Title: Tensor Network Algorithms for 2D Strongly Correlated Systems

Date: Dec 14, 2016 10:00 AM

URL: http://pirsa.org/16120022

Abstract: <p>In this talk I will give a short introduction into Projected Entangled-Pair States (PEPS), and their infinite variant iPEPS, a class of tensor network Ansatz targeted at the simulation of 2D strongly correlated systems. I will present work on two recent</p>

<p>projects: the first will be an application of the iPEPS algorithm to a Kitaev-Heisenberg model, a model which through-out recent years has received a lot of attention due to its potential connection to the physics of a subclass of the so-called Iridate compounds. The second will be work related to the development of the iPEPS method to specifically target cylindrical geometries. Here I will present some preliminary results where we apply the methods to the Heisenberg and Fermi-Hubbard models and evaluate their performance in comparison to infinite Matrix Product States. As a final part of my talk I will, depending on time, elaborate somewhat on potential future topics including (but not restricted to): the main challenges of iPEPS simulations from a numerical perspective and what pre-steps we have experimented with to tackle these, the possibility of applying recent proposals for finite-temperature calculations within the PEPS framework to frustrated spin systems and the use of Tensor Network Renormalization for the study of RG flows.</p>

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Tensor Network Algorithms

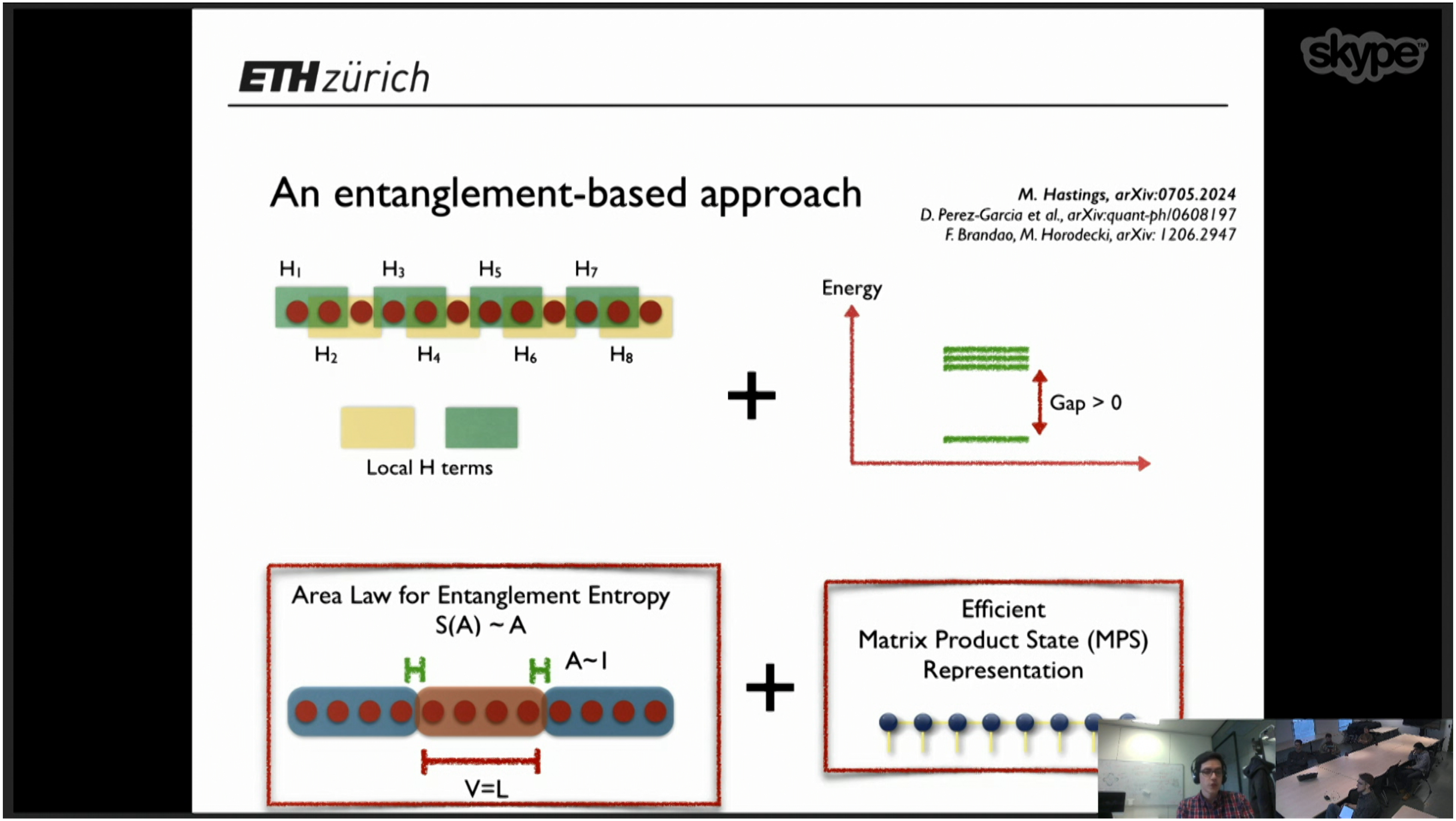
for 2D strongly correlated systems

Juan Osorio Iregui
Computational Physics Group
ETH Zürich

PhD. Advisors

Matthias Troyer
Computational Physics Group
ETH Zürich / Microsoft Research

Philippe Corboz
Institute for Theoretical Physics
University of Amsterdam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An entanglement-based approach
M. Hastings, arXiv:0705.2024
D. Perez-Garcia et al., arXiv:quant-ph/0608197
F. Brandao, M. Horodecki, arXiv: 1206.2947
H1
H3
H5
H7
H2
H4
H6
H8
Local H terms
Energy
Gap > 0
Area Law for Entanglement Entropy
S(A) ~ A
H
H
A~1
V=L
Efficient
Matrix Product State (MPS)
Representation
skype

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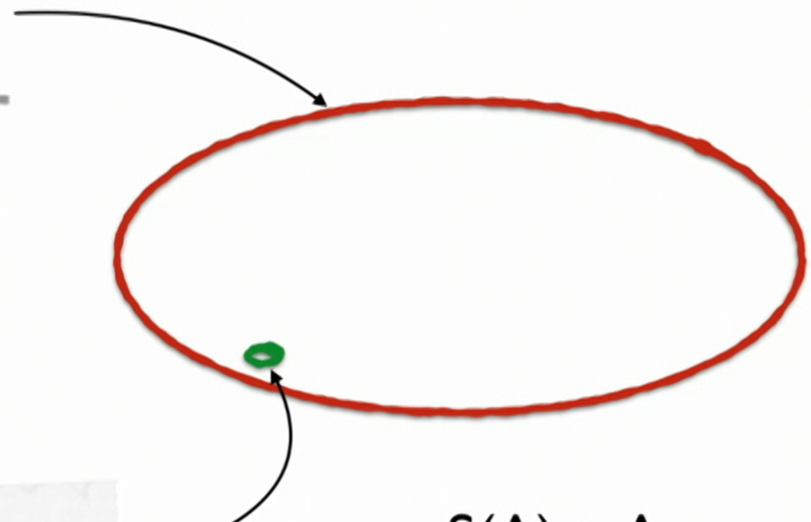
An entanglement-based approach

M. Hastings, arXiv:0705.2024
D. Perez-Garcia et al., arXiv:quant-ph/0608197
F. Brandao, M. Horodecki, arXiv: 1206.2947

Hilbert Space

$H \sim V^N$

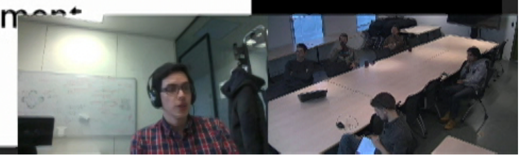
Exponential growth



low entanglement corner

$S(A) \sim A$

Area law for entanglement entropy



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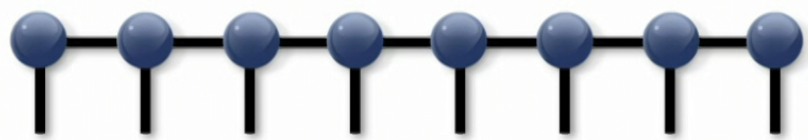
Matrix Product States (MPS)

$$\Psi = \sum_{\{\sigma\}} A_1^{\sigma_1} A_2^{\sigma_2} \dots A_N^{\sigma_N} |\sigma_1 \sigma_2 \dots \sigma_N\rangle$$



Area Law Entanglement Entropy

Efficient encoding

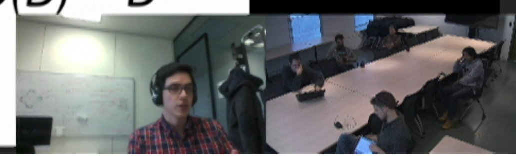
$$Dim\,[A^\sigma] = D \times D$$

Var. Parameters
ND^2

Efficient algorithm

Ops.: O(D) ~ D^3

Memory: O(D) ~ D^2



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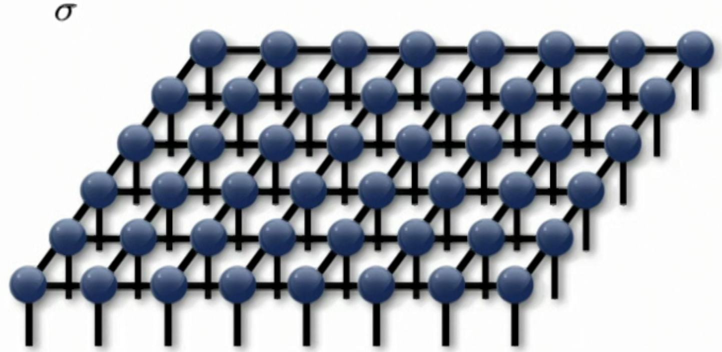
Projected Entangled-Pair States (PEPS)

$$\Psi = \sum_{\sigma} tTr(A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_N}) |\sigma_1 \sigma_2 \dots \sigma_N\rangle$$



Area Law Entanglement Entropy

Efficient encoding

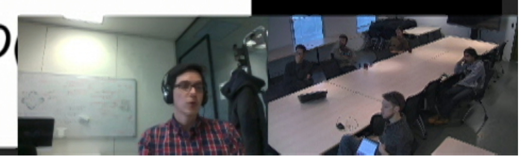
$$Dim\,[A^{\sigma}] = D \times D \times D \times D$$

Var. Parameters
ND^4

Efficient algorithm?

Ops.: O(D) ~ D^W

Memory: O(



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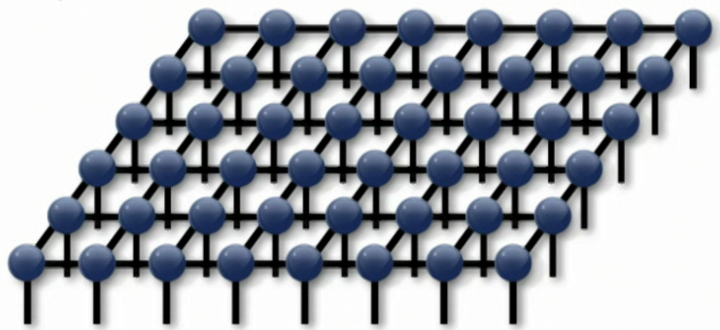
Projected Entangled-Pair States (PEPS)

$$\Psi = \sum_{\sigma} tTr(A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_N}) |\sigma_1 \sigma_2 \ldots \sigma_N\rangle$$



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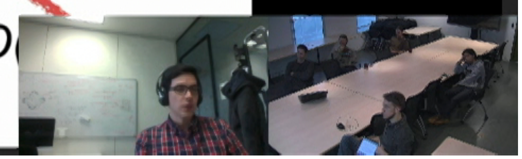
~~Efficient algorithm?~~

~~*Ops.: O(D) ~ D^W*~~

~~*Memory: O(*~~



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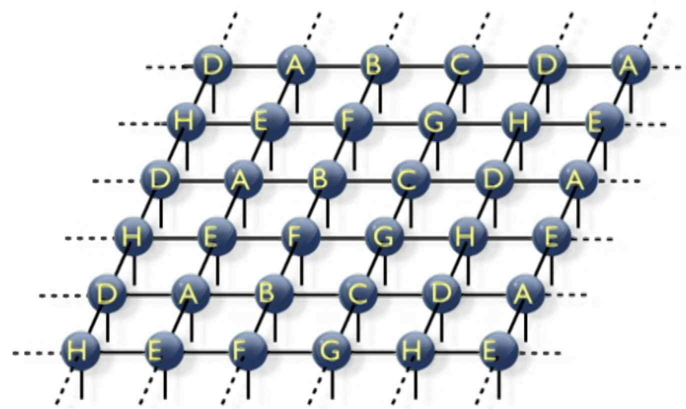
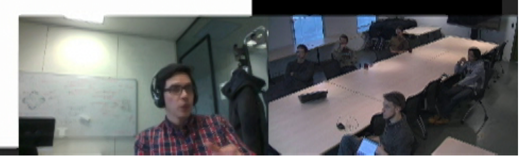
infinite Projected Entangled-Pair States (iPEPS)

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





Juan
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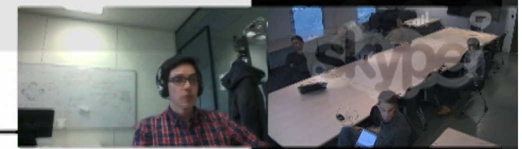

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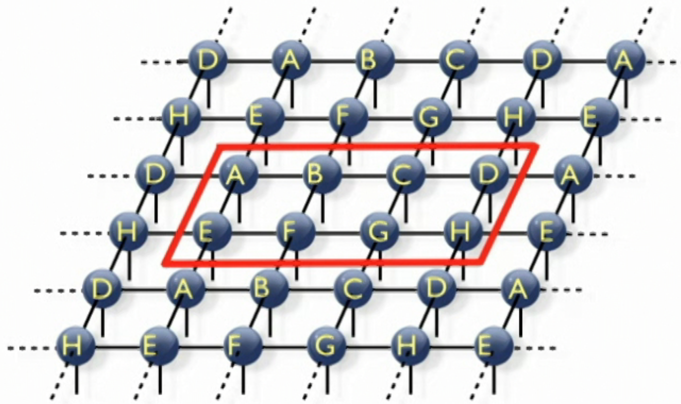

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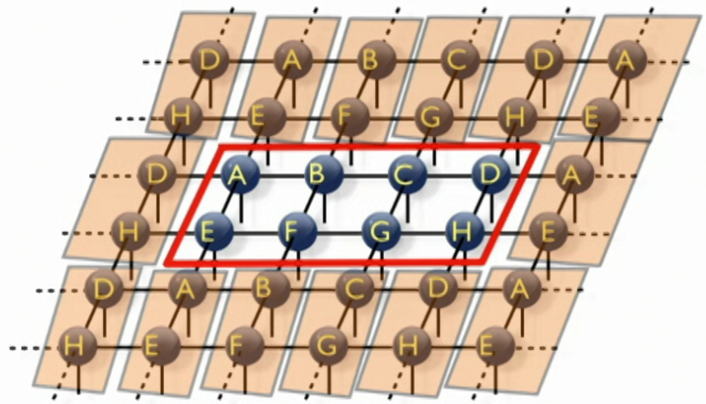

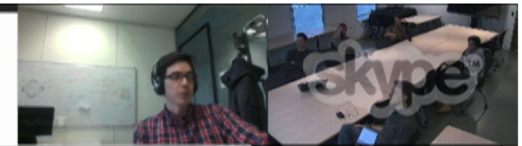

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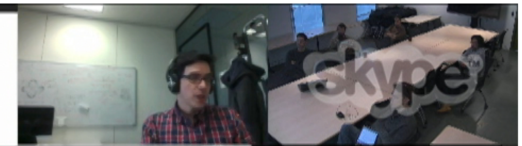

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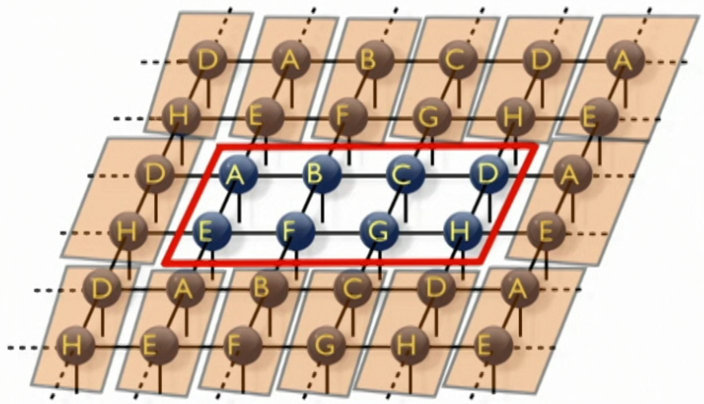

Area Law Entanglement Entropy

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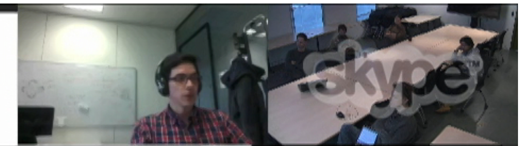

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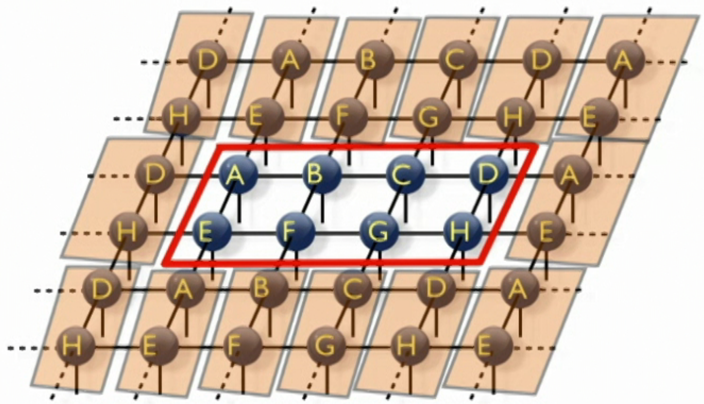
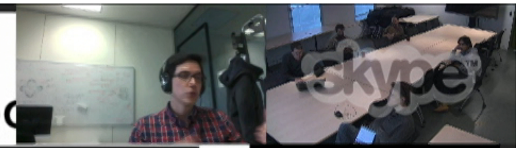


Introduce
Contraction Schemes

~~Efficient algorithm?~~

~~*Ops.: O(D) ~ D^W*~~

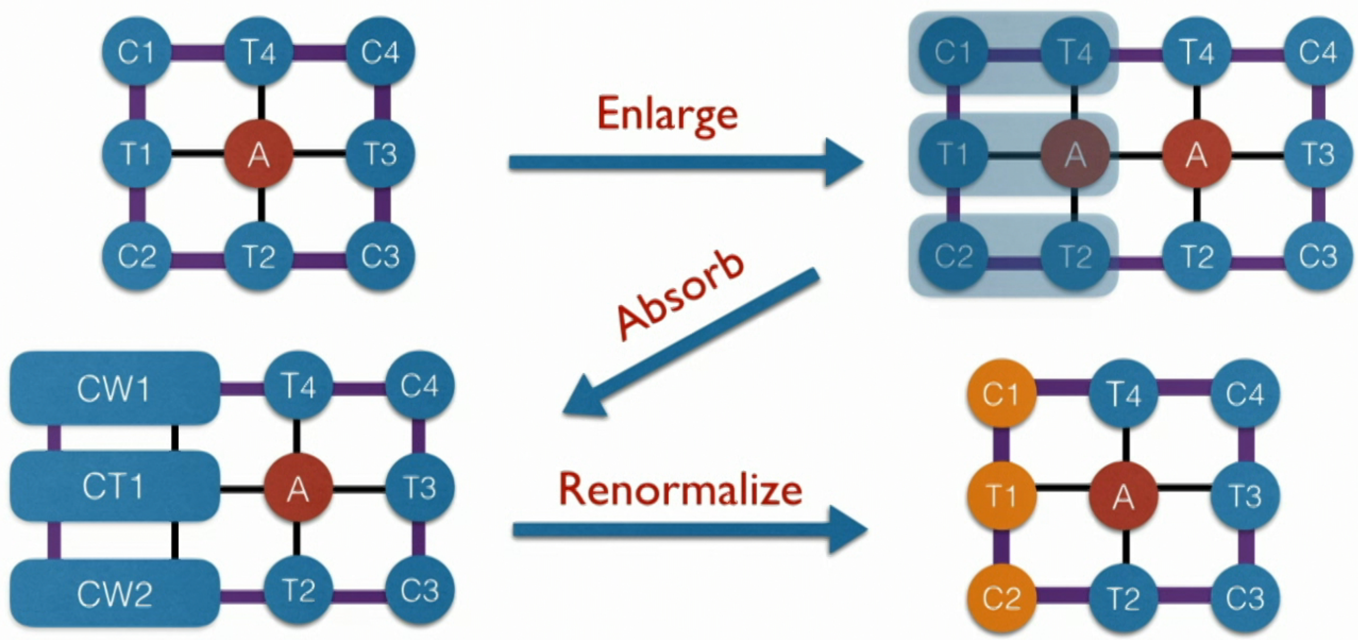
~~*Memory: O(D) ~ D^4*~~



Contraction Scheme

Nishino, Okunishi, JPSJ65 (1996)
Orus, Vidal, PRB 80 (2009)
Corboz, arXiv:1402.2859v2

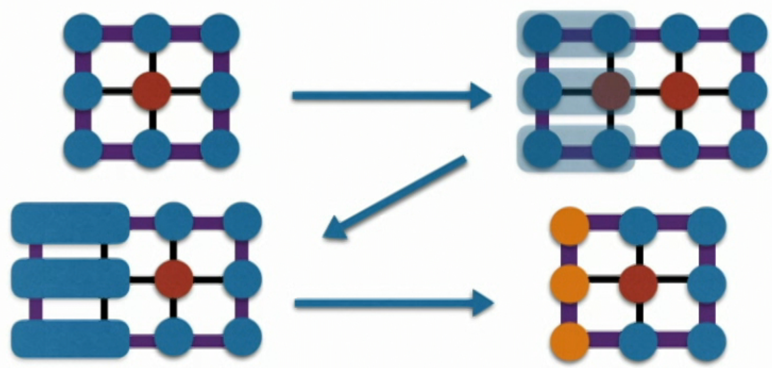
Corner Transfer Matrix (CTM)



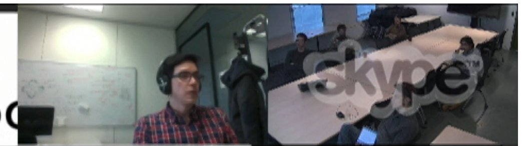
Contraction Scheme

Nishino, Okunishi, JPSJ65 (1996)
Orus, Vidal, PRB 80 (2009)
Corboz, arXiv:1402.2859v2

Corner Transfer Matrix (CTM)



Computational Cost $\sim O(X^3D^6)$ ⟵ Double Layer ⟶ Memory Cost $\sim O(X^2D^2)$



Optimization Scheme

Imaginary-Time Evolution

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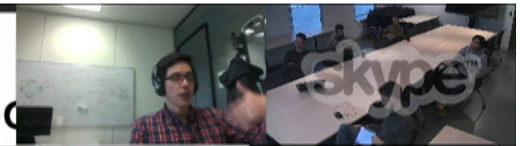
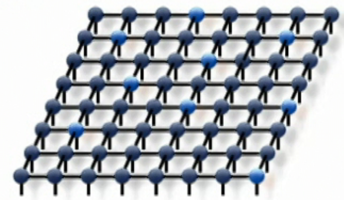
iPEPS - A short intro



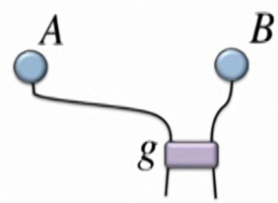
Optimization Scheme

Imaginary-Time Evolution

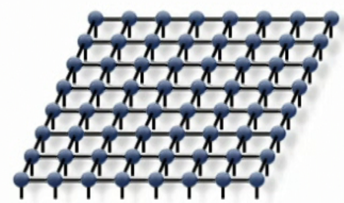
$|\psi_0\rangle$ Trial state



$$|\psi_{k+1}\rangle = \frac{\mathrm{e}^{-\tau \hat{H}}|\psi_k\rangle}{\|\mathrm{e}^{-\tau \hat{H}}|\psi_k\rangle\|}$$



$|\Psi\rangle$ Ground state



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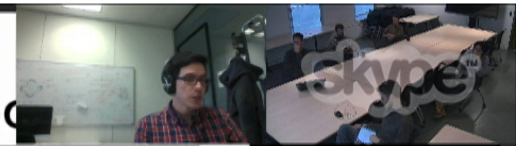
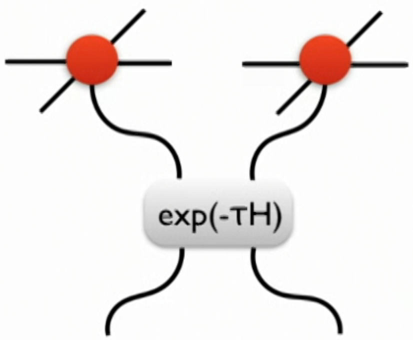
iPEPS - A short introd



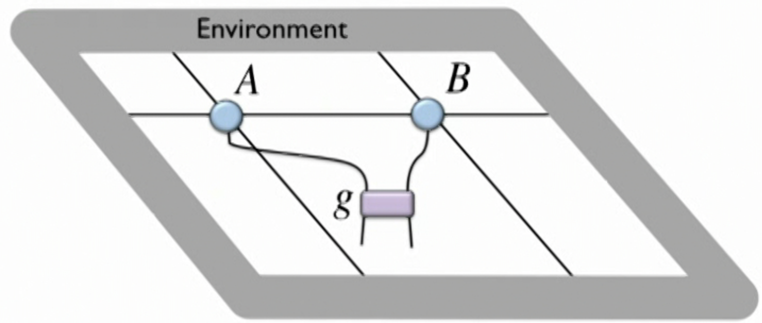
Optimization Scheme

Imaginary-Time Evolution

Simple Update



Full Update



Variational Optimization

P. Corboz, arXiv:1605.03006v1

Vanderstraeten et al., arXiv:1606.09170v2

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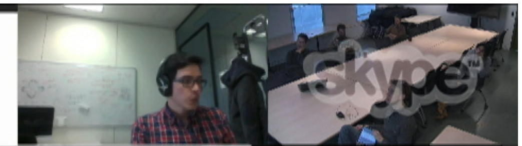

iPEPS

Kitaev-Heisenberg Model

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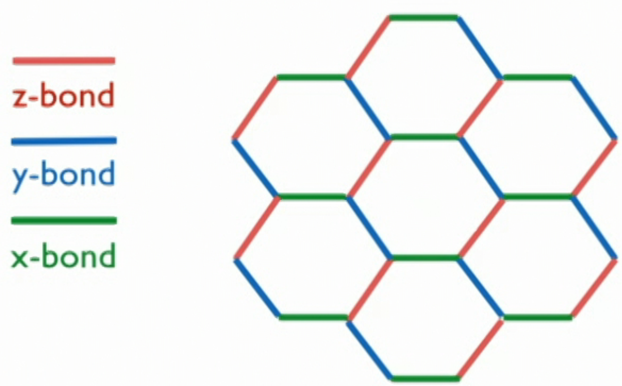
Kitaev's Honeycomb model

A. Kitaev, Annals of Physics 321 (2006).

$$H = -J_x \sum_{x\text{-links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-links}} \sigma_j^z \sigma_k^z$$



- Bond dependent Ising couplings.
- Strongly frustrated.
- Exactly soluble.
- Z_2 spin-liquid ground state

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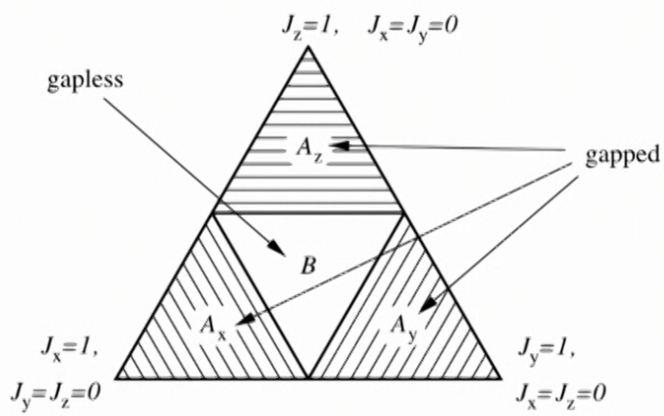
Kitaev's Honeycomb

Phase Diagram

A. Kitaev, Annals of Physics 321 (2006).

$$H = -J_x \sum_{x\text{-links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-links}} \sigma_j^z \sigma_k^z$$



Gapped (A) phase can be mapped to the toric code.

Gapless (B) phase hosts non-abelian anyonic excitations.

We expect iPEPS to perform well inside gapped (A phase) region. What about the gapless region?

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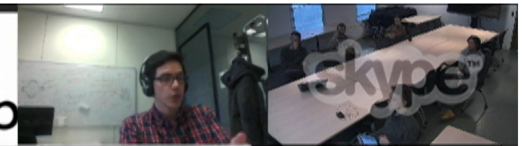
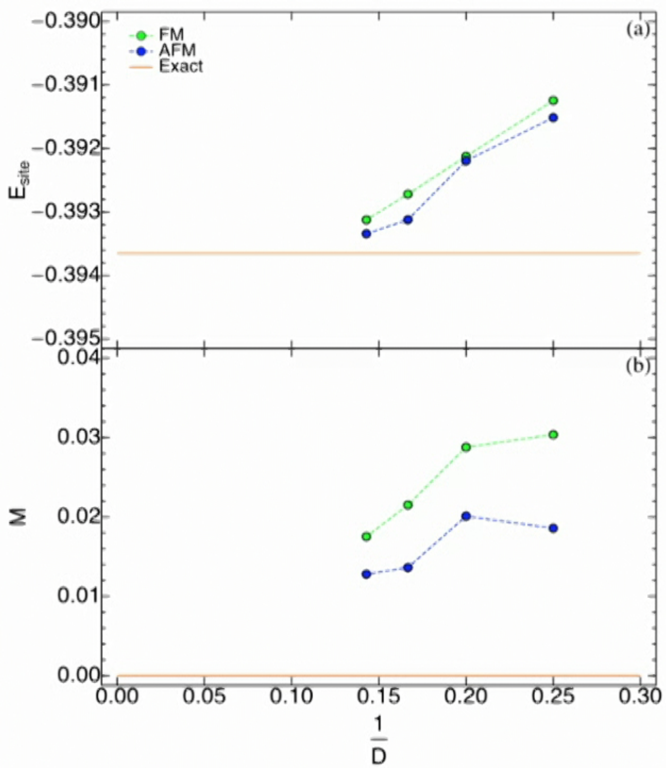
Kitaev's Honeycomb



Energy/Magnetization



- Isotropic $J_x=J_y=J_z$ point (B-phase).
- Exact energy per site: -0.3936.
- iPEPS energy:
  - D=7 (AFM): -0.3933
  - D=7 (FM): -0.3931
- Monotonic decrease with D.

- Spin liquid ground state > Zero magnetization expected.
- iPEPS results:
  - D=7 (AFM): 0.01
  - D=7 (FM): 0.02
- Monotonic decrease with D.
- Infinite D extrapolation yields vanishing magnetization.

A. Kitaev, Annals of Physics 321 (2006).
G.Baskaran, S.Mandal, R. Shankar, PRL 98 (2007).
JOI, P. Corboz, M. Troyer, arXiv:1408.4020.

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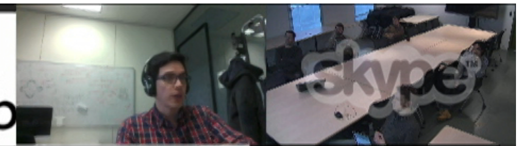
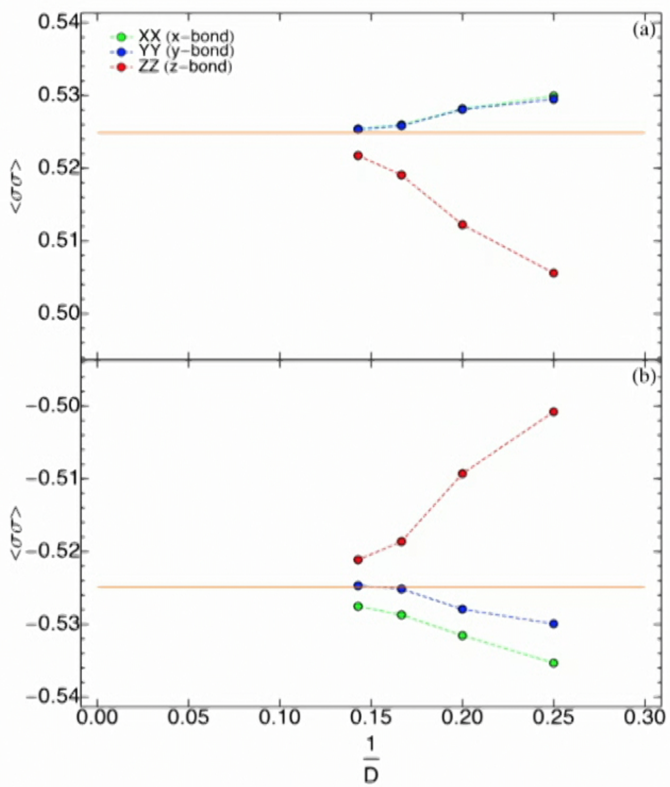
Kitaev's Honeycomb



Spin-Spin Correlations



- Only NN correlations of corresponding bond type are non-vanishing, eg.

$$\gamma(i,j) = x \rightarrow \langle \sigma_i^x \sigma_j^x \rangle = 0.525$$
$$\langle \sigma_i^y \sigma_j^y \rangle = 0$$
$$\langle \sigma_i^z \sigma_j^z \rangle = 0$$

- Data not shown < 10^{-3}.
- Systematic improvement upon increasing bond dimension.

G.Baskaran, S.Mandal, R. Shankar, PRL 98 (2007).
JOI, P. Corboz, M.Troyer, arXiv:1408.4020.

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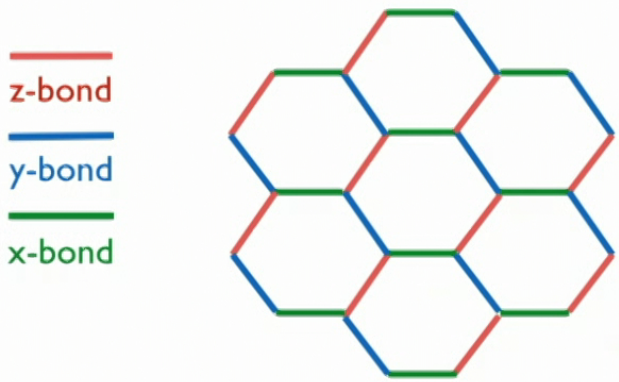
Kitaev-Heisenberg model

J. Chaloupka, G. Jackeli, G. Khaliullin, arXiv:1004.2964v2.
J. Chaloupka, G. Jackeli, G. Khaliullin, PRL 110 (2013).

$$H_{i,j}^{(\gamma)} = \cos\varphi \, \vec{S}_i \cdot \vec{S}_j + 2\sin\varphi \, S_i^{(\gamma)} S_j^{(\gamma)}$$



- Proposed by Chaloupka et al. as effective model for (layered) Iridate compounds A_2IrO_3 (A = Li,Na).
- Nearest-neighbor (pseudo-)spin interactions composed of isotropic Heisenberg + anisotropic Kitaev terms.
- Small system studies show that (zigzag) magnetic order found in Iridate compounds is natural ground state of KH model.

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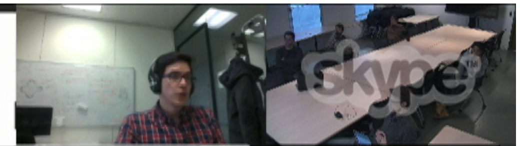

Previous Results

$$H_{i,j}^{(\gamma)} = \cos\varphi\, \vec{S}_i \cdot \vec{S}_j + 2\sin\varphi\, S_i^{(\gamma)} S_j^{(\gamma)}$$

- Type of transition observed in 4th quadrant differed for small systems vs SP Mean-Field study.
- Survival of QSL phases in TD limit remained under debate.
- Type of phase transitions from AQSL to symmetry broken not certain.

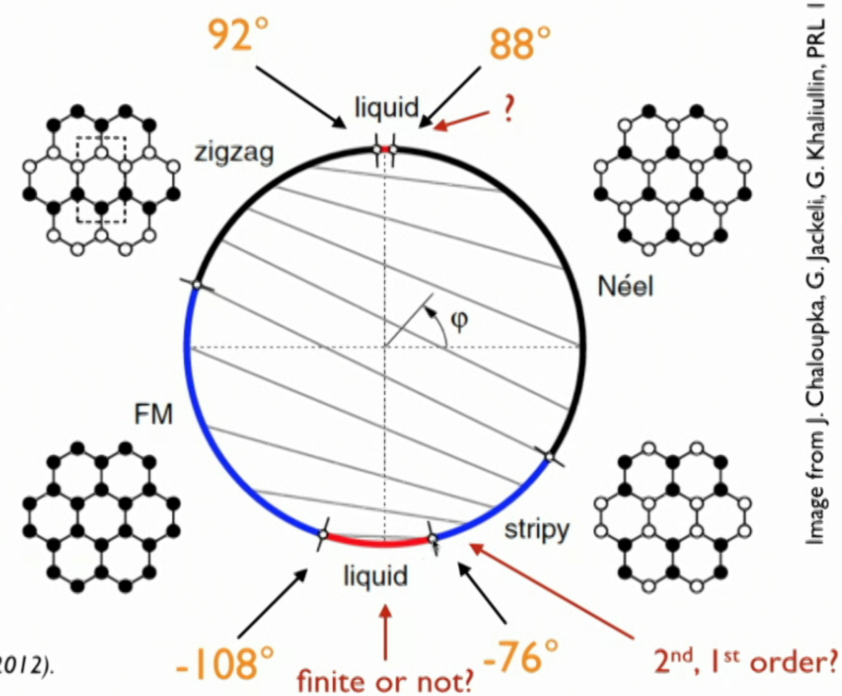

Image from J. Chaloupka, G. Jackeli, G. Khaliullin, PRL 110 (2013).

J. Chaloupka, G. Jackeli, G. Khaliullin, PRL 110 (2013).
J. Chaloupka, G. Jackeli, G. Khaliullin, arXiv:1004.2964v2.
R. Schaer, S. Bhattacharjee, and Y. B. Kim, Phys. Rev. B 86, 224417 (2012).
Jiang et al., arXiv:1101.1145v1.
Z. Wang, C. Li, Y. Han, and G. Guo, arXiv:1303.2431 (2013)

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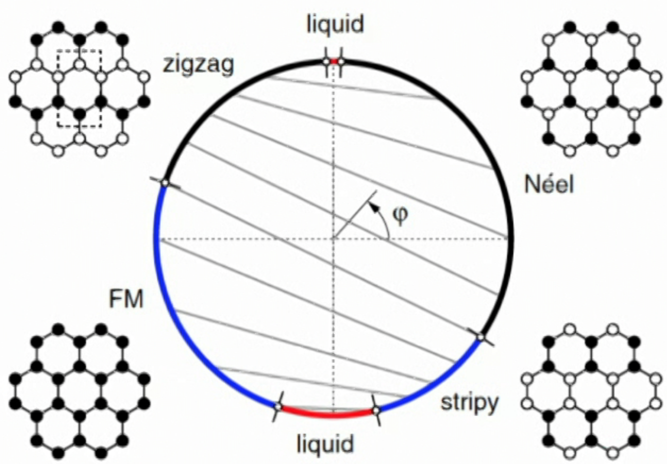
Kitaev-Heisenberg

iPEPS Approach

Energy crossing + OP analysis

JOI, P. Corboz, M. Troyer, arXiv:1408.4020.



- Perform initial runs mapping out phases arising in phase diagram.
- Find representative states deep inside each phase.
- Compare energies + OP of different phases in the vicinity of phase transitions.
- "Hysteretic" behavior will hint towards 1st order type transitions.

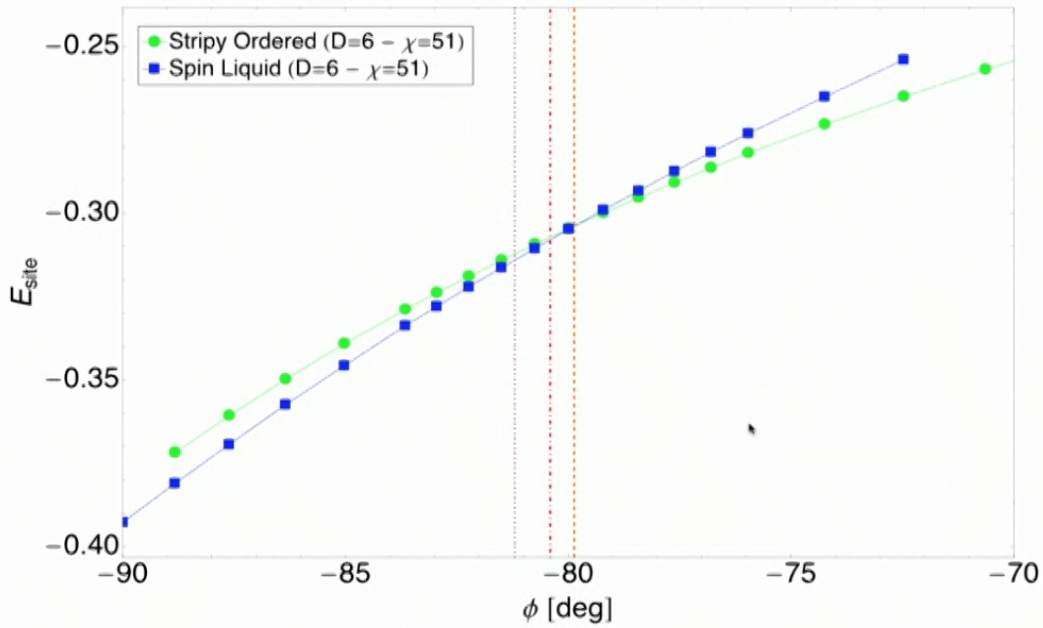
Image from J. Chaloupka, G. Jackeli, G. Khaliullin, PRL 110 (2013).

ETH zürich **Kitaev-Heisenberg**

Spin Liquid to Stripy Transition

Energy Crossings

JOI, P. Corboz, M. Troyer, arXiv:1408.4020.



- Weak energy crossing at φ ~ -80° (D=6) suggests 1st order phase transition.
- Transition point shifts towards lower φ with increasing D.

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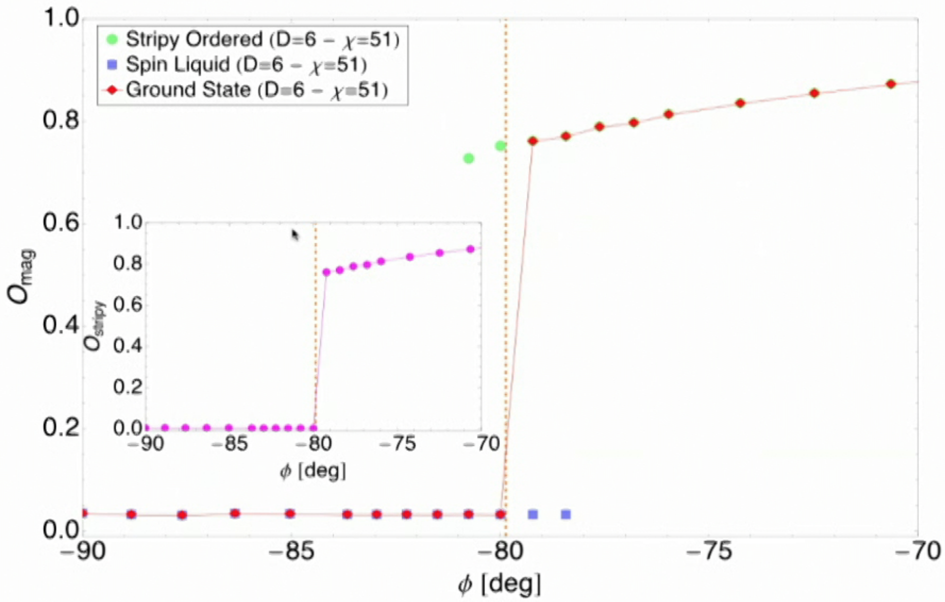
Kitaev-Heisenberg

Spin Liquid to Stripy Transition

Magnetic Order Parameters

JOI, P. Corboz, M. Troyer, arXiv:1408.4020.



- Discontinuous behavior for Magnetization/Stripy order parameters in GS (red diamonds/cyan circles).
- Green/blue data show OP values for each of the phases.
- Discontinuity expected to remain finite in infinite D limit.

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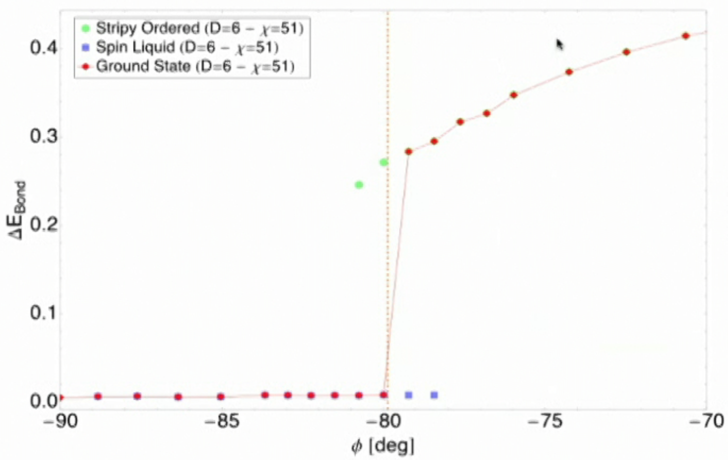
Kitaev-Heisenberg

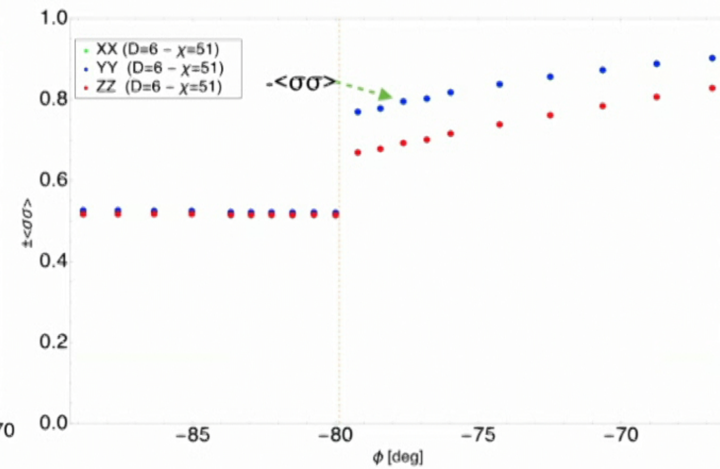
Spin Liquid to Stripy Transition

JOI, P. Corboz, M. Troyer, arXiv:1408.4020.

Bond Order Parameter



Dominant NN Correlations



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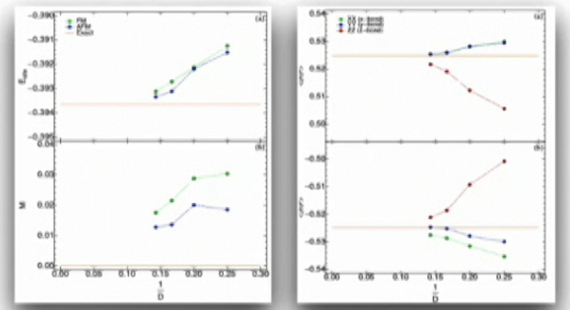
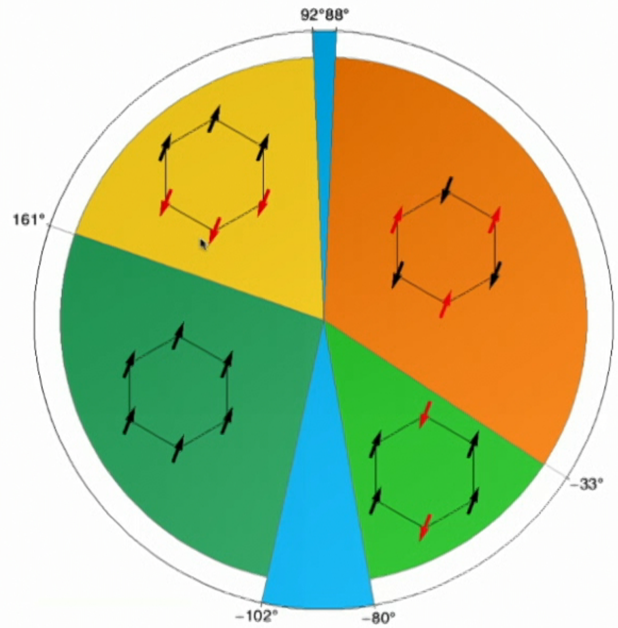
Kitaev-Heisenberg

Summary



	iPEPS	Lanczos
ASL - Néel	$88°$	$88°$
ASL - Zigzag	$92°$	$92°$
FSL - Stripy	$-80°$	$-76°$
FSL - Ferro	$-102°$	$-108°$
Ferro - Zigzag	$161°$	$162°$
Stripy - Néel	$-33°$	$-34°$



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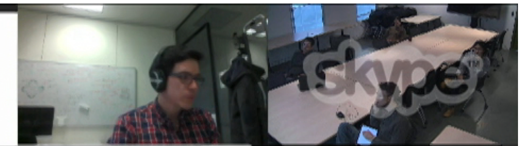
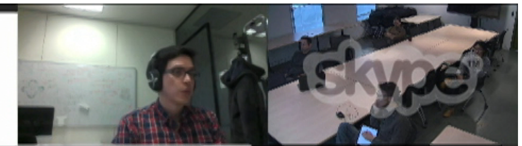


iMPS vs iPEPS

on infinite cylinders



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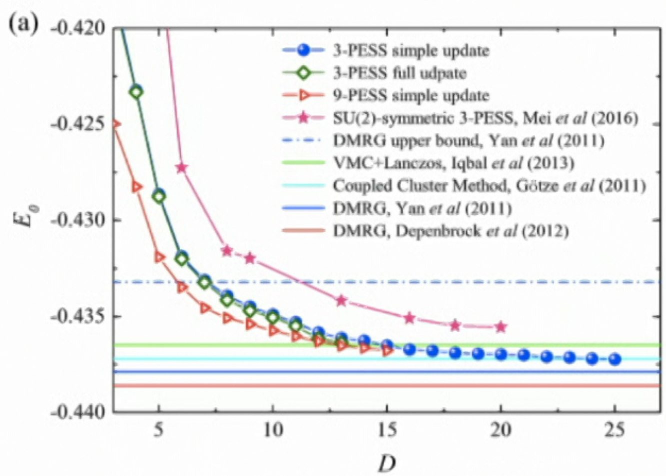
DMRG on cylinders

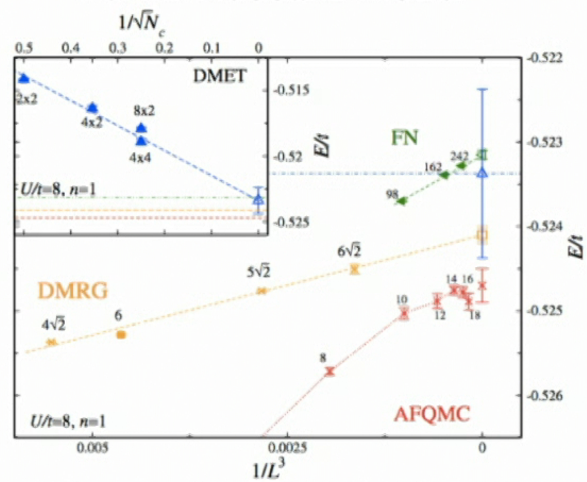
- Golden standard for 1D systems
- State-of-the-art even for 2D!

Kagome Lattice
Heisenberg model



Liao et al., arXiv:1610.04727v1

Square Lattice
Fermi-Hubbard model



LeBlanc et al., Phys. Rev. X 5, 041041 (2015)

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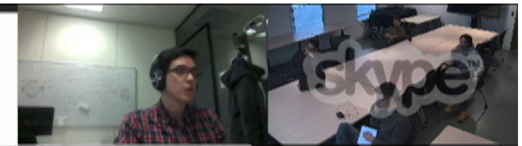
DMRG on cylinders

Can we improve on this? We should. In principle.



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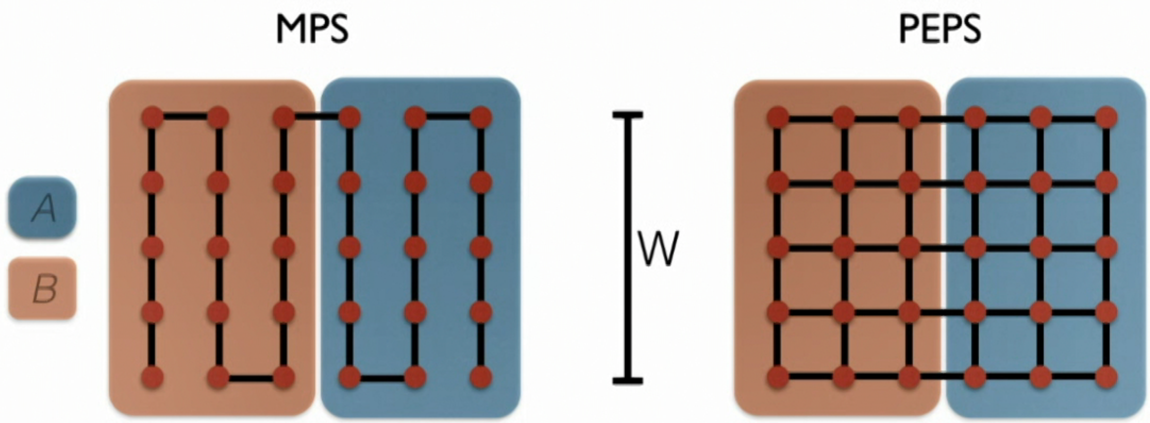
DMRG on cylinders

Can we improve on this? We should. In principle.

MPS are no longer efficient in 2D.



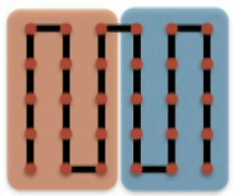
$S_{MPS} \sim \log(D)$ $S_{PEPS} \sim \log(D^W)$

$D \sim \exp(W)$ $D \sim \text{Const.}$

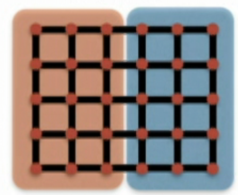
DMRG on cylinders

Where is the crossover?

MPS



PEPS



$S_{MPS} \sim \log(D_{MPS})$

$D_{MPS} \sim \exp(W)$

$S_{PEPS} \sim \log(D_{PEPS}^{W})$

$D_{PEPS} \sim$ Const.

$D_{MPS} = 65k$ ← $D_{PEPS} = 4$ & $W = 8$

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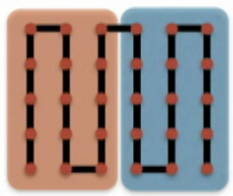
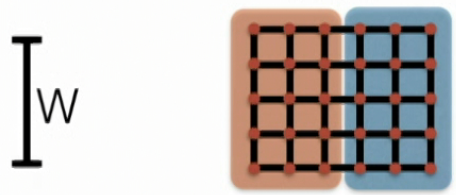
DMRG on cylinders

Where is the crossover?

MPS



PEPS



$S_{MPS} \sim \log(D_{MPS})$

$S_{PEPS} \sim \log(D_{PEPS}^{W})$

$D_{MPS} \sim \exp(W)$

$D_{PEPS} \sim$ Const.

D_{MPS} = 65k

$D_{PEPS} = 4$
&
$W = 8$

Current state-of-the-art ~ 20-30k

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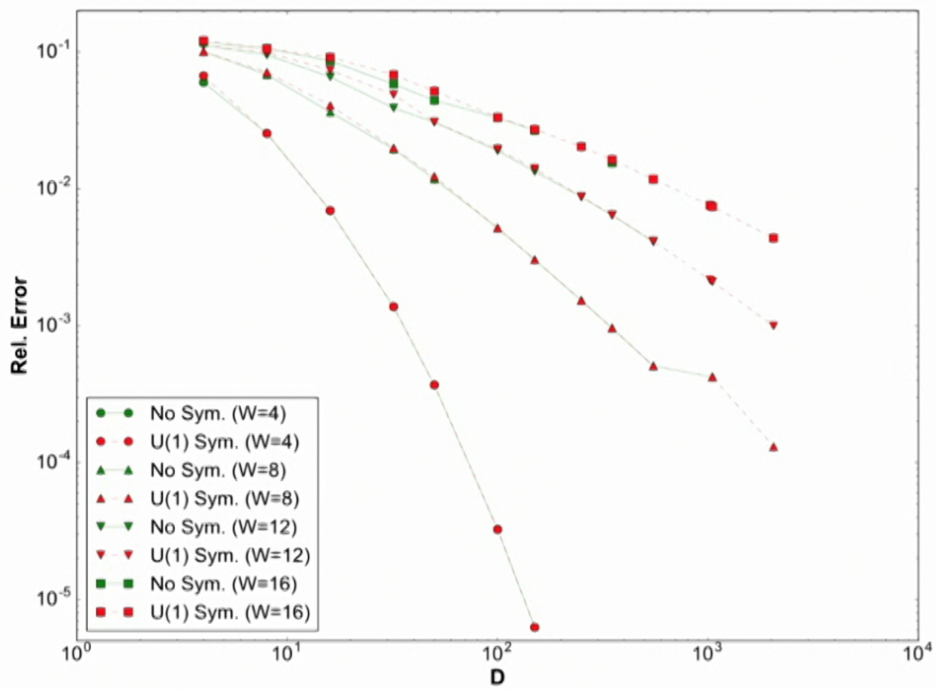
iMPS on cylinders

Square Lattice Heisenberg Model

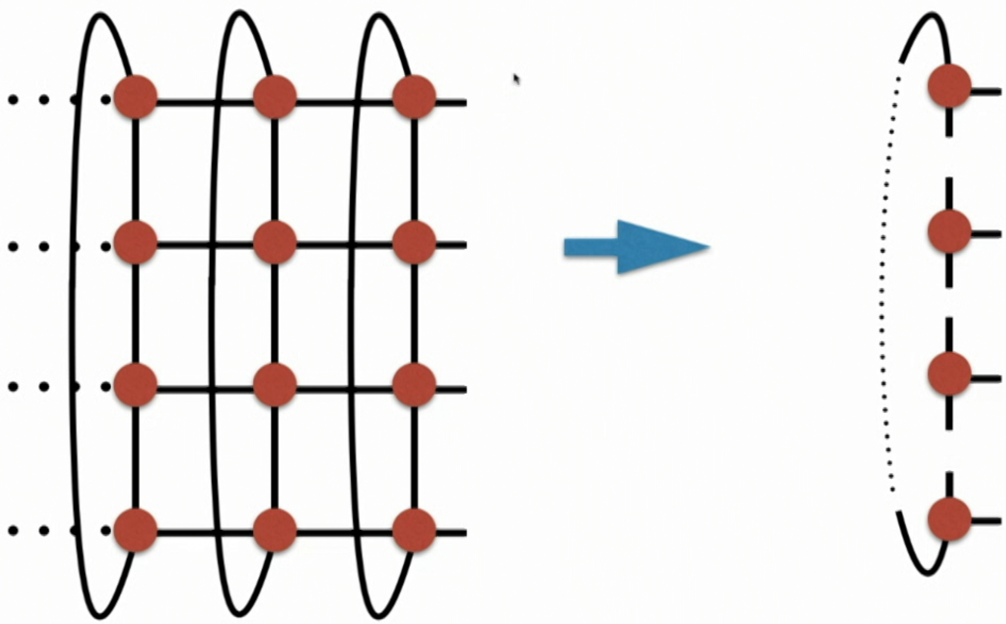


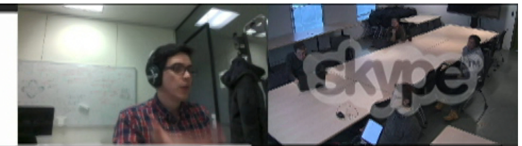
- Loop QMC data as reference.
- Exponential decay visible for thin cylinders
- Flattening of larger width curves due to closing of the gap.

JOI, M. Dolfi , M. Troyer (in preparation)

iPEPS on cylinders

How do we manipulate the iPEPS?





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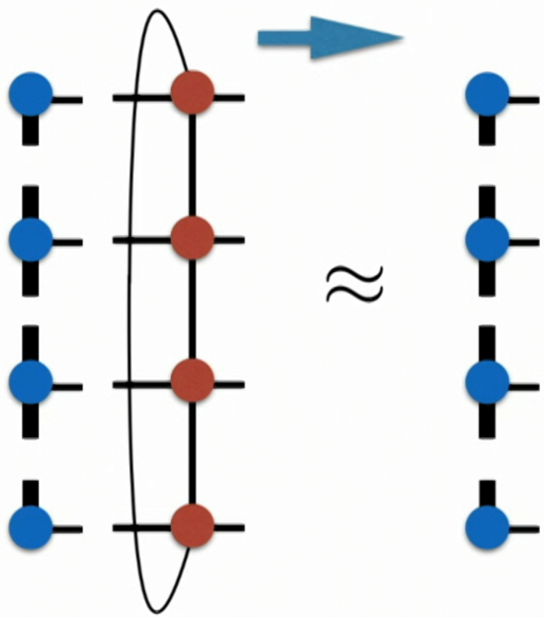
iPEPS on cylinders

How do we manipulate the iPEPS?

Boundary Construction

MPS Comp.



Minimize cost function

$$||O_{MPO}|\psi\rangle - |\tilde{\psi}\rangle||^2$$

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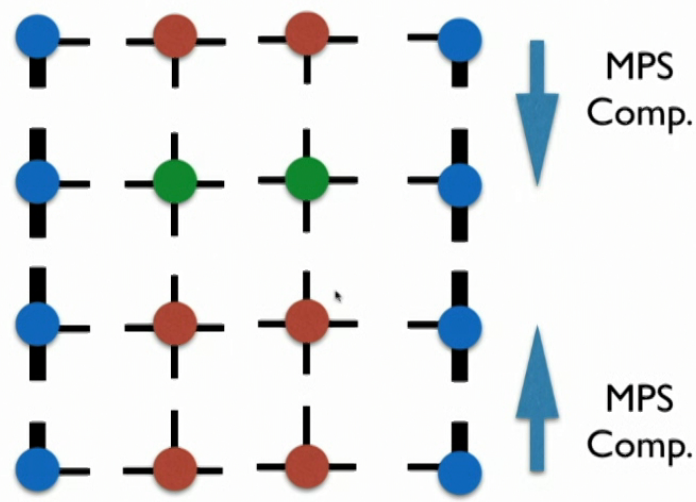
iPEPS on cylinders

How do we manipulate the iPEPS?

Observable Evaluation



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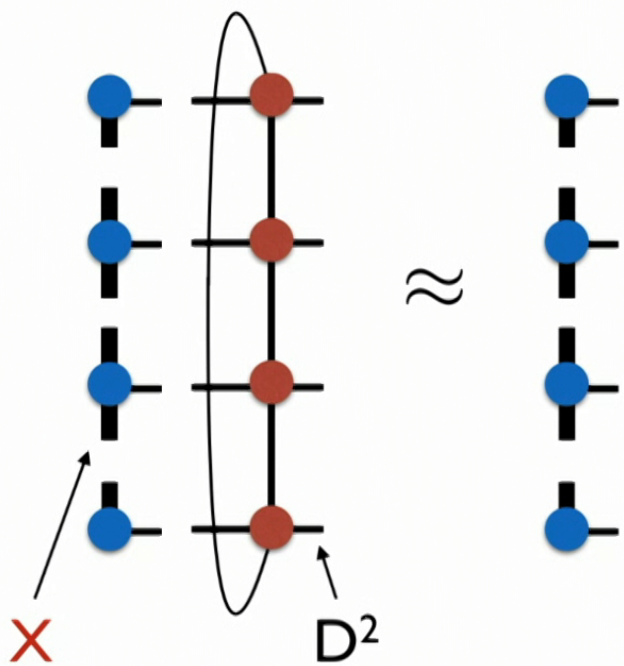
iPEPS on cylinders

How do we manipulate the iPEPS?



Procedure # 1 (OBC MPS)

Advantages

- Profit from stable/well-behaved MPS optimisation procedure.
- Longer ranged observable evaluations manageable.

Disadvantages

- Breaks translational symmetry.

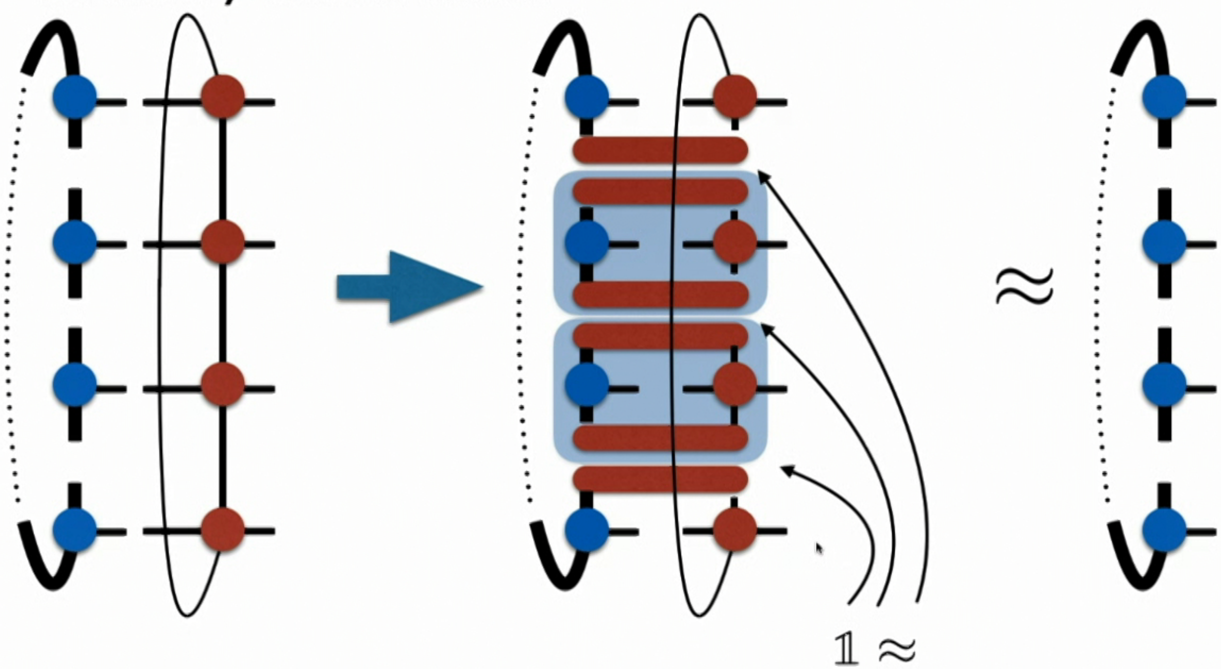
Computational scaling

$\sim O(\chi^3 D^6)$ $\chi \sim O(D^4)$

iPEPS on cylinders

How do we manipulate the iPEPS?

Boundary Construction



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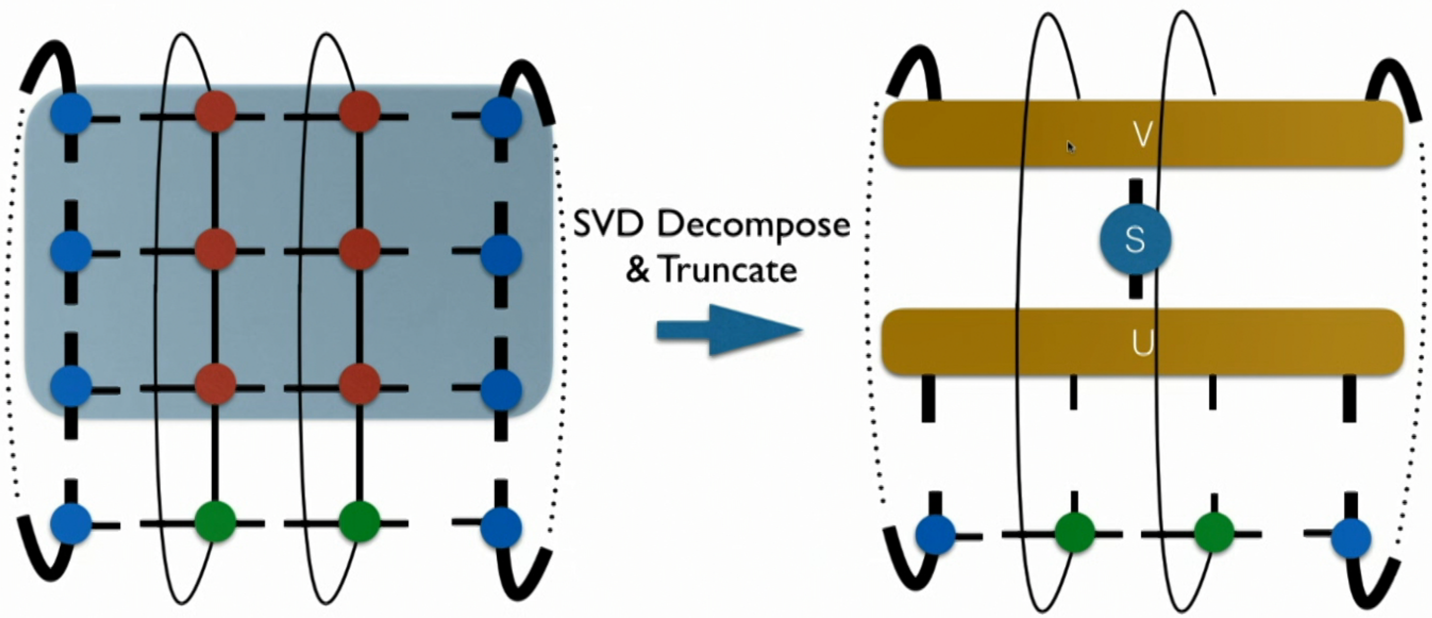
iPEPS on cylinders

How do we manipulate the iPEPS?

Observable Evaluation



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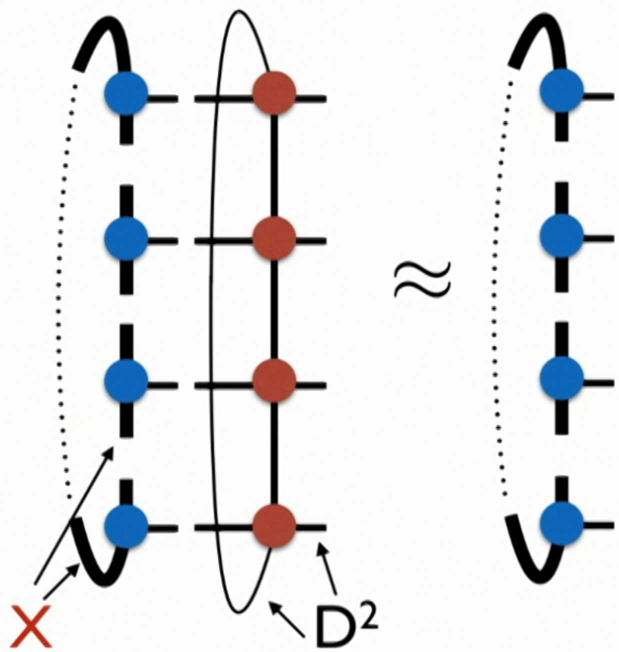
iPEPS on cylinders

How do we manipulate the iPEPS?



Procedure # 2 (PBC MPS)

Advantages

- Preserves translational symmetry.
- Allows recycling of objects from infinite size simulation.

Disadvantages

- Only local observables manageable.
- Potential bias towards infinite size result.

Computational scaling

$\sim O(X^3 D^8)$ $\quad X \sim O(D^2)$

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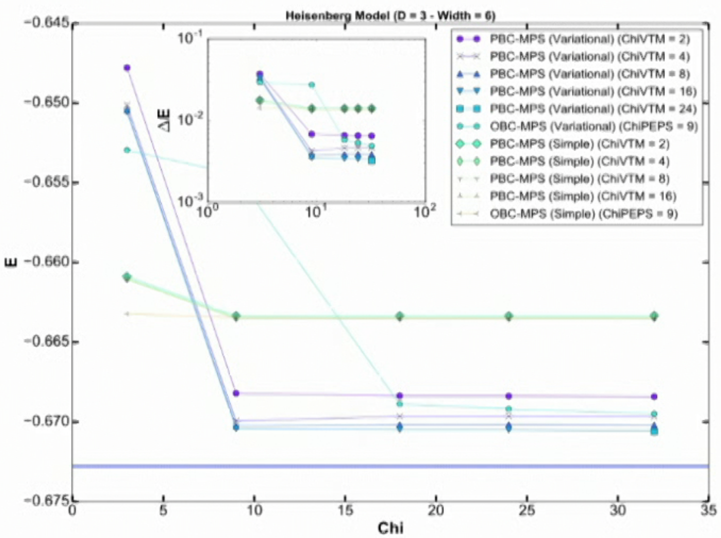
iPEPS on cylinders

JOI, M. Troyer, P. Corboz (in preparation)

Convergence properties

Procedure # 1 (OBC-MPS) vs Procedure # 2 (PBC-MPS)

Heisenberg Model - Ground State Energy



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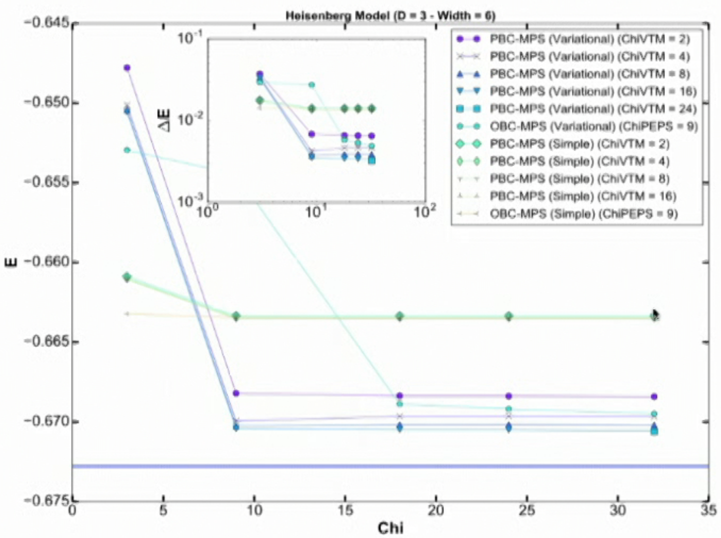
iPEPS on cylinders

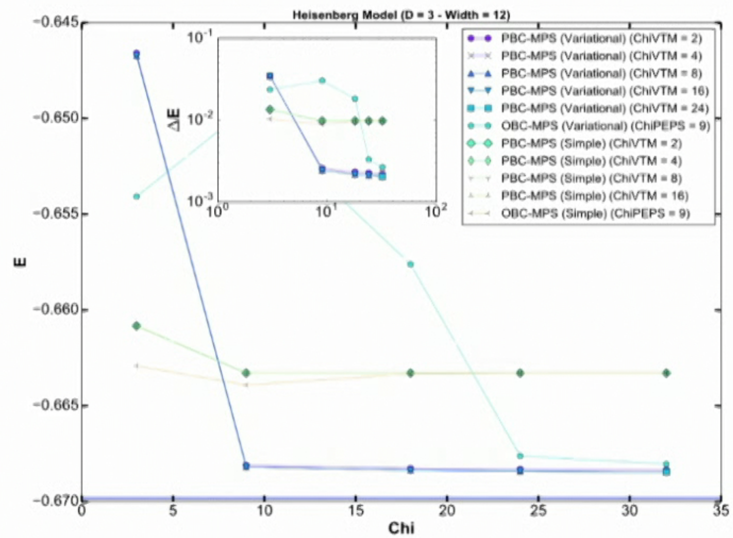
JOI, M. Troyer, P. Corboz (in preparation)

Convergence properties

Procedure # 1 (OBC-MPS) vs Procedure # 2 (PBC-MPS)

Heisenberg Model - Ground State Energy





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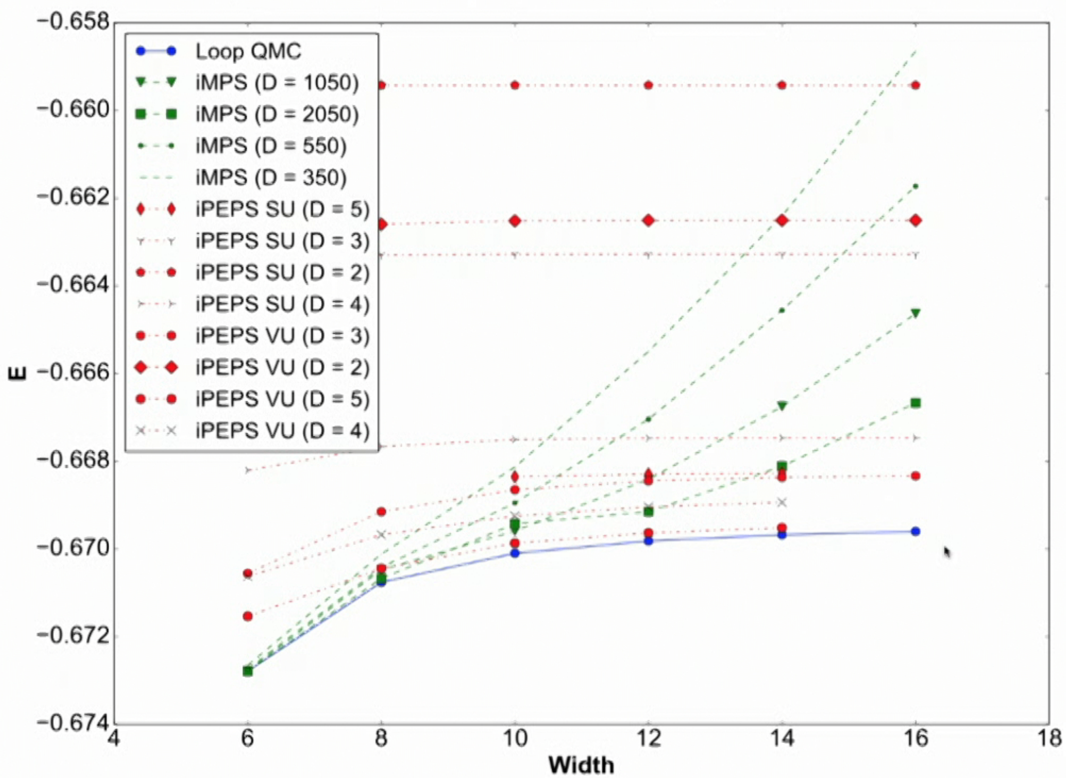
iMPS vs iPEPS

JOI, M. Troyer, P. Corboz (in preparation)

Square Lattice Heisenberg Model



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iMPS vs iPEPS

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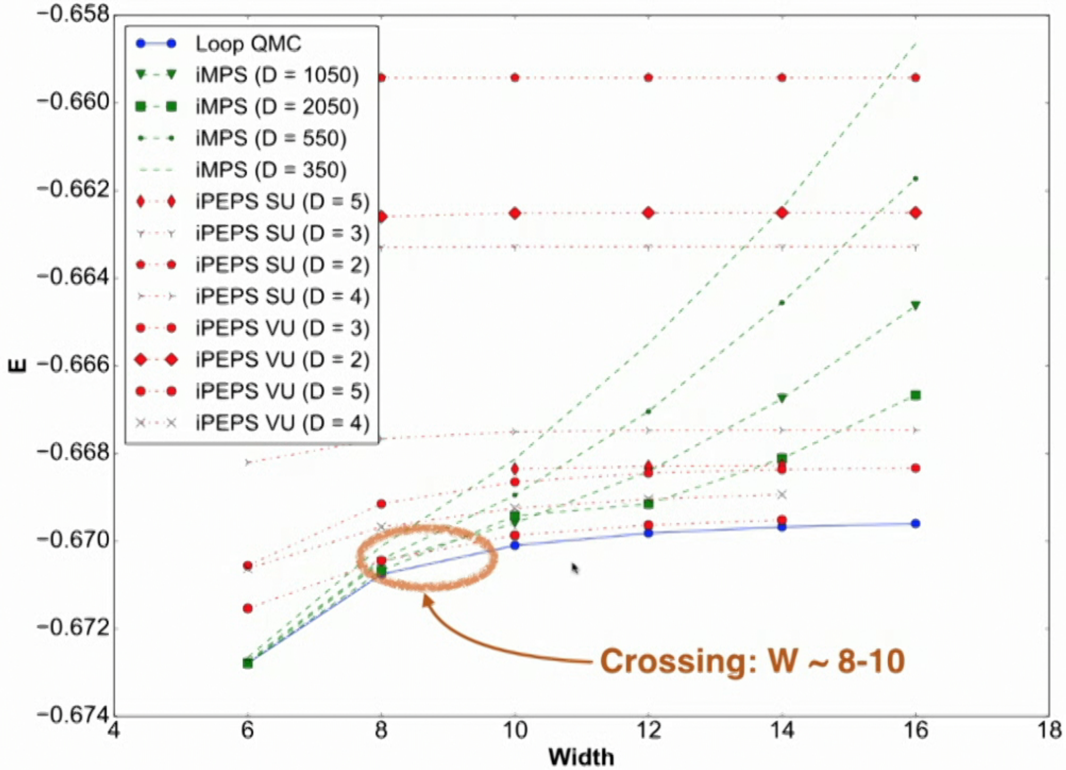

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iMPS vs iPEPS

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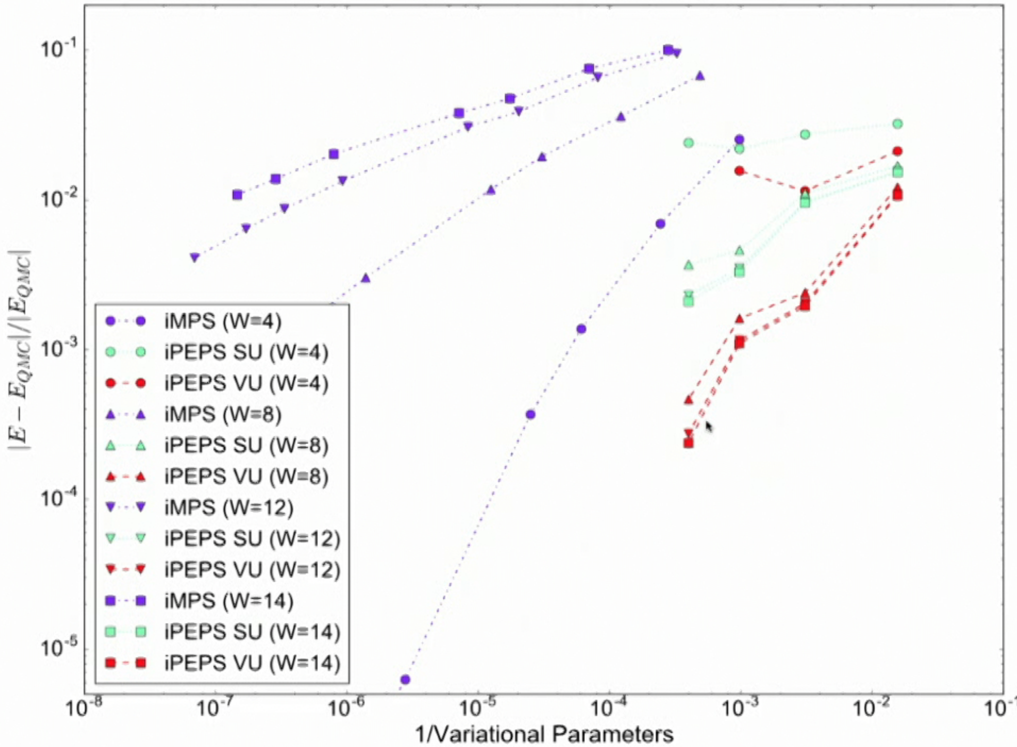

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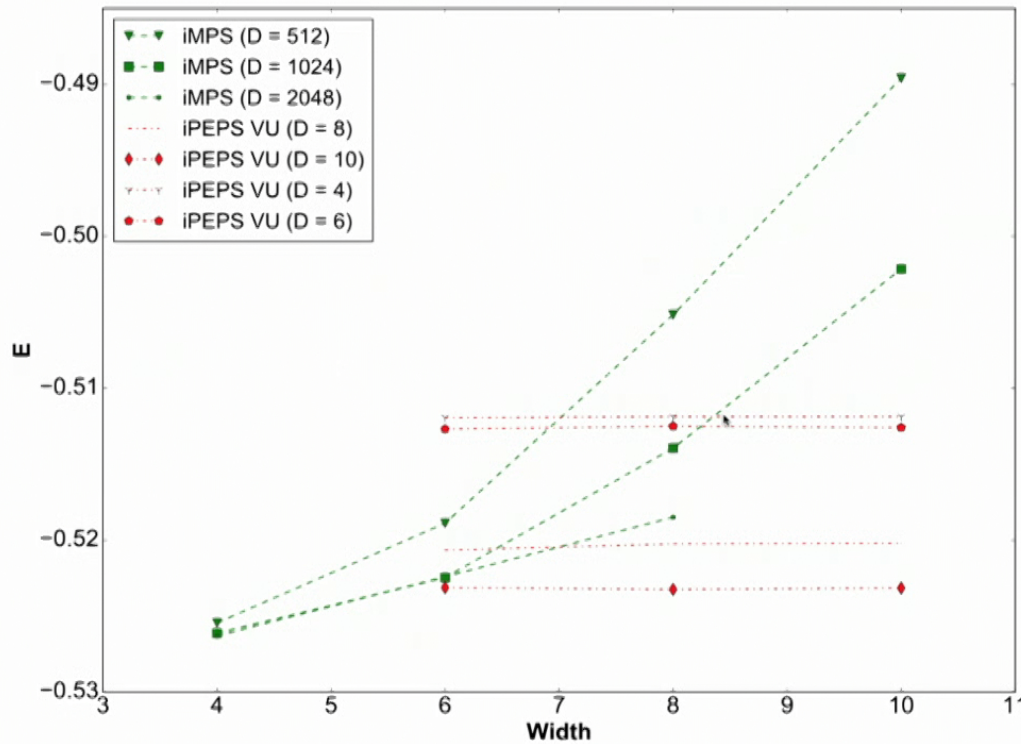
iMPS vs iPEPS

JOI, M. Troyer, P. Corboz (in preparation)

Fermi-Hubbard Model
(U/t = 8 - n = 1.0)



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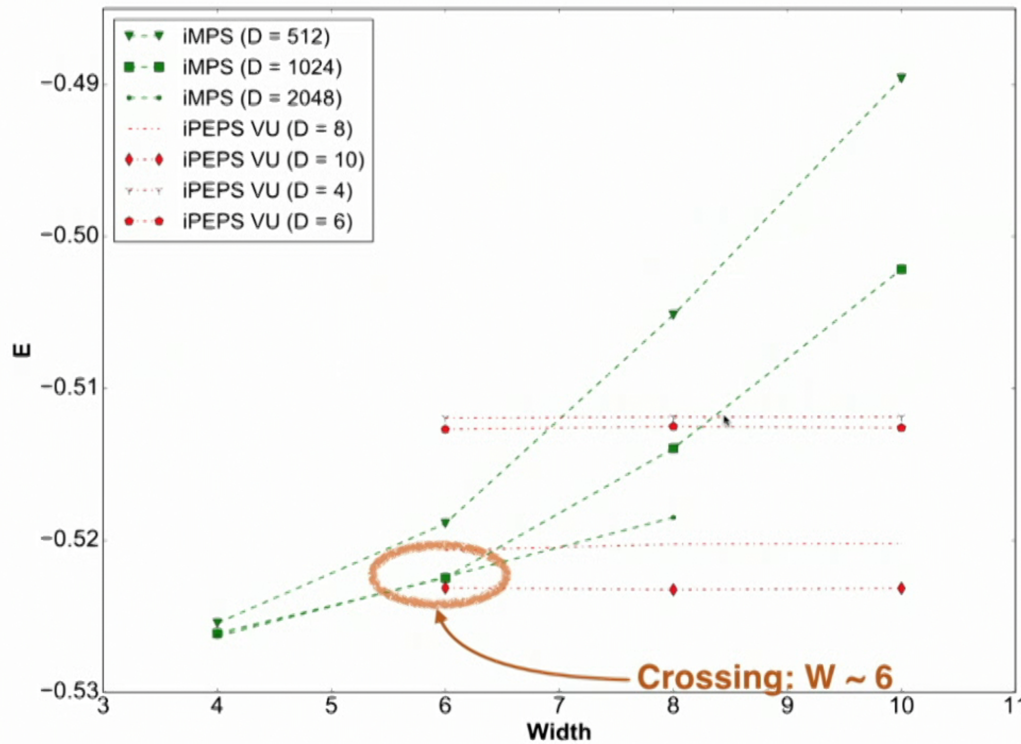
iMPS vs iPEPS

JOI, M. Troyer, P. Corboz (in preparation)

Fermi-Hubbard Model
(U/t = 8 - n = 1.0)



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iMPS vs iPEPS

Summary and Outlook

- iMPS/iPEPS crossover clearly visible.
- Room for improvement with appropriately optimized tensors.
- Work underway to fully determine whether approaching thermodynamic limit from finite-width cylinders will prove to be feasible approach.

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iPEPS

Where do we go from here?

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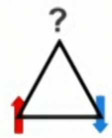
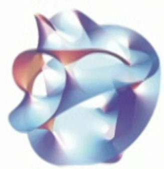
iPEPS

Where do we go from here?



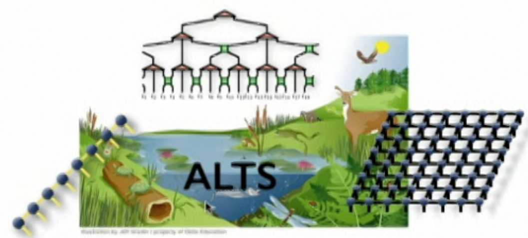
Frustrated magnetism



TNR for RG flows, etc…

Finite temperature

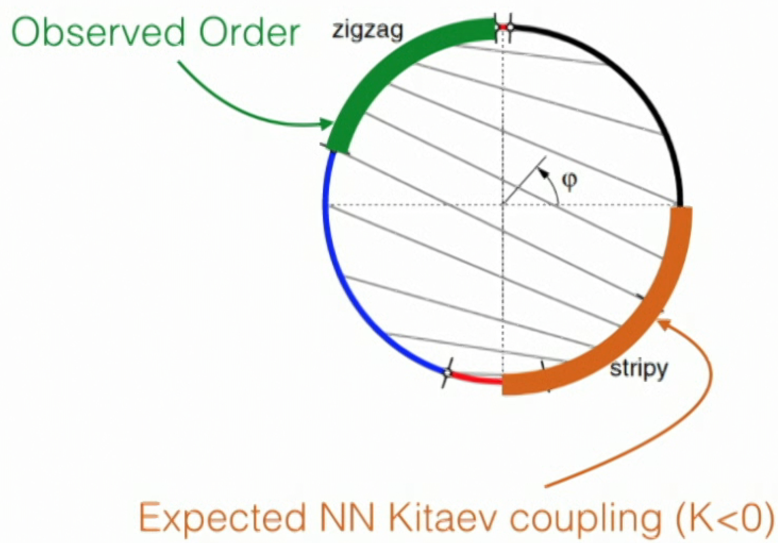
Entering the HPC world



Common ecosystem

Beyond Kitaev-Heisenberg

Additional theoretical/experimental work shows that K-H model does not provide an adequate description of Li/Na_2IrO_3.



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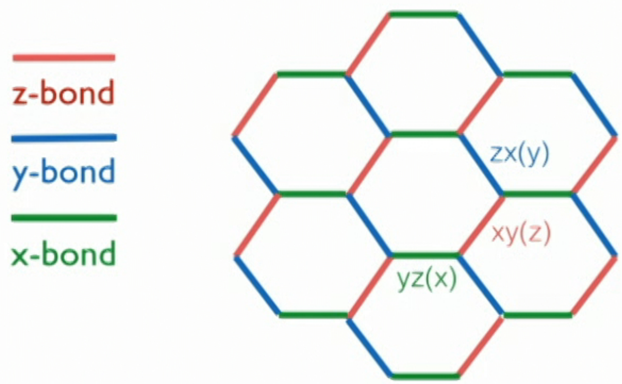
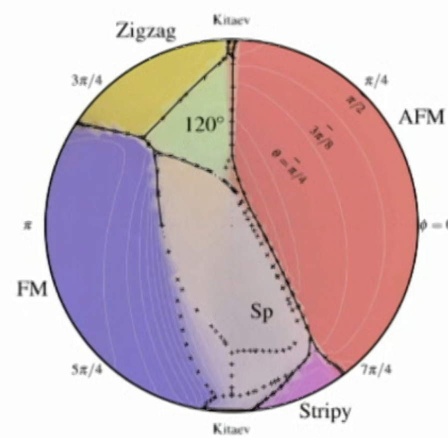
Beyond Kitaev-Heisenberg

Proposed extensions

J-K-Γ model

$$\mathcal{H} = \sum_{\langle i,j \rangle \in \alpha\beta(\gamma)} \left[J S_i \cdot S_j + K S_i^{\gamma_{i,j}} S_j^{\gamma_{i,j}} + \Gamma (S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) \right]$$





Rau, et al., **Phys. Rev. Lett.** ***112, 077204 (2014)***

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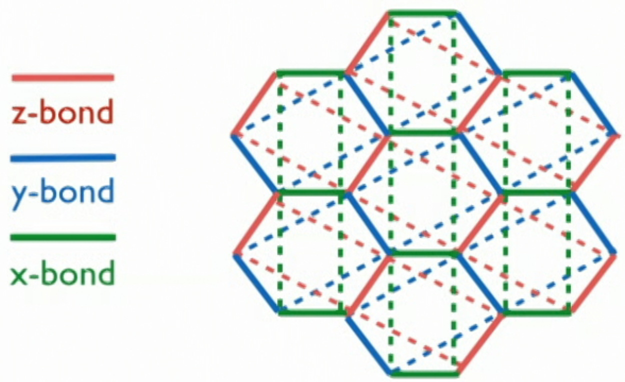
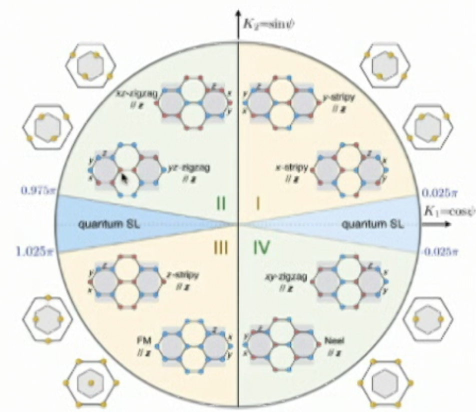
Beyond Kitaev-Heisenberg

Proposed extensions

K1-K2 model

$$\mathcal{H} = K_1 \sum_{\langle i,j \rangle} S_i^{\gamma_{i,j}} S_j^{\gamma_{i,j}} + K_2 \sum_{\langle\langle i,j \rangle\rangle} S_i^{\lambda_{i,j}} S_j^{\lambda_{i,j}}$$





Rousochatzakis, et al., Phys. Rev. X 5, 041035 (2015)

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PEPS - Finite Temp

PEPS have been shown to provide efficient representations of Gibbs states of Local Hamiltonians.

$$D = (N/\epsilon)^{O(\beta)}$$

Most proposals so far only tested in benchmark scenarios, eg. transverse field Ising model, or remain at theoretical level.

Systematic tests in more challenging scenarios are required to determine which approaches are most promising.

Molnar, et al., Phys. Rev. B *91, 045138 (2015)*
Czarnik, et al., Phys. Rev. B 92, 035152 (2015)
Evenbly & Vidal, arXiv:1412.0732v3
Zhao et al., arXiv:1510.03333v1

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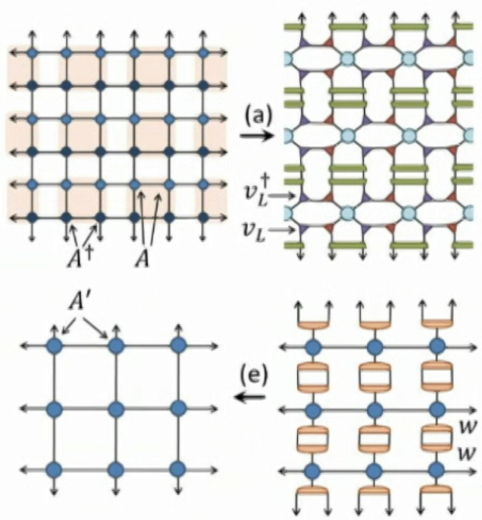
PEPS - Finite Temp

2D TNR



3D TNR

?

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iPEPS - Addressing the con

- Computational cost of algorithm depends on lattice geometry, optimization/contraction scheme, e.g. for a single-layer square lattice:

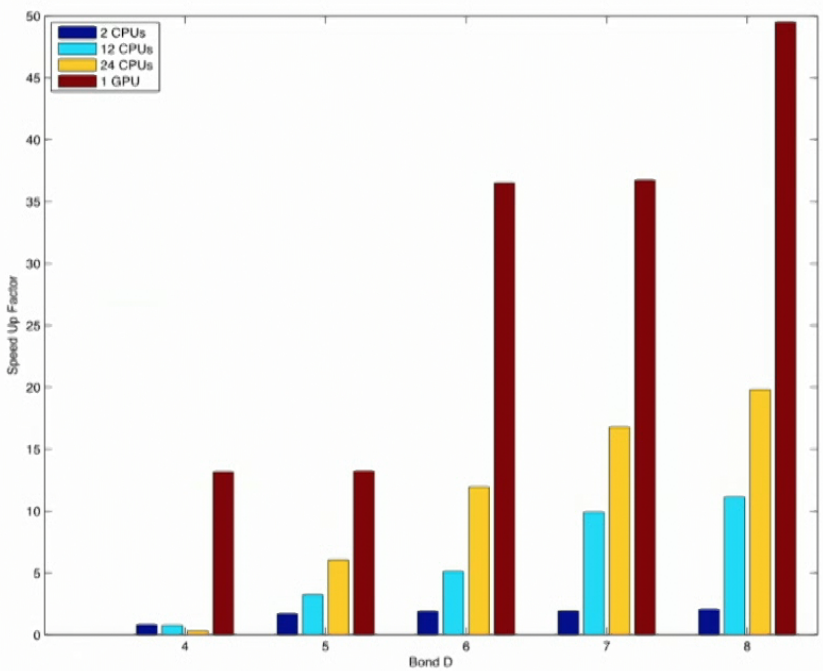
CTM	X^3D^2
TERG	X^6
HOTRG	X^7

Compare to D^3 of MPS methods.

Evaluation of observables requires a double layer set-up increasing computational cost (CTM - X^3D^6). Currently affordable values of D ~ 7 without symmetries.

Hardware Acceleration

Timings - Leading Tensor Contraction



- Leading complexity operation of CTM algorithm.
- Computational Cost ~ $O(\chi^3 D^6)$
- Computations performed using MATLAB.
- CPU computations performed on AMD Opteron 6174.
- GPU computations performed on NVIDIA Tesla M2050 (Fermi)

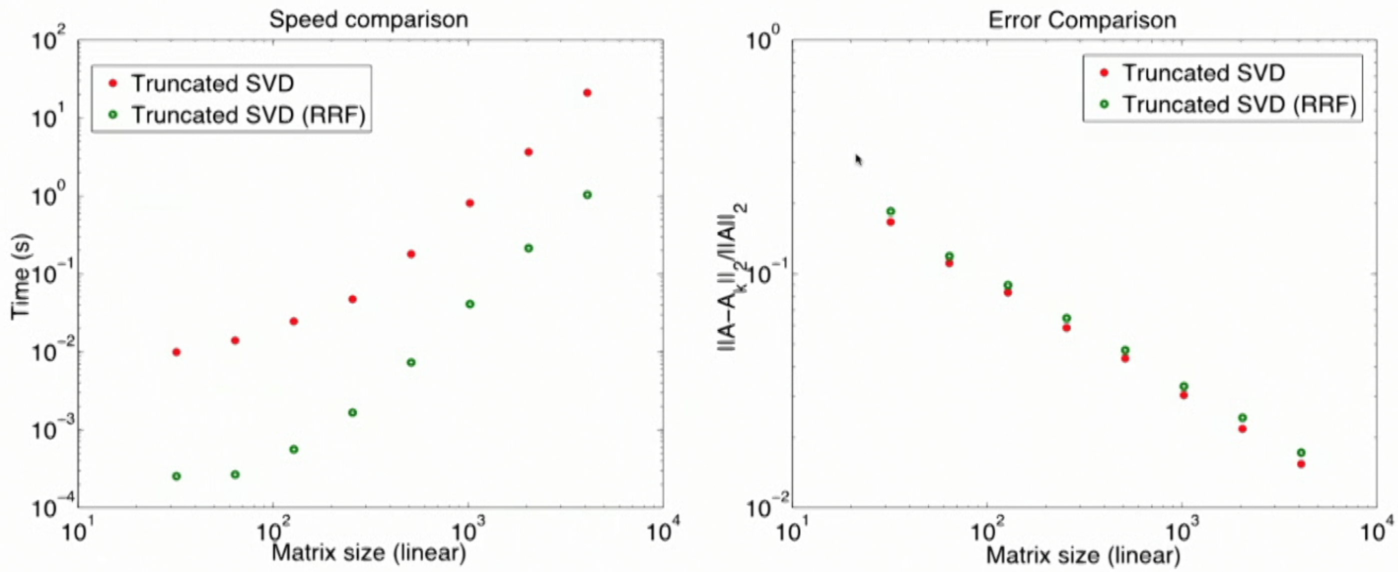
Speed-up factor ~ 2.5x-50x.

ETH zürich iPEPS - Addressing the con

Algorithmic Acceleration

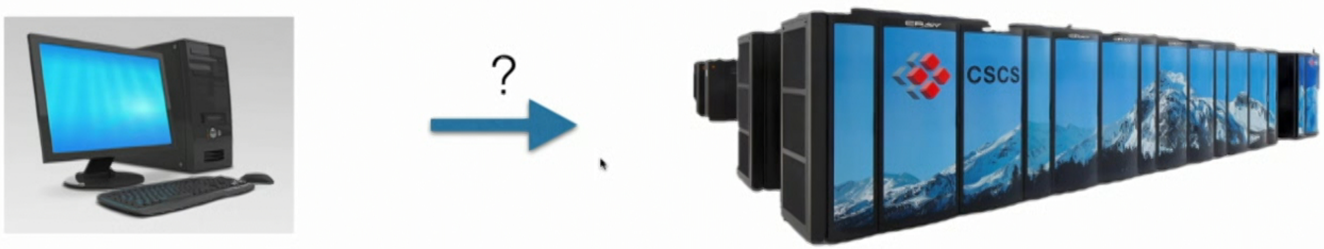
Randomized Range Finder - Timings & Error

Polynomially decaying singular values

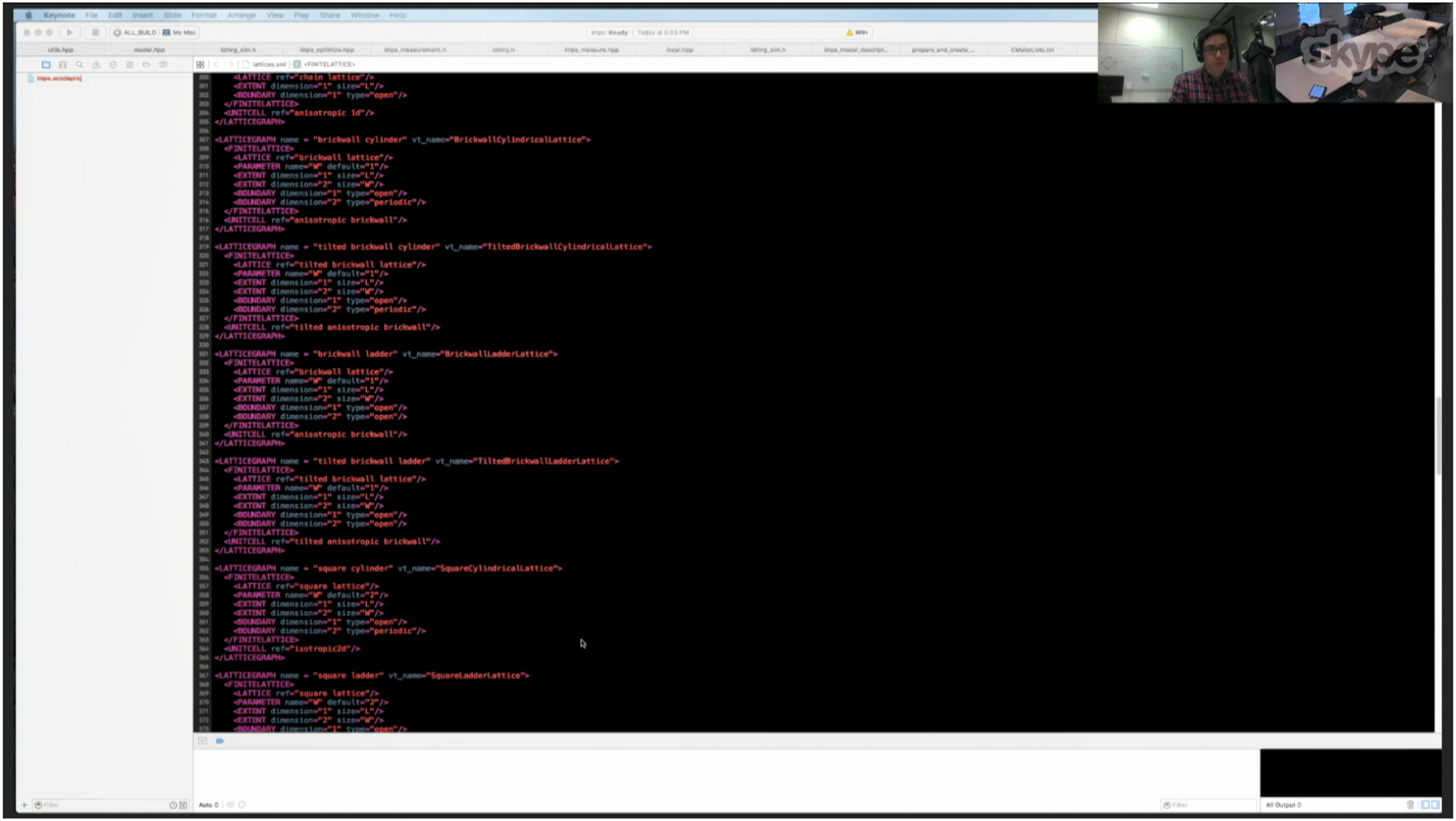


ETH zürich iPEPS - Addressing the con

Entering the HPC world



- Simple Update: easily parallelizable.
- Full/Variational Update: clear opportunities as unit cell gets larger.
- Parallelism at single unit cell level not so straight forward/clear.



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