How did I earn an Erdős number of 2?

Lei Wang Institute of Physics

2016.04 @ CSRC

1913.3.26–1996.9.20



• One of the most prolific math problem solver in history

combinatorics, graph theory, number theory, classical analysis, approximation theory, set theory, and probability theory.

• Over 1500 published papers and more than 500 collaborators

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- 1 ...
- 2 Einstein, Glashow, S.-S. Chern, Freedman, Knuth, Shor ...

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- 1 ... +
- 2 Einstein, Glashow, S.-S. Chern, Freedman, Knuth, Shor ...
- 3 Bethe, Schrödinger, Fermi, Pauli, Feynman, Wilczek, Witten, Kohn, C.-N. Yang ...

How did I earn an Erdős number of 2? —new adventures of quantum Monte Carlo

Lei Wang Institute of Physics

2016.04 @ CSRC



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

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Time

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Entanglement & Fidelity

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

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LCT-QMC methods

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



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

$$\det M \ge 0 \quad \text{if} \quad \begin{array}{l} \Theta M \Theta^{-1} = M \\ \Theta^2 = -1 \end{array}$$

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



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



And more ...





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



Spin-fermion models

Berg, Metliski and Sachdev, Science 2012



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

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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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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,*} 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 ¹Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland ²Institute for Theoretical Physics, University of Amsterdam, Science Park 904 Postbus 94485, 1090 GL Amsterdam, The Netherlands

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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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Wei, Wu, Li, Zhang, Xiang, arXiv:1601.01994

> Li, Jiang Yao, arXiv:1601.05780

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

Free fermions with an effective imaginary-time dependent Hamiltonian

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

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



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 many 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



MICHAEL NIELSEN

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 $\eta = \operatorname{diag}(I, -I)$

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

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

(n,n)

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



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 $\eta = \operatorname{diag}(I, -I)$
 $\mathcal{T}e^{-\int_0^\beta d\tau H_c(\tau)}$ $\stackrel{O^{+-}(n,n)}{\longrightarrow} \equiv 0$ $\stackrel{O^{++}(n,n)}{\longrightarrow} \geq 0$
Then $\operatorname{det}(I+M)$ $\stackrel{has a definite sign}{\longrightarrow}$ for each component ! $\stackrel{O^{--}(n,n)}{\longrightarrow} < 0$ $\stackrel{O^{-+}(n,n)}{\longrightarrow} \equiv 0$

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

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

 $\mathcal{T}e^{-\int_0^\beta d\tau H_{\mathcal{C}}(\tau)}$ (n, n)(n, n)()Then $\det\left(I+M\right)$ has a definite sign (n, n)(n,n)for each component ! spin nematicity **SU(3)** spinless fermions split Dirac cone LW, Troyer, PRL 2014 Liu and LW, PRB 2015 LW, Corboz, Troyer, NJP 2014 LW, Iazzi, Corboz, Troyer, PRB, 2015

LW, Liu and Troyer, PRB 2016

1.0

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

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





spin nematicity



SU(3)

Liu and LW, PRB 2015



cf Li, Jiang, Yao 2015 Hesselmann and Wessel 2016





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

- Realization: mixture of ultracold fermions (e.g. ⁶Li and ⁴°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

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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

 $\ll U$





XXZ model with Ising anisotropy















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

It is an exciting time







better scaling

entanglement & fidelity

sign problem

Thanks to my collaborators!





Discrete Mathematics 200 (1999) 95-99

Popular distances in 3-space

DISCRETE

MATHEMATICS

Paul Erdős^a, Gergely Harcos^b, János Pach^{a,c,*}

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Received 19 April 1998; accepted 9 June 1998





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计计

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International Summer School on Computational Approaches for Quantum Many Body Systems 2016.08.01-2016.08.21 Lecture + Seminar + Tutorial

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Fakher Assaad Bela Bauer Erez Berg Jan Gukelberger Andreas Lauchli David Luitz Lode Pollet Marcos Rigol Anders Sandvik Phillip Werner Stefan Wessel

Speakers

Xi Dai Youjin Deng Wenan Guo Li Huang Zi Yang Meng Ninghua Tong Lei Wang Yilin Wang Tao Xiang Zhiyuan Xie

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