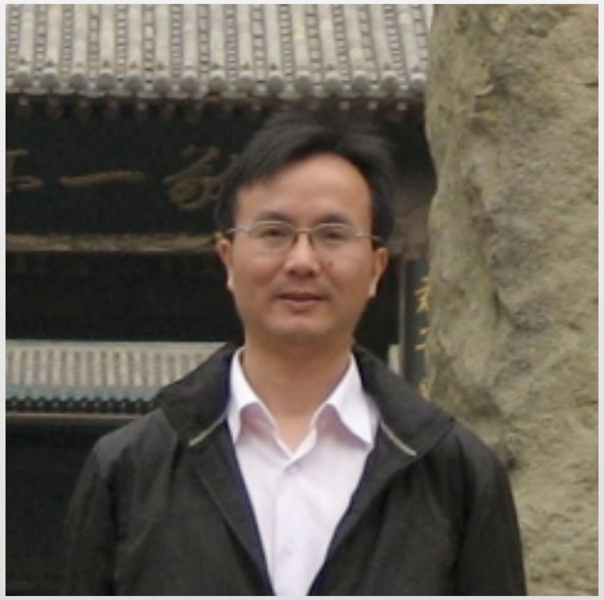
Received 20 August 2010

We review the quantum fidelity approach to quantum phase transitions in a pedagogical manner. We try to relate all established but scattered results on the leading term of the fidelity into a systematic theoretical framework, which might provide an alternative paradigm for understanding quantum critical phenomena. The definition of the fidelity and the scaling behavior of its leading term, as well as their explicit applications to the one-dimensional transverse-field Ising model and the Lipkin–Meshkov–Glick model, are introduced at the graduate-student level. Besides, we survey also other types of fidelity approach, such as the fidelity per site, reduced fidelity, thermal-state fidelity, operator fidelity, etc; as well as relevant works on the fidelity approach to quantum phase transitions occurring in various many-body systems.

Keywords: Fidelity; fidelity susceptibility; quantum phase transitions.



顧世建教授

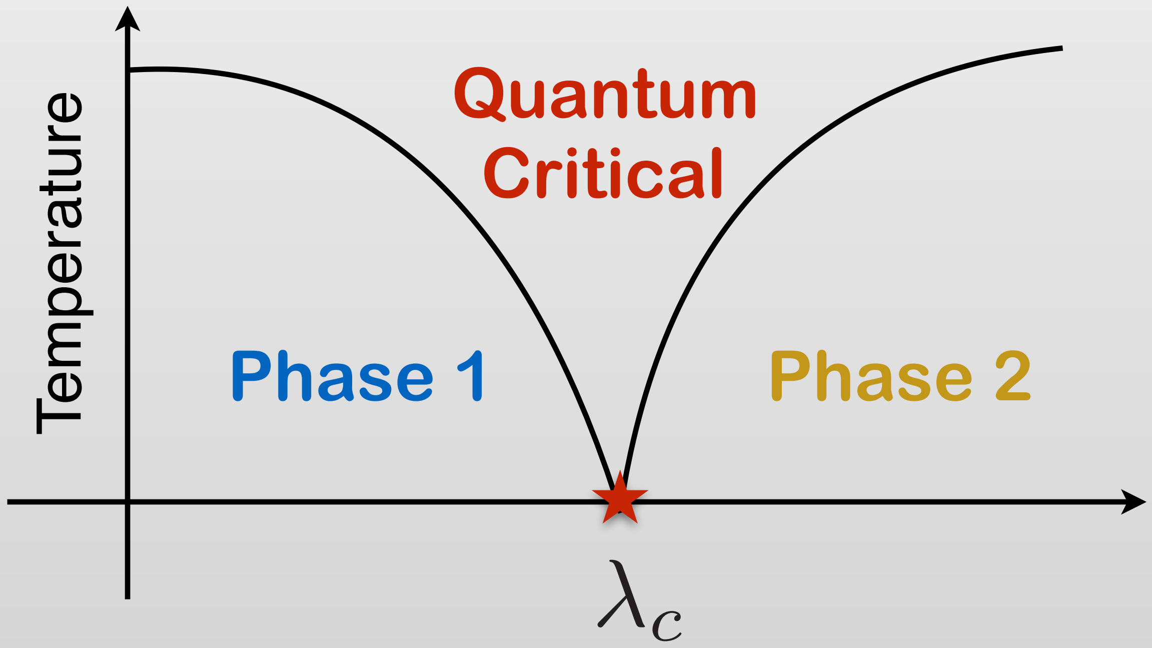
News on Fidelity Susceptibility

LW, Liu, Imriška, Ma and Troyer, PRX 2015
LW, Shinaoka and Troyer, PRL 2015

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



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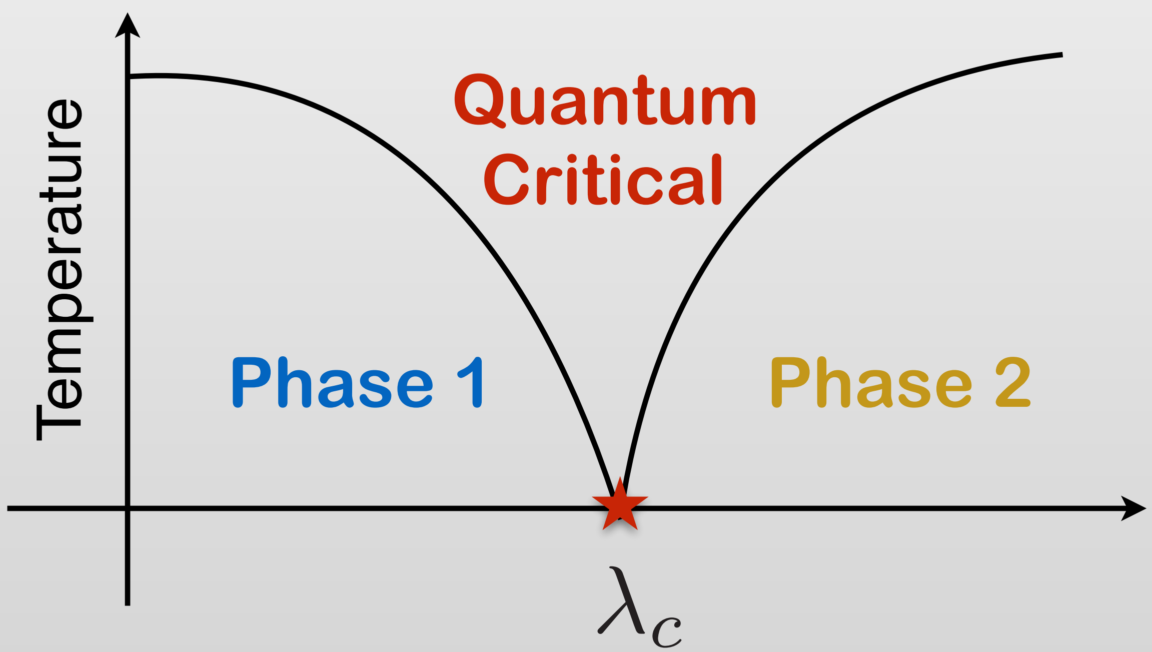

Fidelity $F(\lambda, \epsilon) = |\langle \Psi_0(\lambda) | \Psi_0(\lambda + \epsilon) \rangle|$

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

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

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

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A general indicator of quantum phase transitions

No need for local order parameters 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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Fulfills scaling law around QCP Gu et al 2009, Albuquerque et al 2010

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

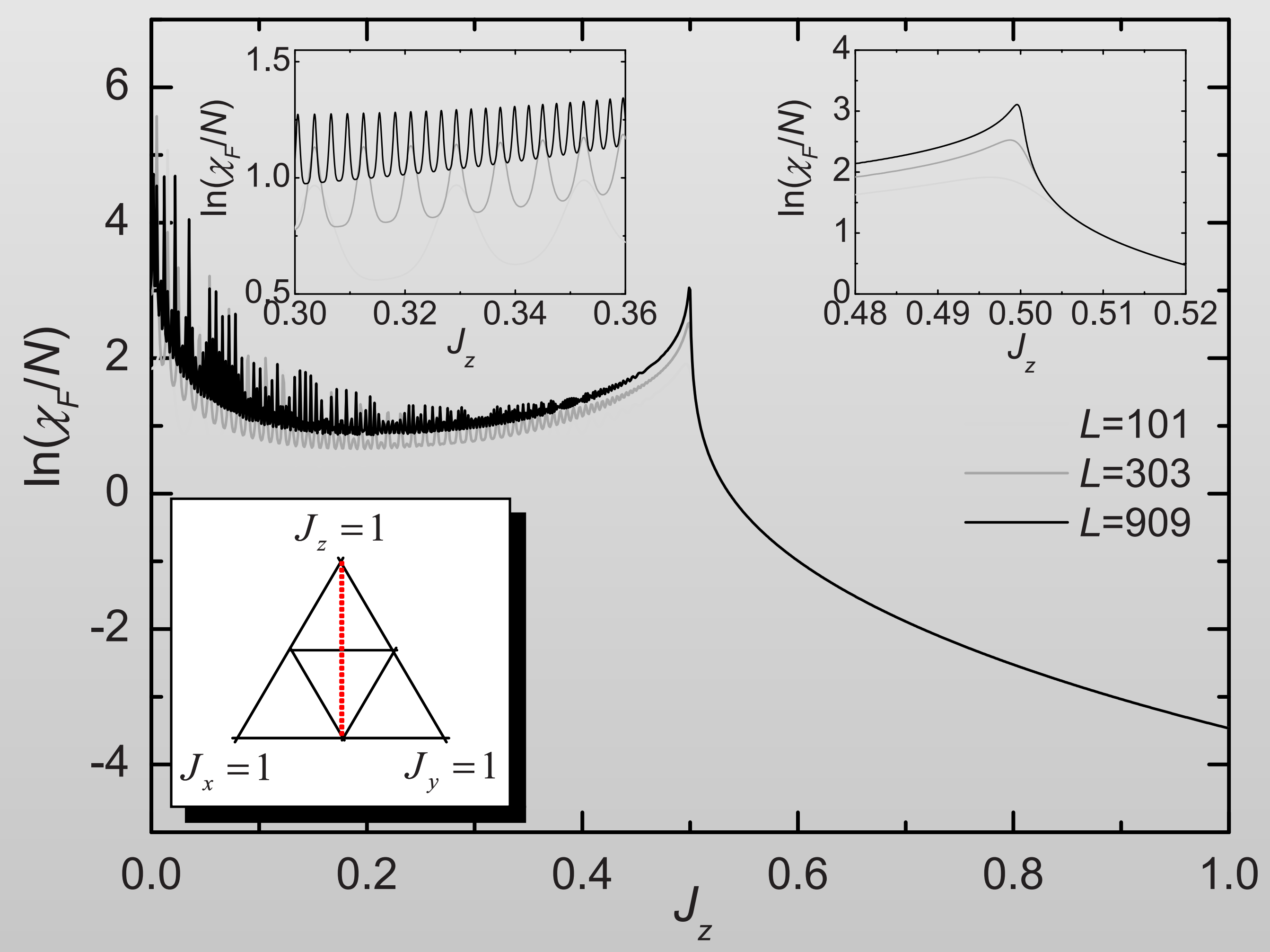
PHYSICAL REVIEW A **78**, 012304 (2008)

Fidelity susceptibility and long-range correlation in the Kitaev honeycomb model

Shuo Yang,[1,2] Shi-Jian Gu,[1,*] Chang-Pu Sun,[2] and Hai-Qing Lin[1]
[1]*Department of Physics and ITP, The Chinese University of Hong Kong, Hong Kong, China*
[2]*Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, 100080, China*
(Received 27 March 2008; published 2 July 2008)

- Exactly solvable model
- A simple analytical formula for χ_F

$$\chi_F = \frac{1}{16}\sum_{\mathbf{q}}\left(\frac{\sin q_x + \sin q_y}{\epsilon_{\mathbf{q}}^2 + \Delta_{\mathbf{q}}^2}\right)^2.$$



PHYSICAL REVIEW B **80**, 094529 (2009)

Fidelity and superconductivity in two-dimensional *t-J* models

Marcos Rigol
Department of Physics, Georgetown University, Washington, DC 20057, USA

B. Sriram Shastry
Department of Physics, University of California, Santa Cruz, California 95064, USA

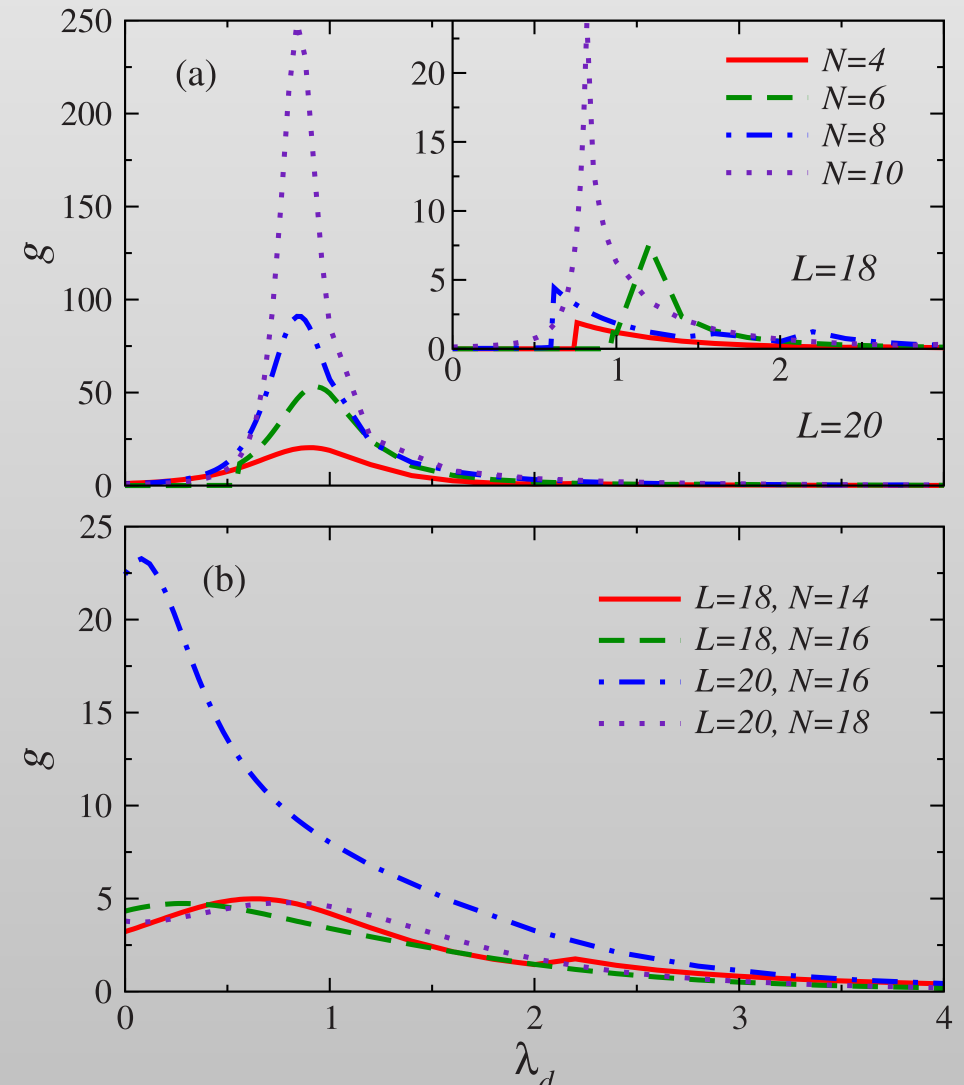
Stephan Haas
Department of Physics and Astronomy, University of Southern California, Los Angeles, California 90089, USA

(Received 29 June 2009; revised manuscript received 25 August 2009; published 29 September 2009)

Exact diagonalization on small clusters

$$g(\lambda, \delta\lambda) \equiv \frac{2}{L}\frac{1-F(\lambda,\delta\lambda)}{\delta\lambda^2}$$

$$\delta\lambda = 10^{-5}$$



Is there a general way to compute χ_F ?

Fidelity Susceptibility

Yu, et al., PRE, **76** 022101 (2007)

Differential form

L. Campos Venuti, et al., PRL **99**,095701 (2007)

$$\chi_F = \frac{\langle \partial_\lambda \Psi_0 | \partial_\lambda \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} - \frac{\langle \Psi_0 | \partial_\lambda \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \frac{\langle \partial_\lambda \Psi_0 | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

Real part of "quantum geometric tensor"

Fidelity Susceptibility

Yu, et al., PRE, **76** 022101 (2007)

Differential form

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Real part of "quantum geometric tensor"

Fidelity Susceptibility

Yu, et al., PRE, **76** 022101 (2007)

Perturbative form

$$\chi_F = \sum_{n \neq 0} \frac{| \langle \Psi_n | \hat{H}_1 | \Psi_0 \rangle |^2}{(E_0 - E_n)^2}$$

Related to second order derivative of energy

Differential form

L. Campos Venuti, et al., PRL **99**,095701 (2007)

$$\chi_F = \frac{\langle \partial_\lambda \Psi_0 | \partial_\lambda \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} - \frac{\langle \Psi_0 | \partial_\lambda \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \frac{\langle \partial_\lambda \Psi_0 | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

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Yu, et al., PRE, **76** 022101 (2007)

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Related to second order derivative of energy

Kubo form

$$\chi_F = \int_0^\infty d\tau \left[\langle \hat{H}_1(\tau) \hat{H}_1 \rangle - \langle \hat{H}_1 \rangle^2 \right] \tau$$

Extension to finite-temperature

Differential form

L. Campos Venuti, et al., PRL **99**,095701 (2007)

$$\chi_F = \frac{\langle \partial_\lambda \Psi_0 | \partial_\lambda \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} - \frac{\langle \Psi_0 | \partial_\lambda \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \frac{\langle \partial_\lambda \Psi_0 | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle}$$

Real part of "quantum geometric tensor"

Fidelity Susceptibility

Yu, et al., PRE, **76** 022101 (2007)

Perturbative form

$$\chi_F = \sum_{n \neq 0} \frac{| \langle \Psi_n | \hat{H}_1 | \Psi_0 \rangle |^2}{(E_0 - E_n)^2}$$

Related to second order derivative of energy

Kubo form

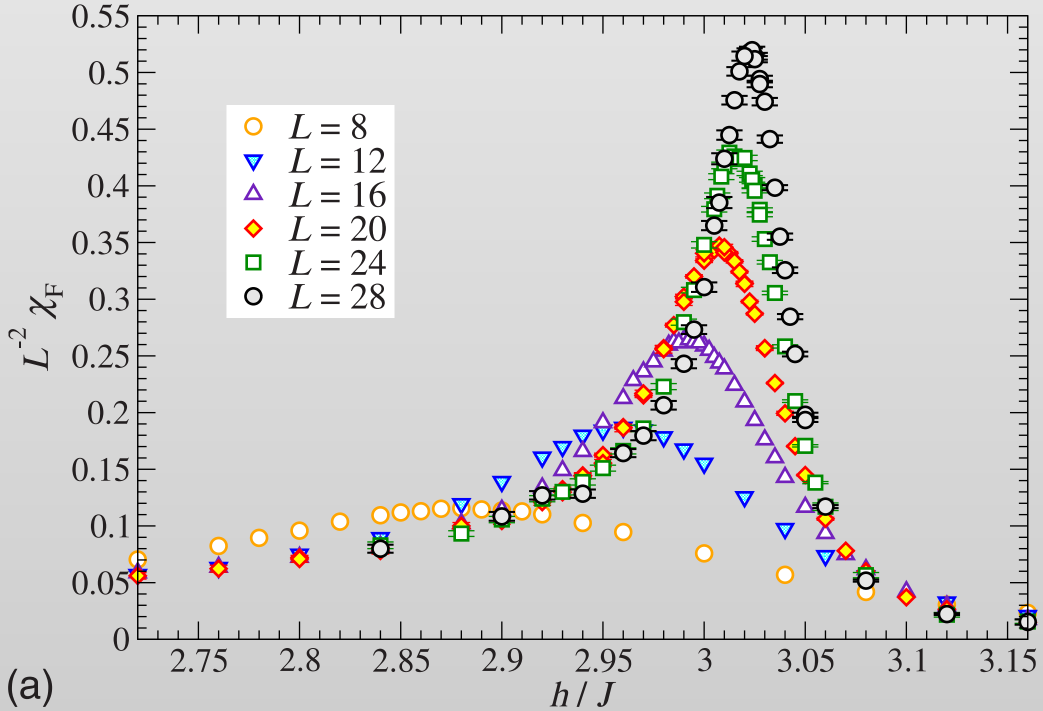
$$\chi_F = \int_0^{\beta/2} d\tau \left[\langle \hat{H}_1(\tau) \hat{H}_1 \rangle - \langle \hat{H}_1 \rangle^2 \right] \tau$$

Extension to finite-temperature

PHYSICAL REVIEW B **81**, 064418 (2010)

Quantum critical scaling of fidelity susceptibility

A. Fabricio Albuquerque, Fabien Alet, Clément Sire, and Sylvain Capponi
Laboratoire de Physique Théorique, (IRSAMC), Université de Toulouse (UPS), F-31062 Toulouse, France and LPT (IRSAMC), CNRS, F-31062 Toulouse, France
(Received 18 December 2009; published 18 February 2010)



2D transverse field
Ising model

PHYSICAL REVIEW B **81**, 064418 (2010)

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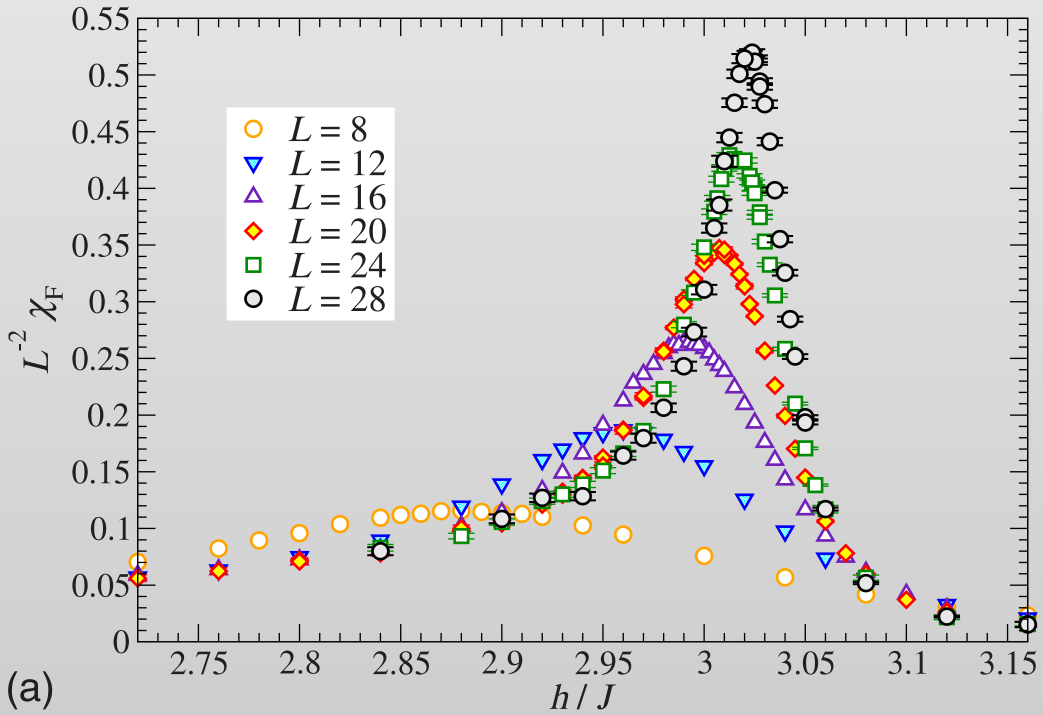


2D transverse field Ising model

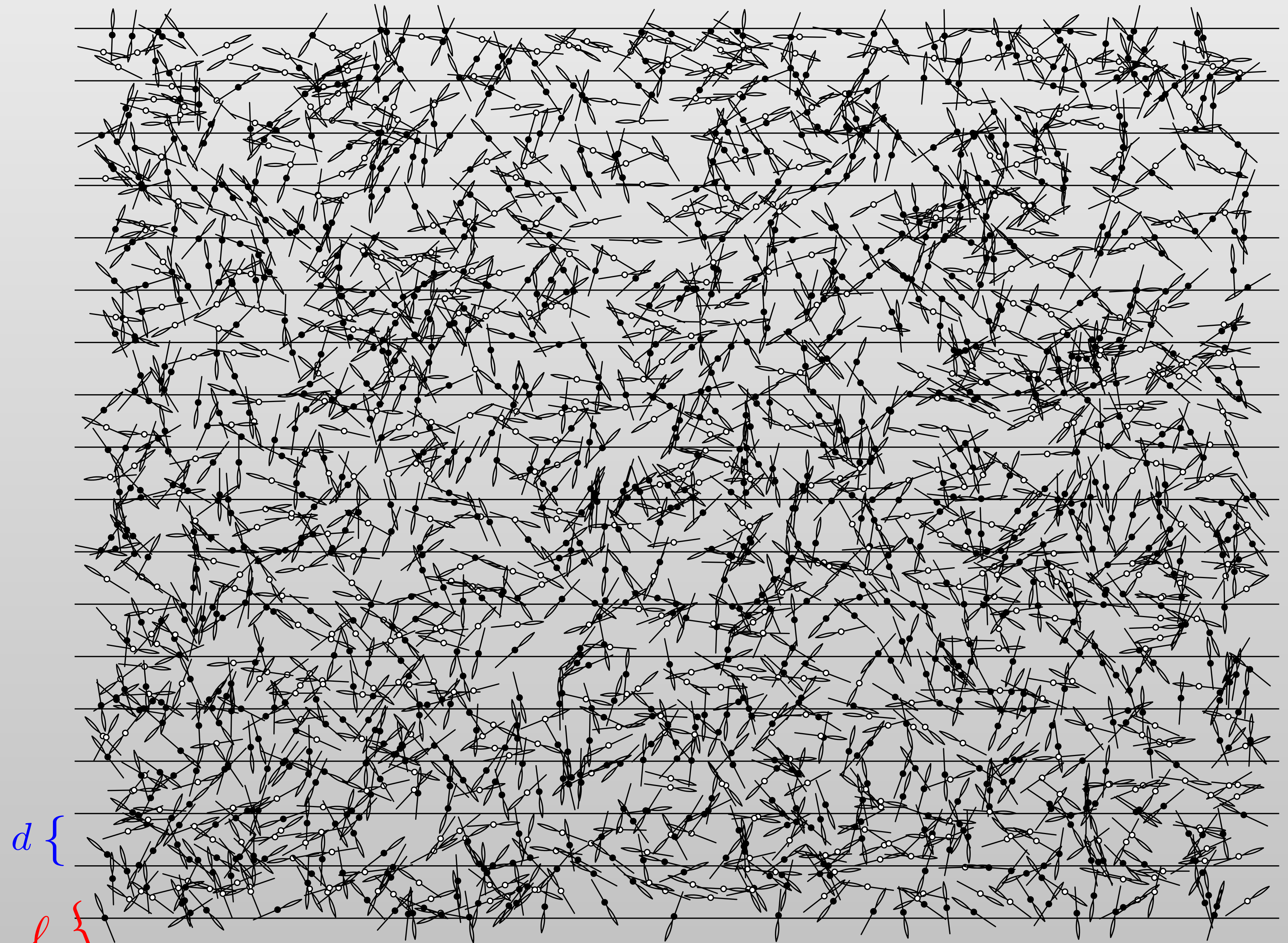
Imaginary-time correlator in stochastic series expansion

$$g^2\langle H_1(\tau)H_1(0)\rangle = \sum_{m=0}^{n-2} \frac{(n-1)!}{(n-m-2)!m!}\beta^{-n}(\beta-\tau)^{n-m-2}\tau^m\langle N_{gH_1}(m)\rangle_W$$

Can we do even better ?

The first recorded Monte Carlo simulation

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



Buffon 1777

Statistical Mechanics: Algorithms and Computations
Werner Krauth

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)

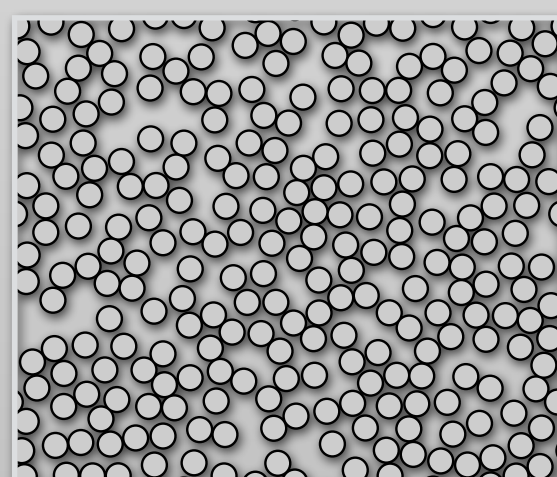
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional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

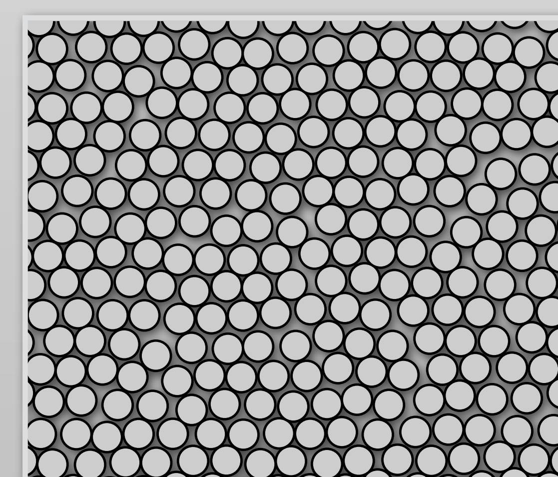
I. INTRODUCTION

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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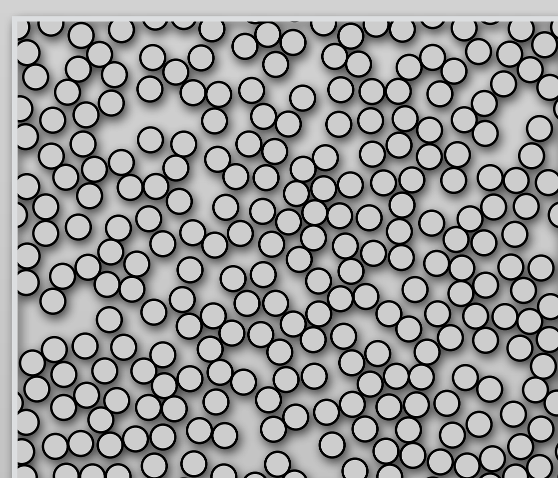
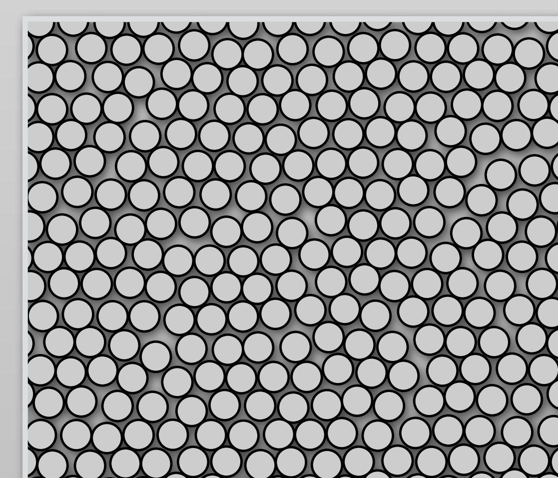


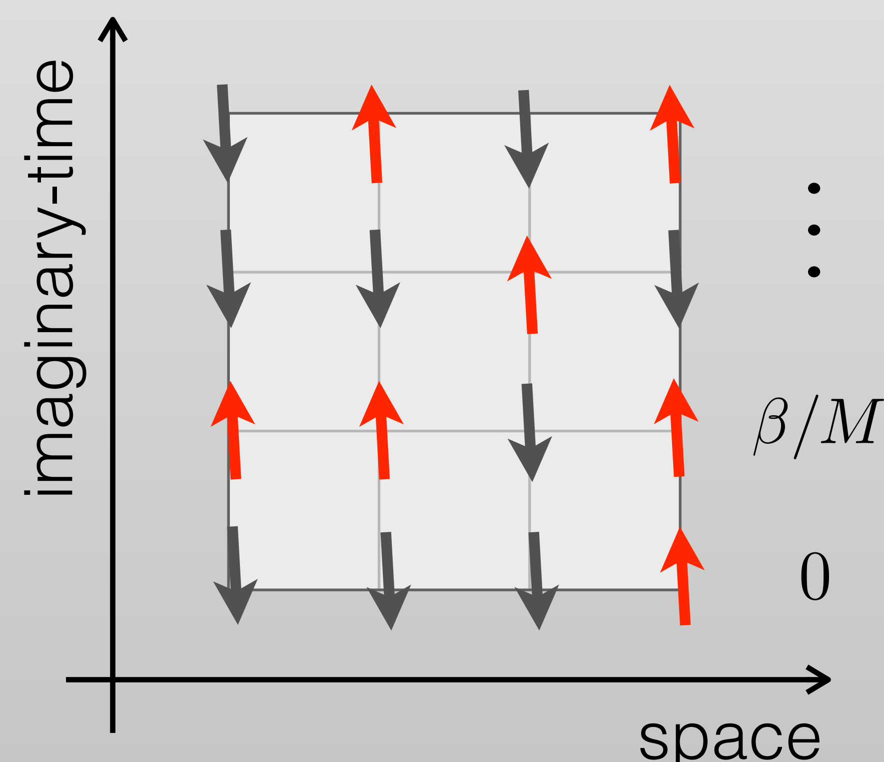


Quantum to classical mapping

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

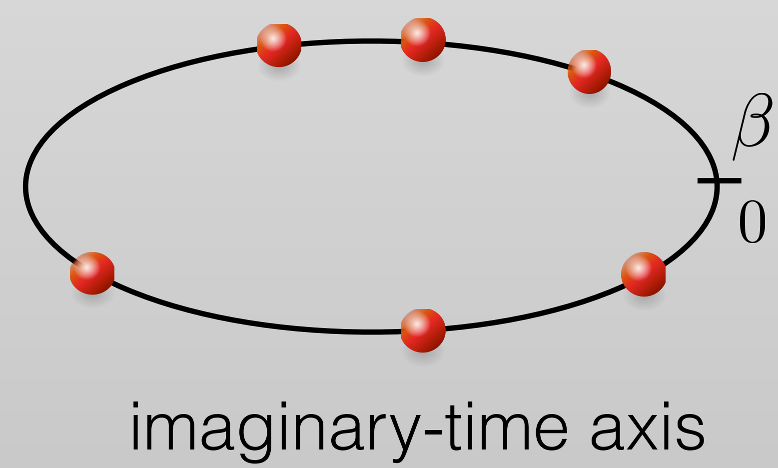
Trotterization

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



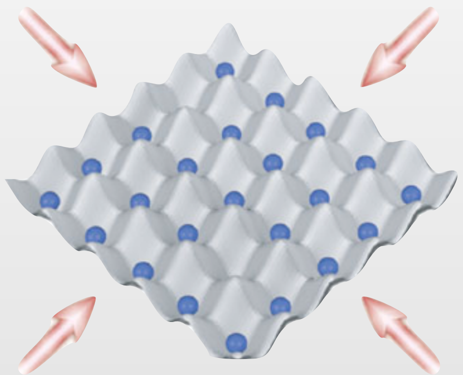
Diagrammatic approach

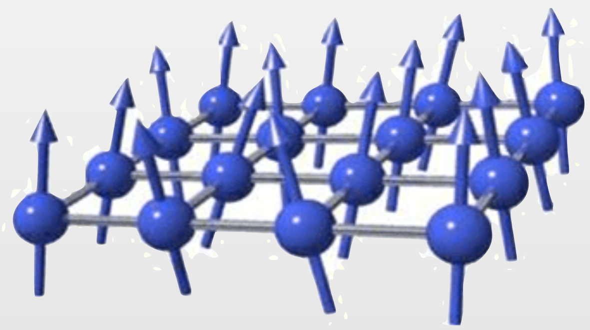
$$Z = \sum_{k=0}^{\infty} \lambda^k \int_0^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^{\beta} d\tau_k \times$$
$$\mathrm{Tr}\left[(-1)^k e^{-(\beta-\tau_k)\hat{H}_0} \hat{H}_1 \ldots \hat{H}_1 e^{-\tau_1 \hat{H}_0}\right]$$

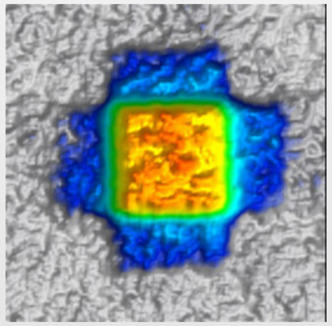


Beard and Wiese, 1996
Prokof'ev, Svistunov, Tupitsyn,1996

Diagrammatic approaches







bosons

World-line Approach

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

quantum spins

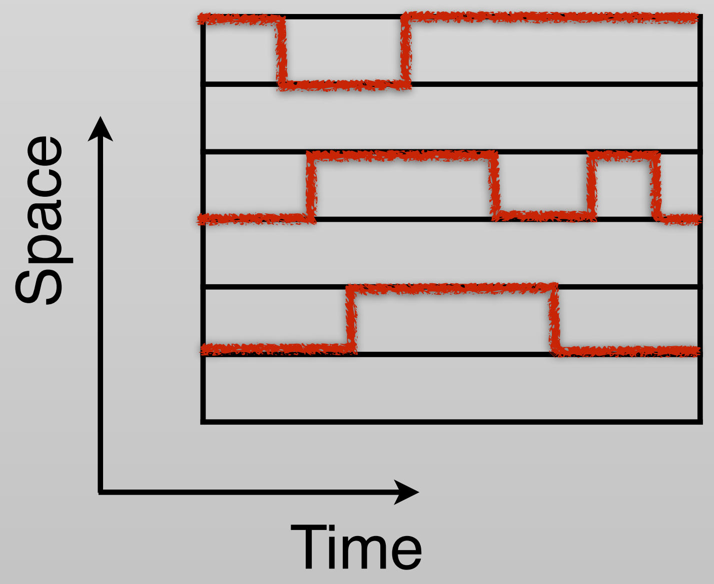
Stochastic Series Expansion

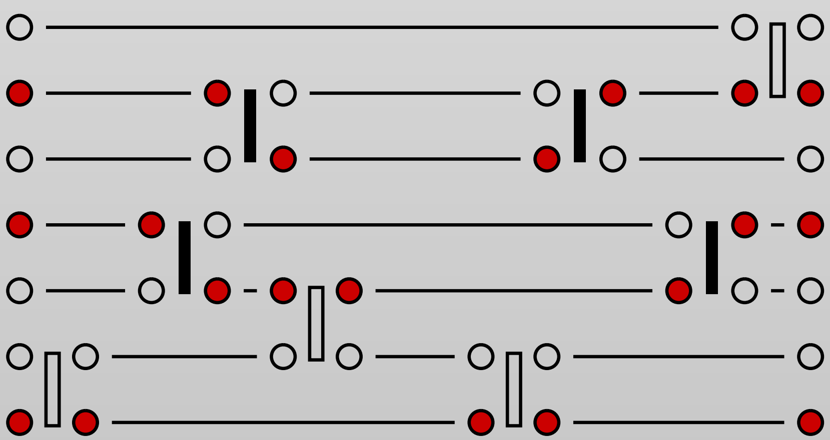
Sandvik et al, PRB, **43**, 5950 (1991)

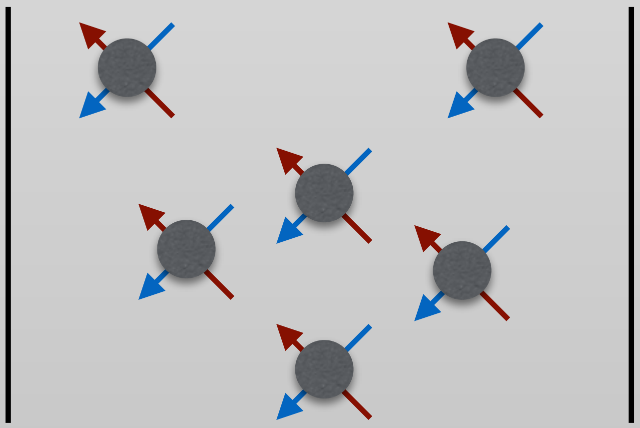
fermions

Determinantal Methods

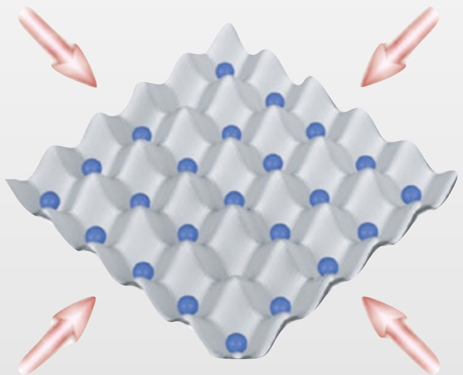
Gull et al, RMP, **83**, 349 (2011)

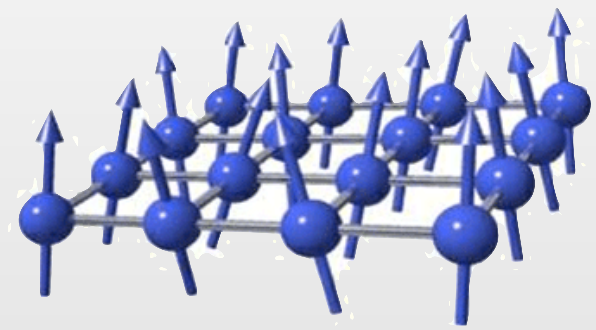


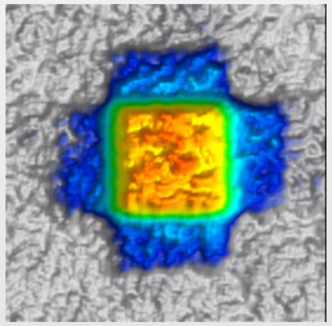




Diagrammatic approaches







bosons

World-line Approach

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

quantum spins

Stochastic Series Expansion

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fermions

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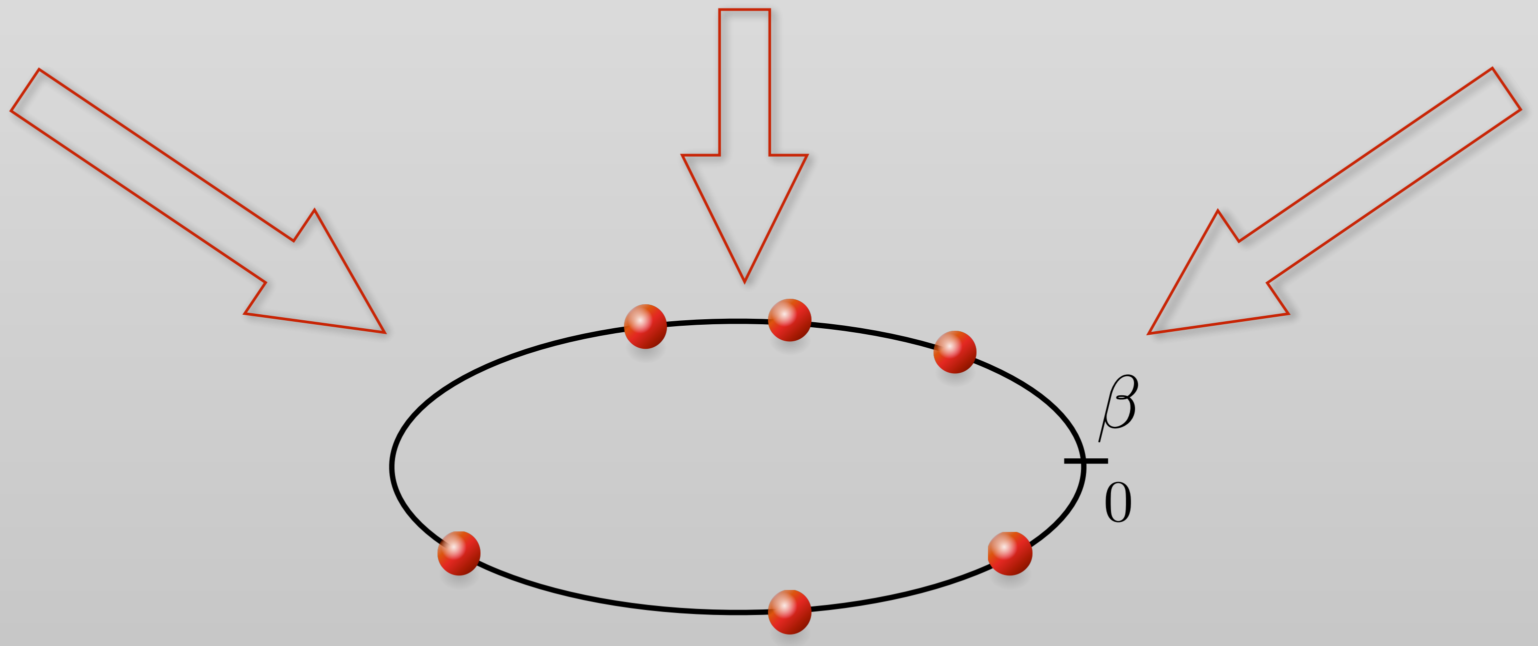

Diagrammatic determinant QMC

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

$$= \sum_{k=0}^{\infty} \lambda^k \sum_{\mathcal{C}_k} w(\mathcal{C}_k)$$

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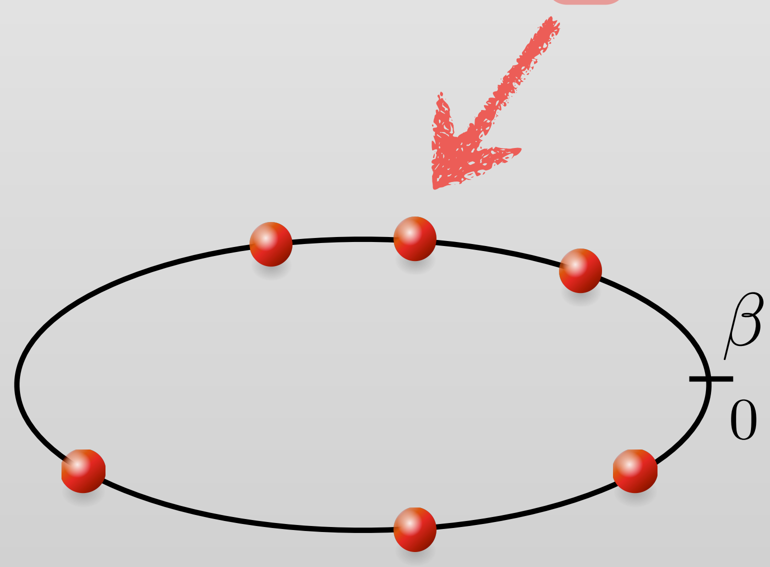

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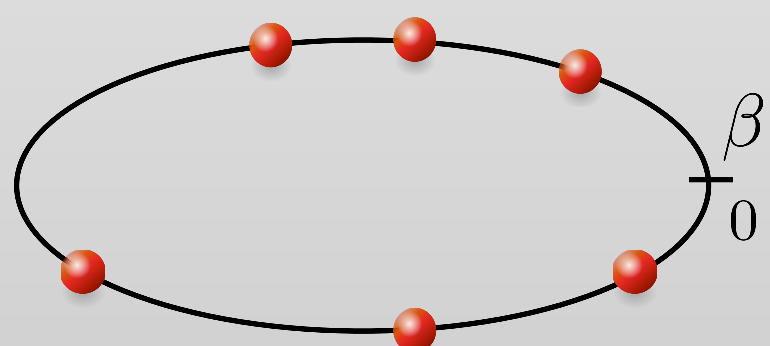

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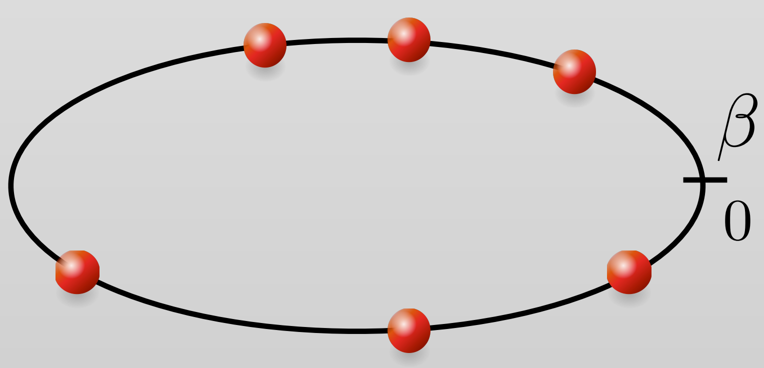
$$= \sum_{k=0}^{\infty} \lambda^k \sum_{\mathcal{C}_k} w(\mathcal{C}_k)$$

Rubtsov et al, PRB 2005   Gull et al, RMP 2011

$$\det\begin{pmatrix}\text{Noninteracting} \\ \text{Green's functions}\end{pmatrix}_{k\times k}$$

$\langle k \rangle \sim \beta\lambda N,$ scales as $\mathcal{O}(\beta^3\lambda^3N^3)$



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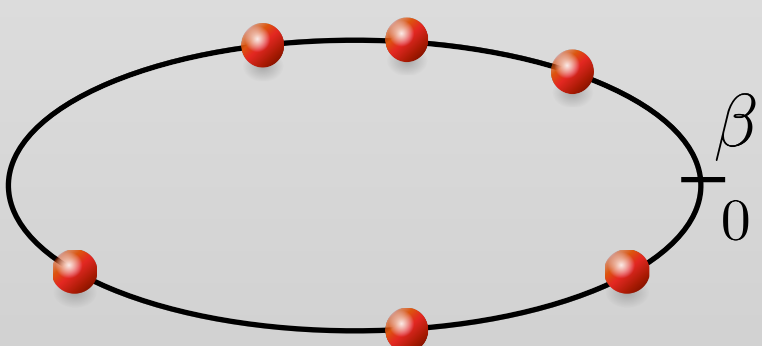


Rombouts, Heyde and Jachowicz, PRL 1999
Iazzi and Troyer, PRB 2015   LW, Iazzi, Corboz and Troyer, PRB 2015

LCT-QMC Methods

$$\det \left(I + \mathcal{T} e^{-\int_0^\beta d\tau H_{\mathcal{C}_k}(\tau)}\right)_{N \times N}$$

thus achieving $\mathcal{O}(\beta \lambda N^3)$ scaling!

More advantages

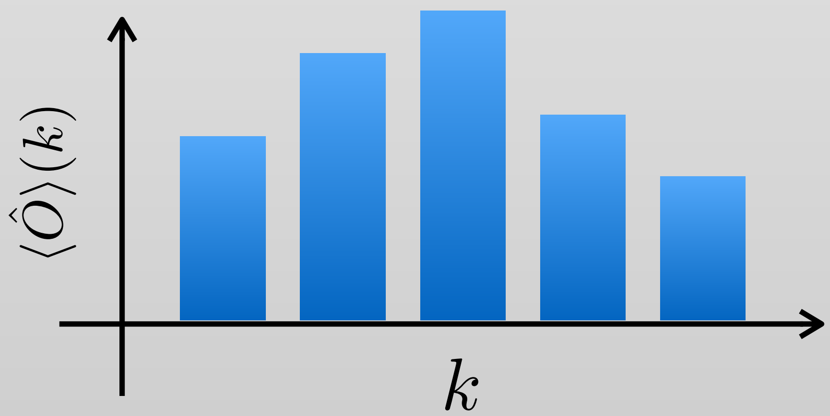
$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_k \boxed{\lambda^k} \sum_{\mathcal{C}_k} w(\mathcal{C}_k) O(\mathcal{C}_k)$$

Observable derivatives

$$\boxed{\frac{\partial \langle \hat{O} \rangle}{\partial \lambda} = \frac{\langle \hat{O} k \rangle - \langle \hat{O} \rangle \langle k \rangle}{\lambda}}$$

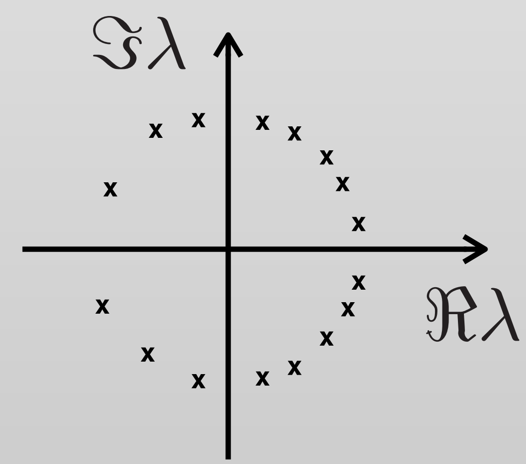
Directly sample *derivatives* of any observable

Histogram reweighing



Can obtain observables in a *continuous range* of coupling strengths

Lee-Yang zeros



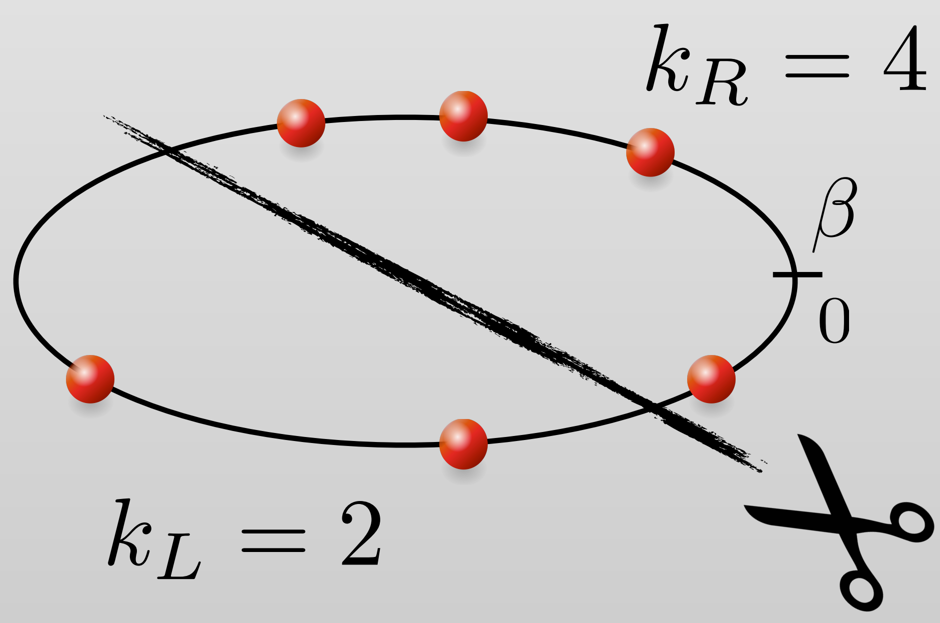
Partition function zeros in the *complex coupling strength* plane

Ferrenberg et al, 1988 Wang and Landau, 2001 Troyer et al, 2003

Fidelity susceptibility made simple!

LW, Liu, Imriška, Ma and Troyer, PRX 2015

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



Cut and count, that's it!

Fidelity susceptibility made simple!

LW, Liu, Imriška, Ma and Troyer, PRX 2015

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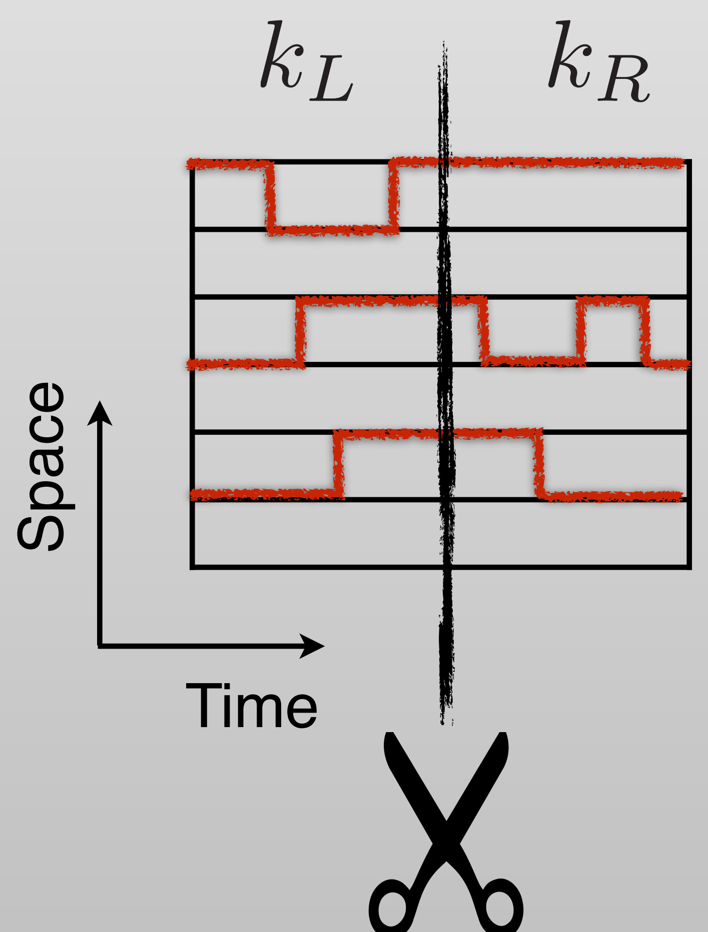
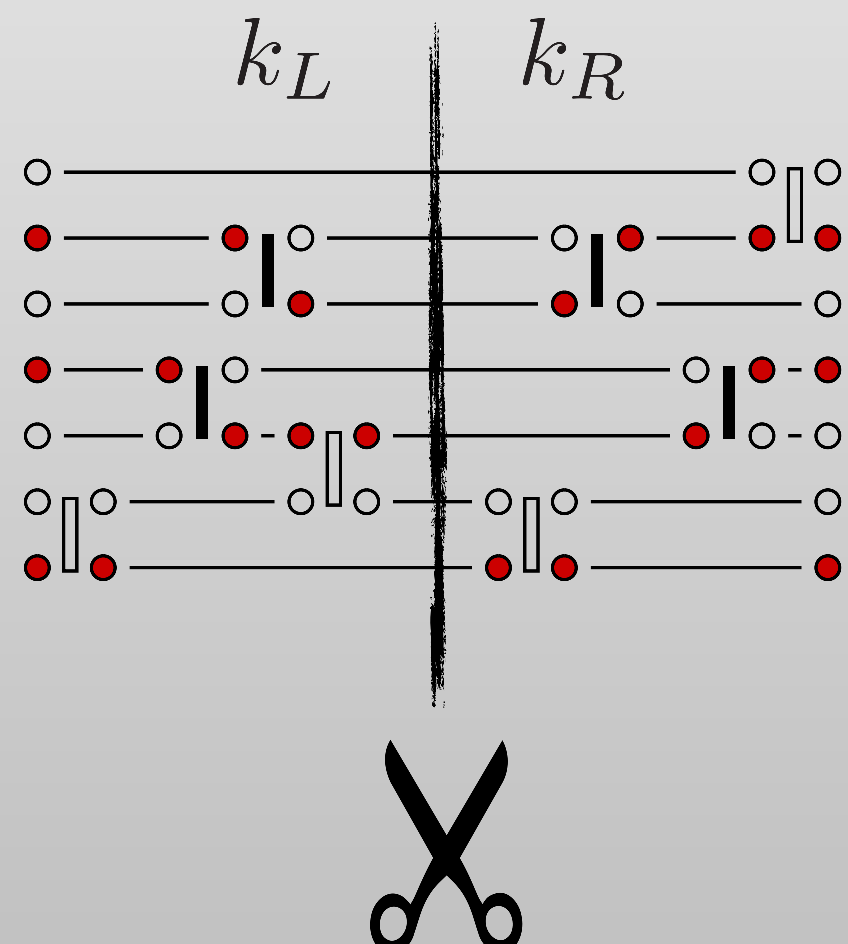
Worldline Algorithms

(bosons)



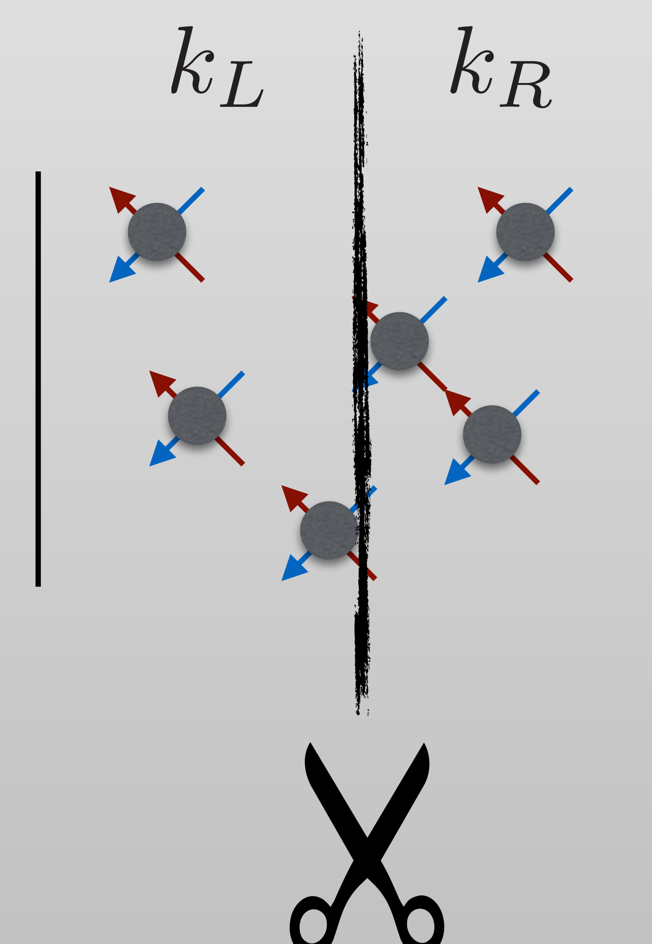
Stochastic Series Expansion

(quantum spins)



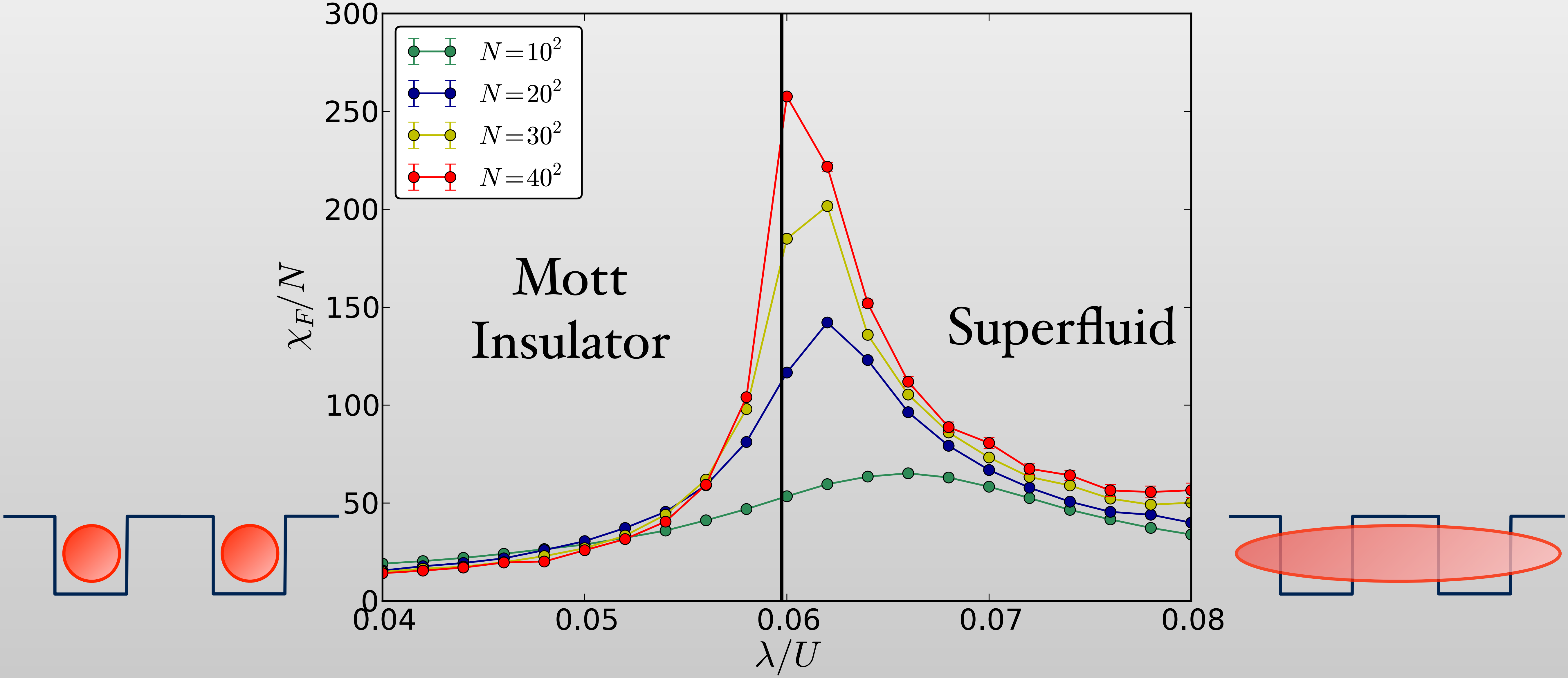
Determinantal Methods

(fermions)



Bose-Hubbard Model

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

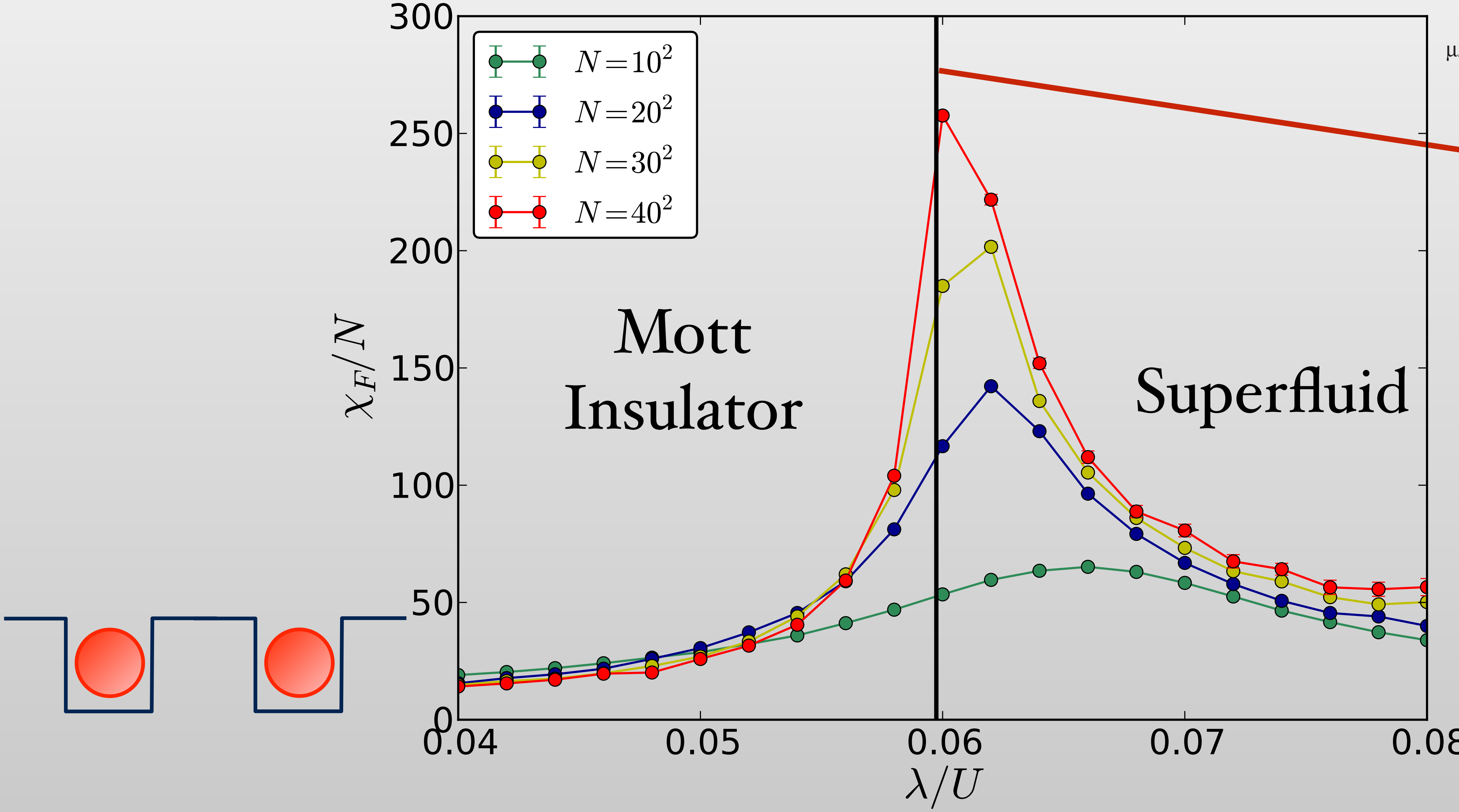


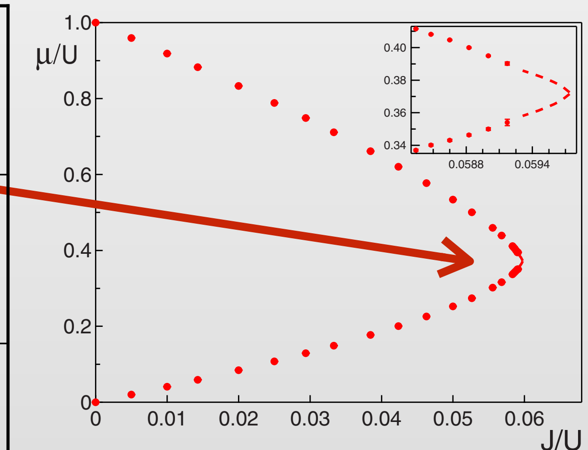
Divergence of fidelity susceptibility

correctly single out the quantum critical point

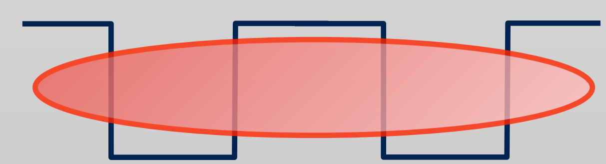
Bose-Hubbard Model

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





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

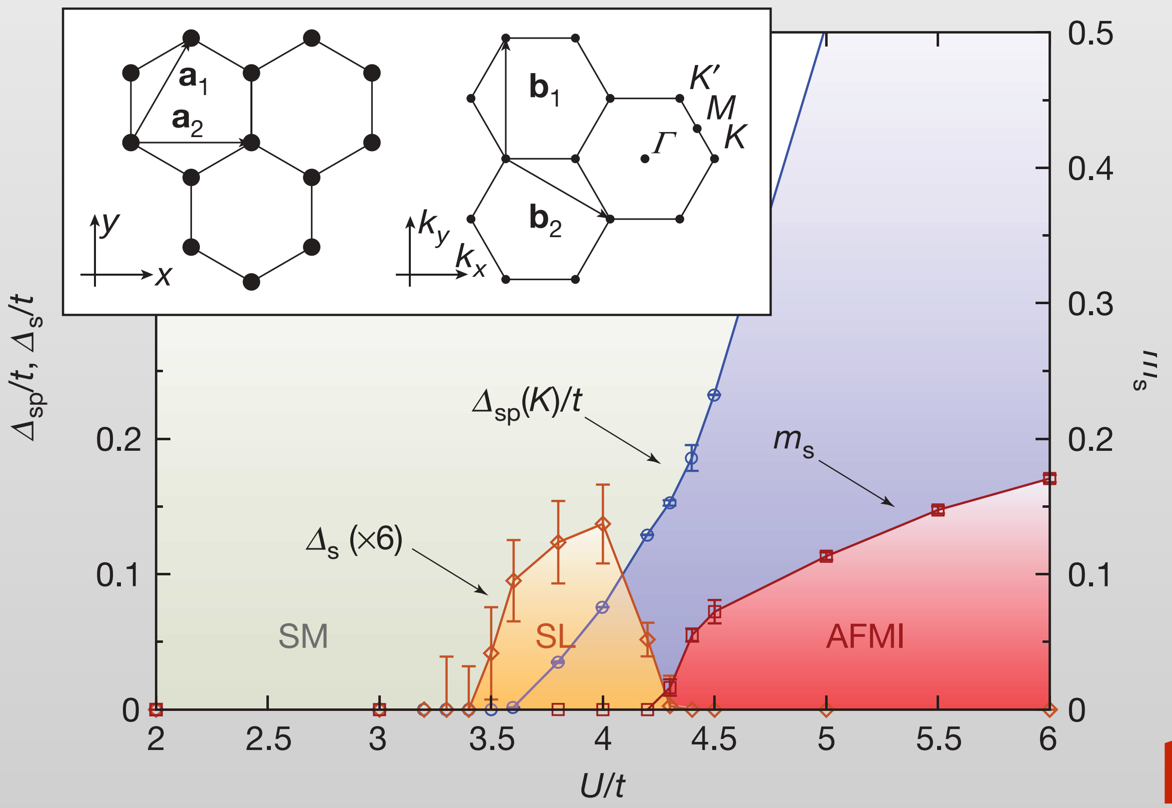


Divergence of fidelity susceptibility correctly single out the quantum critical point

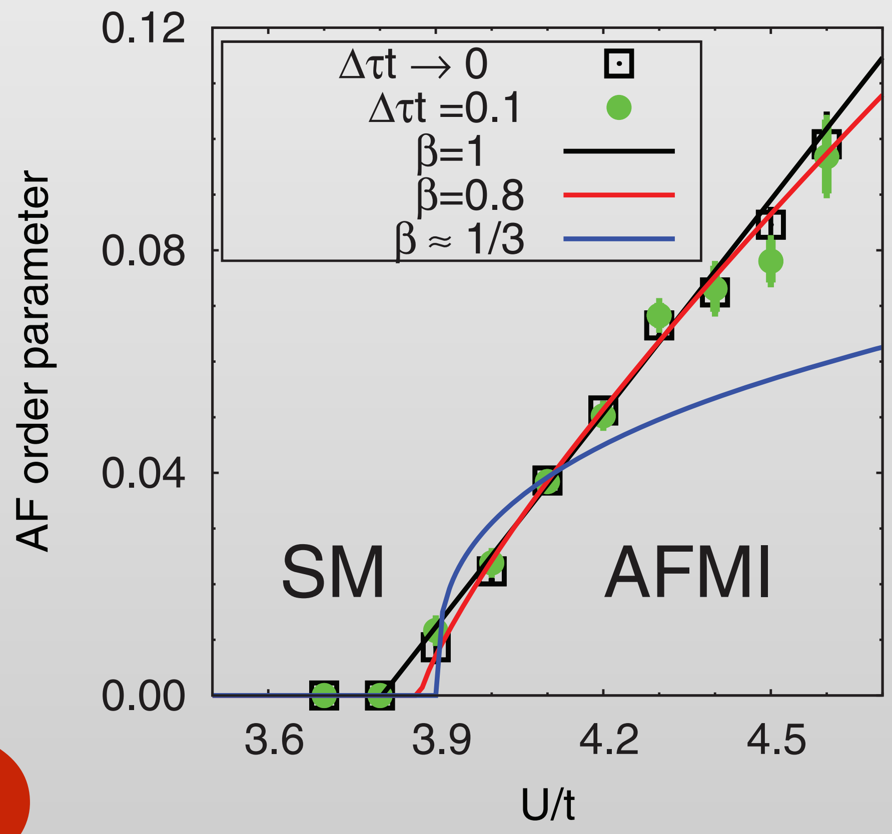
Honeycomb Hubbard Model

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

Meng et al, Nature 2010



Sorella et al, Sci.Rep 2012



?

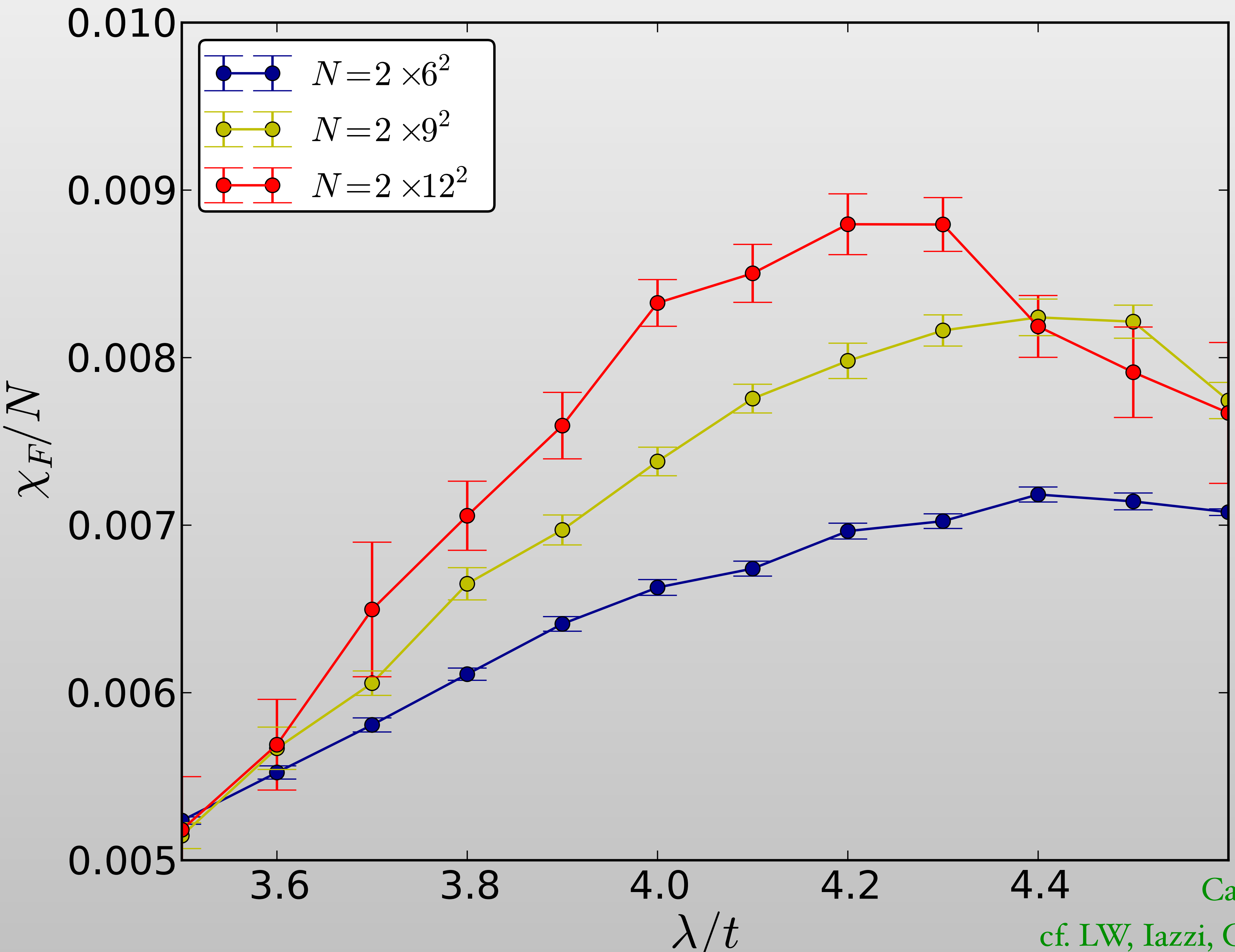
cf. Assaad et al, PRX 2013
Toldin et al, PRB 2014

A hotly debated problem in recent years

There is only one peak !

Suggesting a single phase transition,

i.e. no intermediate phase

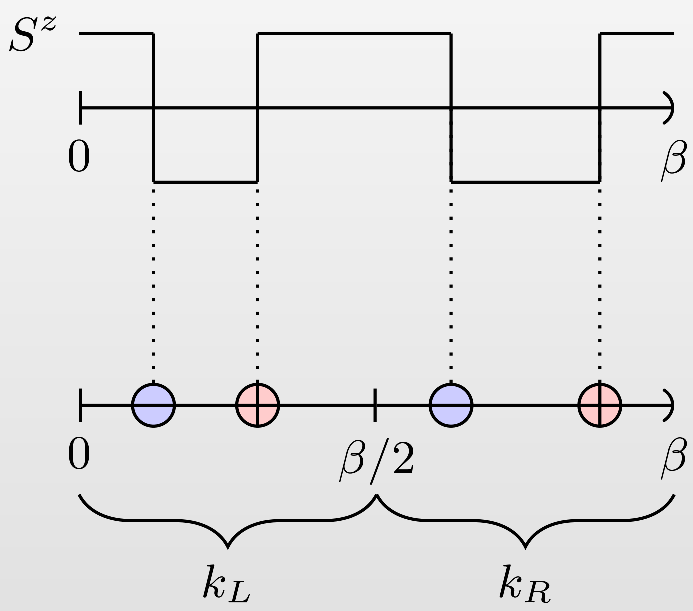


Calculated using LCT-INT

cf. LW, Iazzi, Corboz, Troyer PRB 2015

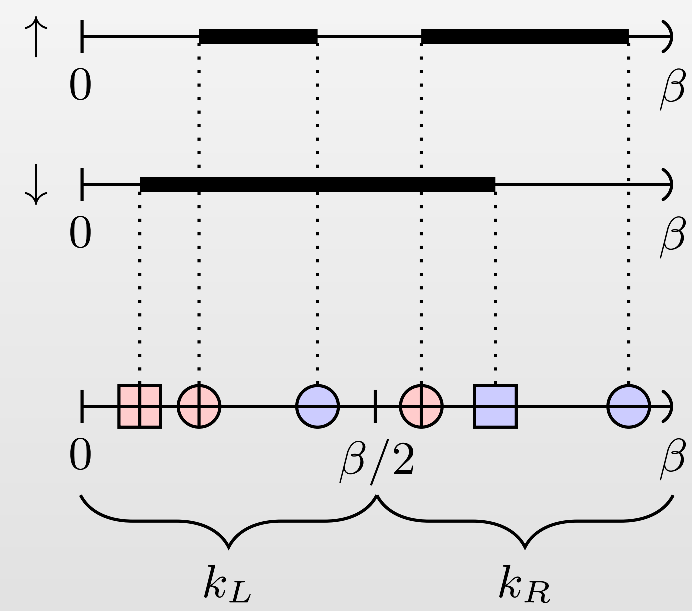
Impurity QPT

LW, Shinaoka and Troyer, PRL 2015



Anderson and Yuval, 1969

Maps the Kondo model to a classical Coulomb gas

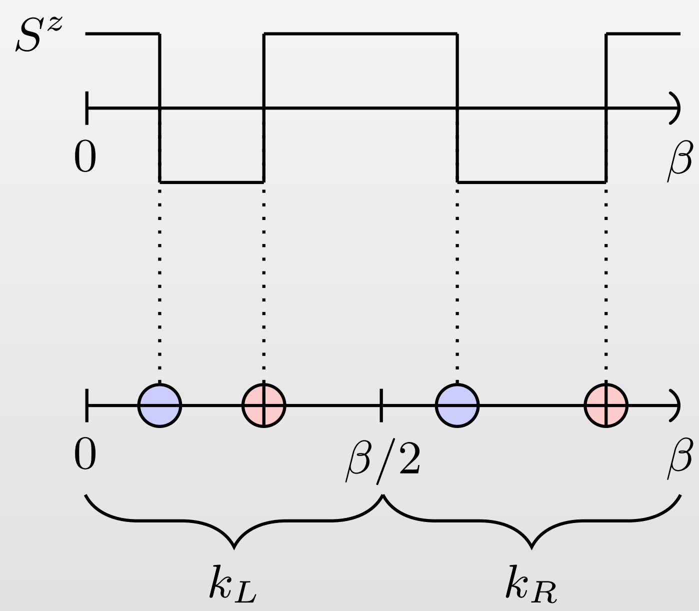


Werner el al 2006

Hybridization expansion QMC performs a similar mapping for the Anderson impurity models

Impurity QPT

LW, Shinaoka and Troyer, PRL 2015



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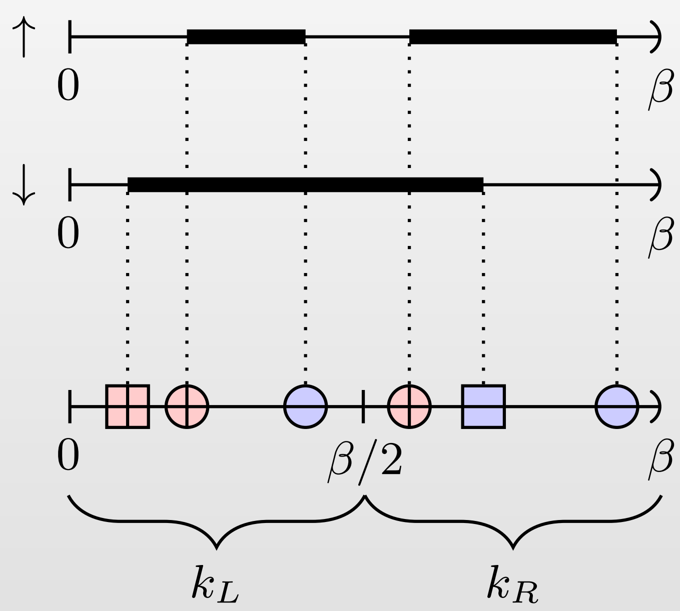
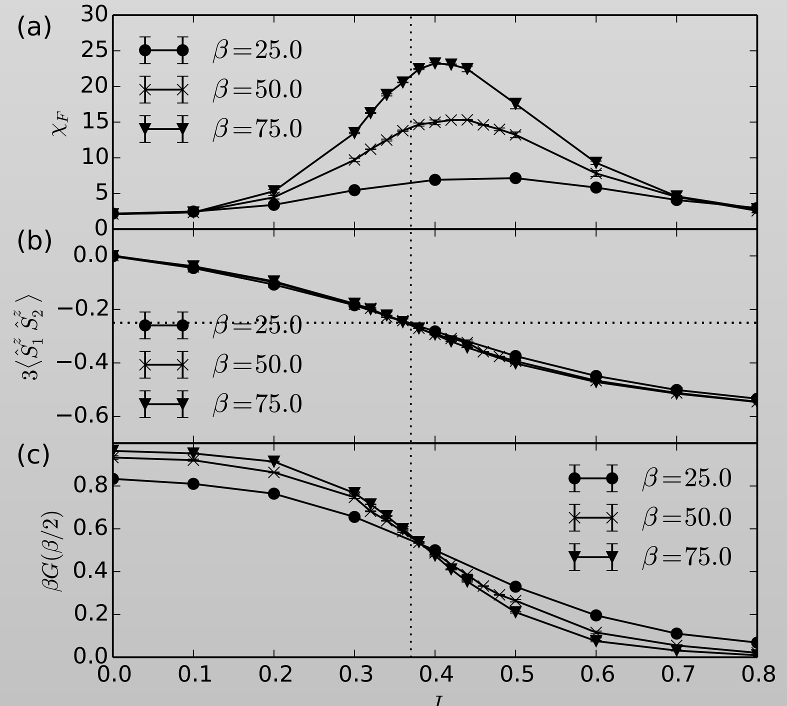
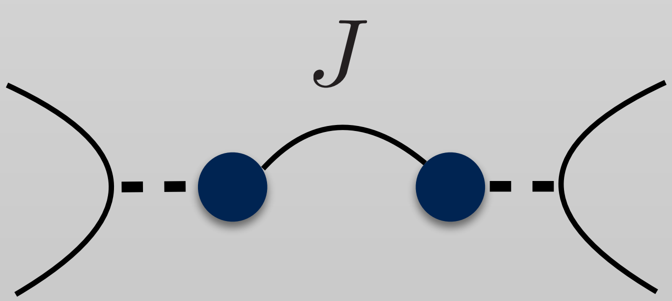


Werner el al 2006

Hybridization expansion QMC performs a similar mapping for the Anderson impurity models





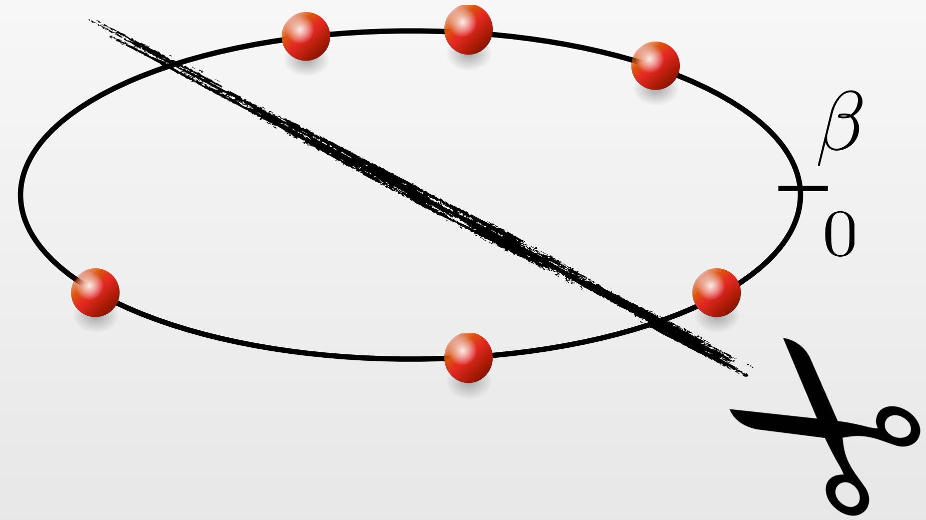
Two-impurity Anderson model

Why it works ?

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

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

fugacity



Quantum Phase Transition

$d(\text{Free Energy})/d\lambda = \langle \hat{H}_1 \rangle$

$d^2(\text{Free Energy})/d\lambda^2$

Fidelity Susceptibility

Classical Particle Condensation

Particle number $\langle k \rangle$

Compressibility $\langle k^2 \rangle - \langle k \rangle^2$

$\langle k_L k_R \rangle - \langle k_L \rangle \langle k_R \rangle$

How to experimentally measure χ_{F} ?

How to experimentally measure χ_F ?

Dynamical response functions

Hauke, et al Nat. Phys. 2016

Gu, et al EPL 2014

Excitations after an adiabatic ramp

Kolodrubetz, et al PRB 2013

De Grandi, et al PRB 2010

Polkovnikov et al RMP 2011

Islam et al, Nature 2015

Measure fidelity by interferencing two copies of many-body system ?

χ_F in AdS-CFT

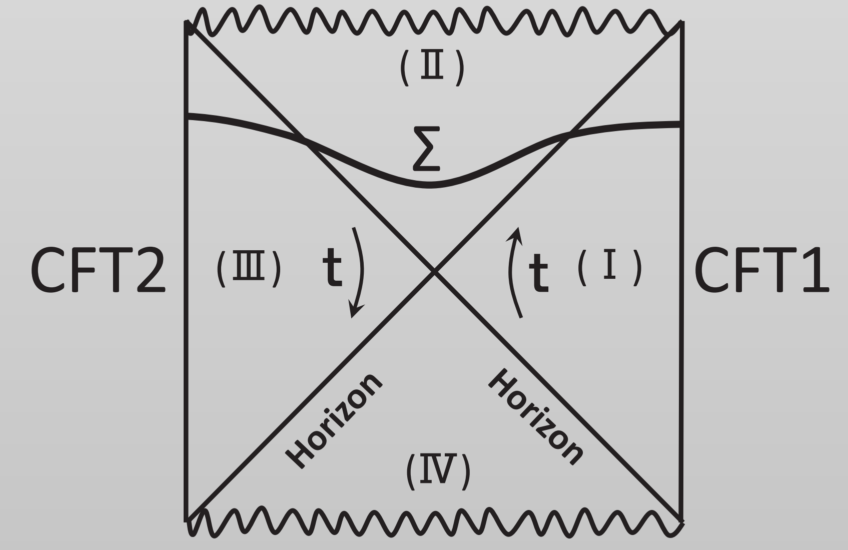
PRL **115,** 261602 (2015) PHYSICAL REVIEW LETTERS week ending 31 DECEMBER 2015

Distance between Quantum States and Gauge-Gravity Duality

Masamichi Miyaji,[1] Tokiro Numasawa,[1] Noburo Shiba,[1] Tadashi Takayanagi,[1,2] and Kento Watanabe[1]
[1]*Yukawa Institute for Theoretical Physics, Kyoto University, Kitashirakawa Oiwakecho, Sakyo-ku, Kyoto 606-8502, Japan*
[2]*Kavli Institute for the Physics and Mathematics of the Universe, University of Tokyo, Kashiwa, Chiba 277-8582, Japan*
(Received 3 August 2015; revised manuscript received 5 October 2015; published 22 December 2015)

We study a quantum information metric (or fidelity susceptibility) in conformal field theories with respect to a small perturbation by a primary operator. We argue that its gravity dual is approximately given by a volume of maximal time slice in an anti–de Sitter spacetime when the perturbation is exactly marginal. We confirm our claim in several examples.

Don’t ask me what’s on the right ➔

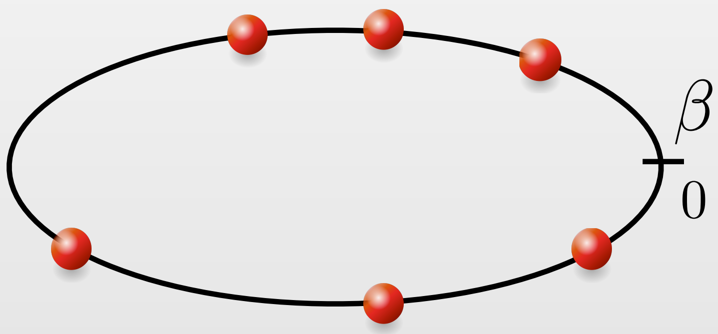


Monte Carlo simulations can be painfully slow

A Comparison of two Markov Chain Monte Carlo samplers

Recommender engine for QMC

1. Collect configuration data



2. Train a classical Stat-Mech model

$$E(\{\tau_i\}) = -\sum_{i<j}^{k} V(\tau_i - \tau_j) - \mu k$$

3. Use it as a recommender engine!

Huang and LW, 1610.02746 Liu, Qi, Meng and Fu, 1610.03137

and more to come...

Take home message

Fidelity Susceptibility: A general purpose indicator of quantum phase transition

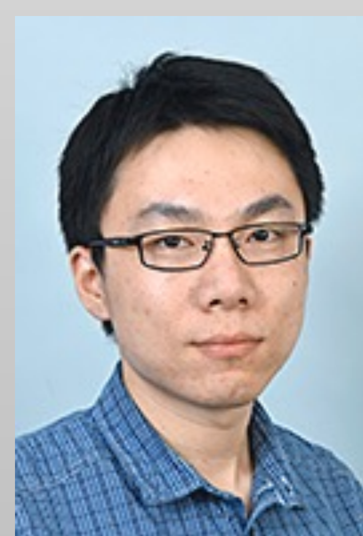
Quantum Monte Carlo: New developments are around the horizon

Thanks to my collaborators!

Mauro Iazzi

Philippe Corboz

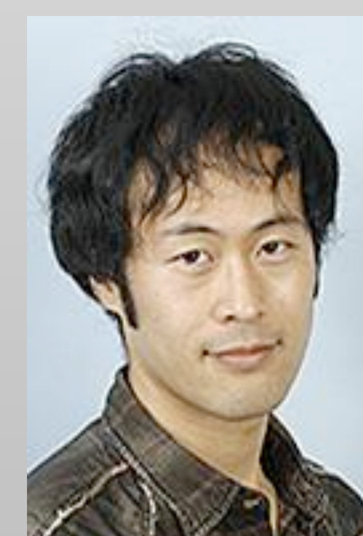
Ye-Hua Liu



Jakub Imriška

Ping Nang Ma

Hiroshi Shinaoka



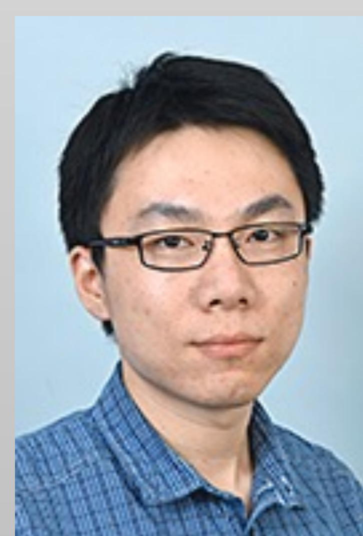
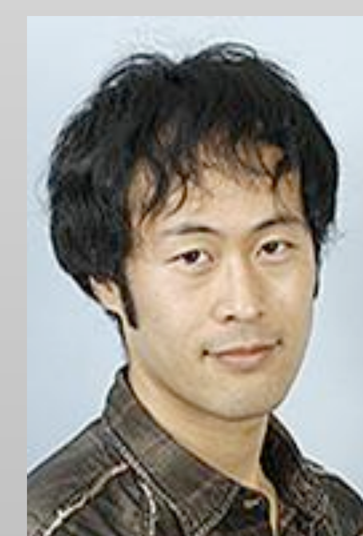
Matthias Troyer

Take home message

Fidelity Susceptibility: A general purpo
quantum phase transition

Quantum Monte Carlo: New developments are around the horizon

Thanks to my collaborators!

Mauro Iazzi	Philippe Corboz	Ye-Hua Liu	Jakub Imriška	Ping Nang Ma	Hiroshi Shinaoka	Matthias Troyer
						

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欢迎本科生毕业设计, 博士生, 博士后

wanglei@iphy.ac.cn　　010-82649853