Fermionic tensor networks

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P. Corboz, G. Evenbly, F. Verstraete, G. Vidal, PRA 81, 010303(R) (2010)
P. Corboz, G. Vidal, Phys. Rev. B 80, 165129 (2009)
P. Corboz, R. Orus, B. Bauer, G. Vidal. PRB 81, 165104 (2010)
Attack the sign problem

\[ \text{cost} \sim \exp \left( \frac{N}{k_B T} \right) \]
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
- ...

2D

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

2D MERA

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

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Fermions in 2D & tensor networks

Simulate fermions in 2D?

Before April 2009: **NO!**

Since April 2009: **YES!**

C. V. Kraus, N. Schuch, F. Verstraete, J. I. Cirac, arXiv:0904.4667
P. Corboz, G. Vidal, Phys. Rev. B 80, 165129 (2009)
T. Barthel, C. Pineda, J. Eisert, PRA 80, 042333 (2009)
P. Corboz, R. Orus, B. Bauer, G. Vidal, PRB 81, 165104 (2010)
...

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Outline

- Short introduction to tensor networks
  - Idea: efficient representation of quantum many-body states
  - Examples: Tree Tensor Network, MERA, MPS, PEPS

- Fermionic systems in 2D & tensor networks
  - Simple rules
  - Computational cost compared to bosonic systems

- Results (iPEPS) & comparison with other methods
  - Free and interacting spinless fermions
  - t-J model

- Summary: What’s the status?
Tensor networks: Efficient representation of QMB states

\[ |\Psi\rangle = \sum \Psi_{i_1 i_2 i_3 i_4 i_5 i_6} |i_1 \otimes i_2 \otimes i_3 \otimes i_4 \otimes i_5 \otimes i_6\rangle \]

6 site system

Why is this possible??
Tree Tensor Network (1D)
The MERA \textbf{(The Multi-scale Entanglement Renormalization Ansatz)}


\[
\chi = d
\]

\[
\chi_0 = d
\]

\begin{itemize}
  \item \textbf{KEY:} Disentanglers reduce the amount of short-range entanglement
  \item \textbf{Efficient ansatz} for critical and non-critical systems in 1D
\end{itemize}

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2D MERA (top view)

Original lattice → Apply disentanglers → Apply isometries

Accounts for area-law in 2D systems

\[ S(L) \sim L \]

\[ \chi_\tau = \text{const} \]

Evenbly, Vidal. PRL 102, 180406 (2009)
2D MERA represented as a 1D MERA

Typical network

Crossing lines play an important role for fermions!
MPS & PEPS

**1D**

**MPS**
Matrix-product state  
*(Related to DMRG)*

![Diagram of 1D MPS](image)

Physical indices (lattices sites)

S. R. White, PRL 69, 2863 (1992)
Fannes et al., CMP 144, 443 (1992)
Östlund, Rommer, PRL 75, 3537 (1995)

✓ Reproduces area-law in 1D  
\[ S(L) = \text{const} \]

**2D**

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

![Diagram of 2D PEPS](image)

F. Verstraete, J. I. Cirac, cond-mat/0407066

✓ Reproduces area-law in 2D  
\[ S(L) \sim L \]
Summary: Tensor network algorithms

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
Bosons vs Fermions

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

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

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

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

Crossings in a tensor network ignore crossings take care!

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The swap tensor

# Fermions

Even Even Odd Even Even Odd Odd

Parity $P$ of a state:

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

Replace crossing by swap tensor

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

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

Use parity preserving tensors:

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

Bosonic tensor network

Fermionic tensor network

EASY!!!
Fermionic “operator networks”

State of 4 site system \( |\Psi\rangle = \sum_{i_1i_2i_3i_4} \Psi_{i_1i_2i_3i_4} |i_1i_2i_3i_4\rangle \)

\( \{0\}, \{1\} \)

\( \hat{A} = A_{i_1i_2}^{j_1} |i_1i_2\rangle \langle j_1| = A_{i_1i_2}^{j_1} \hat{c}_1^\dagger \hat{c}_2^\dagger |0\rangle \langle 0| \hat{c}_1^{j_1} \)
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??

NO!

Same computational cost
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

now contract as usual!

absorb

absorb
Message:

- Taking fermionic statistics into account is easy!
- Replace crossings by swap tensors & use parity preserving tensors
- Computational cost does not depend a priori on the particle statistics, but on the amount of entanglement in the system!
Computational cost

- Leading cost: $O(D^k)$
- How large does $D$ have to be?

**MPS:** $k = 3$

**PEPS:** $k \approx 10 \ldots 12$ (polynomial scaling but large exponent!)

**2D MERA:** $k = 16$

It depends on the amount of entanglement in the system!

Bond dimension: $D$
Classification by entanglement

**Entanglement**

- **low**
  - gapped systems
    - band insulators,
      - valence-bond crystals,
      - s-wave superconductors,
      - ... 
    - Heisenberg model,
      - p-wave superconductors,
      - Dirac Fermions,
      - ...

- **high**
  - gapless systems
    - systems with “1D fermi surface”
      - free Fermions, Fermi-liquid type phases, bose-metals?

\[ S(L) \sim L \log L \]
Overview: Results / benchmarks

- Free spinless fermions
  - Finite systems (MERA, TTN)
  - Finite systems (PEPS)
  - Infinite systems (iPEPS)
    - Corboz, Evenbly, Verstraete, Vidal, PRA 81, 010303(R) (2010),
    - Corboz, Vidal, PRB 80, 165129 (2009)
    - Pineda, Barthel, Eisert, arXiv:0905.0669
    - Kraus, Schuch, Verstraete, Cirac, arXiv:0904.4667
    - Pizorn, Verstraete. arXiv:1003.2743

- Interacting spinless fermions
  - Finite systems (MERA, TTN)
  - Finite systems (PEPS)
  - Phase diagram of t-V model (iPEPS)
    - Corboz, Orus, Bauer, Vidal, PRB 81, 165104 (2010)
    - Shi, Li, Zhao, Zhou, arXiv:0907.5520

- t-J model
  - Benchmark (iPEPS)
  - Phase diagram (iPEPS)
Non-interacting spinless fermions: infinite systems (iPEPS)

\[ H_{\text{free}} = \sum_{\langle rs \rangle} [c_r^c c_s + c_s^c c_r - \gamma (c_r^c c_s^c + c_s c_r)] - 2\lambda \sum_r c_r^r c_r \]

Li et al., PRB 74, 073103 (2006)

Fast convergence with D in gapped phases

Slow convergence in phase with 1D Fermi surface
Correlators

\[ C(\vec{r}) = \langle c_{\vec{r}_0}^{\dagger} c_{\vec{r}_0 + \vec{r}} \rangle \]
Phase diagram of interacting spinless fermions (iPEPS)

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

iPEPS vs Hartree-Fock

Corboz, Orus, Bauer, Vidal. PRB 81, 165104 (2010)

Phase boundary moves away from HF result with increasing D

qualitative agreement
iPEPS vs Hartree-Fock

D=4 result ~ HF result

D=6: lower (better) energies in the metal phase

Corboz, Orus, Bauer, Vidal. PRB 81, 165104 (2010)
Adding a next-nearest neighbor hopping

\[ \hat{H} = -t \sum_{\langle i,j \rangle} \left[ \hat{c}^\dagger_i \hat{c}_j + H.c. \right] - \mu \sum_i \hat{c}^\dagger_i \hat{c}_i + V \sum_{\langle i,j \rangle} \hat{c}^\dagger_i \hat{c}_i \hat{c}^\dagger_j \hat{c}_j - t' \sum_{\langle\langle i,j \rangle\rangle} \left[ \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + H.c. \right] \]


\[ V = 2 \quad t' = -0.4 \]

Is there a stable doped CDW phase beyond Hartree-Fock?

**NO**... (at least not for these parameters)
Adding a next-nearest neighbor hopping

Corboz, Jordan, Vidal, arXiv:1008:3937

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![Graph showing the relationship between $E_s$ and $\mu$ for different systems, with markers indicating various densities and wave numbers. The graph highlights the doped CDW region.](image)

- HF metal
- HF CDW
- D=4 metal
- D=4 CDW
- D=6 metal
- D=6 CDW
- D=8 metal
- D=8 CDW

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Adding a next-nearest neighbor hopping

Corboz, Jordan, Vidal, arXiv:1008:3937

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**t-t’-J model**

\[ H_{t-J} = -t \sum_{\langle ij \rangle \sigma} \tilde{c}_{i \sigma}^\dagger \tilde{c}_{j \sigma} - t' \sum_{\langle \langle ij \rangle \rangle \sigma} \tilde{c}_{i \sigma}^\dagger \tilde{c}_{j \sigma} + J \sum_{\langle ij \rangle} (S_i S_j - \frac{1}{4} n_i n_j) - \mu \sum_i n_i \]

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

**How about striped phases??**

- need larger unit cell!!

**D=8 results in between VMC and FNMC**

Corboz, Jordan, Vidal, arXiv:1008:3937

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Summary: status

YES, we have the holy grail! We can now solve everything!

This is useless! $D^{12}$ scaling is as bad as exponential!
Summary: status

✓ Variational ansatz with no (little) bias & controllable accuracy. Accuracy depends on the amount of entanglement in the system

✓ Accurate results for gapped systems

✓ Competitive compared to other variational wave functions

✓ Systematic improvement upon mean-field solution

- For which bond dimension is it converged?
- Limited accuracy for gapless systems
- no L log L scaling
- High computational cost

› 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