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

sign problem
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Li, Jiang and Yao, PRB 2015
LW, Liu, Iazzi, Troyer and Harcos, 1506.05349
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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

\[ \langle N_{\text{hits}} \rangle = \frac{2 \ell}{\pi d} \]
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,
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

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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

\[ Z = \text{Tr} \left( e^{-\beta \hat{H}} \right) \quad \hat{H} = \hat{H}_0 + \lambda \hat{H}_1 \]

Trotterization

\[ Z = \text{Tr} \left( e^{-\frac{\beta}{M} \hat{H}} \ldots e^{-\frac{\beta}{M} \hat{H}} \right) \]

Diagrammatic approach

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

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)
Diagrammatic approaches

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

\[ = \sum_{k=0}^{\infty} \lambda^k \sum_{C_k} w(C_k) \]
Diagrammatic determinant QMC

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

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

\[ = \sum_{k=0}^{\infty} \lambda^k \sum_{C_k} w(C_k) \]

\[ \det \left( \begin{array}{ccc} \text{Noninteracting} \\ \text{Green's functions} \end{array} \right)_{k \times k} \]

\[ \langle k \rangle \sim \beta \lambda N, \text{ scales as } O(\beta^3 \lambda^3 N^3) \]
Diagrammatic determinant QMC

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

\[ = \sum_{k=0}^{\infty} \lambda^k \sum_{C_k} w(C_k) \]

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

LCT-QMC Methods

\[ \text{det} \left( I + T e^{-\int_0^\beta d\tau H c_k(\tau)} \right)_{N \times N} \]

thus achieving \( \mathcal{O}(\beta \lambda N^3) \) scaling!
Fidelity susceptibility made simple!

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

Signifies quantum phase transitions without need of the local order parameter.
Fidelity susceptibility made simple!

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

Signifies quantum phase transitions without need of the local order parameter

Worldline Algorithms  Stochastic Series Expansion  Determinantal Methods

(bosons)  (quantum spins)  (fermions)

\[ k_L \quad k_R \]

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\[ k_L \quad k_R \]
More advantages

\[ \langle \hat{O} \rangle = \frac{1}{Z} \sum_k \lambda^k \sum_{C_k} w(C_k) O(C_k) \]

Observable derivatives

\[ \frac{\partial \langle \hat{O} \rangle}{\partial \lambda} = \langle \hat{O} \rangle_k - \langle \hat{O} \rangle \langle k \rangle \]

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

What about the sign problem?

Sign problem free

time-reversal symmetry

\[ w(C_k) = \det M_\uparrow \times \det M_\downarrow \]

\[ = |\det M_\uparrow|^2 \geq 0 \]
What about the sign problem?

Sign problem free

time-reversal symmetry

\[ \omega(C_k) = \det M_{\uparrow} \times \det M_{\downarrow} \]

\[ = |\det M_{\uparrow}|^2 \geq 0 \]

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

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
What about the sign problem?

Sign problem free

time-reversal symmetry

\[ w(C_k) = \det M_\uparrow \times \det M_\downarrow \]
\[ = |\det M_\uparrow|^2 \geq 0 \]

But, how about this?

spinless fermions

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

\[ w(C_k) = \det M \]

Meron cluster approach, Chandrasekharan and Wiese, PRL 1999

= |det \( M_\uparrow \)|^2 \geq 0

Hands et al, EPJC, 2000

Koonin et al, Phys. Rep, 1997

Wu et al, PRB, 2005


Scalapino et al, PRB 1984

Gubernatis et al, PRB 1985

up to 8*8 square lattice and T \geq 0.3t

solves sign problem for V \geq 2t
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)

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

Zi-Xiang Li, 1 Yi-Fan Jiang,1,2 and Hong Yao1,3,*
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)

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
1Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland
2Institute 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)
A tale of open science

\[ \omega(C_k) \sim \det \left( I + \mathcal{T} e^{-\int_0^\beta d\tau H_{C_k}(\tau)} \right) \]

Free fermions with an effective imaginary-time dependent
A tale of open science

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

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

Free fermions with an effective imaginary-time dependent

$w(C_k) \sim \det \left( I + T e^{-\int_0^\beta d\tau H_{C_k}(\tau)} \right)$
A tale of open science

\[ w(C_k) \sim \det \left( I + T e^{-\int_0^\beta d\tau H_{C_k}(\tau)} \right) \]

Free fermions with an effective imaginary-time dependent

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

mathoverflow

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
Maths whizz solves a master's riddle

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

Chris Cesare

25 September 2015

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Tao and Paul Erdős in 1985
A new design principle

If \( M^T \eta M = \eta \) where \( \eta = \text{diag}(I, -I) \)
A new design principle

If \( M^T \eta M = \eta \)

where \( \eta = \text{diag}(I, -I) \)

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

split orthogonal group
A new de-sign principle

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

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 design principle

\[ M^T \eta M = \eta \quad \text{where} \quad \eta = \text{diag}(I, -I) \]

If \( M^T \eta M = \eta \) then \( \det(I + M) \) has a definite sign for each component!
A new de-sign principle

If \( M^T \eta M = \eta \)

where \( \eta = \text{diag}(I, -I) \)

Then \( \det (I + M) \)

has a definite sign

for each component!

\[ \mathcal{T} e^{-\int_0^\beta d\tau H_{C_k}(\tau)} \]

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

spinless fermions

split Dirac cone

spin nematicity

\( SU(3) \)

LW, Liu, Iazzi, Troyer and Harcos 1506.05349

LW, Corboz, Troyer, NJP 2014
LW, Iazzi, Corboz, Troyer, PRB, 2015

Liu and LW, 1510.00715
A new de-sign principle

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\[ O^{+-}(n,n) \equiv 0 \]

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\[ O^{-+}(n,n) \equiv 0 \]

\[ T \]

spinless fermions

split Dirac cone

spin nematicity

SU(3)

LW, Liu, Iazzi, Troyer and Harcos 1506.05349

Liu and LW, 1510.00715

LW, Troyer, PRL 2014

LW, Corboz, Troyer, NJP 2014

LW, Iazzi, Corboz, Troyer, PRB, 2015
Asymmetric Hubbard model

Realization: mixture of ultracold fermions (e.g.
Now, continuously tunable by

\[ \frac{t_\downarrow}{t_\uparrow} \in (-\infty, \infty) \]

\[ J_{\text{eff}} / J \]

Dirac fermions with unequal Fermi velocities

Lignier et al, PRL 2007 and many others

Dirac fermions with unequal Fermi velocities
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Lignier et al, PRL 2007 and many others

Dirac fermions with unequal Fermi velocities

Jotzu et al, PRL 2015
Two limiting cases

Falicov-Kamaball 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.

Strong Coupling Limit

Long-range spin order on bipartite lattices with infinitesimal repulsion

Kennedy and Lieb

“Fruit fly” of DMFT

Freericks and Zlatić, RMP, 2003

XXZ model with

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

\[ \frac{4t_+ t_-}{U} \leq \frac{2(t_+^2 + t_-^2)}{U} \]
Phase diagram

\[ \frac{t}{t} \uparrow \]

\[ \frac{U}{t} \uparrow \]

0
Phase diagram

$U/t$ →

$\downarrow t/\uparrow t$

Dirac

Fermions
Phase diagram

- Dirac Fermions
- AF-Ising
- Falicov-Kimball limit

Parameters:
- $t_{\downarrow}/t$
- $U/t$
Phase diagram

- **Falicov-Kimball limit**
- **AF-Ising**
- **Dirac Fermions**
- **XXZ limit**

Parameters:
- $t_{\downarrow}/t_{\uparrow}$
- $U/t_{\uparrow}$

Regions:
- **Falicov-Kimball limit**
- **Dirac Fermions**
- **XXZ limit**
Phase diagram

- Falicov-Kimball limit
- AF-Ising
- Dirac
- Fermions
- AF-Heisenberg
- XXZ limit
Phase diagram

- Falicov-Kimball limit
- AF-Ising
- Dirac
- Fermions
- AF-Heisenberg
- XXZ limit

Meng et al 2010
Sorella et al 2012
Assaad et al 2013

\[ U/t \approx 3.8 \]
Phase diagram

How to connect the phase boundary?
What is the

AF-Heisenberg
Dirac Fermions
Falicov-Kimball limit

XXZ limit

AF-Ising

Meng et al 2010
Sorella et al 2012
Assaad et al 2013

\[ \approx 3.8 \]

$U/t$

$U/t$
Binder ratio \( t_{\downarrow}/t_{\uparrow} = 0.15 \)

\[
M_2 = \left\langle \left( \frac{1}{N} \sum_r e^{i Q \cdot r} \hat{n}_{r \uparrow} - \hat{n}_{r \downarrow} \right)^2 \right\rangle \quad M_4 = \left\langle \left( \frac{1}{N} \sum_r e^{i Q \cdot r} \hat{n}_{r \uparrow} - \hat{n}_{r \downarrow} \right)^4 \right\rangle
\]
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