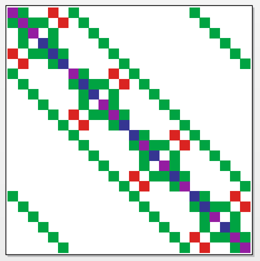
New adventures of QMC for fermions

Lei Wang
Institute of Physics
http://wangleiphy.github.io/

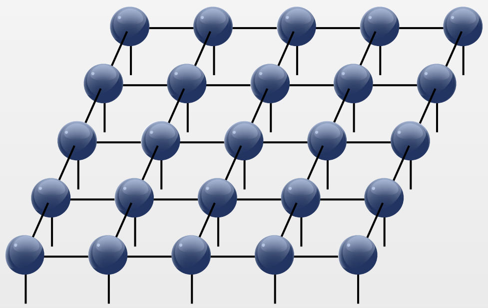
International Summer School on
Computational Approaches for Quantum Many Body Systems

Algorithms for quantum many-body systems

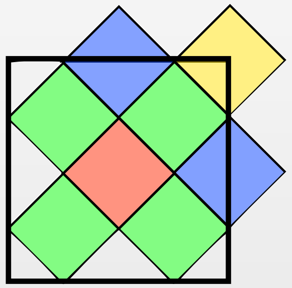


exact
diagonalization

quantum
Monte Carlo

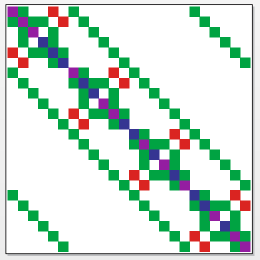


tensor network
states



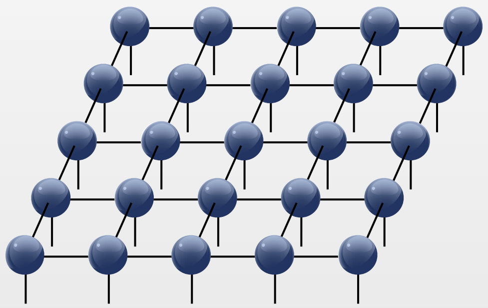
dynamical mean
field theories

Algorithms for quantum many-body systems

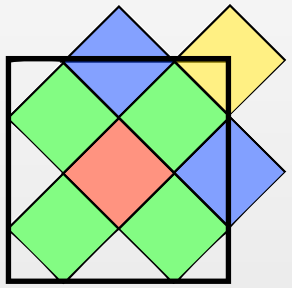


exact diagonalization

quantum Monte Carlo



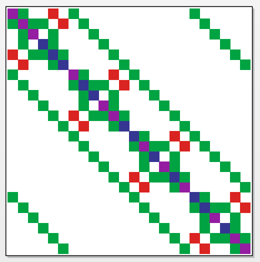
tensor network states



dynamical mean field theories

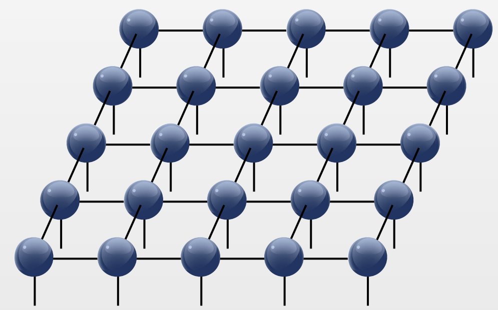
Algorithmic improvement in past 20 years outperformed Moore's law

Algorithms for quantum many-body systems

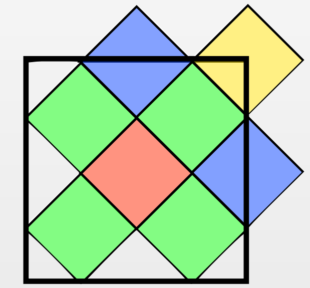


exact diagonalization

quantum Monte Carlo



tensor network states



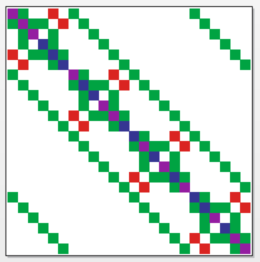
dynamical mean field theories

Modern algorithm

is faster than

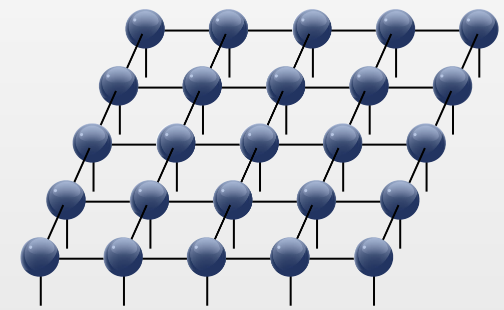
Traditional algorithm

Algorithms for quantum many-body systems

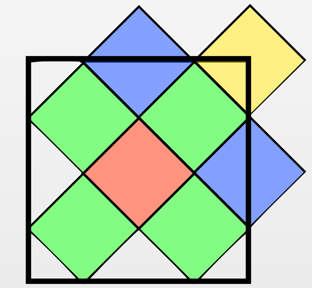


exact diagonalization

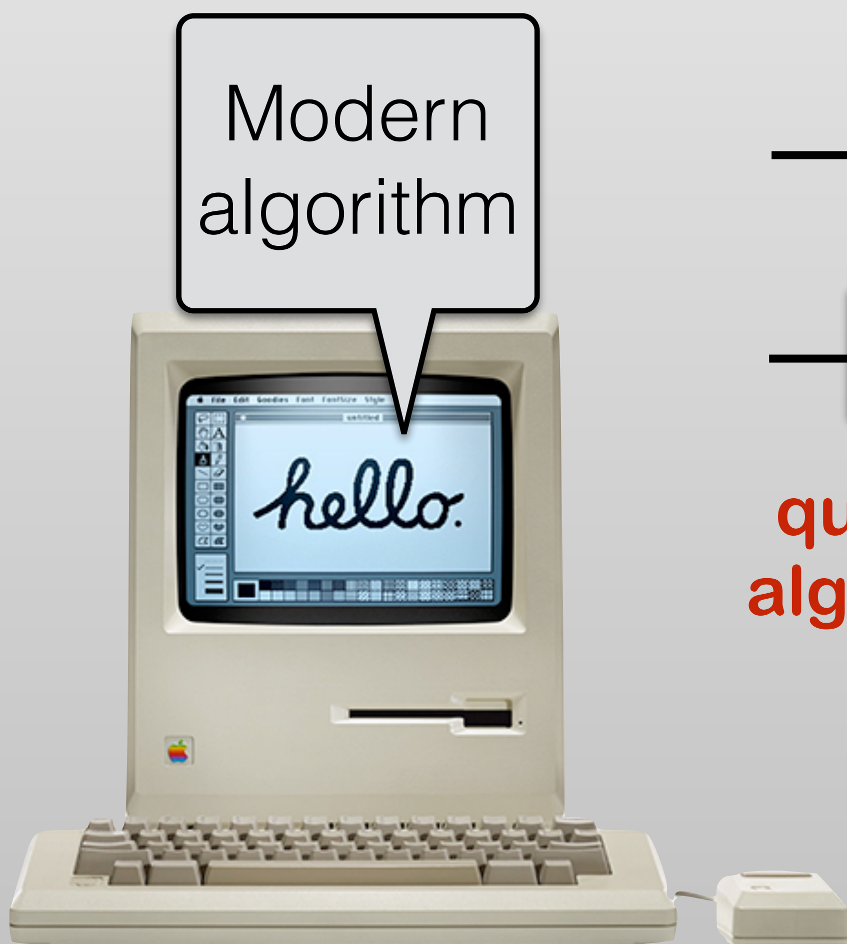
quantum Monte Carlo

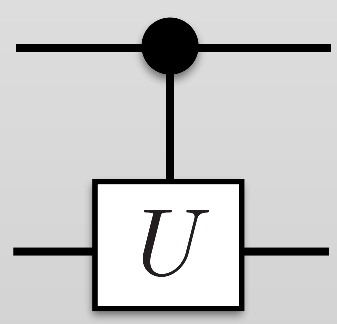


tensor network states

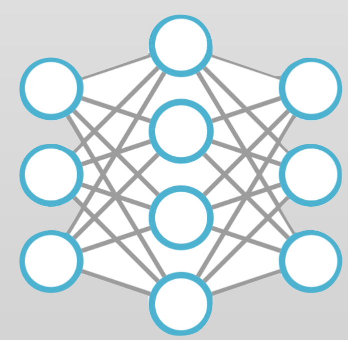


dynamical mean field theories

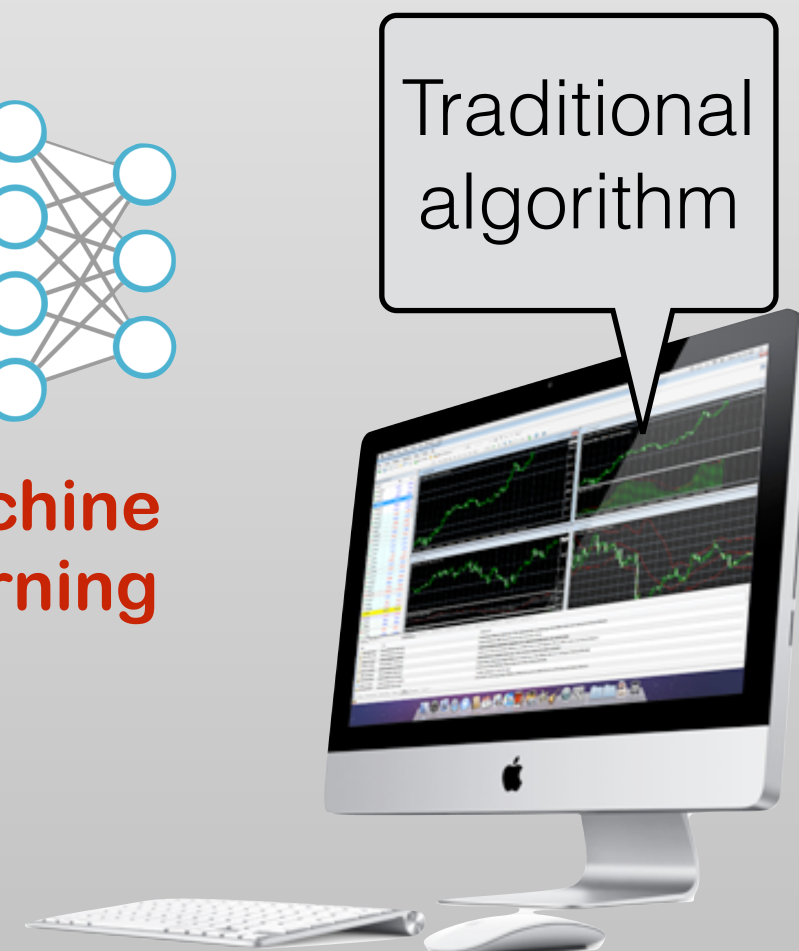


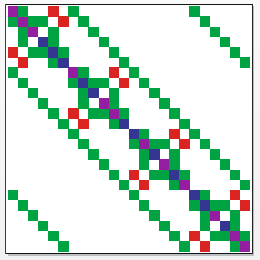


quantum algorithms



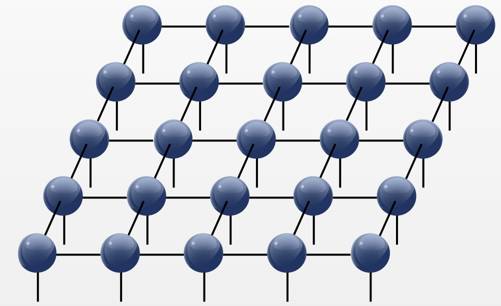
machine learning



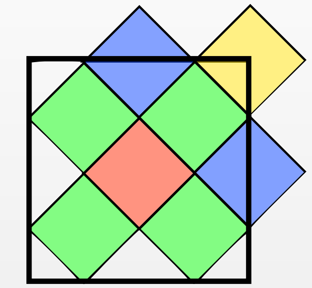


exact diagonalization

quantum Monte Carlo



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

To put it in the context...

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

	Lattice models				Impurity models			
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

To put it in the context...

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

1981

	Lattice models				Impurity models			
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

To put it in the context...

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

1981

	Lattice models				Impurity models			
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

Meng, Assaad
Xu, He

To put it in the context...

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

	1981 Lattice models				1986 Impurity models			
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

Meng, Assaad
Xu, He

To put it in the context...

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

	1981	1999 models			1986	Impurity models		
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

Meng, Assaad
Xu, He

To put it in the context...

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

	1981	1999 models			1986	2005 ty models		
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

Meng, Assaad
Xu, He

To put it in the context...

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

	1981	1999	models		1986	2005 ty m	2008	
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

Meng, Assaad
Xu, He

To put it in the context...

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

	1981	1999 models			1986	2005 ty m	2008	2006
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

Meng, Assaad
Xu, He

To put it in the context...

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

	1981	1999	models		1986	2005	ty m 2008	2006
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

Meng, Assaad
Xu, He

Tong, Huang

To put it in the context…

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

	1981	1999	2015 models		1986	2005 ty m	2008	2006
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

Meng, Assaad
Xu, He

Tong, Huang

To put it in the context...

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

	1981	1999 models	2015		1986	2005 ty m	2008	2006
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

Meng, Assaad
Xu, He

This lecture

Tong, Huang

To put it in the context...

Table from LW, Iazzi, Corboz and Troyer, PRB 91, 235151 (2015)

TABLE I. Comparison between various determinantal QMC methods for fermions. The ground state methods are extensions of the corresponding finite temperature methods. They have similar scalings when replacing the inverse temperature β by the projection time Θ. N denotes the number of correlated sites and V denotes the interaction strength.

	1981	1999 models	2015		1986	2005 ty m	2008	2006
Method name	BSS	–	LCT-INT	LCT-AUX	Hirsch-Fye	CT-INT	CT-AUX	CT-HYB
Finite temperature	Ref. [22]	Ref. [29]	Ref. [30]		Ref. [27]	Ref. [31]	Ref. [32]	Ref. [33]
Ground state	Refs. [23,34,35]		This paper	–	Ref. [36]	Ref. [37]	–	–
Trotter error	Yes	No	No	No	Yes	No	No	No
Auxiliary field	Yes	Yes	No	Yes	Yes	No	Yes	No
Scaling	$\beta V N^3$ [a]	[b]	$\beta V N^3$	$\beta V N^3$	$(\beta V N)^3$	$(\beta V N)^3$	$(\beta V N)^3$	e^N

Meng, Assaad
Xu, He

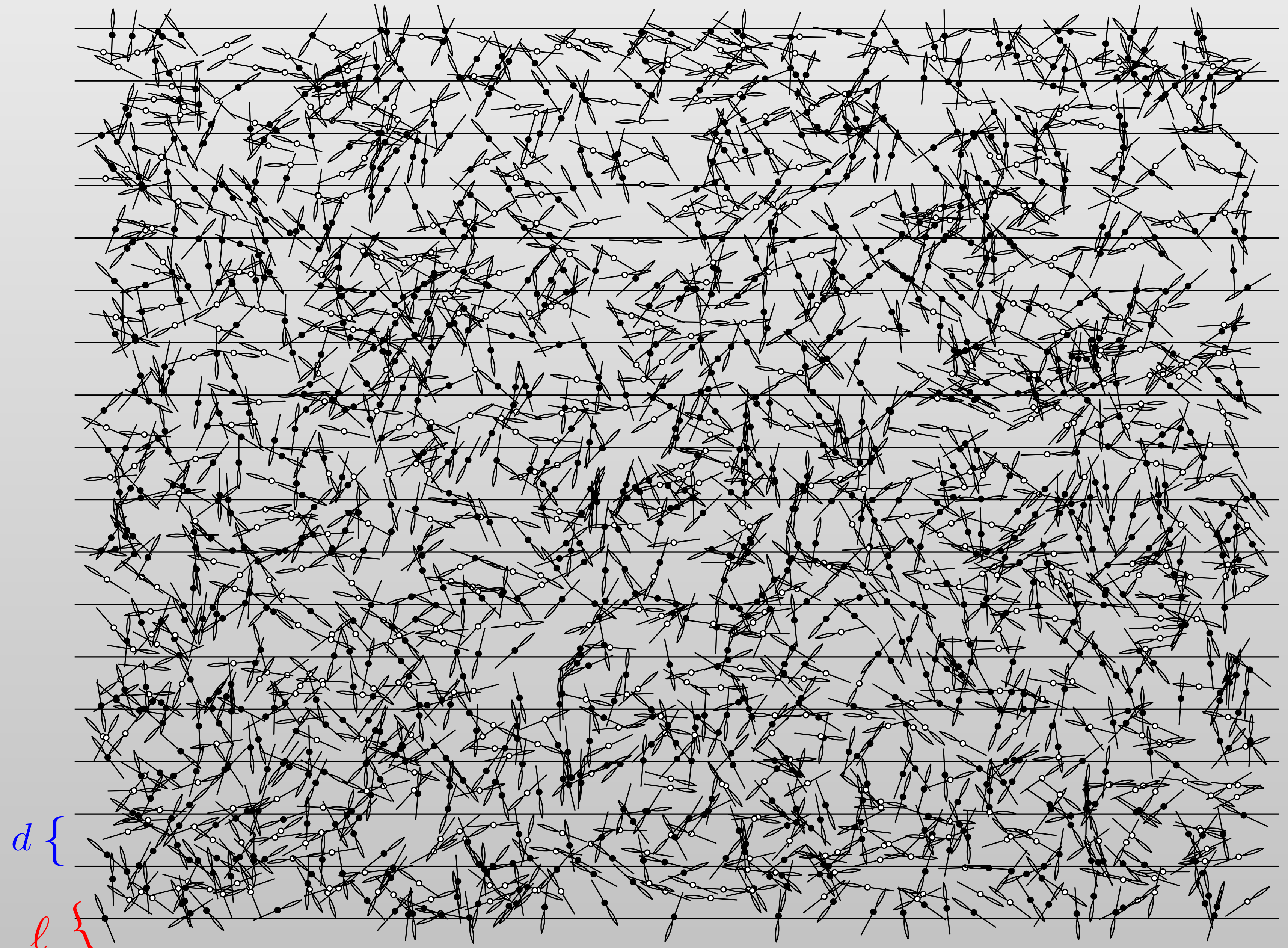
This lecture

Tong, Huang

A unified framework with
worldline QMC & SSE for bosons/spins

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)

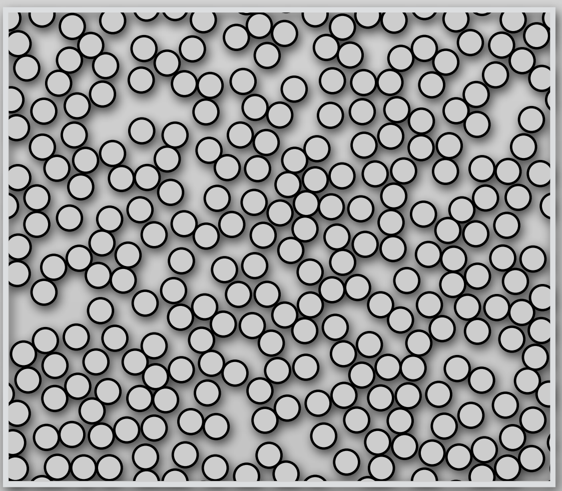
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional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

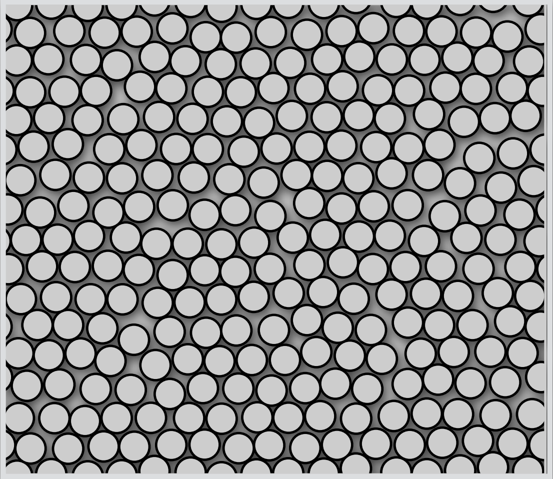
I. INTRODUCTION

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-





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)

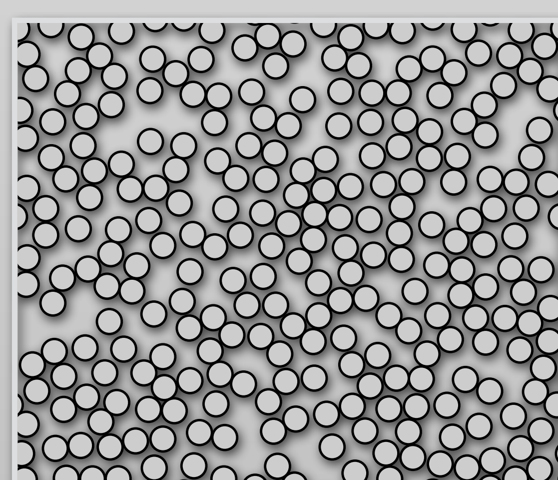
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional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

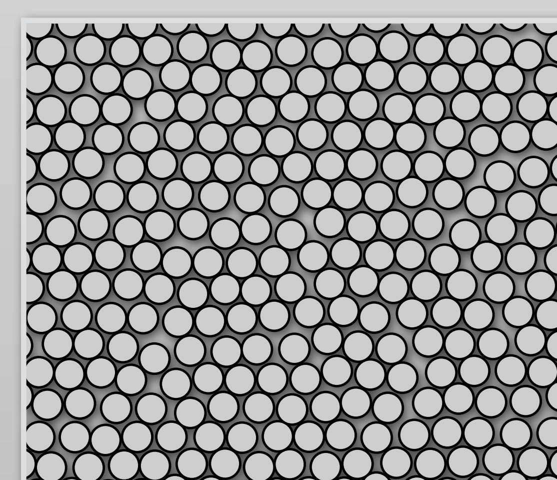
I. INTRODUCTION

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-



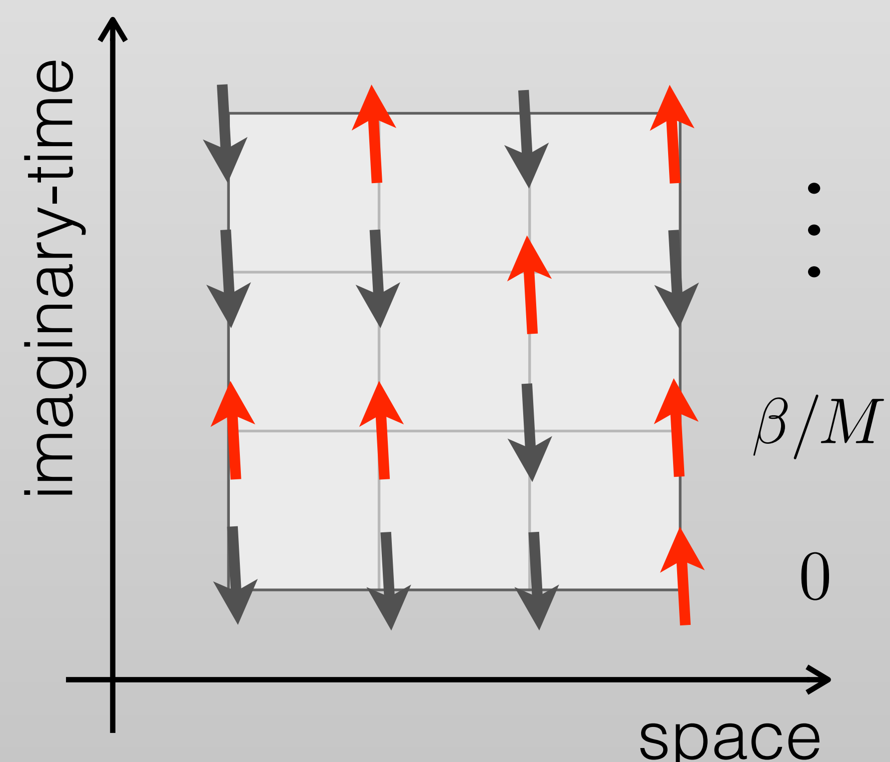


Quantum to classical mapping

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

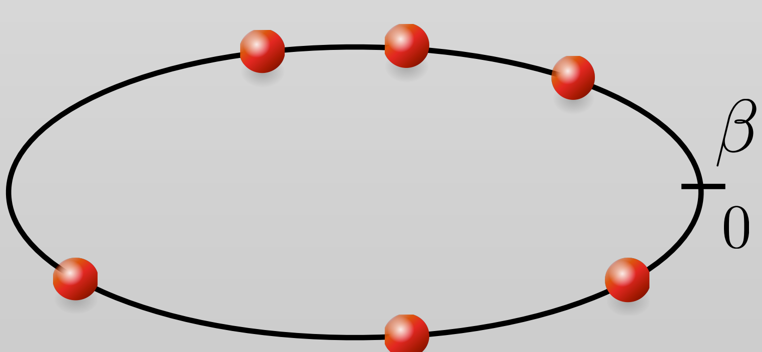
Trotterization

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



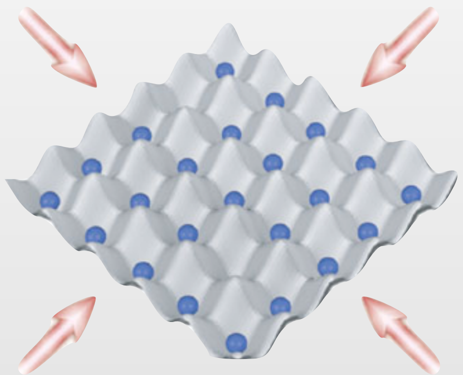
Diagrammatic approach

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



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

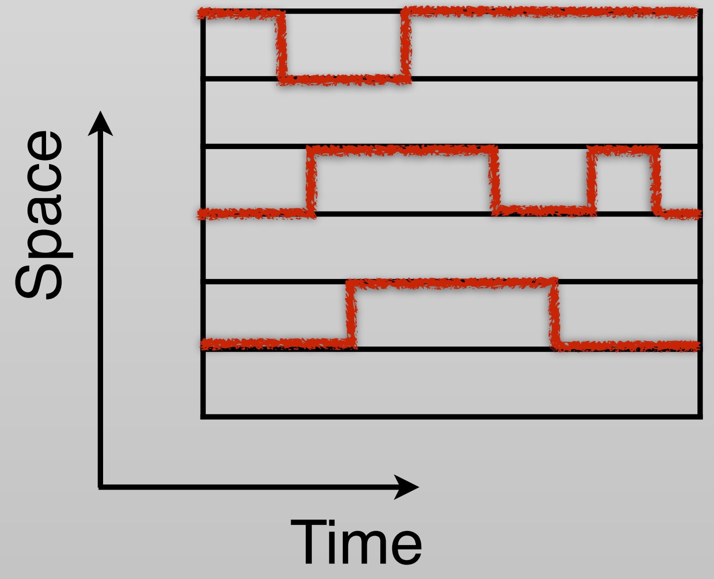
Diagrammatic approaches

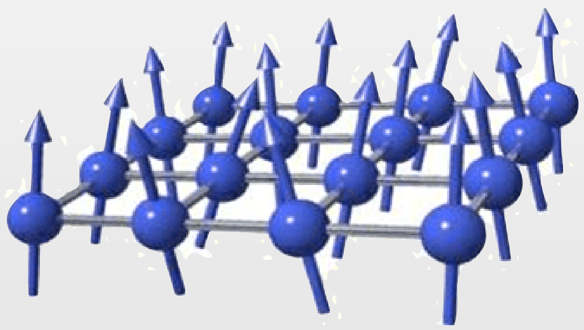


bosons

World-line Approach

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

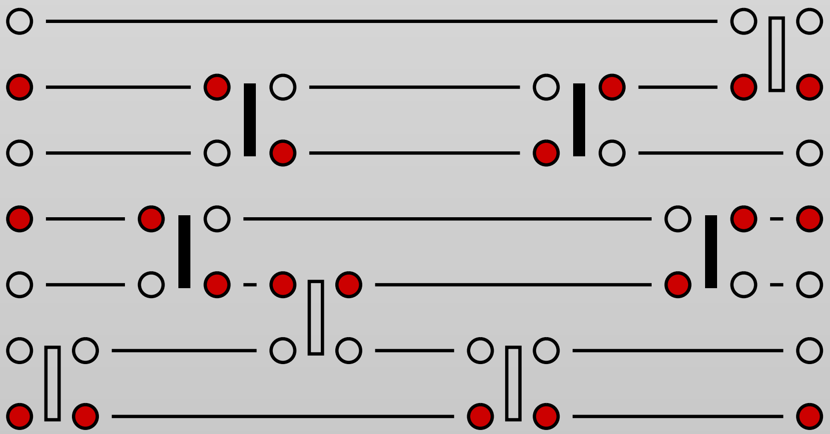


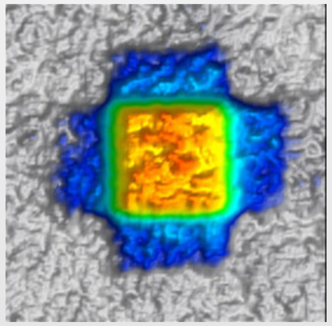


quantum spins

Stochastic Series Expansion

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

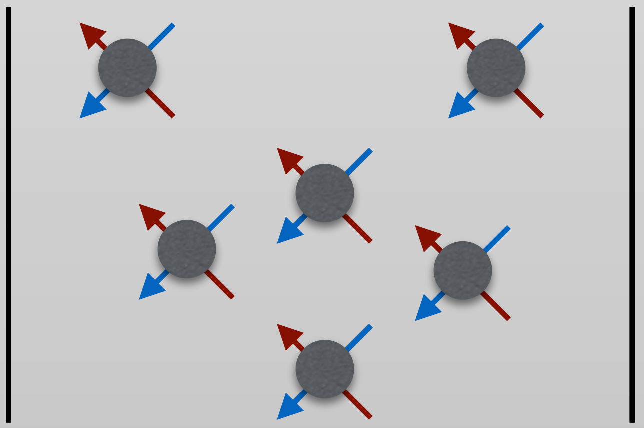




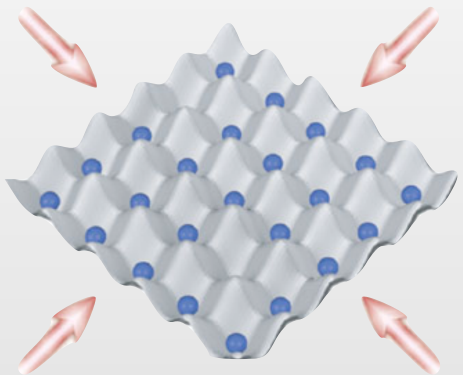
fermions

Determinantal Methods

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



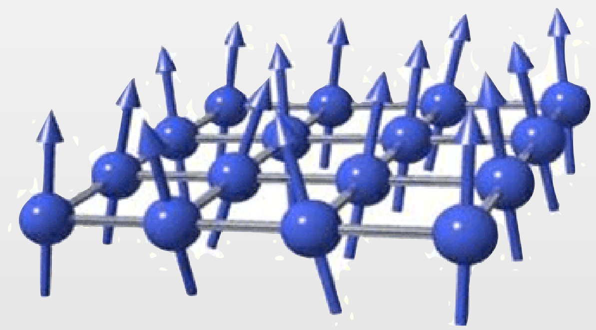
Diagrammatic approaches



bosons

World-line Approach

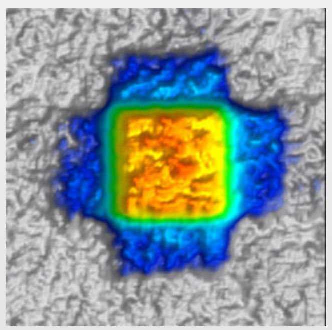
Prokof'ev et al, JETP, **87**, 310 (1998)



quantum spins

Stochastic Series Expansion

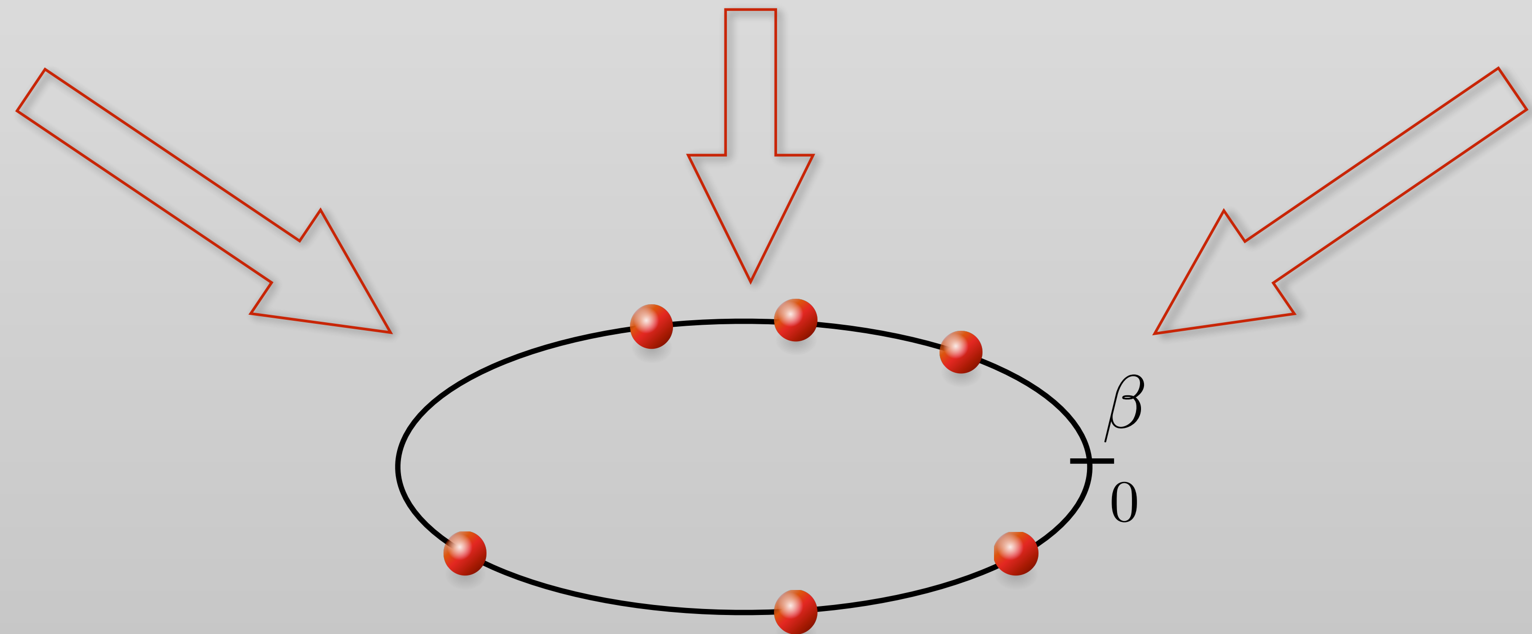
Sandvik et al, PRB, **43**, 5950 (1991)



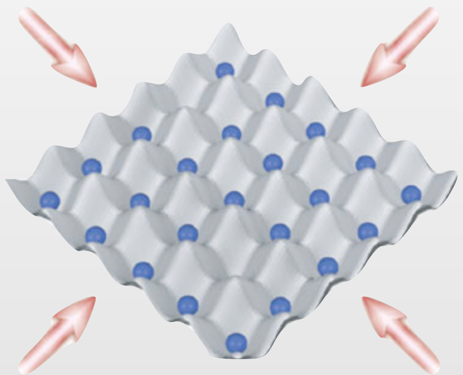
fermions

Determinantal Methods

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



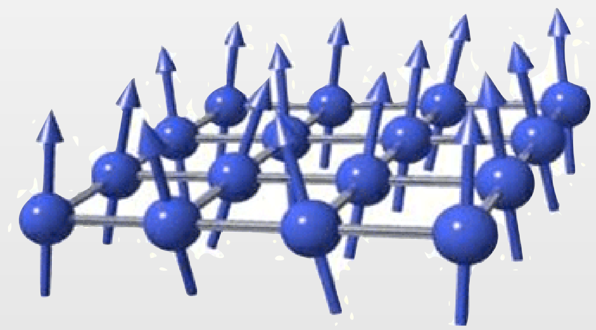
Diagrammatic approaches



bosons

World-line Approach

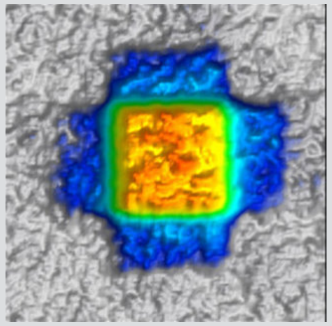
Prokof'ev et al, JETP, **87**, 310 (1998)



quantum spins

Stochastic Series Expansion

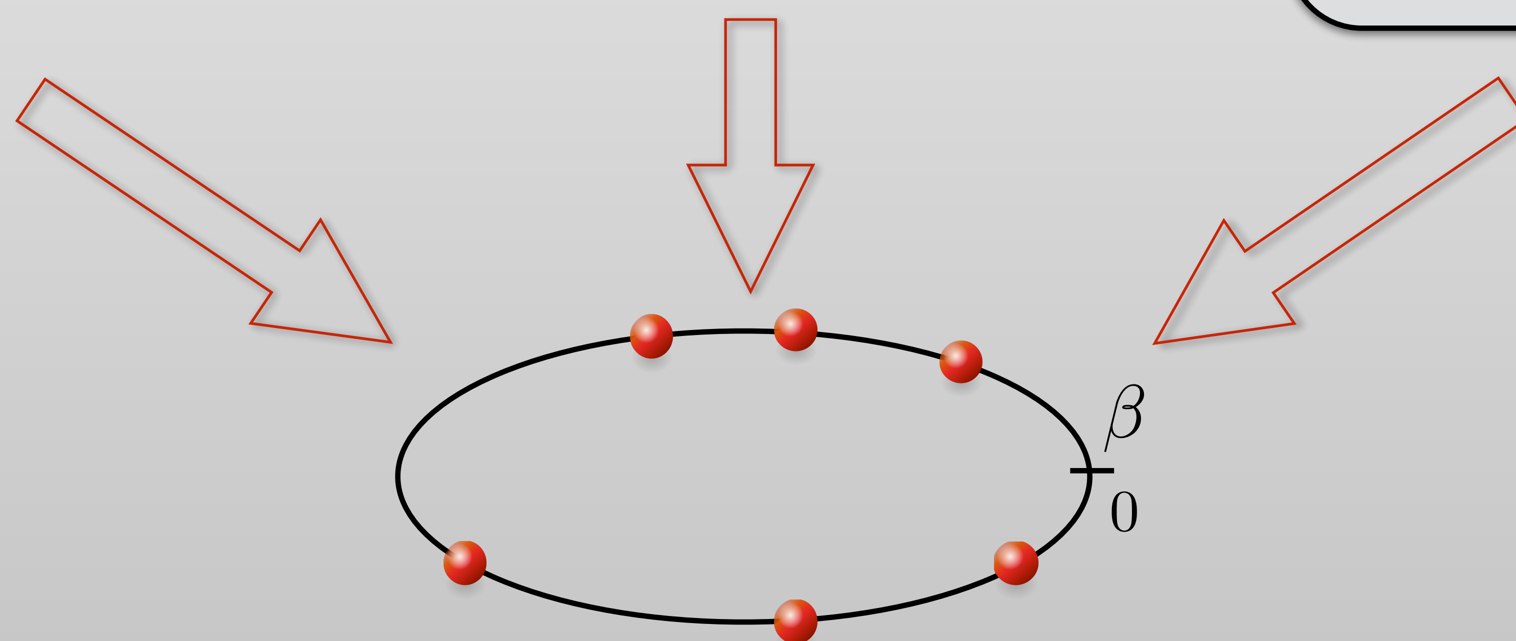
Sandvik et al, PRB, **43**, 5950 (1991)



fermions

Determinantal Methods

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



Diagrammatic determinant QMC

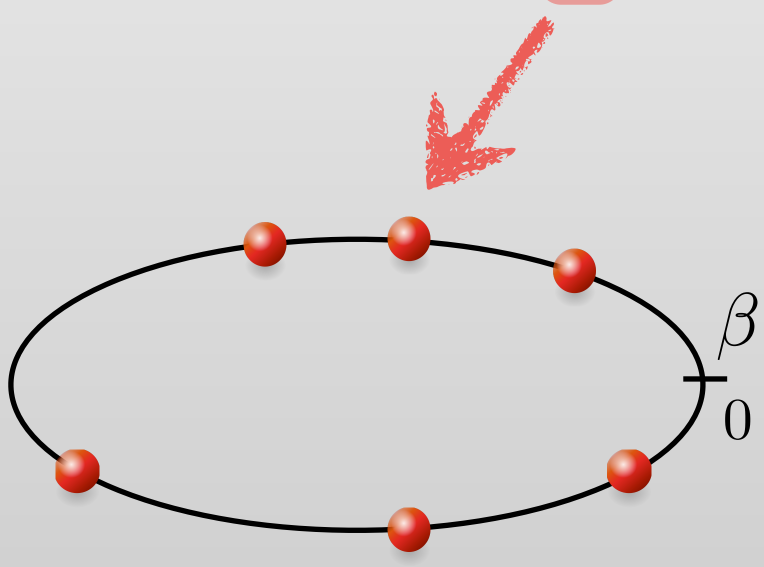
$$Z = \sum_{k=0}^{\infty} \lambda^k \int_0^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^{\beta} d\tau_k \,\mathrm{Tr}\left[(-1)^k e^{-(\beta-\tau_k)\hat{H}_0} \hat{H}_1 \ldots \hat{H}_1 e^{-\tau_1 \hat{H}_0}\right]$$

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

Diagrammatic determinant QMC

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

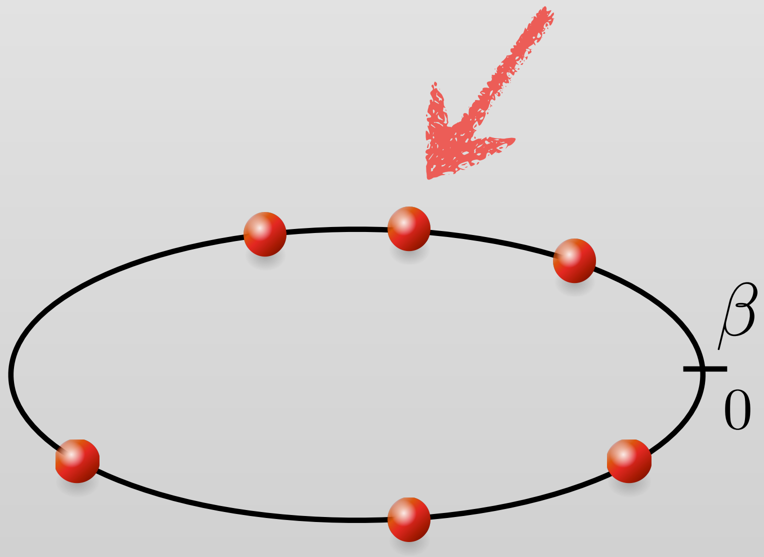
$$= \sum_{k=0}^{\infty} \lambda^k \sum_{\mathcal{C}_k} w(\mathcal{C}_k)$$



Diagrammatic determinant QMC

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

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



Diagrammatic determinant QMC

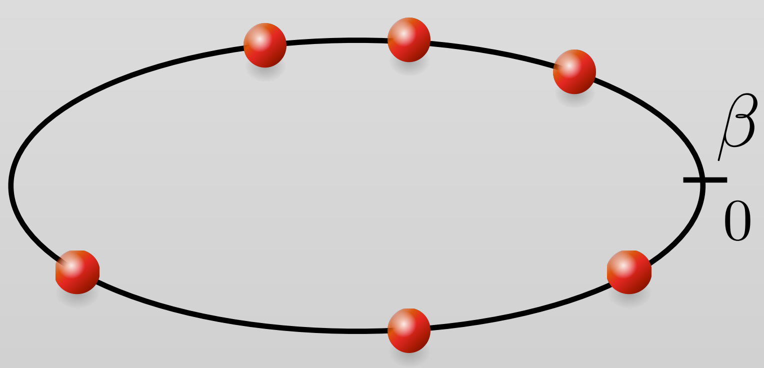
$$Z = \sum_{k=0}^{\infty} \lambda^k \int_0^\beta d\tau_1 \ldots \int_{\tau_{k-1}}^{\beta} d\tau_k \, \mathrm{Tr}\left[(-1)^k e^{-(\beta-\tau_k)\hat{H}_0}\hat{H}_1 \ldots \hat{H}_1 e^{-\tau_1 \hat{H}_0}\right]$$

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

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 $\mathcal{O}(\beta^3\lambda^3N^3)$



Diagrammatic determinant QMC

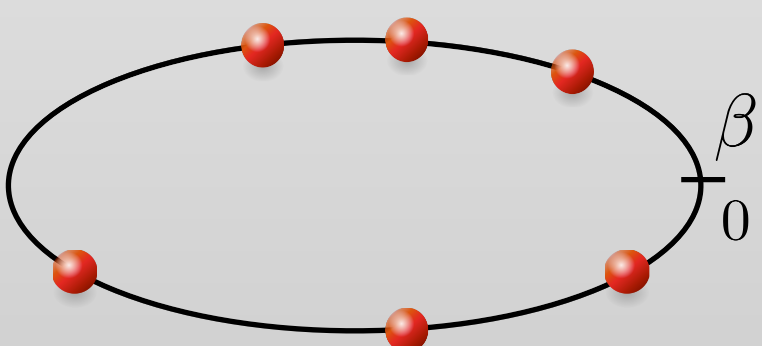
$$Z = \sum_{k=0}^{\infty} \lambda^k \int_0^{\beta} d\tau_1 \ldots \int_{\tau_{k-1}}^{\beta} d\tau_k \, \mathrm{Tr}\left[(-1)^k e^{-(\beta-\tau_k)\hat{H}_0} \hat{H}_1 \ldots \hat{H}_1 e^{-\tau_1 \hat{H}_0}\right]$$

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

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 $\mathcal{O}(\beta^3\lambda^3N^3)$



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

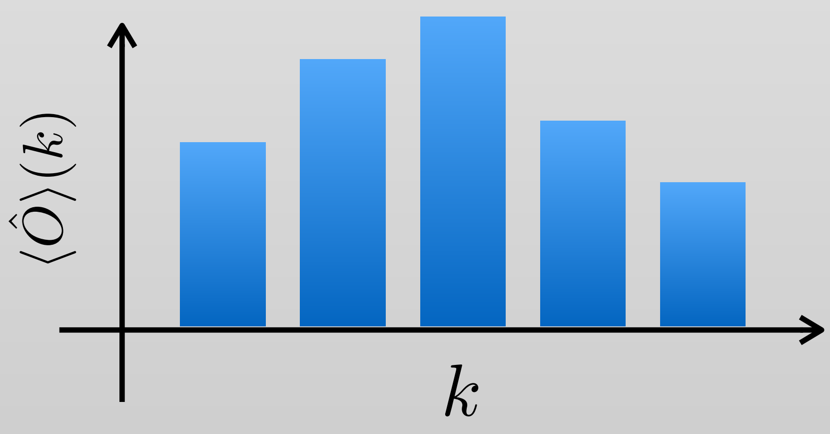
$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_k \lambda^k \sum_{\mathcal{C}_k} w(\mathcal{C}_k) O(\mathcal{C}_k)$$

Observable derivatives

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

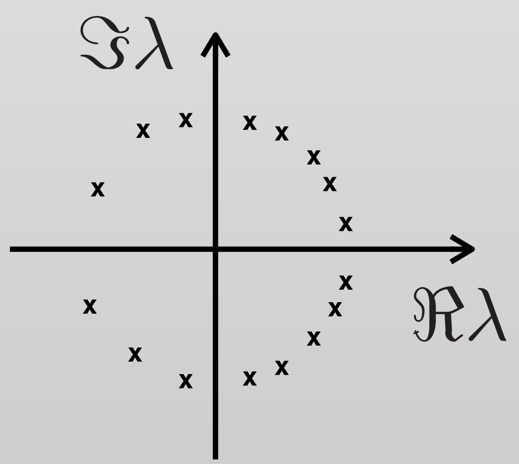
Directly sample *derivatives* of any observable

Histogram reweighing



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

Lee-Yang zeros



Partition function zeros in the *complex coupling strength* plane

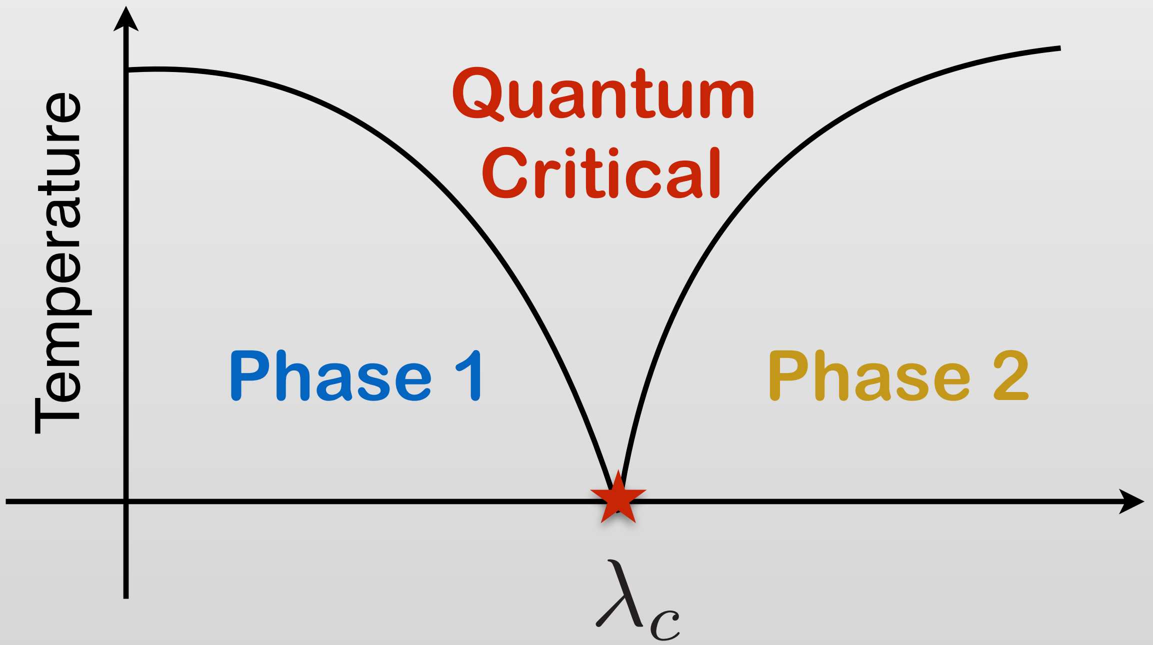
Ferrenberg et al, 1988 Wang and Landau, 2001 Troyer et al, 2003

Fidelity Susceptibility

What's that ? Why should I care ?

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

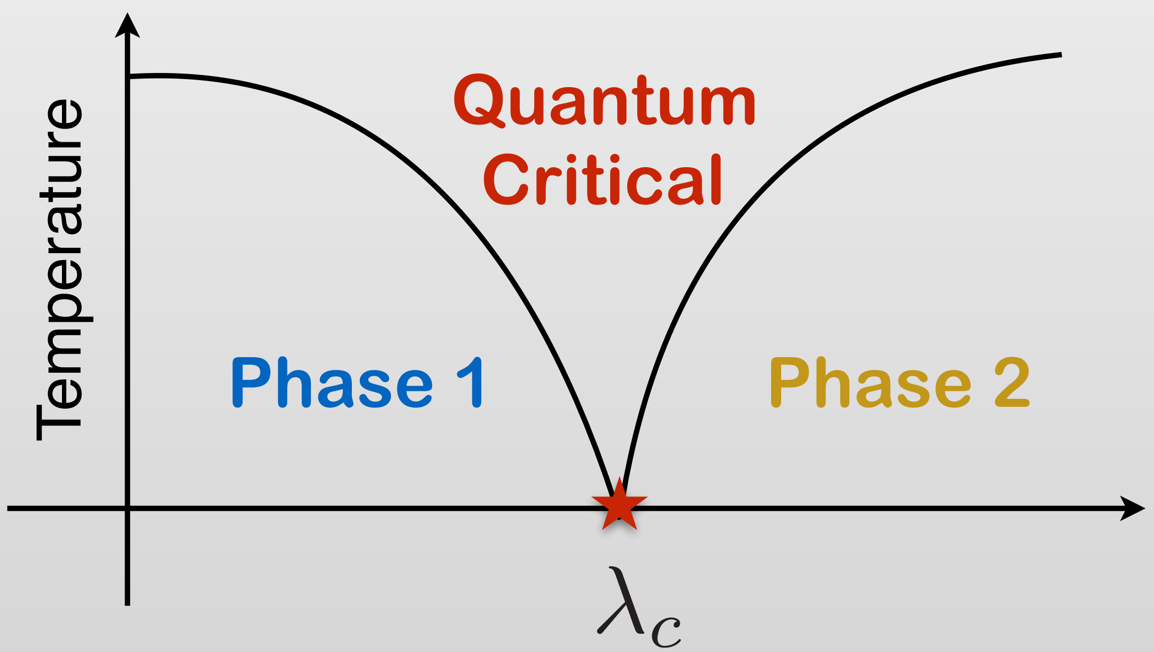
You, Li, and Gu, 2007
Campos Venuti et al, 2007



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



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 ?

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

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

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 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

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 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

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

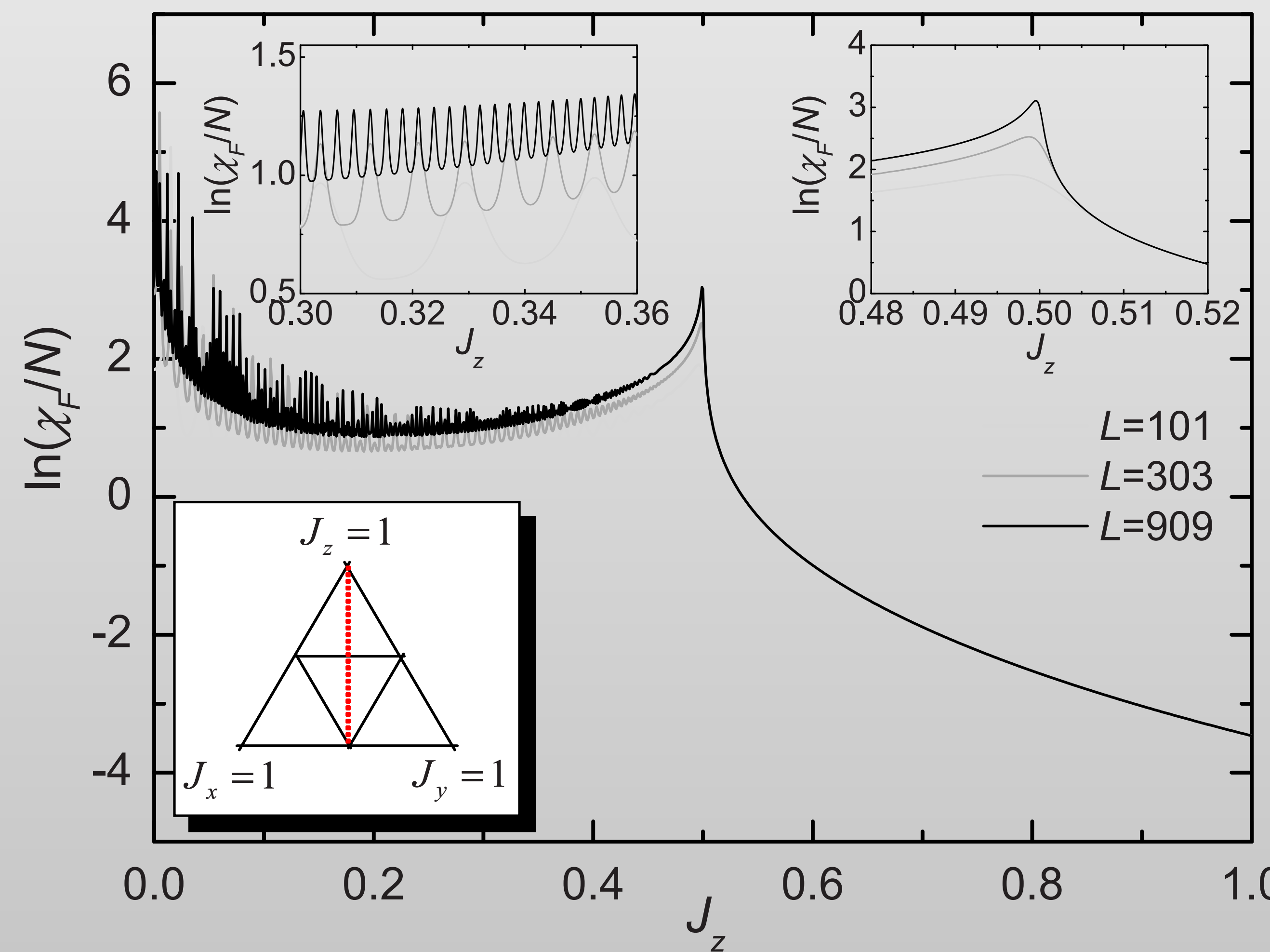
PHYSICAL REVIEW A **78**, 012304 (2008)

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

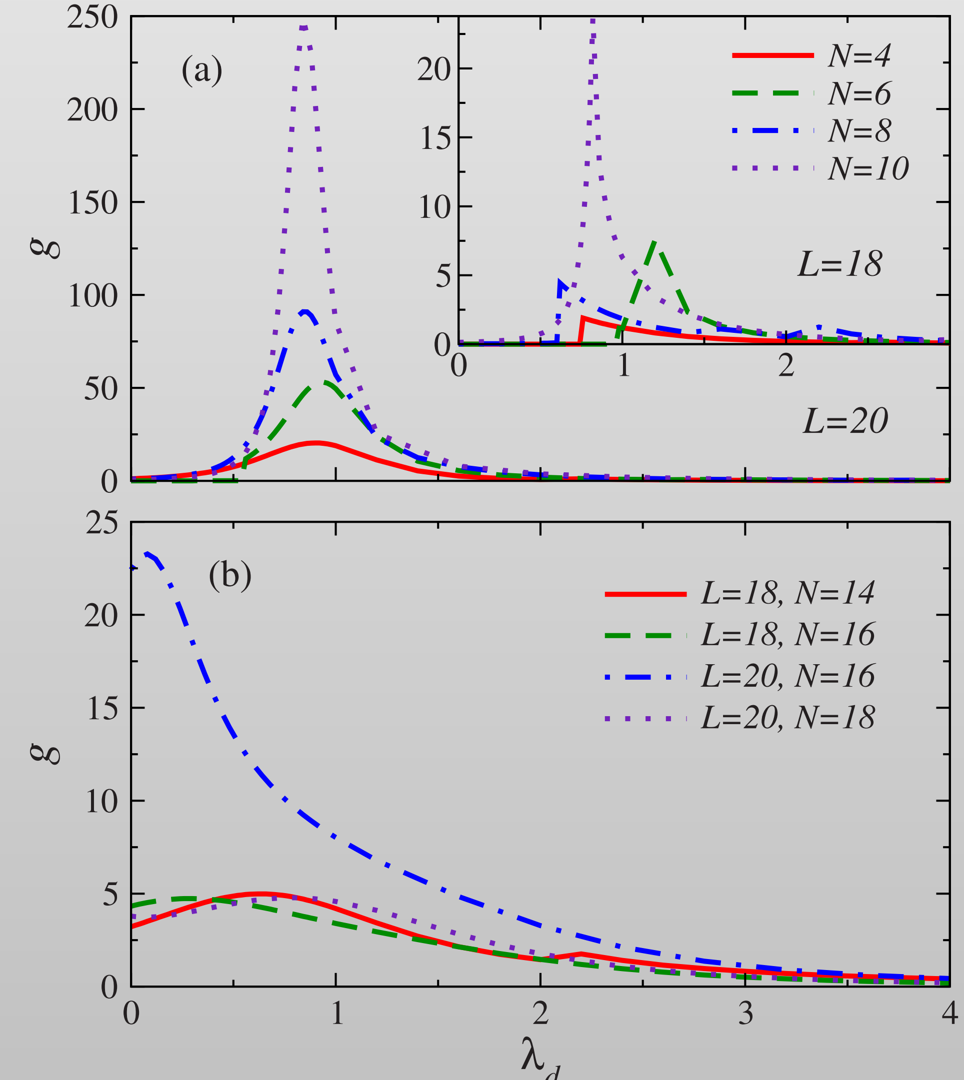
Stephan Haas
Department of Physics and Astronomy, University of Southern California, Los Angeles, California 90089, USA

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

Exact diagonalization on small clusters

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

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



Finite-Temperature Fidelity Susceptibility for One-Dimensional Quantum Systems

J. Sirker
Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, D-67663 Kaiserslautern, Germany
(Received 13 June 2010; revised manuscript received 18 July 2010; published 8 September 2010)

We can generalize (1) to finite temperatures so that $F_T(0) = 1$ and $\lim_{T\to 0} F_T(\lambda) = F_0(\lambda)$ by

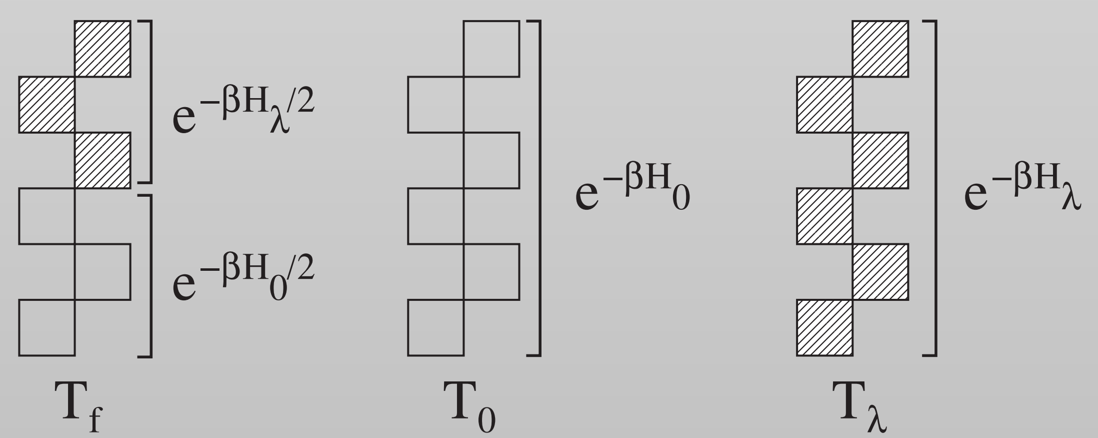
$$F_T(\lambda) = \sqrt{\mathrm{Tr}\{e^{-\beta\hat{H}_0/2}e^{-\beta\hat{H}_\lambda/2}\}}/(Z_0 Z_\lambda)^{1/4} \qquad (2)$$

where $\beta = 1/T$, $Z_0 = \mathrm{Tr}e^{-\beta\hat{H}_0}$, and $Z_\lambda = \mathrm{Tr}e^{-\beta\hat{H}_\lambda}$. For a

Finite-T generalization based on density matrices

Apart from the two different Boltzmann weights necessary to form the three transfer matrices depicted in Fig. 1 the algorithm can therefore proceed in exactly the same way as the TMRG algorithm to calculate thermodynamic

Computed fidelity in TDL using TMRG



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

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

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

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

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

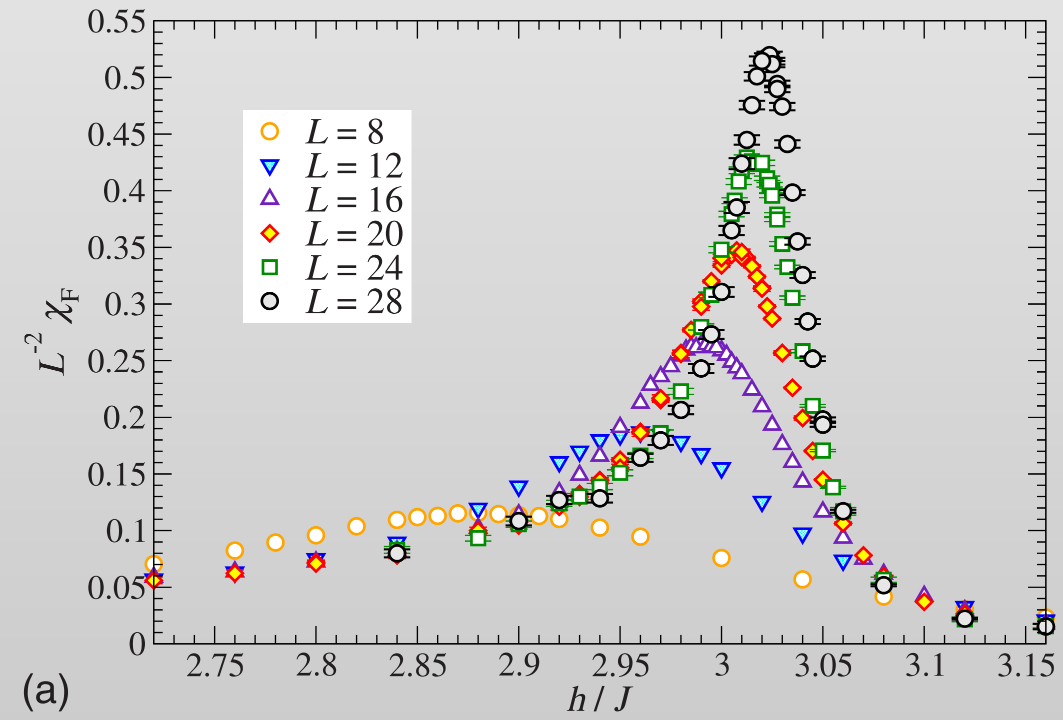
PHYSICAL REVIEW B **81**, 064418 (2010)

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)

SSE estimator of the imaginary-time correlator

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



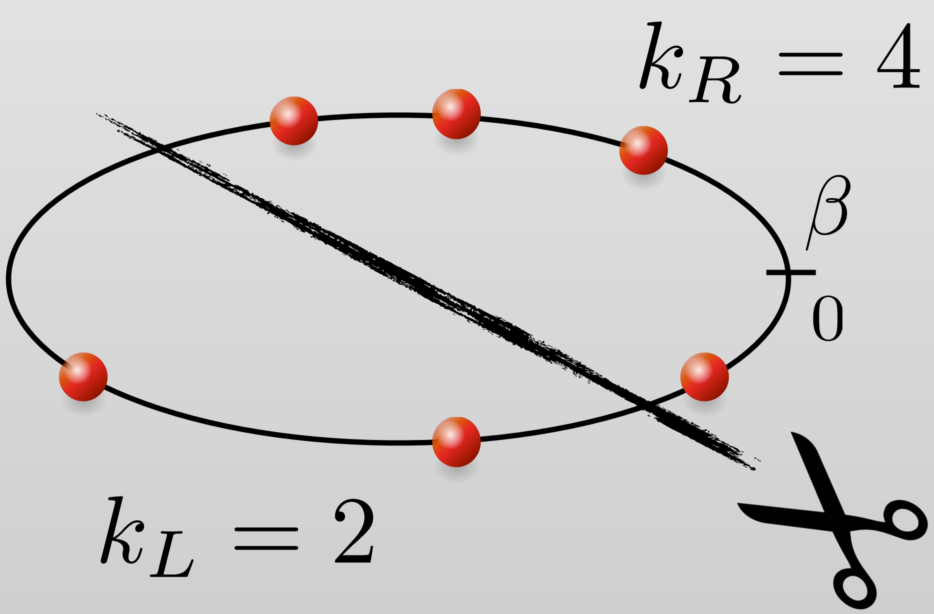
2D TFIM

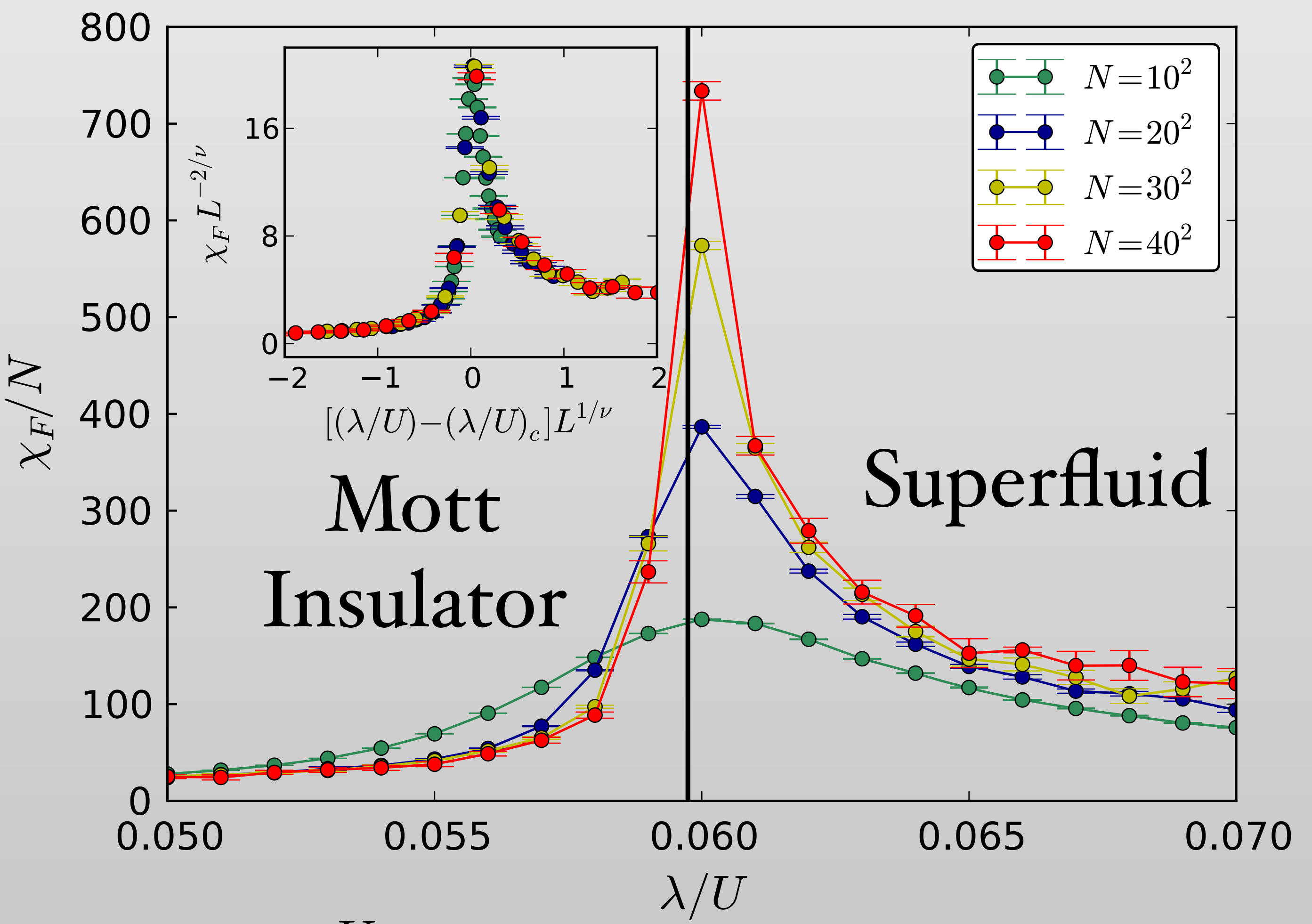
Can we do even better ?

Fidelity susceptibility made simple!

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

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





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

Cut and count, that's it!

Calculated using directed worm algorithm

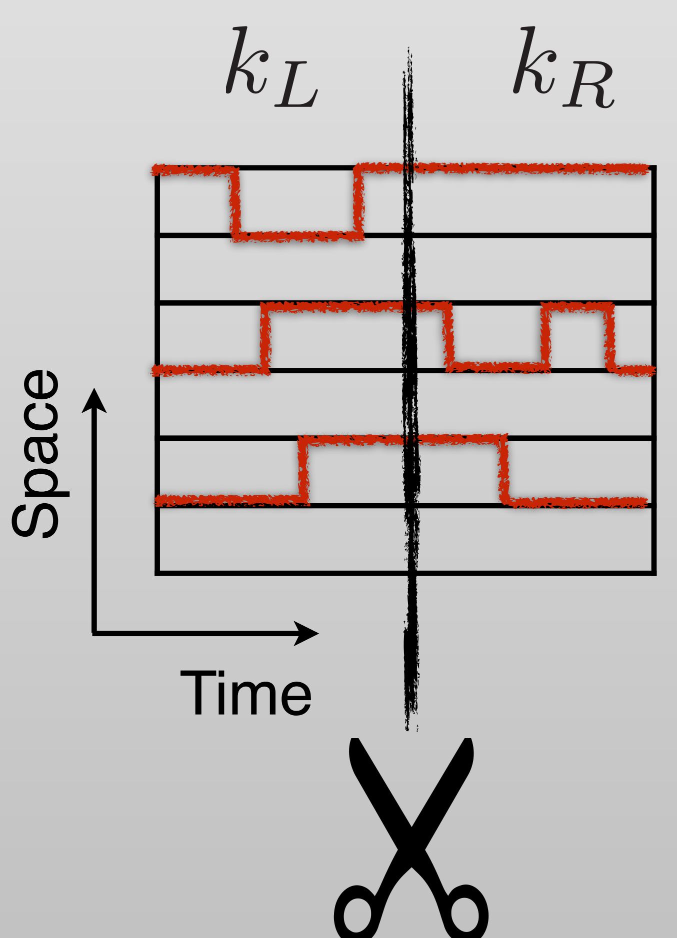
Fidelity susceptibility made simple!

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

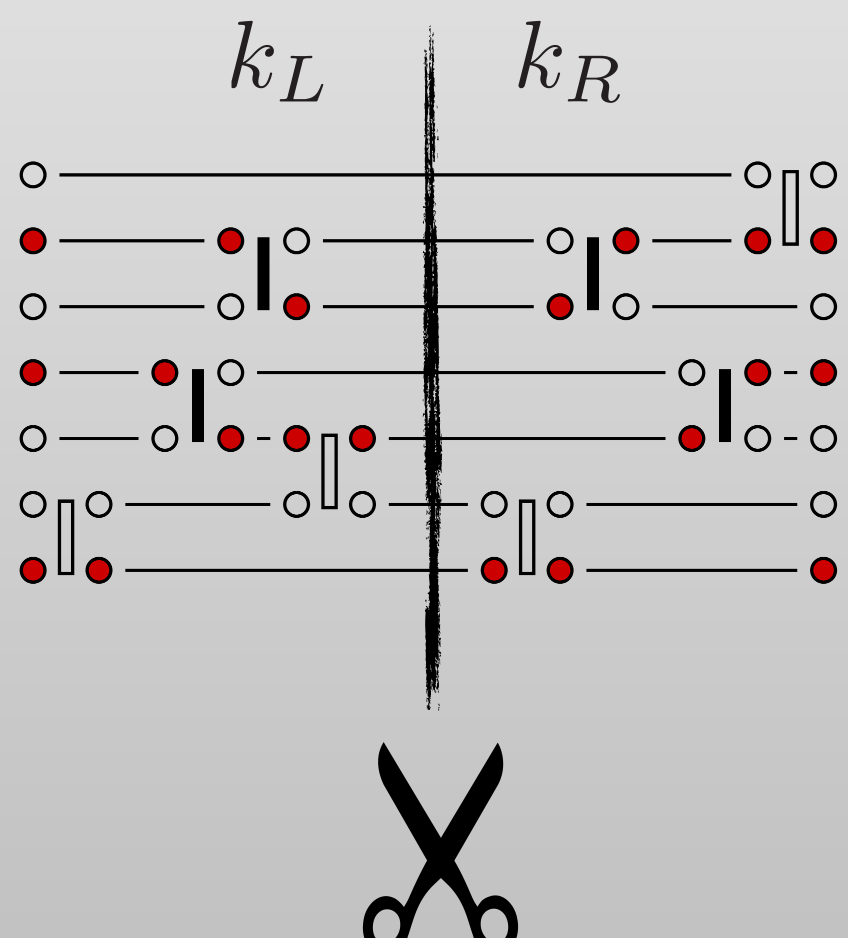
$$\chi_F = \frac{\langle k_L k_R \rangle - \langle k_L \rangle \langle k_R \rangle}{2\lambda^2}$$

```
kL = std::count_if(worldlines.begin(), wordlines.end(), IsLeft)
```

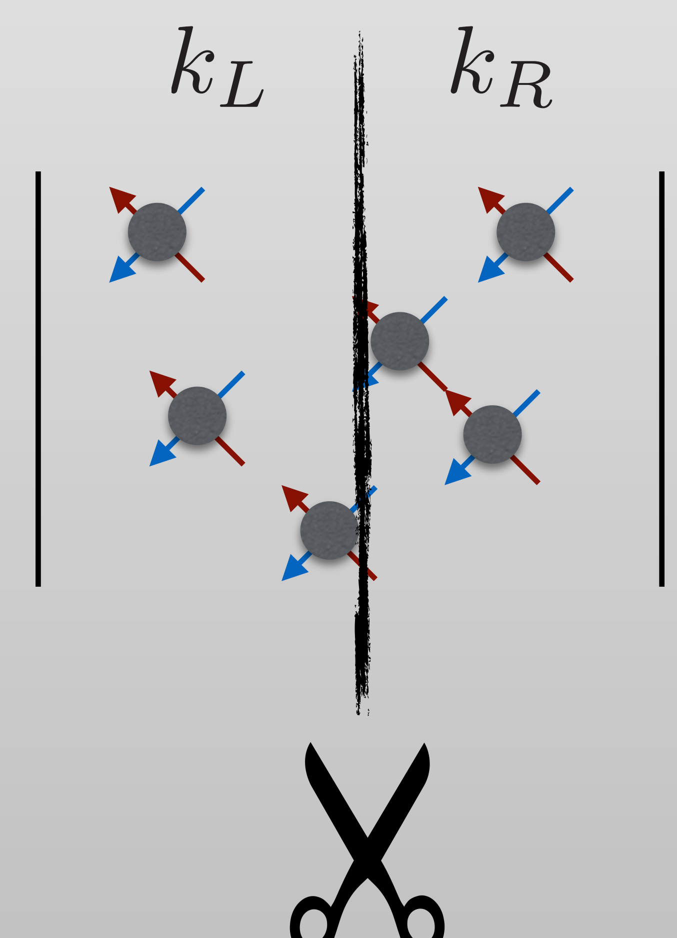
Worldline Algorithms **(bosons)**



Stochastic Series Expansion **(quantum spins)**



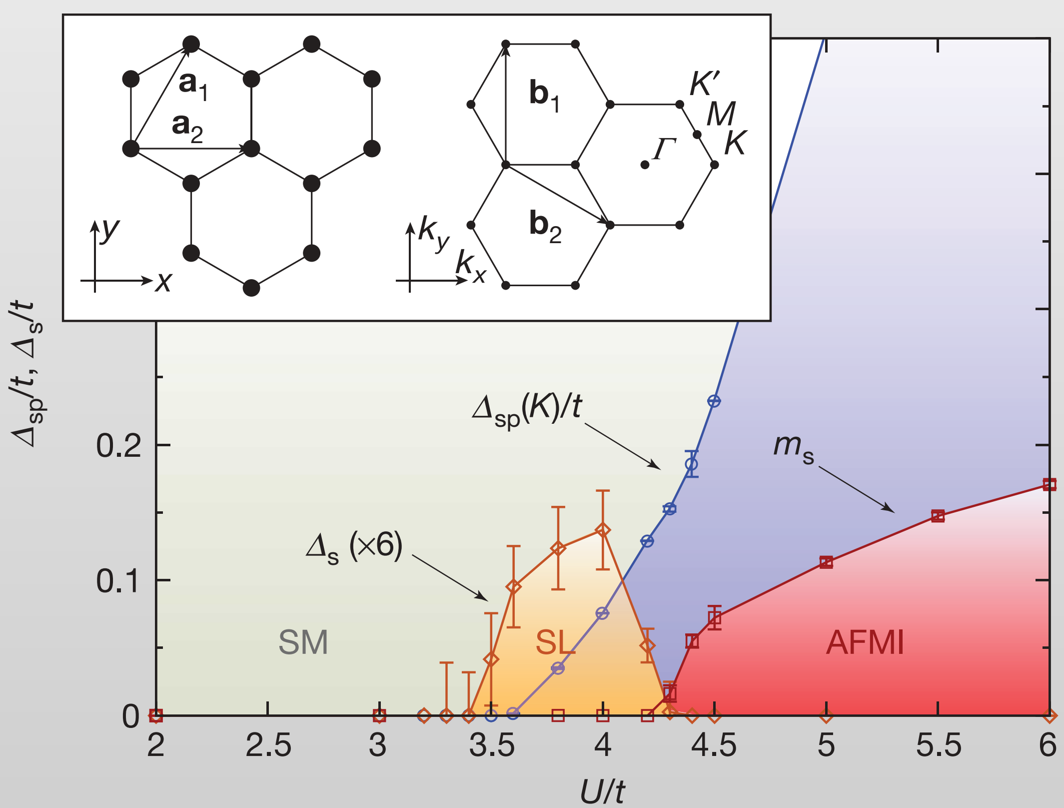
Determinantal Methods **(fermions)**



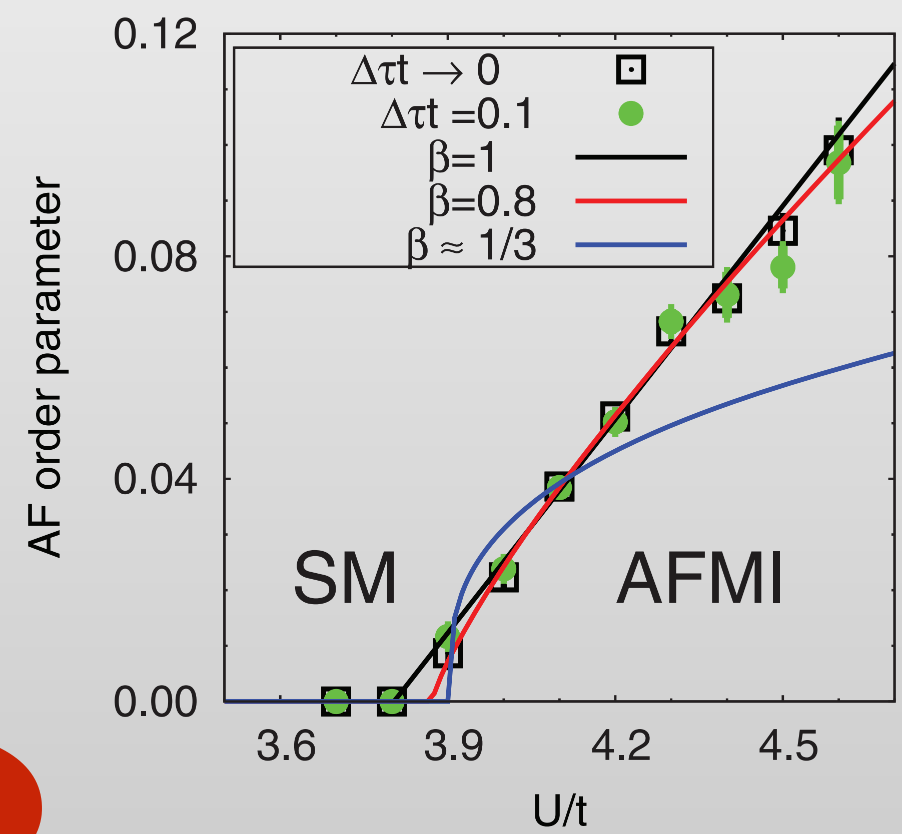
Honeycomb Hubbard Model

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

Meng et al, Nature 2010



Sorella et al, Sci.Rep 2012



?

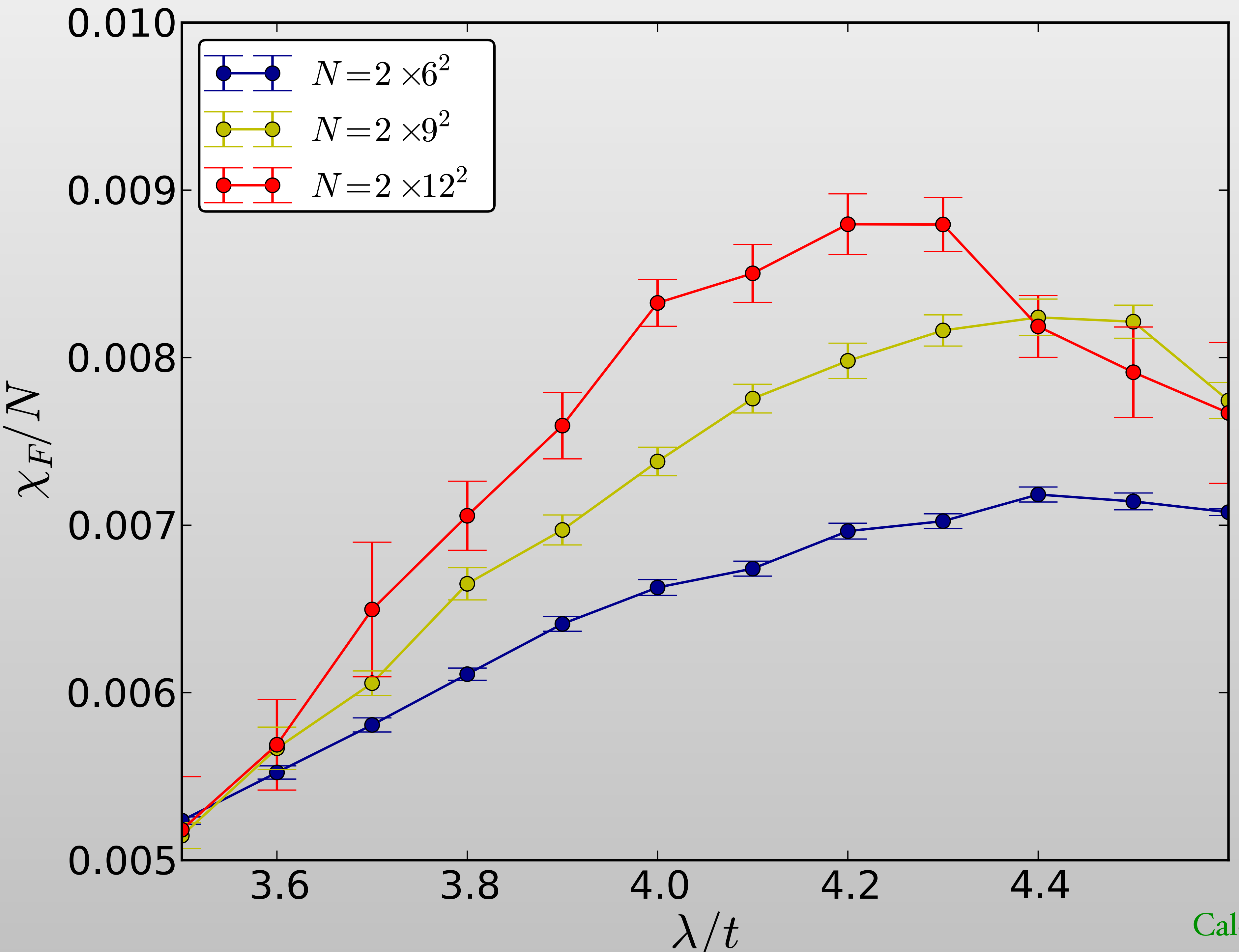
cf. Assaad et al, PRX 2013
Otsuka et al, PRX 2016

Debates in the past few years

There is only one peak !

Suggesting a single phase transition,

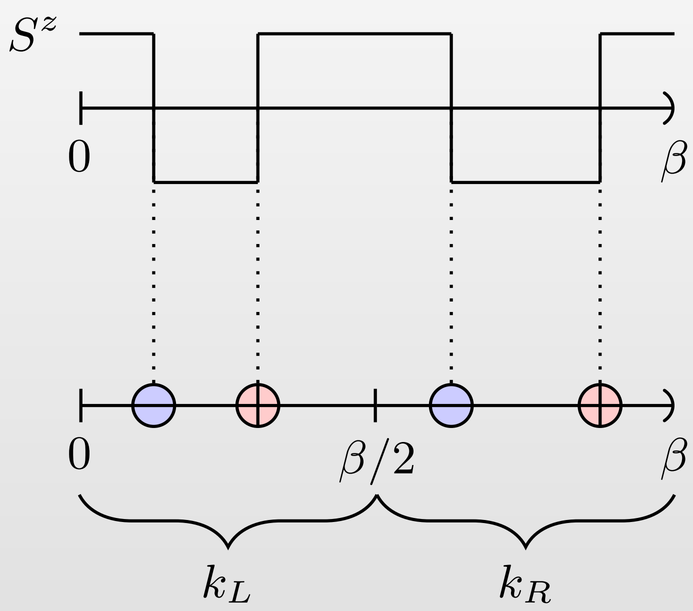
i.e. no intermediate phase



Calculated using LCT-INT

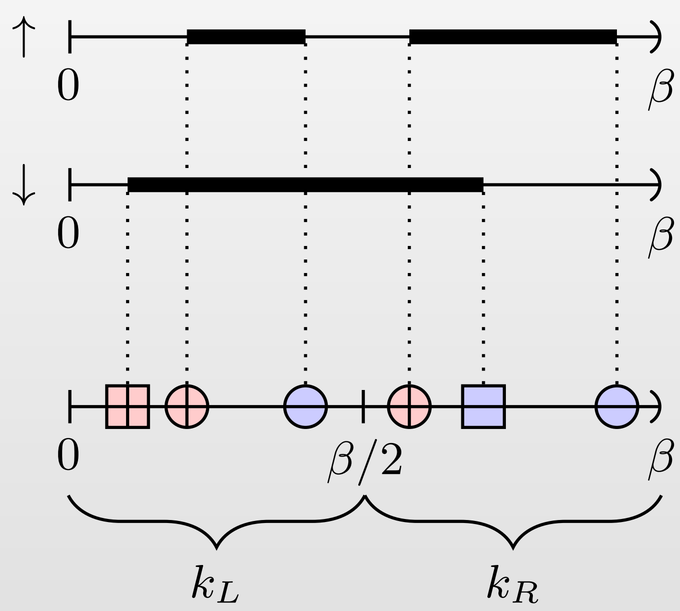
Impurity QPT

LW, Shinaoka and Troyer, PRL 2015



Anderson and Yuval, 1969

Maps the Kondo model to a classical Coulomb gas



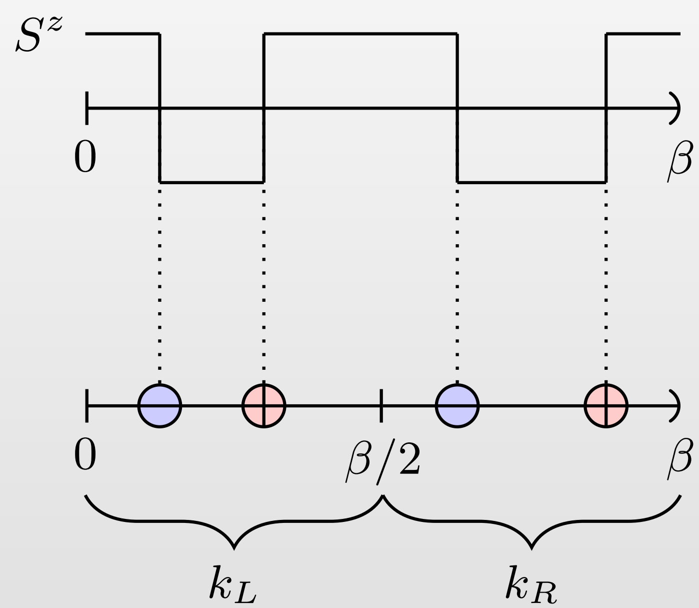
Werner el al 2006

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

Calculated using CT-HYB

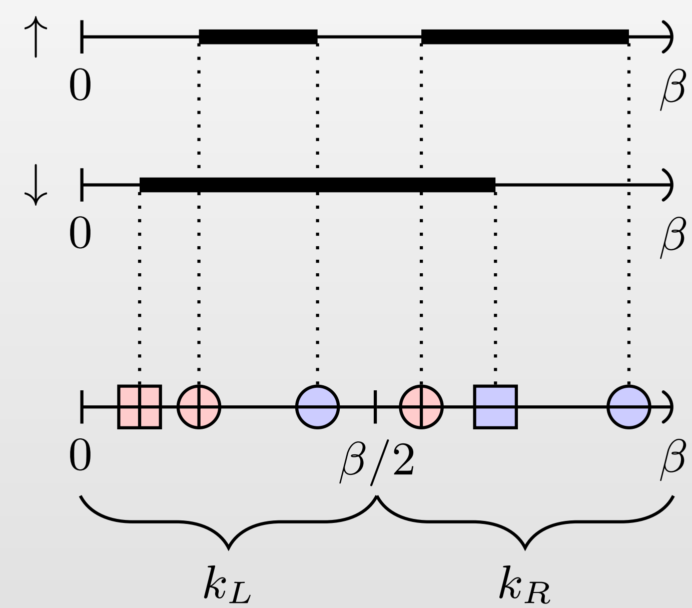
Impurity QPT

LW, Shinaoka and Troyer, PRL 2015



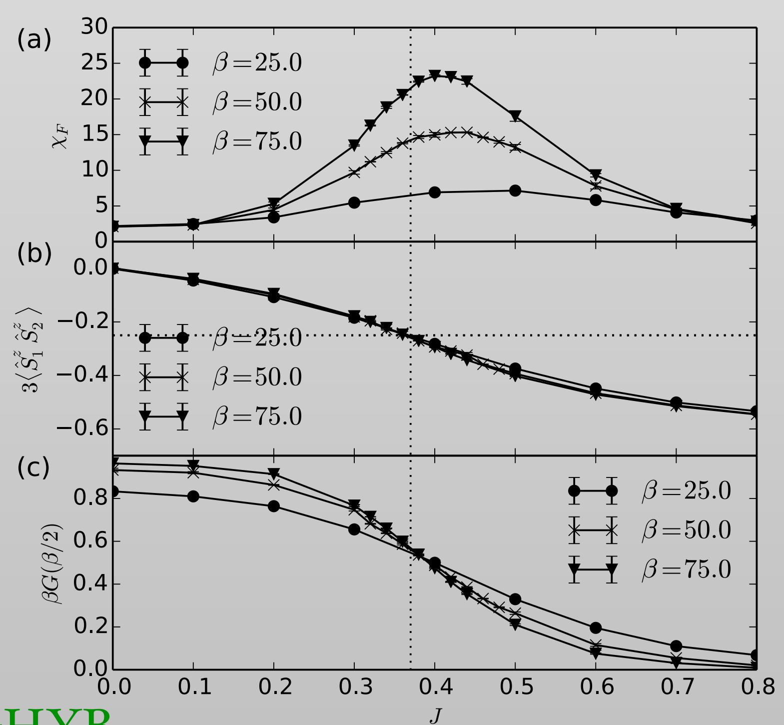
Anderson and Yuval, 1969

Maps the Kondo model to a classical Coulomb gas

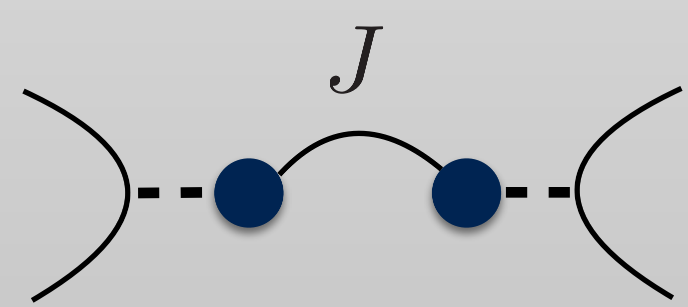


Werner el al 2006

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



Calculated using CT-HYB



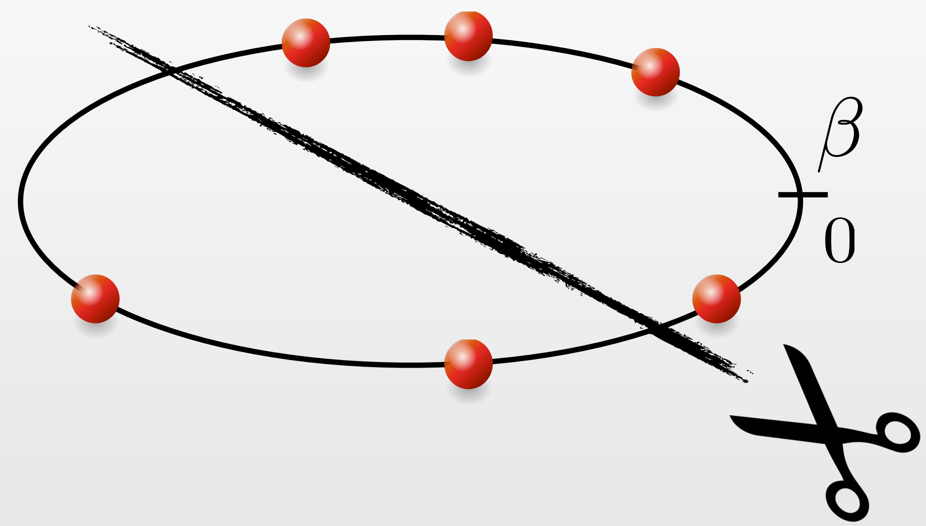
Two-impurity Anderson model

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

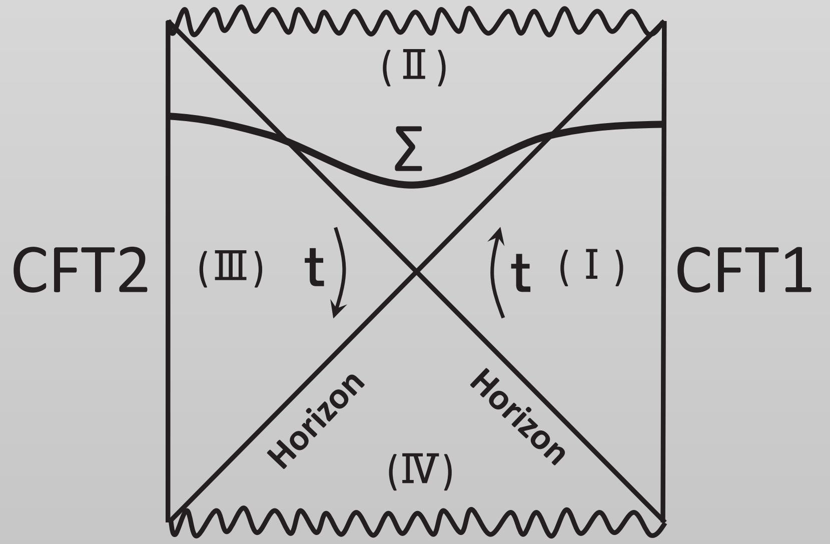
PRL **115,** 261602 (2015) PHYSICAL REVIEW LETTERS week ending 31 DECEMBER 2015

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 ➔



What about the sign problem ?

Sign problem free: Kramers pairs due to the time-reversal symmetry

$$M_{\uparrow} = M_{\downarrow}^{*}$$

Lang et al, Phys. Rev. C, 1993
Koonin et al, Phys. Rep, 1997
Hands et al, EPJC, 2000
Wu et al, PRB, 2005

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

What about the sign problem ?

Sign problem free: Kramers pairs due to the time-reversal symmetry

$$M_\uparrow = M_\downarrow^*$$

Lang et al, Phys. Rev. C, 1993
Koonin et al, Phys. Rep, 1997
Hands et al, EPJC, 2000
Wu et al, PRB, 2005

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

- Attractive interaction at any filling on any lattice
- Repulsive interaction at half-filling on bipartite lattices

What about the sign problem ?

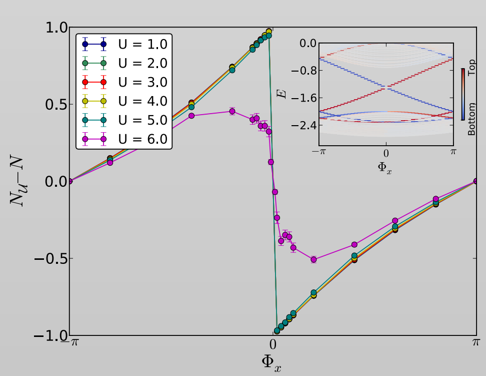
Sign problem free: Kramers pairs due to the time-reversal symmetry

$$M_{\uparrow} = M_{\downarrow}^{*}$$

Lang et al, Phys. Rev. C, 1993
Koonin et al, Phys. Rep, 1997
Hands et al, EPJC, 2000
Wu et al, PRB, 2005

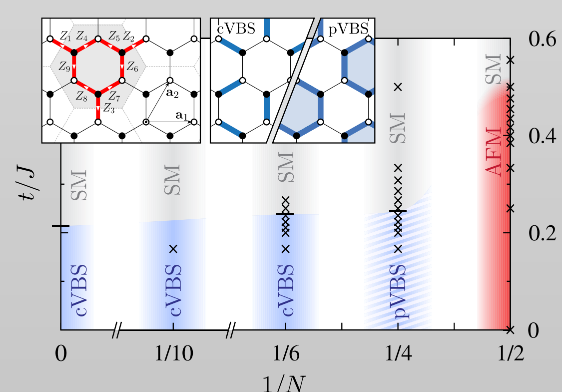
$$w(\mathcal{C}_k) = \det M_{\uparrow} \times \det M_{\downarrow}$$
$$= |\det M_{\uparrow}|^2 \geq 0$$

- Attractive interaction at any filling on any lattice
- Repulsive interaction at half-filling on bipartite lattices
- And more ...



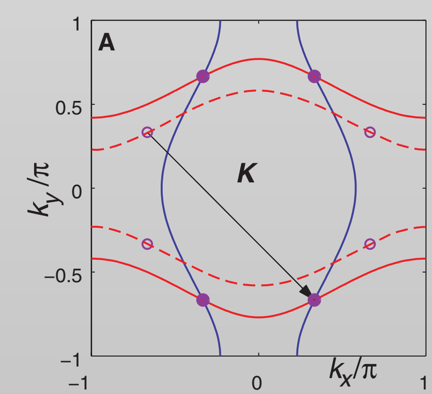
Hofstadter model

LW, Hung and Troyer, PRB 2014



SU(2N) models

Lang, Meng, Muramatsu, Wessel and Assaad, PRL 2013



Spin-fermion models

Berg, Metliski and Sachdev, Science 2012

What about the sign problem ?

Sign problem free: Kramers pairs due to the time-reversal symmetry

$$M_\uparrow = M_\downarrow^*$$

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

Lang et al, Phys. Rev. C, 1993
Koonin et al, Phys. Rep, 1997
Hands et al, EPJC, 2000
Wu et al, PRB, 2005

But, how about this ?

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

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

Scalapino et al, PRB 1984 Gubernatis et al, PRB 1985
up to 8*8 square lattice and T≥0.3t

Meron cluster approach, Chandrasekharan and Wiese, PRL 1999
solves sign problem for V ≥ 2t

Solutions !

PHYSICAL REVIEW B **89**, 111101(R) (2014)

Solution to sign problems in half-filled spin-polarized electronic systems

Emilie Fulton Huffman and Shailesh Chandrasekharan
Department of Physics, Duke University, Durham, North Carolina 27708, USA
(Received 19 December 2013; revised manuscript received 14 February 2014; published 12 March 2014)

Solutions !

PHYSICAL REVIEW B **89**, 111101(R) (2014)

Solution to sign problems in half-filled spin-polarized electronic systems

Emilie Fulton Huffman and Shailesh Chandrasekharan
Department of Physics, Duke University, Durham, North Carolina 27708, USA
(Received 19 December 2013; revised manuscript received 14 February 2014; published 12 March 2014)

PHYSICAL REVIEW B **91**, 241117(R) (2015)

Solving the fermion sign problem in quantum Monte Carlo simulations by Majorana representation

Zi-Xiang Li,[1] Yi-Fan Jiang,[1,2] and Hong Yao[1,3,*]
[1]*Institute for Advanced Study, Tsinghua University, Beijing 100084, China*
[2]*Department of Physics, Stanford University, Stanford, California 94305, USA*
[3]*Collaborative Innovation Center of Quantum Matter, Beijing 100084, China*
(Received 27 August 2014; revised manuscript received 13 October 2014; published 30 June 2015)

PHYSICAL REVIEW B **91**, 235151 (2015)

Efficient continuous-time quantum Monte Carlo method for the ground state of correlated fermions

Lei Wang,[1] Mauro Iazzi,[1] Philippe Corboz,[2] and Matthias Troyer[1]
[1]*Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*
[2]*Institute for Theoretical Physics, University of Amsterdam, Science Park 904 Postbus 94485, 1090 GL Amsterdam, The Netherlands*
(Received 12 January 2015; revised manuscript received 13 March 2015; published 30 June 2015)

Solutions !

PHYSICAL REVIEW B **89**, 111101(R) (2014)

Solution to sign problems in half-filled spin-polarized electronic systems

Emilie Fulton Huffman and Shailesh Chandrasekharan
Department of Physics, Duke University, Durham, North Carolina 27708, USA
(Received 19 December 2013; revised manuscript received 14 February 2014; published 12 March 2014)

PHYSICAL REVIEW B **91**, 241117(R) (2015)

Solving the fermion sign problem in quantum Monte Carlo simulations by Majorana representation

Zi-Xiang Li,[1] Yi-Fan Jiang,[1,2] and Hong Yao[1,3,*]
[1]*Institute for Advanced Study, Tsinghua University, Beijing 100084, China*
[2]*Department of Physics, Stanford University, Stanford, California 94305, USA*
[3]*Collaborative Innovation Center of Quantum Matter, Beijing 100084, China*
(Received 27 August 2014; revised manuscript received 13 October 2014; published 30 June 2015)

PHYSICAL REVIEW B **91**, 235151 (2015)

Efficient continuous-time quantum Monte Carlo method for the ground state of correlated fermions

Lei Wang,[1] Mauro Iazzi,[1] Philippe Corboz,[2] and Matthias Troyer[1]
[1]*Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*
[2]*Institute for Theoretical Physics, University of Amsterdam, Science Park 904 Postbus 94485, 1090 GL Amsterdam, The Netherlands*
(Received 12 January 2015; revised manuscript received 13 March 2015; published 30 June 2015)

PRL **115,** 250601 (2015) PHYSICAL REVIEW LETTERS week ending 18 DECEMBER 2015

Split Orthogonal Group: A Guiding Principle for Sign-Problem-Free Fermionic Simulations

Lei Wang,[1] Ye-Hua Liu,[1] Mauro Iazzi,[1] Matthias Troyer,[1] and Gergely Harcos[2]
[1]*Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*
[2]*Alfréd Rényi Institute of Mathematics, Reáltanoda utca 13-15., Budapest H-1053, Hungary*

Solutions !

PHYSICAL REVIEW B **89**, 111101(R) (2014)

Solution to sign problems in half-filled spin-polarized electronic systems

Emilie Fulton Huffman and Shailesh Chandrasekharan
Department of Physics, Duke University, Durham, North Carolina 27708, USA
(Received 19 December 2013; revised manuscript received 14 February 2014; published 12 March 2014)

PHYSICAL REVIEW B **91**, 241117(R) (2015)

Solving the fermion sign problem in quantum Monte Carlo simulations by Majorana representation

Zi-Xiang Li,[1] Yi-Fan Jiang,[1,2] and Hong Yao[1,3,*]
[1]*Institute for Advanced Study, Tsinghua University, Beijing 100084, China*
[2]*Department of Physics, Stanford University, Stanford, California 94305, USA*
[3]*Collaborative Innovation Center of Quantum Matter, Beijing 100084, China*
(Received 27 August 2014; revised manuscript received 13 October 2014; published 30 June 2015)

PHYSICAL REVIEW B **91**, 235151 (2015)

Efficient continuous-time quantum Monte Carlo method for the ground state of correlated fermions

Lei Wang,[1] Mauro Iazzi,[1] Philippe Corboz,[2] and Matthias Troyer[1]
[1]*Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*
[2]*Institute for Theoretical Physics, University of Amsterdam, Science Park 904 Postbus 94485, 1090 GL Amsterdam, The Netherlands*
(Received 12 January 2015; revised manuscript received 13 March 2015; published 30 June 2015)

PRL **115,** 250601 (2015) PHYSICAL REVIEW LETTERS week ending 18 DECEMBER 2015

Split Orthogonal Group: A Guiding Principle for Sign-Problem-Free Fermionic Simulations

Lei Wang,[1] Ye-Hua Liu,[1] Mauro Iazzi,[1] Matthias Troyer,[1] and Gergely Harcos[2]
[1]*Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*
[2]*Alfréd Rényi Institute of Mathematics, Reáltanoda utca 13-15., Budapest H-1053, Hungary*

Latest update

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

A tale of open science

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

Free fermions with an effective imaginary-time dependent Hamiltonian

A tale of open science

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

Free fermions with an effective imaginary-time dependent Hamiltonian

Let real matrices $A_i = \begin{pmatrix} 0 & B_i \\ B_i^T & 0 \end{pmatrix}$

then $\det\left(I + e^{A_1} e^{A_2} \ldots e^{A_N}\right) \geq 0$

http://mathoverflow.net/questions/204460/how-to-prove-this-determinant-is-positive

A tale of open science

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

Free fermions with an effective imaginary-time dependent Hamiltonian

Let real matrices $A_i = \begin{pmatrix} 0 & B_i \\ B_i^T & 0 \end{pmatrix}$

then $\det\left(I + e^{A_1} e^{A_2} \dots e^{A_N}\right) \geq 0$

http://mathoverflow.net/questions/204460/how-to-prove-this-determinant-is-positive

mathoverflow

The conjecture was proved by Gergely Harcos and Terence Tao, with inputs from many others

https://terrytao.wordpress.com/2015/05/03/the-standard-branch-of-the-matrix-logarithm/

Tao and Paul Erdős in 1985

A tale of open science

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

Free fermions with an effective imaginary-time dependent Hamiltonian

Let real matrices $A_i = \begin{pmatrix} 0 & B_i \\ B_i^T & 0 \end{pmatrix}$

then $\det\left(I + e^{A_1} e^{A_2} \dots e^{A_N}\right) \geq 0$

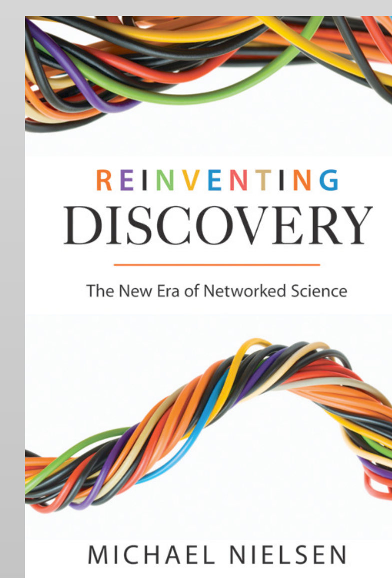
http://mathoverflow.net/questions/204460/how-to-prove-this-determinant-is-positive

mathoverflow

The conjecture was proved by Gergely Harcos and Terence Tao, with inputs from many others

https://terrytao.wordpress.com/2015/05/03/the-standard-branch-of-the-matrix-logarithm/

Tao and Paul Erdős in 1985



A tale of open science

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

Free fermions with an effective imaginary-time dependent Hamiltonian

Let real matrices $A_i = \begin{pmatrix} 0 & B_i \\ B_i^T & 0 \end{pmatrix}$

then $\det\left(I + e^{A_1} e^{A_2} \ldots e^{A_N}\right) \geq 0$

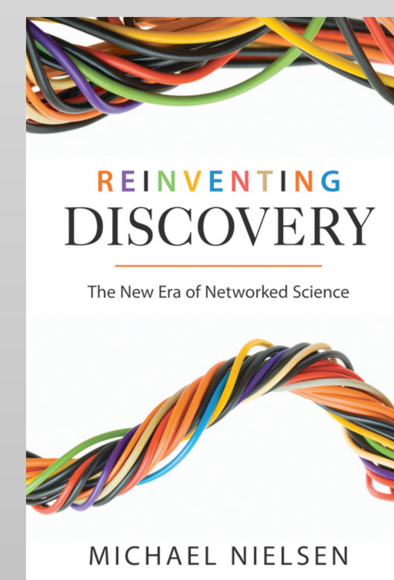
http://mathoverflow.net/questions/204460/how-to-prove-this-determinant-is-positive

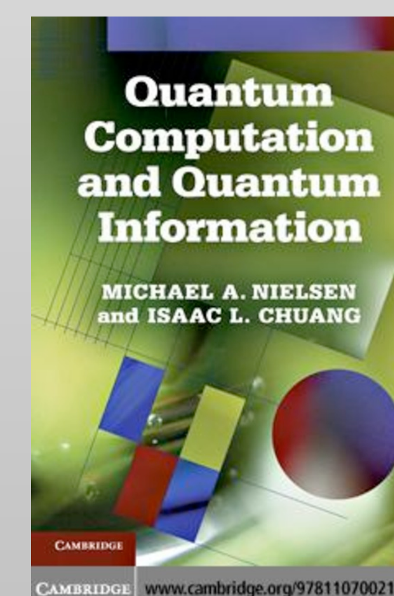
mathoverflow

The conjecture was proved by Gergely Harcos and Terence Tao, with inputs from many others

https://terrytao.wordpress.com/2015/05/03/the-standard-branch-of-the-matrix-logarithm/

Tao and Paul Erdős in 1985





A new “de-sign” principle

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

If $M^T \eta M = \eta$ where $\eta = \mathrm{diag}(I, -I)$

A new "de-sign" principle

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

If $M^T \eta M = \eta$ where $\eta = \mathrm{diag}(I, -I)$

Then $M \in O(n,n)$

split orthogonal group

$O^{+-}(n,n)$

$O^{++}(n,n)$

$O^{--}(n,n)$

$O^{-+}(n,n)$

A new "de-sign" principle

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

If $M^T \eta M = \eta$ where $\eta = \mathrm{diag}(I, -I)$

Then $\det\left(I + M\right)$

has a definite sign

for each component !

$O^{+-}(n,n)$

$\equiv 0$

$O^{++}(n,n)$

≥ 0

$O^{--}(n,n)$

≤ 0

$O^{-+}(n,n)$

$\equiv 0$

A new “de-sign” principle

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

If $M^T \eta M = \eta$ **where** $\eta = \mathrm{diag}(I, -I)$

$\mathcal{T} e^{-\int_0^\beta d\tau H_{\mathcal{C}_k}(\tau)}$

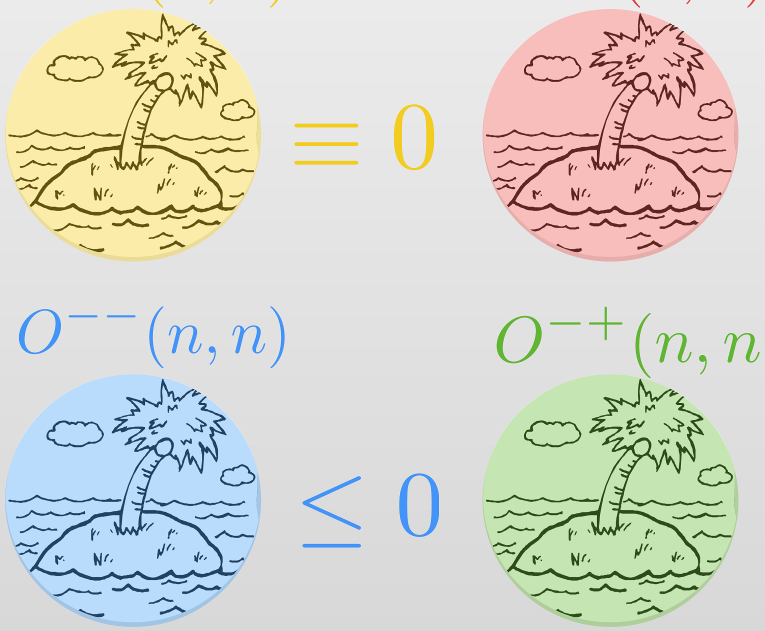
Then $\det(I + M)$

has a definite sign

for each component !

$O^{+-}(n,n) \equiv 0$ $\quad O^{++}(n,n) \geq 0$

$O^{--}(n,n) \leq 0$ $\quad O^{-+}(n,n) \equiv 0$



A new "de-sign" principle

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

If $\quad M^T \eta M = \eta \quad$ where $\quad \eta = \mathrm{diag}(I, -I)$

Then $\quad \det\left(I + M\right)$ — with $M = \mathcal{T} e^{-\int_0^\beta d\tau H_{\mathcal{C}_k}(\tau)}$

has a definite sign

for each component !

$O^{+-}(n,n)$

$\equiv 0$

$O^{++}(n,n)$

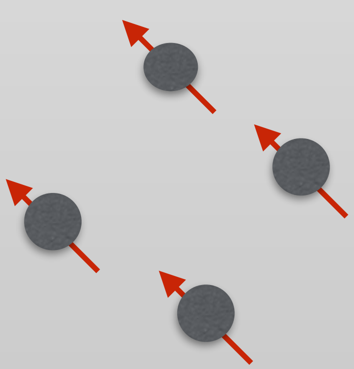
≥ 0

$O^{--}(n,n)$

≤ 0

$O^{-+}(n,n)$

$\equiv 0$



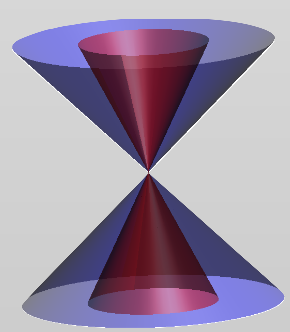
spinless fermions

LW, Troyer, PRL 2014

LW, Corboz, Troyer, NJP 2014

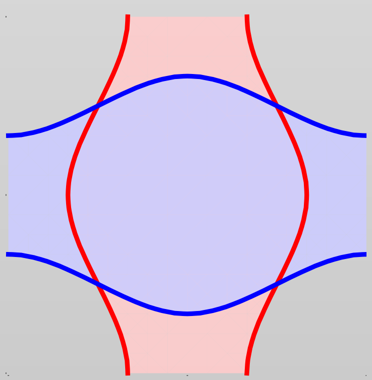
LW, Iazzi, Corboz, Troyer, PRB 2015

LW, Liu and Troyer, PRB 2016

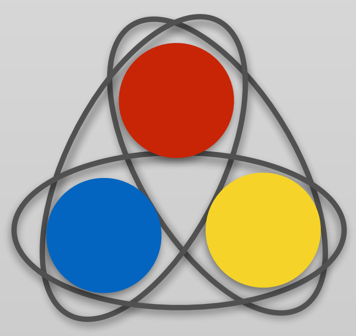


split Dirac cone

Liu and LW, PRB 2015



spin nematicity



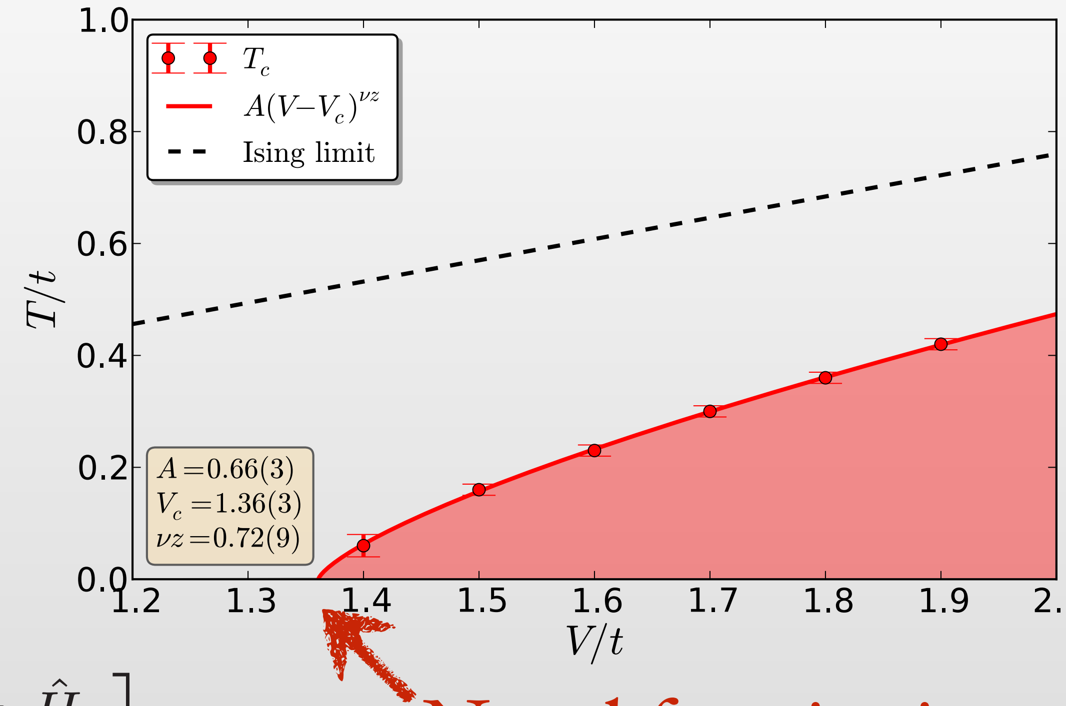
SU(3)

Solutions to the spinless t-V model

$$\hat{H}_0 = -t \sum_{\langle i,j \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right)$$

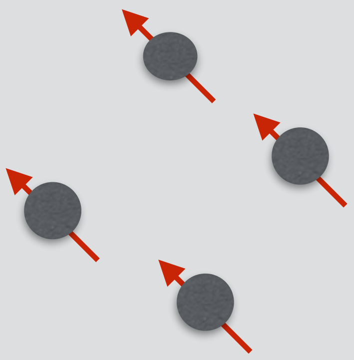
$$\hat{H}_1 = V \sum_{\langle i,j \rangle} \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_j - \frac{1}{2} \right)$$

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



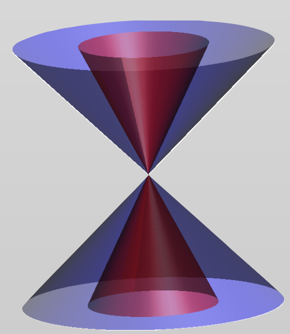
Novel fermionic quantum critical point

cf Li, Jiang, Yao 2015 Hesselmann and Wessel 2016



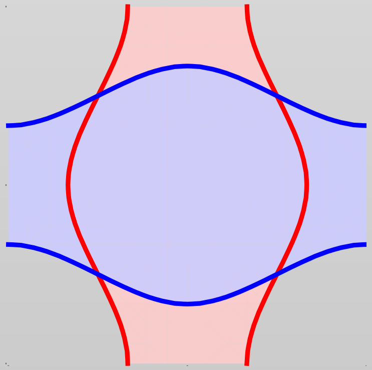
spinless fermions

LW, Troyer, PRL 2014
LW, Corboz, Troyer, NJP 2014
LW, Iazzi, Corboz, Troyer, PRB 2015
LW, Liu and Troyer, PRB 2016

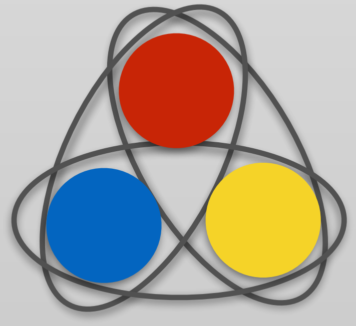


split Dirac cone

Liu and LW, PRB 2015



spin nematicity



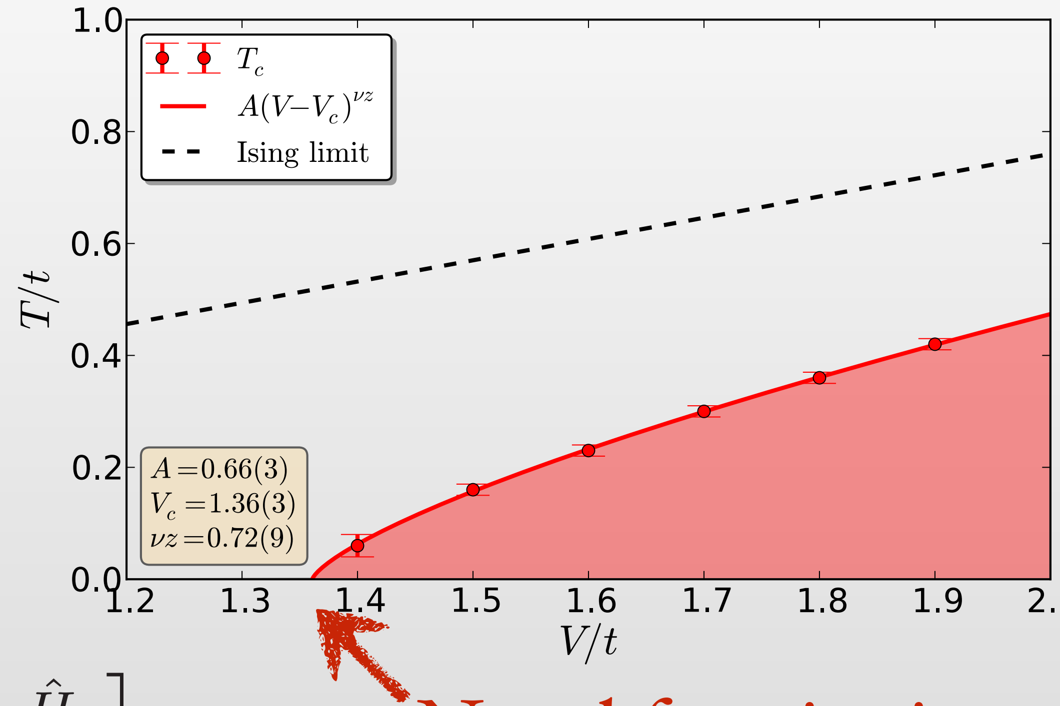
SU(3)

Solutions to the spinless t-V model

$$\hat{H}_0 = -t \sum_{\langle i,j \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right)$$

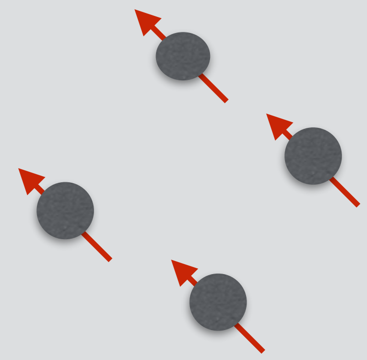
$$\hat{H}_1 = \frac{V}{4} \sum_{\langle i,j \rangle} e^{i\pi(\hat{n}_i + \hat{n}_j)}$$

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



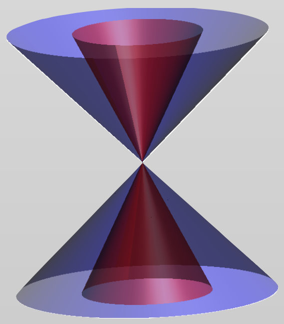
Novel fermionic quantum critical point

cf Li, Jiang, Yao 2015 Hesselmann and Wessel 2016



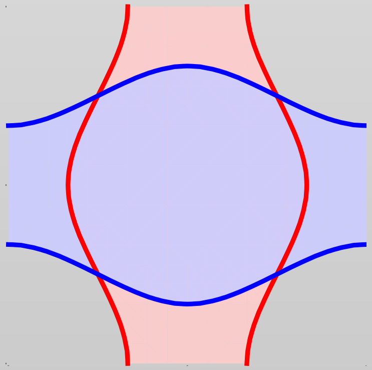
spinless fermions

LW, Troyer, PRL 2014
LW, Corboz, Troyer, NJP 2014
LW, Iazzi, Corboz, Troyer, PRB 2015
LW, Liu and Troyer, PRB 2016

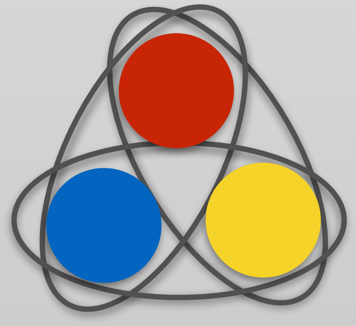


split Dirac cone

Liu and LW, PRB 2015



spin nematicity



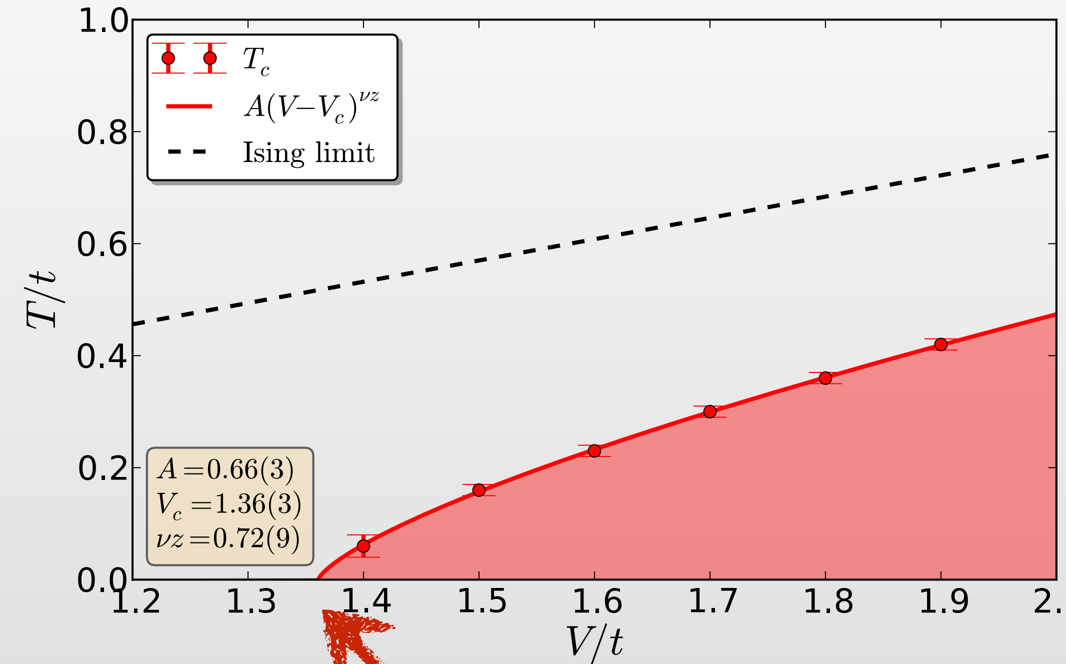
SU(3)

Solutions to the spinless t-V model

$$\hat{H}_0 = -t \sum_{\langle i,j \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right)$$

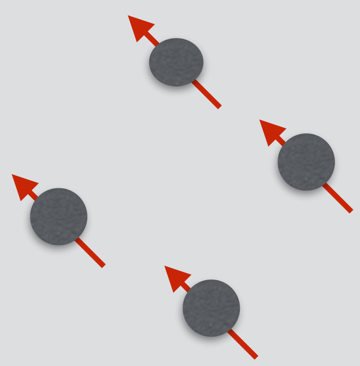
$$\hat{H}_1 = \frac{V}{4} \sum_{\langle i,j \rangle} e^{i\pi(\hat{n}_i + \hat{n}_j)}$$

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



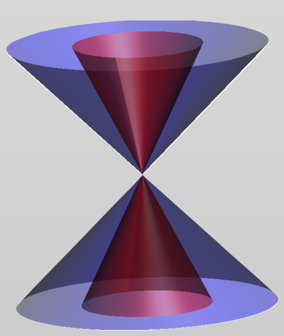
Novel fermionic quantum critical point

cf Li, Jiang, Yao 2015 Hesselmann and Wessel 2016



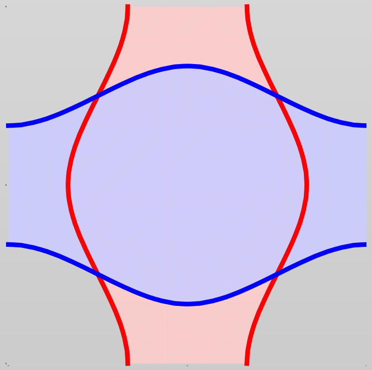
spinless fermions

LW, Troyer, PRL 2014
LW, Corboz, Troyer, NJP 2014
LW, Iazzi, Corboz, Troyer, PRB 2015
LW, Liu and Troyer, PRB 2016

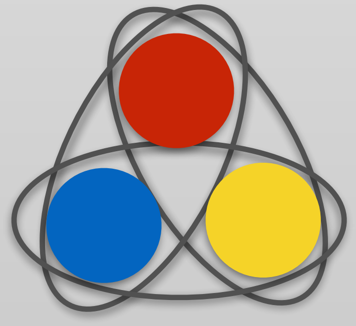


split Dirac cone

Liu and LW, PRB 2015



spin nematicity



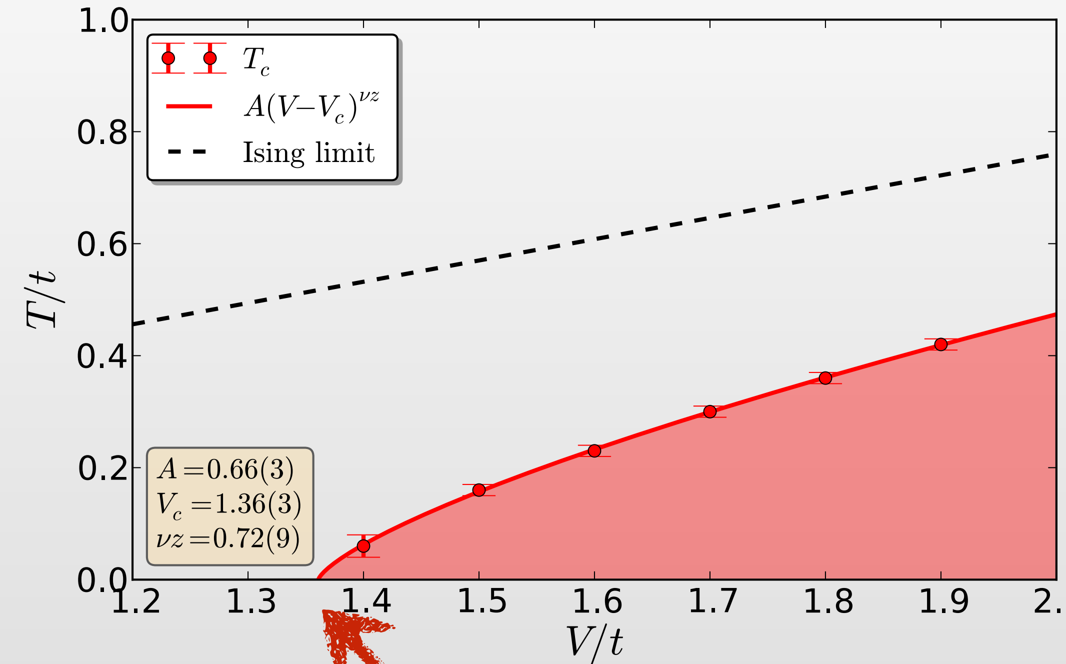
SU(3)

Solutions to the spinless t-V model

$$\hat{H}_0 = -t \sum_{\langle i,j \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right)$$

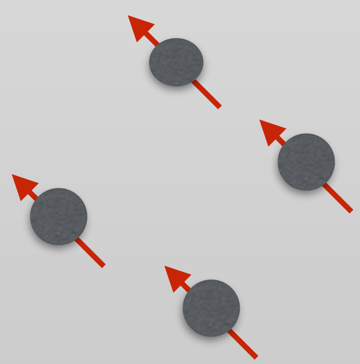
$$\hat{H}_1 = \frac{V}{4} \sum_{\langle i,j \rangle} e^{i\pi(\hat{n}_i + \hat{n}_j)}$$

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



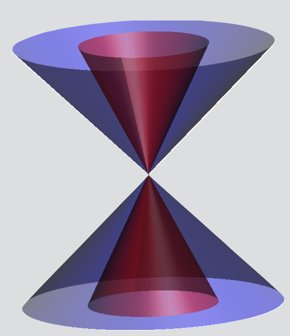
Novel fermionic quantum critical point

cf Li, Jiang, Yao 2015 Hesselmann and Wessel 2016



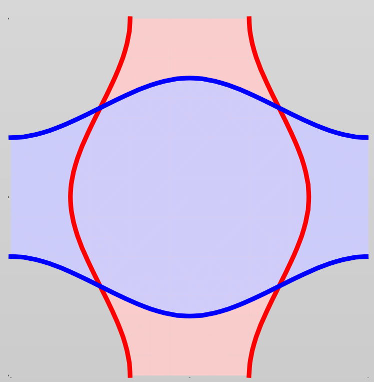
spinless fermions

LW, Troyer, PRL 2014
LW, Corboz, Troyer, NJP 2014
LW, Iazzi, Corboz, Troyer, PRB 2015
LW, Liu and Troyer, PRB 2016

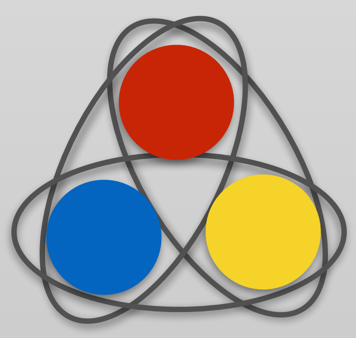


split Dirac cone

Liu and LW, PRB 2015

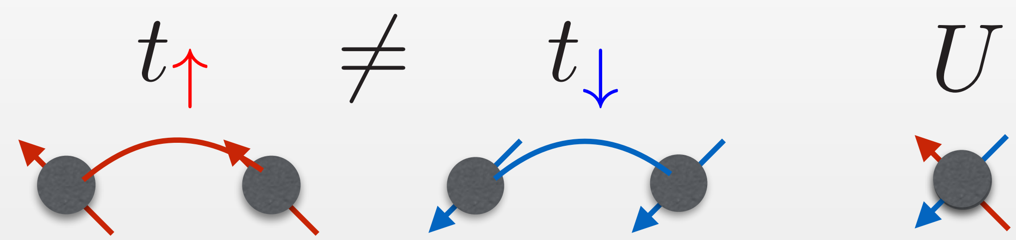


spin nematicity



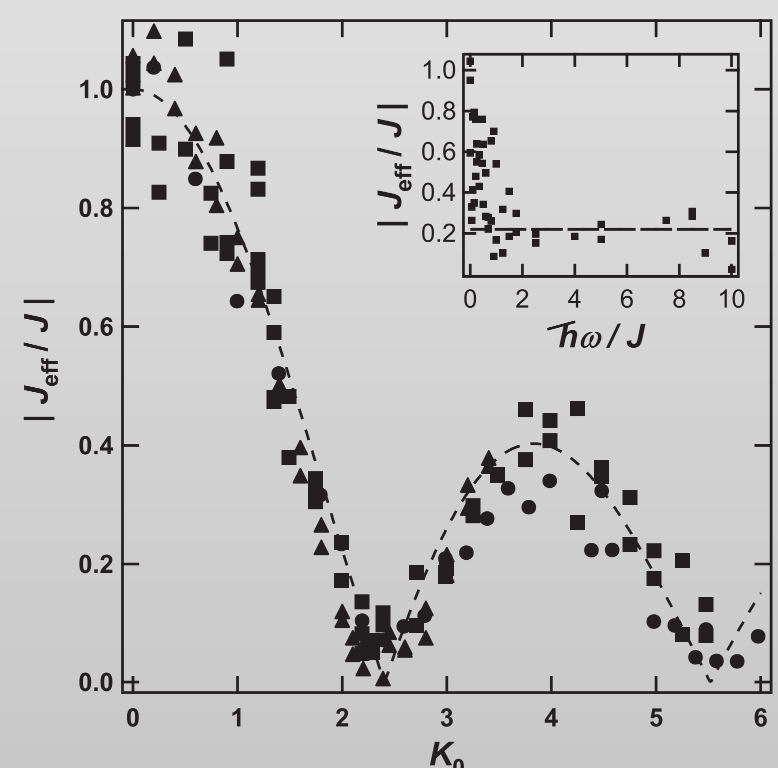
SU(3)

Asymmetric Hubbard model

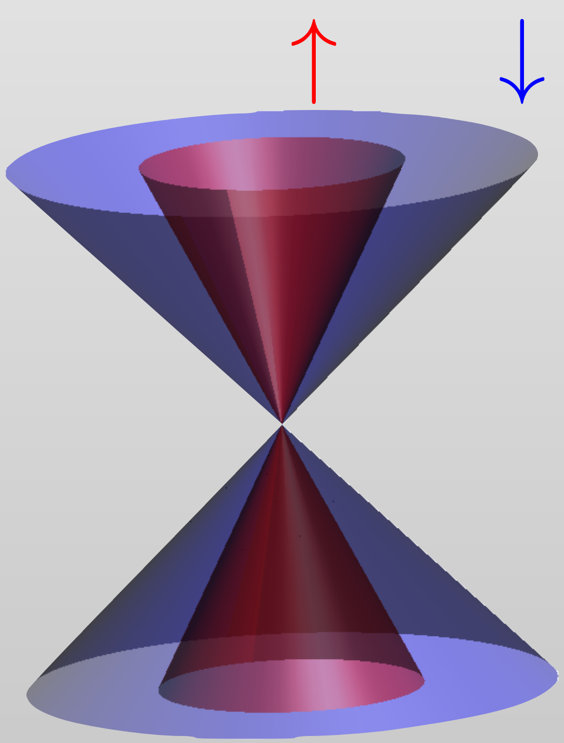


- Realization: mixture of ultracold fermions (e.g. ^{6}Li and ^{40}K)
- Now, continuously tunable by spin-dependent modulations Jotzu et al, PRL 2015

$$t_{\downarrow}/t_{\uparrow} \in (-\infty, \infty)$$



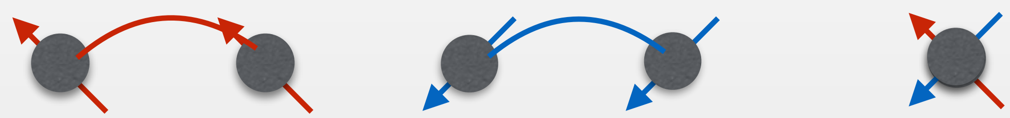
Lignier et al, PRL 2007 and many others



Dirac fermions with unequal Fermi velocities

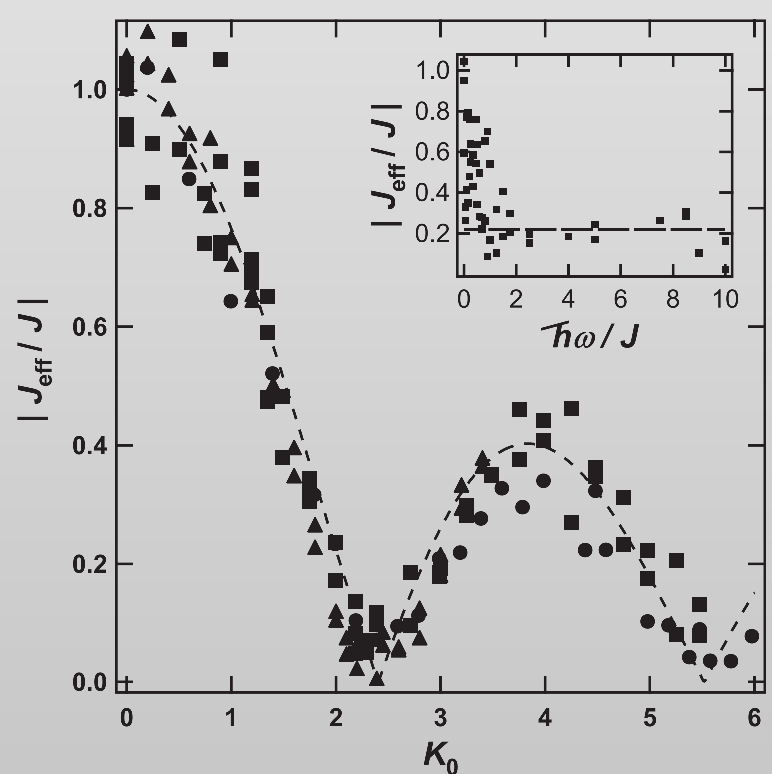
Asymmetric Hubbard model

$t_{\uparrow} \neq t_{\downarrow} \qquad U$

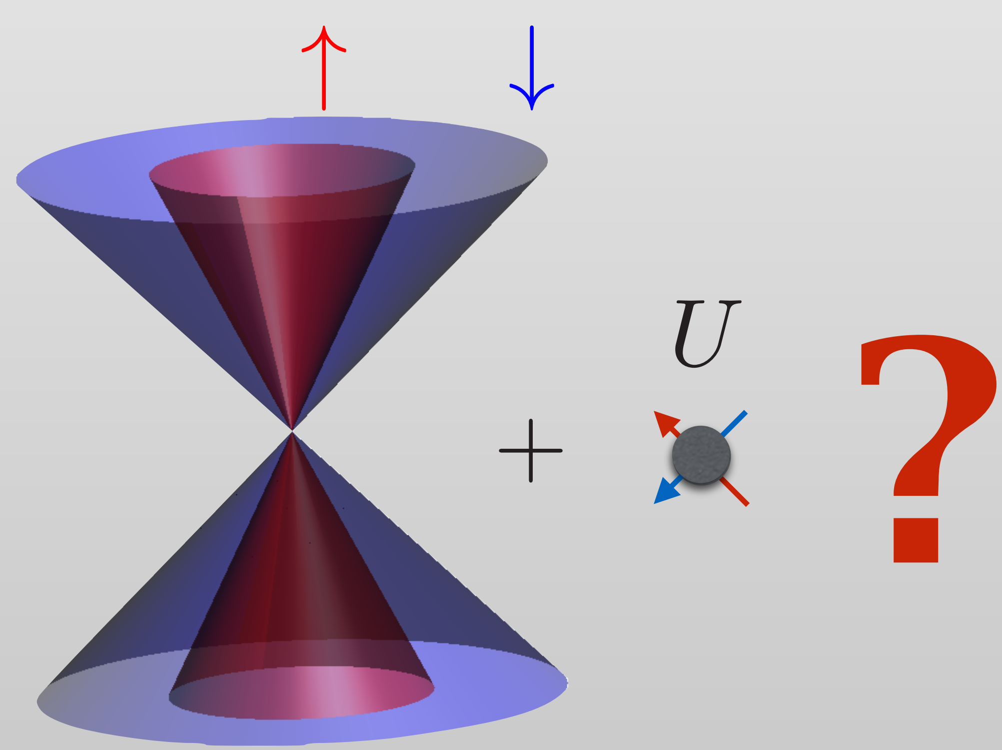


- Realization: mixture of ultracold fermions (e.g. ^{6}Li and ^{40}K)
- Now, continuously tunable by spin-dependent modulations Jotzu et al, PRL 2015

$$t_{\downarrow}/t_{\uparrow} \in (-\infty, \infty)$$

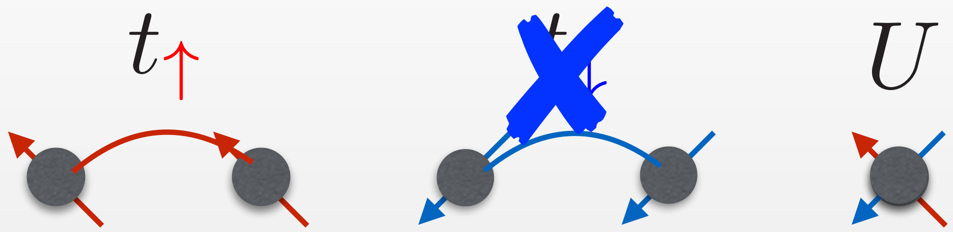


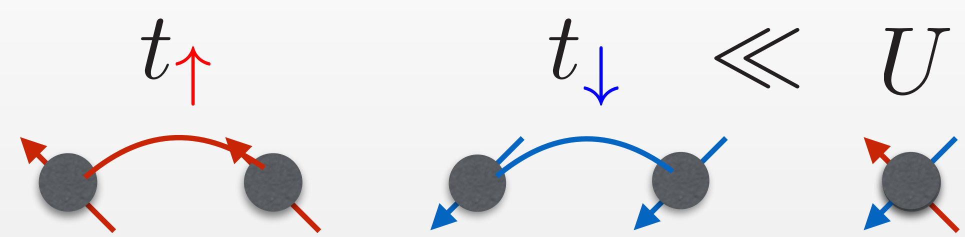
Lignier et al, PRL 2007 and many others



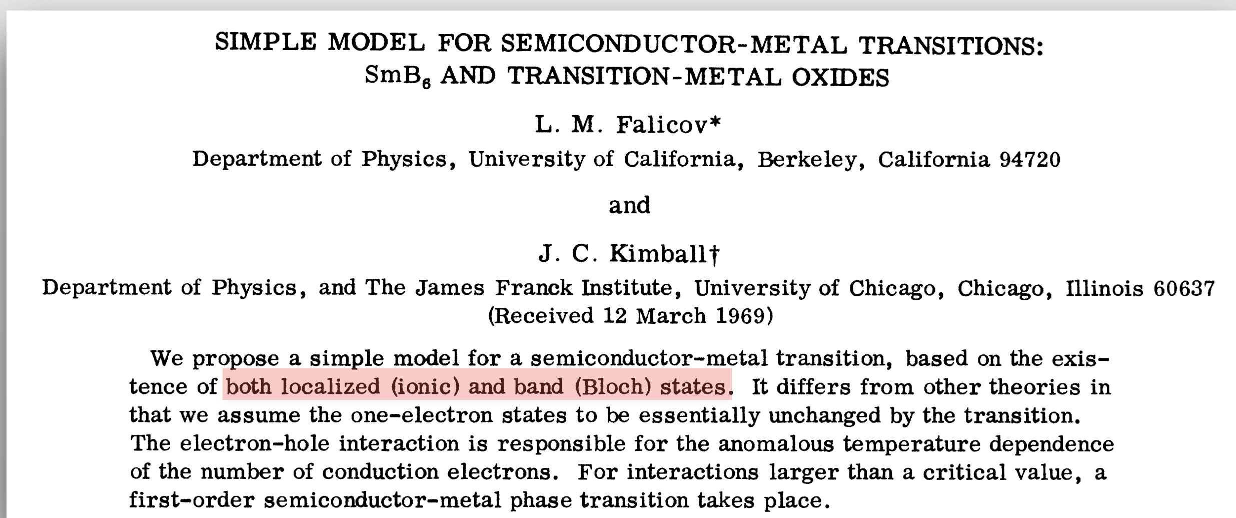
Dirac fermions with unequal Fermi velocities

Two limiting cases





Falicov-Kamball Limit



SIMPLE MODEL FOR SEMICONDUCTOR-METAL TRANSITIONS: SmB_6 AND TRANSITION-METAL OXIDES

L. M. Falicov*
Department of Physics, University of California, Berkeley, California 94720

and

J. C. Kimball†
Department of Physics, and The James Franck Institute, University of Chicago, Chicago, Illinois 60637

(Received 12 March 1969)

We propose a simple model for a semiconductor-metal transition, based on the existence of both localized (ionic) and band (Bloch) states. It differs from other theories in that we assume the one-electron states to be essentially unchanged by the transition. The electron-hole interaction is responsible for the anomalous temperature dependence of the number of conduction electrons. For interactions larger than a critical value, a first-order semiconductor-metal phase transition takes place.

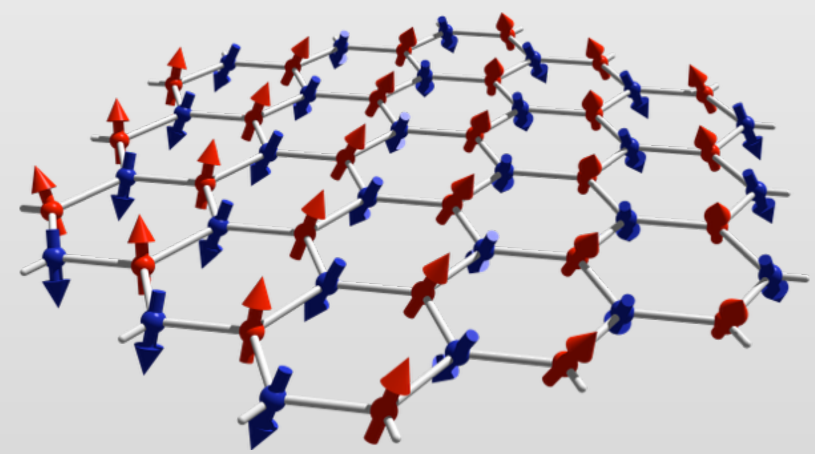
Long-range spin order on bipartite lattices with infinitesimal repulsion

Kennedy and Lieb 1986

“Fruit fly” of DMFT

Freericks and Zlatić, RMP, 2003

Strong Coupling Limit

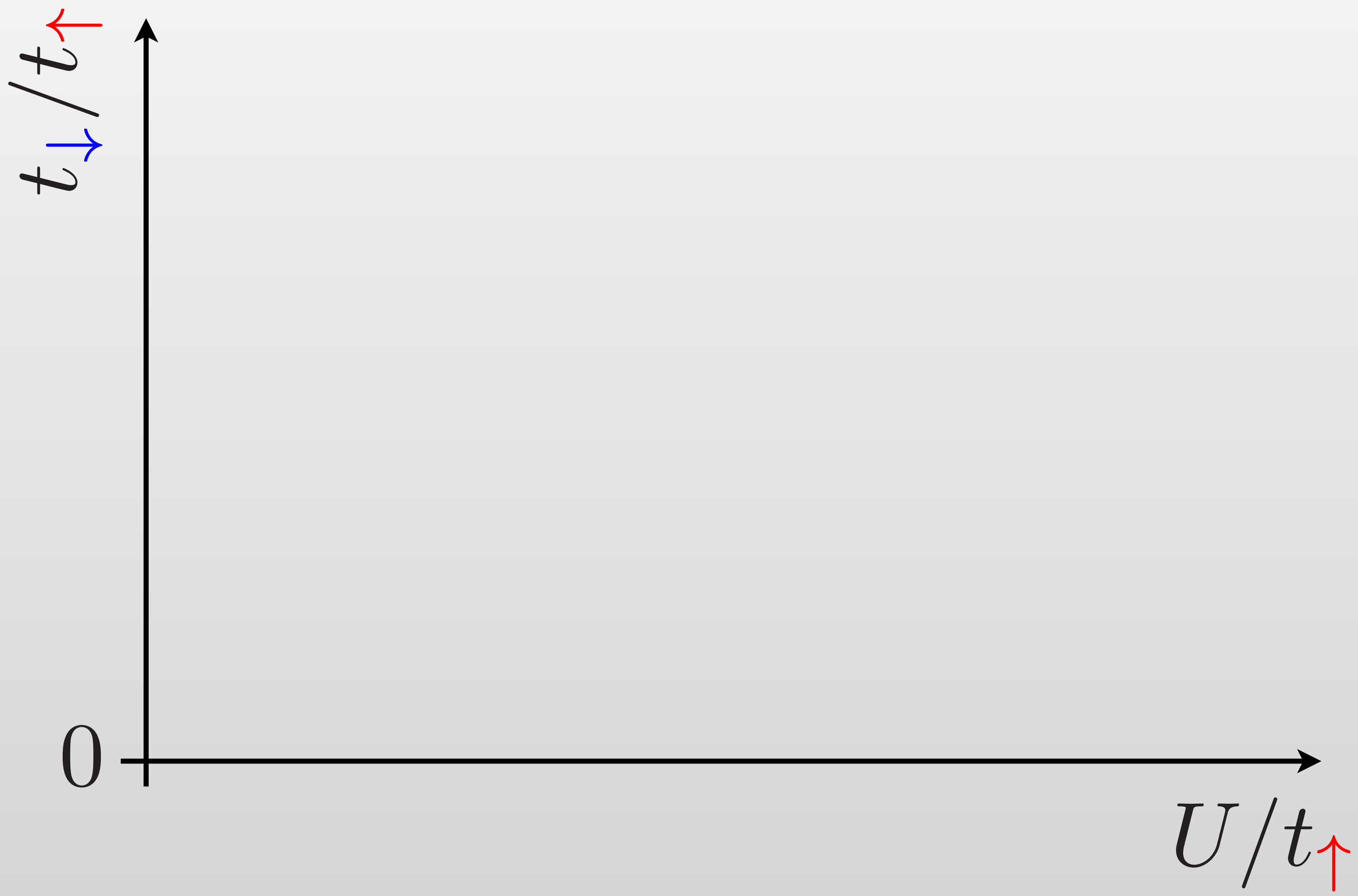


$$J_{xy}\left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y\right) + J_z \hat{S}_i^z \hat{S}_j^z$$

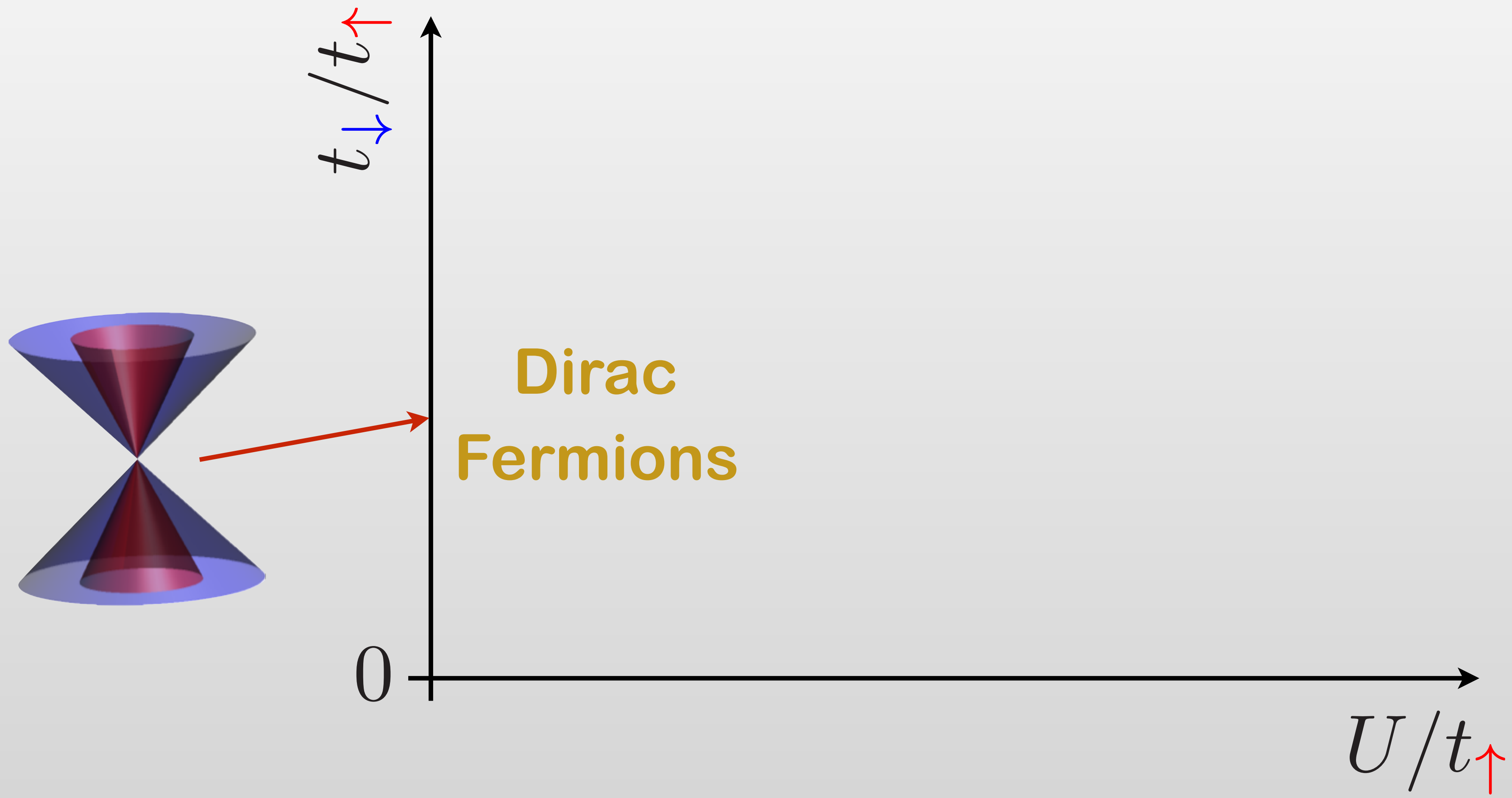
$$\frac{4t_\uparrow t_\downarrow}{U} \le \frac{2(t_\uparrow^2 + t_\downarrow^2)}{U}$$

XXZ model with Ising anisotropy

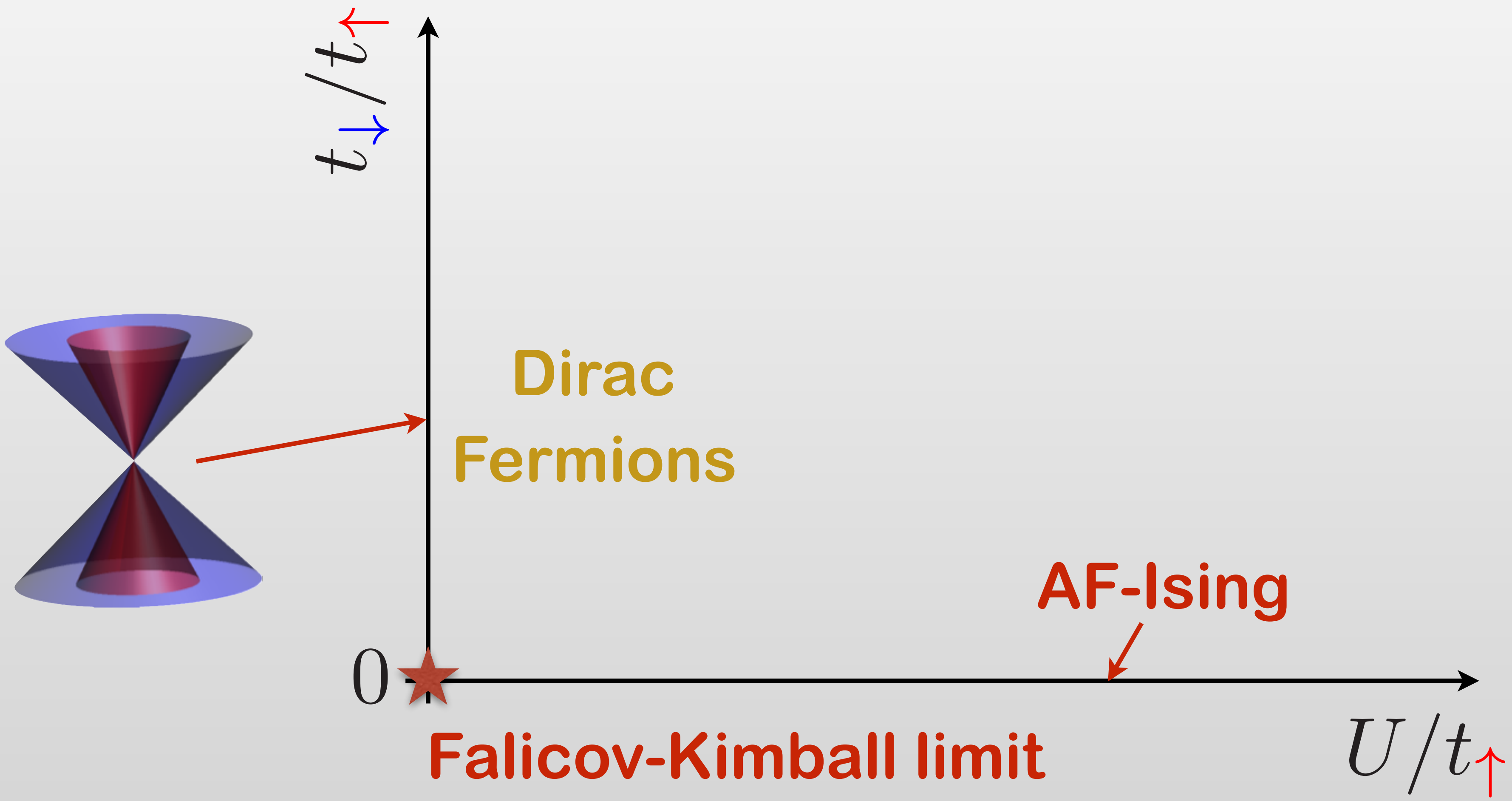
Phase diagram



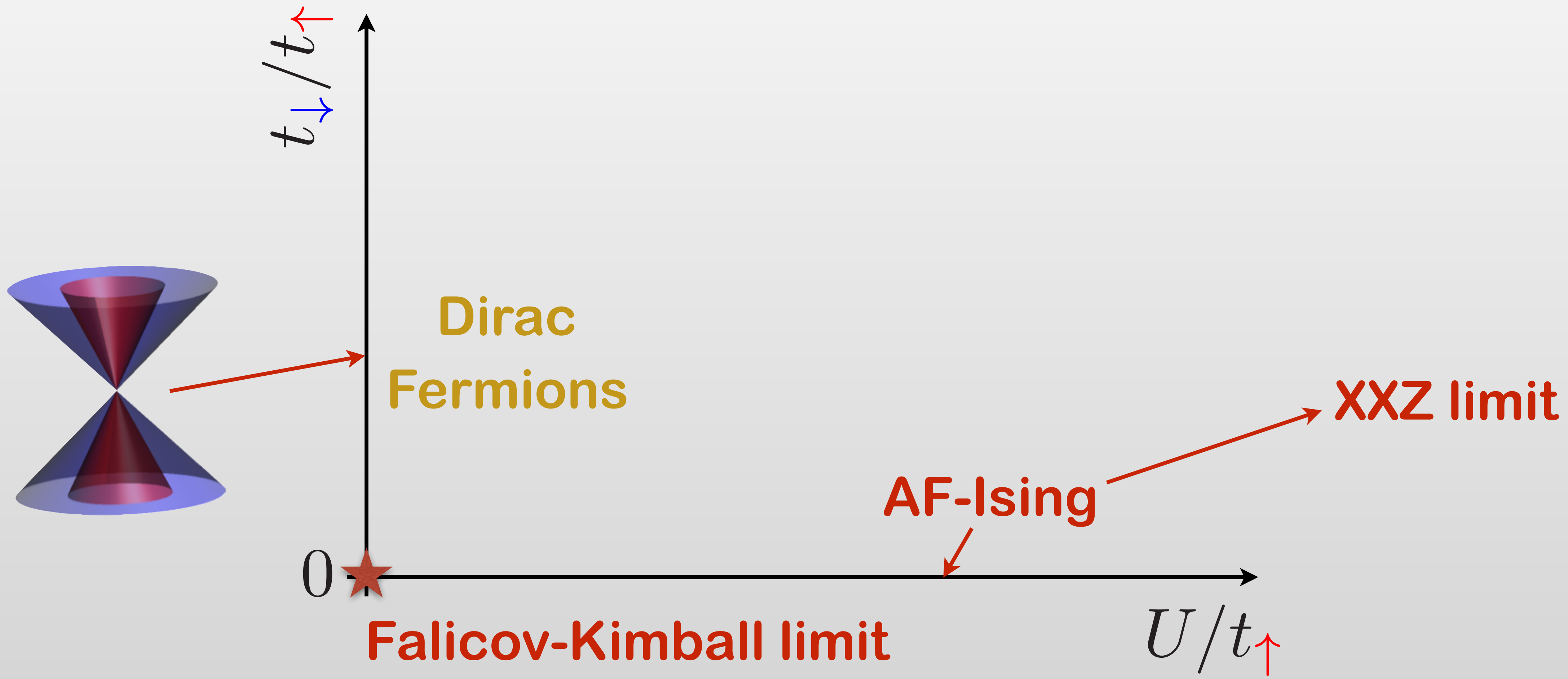
Phase diagram



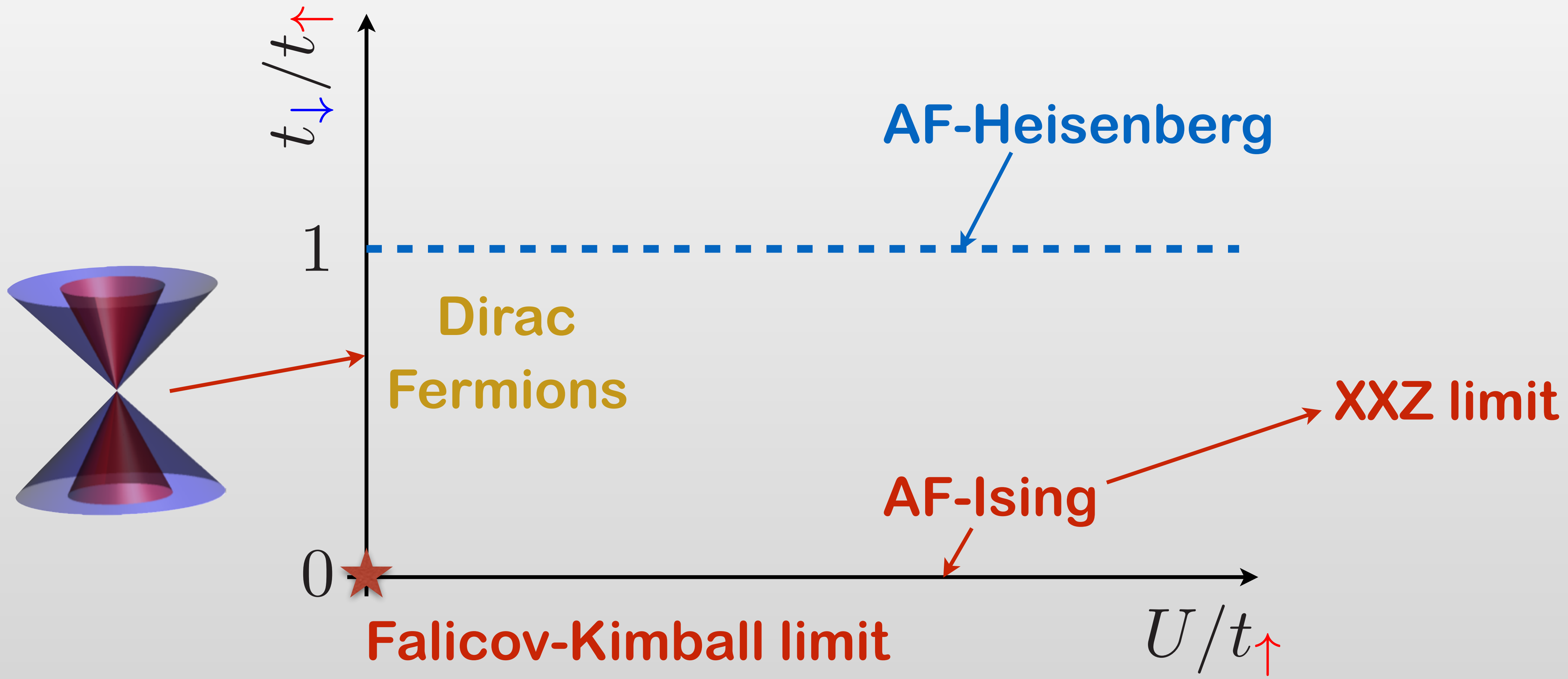
Phase diagram



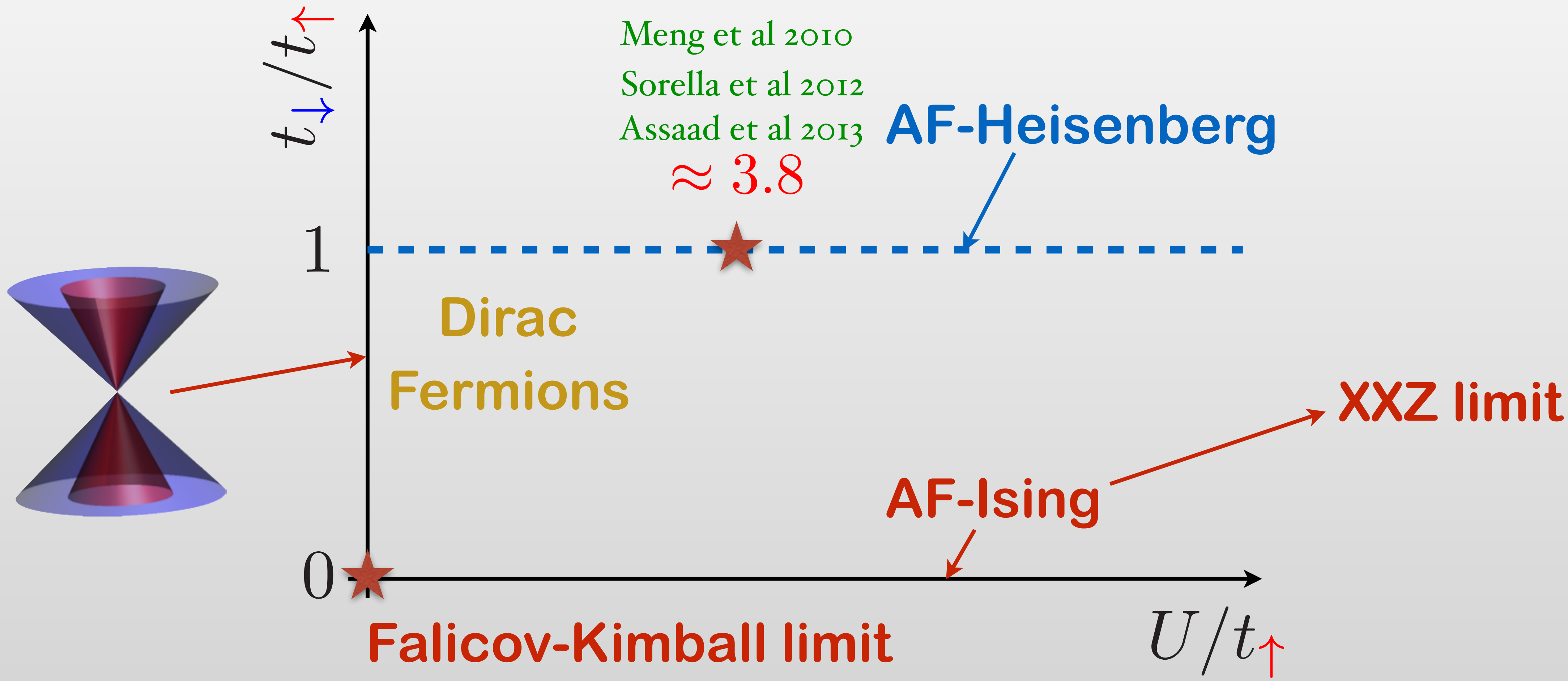
Phase diagram



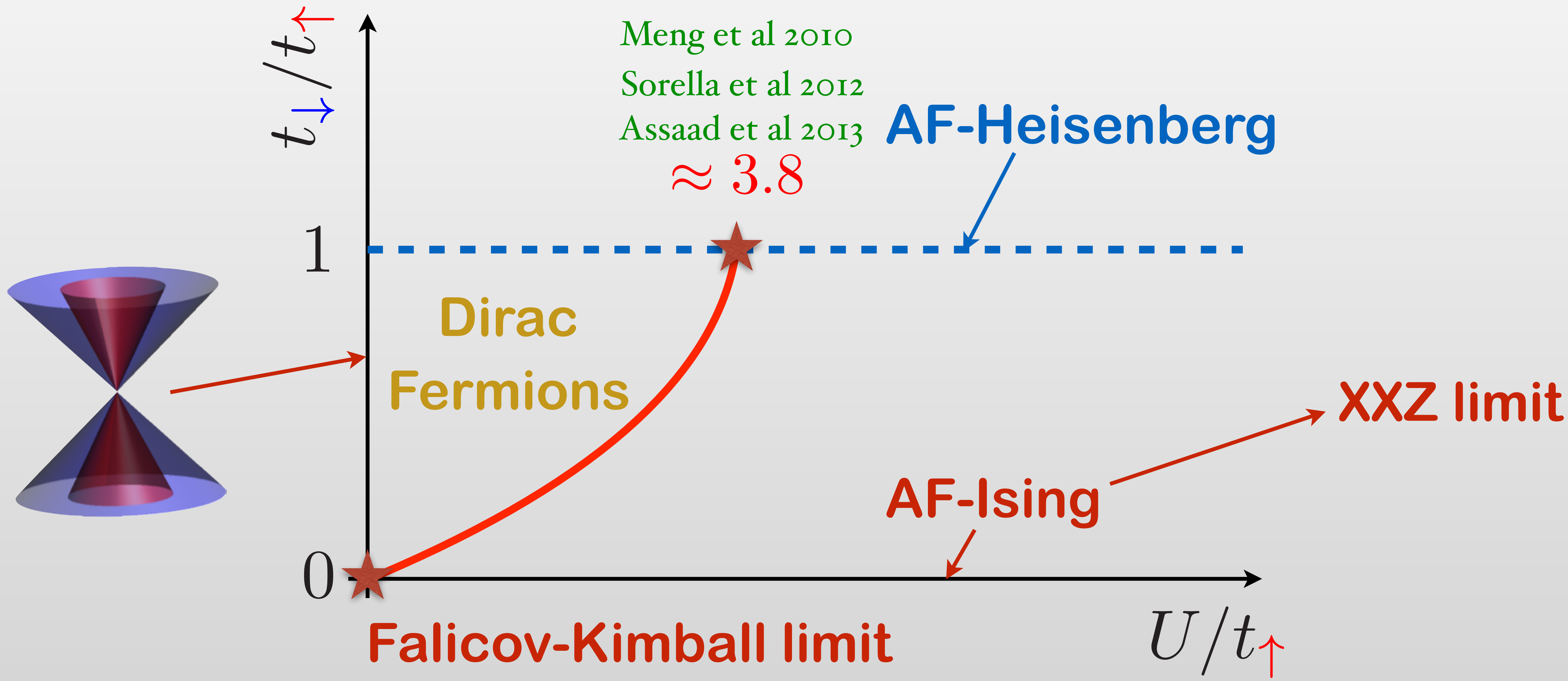
Phase diagram



Phase diagram



Phase diagram

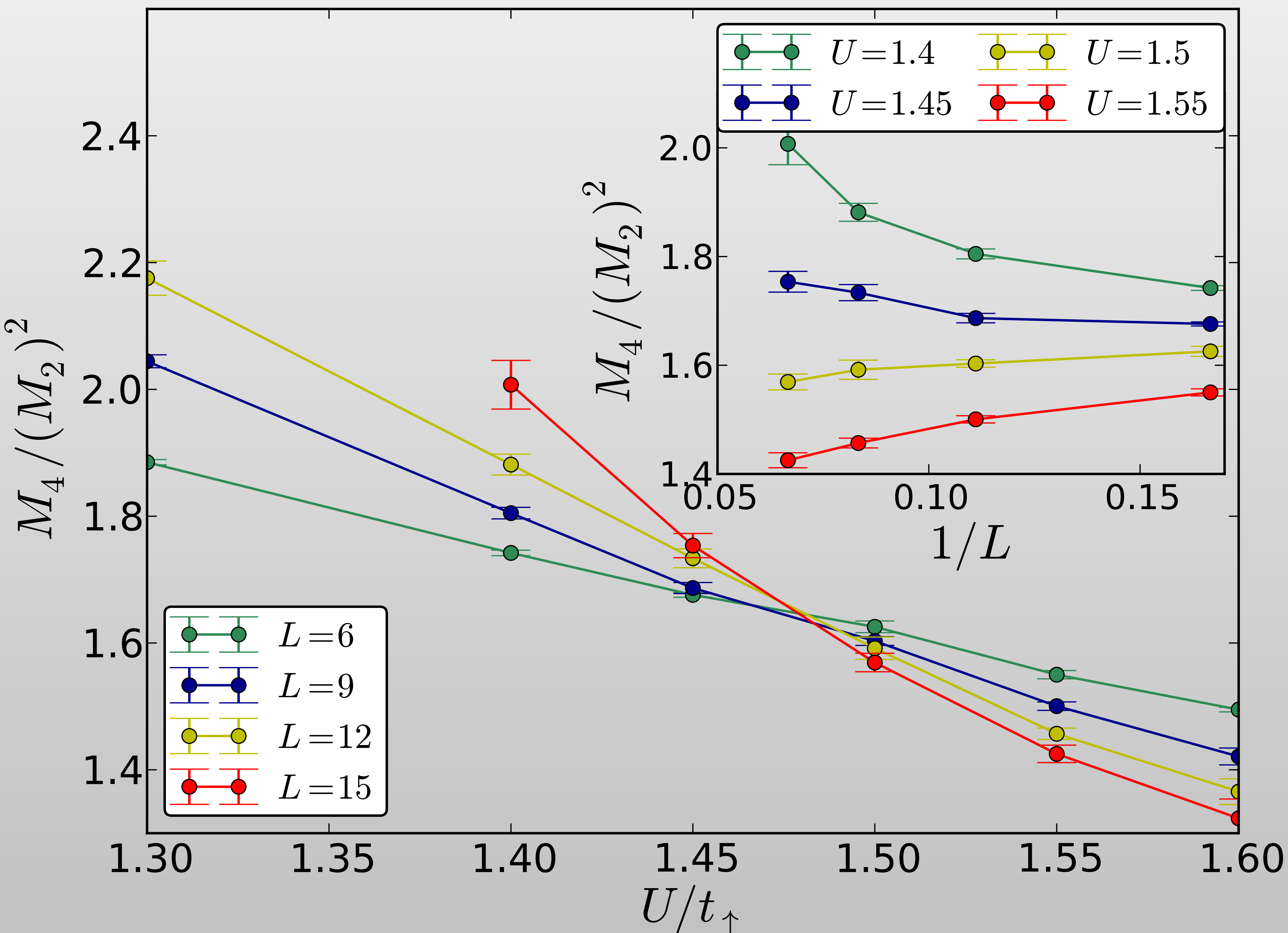


- How to connect the phase boundary ?
- What is the universality class ?

Binder ratio

$t_\downarrow / t_\uparrow = 0.15$

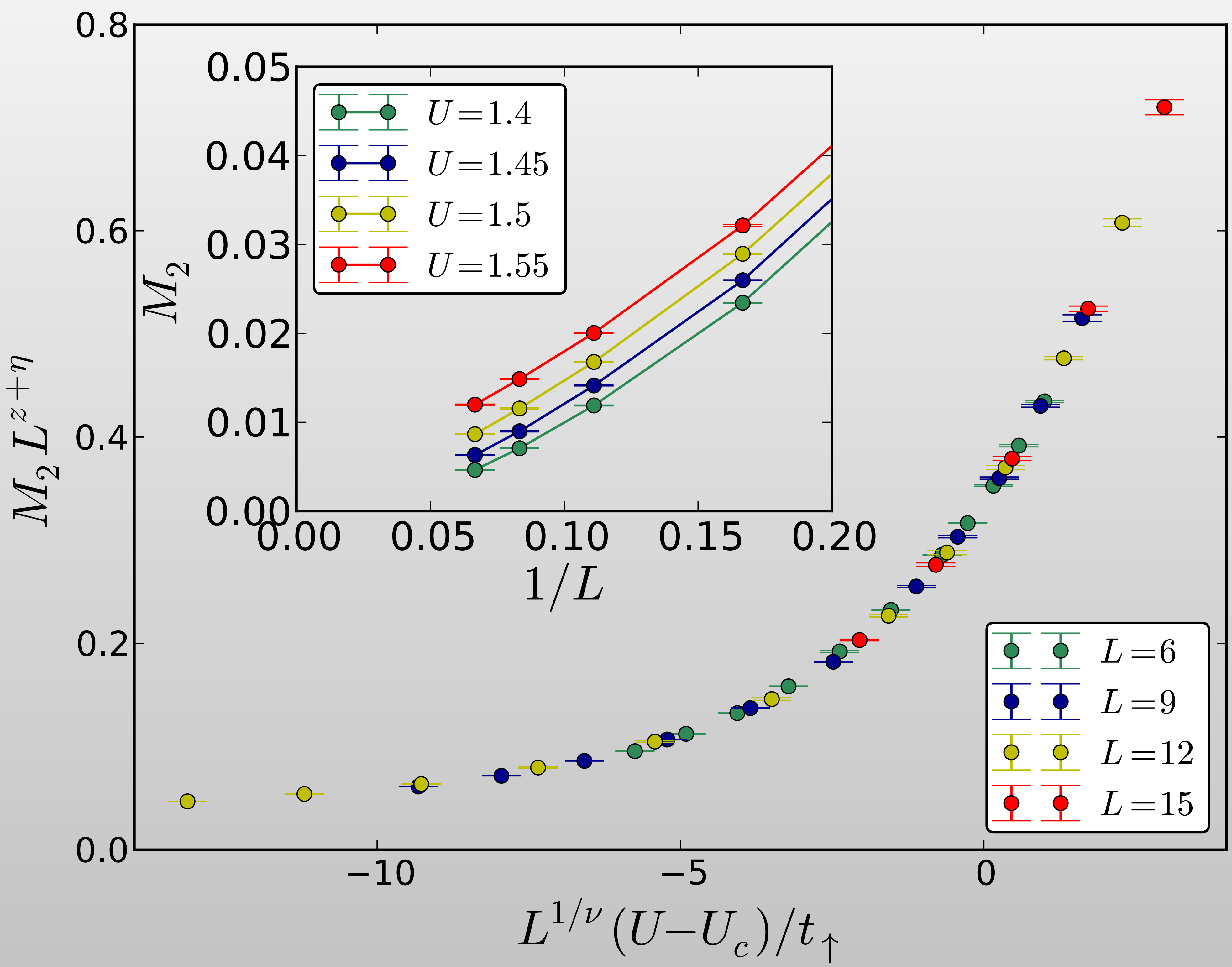
$$M_2 = \left\langle \left(\frac{1}{N} \sum_{\mathbf{r}} e^{i\mathbf{Q}\cdot\mathbf{r}} \frac{\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow}}{2} \right)^2 \right\rangle \qquad M_4 = \left\langle \left(\frac{1}{N} \sum_{\mathbf{r}} e^{i\mathbf{Q}\cdot\mathbf{r}} \frac{\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow}}{2} \right)^4 \right\rangle$$



Liu and Wang, PRB 2015

Scaling analysis

$$\nu = 0.84(4)$$
$$z + \eta = 1.395(7)$$



Liu and Wang, PRB 2015

Summary

Exciting time!

Thanks to my collaborators!

Mauro Iazzi

Philippe Corboz

Jakub Imriška

Ping Nang Ma

Gergely Harcos

Ye-Hua Liu

Matthias Troyer

中国科学院物理研究所
Institute of Physics Chinese Academy of Sciences

广告

欢迎本科生毕业设计，博士生，博士后

wanglei@iphy.ac.cn   010-82649853