Simulation of strongly correlated systems in 2D with iPEPS

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam

PC, F. Mila, PRL 112, 147203 (2014)
PC, T. M. Rice, and M. Troyer, PRL 113, 046402 (2014)
Outline

- iPEPS ansatz
- Benchmarks: Heisenberg model

- iPEPS can outperform state-of-the-art variational Monte Carlo methods
  - t-J model: Extreme competition between uniform and stripe states
  - Hubbard model: Benchmark comparisons with other methods

- Discover new physics thanks to (largely) unbiased simulations
  - Shastry-Sutherland model: Breakthrough in the understanding of the magnetization process in SrCu$_2$(BO$_3$)$_2$

- Conclusion
MPS & PEPS

1D MPS
Matrix-product state

Physical indices (lattices sites)

2D Snake MPS

Computational cost:
$\propto \exp(L)$

Bond dimension $D$
**MPS & PEPS**

**1D**
Matrix-product state

**2D**
Projected entangled-pair state

Bond dimension \( D \)

Verstraete and Cirac, cond-mat/0407066
Infinite PEPS (iPEPS)

**1D**

IMPS

infinite matrix-product state

**2D**

iPEPS

infinite projected entangled-pair state

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Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)

★ Work directly in the thermodynamic limit:

**No finite size and boundary effects!**
iPEPS with arbitrary unit cells

**1D**

**iMPS**

infinite matrix-product state

**2D**

**iPEPS**

with arbitrary unit cell of tensors

here: 4x2 unit cell

Corboz, White, Vidal, Troyer, PRB 84 (2011)

★ Run simulations with different unit cell sizes and compare variational energies
Benchmark $S=1/2$ Heisenberg model

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

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

Accuracy checks:
- Sandvik & Evertz, PRB 82 (2010)

Graphical representation:
- Staggered magnetization
  - QMC from $M_s^2$
  - QMC from $C(L/2,L/2)$
  - QMC extrapolation

- Strong finite size effects
- Strong finite $D$ effects
- Accurate extrapolation
- How to extrapolate?

A. Sandvik, PRB 56 (1997)
**t-J model**

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

- Nearest-neighbor hopping
- Heisenberg interaction

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

\[ J/t = 0.4 \]

Does it reproduce the stripe states observed in some of the cuprates?

**DMRG (cylinders)**: **YES!**

**Variational Monte Carlo**

**Fixed-node Monte Carlo** **NO!**

\[ \Rightarrow \text{uniform } d\text{-wave state!} \]

- White & Scalapino, PRL 80 (1998)
- White & Scalapino, PRB 60 (1999)
- Hu, Becca & Sorella, PRB 85 (2012)
- ... and more ...
Uniform d-wave SC state (+AF order)

\[ J/t = 0.4 \]

- \( \delta_i \) hole density
- \( m_i \) magnetic moment
- \( \Delta_{ij} \) nearest-neighbor singlet pairing amplitude

★ Finite d-wave pairing for any finite doping
★ Coexisting with AF order for \( \delta \lesssim 0.1 \)
★ In agreement with previous studies
  [Himeda et al. '02, Ogata et al. '03, Ivanov '04, Shih et al. '04, Lugas et al. '06, Spanu et al. '08, Hu '12]
★ Lower energy than best VMC result, e.g.
  -1.578t (D=14 iPEPS) vs
  -1.546t (FNMC+2L), for \( \delta = 0.12 \)
Vertical stripe state

iPEPS result 5x2 cell

- $\delta_i$
- $m_i$
- $\Delta_{ij}$

★ Modulation in the hole-density, AF and SC order
★ “Site-centered” stripe (not bond-centered)
★ $\pi$-phase shift in the AF order
★ Preferred stripe width depends on doping
  (width-5 stripe lowest around $\delta = 0.12$)
Diagonal stripe states

★ Insulating with a filling of 1 hole per unit length per stripe
★ Competing state, but higher in energy for large D
uniform d-wave vs stripe
Uniform vs stripe state

\[ J/t = 0.4 \quad \delta = 0.12 \]

States are still competing at very low energies!

★ Close to a phase transition?
★ Small additional terms (material dependent) may stabilize one of the two states
★ May explain why stripes are found only in certain cuprates

VMC+fixed node for N=162
Lugas et al., PRB 74 (2006)

VMC+FN+2 Lanczos steps, for N=162
Hu et al. PRB 85 (2012)
Outlook: beyond simple $t$-$J$

**Next:** Go beyond the simple $t$-$J$ model towards more realistic models:

- Include longer range interactions / hoppings
- Single-band Hubbard model
- Multi-band Hubbard model
- Study of additional ingredients, e.g. coupled CuO planes, disorder, ...

★ Effect on the competing phases?
★ Other low-energy states in more realistic models?
★ Effect on superconductivity? Enhancing? Suppressing?

- **Systematic study** will help to get a better understanding of the various competing phases in the cuprates
Hubbard model: results $U/t=10$ (unpublished)

**Half-filled case (n=1):**
- Relative error in the TL: $O(0.05\%)$ (D=14 without extrapolation!)
- QMC estimate by S. Sorella (unpublished)

**Doped case:**
- Similar competition as in $t$-$J$ model!
- Lower than best FNMC data [Tocchio&Becca&Sorella, unpublished]
- can still be further improved (using larger D & extrapolation)
Benchmark comparison Hubbard model $U/t=8$, $n=1$

(preliminary results)

**Figure from LeBlanc, et al., arXiv:1505.02290**

**Double occupancy:**
- **iPEPS (D=16)**
  - without extrapolation: 0.0539
  - extrapolated AFQMC result (exact): -0.5247 +/- 0.0002
The Shastry-Sutherland model

\[ \hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\text{dimer}}} S_i \cdot S_j \]

SrCu$_2$(BO$_3$)$_2$

Spin-gap system (~35K)


Kageyama et al. PRL 82 (1999)

C carries S=1/2

same lattice!
The Shastry-Sutherland model

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\( \hat{H} \) carries \( S=1/2 \)

\( \mathbf{C} \) carries \( S=1/2 \)

SrCu\(_2\)(BO\(_3\))\(_2\) Spin-gap system (~35K)

Kageyama et al. PRL 82 (1999)

Dimer phase

Néel phase

helical?

columnar-dimer?

plaquette?

spin-liquid?

...
The Shastry-Sutherland model

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**SrCu$_2$(BO$_3$)$_2$**
Spin-gap system (~35K)

"C carries S=1/2"

previously found in:
- Koga and Kawakami, PRL 84 (2000)
- Takushima et al., JPSJ 70 (2001)
- Chung et al., PRB 64 (2001)
- Läuchli et al., PRB 66 (2002)

\[ \hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\text{dimer}}} S_i \cdot S_j \]

Dimer phase
Plaquette phase
Néel phase

Corboz and Mila, PRB 87 (2013)
Magnetization plateaus

SrCu$_2$(BO$_3$)$_2$ in a magnetic field exhibits several magnetization plateaus

The SSM has almost localized triplet excitations [Miyahara & Ueda’99, Kageyama et al. ’00]

Triplets repel each other (on the mean-field level)

Intuition: The magnetization plateaus corresponds to crystals of localized triplets! (Mott insulators)

Crystals of localized triplets
Magnetization plateaus

- Many experiments and theoretical works over the last 15 years
- Experiments: $1/8, 2/15, 1/6, 1/4, 1/3, 1/2$
- Theory: $1/9, 2/15, 1/6, 1/4, 1/3, 1/2$
- What about the $1/8$ plateau?
- Complicated structures for the $2/15$ plateau...
- Big puzzle for many years...

★ Ideal problem for iPEPS: simulating large unit cell embedded in infinite system and compare variational energies of the proposed crystals
BUT!

SURPRISE!
The assumption that plateaus correspond to crystals of triplets is wrong! (for the plateaus below 1/4)

- Crystals of bound states instead of crystals of triplets??

Bound state of two triplets!
Example: 1/8 plateau

- All the proposed triplet crystals have a higher energy than the crystals made of bound states!
- Similar results found for other plateaus below 1/4

\[
J'/J = 0.63
\]
2/15 plateau

Unit cell with 30 tensors (60 sites)
Sizable plateaus found at: 1/8, 2/15, 1/6, 1/5, 1/4, 1/3, 1/2
[1/5 plateau vanishes upon adding a small (but realistic) DM interaction]

Sequence in agreement with experiments

New understanding of the magnetization process in SrCu$_2$(BO$_3$)$_2$

- see also related work: SSM in high fields: Matsuda et al. PRL 111 (2013)
**SU(N) Heisenberg models**

**SU(3) square/triangular:**
*3-sublattice Néel order*
Bauer, PC, et al., PRB 85 (2012)

**SU(3) honeycomb:**
*Plaquette state*
PC, Läuchli, Penc, Mila, PRB 87 (2013)

**SU(3) kagome:**
*Simplex solid state*
PC, Penc, Mila, Läuchli, PRB 86 (2012)

**SU(4) square:**
*Dimer-Néel order*
PC, Läuchli, Penc, Troyer, Mila, PRL 107 (‘11)

**SU(4) honeycomb:**
*spin-orbital (4-color) liquid*
PC, Lajkó, Läuchli, Penc, Mila, PRX 2 (‘12)

**3-color quantum Potts:**
*superfluid phases*
Messio, PC, Mila, PRB 88 (2013)
Conclusion

✓ **2D TN** algorithms are challenging, but a lot of recent progress
  ★ iPEPS can outperform state-of-the-art variational methods
  ★ New insights into the competing uniform and stripe states in the \( t-J \) model
  ★ Breakthrough in understanding the magnetization process in \( \text{SrCu}_2(\text{BO}_3)_2 \)

✓ Big room for improvement (e.g. better optimization/contraction schemes, ...)
✓ Many possible extensions (e.g. finite \( T \), excitations, real-time evolution, ...)

One of the most promising routes to solve challenging open problems in 2D

Thank you for your attention!