Title: Simulation of Fermionic and Frustrated Systems with 2D Tensor Networks

Date: Oct 24, 2011  10:00 AM

URL: http://pirsa.org/11100084

Abstract: The study of fermionic and frustrated systems in two dimensions is one of the biggest challenges in condensed matter physics. Among the most promising tools to simulate these systems are 2D tensor networks, including projected entangled-pair states (PEPS) and the 2D multi-scale entanglement renormalization ansatz (MERA), which have been generalized to fermionic systems recently.

In the first part of this talk I will present a simple formalism how to include fermionic statistics into 2D tensor networks. The second part covers recent simulation results showing that infinite PEPS (iPEPS) can compete with the best known variational methods. In particular, for the t-J model and the SU(4) Heisenberg model iPEPS yields better variational energies than obtained in previous variational- and fixed-node Monte Carlo studies. Future perspectives and open problems are discussed.
Simulation of fermionic and frustrated lattice models with 2D tensor networks

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Motivation: Strongly correlated quantum many-body systems

- High-temperature superconductivity
- Fractional QH Effect
- Quantum magnetism / spin liquids
Motivation: Strongly correlated quantum many-body systems

High-temperature superconductivity

Fractional QH Effect

Quantum magnetism / spin liquids

Challenging!
Quantum Monte Carlo

Main idea: **Statistical sampling** of
the exponentially large configuration space

☑️ **Very powerful!**
Strongly correlated fermionic systems

**2D Hubbard model**

\[ \hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \]

- Hopping between nearest-neighbor sites
- On-site repulsion between electrons with opposite spin
Strongly correlated fermionic systems

2D Hubbard model

\[ \hat{H} = -t \sum_{\langle i, j \rangle, \sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \]

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Is it the relevant model of high-temperature superconductors?
Strongly correlated fermionic systems

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Is it the relevant model of high-temperature superconductors?

Methods to study strongly correlated fermions in 2D

- Exact diagonalization of small systems
- Density matrix renormalization group (small 2D systems / ladders)
- Variational approaches
- (Cluster) dynamical mean field theory
- Fixed-node Monte Carlo
- Diagrammatic Monte Carlo
- Gaussian Monte Carlo
- ... and more ...
Strongly correlated fermionic systems

2D Hubbard model

\[ \hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \hat{c}_{i \sigma}^{\dagger} \hat{c}_{j \sigma} + U \sum_{i} \hat{n}_{i \uparrow} \hat{n}_{i \downarrow} \]

- Hopping between nearest-neighbor sites
- On-site repulsion between electrons with opposite spin

Is it the relevant model of high-temperature superconductors?

⇒ Still controversial!!
Overview: tensor networks in 1D and 2D

**1D**

MPS
Matrix-product state

1 2 3 4 5 6 7 8

Related to the famous density-matrix renormalization group (DMRG) method
Overview: tensor networks in 1D and 2D

**1D MPS**
Matrix-product state

Related to the famous density-matrix renormalization group (DMRG) method

**1D MERA**
Multi-scale entanglement renormalization ansatz

*and more*
- 1D tree tensor network
- ...

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*Pirsa: 11100084*
Overview: tensor networks in 1D and 2D

1D

**MPS**
Matrix-product state

Related to the famous density-matrix renormalization group (DMRG) method

ID MERA
Multi-scale entanglement renormalization ansatz

and more
- 1D tree tensor network
- ...

2D

**(i)PEPS**
(infinite) projected entangled-pair state

2D MERA

and more
- 2D tree tensor network
- String-bond states
- Entangled-plaquette states
- ...

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Fermions with 2D tensor networks

Simulate fermions in 2D?
Fermions with 2D tensor networks

Simulate fermions in 2D?

Before April 2009: NO!

Since April 2009: YES!

Different formulations:

P. Corboz and G. Vidal, Phys. Rev. B 80, 165129 (2009)
P. Corboz, R. Orus, B. Bauer, G. Vidal, PRB 81, 165104 (2010)
Summary: Tensor network algorithms

2D MERA

1D MERA

MPS

PEPS

Structure (ansatz)
Summary: Tensor network algorithms

Structure (ansatz)

Find the best (ground) state $|\tilde{\Psi}\rangle$

- Iterative optimization of individual tensors (energy minimization)
- Imaginary time evolution

2D MERA

1D MERA

MPS

PEPS
Summary: Tensor network algorithms

- 2D MERA
- MPS
- PEPS

Structure (ansatz)

Find the best (ground) state $|\tilde{\Psi}\rangle$

- Iterative optimization of individual tensors (energy minimization)
- Imaginary time evolution

Compute observables $\langle \tilde{\Psi} | O | \tilde{\Psi} \rangle$

- Contraction of the tensor network exact / approximate
Outline

- Motivation

- **Part I:** Fermionic tensor networks
  - Formalism to take fermionic statistics in 2D tensor networks into account!

- **Part II:** Benchmark results (exactly solvable model)
  - Accuracy depends on the amount of entanglement in the system

- **Part III:** Recent studies with iPEPS
  - Infinite PEPS can compete with the best known variational methods
  - t-J model: stripes
  - SU(4) Heisenberg model: new prediction for the ground state

- Summary
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  - Infinite PEPS can compete with the best known variational methods
  - t-J model: *stripes*
  - SU(4) Heisenberg model: *new prediction for the ground state*

- Summary
Crossings in 2D tensor networks
Crossings in 2D tensor networks

Example network of the 2D MERA

$\langle \Psi | \Psi^+ \rangle$
\[ \Psi_B(x_1, x_2) = \Psi_B(x_2, x_1) \]

Symmetric!

\[ \Psi_F(x_1, x_2) = -\Psi_F(x_2, x_1) \]

Antisymmetric!
Bosons vs Fermions

\[ \Psi_B(x_1, x_2) = \Psi_B(x_2, x_1) \]

\textit{symmetric!}

\[ \Psi_F(x_1, x_2) = -\Psi_F(x_2, x_1) \]

\textit{antisymmetric!}
\[ \Psi_B(x_1, x_2) = \Psi_B(x_2, x_1) \]

\text{symmetric!}

\[ \hat{b}_i \hat{b}_j = \hat{b}_j \hat{b}_i \]

\text{operators commute}

\[ \Psi_F(x_1, x_2) = -\Psi_F(x_2, x_1) \]

\text{antisymmetric!}

\[ \hat{c}_i \hat{c}_j = -\hat{c}_j \hat{c}_i \]

\text{operators anticommutate}
Bosons vs Fermions

\[ \Psi_B(x_1, x_2) = \Psi_B(x_2, x_1) \]

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operators anticommute
Bosons vs Fermions

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antisymmetric!

\[ \hat{c}_i \hat{c}_j = -\hat{c}_j \hat{c}_i \]
operators anticommutate

Crossings in a tensor network

ignore crossings

+ 

take care!
The swap tensor

# Fermions

even  even  odd  even  even  odd  odd  odd  → Parity

RULE:

+  +  +  −
The swap tensor

RULE:

Parity $P$ of a state:

\[
\begin{align*}
P &= +1 & \text{ (even parity), even number of particles} \\
P &= -1 & \text{ (odd parity), odd number of particles}
\end{align*}
\]
The swap tensor

# Fermions

even  even  odd  even  even  odd  odd  odd  ← Parity

RULE:

Parity $P$ of a state:

$$P = +1 \quad \text{(even parity), even number of particles}$$

$$P = -1 \quad \text{(odd parity), odd number of particles}$$

Replace crossing by swap tensor

$$B_{j_2,j_1}^{i_1,i_2} = \delta_{i_1,j_1} \delta_{i_2,j_2} S(P(i_1), P(i_2))$$

$$S(P(i_1), P(i_2)) = \begin{cases} 
-1 & \text{if } P(i_1) = P(i_2) = -1 \\
+1 & \text{otherwise}
\end{cases}$$
Parity symmetry

- Fermionic systems exhibit **parity symmetry**! \[ [\hat{H}, \hat{P}] = 0 \]

- Choose all tensors to be **parity preserving**!

\[ T_{i_1i_2...i_M} = 0 \quad \text{if} \quad P(i_1)P(i_2)...P(i_M) \neq 1 \]
Parity symmetry

- Fermionic systems exhibit **parity symmetry**! \([\hat{H}, \hat{P}] = 0\)

- Choose all tensors to be **parity preserving**!

\[ T_{i_1 i_2 \ldots i_M} = 0 \quad \text{if} \quad P(i_1)P(i_2)\ldots P(i_M) \neq 1 \]

- Decomposing local Hilbert spaces into even and odd parity sectors

\[ \mathbb{V} = \mathbb{V}^+ \oplus \mathbb{V}^- \]

- Label state by a composite index

\[ i = (p, \alpha_p) \]

⇒ tensor with a block structure (similar to a block diagonal matrix)
⇒ Easy identification of the parity of a state!
Example

Bosonic tensor network
Example

Bosonic tensor network

Fermionic tensor network

EASY!!!
Fermionic “operator networks”

State of 4 site system \( |\Psi\rangle = \sum_{i_1 i_2 i_3 i_4} \Psi_{i_1 i_2 i_3 i_4} |i_1 i_2 i_3 i_4\rangle \)

\{ |0\rangle, |1\rangle \}
Fermionic “operator networks”

State of 4 site system

\[ |\Psi\rangle = \sum_{i_1i_2i_3i_4} \Psi_{i_1i_2i_3i_4} |i_1i_2i_3i_4\rangle \]

\{ |0\rangle, |1\rangle \}

Bosons

Tensor

\[ \Psi_{i_1i_2i_3i_4} \]

\[ i_1 \quad i_2 \quad i_3 \quad i_4 \]

Bosonic tensor network

\[ D_{j_1j_2} \]

\[ A_{j_1}^{i_1i_2} \]

\[ i_1 \quad i_2 \]

\[ j_1 \]

\[ B_{j_2}^{i_3i_4} \]

\[ i_3 \quad i_4 \]

\[ j_2 \]

Contract
Fermionic “operator networks”

State of 4 site system \[ |\Psi\rangle = \sum_{i_1i_2i_3i_4} \Psi_{i_1i_2i_3i_4} |i_1i_2i_3i_4\rangle \]

\[\{0,1\}\]

\[A = A^{j_1}_{i_1i_2} |i_1i_2\rangle \langle j_1| = A^{j_1}_{i_1i_2} \hat{c}^{\dagger i_1}_1 \hat{c}^{\dagger i_2}_2 |0\rangle \langle 0| \hat{c}^{j_1}_1\]

Contract + operator calculus
Fermionic “operator network”

Use anticommutation rules to evaluate fermionic operator network:
Fermionic “operator network”

Use anticommutation rules to evaluate fermionic operator network:

Easy solution: Map it to a tensor network by replacing crossings by swap tensors
Cost of fermionic tensor networks??

First thought:
Many crossings $\rightarrow$ many more tensors
$\rightarrow$ larger computational cost??
The “jump” move
The “jump” move

- Jumps over tensors leave the tensor network **invariant**
- Follows form parity preserving tensors

$$[\hat{T}, \hat{c}_k] = 0, \quad \text{if } k \notin \text{sup}[\hat{T}]$$
The “jump” move

- Jumps over tensors leave the tensor network invariant
- Follows form parity preserving tensors

\[ [\hat{T}, \hat{c}_k] = 0, \quad \text{if } k \notin \text{sup}[\hat{T}] \]

- Allows us to simplify the tensor network
- Final cost is the same as in a bosonic tensor network
Example of the “jump” move
Example of the “jump” move

now
contract as usual!
Fermionic (i)PEPS

\[ \langle \Psi | \hat{\Psi} \rangle \rightarrow \hat{\Psi} \]
Fermionic (i)PEPS

\[ \langle \Psi | \hat{\Psi} \rangle \]
Fermionic (i)PEPS

\[ \langle \Psi | \Phi \rangle \]

\[ \Psi \]

\[ \Psi^\dagger \]

Diagram showing the transition from one state to another in a fermionic PEPS representation.
Fermionic (i)PEPS

\[ |\Psi\rangle |\Psi^+\rangle \rightarrow \rightarrow \rightarrow \]

\[\equiv\]

\[\downarrow\]
Fermionic (i)PEPS

\( |\Psi^\dagger\Psi\rangle \)
Fermionic (i)PEPS

$\langle \Omega | \Omega \rangle$

$\Psi$

$\Psi^+$

- Fermionic character taken into account **locally!**

- **No** crossings left!
Summary Part 1:

→ Simulate fermionic systems with 2D tensor networks
Computational cost

- Leading cost: $O(D^k)$
**Computational cost**

- Leading cost: $O(D^k)$
  - MPS: $k = 3$
  - PEPS: $k \approx 10 \ldots 12$
  - 2D MERA: $k = 16$

- How large does $D$ have to be?

> It depends on the amount of entanglement in the system!

**MERA**

**(i)PEPS**

Bond dimension $D$
The $t$-$J$ model is given by:

$$H_{t,J} = -t \sum_{\langle ij \rangle} \tilde{c}_{i \sigma}^{\dagger} \tilde{c}_{j \sigma} + H.c. + J \sum_{\langle ij \rangle} (S_i S_j - \frac{1}{4} n_i n_j)$$

**constraint:** only one electron per site!
The **t-J model** is described by the Hamiltonian:

\[
H_{t-J} = -t \sum_{\langle ij \rangle \sigma} \tilde{c}_{i\sigma}^\dagger \tilde{c}_{j\sigma} + H.c. + J \sum_{\langle ij \rangle} (S_i S_j - \frac{1}{4} n_i n_j)
\]

- **Nearest-neighbor hopping**
- **Antiferro interaction**

**Constraint:** only one electron per site!
Evidence for stripe correlations of spins and holes in copper oxide superconductors

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One of the long-standing mysteries associated with the high-temperature copper oxide superconductors concerns the anomalous suppression of certain superconducting properties. Here we present evidence from neutron diffraction that in the compound La$_{1.6-x}$Nd$_x$Sr$_x$CuO$_4$, with $x=0.12$, a static analogue of the dynamical stripe phase is present, and is associated with an anomalous suppression of superconductivity. Our results thus provide an explanation for the "50%" conundrum, and also support the suggestion that spatial modulations of spin and charge density are related to superconductivity in the copper oxides.

constraint: only one electron per site!

Does it reproduce "striped" states observed in some cuprates?
**t-J model**

\[
H_{t-J} = -t \sum_{\langle ij \rangle \sigma} \tilde{c}_{i \sigma}^\dagger \tilde{c}_{j \sigma} + H.c. + J \sum_{\langle ij \rangle} (S_i S_j - \frac{1}{4} n_i n_j)
\]

**constraint:** only one electron per site!

- Nearest-neighbor hopping
- Antiferro interaction

Does it reproduce “striped” states observed in some cuprates?

**DMRG (wide ladders):** YES!

**Variational Monte Carlo**

**Fixed-node Monte Carlo:** NO!
**t-J model: iPEPS results**

- **Comparison with:** M. Lugas, L. Spanu, F. Becca, S. Sorella. PRB 74, 165122 (2006)
  - variational Monte Carlo (VMC) (Gutzwiller projected wavefunctions)
  - state-of-the-art fixed node Monte Carlo (FNMC)

![Graph showing energy per hole versus delta for J/t = 0.4](image)

- **Equation:** 
  
  \[ E_{\text{hole}} = \text{function of } \delta \text{ for } J/t = 0.4 \]

- **Legend:**
  - VMC
  - FNMC
  - iPEPS D=8 2x2 unit cell

Corboz, White, Vidal, Troyer, arXiv:1104.5463
  - variational Monte Carlo (VMC) (Gutzwiller projected wavefunctions)
  - state-of-the-art fixed node Monte Carlo (FNMC)

**t-J model: iPEPS results**

\[ J/t = 0.4 \]

**iPEPS with 2x2 unit cell**

- $E_{\text{hole}}$ vs. $\delta$
- $J/t = 0.4$
- VMC
- FNMC
- iPEPS D=8 2x2 unit cell

Diagram showing the energy per hole ($E_{\text{hole}}$) as a function of the parameter $\delta$ for different methods and unit cells.
**t-j model: iPEPS results**

  - variational Monte Carlo (VMC) (Gutzwiller projected wavefunctions)
  - state-of-the-art fixed node Monte Carlo (FNMC)

\[ J/t = 0.4 \]

\[ E_{\text{hole}} \]

**iPEPS:** lower (better) variational energy: **stripes!**
  - variational Monte Carlo (VMC) (Gutzwiller projected wavefunctions)
  - state-of-the-art fixed node Monte Carlo (FNMC)

Large hole density

AF order

DMRG, 18x10, cylindric BC, m=5000

iPEPS: lower (better) variational energy: stripes!
SU(N) Heisenberg models (square lattice)

- $N=2$: $H = \sum_{\langle i,j \rangle} S_i S_j$

local basis states: $|\uparrow\rangle, |\downarrow\rangle$

Néel order
SU(N) Heisenberg models (square lattice)

• N=2: \[ H = \sum_{\langle i,j \rangle} P_{ij} \]

local basis states: \[ |\downarrow\rangle, |\uparrow\rangle \]

Néel order

• N=3

• N=4

Ground state??
Two-orbital $SU(N)$ magnetism with ultracold alkaline-earth atoms

A. V. Gorshkov$^1$, M. Hermele$^2$, V. Gurarie$^2$, C. Xu$^1$, P. S. Julienne$^3$, J. Ye$^4$, P. Zoller$^{5,6}$, E. Demler$^{1,7}$, M. D. Lukin$^{1,7}$ and A. M. Rey$^4$

$^{87}Sr$: $I = 9/2 \rightarrow N_{max} = 2I + 1 = 10$

- $N=3$
- $N=4$

Ground state??
SU(2): Comparison with Quantum Monte Carlo

Energy:  
QMC (extrap.): $-0.669437(5)J$  
iPEPS (D=10): $-0.66939J$  

rel. error $< 10^{-4}$

A. Sandvik, PRB56, 11678 (1997)
SU(2): Comparison with Quantum Monte Carlo

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  rel. error $< 10^{-4}$

**QMC study:** Sandvik & Evertz, PRB82, 024407 (2010): system sizes up to 256x256

![Graph of staggered magnetization vs 1/L]

- $m = 0.30743(1)$
- strong finite size effects
- accurate extrapolation
**SU(2): Comparison with Quantum Monte Carlo**

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**QMC study:** Sandvik & Evertz, PRB82, 024407 (2010): system sizes up to 256x256

- **strong finite size effects**
  \[ m = 0.30743(1) \]
  accurate extrapolation

- **strong finite D effects**

\[ \text{linear fits} \]
\[ \text{quadratic fits} \]
SU(N) Heisenberg models (square lattice)

• \( N=2 \): \[ H = \sum_{\langle i,j \rangle} P_{ij} \]

local basis states: \( | \bullet \rangle, | \circ \rangle \)

• \( N=3 \)

• \( N=4 \)

Néel order

Cannot use QMC because of the sign problem!!!
SU(N) Heisenberg models (square lattice)

- $N=2$: $H = \sum_{\langle i,j \rangle} P_{ij}$
  - Local basis states: $|\cdot\rangle$, $|\circ\rangle$
  - Néel order

- $N=3$
  - 3 sub-lattice
  - Néel order

- $N=4$
  - ED & flavor-wave theory (Toth et al.)
  - iPEPS & DMRG (Bauer et al.)
SU(4) Heisenberg model: iPEPS results

Corboz, Läuchli, Mila, Penc, Troyer, arXiv:1108.2857
SU(4) Heisenberg model: iPEPS results

Corboz, Läuchli, Mila, Penc, Troyer, arXiv:1108.2857

![Graph showing energy vs. inverse aspect ratio](image)

- 2x2 unit cell
- 4x2 u.c.
- 4x4 u.c.
- VMC

Spin-orbital liquid
Wang & Vishwanath '09

"Dimer-Néel" order

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SU(4): Study as a function of bond dimension

- Infinite ground state degeneracy

Plaquette state

\(D = 1\)
Product state (mean-field)

\(D = 2\)
Add quantum fluctuations on top of product state; same solution as linear flavor-wave theory
SU(4): Study as a function of bond dimension

- Infinite ground state degeneracy
- Plaquette state
- Dimer-Néel ordered state

- Studying extrapolations of the data for $D=5-16$ suggests that state is stable

- $D=1$ product state (mean-field)
- $D=2$ add quantum fluctuations on top of product state same solution as linear flavor-wave theory
- $D=5$ largest $D$ tested in this study

Increase quantum fluctuations / increase entanglement
Summary: tensor networks in 2D

- Variational ansatz with no (little) bias & controllable accuracy for bosonic/spin and fermionic systems

Recent progress with iPEPS: competitive method!

- t-J model: striped state with better variational energy than variational and fixed-node Monte Carlo
- SU(4) Heisenberg: New type of ground state (Dimer-Néel ordered)
Summary: tensor networks in 2D

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Open problems:
- Quantities not converged (yet) in the bond dimension D. Extrapolation?
- High computational cost
Summary: tensor networks in 2D

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Open problems:
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- High computational cost

Ways to improve the efficiency:
- Combine with Monte Carlo sampling (Schuch et al., Sandvik&Vidal, Wang et al.)
- Exploit symmetries of a model (Singh et al., Bauer et al.)
- Improve optimization/contraction schemes (Pizorn et al., Vidal et al.)