Simulation of Hubbard Models in the Era of Synthetic Gauge Field

### Lei Wang Institute of Physics

第十届冷原子物理青年学者学术讨论会 2016.7

## Hubbard Model



**Optical lattices** 

# Hubbard Model

$$\hat{H} = -\sum_{i,j,\sigma} t_{ij} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$\overset{d\text{-wave SC}}{\text{Mott physics}}_{\text{Magnetism}}_{\text{BCS-BEC}}$$

$$\underset{\dots}{\text{als}}$$

$$\text{Optical lattices}$$

Solid materials

### Algorithms for quantum many body systems





exact diagonalization

quantum Monte Carlo



tensor network states



# Hubbard Model



Solid materials

### Algorithms for quantum many body systems



exact diagonalization



**Monte Carlo** 



tensor network states





### 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



exact diagonalization



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#### 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<sup>†</sup> con-



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# Diagrammatic approaches







#### bosons **World-line Approach**

**Stochastic Series Expansion** 

quantum spins

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

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



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







Time

## Diagrammatic approaches







#### bosons **World-line Approach**

### **Stochastic Series Expansion**

### fermions **Determinantal Methods**

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quantum spins

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# Aspects of QMC

Unbiased method with statistical error more accurate if you run it longer

- Quite flexible in terms of temperature, dimension and range of interactions
- Frontier: compute quantum information quantities LW and Troyer, PRL 2014 LW, Liu, Imriška, Ma and Troyer, PRX 2015 LW, Shinaoka and Troyer, PRL 2015
- Can simulate millions of bosons/quantum spins on a PC,
   thousands of fermions on a cluster

... if there is no sign problem!

### Calibrator

Model all details of the experiment

- Accurate microscopic model (including the trap)
- Actual size simulation (-300,000 bosons)
- Calculate what the experiment should see

Time of flight image

Trotzky, Pollet et al, Nat. Phys, 2010



### Thermometer



### n.n. spin correlation

### spin structure factor



## Theoretical guidance

Critical temperatures Staudt, Kent, Kozik...

Equation of states

Fuchs, LeBlanc, Rigol, Scalettar ...

Isentropic curves

Pollet, Cai, Wang...



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

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

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Bosons: no sign problem if there is no frustration QMC works for any filling, any lattice and any interactions

### How about fermions?

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

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$$= \sum_{k=0}^{\infty} \sum_{\mathcal{C}_{k}} w(\mathcal{C}_{k}) \longrightarrow \left[ \operatorname{det} \left( \begin{array}{c} \operatorname{Noninteracting} \\ \operatorname{Green's functions} \end{array} \right)_{k \times k} \right]$$

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

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Rubisov et al, PRB 2005 Gull et al, RMP 2011
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Rombouts, Heyde and Jachowicz, PRL 1999
$$\operatorname{Izzi and Troyer, PRB 2015 LW, Iazzi, Corboz and T$$

# Fermion sign problem

Spinful fermions: no sign problem thanks to the time-reversal symmetry

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

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

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

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Attractive interaction at any filling on any lattice

Repulsive interaction at half-filling on bipartite lattices

Gauge fields are not impossible for fermions !





### Hofstadter-Hubbard Model when topology meets interaction

Wang, Hung and Troyer, PRB, 2014

## Hofstadter Model



Thouless, Kohmoto, Nightingale and den Nijs, 1982 Chern number of the n-th gap is given by the Diophantine equation





## Hofstadter Model



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$$n = qs + pC$$



### Time-Reversal Invariant Fluxes

### Opposite fluxes for the two spin species

Aidelsburger et al, PRL 2013



### Quantum Spin Hall Insulator if load fermions into the lowest band

cf Miyake et al, PRL 2013 Kennedy et al, PRL 2013 and experiments in NIST, Hamburg ...

# Hofstadter-Hubbard Model



cf. same fluxes Zhai et al, PRL 2010



cf. repulsive interaction Cocks et al, PRL 2012



What's the topological signature of the transition ? LW, Hung and Troyer, PRB 2014

### Locate the transition point

LW, Hung and Troyer, PRB 2014



### Locate the transition point



### What can we say about topology?



# **Topological Pumping**

Laughlin, PRB 1981 Thouless, PRB 1983 LW, Hung and Troyer, PRB 2014

Flux insertion pumps quantized particle in the QSHI



May even be measured in the experiment !

Mancini et al, Science 2015 Stuhl et al, Science 2015 Cooper and Rey, PRA 2015 Zeng, Wang and Zhai, PRL, 2015



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

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

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

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

### 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 $\geq$ 0.3t

Meron cluster approach, Chandrasekharan and Wiese, PRL 1999 solves sign problem for  $V \ge 2t$
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)



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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,<sup>1</sup> Yi-Fan Jiang,<sup>1,2</sup> and Hong Yao<sup>1,3,\*</sup> <sup>1</sup>Institute for Advanced Study, Tsinghua University, Beijing 100084, China <sup>2</sup>Department of Physics, Stanford University, Stanford, California 94305, USA <sup>3</sup>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)

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

Lei Wang,<sup>1</sup> Mauro Iazzi,<sup>1</sup> Philippe Corboz,<sup>2</sup> and Matthias Troyer<sup>1</sup> <sup>1</sup>Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland tiogl Physics, University of Amstendam, Spience, Park 004 Posthus 04485, 1000 CL Amste

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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,<sup>1</sup> Ye-Hua Liu,<sup>1</sup> Mauro Iazzi,<sup>1</sup> Matthias Troyer,<sup>1</sup> and Gergely Harcos<sup>2</sup> <sup>1</sup>Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland <sup>2</sup>Alfréd Rényi Institute of Mathematics, Reáltanoda utca 13-15., Budapest H-1053, Hungary

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### Latest update

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



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

Free fermions with an effective imaginary-time dependent Hamiltonian

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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  $(I + e^{A_1} e^{A_2} \dots e^{A_N}) \ge 0$ 



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

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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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Tao and Paul Erdős in 1985



Quantum Computation and Quantum Information

MICHAEL A. NIELSEN and ISAAC L. CHUANG



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

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

A new "de-sign" principle

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

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

(n,n)

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



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

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

Then det(I + M)has a definite sign for each component !



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

If 
$$M^T \eta M = \eta$$
 where  $\eta = \operatorname{diag}(I, -I)$   
 $\mathcal{T}_e^{-\int_0^\beta d\tau H_{c_k}(\tau)}$   
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for each component !  
 $\eta = \operatorname{diag}(I, -I)$   
 $\eta = \operatorname{dia$ 

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

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

 $\mathcal{T}e^{-\int_0^\beta d\tau H_{\mathcal{C}_k}(\tau)}$ Then  $\det\left(I+M\right)$ has a definite sign for each component !



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

spinless fermions

Liu and LW, PRB 2015

1.0

$$\begin{split} \hat{H}_{0} &= -t \sum_{\langle i,j \rangle} \left( \hat{c}_{i}^{\dagger} \hat{c}_{j} + \hat{c}_{j}^{\dagger} \hat{c}_{i} \right) \\ \hat{H}_{1} &= V \sum_{\langle i,j \rangle} \left( \hat{n}_{i} - \frac{1}{2} \right) \left( \hat{n}_{j} - \frac{1}{2} \right) \\ w(\mathcal{C}_{k}) &\sim \operatorname{Tr} \left[ (-1)^{k} e^{-(\beta - \tau_{k})\hat{H}_{0}} \hat{H}_{1} \dots \hat{H}_{1} e^{-\tau_{1}\hat{H}_{0}} \right] \\ \end{split}$$

see also Li, Jiang, Yao 2015 Hesselmann and Wessel 2016





see also Li, Jiang, Yao 2015 Hesselmann and Wessel 2016





see also Li, Jiang, Yao 2015 Hesselmann and Wessel 2016





# Asymmetric Hubbard model $t_{\uparrow} \neq t_{\downarrow} \quad U$

- Realization: mixture of ultracold fermions (e.g. <sup>6</sup>Li and <sup>4</sup>°K)
- Solve Now, continuously tunable by spin-dependent modulations  $t_{\downarrow}/t_{\uparrow} \in (-\infty, \infty)$



Lignier et al, PRL 2007 and many others

Jotzu et al, PRL 2015

### 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**





XXZ model with Ising anisotropy

### Physics on a square lattice











Finite T<sub>c</sub> in 2D because of broken discrete Z2 symmetry
 Advantage in 3D ? Sotnikov et al, PRL 2012

### Locate the critical temperature

Liu and LW, PRB 2015

















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

### **Binder ratio** $t_{\downarrow}/t_{\uparrow} = 0.15$





Liu and Wang, PRB 2015

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



Liu and Wang, PRB 2015



exact diagonalization







tensor network states



dynamical mean field theories



exact diagonalization







tensor network states



dynamical mean field theories

Algorithmic improvement in past 20 years outperformed Moore's law



exact diagonalization



quantum Monte Carlo



tensor network states



dynamical mean field theories





exact diagonalization



quantum Monte Carlo



tensor network states



dynamical mean field theories







dynamical mean field theories

### Thanks to my collaborators!





# 欢迎本科生毕业设计,博士生,博士后 wanglei@iphy.ac.cn 010-82649853

State of the second second

广告

M