Monte Carlo methods in continuous time for lattice Hamiltonians

Emilie Huffman with Shailesh Chandrasekharan

Duke University

The 34th annual International Symposium on Lattice Field Theory

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- We have discovered new sign problems solvable in CT-INT formalism, defined below for $H = H_0 + H_{\rm int}$.

$$Z = \sum_k \int [dt] \, (-1)^k \, Tr \left(e^{-(\beta - t)H_0} H_{\rm int} e^{-(t_1 - t_2)H_0} H_{\rm int} \ldots \right), \tag{1}$$

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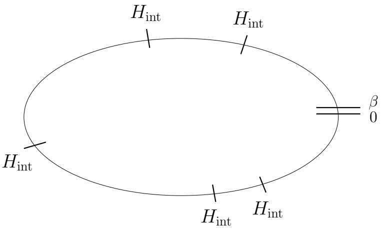

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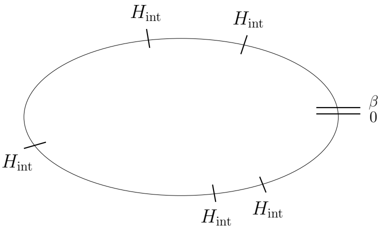

- We can discretize in time as well for these solutions.

The New Solutions

- *CT-INT* is key to most of these solutions. Most of these models involve interactions between fermions and quantum spins. (Non-interacting: *Continuous-time QMC Solvers for Electronic Systems in Fermionic and Bosonic Baths* (Assaad 2014))

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- Key idea previously used for lattice field theories. (Chandrasekharan, PRD 2012)

RAPID COMMUNICATIONS

PHYSICAL REVIEW D **86**, 021701(R) (2012)

Solutions to sign problems in lattice Yukawa models

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Department of Physics, Duke University, Durham, North Carolina 27708, USA
(Received 22 May 2012; published 3 July 2012)

The New Solutions

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- Effective for many interesting models, including antiferromagnets and Kondo models. Also plays well with Meron Cluster technique, extending parameter space.

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Meron-Cluster Solution of Fermion Sign Problems

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[2]*Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139*
(Received 10 February 1999)

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- Key idea previously used for lattice field theories. (Chandrasekharan, PRD 2012)
- Effective for many interesting models, including antiferromagnets and Kondo models. Also plays well with Meron Cluster technique, extending parameter space.
- Also simple $\mathbb{Z}_2$ gauge theories.
- Algorithms available in (L. Wang, et. al. PRB 2015) that scale as:

	Lattice models	
	CT-INT	**CT-AUX**
Scaling	βN^3	βN^3

General Model

- The newly solvable interacting spinless fermion and quantum spin models have this general form:

$$
\begin{aligned}
H = & -t \sum_{\langle xy \rangle} \left(c_x^\dagger c_y + c_y^\dagger c_x \right) + V \sum_{\langle xy \rangle} \left(n_x - \frac{1}{2} \right) \left(n_y - \frac{1}{2} \right) \\
& + \sum_{xy} \left(J_{\text{perp}} \left(S_x^1 S_y^1 + S_x^2 S_y^2 \right) \pm J_3 S_x^3 S_y^3 \right) - \sum_x h_x \left(n_x - \frac{1}{2} \right) S_x^1
\end{aligned}
\tag{2}
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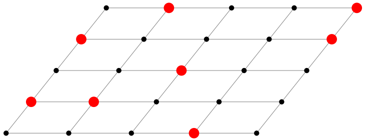
$$H = \overbrace{-t \sum_{\langle xy \rangle} \left(c_x^\dagger c_y + c_y^\dagger c_x \right)}^{H_0^f} + V \sum_{\langle xy \rangle} \left(n_x - \frac{1}{2} \right) \left(n_y - \frac{1}{2} \right)$$
$$+ \sum_{xy} \left(J_{\mathrm{perp}} \left(S_x^1 S_y^1 + S_x^2 S_y^2 \right) \pm J_3 S_x^3 S_y^3 \right) - \sum_x h_x \left(n_x - \frac{1}{2} \right) S_x^1 \qquad (2)$$

- Here, H_0^f is the tight-binding Hamiltonian.



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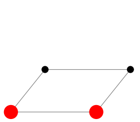
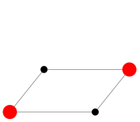
- H_{int}^b is the fermion interaction term from the t-V model.





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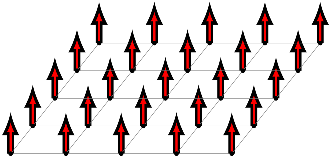
H_0^b

- Then H_0^b is a somewhat general spin model.



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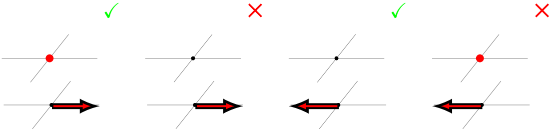
- And H_{int}^{fb} is interaction between the fermions and spins.



Physics Motivation: Fermion Part

- Even with the simplest quantum spin interaction, where $H_0^b = J\sum_{\langle x,y\rangle} S_x^3 S_y^3$, we see potentially interesting physics.

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- t-V part solvable in both *CT-INT* (Huffman, Chandrasekharan, PRB 2014) and *CT-AUX* (Li et. al. PRB 2015).

RAPID COMMUNICATIONS

PHYSICAL REVIEW B **89**, 111101(R) (2014)

Solution to sign problems in half-filled spin-polarized electronic systems

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Department of Physics, Duke University, Durham, North Carolina 27708, USA
(Received 19 December 2013; revised manuscript received 14 February 2014; published 12 March 2014)

RAPID COMMUNICATIONS

PHYSICAL REVIEW B **91**, 241117(R) (2015)

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

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[2]*Department of Physics, Stanford University, Stanford, California 94305, USA*
[3]*Collaborative Innovation Center of Quantum Matter, Beijing 100084, China*
(Received 27 August 2014; revised manuscript received 13 October 2014; published 30 June 2015)

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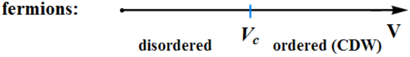

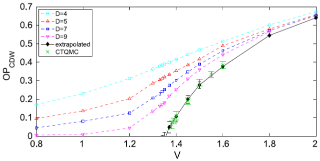

Figure: L. Wang, P. Corboz, M. Troyer, *New J. Phys. 16, 103008.*

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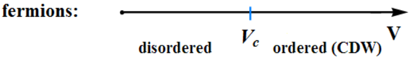

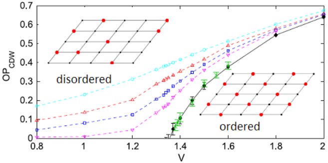

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Physics Motivation: Suspected Phase Diagram

- But remember, spins are correlated with fermions:

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\end{aligned} \tag{4}
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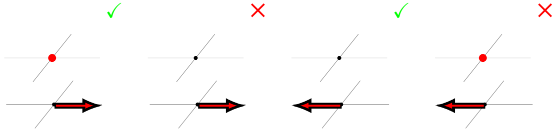

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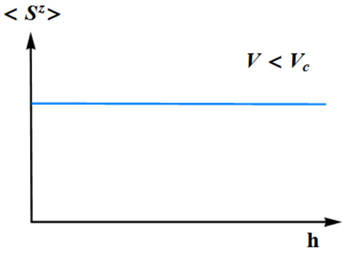
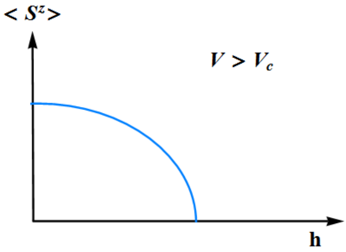
- Thus we propose:





- What happens at the critical point V_c?

A note on the fermionic part

- We know that the t-V model has no sign problem in *CT-INT* and *CT-AUX*.

$$H_0^f + H_{\mathrm{int}}^b = -t \sum_{\langle xy \rangle} \left(c_x^\dagger c_y + c_y^\dagger c_x \right) + V \sum_{\langle xy \rangle} \left(n_x - \frac{1}{2} \right) \left(n_y - \frac{1}{2} \right), \tag{5}$$

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- All continuous-time Hamiltonian solutions so far allow for the following addition:

$$H_{\mathrm{stagg}} = \sum_x \eta_x h_x \left(n_x - \frac{1}{2}\right) \tag{6}$$

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- We show in the following slides how instead adding the spin sector portion $H_{\text{int}}^{fb} = \sum_x h_x \left(n_x - \frac{1}{2} \right) S_x^1$ results in no sign problem for *CT-INT* specifically.

Model 1: Factorization

$$
\begin{aligned}
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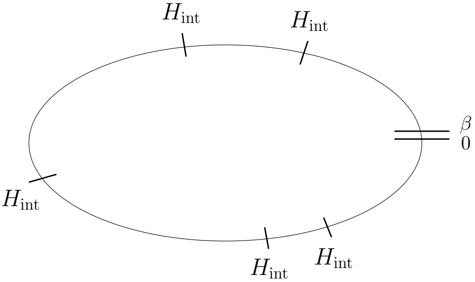
& + J \sum_{xy} S_x^3 S_y^3 - \sum_x h_x \left(n_x - \frac{1}{2} \right) S_x^1
\end{aligned} \tag{7}
$$

- The expansion will consist of terms of this form,

$$
(-1)^k \, \mathrm{Tr} \left(e^{-(\beta - t_1) H_0} H_{\text{int}} e^{-(t_1 - t_2) H_0} H_{\text{int}} \ldots H_{\text{int}} e^{-t_k H_0} \right) , \tag{8}
$$

where $H_0 = H_0^f + H_0^b$ and $H_{\text{int}} = H_{\text{int}}^f + H_{\text{int}}^{fb}$.



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- Example term:

$$h_x (-1)^{2+1} \, \mathrm{Tr} \left(e^{-(\beta - t_1) H_0} H_{\mathrm{int}}^f e^{-(t_1 - t_2) H_0} \left(n_x - \frac{1}{2} \right) S_x^1 e^{-t_2 H_0} \right). \tag{9}$$

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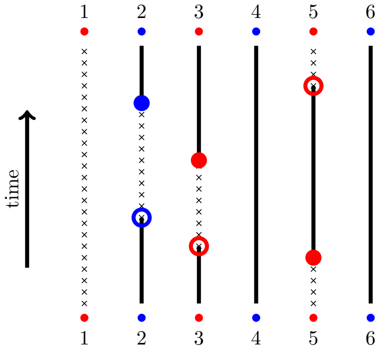
- We can rewrite

$$h_i (-1)^{2+1} \operatorname{Tr}_b \left(e^{-(\beta - t_2) H_0^b} S_x^1 e^{-t_2 H_0^b} \right) \times \operatorname{Tr}_f \left(e^{-(\beta - t_1) H_0^f} H_{\text{int}}^f e^{-(t_1 - t_2) H_0^f} \left(n_x - \frac{1}{2} \right) e^{-t_2 H_0^f} \right). \quad (10)$$

Worldline Approach: The Spin Part

- Key idea: Use the z-basis for spin states. Particles are spin z-up and holes are spin z-down.



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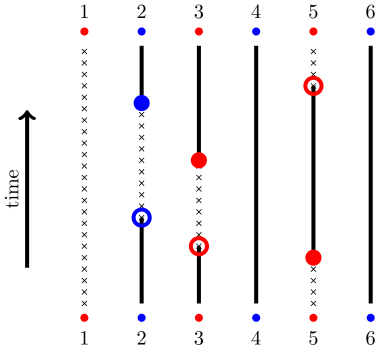

Worldline Approach: The Spin Part

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$$\langle\downarrow\uparrow\uparrow\uparrow\downarrow\uparrow|\, e^{-(\beta-t_6)H_0^b} S_{\color{red}5}^1 e^{-(t_6-t_5)H_0^b} S_{\color{blue}2}^1 e^{-(t_5-t_4)H_0^b} S_{\color{red}3}^1 e^{-(t_4-t_3)H_0^b}$$

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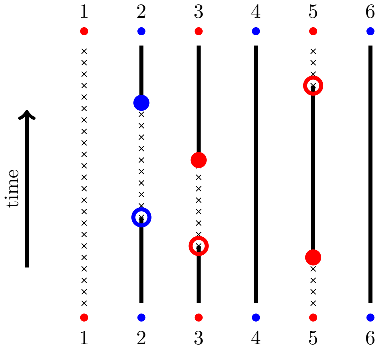
- If we flip a spin, we must flip it back again.



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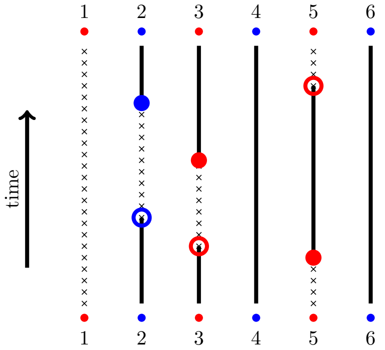
- If we flip a spin, we must flip it back again.
- We need an even number of every S_x^1 operator.



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- And thus most generally the Ising model coupled with fermions

$$\begin{aligned} H = & - t \sum_{\langle xy \rangle} \left(c_x^\dagger c_y + c_y^\dagger c_x \right) + V \sum_{\langle xy \rangle} \left(n_x - \frac{1}{2} \right) \left(n_y - \frac{1}{2} \right) \\ & \pm J \sum_{xy} S_x^3 S_y^3 - \sum_x h_x \left(n_x - \frac{1}{2} \right) S_x^1 \end{aligned} \tag{13}$$

has no sign problem for any h_x.

Model 2: The Heisenburg Antiferromagnet

- We add a bit more complexity to the spin section for this second model, considering

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- The new H_{int} is

$$
H_{\text{int}} = H_{\text{int}}^f + H_{\text{int}}^b + H_{\text{int}}^{fb}. \tag{15}
$$

Antiferromagnetic Heisenburg Model

- How does H_{int}^{b} affect the spin space?

Antiferromagnetic Heisenberg Model

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- For two nearest neighbors, x and y, using the basis states $(\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow)$, we have

$$H^b_{\text{int},xy} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -J/2 & J/2 & 0 \\ 0 & J/2 & -J/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{16}$$

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- Therefore, every time the Hamiltonian flips a nearest neighbor spin pair, the overall matrix element takes on an extra minus sign.

Worldline Approach: With H^{fb}_{int} insertions

Contribution to $\langle\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow|\, e^{-(\beta-t_6)H_0^b} S^1_6\, e^{-(t_6-t_5)H_0^b} S^1_3\, e^{-(t_5-t_4)H_0^b} S^1_5$

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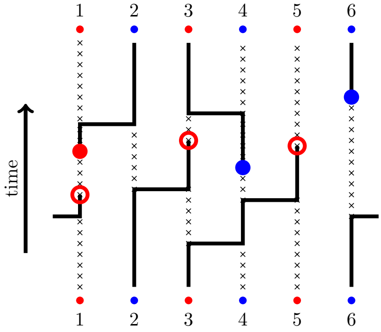
- Now our insertions can hop before being annihilated.



Worldline Approach: With $H_{\rm int}^{fb}$ insertions

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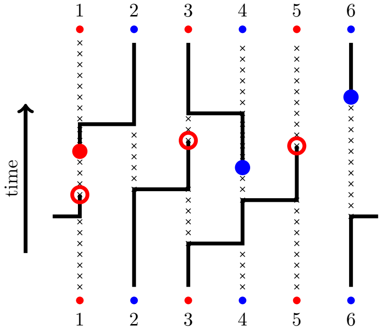
- Now our insertions can hop before being annihilated.
- Odd-even (even-odd) creation-annihilation has odd number of hops. Odd-odd (even-even) creation-annihilation has even number of hops.



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- The antiferromagnet coupled with fermions has no sign problem in the CT-INT expansion.

Model 3: $\mathbb{Z}_2$ Gauge Theory

- We can extend the these ideas to gauge theories. A simple example:

$$H = -t\left(\sum_{\langle xy\rangle} c_x^\dagger \sigma_{xy}^3 c_y + c_y^\dagger \sigma_{xy}^3 c_x\right) - h\sum_{\langle xy\rangle}\sigma_{xy}^1 + \sum_{\text{plaquettes}} \sigma_a^3\sigma_b^3\sigma_c^3\sigma_d^3 \tag{19}$$

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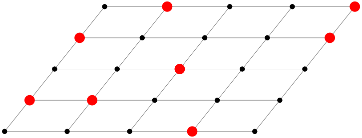
H_0^{fb}

- Here, H_0^{fb} is the free part, coming from the covariant derivative.



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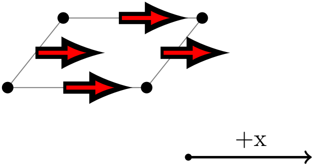
- H_{int}^b is a field in the x-direction.



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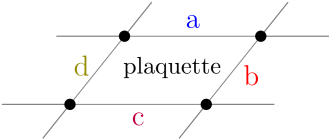
$$+ \underbrace{\sum_{\text{plaquettes}} \sigma^3_a\sigma^3_b\sigma^3_c\sigma^3_d}_{H^p}$$

- H^p is a sum over plaquettes.



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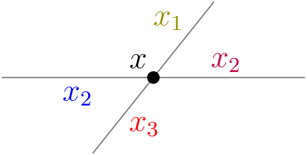
- Invariant under $G_x^\dagger c_x G_x = -c_x$, $G_x^\dagger \sigma_{x_n}^1 G_x \to = \sigma_{x_n}^1$, and $G_x^\dagger \sigma_{x_n}^3 G_x = -\sigma_{x_n}^3$, where $G_x = \sigma_{x_1}^1\sigma_{x_2}^1\sigma_{x_3}^1\sigma_{x_4}^1\eta_x\,(2n_x - 1)$



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- Spinful fermionic version considered by (Gazit, Randeria, Vishwanath (2016)), so there is interest in such models.

Charged fermions coupled to $\mathbb{Z}_2$ gauge fields: Superfluidity, confinement and emergent Dirac fermions.

Snir Gazit,[1] Mohit Randeria,[2] and Ashvin Vishwanath[1,3]
[1]*Department of Physics, University of California, Berkeley, CA 94720, USA*
[2]*Department of Physics, The Ohio State University, Columbus, OH 43210*
[3]*Department of Physics, Harvard University, Cambridge MA 02138, USA*
(Dated: July 15, 2016)

$\mathbb{Z}_2$ Gauge Theories

- We again use *CT-INT*. $\hat{P}$ enforces the Gauss's Law constraint.

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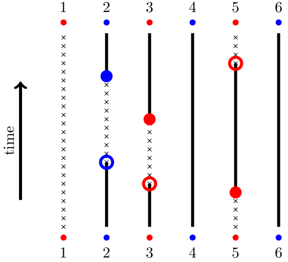

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- Now we cannot factor into separate fermionic and spin factors, but we can use z-basis to replace spin operators with numbers.
- Using a Majorana transformation we can confirm that the fermionic part has no sign problem either.
(Li, Jiang, Yao PRB (2015)), (Wang, Iazzi, Corboz, Troyer PRL (2015)), (Wei, Wu, Li, Zhang, Xiang, PRL (2016)), (Li, Jiang, Yao, 1601.05780).

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- The *CT-INT* formalism also plays well with other techniques, such as the Meron Cluster method.
- We can also apply these techniques to simple gauge theories, such as the $\mathbb{Z}_2$ gauge theory we have shown here.