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



Optical lattices

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



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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[†] 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)

fermions **Determinantal Methods**

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







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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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Is it all positive ?

General solution implies P=NP! Troyer and Wiese, 2005



 ∞

 $=\sum\sum w(\mathcal{C}_k)$

k=0 C_k



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



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

How about fermions?

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

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

How about fermions?

How about fermions?

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



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





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







 $\hat{H} = \hat{H}_{\uparrow}(\phi) + \hat{H}_{\downarrow}(-\phi) - U \sum \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$

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





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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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,*} ¹Institute for Advanced Study, Tsinghua University, Beijing 100084, China ²Department of Physics, Stanford University, Stanford, California 94305, USA ³Collaborative 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,¹ Mauro Iazzi,¹ Philippe Corboz,² and Matthias Troyer¹ ¹*Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*

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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,¹ Ye-Hua Liu,¹ Mauro Iazzi,¹ Matthias Troyer,¹ and Gergely Harcos² ¹Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland ²Alfréd 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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math**overflow**

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

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



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 $\eta = \operatorname{diag}(I, -I)$
 $\mathcal{T}_e^{-\int_0^\beta d\tau H_{c_k}(\tau)}$
Then $\operatorname{det}(I + M)$
has a definite sign
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 $\eta = \operatorname{diag}(I, -I)$

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

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. ⁶Li and ⁴°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_c 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

Summary



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







tensor network states



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

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广告

M