Recent progresses on diagrammatic determinant QMC

Lei Wang, ETH Zürich

Trento 2015.10

better scaling

Iazzi and Troyer, PRB 2015
LW, Iazzi, Corboz and Troyer, PRB 2015

entanglement & fidelity

LW and Troyer, PRL 2014
LW, Liu, Imriška, Ma and Troyer, PRX 2015
LW, Shinaoka and Troyer, PRL 2015

sign problem

Huffman and Chandrasekharan, PRB 2014
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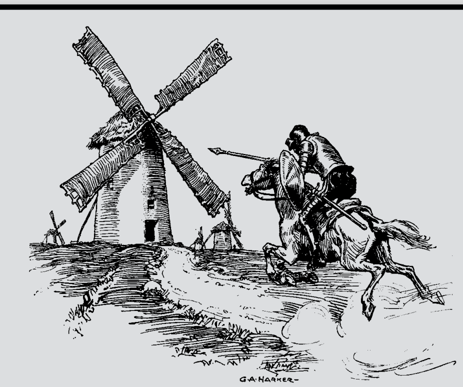

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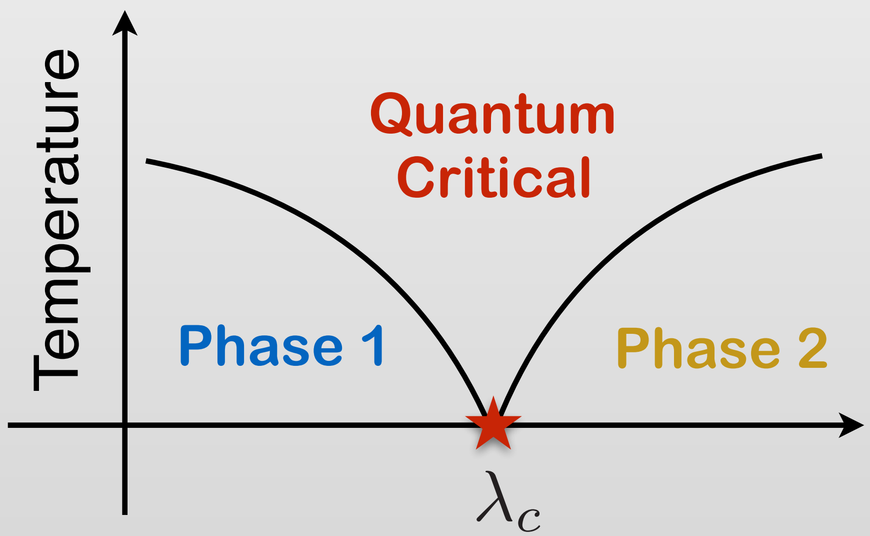
About me

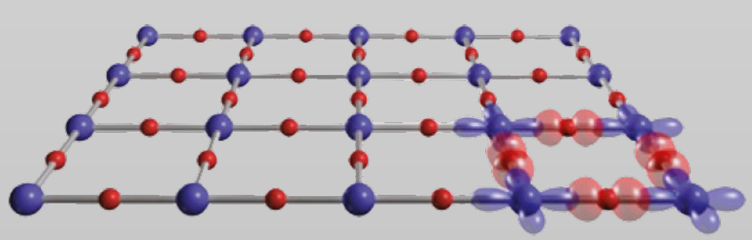
- Background: condensed matter physics

Please forgive my ignorance!

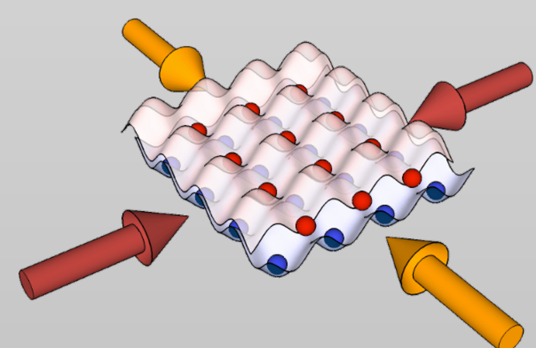
- Interested in quantum many-body systems, quantum phase transitions, etc



- Hubbard model of fermions in this talk



Solid materials

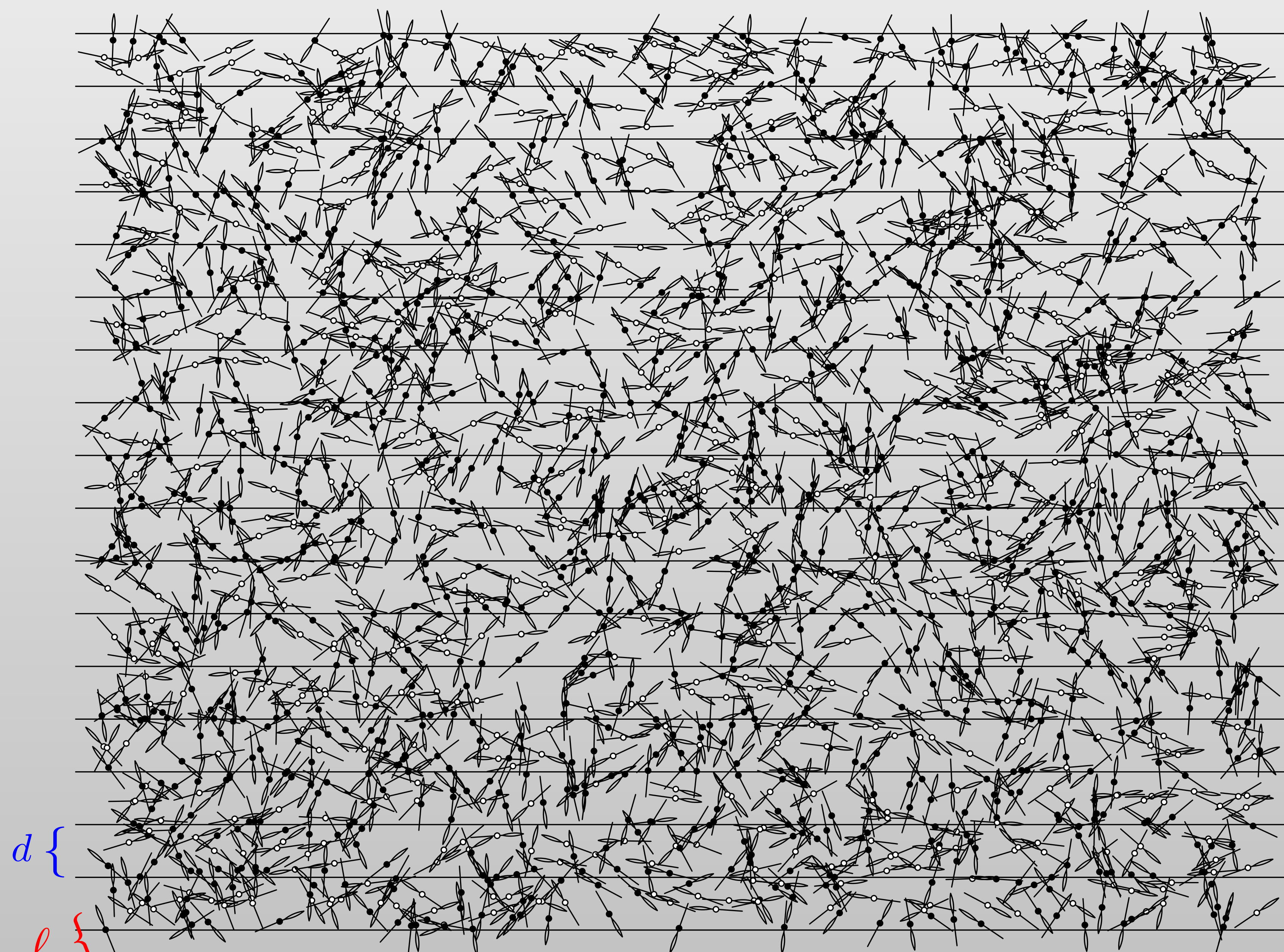


Optical lattices

Quantum Monte Carlo

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)

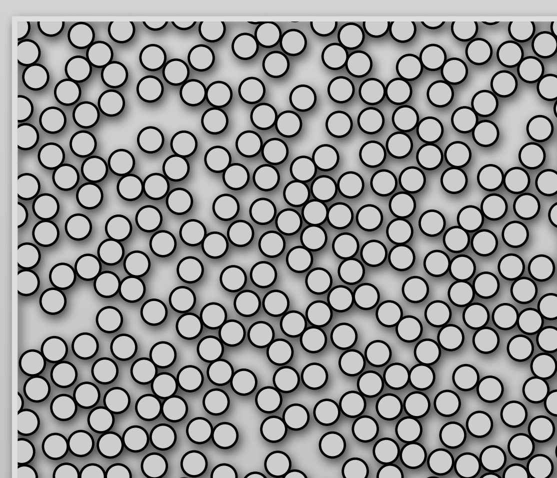
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional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

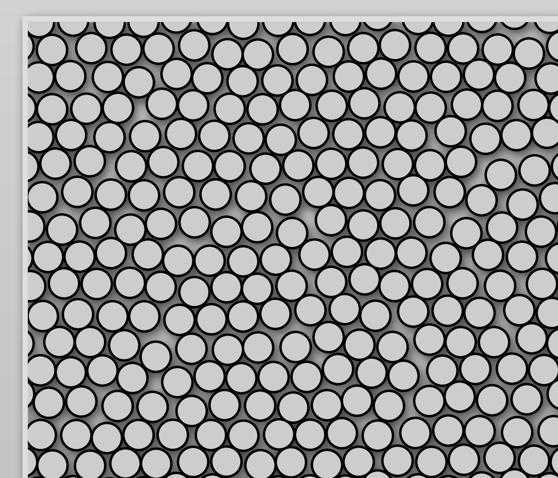
I. INTRODUCTION

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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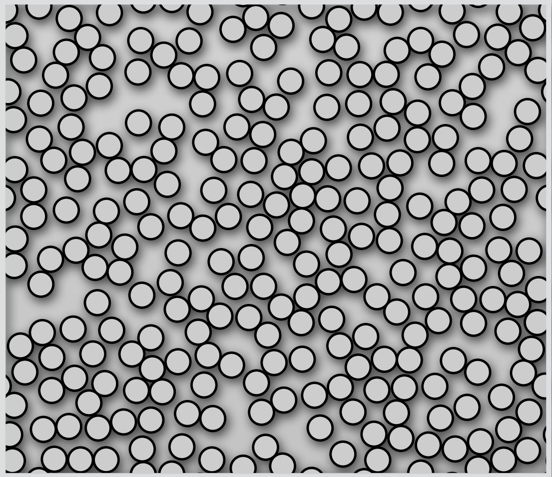
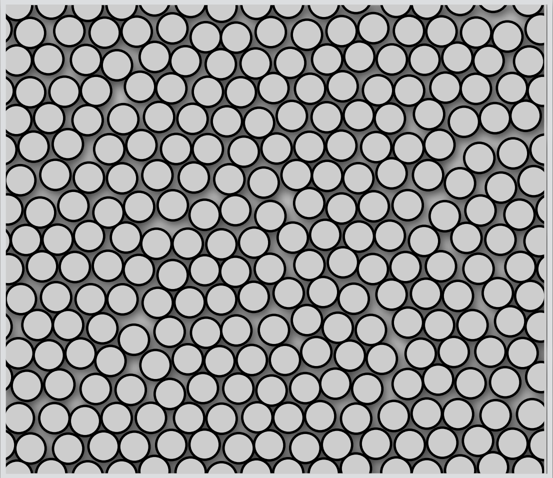


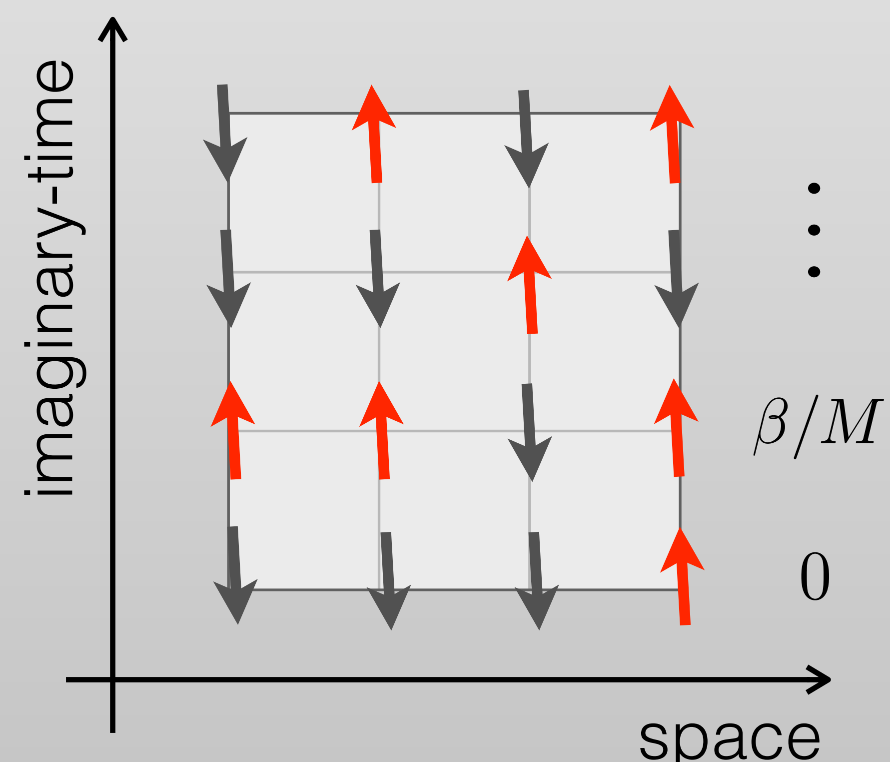


Quantum to classical mapping

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

Trotterization

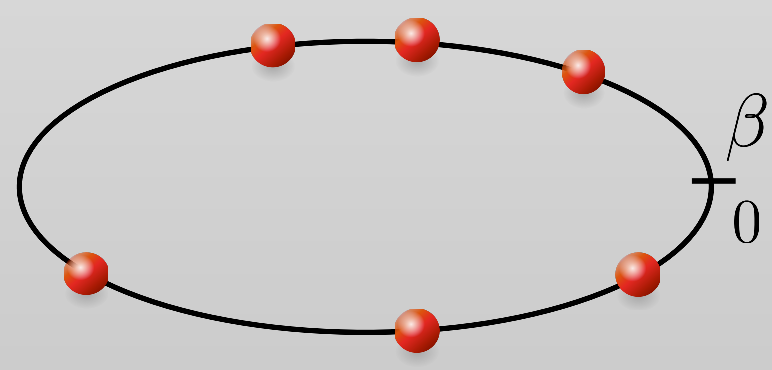
$$Z = \mathrm{Tr}\left(e^{-\frac{\beta}{M}\hat{H}} \dots e^{-\frac{\beta}{M}\hat{H}}\right)$$



Diagrammatic approach

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

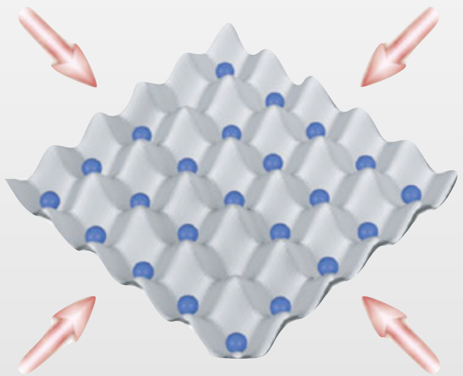
$$\mathrm{Tr}\left[(-1)^k e^{-(\beta-\tau_k)\hat{H}_0} \hat{H}_1 \dots \hat{H}_1 e^{-\tau_1 \hat{H}_0}\right]$$



imaginary-time axis

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

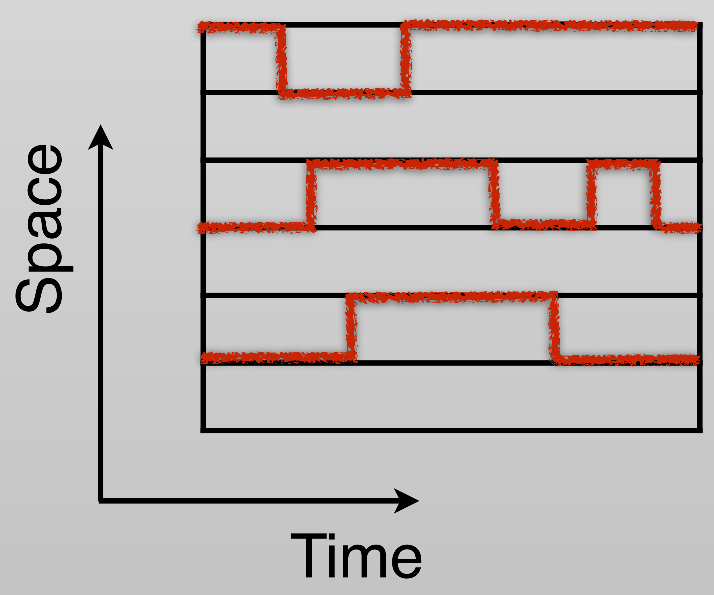
Diagrammatic approaches

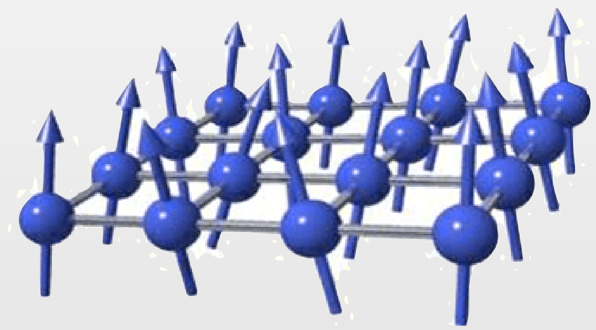


bosons

World-line Approach

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

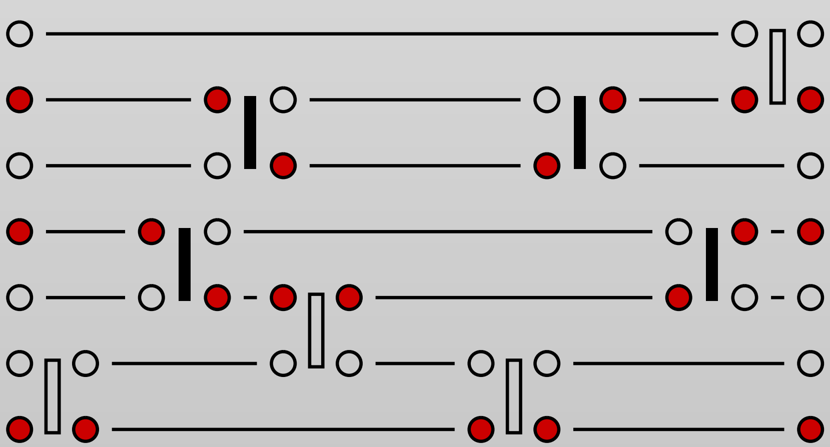


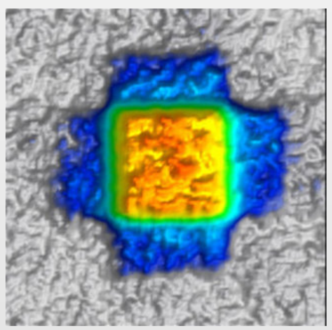


quantum spins

Stochastic Series Expansion

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

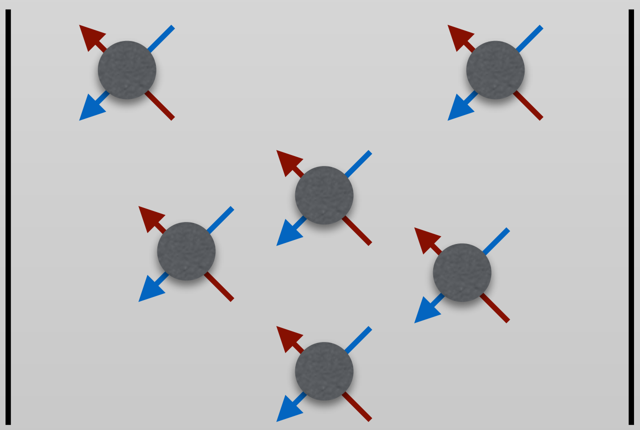




fermions

Determinantal Methods

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



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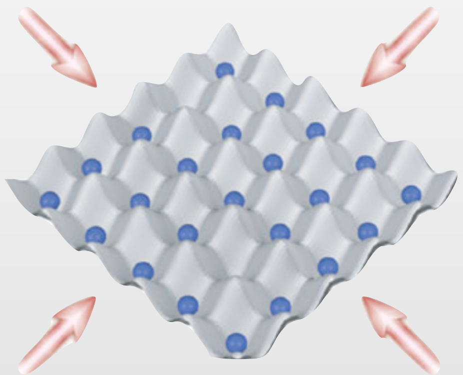

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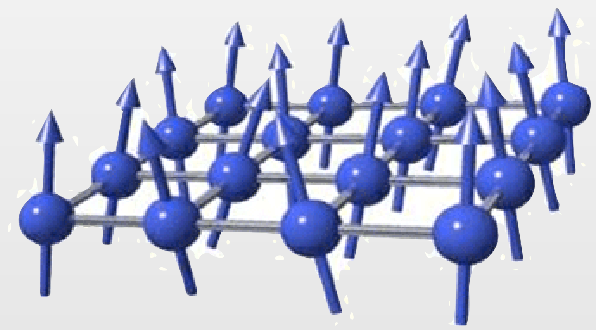

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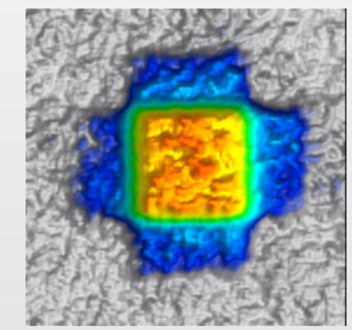

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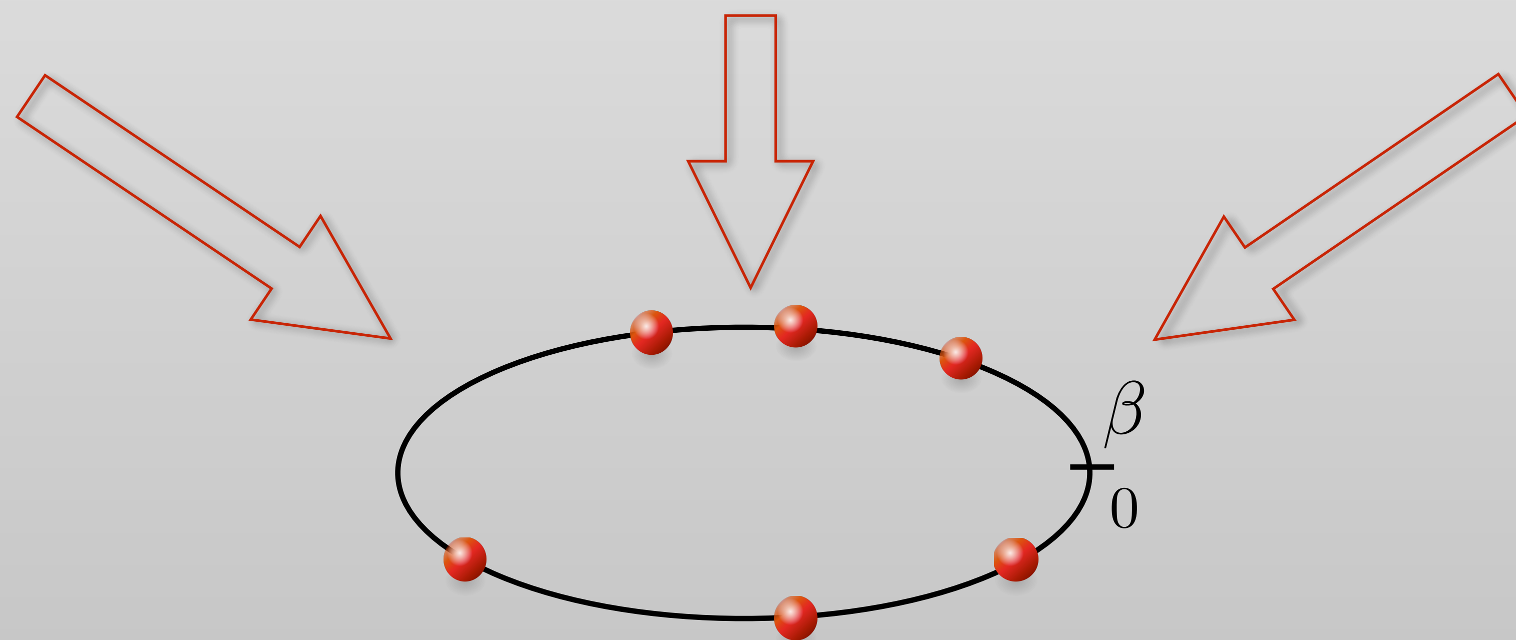

Diagrammatic determinant QMC

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

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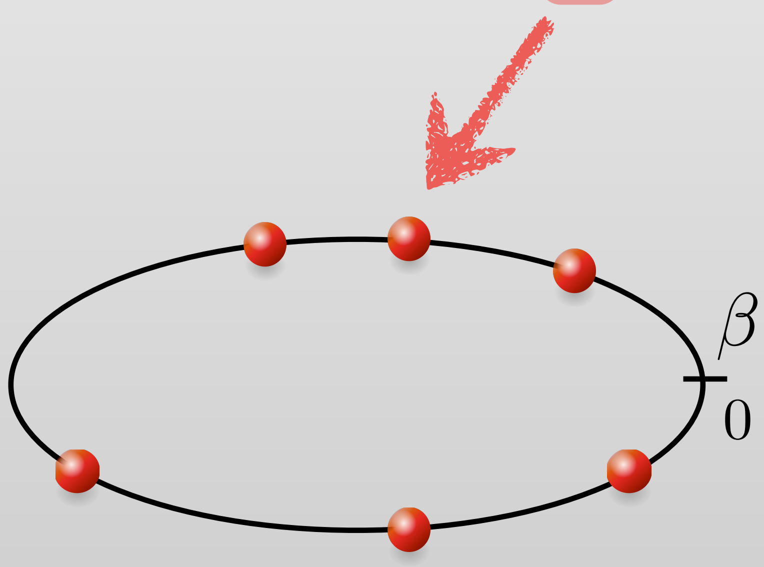

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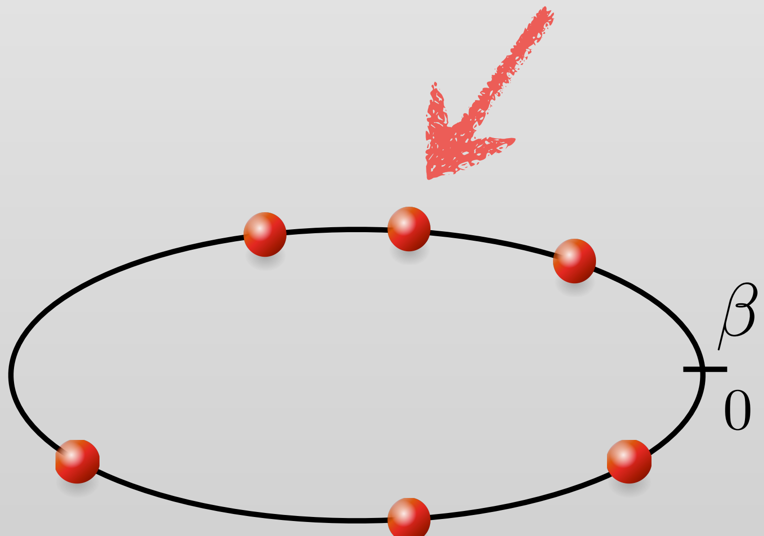

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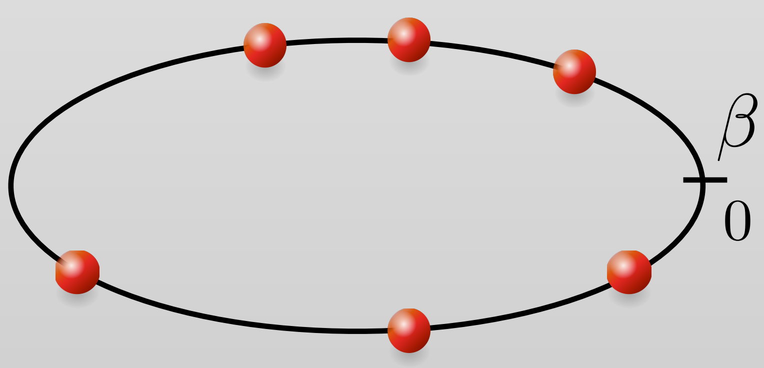
Rubtsov et al, PRB 2005 Gull et al, RMP 2011

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

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



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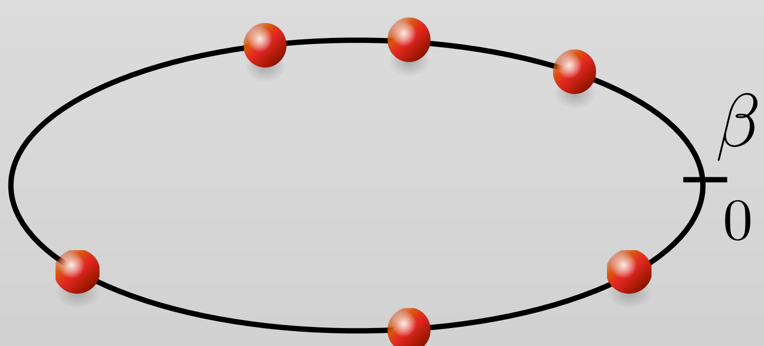


Rombouts, Heyde and Jachowicz, PRL 1999
Iazzi and Troyer, PRB 2015   LW, Iazzi, Corboz and Troyer, PRB 2015

LCT-QMC Methods

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

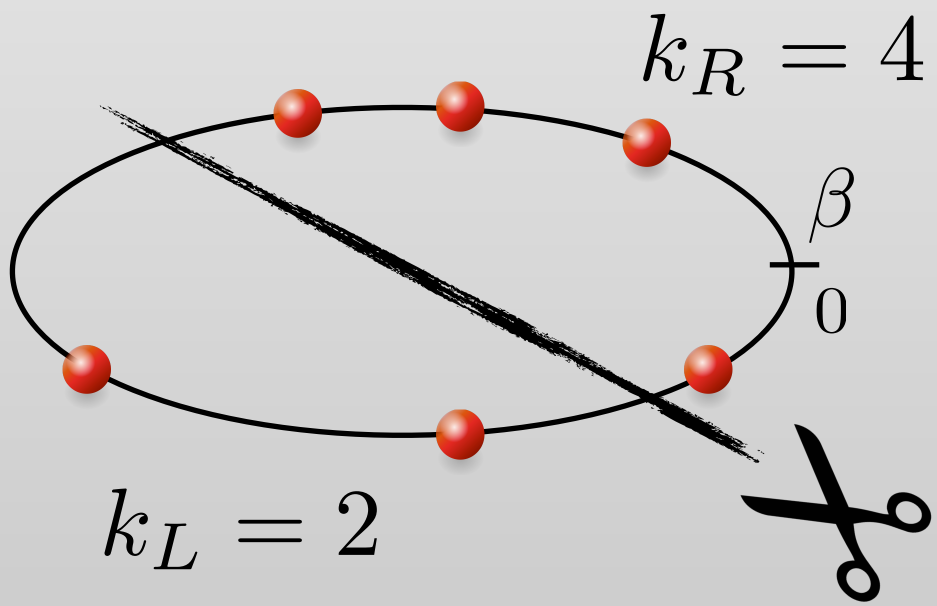
thus achieving $\mathcal{O}(\beta \lambda N^3)$ scaling!

Fidelity susceptibility made simple!

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

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

Signifies quantum phase transitions without need of the local order parameter



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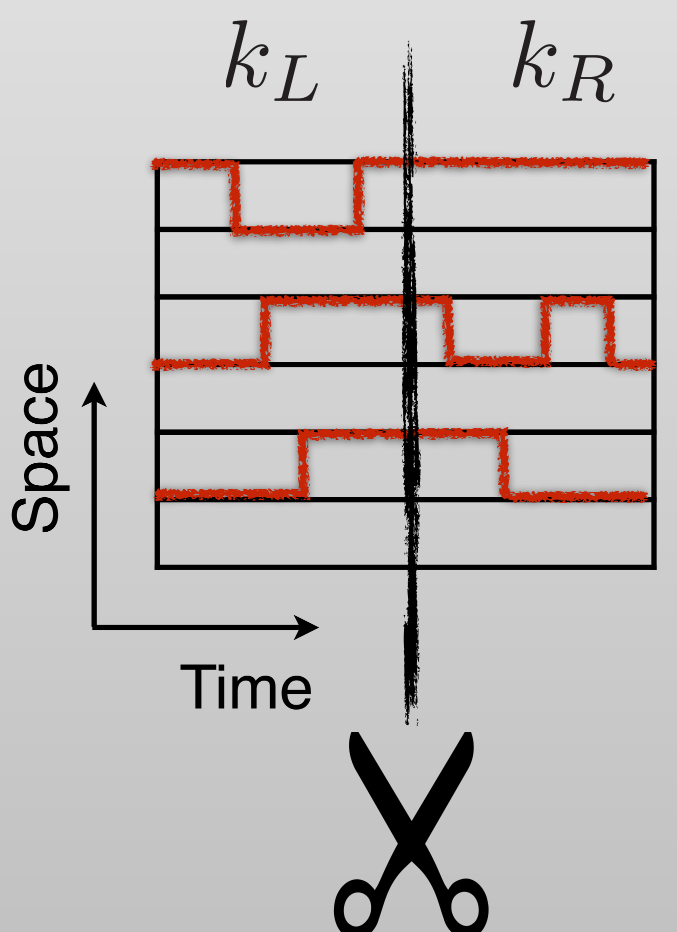
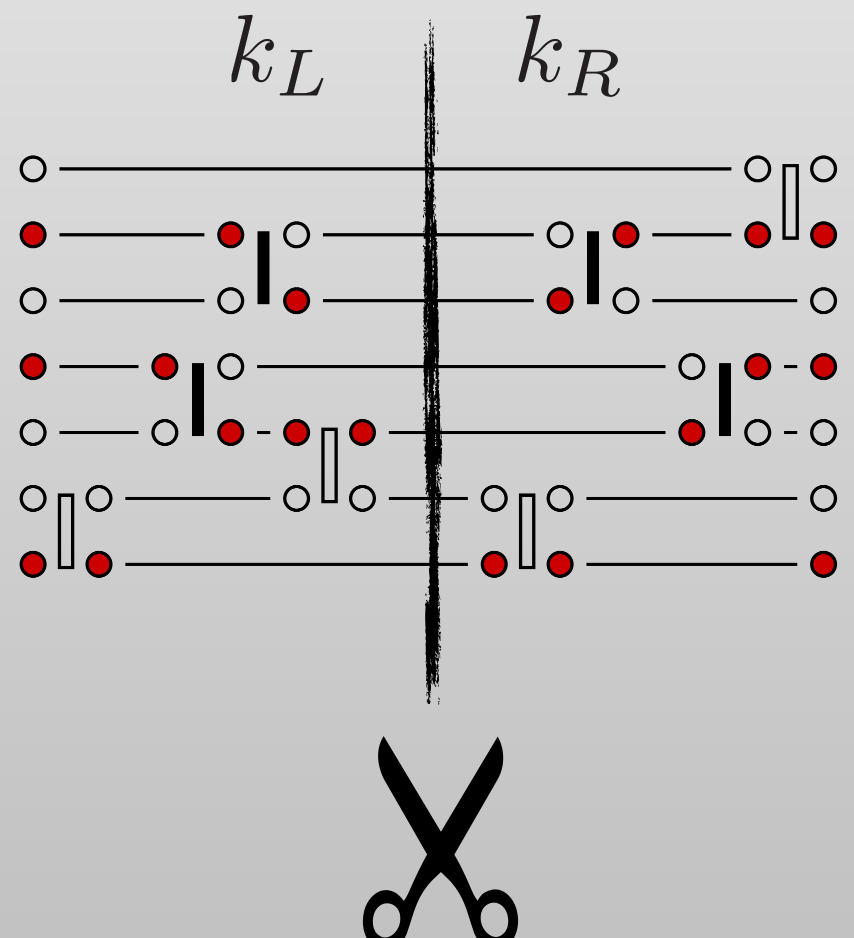
Worldline Algorithms

(bosons)



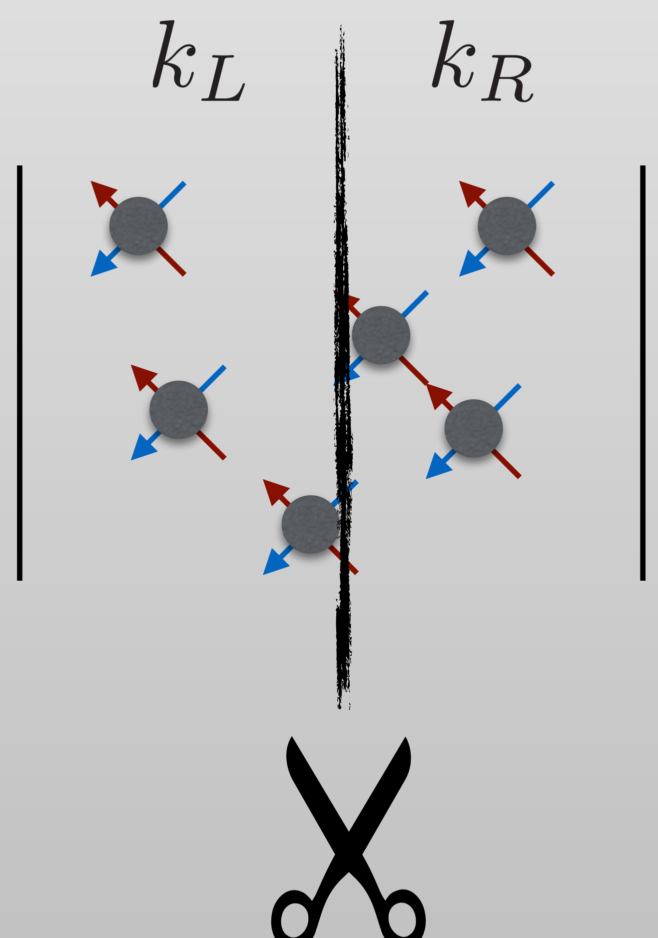
Stochastic Series Expansion

(quantum spins)



Determinantal Methods

(fermions)



More advantages

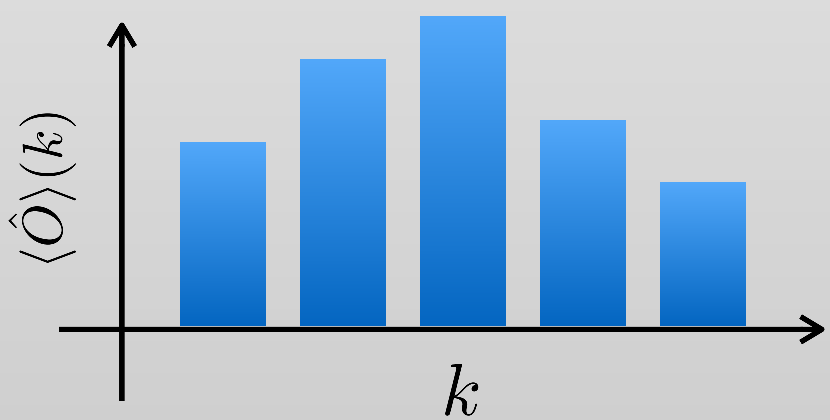
$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_k \lambda^k \sum_{\mathcal{C}_k} w(\mathcal{C}_k) O(\mathcal{C}_k)$$

Observable derivatives

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

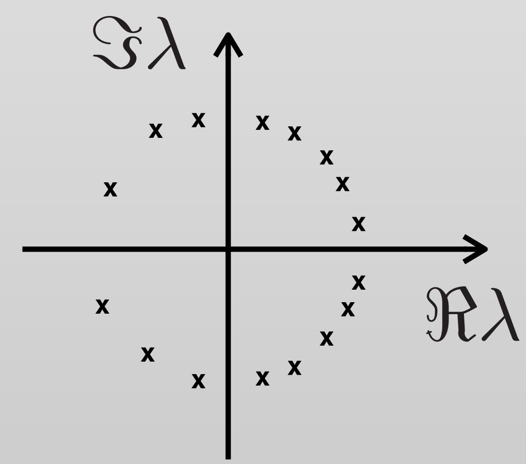
Directly sample *derivatives* of any observable

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

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
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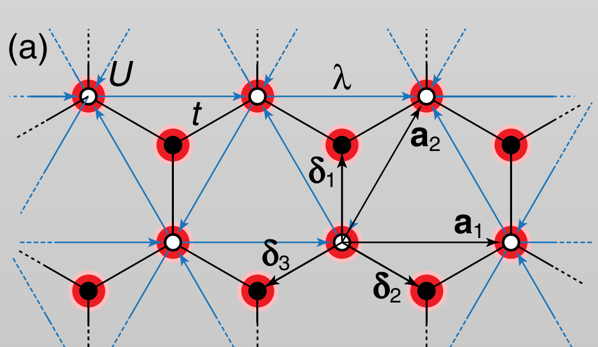
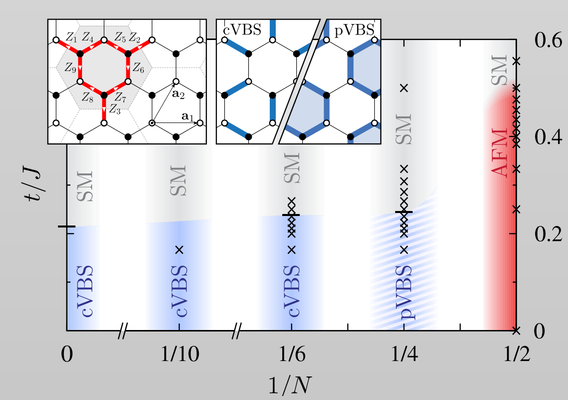
Wu et al, PRB, 2005

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



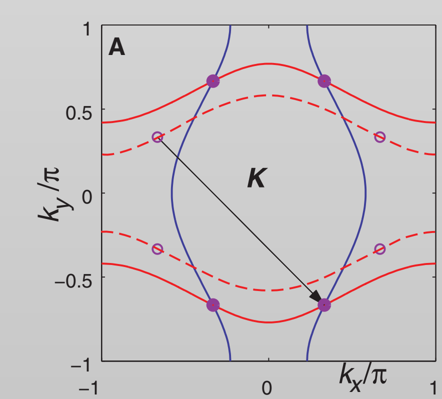
Topological insulators

Hohenadler, Lang and Assaad, PRL 2011



SU(2N) models

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



Two-orbital model

Berg, Metliski and Sachdev, Science 2012

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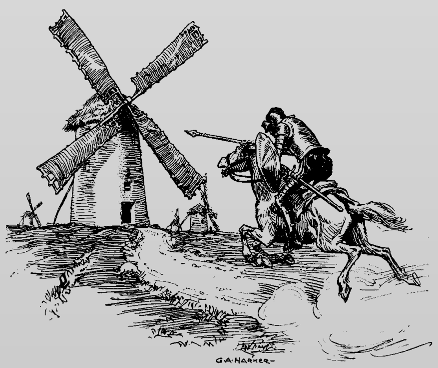
Lang et al, Phys. Rev. C, 1993
Koonin et al, Phys. Rep, 1997
Hands et al, EPJC, 2000
Wu et al, PRB, 2005

But, how about this ?

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

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



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

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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*
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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*
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1506.05349

**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 and*
[2]*Alfréd Rényi Institute of Mathematics, Reáltanoda utca 13-15., Budapest H-1053, Hungary*

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

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

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

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Tao and Paul Erdős in 1985

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NATURE | BREAKING NEWS

Maths whizz solves a master's riddle

Terence Tao successfully attacks the Erdős discrepancy problem by building on an online collaboration.

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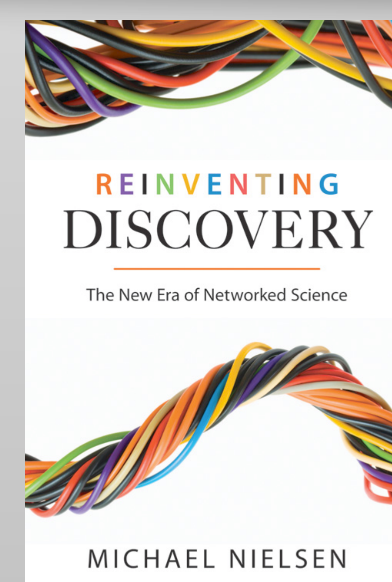

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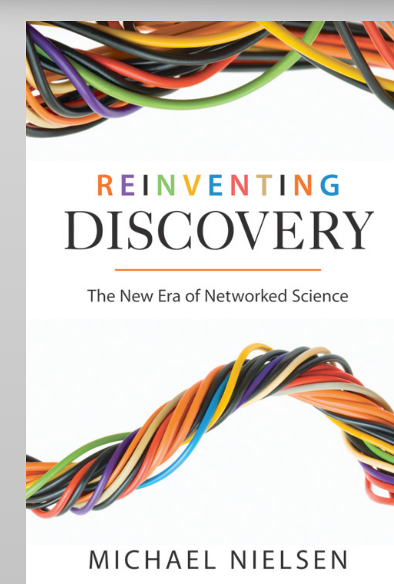

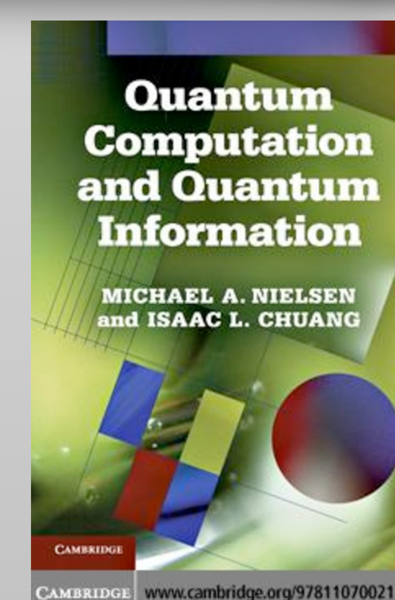

A new de-sign principle

LW, Liu, Iazzi, Troyer and Harcos 1506.05349

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

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

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

split orthogonal group

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

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

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

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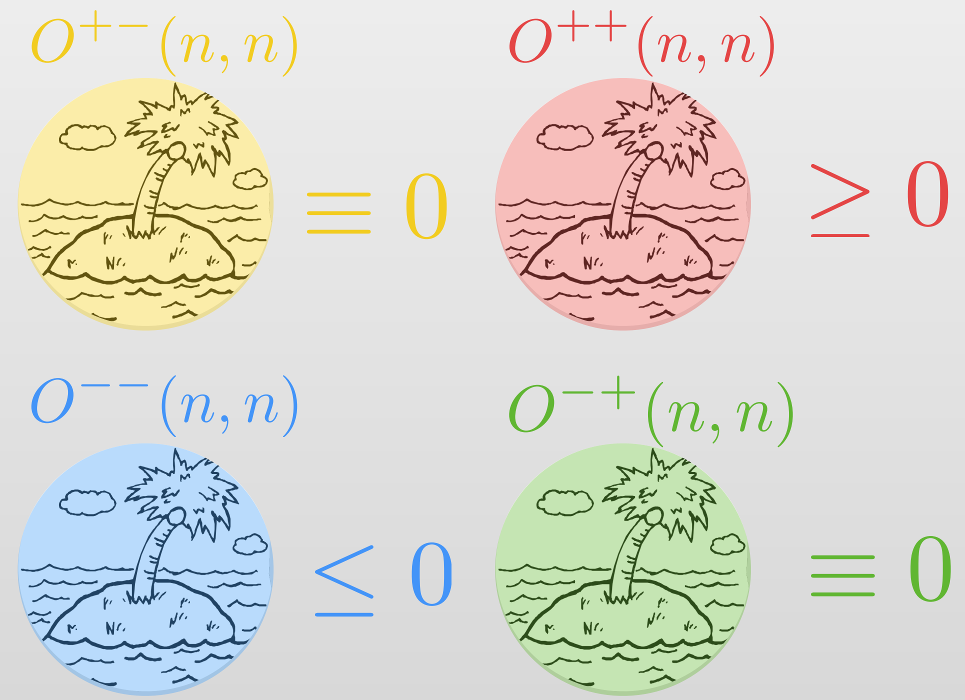
If $M^T \eta M = \eta$ **where** $\eta = \mathrm{diag}(I, -I)$

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

has a definite sign

for each component !



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

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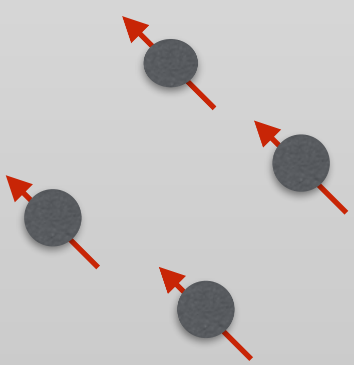
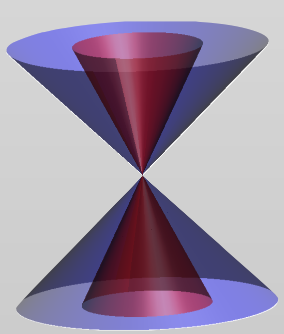


spinless fermions

LW, Troyer, PRL 2014

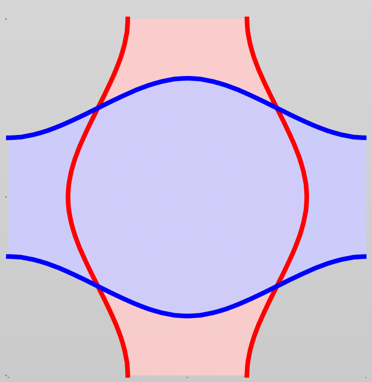
LW, Corboz, Troyer, NJP 2014

LW, Iazzi, Corboz, Troyer, PRB, 2015

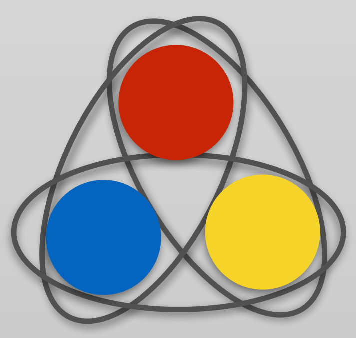


split Dirac cone

Liu and LW, 1510.00715



spin nematicity



SU(3)

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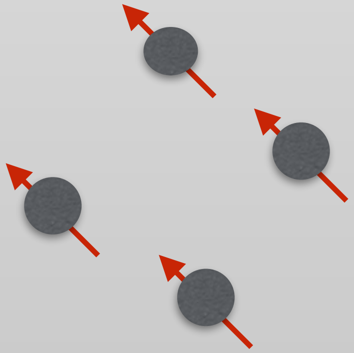

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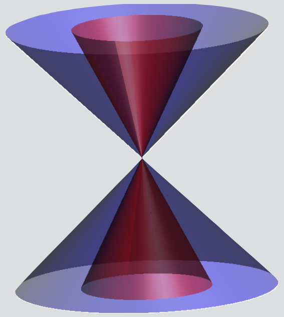

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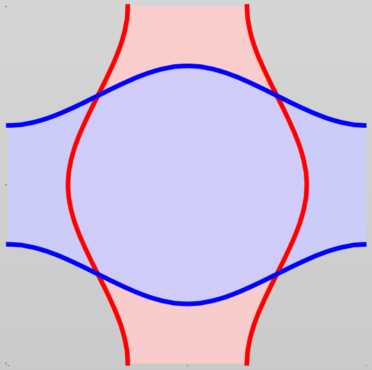
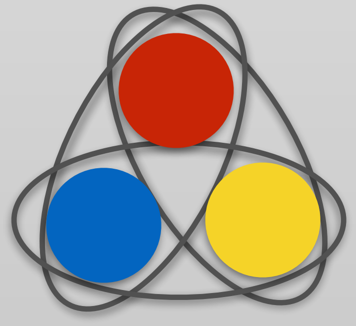
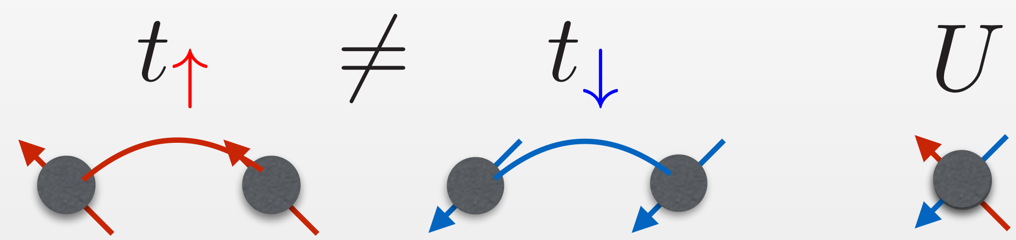


spin nematicity



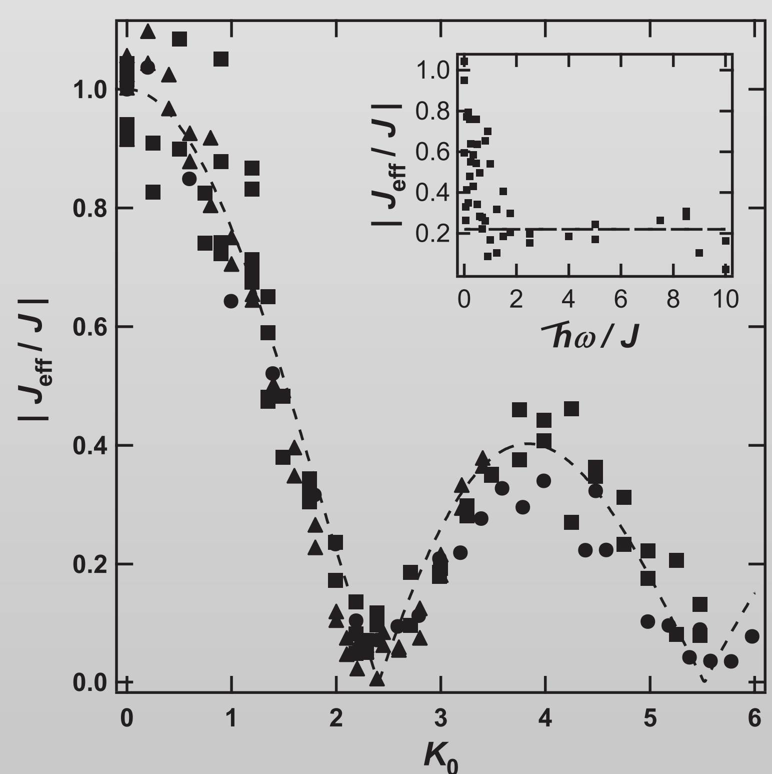
SU(3)

Asymmetric Hubbard model

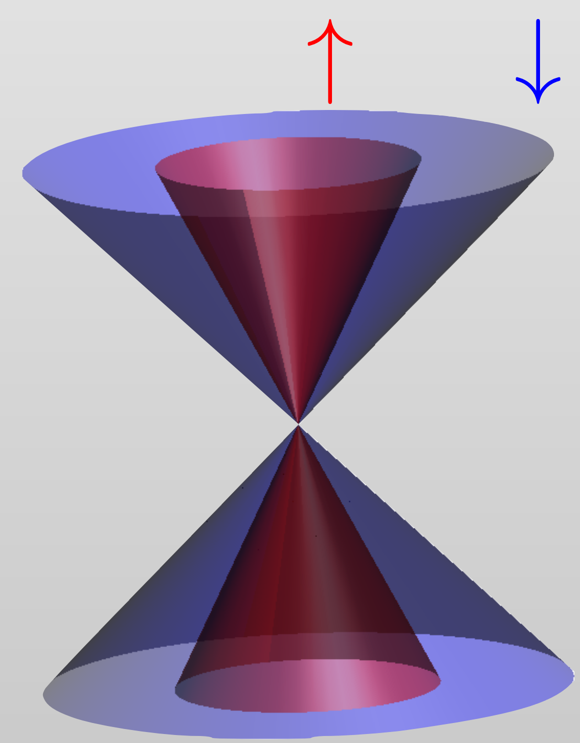


- Realization: mixture of ultracold fermions (e.g. ^{6}Li and ^{40}K)
- Now, continuously tunable by spin-dependent modulations Jotzu et al, PRL 2015

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



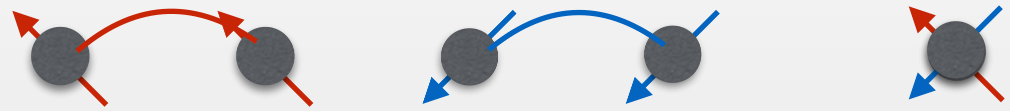
Lignier et al, PRL 2007 and many others



Dirac fermions with unequal Fermi velocities

Asymmetric Hubbard model

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



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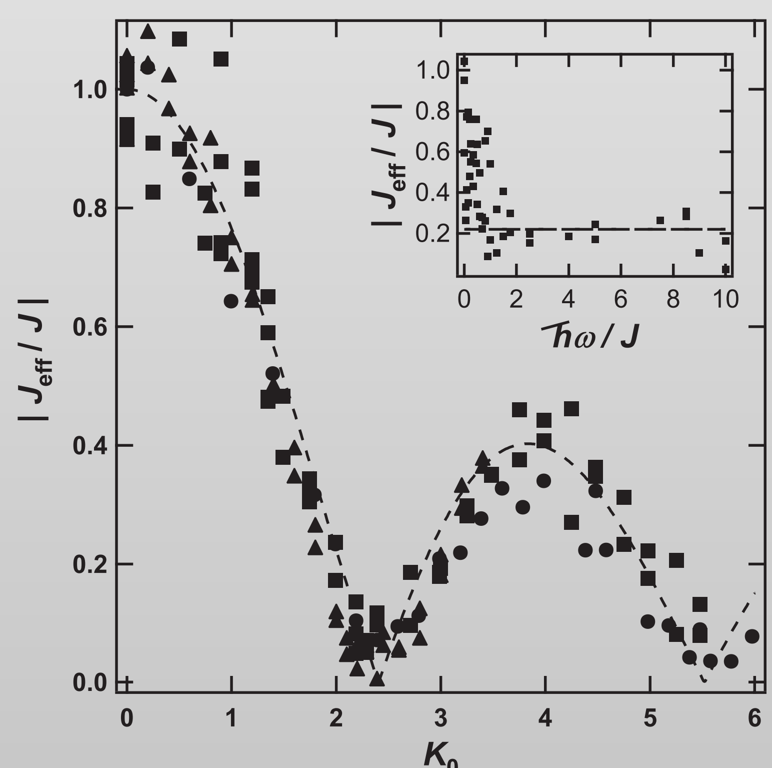

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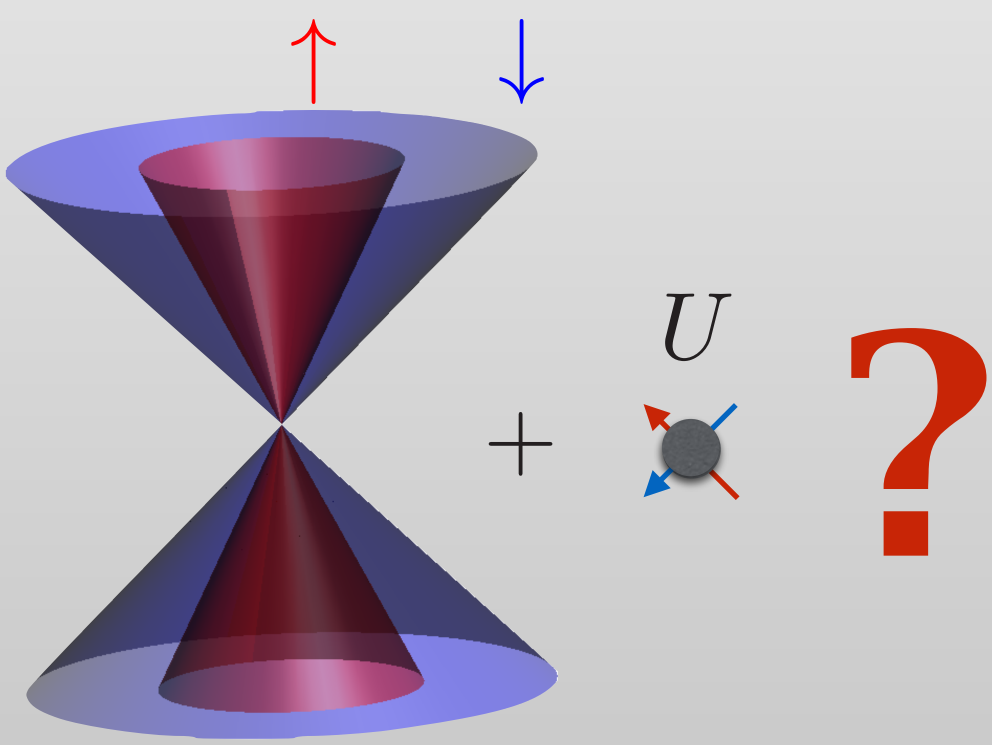
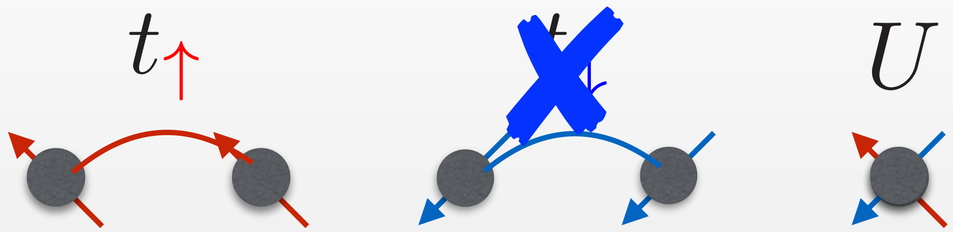
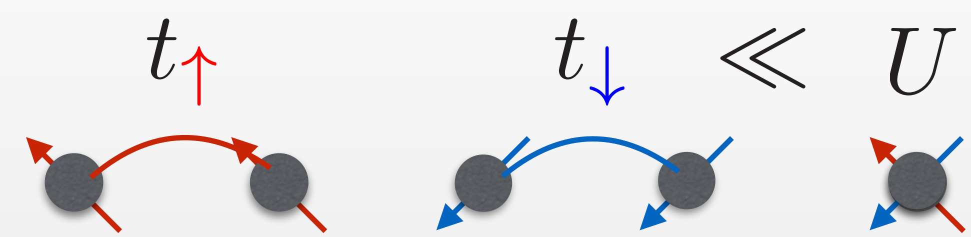


Dirac fermions with unequal Fermi velocities

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.

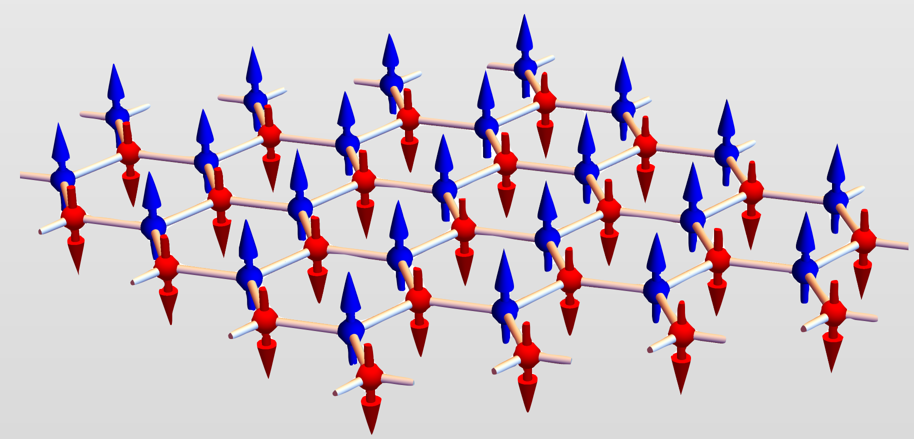
Long-range spin order on bipartite lattices with infinitesimal repulsion

Kennedy and Lieb 1986

“Fruit fly” of DMFT

Freericks and Zlatić, RMP, 2003

Strong Coupling Limit

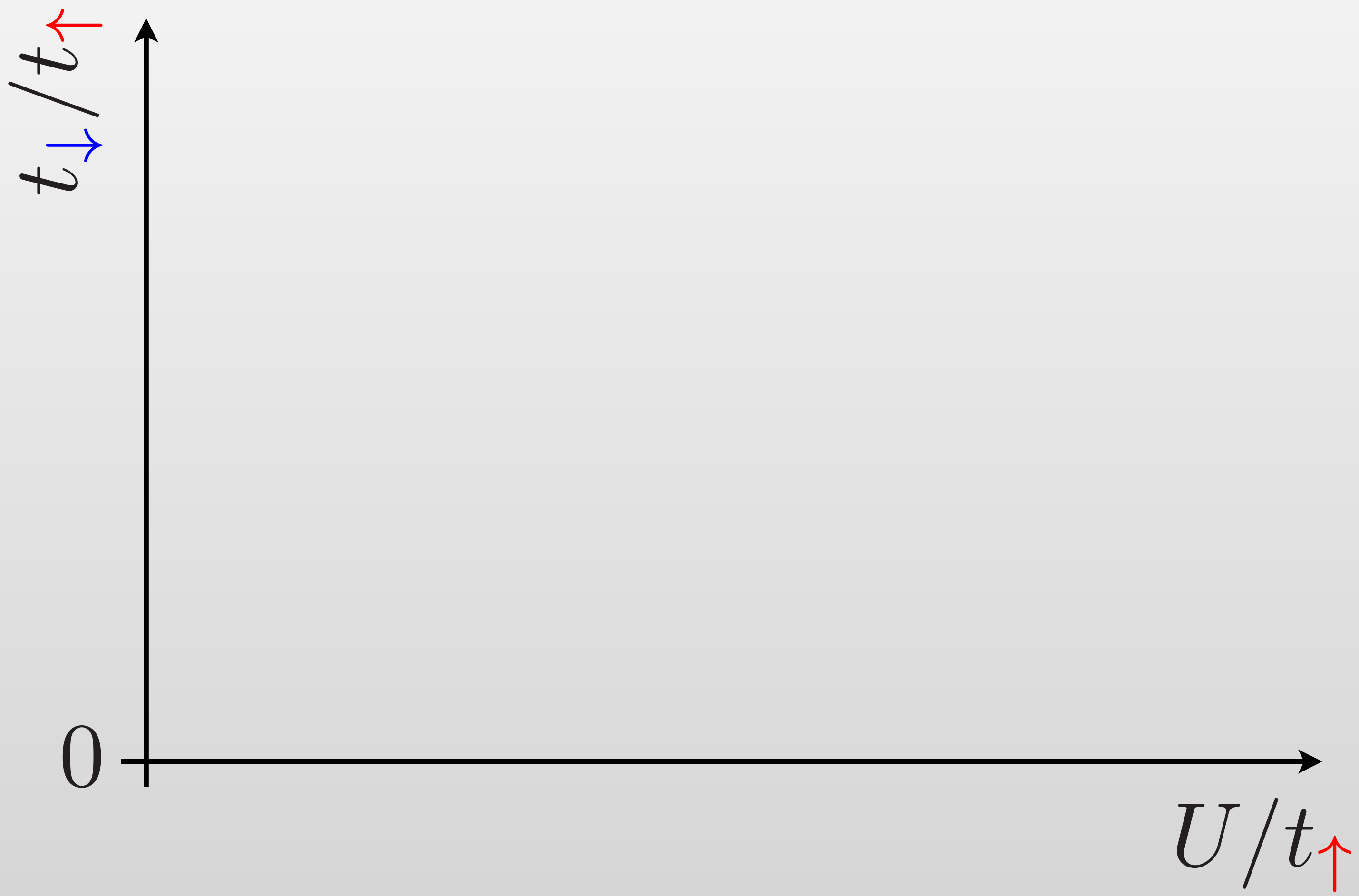


$$J_{xy}\left(\hat{S}_i^x\hat{S}_j^x + \hat{S}_i^y\hat{S}_j^y\right) + J_z\hat{S}_i^z\hat{S}_j^z$$

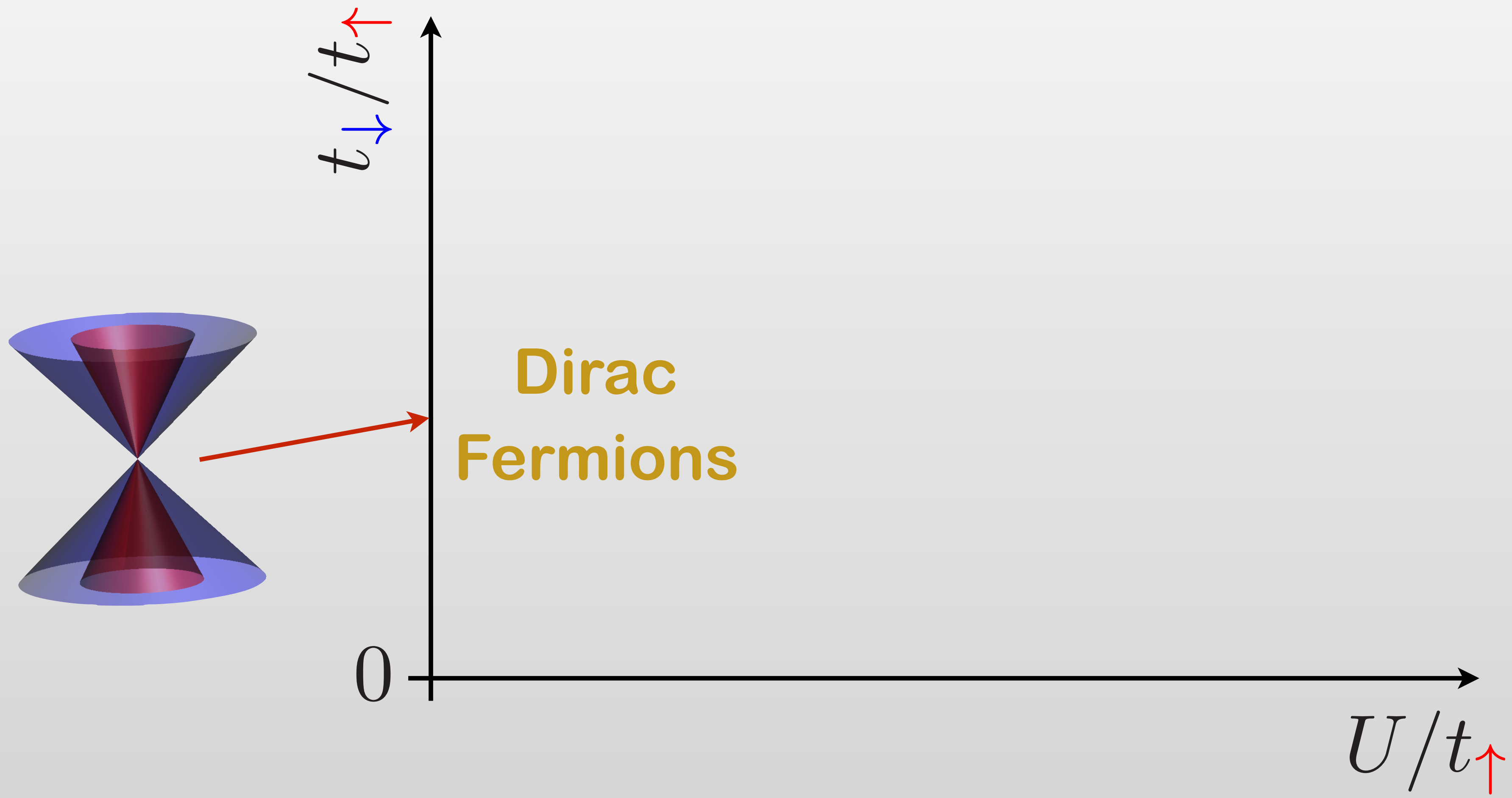
$$\frac{4t_\uparrow t_\downarrow}{U} \leq \frac{2(t_\uparrow^2 + t_\downarrow^2)}{U}$$

XXZ model with Ising anisotropy

Phase diagram



Phase diagram



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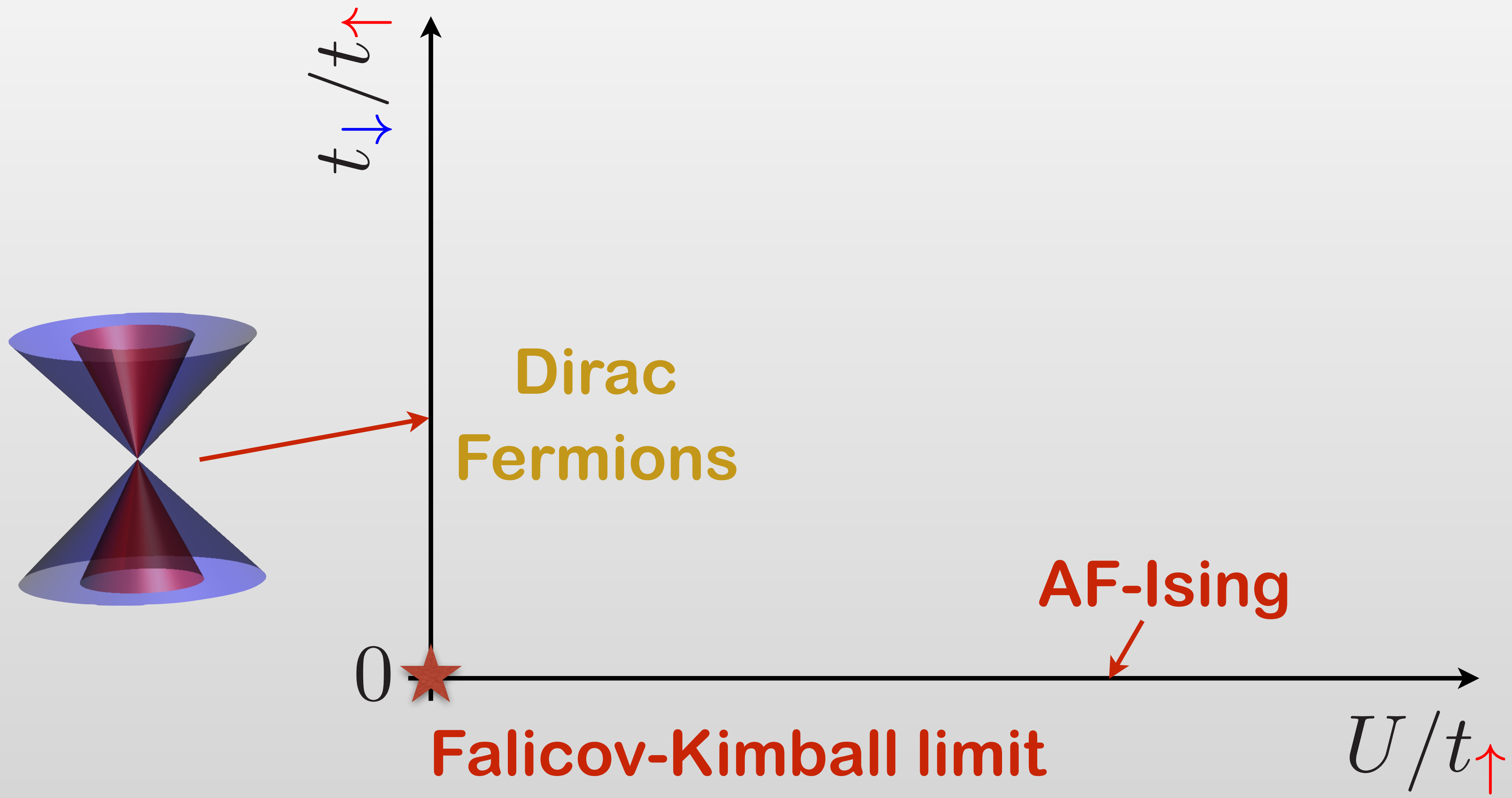

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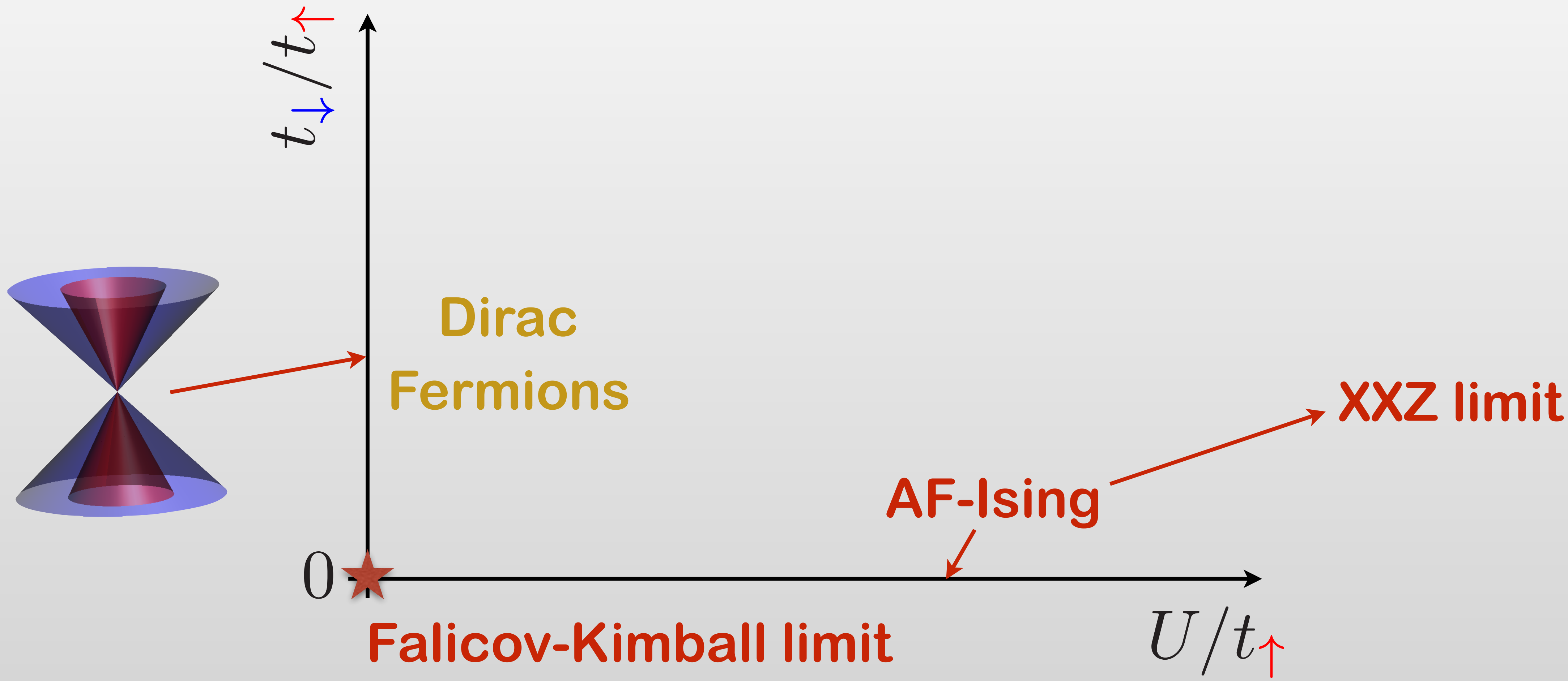

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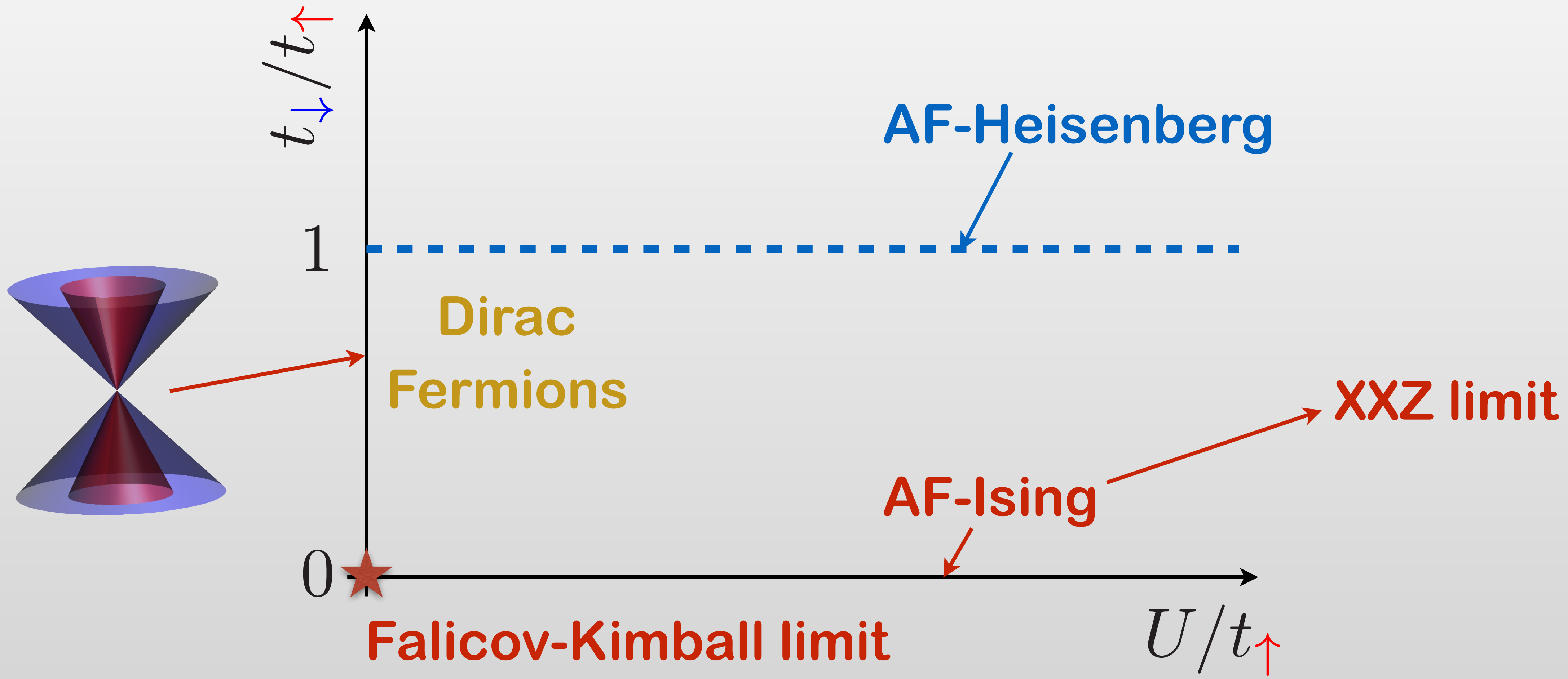

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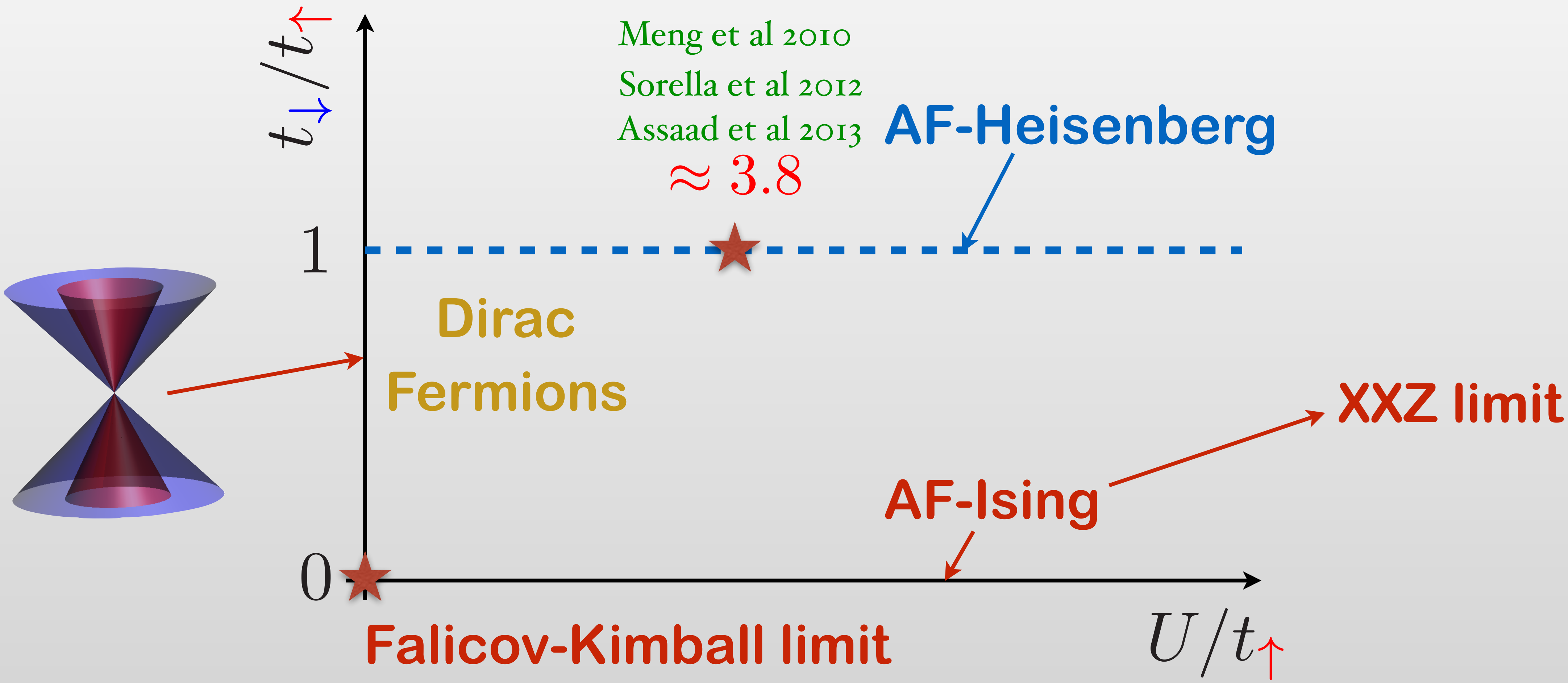

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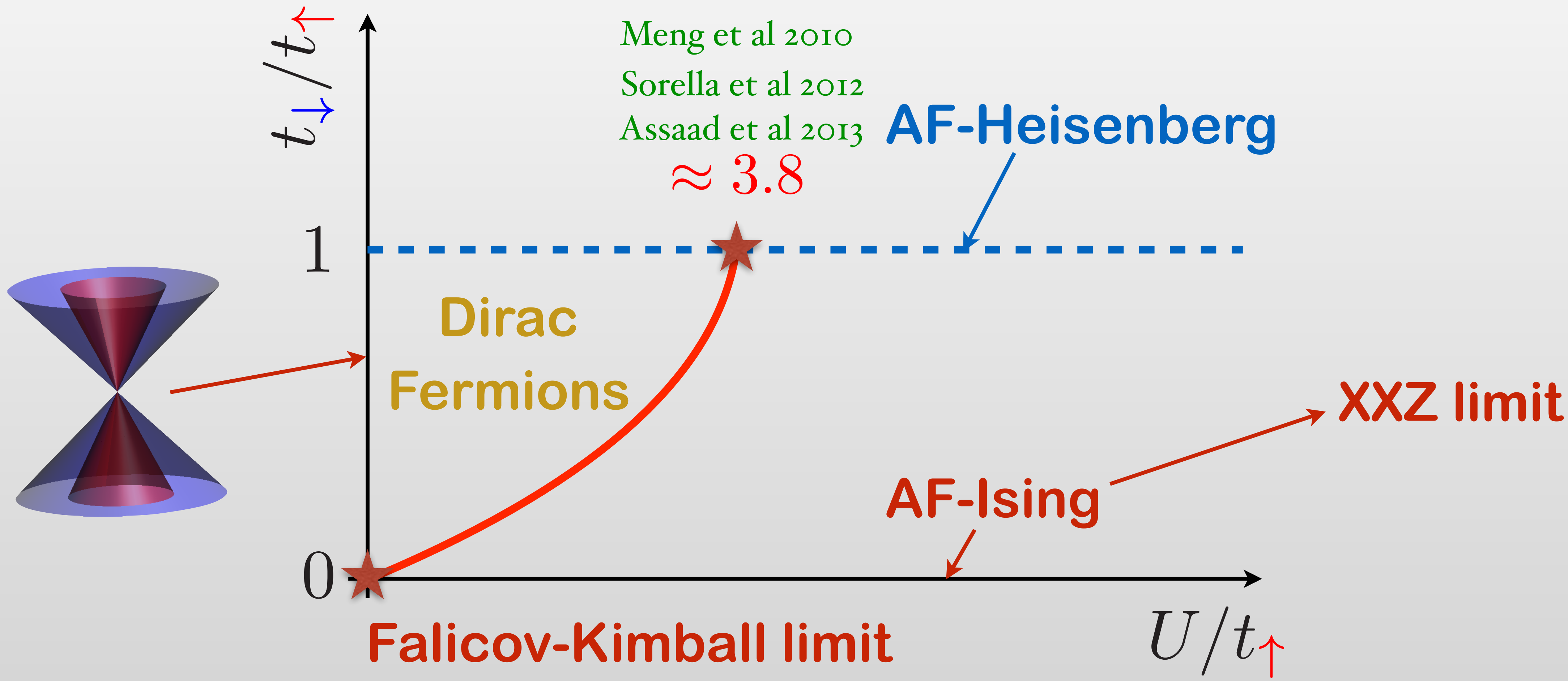
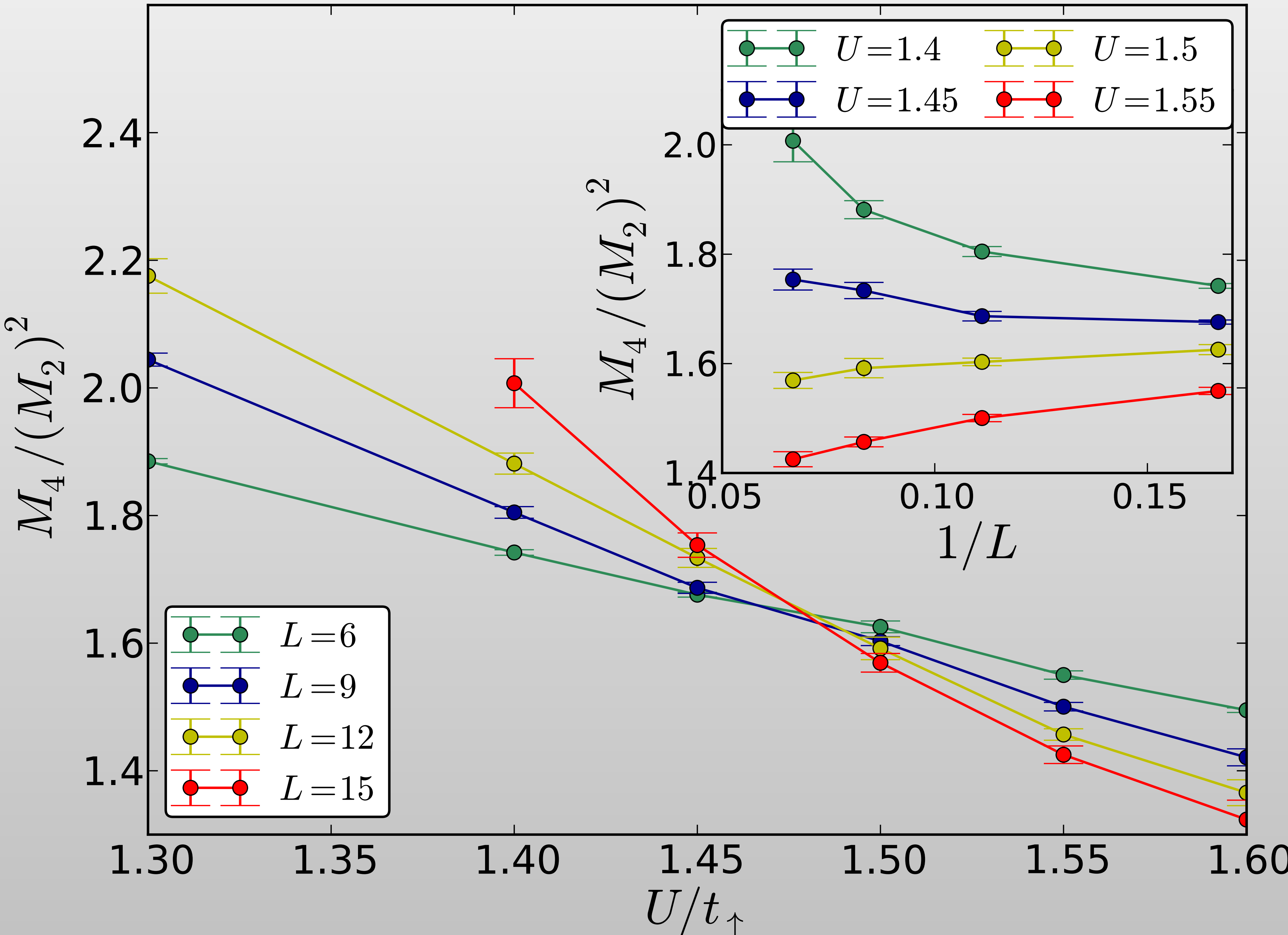


- How to connect the phase boundary ?
- What is the universality class ?

Binder ratio

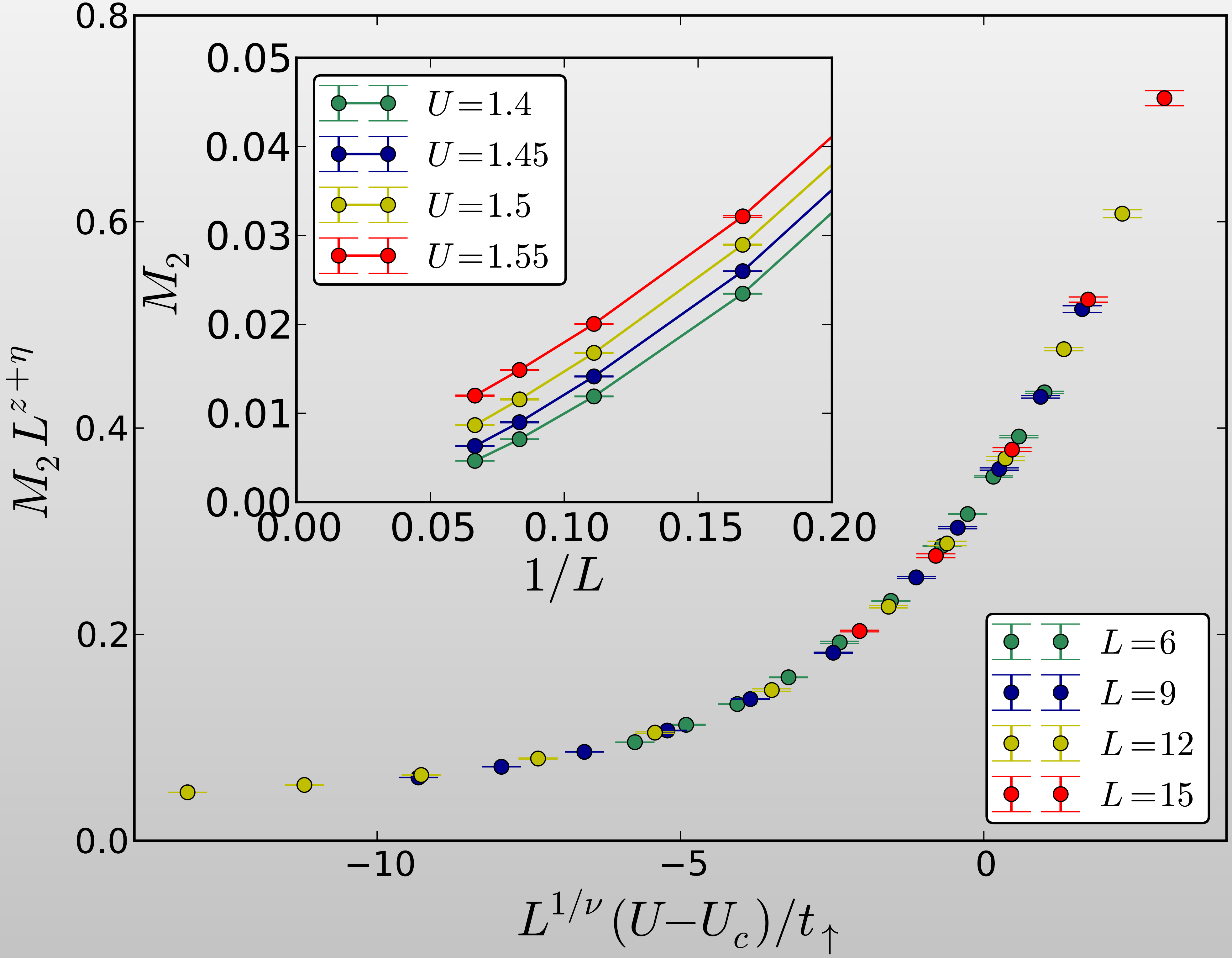
$t_{\downarrow}/t_{\uparrow} = 0.15$

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



Scaling analysis

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



Summary

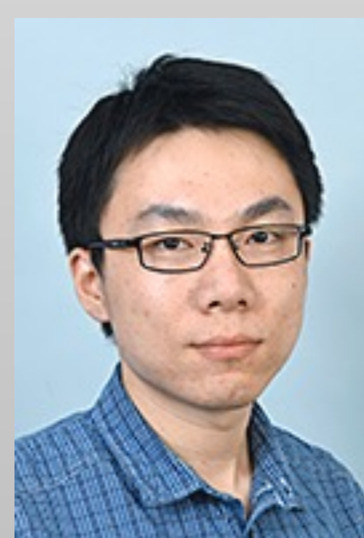
Exciting time for QMC simulation of lattice fermions

Thanks to my collaborators!

Mauro Iazzi

Philippe Corboz

Ye-Hua Liu



Jakub Imriška

Ping Nang Ma

Gergely Harcos

Matthias Troyer