Monte Carlo methods in continuous time for lattice Hamiltonians

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Duke University

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Hamiltonian Formalism: Why use it?

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- Condensed matter problems are naturally formulated in Hamiltonian perspective.

\[ Z = \sum_{k} \int dt \left( -1 \right)^{k} \text{Tr} \left( e^{-\beta (t_2 - t_1) H_0} H_{\text{int}} e^{-t_1 H_0} H_{\text{int}} \right) \]


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- Condensed matter problems are naturally formulated in Hamiltonian perspective.
- We have discovered new sign problems solvable in CT-INT formalism, defined below for \( H = H_0 + H_{\text{int}} \).

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\]

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(1)


- 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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  Solutions to sign problems in lattice Yukawa models

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  (Received 22 May 2012; published 3 July 2012)
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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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(Received 10 February 1999)
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Also simple $\mathbb{Z}_2$ gauge theories.
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- 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:

<table>
<thead>
<tr>
<th></th>
<th>Lattice models</th>
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</thead>
<tbody>
<tr>
<td><strong>Scaling</strong></td>
<td>$\beta N^3$</td>
</tr>
<tr>
<td><strong>CT-INT</strong></td>
<td></td>
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<tr>
<td><strong>CT-AUX</strong></td>
<td></td>
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</tbody>
</table>
The newly solvable interacting spinless fermion and quantum spin models have this general form:

\[
H = -t \sum_{\langle xy \rangle} (c_x^\dagger c_y + c_y^\dagger c_x) + V \sum_{\langle xy \rangle} \left( n_x - \frac{1}{2} \right) \left( n_y - \frac{1}{2} \right)
+ \sum_{xy} (J_{\text{perp}} (S_x^1 S_y^1 + S_x^2 S_y^2) \pm J_3 S_x^3 S_y^3) - \sum_x h_x \left( n_x - \frac{1}{2} \right) S_x^1
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Here, \( H_0^f \) is the tight-binding Hamiltonian.
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Then \( H_0^b \) is a somewhat general spin model.
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\( H_{\text{int}}^{fb} \)

And \( H_{\text{int}}^{fb} \) 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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fermions:  

\[ \text{disordered} \quad V_c \quad \text{ordered (CDW)} \]

Figure: L. Wang, P. Corboz, M. Troyer, New J. Phys. 16, 103008.
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Figure: L. Wang, P. Corboz, M. Troyer, New J. Phys. 16, 103008.
But remember, spins are correlated with fermions:

\[ H = -t \sum_{\langle xy \rangle} \left( c_x^+ c_y + c_y^+ c_x \right) + V \sum_{\langle xy \rangle} \left( n_x - \frac{1}{2} \right) \left( n_y - \frac{1}{2} \right) \]

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Thus we propose:

What happens at the critical point \( V_c \)?
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Thus we propose:

What happens at the critical point \( V_c \)?
We know that the t-V model has no sign problem in \(CT\)-\(INT\) and \(CT\)-\(AUX\).

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H^f_0 + H^b_{\text{int}} = -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),
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All continuous-time Hamiltonian solutions so far allow for the following addition:

\[ H_{\text{stagg}} = \sum_x \eta_x h_x \left( n_x - \frac{1}{2} \right) \]

(6)
A note on the fermionic part

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- For the bipartite lattice, \( \eta_x \) is +1 for one (even) sublattice, and −1 for the other (odd) sublattice.

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

\[ H = -t \sum_{\langle xy \rangle} (c_x^\dagger c_y + c_y^\dagger c_x) + V \sum_{\langle xy \rangle} \left( n_x - \frac{1}{2} \right) \left( n_y - \frac{1}{2} \right) \]

\[ + J \sum_{xy} S_x^3 S_y^3 - \sum_x h_x \left( n_x - \frac{1}{2} \right) S_x^1 \]

The expansion will consist of terms of this form,

\[ (-1)^k \text{Tr} \left( e^{- (\beta - t_1) H_0} H_{\text{int}} e^{-(t_1 - t_2) H_0} H_{\text{int}} \ldots H_{\text{int}} e^{- t_k H_0} \right), \]

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where \( H_0 = H_0^f + H_0^b \) and \( H_{\text{int}} = H_{\text{int}}^f + H_{\text{int}}^b \).

- Example term:

\[ h_x \left( -1 \right)^{2+1} \text{Tr} \left( e^{-(\beta - t_1)H_0} H_{\text{int}}^f e^{-(t_1 - t_2)H_0} \left( n_x - \frac{1}{2} \right) S_x^1 e^{-t_2 H_0} \right). \]  \hspace{1cm} (9)
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- We can rewrite

\[ h_i (-1)^{2+1} \text{Tr}_b \left( e^{-(\beta - t_2)H_0^b} S_x^1 e^{-t_2 H_0^b} \right) \]

\[ \times \text{Tr}_f \left( e^{-(\beta - t_1)H_0^f} H_{\text{int}}^f e^{-(t_1 - t_2)H_0^f} \left( n_x - \frac{1}{2} \right) e^{-t_2 H_0^f} \right). \]
Key idea: Use the $z$-basis for spin states. Particles are spin $z$-up and holes are spin $z$-down.
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\[
\langle \downarrow \uparrow \uparrow \uparrow \downarrow \uparrow | e^{-(\beta - t_6)H_0^b} S_5^1 e^{-(t_6 - t_5)H_0^b} S_2^1 e^{-(t_5 - t_4)H_0^b} S_3^1 e^{-(t_4 - t_3)H_0^b} \times S_2^1 e^{-(t_3 - t_2)H_0^b} S_3^1 e^{-(t_2 - t_1)H_0^b} S_5^1 e^{-(t_1)H_0^b} | \downarrow \uparrow \uparrow \uparrow \downarrow \uparrow \rangle
\]
Key idea: Use the \( z \)-basis for spin states. Particles are spin \( z \)-up and holes are spin \( z \)-down.

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\langle \downarrow \uparrow \uparrow \uparrow \uparrow | e^{-\beta (t_6-t_5)} H_0^b S_5^1 e^{-t_5-t_4} H_0^b S_2^1 e^{-t_4-t_3} H_0^b S_3^1 e^{-t_3-t_2} H_0^b S_2^1 e^{-t_2-t_1} H_0^b S_3^1 e^{-t_1-t_0} H_0^b | \downarrow \uparrow \uparrow \uparrow \uparrow \rangle
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If we flip a spin, we must flip it back again.
Key idea: Use the z-basis for spin states. Particles are spin z-up and holes are spin z-down.

\[
\begin{align*}
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\end{align*}
\]

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

We need an even number of every $S_x^1$ operator.
No Sign Problem

However,

\[ S_x^1 S_x^1 = \eta_x \eta_x S_x^1 S_x^1. \]  \hspace{1cm} (11)
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- Thus it is as if our \( H_{int}^b \) insertion is really
  \[ \sum_x h_x \eta_x \left( n_x - \frac{1}{2} \right) S_x^1. \]  
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  \] \hspace{1cm} (12)

- And thus most generally the Ising model coupled with fermions
  \[
  H = -t \sum_{\langle xy \rangle} \left(c_x^\dagger c_y + c_y^\dagger c_x\right) + V \sum_{\langle xy \rangle} \left(n_x - \frac{1}{2}\right) \left(n_y - \frac{1}{2}\right) 
  \pm J \sum_{xy} S_x^3 S_y^3 - \sum_x h_x \left(n_x - \frac{1}{2}\right) S_x^1. 
  \] \hspace{1cm} (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

$$ H = -t \sum_{\langle xy \rangle} \left( c_x^\dagger c_y + c_y^\dagger c_x \right) + V \sum_{\langle xy \rangle} \left( n_x - \frac{1}{2} \right) \left( n_y - \frac{1}{2} \right) + J \sum_{\langle xy \rangle} \left( \mathbf{S}_x \cdot \mathbf{S}_y - \frac{1}{4} \right) - \sum_x h_x \left( n_x - \frac{1}{2} \right) S_x^1 $$

(14)

This time we treat the spin piece $H_{b0}$ as an interaction piece. We call it $H_{b\text{int}}$.

The new $H_{\text{int}}$ is $H_{\text{int}} = H_{f\text{int}} + H_{b\text{int}} + H_{fb\text{int}}$. (15)
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(14)

- This time we treat the spin piece \( H_0^b \) as an interaction piece. We call it \( H_{\text{int}}^b \).

- The new \( H_{\text{int}} \) is

\[ H_{\text{int}} = H_{\text{int}}^f + H_{\text{int}}^b + H_{\text{int}}^{fb}. \]  

(15)
How does $H^b_{\text{int}}$ affect the spin space?

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

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

At the infinitesimal level, we get for $e^{-\epsilon H^b_{\text{int}}}$:

$$(\uparrow\downarrow, \downarrow\uparrow) = (1 + \epsilon J/2) (0 1 1 0) \tag{17}$$

Therefore, every time the Hamiltonian flips a nearest neighbor spin pair, the overall matrix element takes on an extra minus sign.
How does $H_{\text{int}}^b$ affect the spin space?

For two nearest neighbors, $x$ and $y$, using the basis states $(↑↑, ↑↓, ↓↑, ↓↓)$, we have

$$H_{\text{int,xy}}^b = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -J/2 & J/2 & 0 \\ 0 & J/2 & -J/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$ (16)
Antiferromagnetic Heisenburg Model

- How does $H_{\text{int}}^b$ affect the spin space?
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- At the infinitesimal level, we get for $e^{-\epsilon H}$: $(\uparrow\downarrow, \downarrow\uparrow)$

$$\left(1 + \frac{\epsilon J}{2}\right) I - \frac{\epsilon J}{2} \begin{pmatrix}
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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 $H_{\text{int}}^{fb}$ insertions

Contribution to $\langle \downarrow \uparrow \uparrow \downarrow \downarrow \uparrow | e^{-(\beta - t_6)H_0^b} S_6^1 e^{-(t_6 - t_5)H_0^b} S_3^1 e^{-(t_5 - t_4)H_0^b} S_5^1 \times e^{-(t_4 - t_3)H_0^b} S_1^1 e^{-(t_3 - t_2)H_0^b} S_4^1 e^{-(t_2 - t_1)H_0^b} S_1^1 e^{-t_1 H_0^b} | \downarrow \uparrow \uparrow \downarrow \downarrow \uparrow \rangle$

- Now our insertions can hop before being annihilated.
Worldline Approach: With $H^b_{\text{int}}$ insertions

Contribution to $\langle \downarrow \uparrow \uparrow \downarrow \downarrow \uparrow | e^{-(\beta-t_6)H^b_0} S^1_6 e^{-(t_6-t_5)H^b_0} S^1_3 e^{-(t_5-t_4)H^b_0} S^1_5 \times e^{-(t_4-t_3)H^b_0} S^1_1 e^{-(t_3-t_2)H^b_0} S^1_4 e^{-(t_2-t_1)H^b_0} S^1_1 e^{-t_1 H^b_0} | \downarrow \uparrow \uparrow \downarrow \downarrow \uparrow \rangle$

- 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.
Model 2: The Heisenburg Antiferromagnet

- What does this do for the overall sign?

\[ \sum_{x} h_{x} \eta_{x} \left( n_{x} - \frac{1}{2} \right) S_{1x}. \] (18)

The antiferromagnet coupled with fermions has no sign problem in the CT -INT expansion.
What does this do for the overall sign?

If we have an odd-even (even-odd) pair of \((n_x - 1/2) S_x^1\) insertions, we get an extra negative sign from the bosonic sector.
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Thus again it is as if we are inserting: (unitary transformations can show this explicitly)

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The antiferromagnet coupled with fermions has no sign problem in the CT-INT expansion.
We can extend these ideas to gauge theories. A simple example:

\[
H = -t \left( \sum_{\langle xy \rangle} c_x^\dagger \sigma^3_{xy} c_y + c_y^\dagger \sigma^3_{xy} c_x \right) - h \sum_{\langle xy \rangle} \sigma^1_{xy} \\
+ \sum_{\text{plaquettes}} \sigma^3_a \sigma^3_b \sigma^3_c \sigma^3_d
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\]

Here, \( H_0^{fb} \) is the free part, coming from the covariant derivative.
Model 3: \(\mathbb{Z}_2\) Gauge Theory

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

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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
\]

[19]

- \(H_{\text{int}}^b\) is a field in the \(x\)-direction.
We can extend these ideas to gauge theories. A simple example:

\[ H = -t \left( \sum \langle xy \rangle c_x^\dagger \sigma_3^{xy} c_y + c_y^\dagger \sigma_3^{xy} c_x \right) - h \sum \langle xy \rangle \sigma_1^{xy} \]

\[ + \sum \text{plaquettes} \quad \sigma_a^3 \sigma_b^3 \sigma_c^3 \sigma_d^3 \]

\[ H^p \] is a sum over plaquettes.
Model 3: $\mathbb{Z}_2$ Gauge Theory

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$$+ \sum_{\text{plaquettes}} \sigma_3^a \sigma_3^b \sigma_3^c \sigma_3^d$$

- Invariant under $G_x^\dagger c_x G_x = -c_x$, $G_x^\dagger \sigma_1^{x_n} G_x \rightarrow = \sigma_1^{x_n}$, and $G_x^\dagger \sigma_3^{x_n} G_x = -\sigma_3^{x_n}$, where $G_x = \sigma_1^{x_1} \sigma_1^{x_2} \sigma_1^{x_3} \sigma_1^{x_4} \eta_x (2n_x - 1)$.
Model 3: $\mathbb{Z}_2$ Gauge Theory

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

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

- 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.**

Suir Gazit,1 Mohit Randeria,2 and Ashvin Vishwanath1,3

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

\[
Z = \sum_{\{k\}} (-1)^k \text{Tr} \left( \hat{P} e^{-\left(\beta-t_1\right)H_0} H_{\text{int}} e^{-\left(t_1-t_2\right)H_0} H_{\text{int}} \ldots H_{\text{int}} e^{-t_k H_0} \right)
\]

\[
= \sum_{\{k\}} (-1)^k \text{Tr} \left( \hat{P} e^{-\left(\beta-t_1\right)\left(H^{f}_{b}+H^{p}\right)} H^{b}_{\text{int}} \ldots H^{b}_{\text{int}} e^{-t_k \left(H^{f}_{b}+H^{p}\right)} \right)
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\end{equation}

\begin{equation}
= \sum_{\{k\}} (-1)^k \text{Tr} \left( \hat{P} e^{-(\beta - t_1) \left( H_{0b}^b + H^p \right)} H_{\text{int}}^b \ldots H_{\text{int}}^b e^{-t_k \left( H_{0b}^b + H^p \right)} \right)
\end{equation}

Now we cannot factor into separate fermionic and spin factors, but we can use $z$-basis to replace spin operators with numbers.
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$$= \sum_{\{k\},\{s\}} (-1)^k \text{Tr}_f \left( \hat{P}_f e^{-(\beta - t_1)H_0^f(s_1)} \cdots e^{-t_k H_0^f(s_k)} \right)$$

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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).
Conclusions

- We can now solve a variety of models involving interacting fermions and spins using the CT-INT formalism (in continuous or discrete time).
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- The $CT\text{-}INT$ formalism also plays well with other techniques, such as the Meron Cluster method.
Conclusions

- We can now solve a variety of models involving interacting fermions and spins using the CT-INT formalism (in continuous or discrete time).
- 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.