



Simulating 2d systems with PEPS

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From MPS to PEPS



Matrix Product States (MPS)

1d systems

But we want to go beyond 1d systems!!!





Very painful for DMRG...





PEPS are not your friends... (M. Lubasch)

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MPS



PEPS are not your friends... (M. Lubasch)



PEPS (initially)





PEPS are not your friends... (M. Lubasch)



MPS











...but, after a lot of gymnastics, they can be your allies!





Two exact examples

An exact example: Kitaev's Toric Code



$$H = -J\sum_{s} A_{s} - J\sum_{p} B_{p}$$

$$A_s = \prod_{i \in s} \sigma_i^x$$
 star operator

 $B_p = \prod_{i \in p} \sigma_i^z$ plaquette operator



Simplest known model with "topological order"

Ground state (and in fact all eigenstates) are PEPS with D=2



Resonating Valence Bond State

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Equal superposition of all possible nearest-neighbor singlet coverings of a lattice (spin liquid)

Proposed to understand high-T_C superconductivity





PEPS...



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



and infinite PEPS (iPEPS)



assuming translation invariance

J. Jordan, RO, G. Vidal, F. Verstraete, I. Cirac, Phys. Rev. Lett. 101, 250602 (2008)



PEPS obey 2d area-law















$$\begin{split} \rho_{in} &= \operatorname{tr}_{out} \left(\left| \Psi \right\rangle \left\langle \Psi \right| \right) = \sum_{\overline{\alpha}, \overline{\alpha}'} X_{\overline{\alpha}, \overline{\alpha}'} \left| in(\overline{\alpha}) \right\rangle \left\langle in(\overline{\alpha}') \right| \qquad X_{\overline{\alpha}, \overline{\alpha}'} = \left\langle out(\overline{\alpha}') \right| out(\overline{\alpha}) \right\rangle \\ rank(\rho_{in}) &\leq D^{4L} \qquad S(L) = -\operatorname{tr} \left(\rho_{in} \log \rho_{in} \right) \leq \log(D) 4L \end{split}$$





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Critical correlation functions



F. Verstraete et al, PRL 96, 220601 (2006)

$$|\Psi(\beta)\rangle = \frac{1}{\sqrt{Z(\beta)}} \exp\left(\frac{\beta}{2} \sum_{\langle i,j \rangle} \sigma_z^i \sigma_z^j\right)|+,+...+\rangle$$

Expectation values are those of the classical 2d Ising model

$$\left[\sigma_{z}^{r}\sigma_{z}^{r'}\right]_{\beta} = \frac{1}{Z(\beta)}\sum_{\{s\}} s^{r}s^{r'}\exp\left(\beta\sum_{\langle i,j\rangle}s^{i}s^{j}\right) \quad s = \pm 1$$

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Expectation values are those of the classical 2d Ising model

$$\left\langle \sigma_z^r \sigma_z^{r'} \right\rangle_{\beta} = \frac{1}{Z(\beta)} \sum_{\{s\}} s^r s^{r'} \exp\left(\beta \sum_{\langle i,j \rangle} s^i s^j\right) \quad s = \pm 1$$

It is a PEPS with D=2 (left as exercise):

$$\frac{1}{|+\rangle} \frac{1}{1} = \left(\cosh(\beta/2)\right)^4 \qquad \frac{1}{|-\rangle} \frac{1}{1} = \left(\cosh(\beta/2)\right)^3 \left(\sinh(\beta/2)\right)$$

$$\frac{1}{|+\rangle} \frac{1}{1} = \left(\cosh(\beta/2)\right)^2 \left(\sinh(\beta/2)\right)^2 \qquad \frac{2}{|-\rangle} \frac{1}{1} = \left(\cosh(\beta/2)\right) \left(\sinh(\beta/2)\right)^3$$

$$\frac{2}{|+\rangle} \frac{2}{2} = \left(\sinh(\beta/2)\right)^4 \qquad + \text{permutations}$$

At $\beta_c = \left(\log(1+\sqrt{2})\right)/2$ the correlation length is infinite: $\left\langle \sigma_z^r \sigma_z^{r'} \right\rangle_{\beta_c} \approx \frac{a}{|r-r'|^{1/2}}$

PEPS to/from Hamiltonians

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Comparison



	MPS in 1d 	PEPS in 2d	MERA in 1d
Ent. entropy	S(L) = O(1)	S(L) = O(L)	$S(L) = O(\log L)$
Exact contraction	efficient	inefficient	efficient
Corr. length	finite	finite & infinite	finite & infinite
To/from	1d Ham.	2d Ham.	1d Ham.
Tensors	arbitrary	arbitrary	constrained







PEPS as ansatz: variational optimization





e.g. F. Verstraete, I. Cirac, cond-mat/0407066

Optimize over each tensor individually and sweep over the entire system (as in DMRG)





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e.g. F. Verstraete, I. Cirac, cond-mat/0407066 $\min\left(\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}\right) \qquad \text{Optimize over each tensor individually and} \\ \text{sweep over the entire system (as in DMRG)}$

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$$\frac{\partial}{\partial A^{*i}} \left(\langle \Psi | H | \Psi \rangle - \lambda \langle \Psi | \Psi \rangle \right) = 0$$

Minimization of quadratic function

Variational optimization (e.g. finite PEPS) JG e.g. F. Verstraete, I. Cirac, cond-mat/0407066 $\min\left(\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}\right) \qquad \text{Optimize over each tensor individually and} \\ \text{sweep over the entire system (as in DMRG)}$ $\frac{\partial}{\partial A^{*i}} \left(\langle \Psi | H | \Psi \rangle - \lambda \langle \Psi | \Psi \rangle \right) = 0 \quad \text{Minimization of quadratic function}$ $\mathbf{H}_{eff}^{i}\vec{A}^{i} = \lambda \mathbf{N}^{i}\vec{A}^{i}$ Generalized eigenvalue problem Once \mathbf{H}_{eff}^{i} and \mathbf{N}^{i} are known, we can solve this problem efficiently

Approximate calculation of \mathbf{H}_{eff}^{i} and \mathbf{N}^{i}

e.g. calculation of $\mathbf{N}^i \vec{A}^i$



 $\frac{\partial}{\partial A^{*i}} \left(\left\langle \Psi \middle| H \middle| \Psi \right\rangle - \lambda \left\langle \Psi \middle| \Psi \right\rangle \right) = 0 \qquad \Longrightarrow \qquad \mathbf{H}_{eff}^{i} \vec{A}^{i} = \lambda \mathbf{N}^{i} \vec{A}^{i}$























Time evolution

(real, imaginary)



e.g. J. Jordan et al, PRL 101, 250602 (2008)

Divide into small time-steps $\delta \tau << 1$

$$\left|\Psi_{0}\right\rangle = \lim_{\tau \to \infty} \frac{e^{-\tau H} \left|\Psi\right\rangle}{\left\|e^{-\tau H} \left|\Psi\right\rangle\right\|}$$





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Split the Hamiltonian (e.g. 2-body n.n.)

 $H = H_{hor}^{even} + H_{hor}^{odd} + H_{ver}^{even} + H_{ver}^{odd}$







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$$e^{-\delta\tau H} \approx e^{-\delta\tau H_{hor}^{even}} e^{-\delta\tau H_{hor}^{odd}} e^{-\delta\tau H_{ver}^{even}} e^{-\delta\tau H_{ver}^{odd}} + O(\delta\tau^2)$$

 $e^{-\delta au H_{hor}^{even}}$









Different approaches to this problem: (fast) full update, simplified update, TPVA... **Full update:** $\min \left\| \tilde{\Psi} \right\rangle - \left| \Psi' \right\rangle \right\|^2$

Finite systems: optimize over all tensors in the PEPS (as before)

Infinite systems: optimize over tensors in the PEPS unit cell (iPEPS)

Require *calculations of environments*, like the one shown before.



Environments with infinite PEPS
Infinite systems

e.g. J. Jordan et al, PRL 101, 250602 (2008) R. Orús, G. Vidal, PRB 80 094403 (2009) JGU









Let's put it on the plane of the screen!





Environment calculations



Contraction of this infinite lattice

Contracting the infinite 2d lattice

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Contracting the infinite 2d lattice





Coarse-graining approaches: TRG/SRG, HOSVD, TNR

c.f. T. Xiang's & G. Evenbly's talks



JGU **Contracting the infinite 2d lattice Renormalized Corner Transfer Matrices** Renormalization (numerical) (Baxter, 1968, 1978) 1..*x*

Directional version of the **corner transfer matrix renormalization group** (faster than 1d transfer matrix methods) T. Nishino, K. Okunishi, JPS Jpn. 65, 891 (1996)

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R. Orús, G. Vidal, PRB 80 094403 (2009), R. Orús, PRB 85, 205117 (2012)

Example: left move



R. Orús, G. Vidal, PRB 80 094403 (2009), R. Orús, PRB 85, 205117 (2012)

Example: left move







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R. Orús, G. Vidal, PRB 80 094403 (2009), R. Orús, PRB 85, 205117 (2012)

Example: left move

1) insertion

2) absorption



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R. Orús, G. Vidal, PRB 80 094403 (2009), R. Orús, PRB 85, 205117 (2012)

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Example: left move



R. Orús, G. Vidal, PRB 80 094403 (2009), R. Orús, PRB 85, 205117 (2012)

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A typical example: Toric Code in arbitrary field

S. Dusuel et al., PRL 106, 107203 (2011)

$$H = -J\sum_{s} A_{s} - J\sum_{p} B_{p} - h_{x}\sum_{i} \sigma_{i}^{x} - h_{y}\sum_{i} \sigma_{i}^{y} - h_{z}\sum_{i} \sigma_{i}^{z}$$



Phase diagram

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Fermionic 2d systems



Fermionic systems are extremely interesting physical systems, e.g. the **2d fermionic Hubbard model** may be the key to understand the emergence of **high-T_c superconductivity**

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Unfortunately, fermionic systems are also **amongst the most difficult** to simulate, because of the **sign problem in Quantum MonteCarlo** (sampling of negative probabilities)

Fermionic 2d systems



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Unfortunately, fermionic systems are also **amongst the most difficult** to simulate, because of the **sign problem in Quantum MonteCarlo** (sampling of negative probabilities)

Fermions are a NUMERICAL MONSTER

for Quantum MonteCarlo because of the sign problem!



but there is hope ...

Tensor Networks + Fermions

e.g., P. Corboz, R. Orús, B. Bauer, G. Vidal, PRB 81, 165104 (2010)





$$\Psi_B(x_1, x_2) = \Psi_B(x_2, x_1)$$

Symmetric wavefunction

 $b_i b_j = b_j b_i$

Operators commute





$$\Psi_B(x_1, x_2) = \Psi_B(x_2, x_1)$$

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$$\Psi_F(x_1, x_2) = -\Psi_F(x_2, x_1)$$

Antisymmetric wavefunction

$$C_i C_j = -C_j C_i$$

Operators anticommute







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$$\Psi_F(x_1,x_2) = -\Psi_F(x_2,x_1)$$

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Operators anticommute

Crossings in a TN







Tensor Network "fermionization" rules



Tensor Network "fermionization" rules



Use parity-preserving tensors

$$T_{i_1i_2...i_M} = 0$$
 if $P(i_1)P(i_2)...P(i_M) \neq 1$

Symmetry of the Hamiltonian

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Tensor Network "fermionization" rules

 J_2



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Use parity-preserving tensors $T_{i_1i_2...i_M} = 0$ if $P(i_1)P(i_2)...P(i_M) \neq 1$ Symmetry of the Hamiltonian

Replace crossings by fermionic swap gates $X_{i_2i_1j_1j_2} = \delta_{i_1j_1}\delta_{i_2j_2}S(P(i_1), P(i_2))$ $S(P(i_1), P(i_2)) = \begin{cases} -1 & \text{if } P(i_1) = P(i_2) = -1 \\ +1 & \text{otherwise} \end{cases}$

Fermionic operators anticommute

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Tensor Network "fermionization" rules



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Fermionic operators anticommute

The leading order of the computational cost is the same as in the bosonic case

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fermionic order ~ graphical projection of a PEPS



fermionic order ~ graphical projection of a PEPS







fermionic order ~ graphical projection of a PEPS



physics is independent of the order physics is independent of graphical projection

(different choices of Jordan-Wigner transformation, if mapping to a spin system)



Example: scalar product of 3x3 PEPS



Example: scalar product of 3x3 PEPS
























But... does it work?



But... does it work?



,,Tensor networks provide today the best variational energies for the Hubbard model in the strong coupling limit. iPEPS has really made it".

Matthias Troyer (at the Korrelationstage 2015)

J. Jordan, RO, G. Vidal, F. Verstraete, I. Cirac, PRL **101** 250602 (2008) P. Corboz, RO, B. Bauer, G. Vidal, PRB **81** 165104 (2010)

YES, it does



IGI

FIG. 4. (Color online) iPEPS energy of a period-5 stripe in the doped case in the strongly correlated regime (U/t = 8, n = 0.875) in comparison with other methods.







PEPS & Entanglement Hamiltonians

e.g. I. Cirac et al, PRB 83, 245134 (2011), N. Schuch et al, PRL 111, 090501 (2013)



















(double indices)





Boundary How is physics described here?





 Remember it has double indices...





It is also hermitian and positive by construction (up to finite- χ effects)









Particles and energies from Hamiltonians, and Hamiltonians from networks of entanglement + bulk-boundary correspondence



TNS with symmetries e.g., S. Singh, R. N. C. Pfeifer, G. Vidal, PRA 82, 050301 (2010)

c.f. M. Oshikawa's talk

Symmetric tensors and Schur's lemma

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e.g., S. Singh, R. N. C. Pfeifer, G. Vidal, PRA 82, 050301 (2010)





Structural part depends only on the group properties (intertwiners)

Emergent spin networks

e.g., S. Singh, R. N. C. Pfeifer, G. Vidal, PRA 82, 050301 (2010)



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Emergent spin networks e.g., S. Singh, R. N. C. Pfeifer, G. Vidal, PRA 82, 050301 (2010)





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And AdS/CFT and Ryu-Takayanagi and string theory and ER=EPR and cMERA and spacetime from entanglement and metrics from fidelities and wormholes and blackholes and firewalls and and and...

c.f. T. Takayanagi's talk

Emergent spin networks e.g., S. Singh, R. N. C. Pfeifer, G. Vidal, PRA 82, 050301 (2010)

 $|\Psi\rangle$



States of quantum geometry in loop quantum gravity...



And AdS/CFT and Ryu-Takayanagi and string theory and ER=EPR and cMERA and spacetime from entanglement and metrics from fidelities and wormholes and blackholes and firewalls and and and ...

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c.f. T. Takayanagi's talk

Emergent spin networks

e.g., S. Singh, R. N. C. Pfeifer, G. Vidal, PRA 82, 050301 (2010)



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Global and gauge symmetries are handled naturally

Concerning numerics: HUGE computational savings, e.g., SU(2)-DMRG

Lots of other things:



Lots of other things:



Chiral PEPS Entanglement measures Time evolution Infinite systems Classical systems **Corner Transfer Matrices** Tensor Renormalization Group Variational updates PESS Phases of matter 3d PEPS **Topological systems Excited states** Thermal states & dissipation Continuous tensor networks Tensor Networks & Montecarlo Practical implementations Blablabla...

Ask me if interested!









Thank you!



