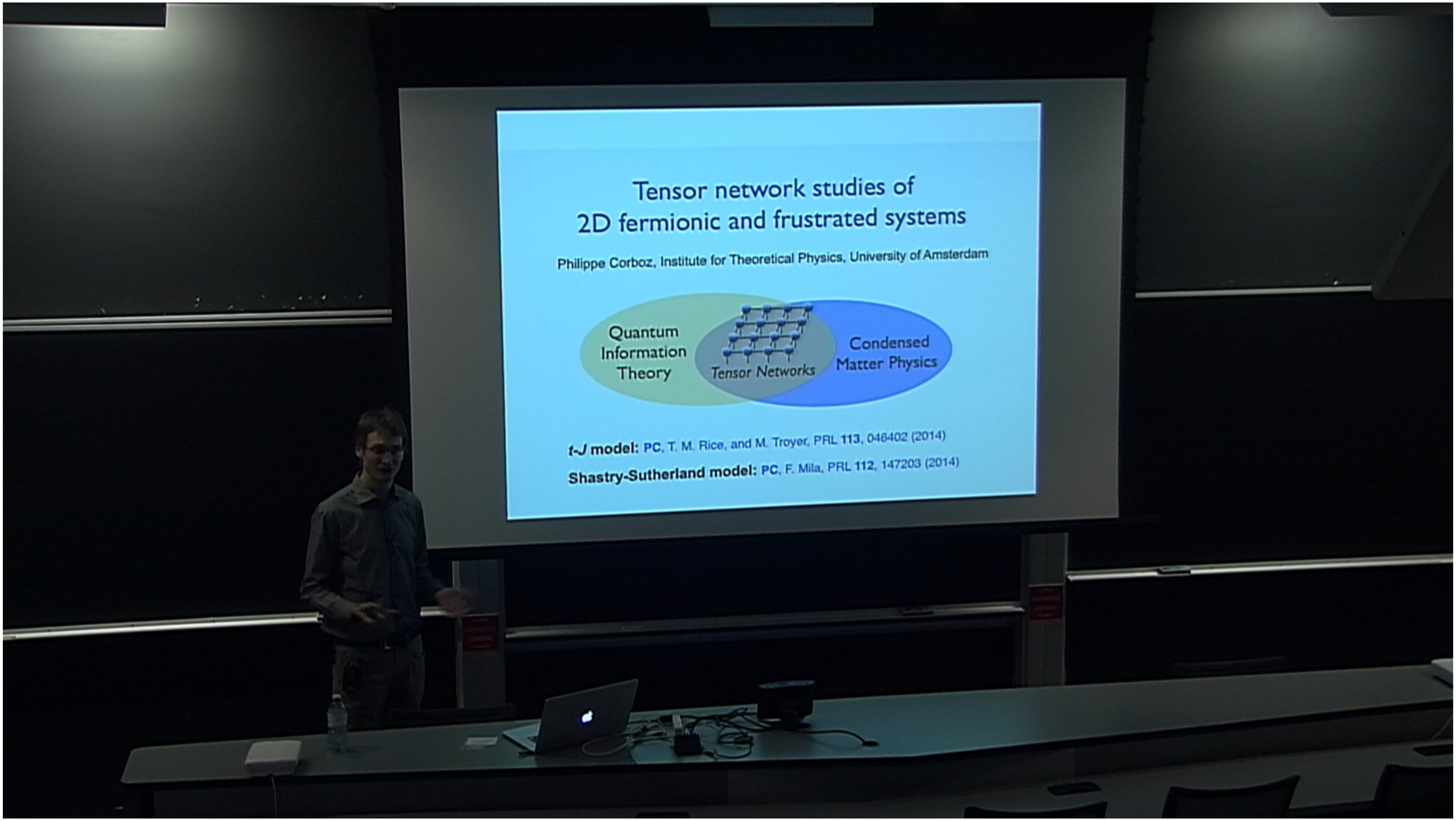
Title: Tensor network studies of 2D fermionic and frustrated systems

Date: Nov 05, 2015 09:05 AM

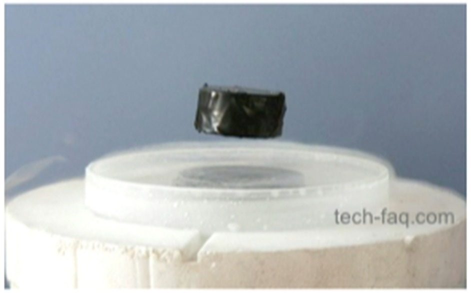
URL: http://pirsa.org/15110067

Abstract:

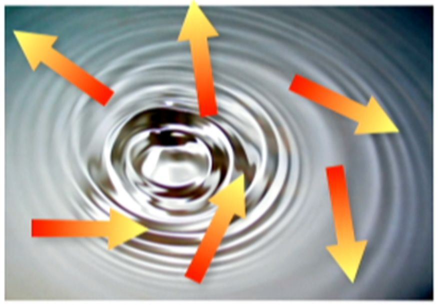

Tensor network studies of
2D fermionic and frustrated systems
Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam
Quantum Information Theory
Tensor Networks
Condensed Matter Physics
t-J model: PC, T. M. Rice, and M. Troyer, PRL 113, 046402 (2014)
Shastry-Sutherland model: PC, F. Mila, PRL 112, 147203 (2014)

Motivation: Strongly correlated quantum many-body systems

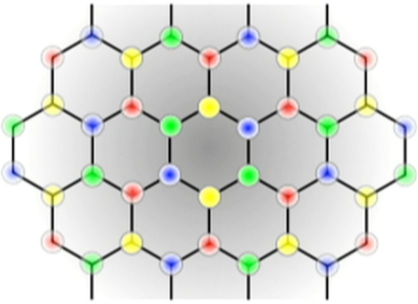
High-Tc superconductivity



Quantum magnetism / spin liquids



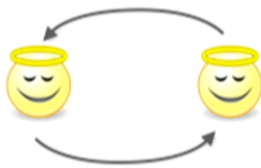
Novel phases with ultra-cold atoms



Quantum Monte Carlo & the negative sign problem

Bosons
(e.g. ^{4}He)

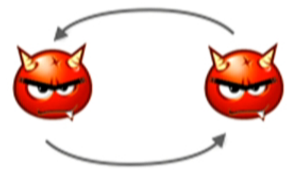
Fermions
(e.g electrons)



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

symmetric!

$$t_{sim} \sim \mathcal{O}(poly(N/T))$$

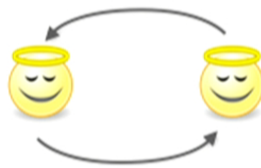


$$\Psi_F(x_1, x_2) = -\Psi_F(x_2, x_1)$$

antisymmetric!

Quantum Monte Carlo & the negative sign problem

Bosons
(e.g. ^{4}He)



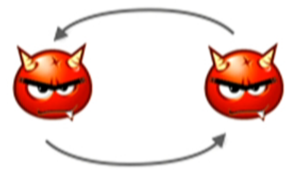
$$\Psi_B(x_1, x_2) = \Psi_B(x_2, x_1)$$

symmetric!

✓

$$t_{sim} \sim \mathcal{O}(poly(N/T))$$

Fermions
(e.g electrons)



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

antisymmetric!

this leads to the infamous negative sign problem

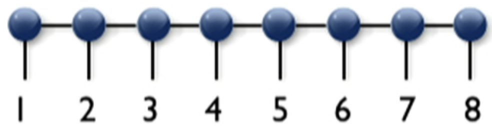
$$t_{sim} \sim \mathcal{O}(\exp(N/T))$$

cannot solve large systems at low temperature!

Overview: tensor networks in 1D and 2D

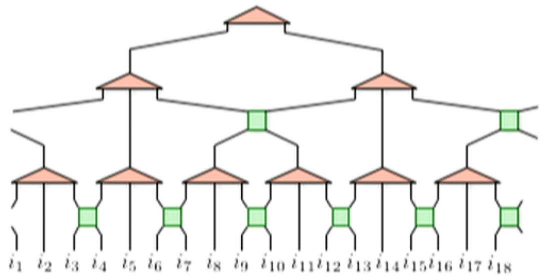
1D

MPS
Matrix-product state



Underlying ansatz of the density-matrix renormalization group (**DMRG**) method

1D MERA
Multi-scale entanglement renormalization ansatz

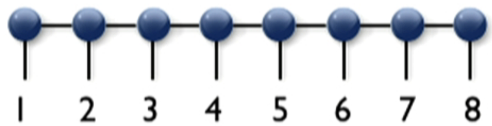


and more
- 1D tree tensor network
- ...

Overview: tensor networks in 1D and 2D

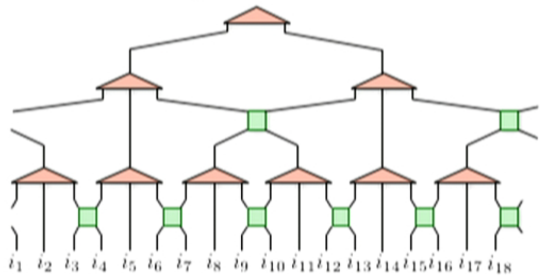
1D

MPS
Matrix-product state



Underlying ansatz of the density-matrix renormalization group (**DMRG**) method

1D MERA
Multi-scale entanglement renormalization ansatz

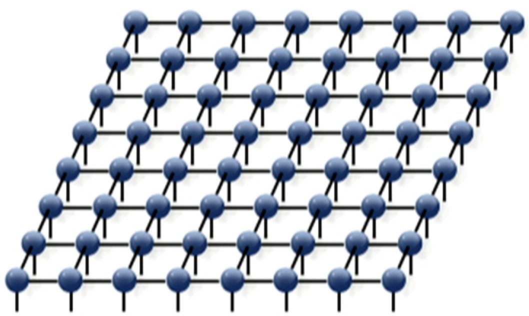


and more

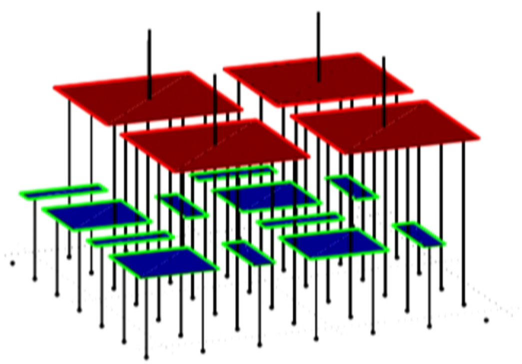
- 1D tree tensor network
- ...

2D

PEPS
projected entangled-pair state

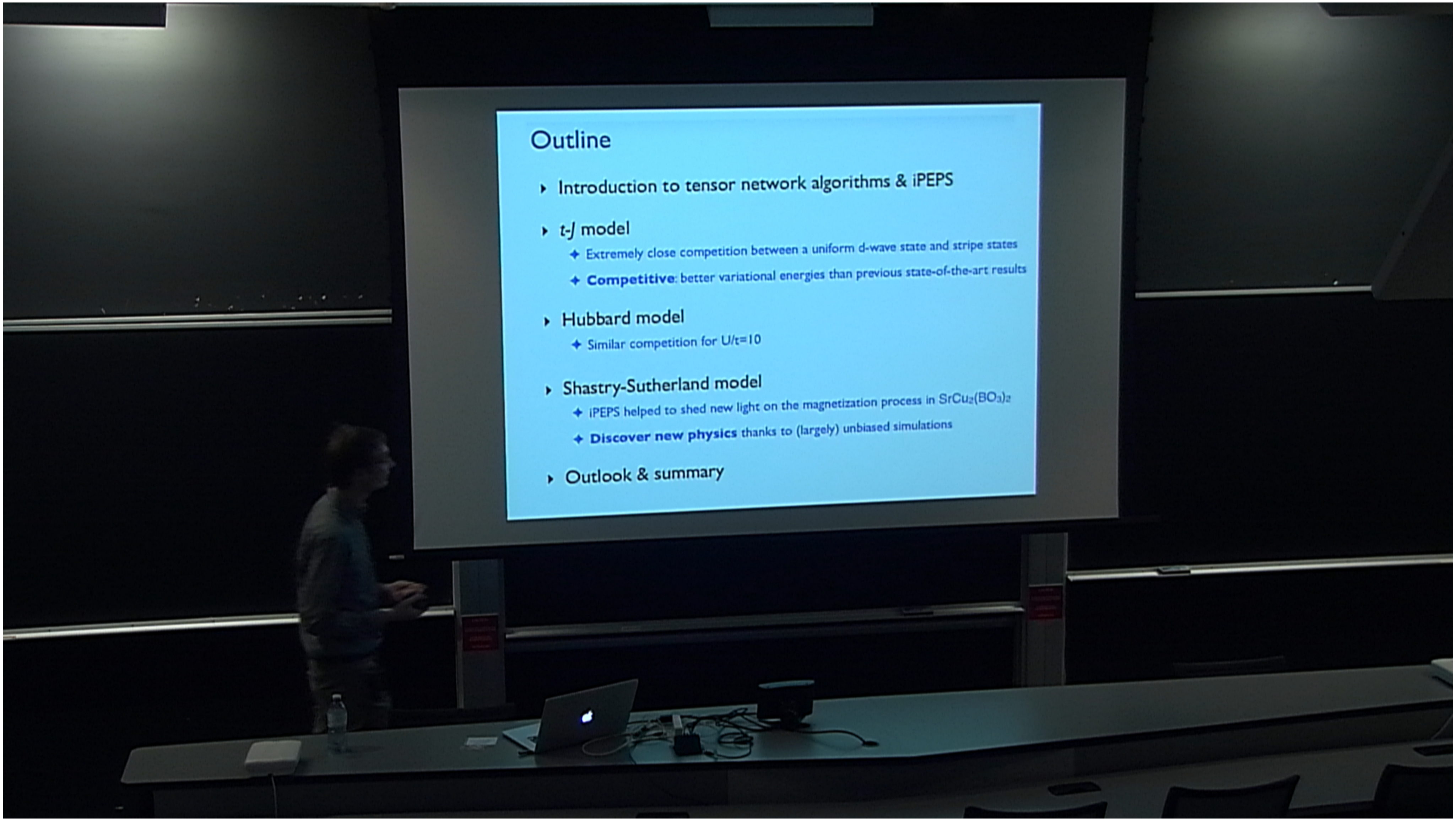


2D MERA



and more

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


Outline
Introduction to tensor network algorithms & iPEPS
t-J model
Extremely close competition between a uniform d-wave state and stripe states
Competitive: better variational energies than previous state-of-the-art results
Hubbard model
Similar competition for U/t=10
Shastry-Sutherland model
iPEPS helped to shed new light on the magnetization process in SrCu2(BO3)2
Discover new physics thanks to (largely) unbiased simulations
Outlook & summary

Outline

- Introduction to tensor network algorithms & iPEPS
- *t-J* model
  - Extremely close competition between a uniform d-wave state and stripe states
  - **Competitive**: better variational energies than previous state-of-the-art results
- Hubbard model
  - Similar competition for U/t=10
- Shastry-Sutherland model
  - iPEPS helped to shed new light on the magnetization process in $SrCu_2(BO_3)_2$
  - **Discover new physics** thanks to (largely) unbiased simulations
- Outlook & summary

Tensor network ansatz for a wave function

Lattice: ● 1 ● 2 ● 3 ● 4 ● 5 ● 6

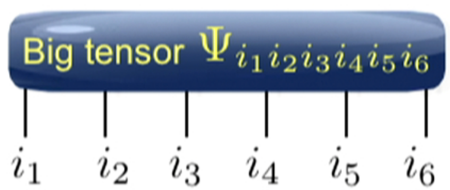
2 basis states per site: $\{|\uparrow\rangle, |\downarrow\rangle\}$

2^6 basis states

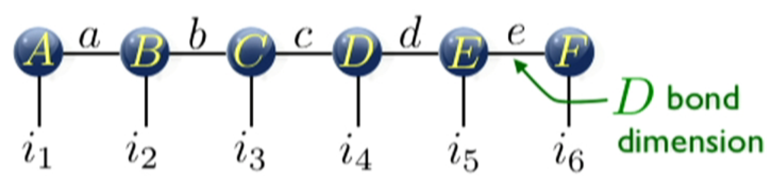
2^6 coefficients

State: $$|\Psi\rangle = \sum_{i_1 i_2 i_3 i_4 i_5 i_6} \Psi_{i_1 i_2 i_3 i_4 i_5 i_6} |i_1 \otimes i_2 \otimes i_3 \otimes i_4 \otimes i_5 \otimes i_6\rangle$$

Tensor/multidimensional array



Tensor network: matrix product state (**MPS**)

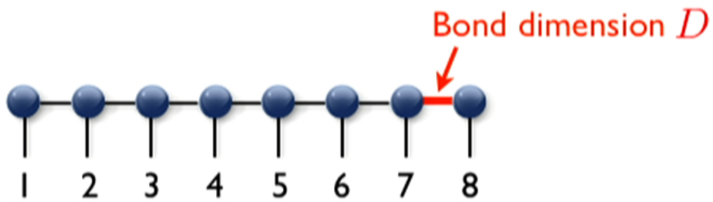


MPS & PEPS

1D

MPS

Matrix-product state
(underlying ansatz of DMRG)



Physical indices (lattices sites)

S. R. White, PRL 69, 2863 (1992)

Fannes et al., CMP 144, 443 (1992)

Östlund, Rommer, PRL 75, 3537 (1995)

MPS & PEPS

1D

MPS

Matrix-product state
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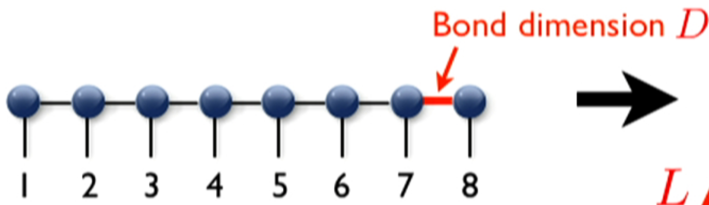


Physical indices (lattices sites)

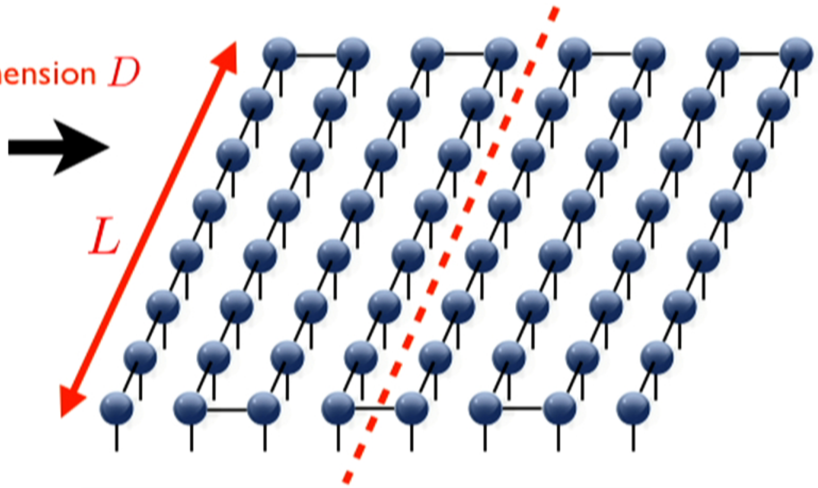
S. R. White, PRL 69, 2863 (1992)

Fannes et al., CMP 144, 443 (1992)

Östlund, Rommer, PRL 75, 3537 (1995)

2D

Snake MPS

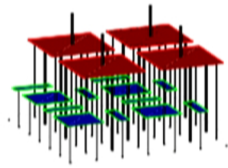


Computational cost:

$\propto \exp(L)$

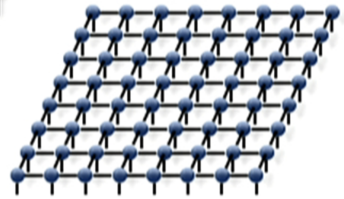
Summary: Tensor network algorithms

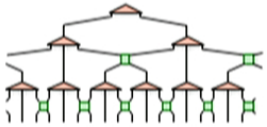
2D MERA



MPS

PEPS





1D MERA

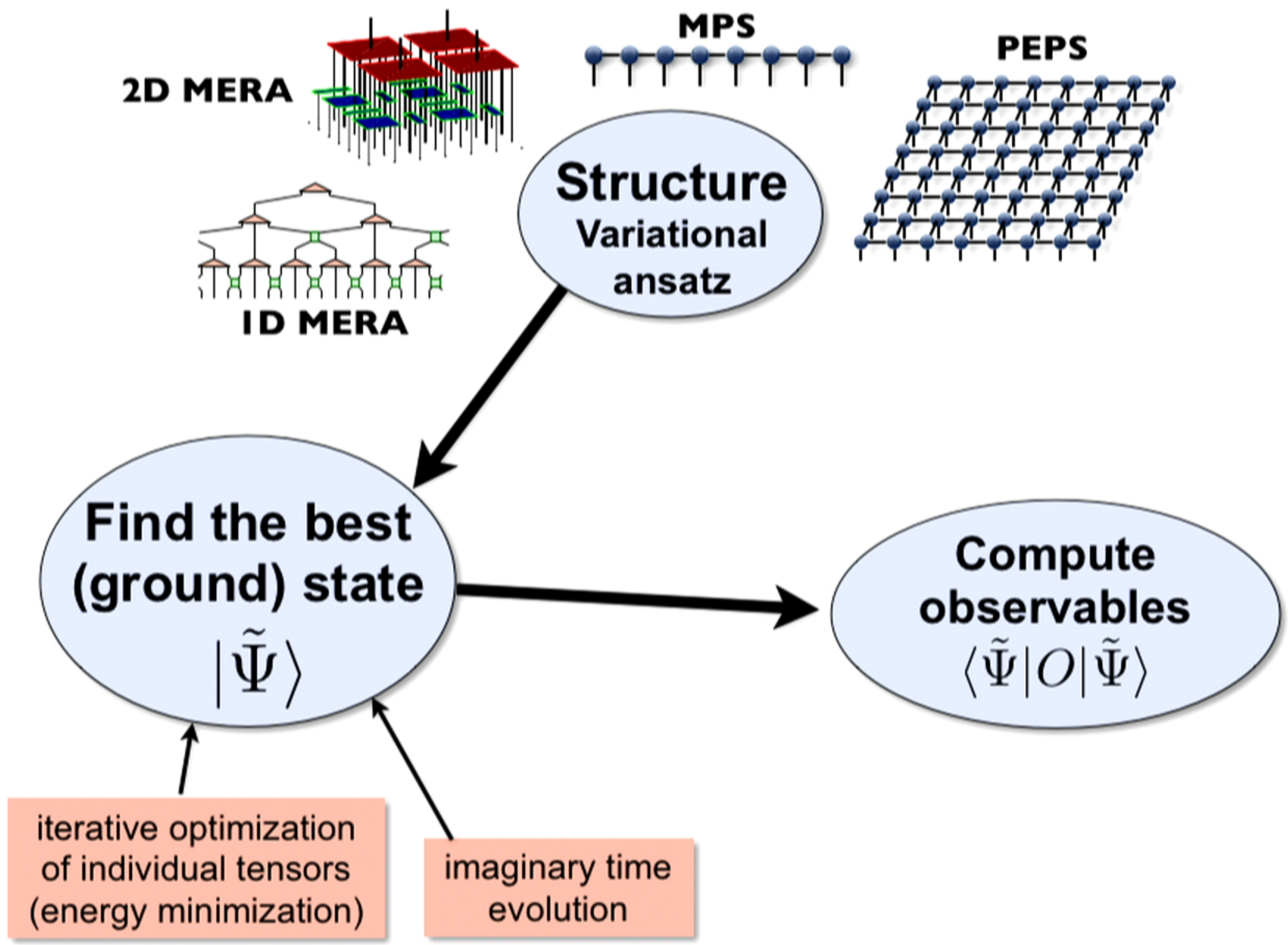
Structure
Variational ansatz

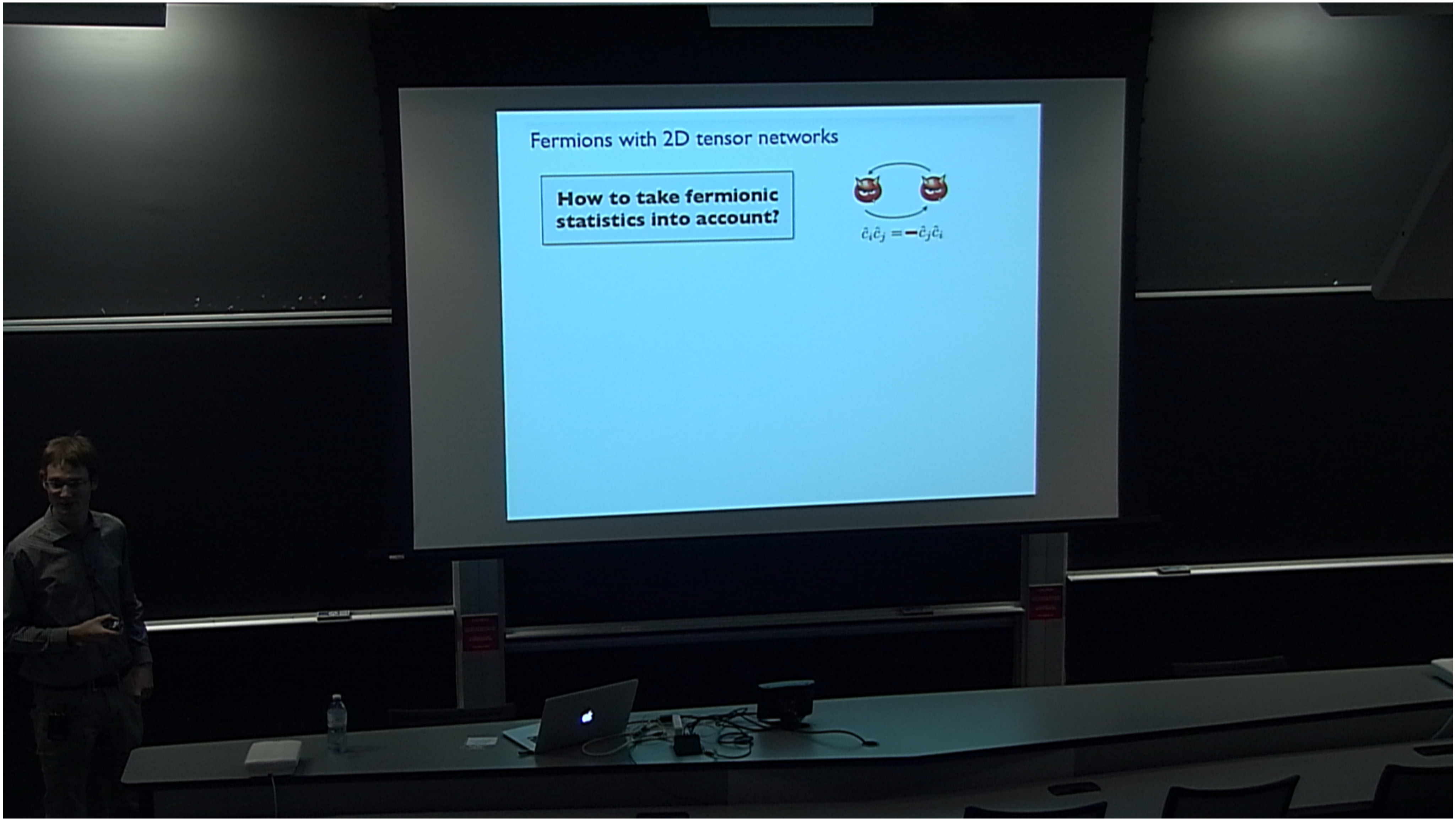
Find the best (ground) state

$$|\tilde{\Psi}\rangle$$

iterative optimization
of individual tensors
(energy minimization)

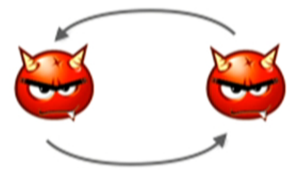
Summary: Tensor network algorithms




Fermions with 2D tensor networks
How to take fermionic statistics into account?
$\hat{c}_i\hat{c}_j = -\hat{c}_j\hat{c}_i$

Fermions with 2D tensor networks

How to take fermionic statistics into account?



$$\hat{c}_i \hat{c}_j = - \hat{c}_j \hat{c}_i$$

Different formulations (but same fermionic ansatz):

PC, Evenbly, Verstraete, Vidal (2009)

Kraus, Schuch, Verstraete, Cirac (2009)

Pineda, Barthel, Eisert (2009)

PC & Vidal (2009)

Barthel, Pineda, Eisert (2009)

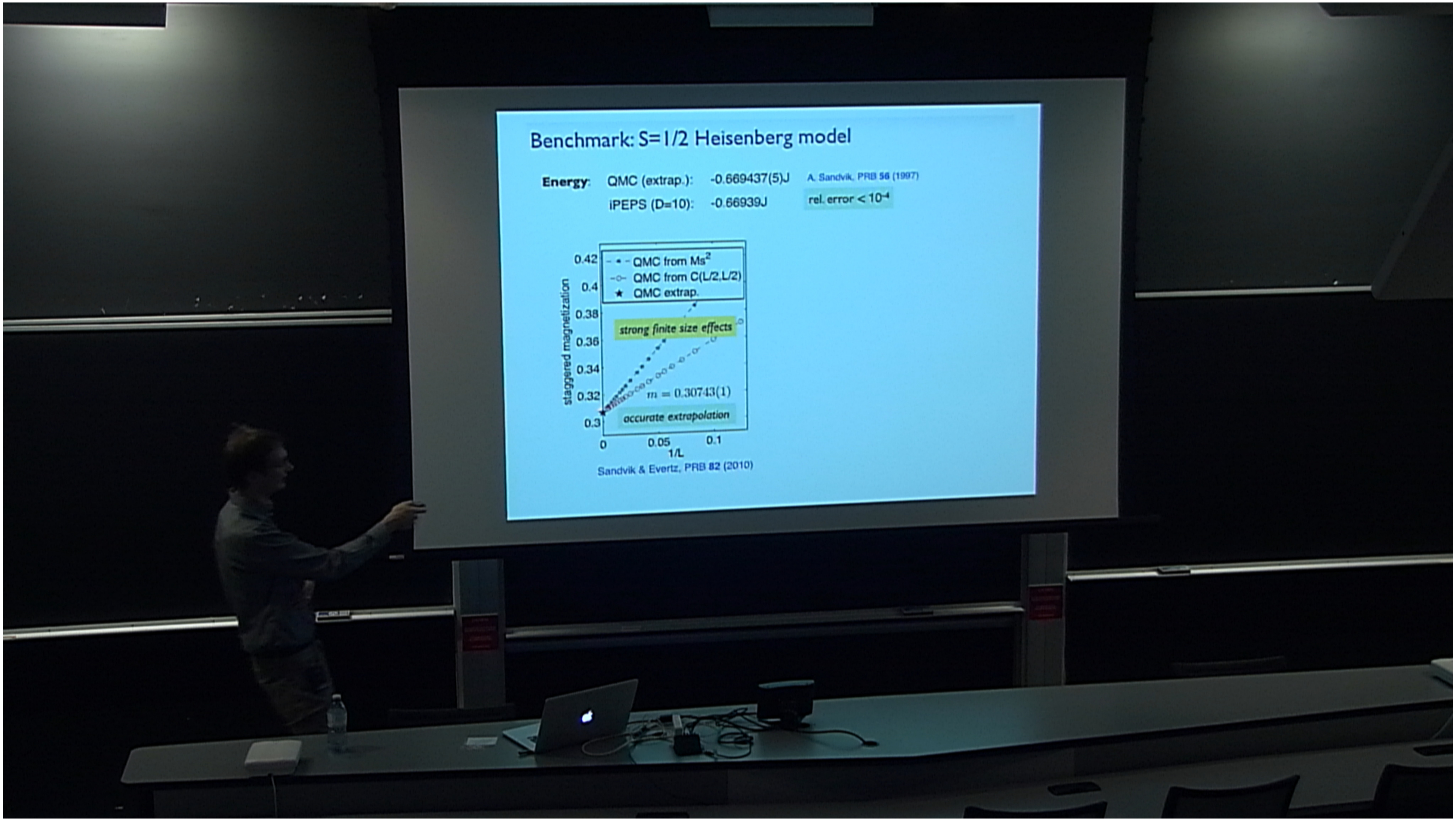
Shi, Li, Zhao, Zhou (2009)

PC, Orus, Bauer, Vidal (2009)

Pizorn, Verstraete (2010)

Gu, Verstraete, Wen (2010)

...


Benchmark: S=1/2 Heisenberg model
Energy: QMC (extrap.): -0.669437(5)J
A. Sandvik, PRB 56 (1997)
iPEPS (D=10): -0.66939J
rel. error < 10-4
QMC from Ms2
QMC from C(L/2,L/2)
QMC extrap.
strong finite size effects
m = 0.30743(1)
accurate extrapolation
staggered magnetization
0.42
0.4
0.38
0.36
0.34
0.32
0.3
0
0.05
0.1
1/L
Sandvik & Evertz, PRB 82 (2010)

t-J model

PC, T. M. Rice, and M. Troyer, PRL **113** (2014)

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

Nearest-neighbor hopping

Heisenberg interaction

constraint: only one electron per site!

$J/t = 0.4$

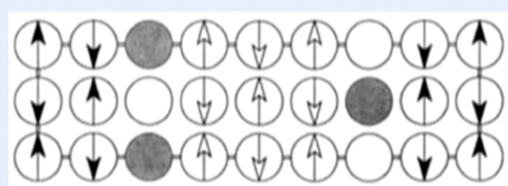
NATURE · VOL 375 · 15 JUNE 1995

Evidence for stripe correlations of spins and holes in copper oxide superconductors

J. M. Tranquada*, B. J. Sternlieb†, J. D. Axe*, Y. Nakamura† & S. Uchida†

* Physics Department, Brookhaven National Laboratory, Upton, New York 11973, USA
† Superconductivity Research Course, The University of Tokyo, Yayoi 2-11-16, Bunkyo-ku, Tokyo 113, Japan

ONE of the long-standing mysteries associated with the high-temperature copper oxide superconductors concerns the anomalous suppr… …ertain relate… …Here we ex… …mical two-di… …the crysta… …O_4 by neutr… …mmen-surabi… …and charg… …s are separated by periodically spaced domain walls to which the holes segregate[5–9]. An ordered stripe phase of this type has recently been observed in hole-doped La_2NiO_4 (refs 10–12). We present evidence from neutron diffraction that in the copper oxide material $La_{1.6-x}Nd_{0.4}Sr_xCuO_4$, with $x = 0.12$, a static analogue of the dynamical stripe phase is present, and is associated with an anomalous suppression of superconductivity[13,14]. Our results thus provide an explanation of the '$\frac{1}{8}$' conundrum, and also support the suggestion[15] that spatial modulations of spin and charge density are related to superconductivity in the copper oxides.



PC, T. M. Rice, and M. Troyer, PRL **113** (2014)

$(S_iS_j - \frac{1}{4}n_in_j)$

…enberg interaction

constraint: only one electron per site!

$J/t = 0.4$

…ce the
…rved in
…rates? ?

t-J model

PC, T. M. Rice, and M. Troyer, PRL **113** (2014)

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

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!**

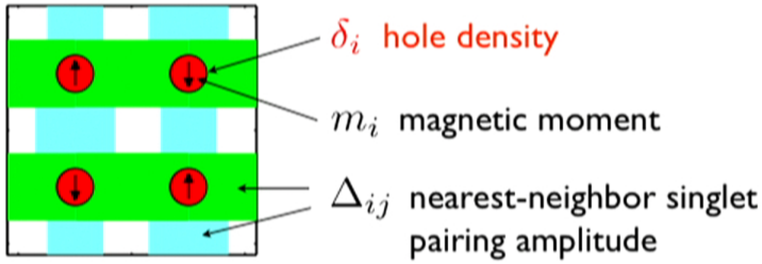
Variational Monte Carlo
Fixed-node Monte Carlo **NO!**
➔ *uniform d-wave state!*

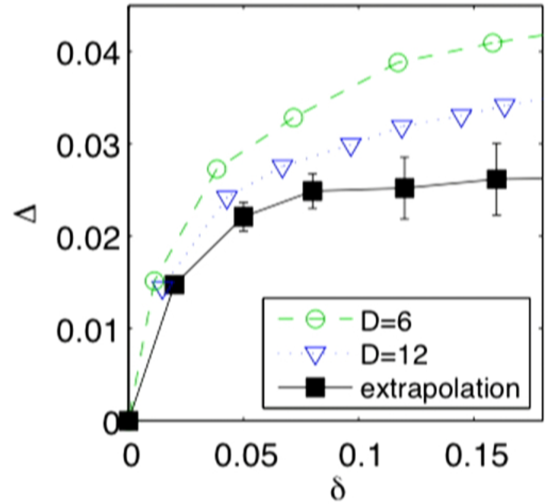
White & Scalapino, PRL **80** (1998)
White & Scalapino, PRB **60** (1999)

Lugas, et al. PRB **74** (2006)
Hu, Becca & Sorella, PRB **85** (2012)
Himeda, Kato & Ogata, PRL **88** (2002)
... and more ...

Uniform d-wave SC state (+AF order)

iPEPS result
2x2 cell





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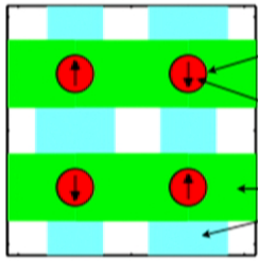


δ_i hole density

m_i magnetic moment

Δ_{ij} nearest-neighbor singlet pairing amplitude

★ Finite d-wave pairing for any finite doping

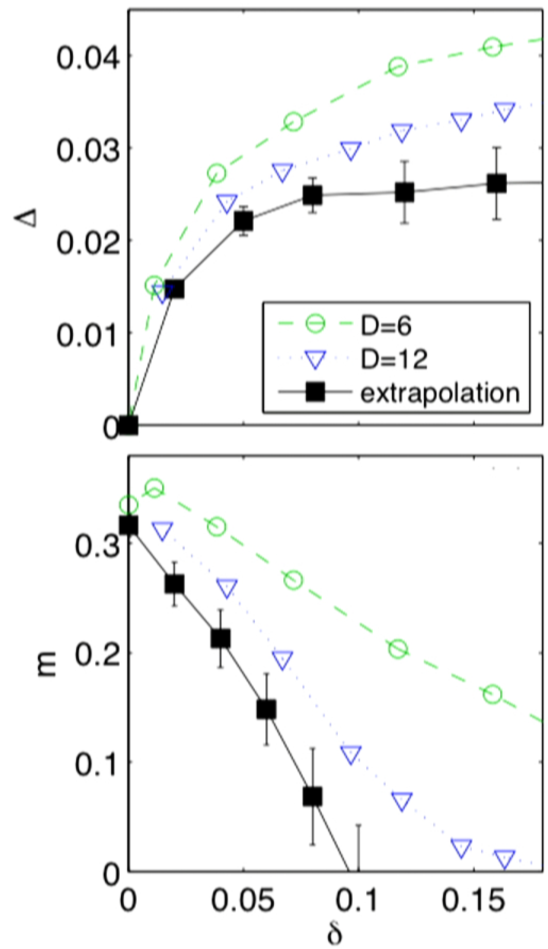
★ Coexisting with AF order for $\delta \lesssim 0.1$

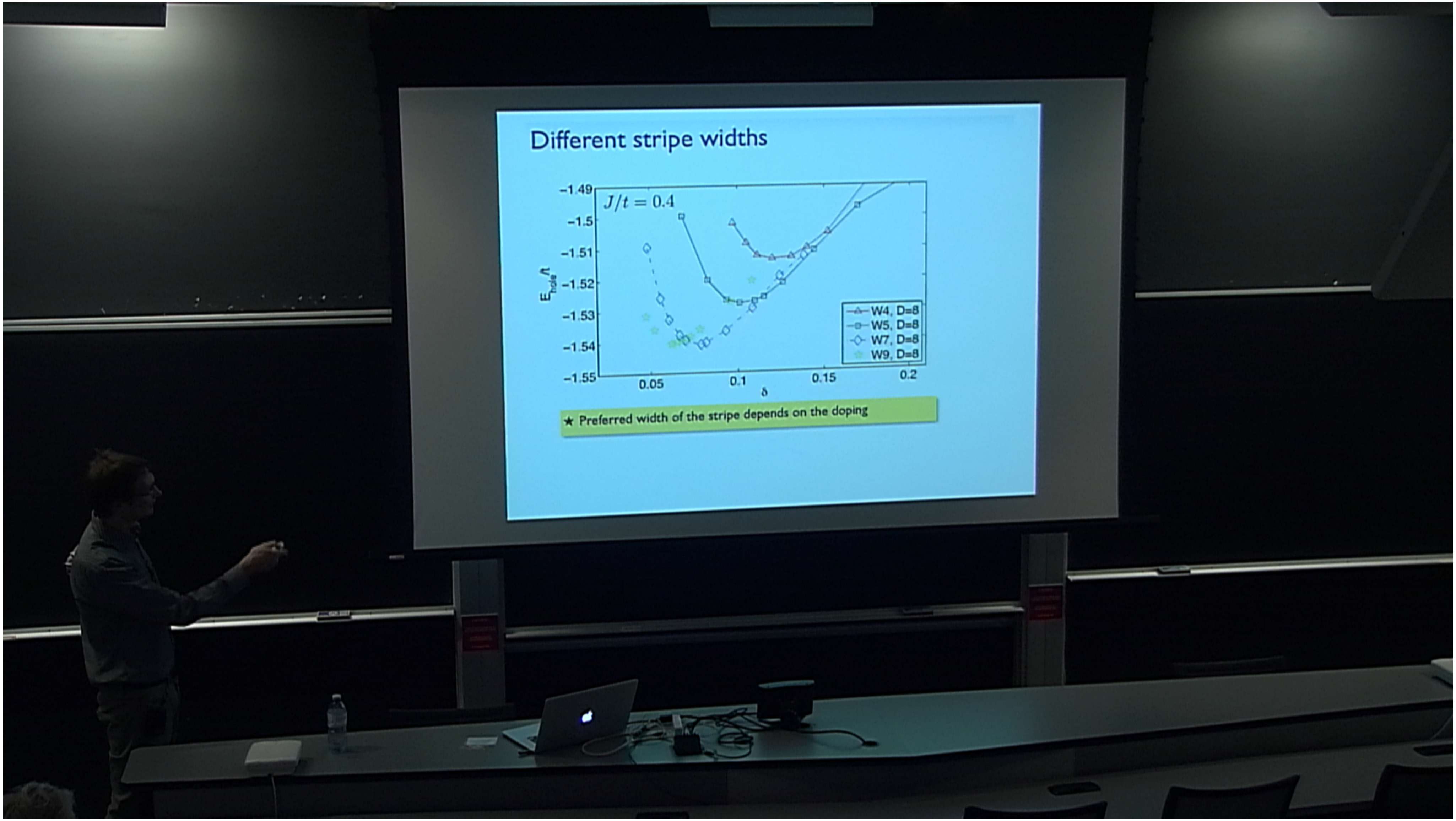
★ In agreement with previous studies
[Himeda et al. '02, Ogata et al. '03, Ivanov '04, Shih et al. '04, Lugas et al. '06, Spanu et al. '08, Hu '12]

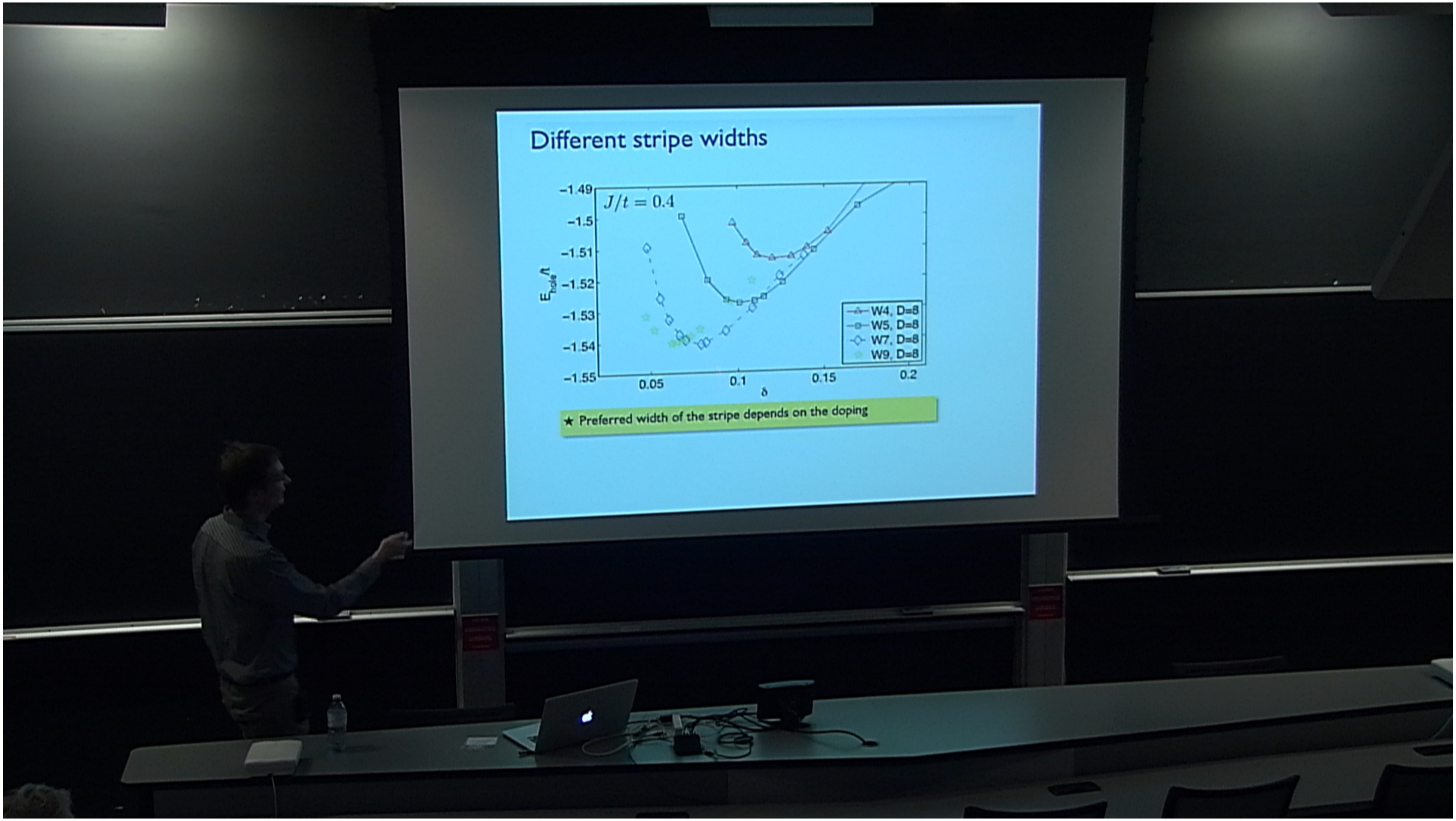
★ **Lower energy than best VMC result**:

FNMC+2L [Hu'12] : -1.546 t
iPEPS (D=14): -1.578 t

$\delta = 0.12$



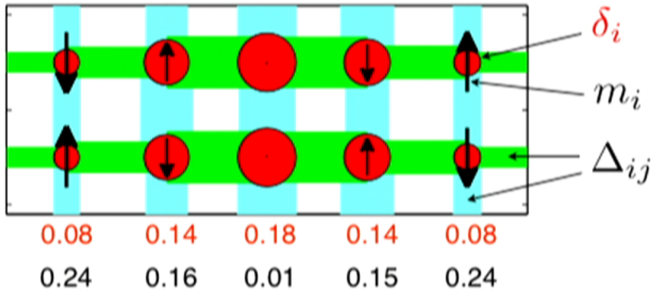

Different stripe widths
J/t = 0.4
E_hole/t
δ
W4, D=8
W5, D=8
W7, D=8
W9, D=8
★ Preferred width of the stripe depends on the doping



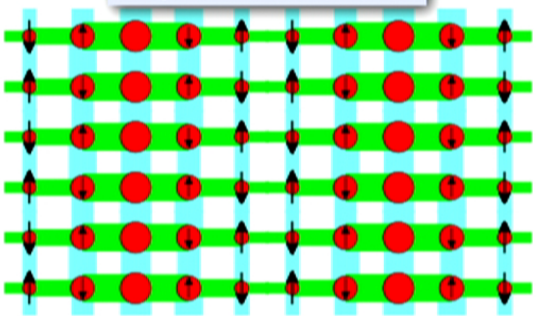
Different stripe widths
J/t = 0.4
E_hole/t
δ
W4, D=8
W5, D=8
W7, D=8
W9, D=8
★ Preferred width of the stripe depends on the doping

Vertical stripe state

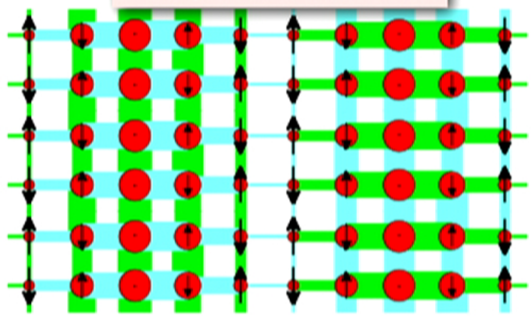
iPEPS result 5x2 cell



in-phase SC order



anti-phase SC order



★ Modulation in the hole-density, AF and SC order

★ "Site-centered" stripe (not bond-centered)

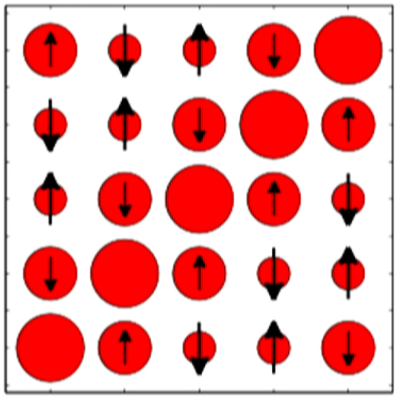
★ π-phase shift in the AF order

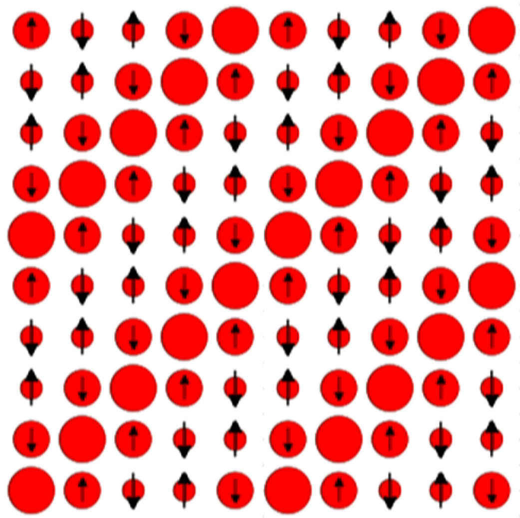
★ Preferred stripe width depends on doping (width-5 stripe lowest around $\delta = 0.12$)

★ *In-phase* and anti-phase stripes have a similar energy (difference: O(0.001t))
Berg et al. '07: Anti-phase stripes lead to effective decoupling between the CuO planes. Explains lack of 3D SC above 4K in $La_{2-x}Ba_xCuO_4$ around x=1/8 [Li et al '07]

Diagonal stripe states

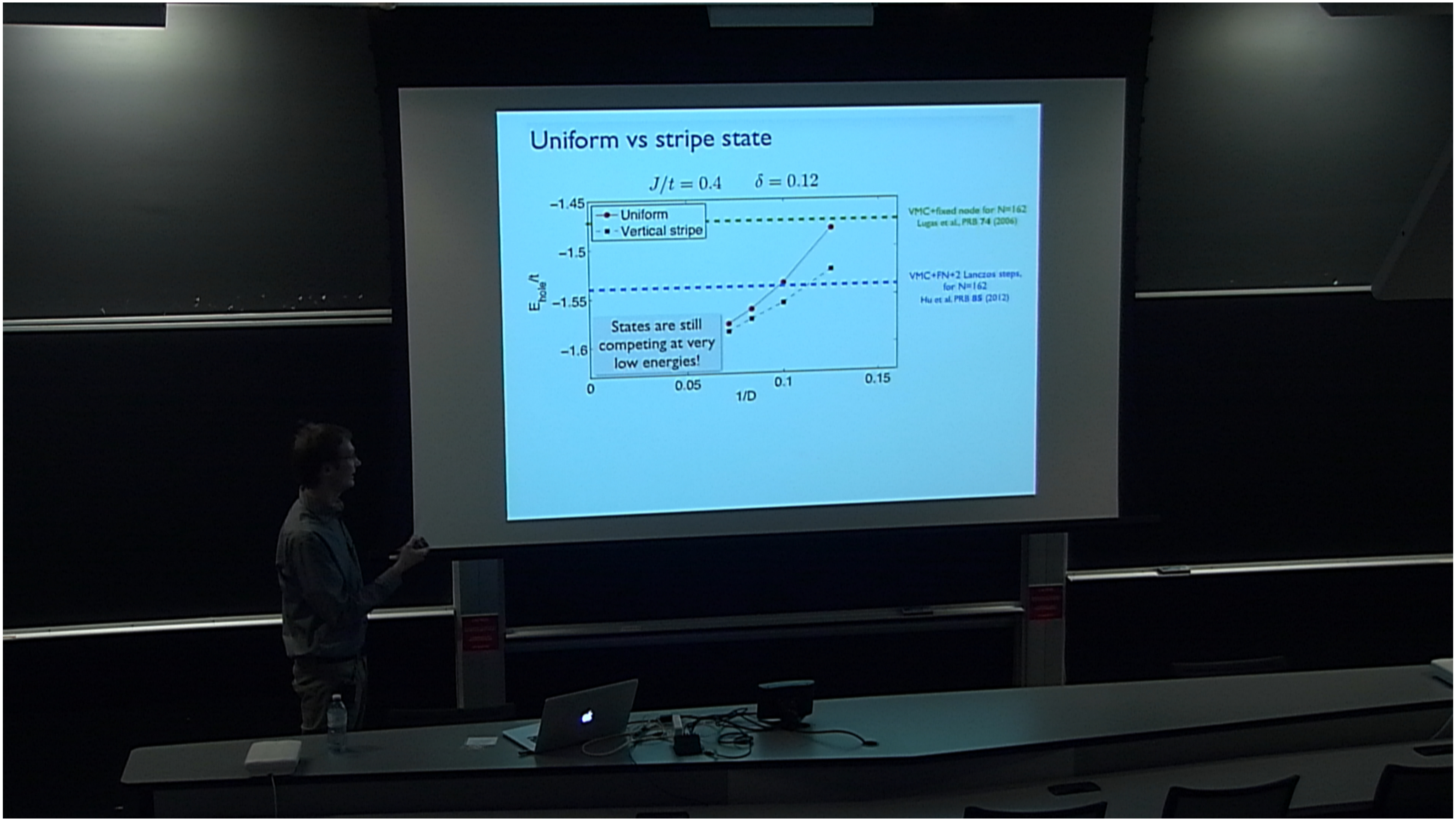
5x5 cell

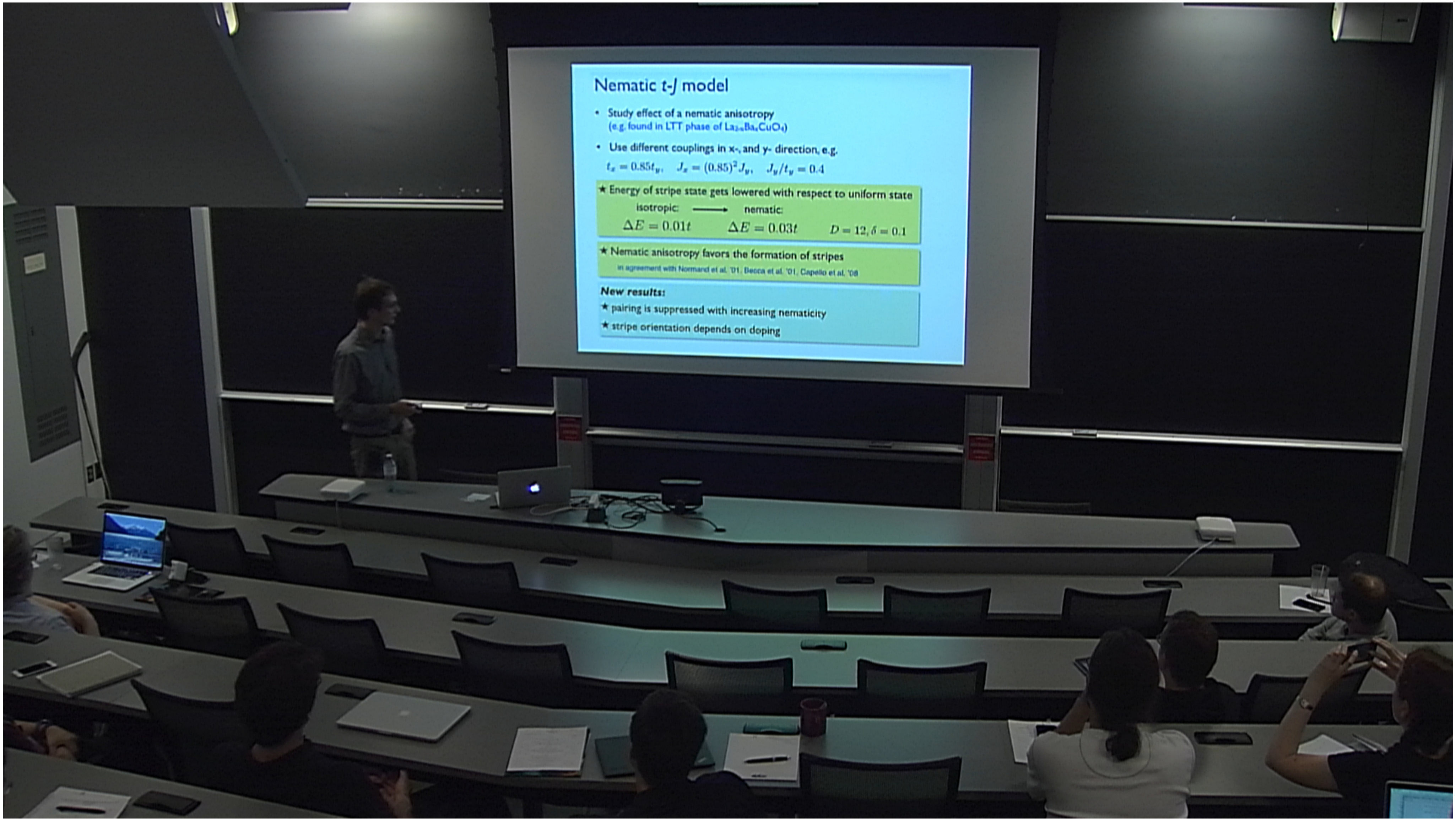


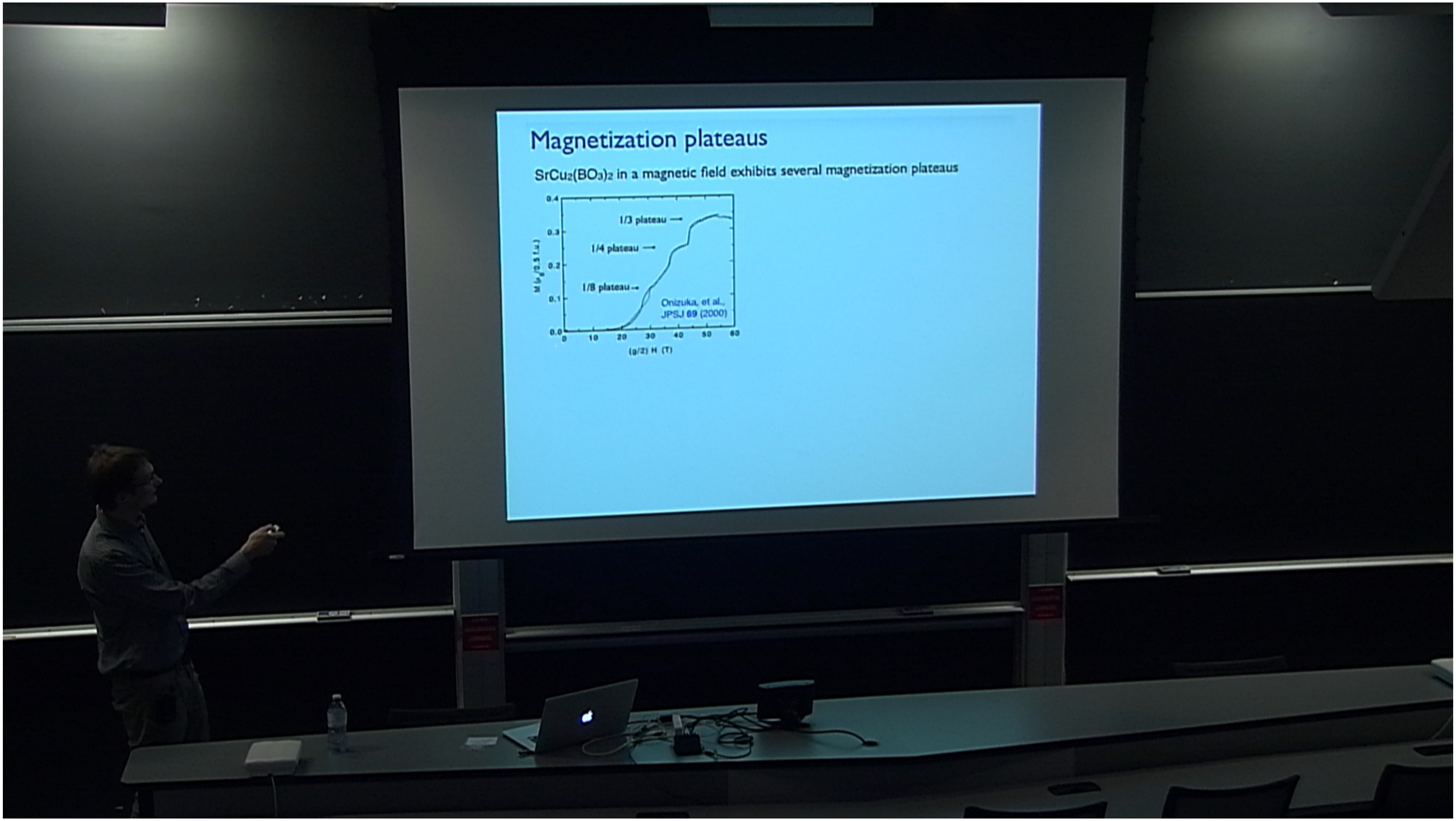


★ Insulating with a filling of 1 hole per unit length per stripe

★ Competing state, but higher in energy for large D

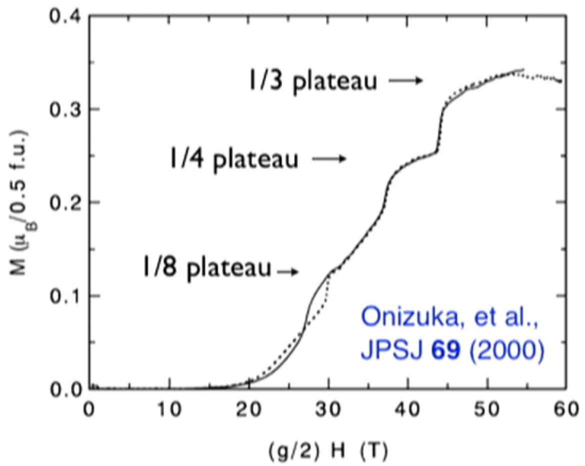

Uniform vs stripe state
$J/t = 0.4$ $\delta = 0.12$
Uniform
Vertical stripe
VMC+fixed node for N=162
Lugas et al., PRB 74 (2006)
VMC+FN+2 Lanczos steps,
for N=162
Hu et al. PRB 85 (2012)
E_{hole}/t
−1.45
−1.5
−1.55
−1.6
0
0.05
0.1
0.15
1/D
States are still competing at very low energies!


Nematic t-J model
• Study effect of a nematic anisotropy
(e.g. found in LTT phase of $La_{2-x}Ba_xCuO_4$)
• Use different couplings in x-, and y- direction, e.g.
$t_x = 0.85 t_y, \quad J_x = (0.85)^2 J_y, \quad J_y/t_y = 0.4$
★ Energy of stripe state gets lowered with respect to uniform state
isotropic: ⟶ nematic:
$\Delta E = 0.01t$ $\Delta E = 0.03t$ $D = 12, \delta = 0.1$
★ Nematic anisotropy favors the formation of stripes
in agreement with Normand et al. '01, Becca et al. '01, Capello et al. '08
New results:
★ pairing is suppressed with increasing nematicity
★ stripe orientation depends on doping


Magnetization plateaus
SrCu2(BO3)2 in a magnetic field exhibits several magnetization plateaus
1/3 plateau
1/4 plateau
1/8 plateau
Onizuka, et al., JPSJ 69 (2000)
(g/2) H (T)

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)

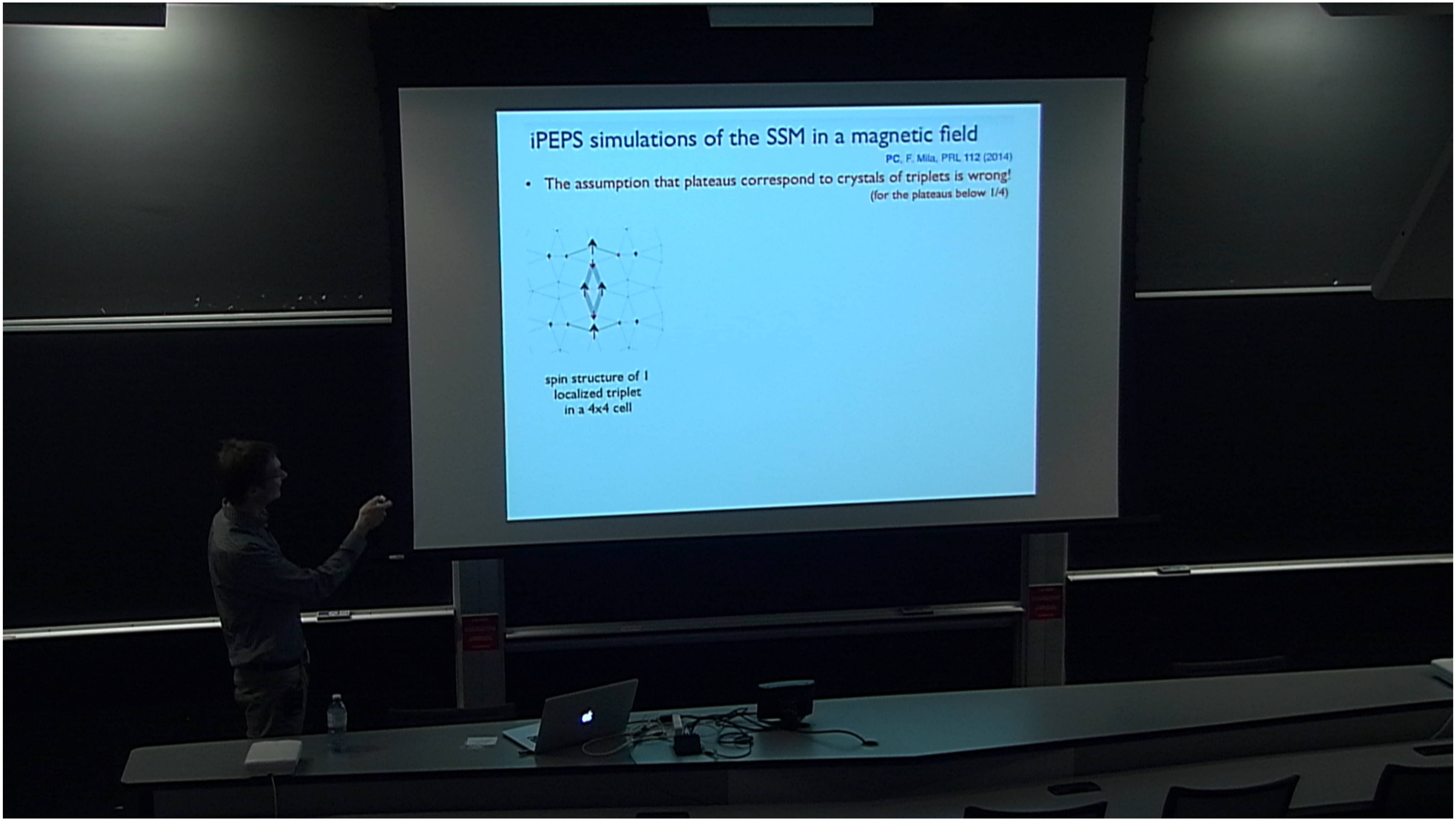
Magnetization plateaus

- 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...

Kageyama et al, PRL **82** (1999)
Onizuka et al, JPSJ **69** (2000)
Kageyama et al, PRL **84** (2000)
Kodama et al, Science **298** (2002)
Takigawa et al, Physica **27** (2004)
Levy et al, EPL **81** (2008)
Sebastian et al, PNAS **105** (2008)
Isaev et al, PRL **103** (2009)
Jaime et al, PNAS **109** (2012)
Takigawa et al, PRL **110** (2013)
Matsuda et al, PRL **111** (2013)
Miyahara and K. Ueda, PRL **82** (1999)
Momoi and Totsuka, PRB **61** (2000)
Momoi and Totsuka, PRB **62** (2000)
Fukumoto and Oguchi, JPSJ **69** (2000)
Fukumoto, JPSJ **70** (2001)
Miyahara and Ueda, JPCM **15** (2003)
Miyahara, Becca and Mila, PRB **68** (2003)
Dorier, Schmidt, and Mila, PRL **101** (2008)
Abendschein & Capponi, PRL **101** (2008)
Takigawa et al, JPSJ **79** (2010).
Nemec et al, PRB **86** (2012).
Lou et al, arXiv:1212.1999.
...

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


iPEPS simulations of the SSM in a magnetic field
PC, F. Mila, PRL 112 (2014)
• The assumption that plateaus correspond to crystals of triplets is wrong!
(for the plateaus below 1/4)
spin structure of 1
localized triplet
in a 4x4 cell

iPEPS simulations of the SSM in a magnetic field

PC, F. Mila, PRL **112** (2014)

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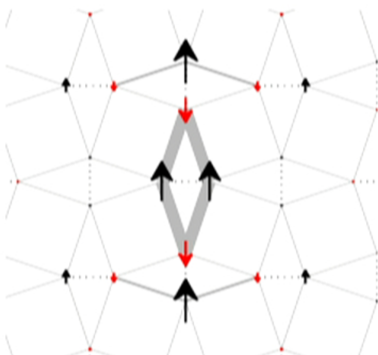
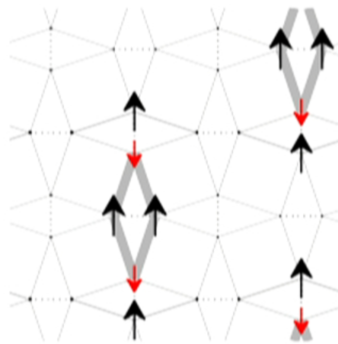
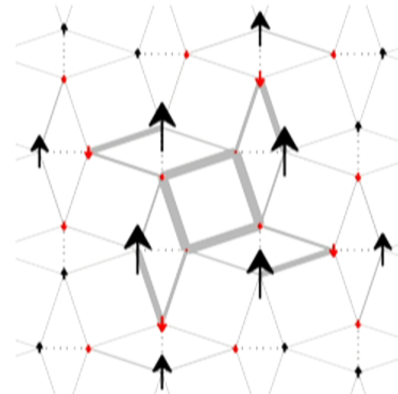


spin structure of 1
localized triplet
in a 4x4 cell



expected spin structure
of 2 localized triplets
in a 4x4 cell

obtained with iPEPS
for small D

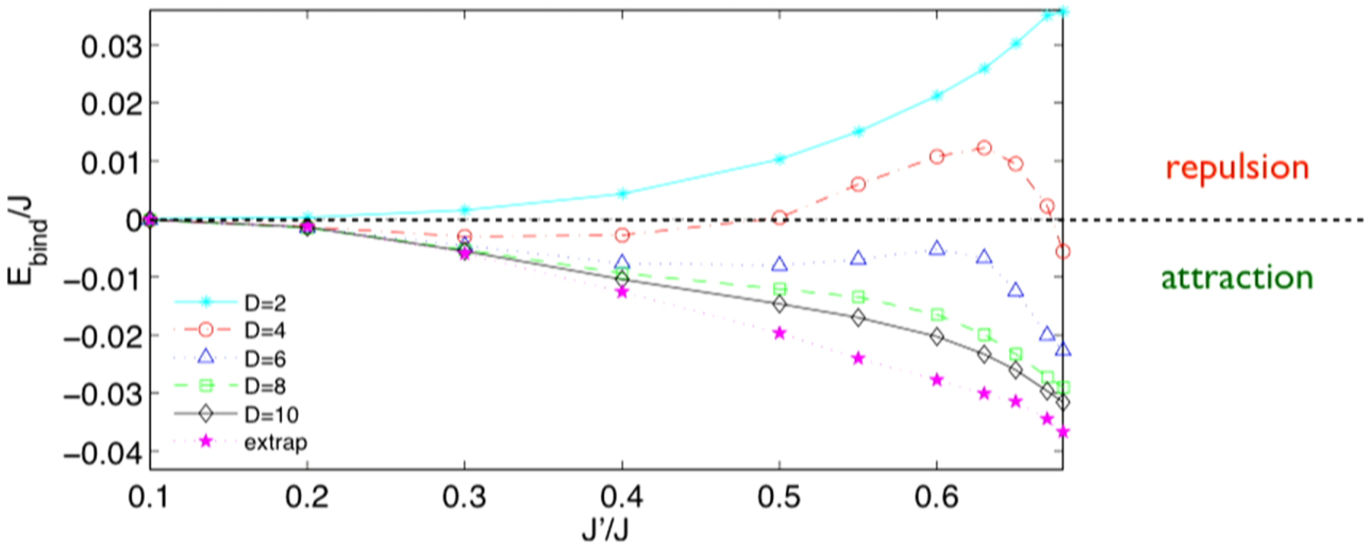


spin structure of a Sz=2
excitation in a 4x4 cell

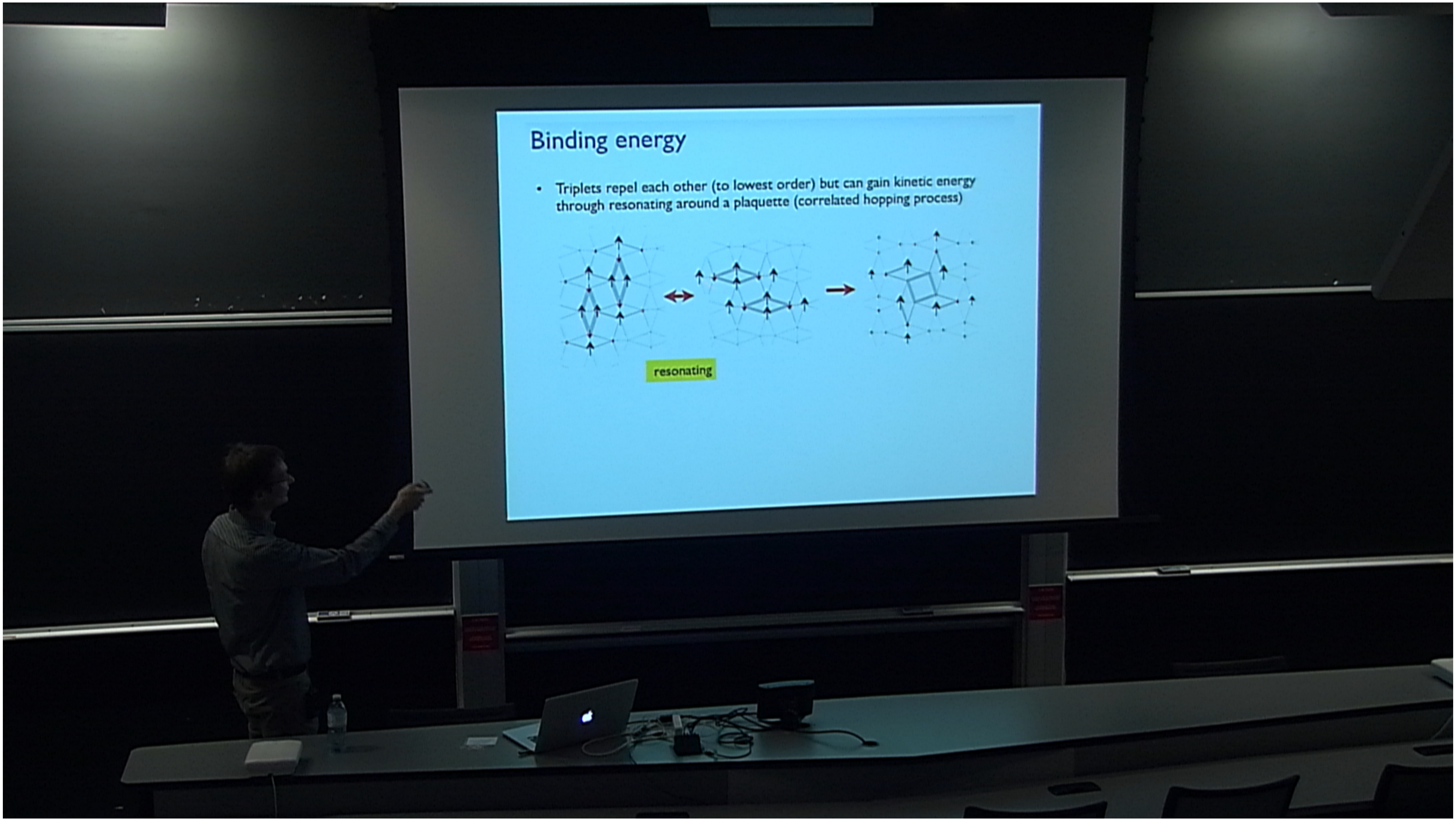
obtained with iPEPS
for D>4

Binding energy

- Compute binding energy of localized bound state: $E^{loc}_{bind} = E^{loc}_{bs} - 2E^{loc}_{triplet}$

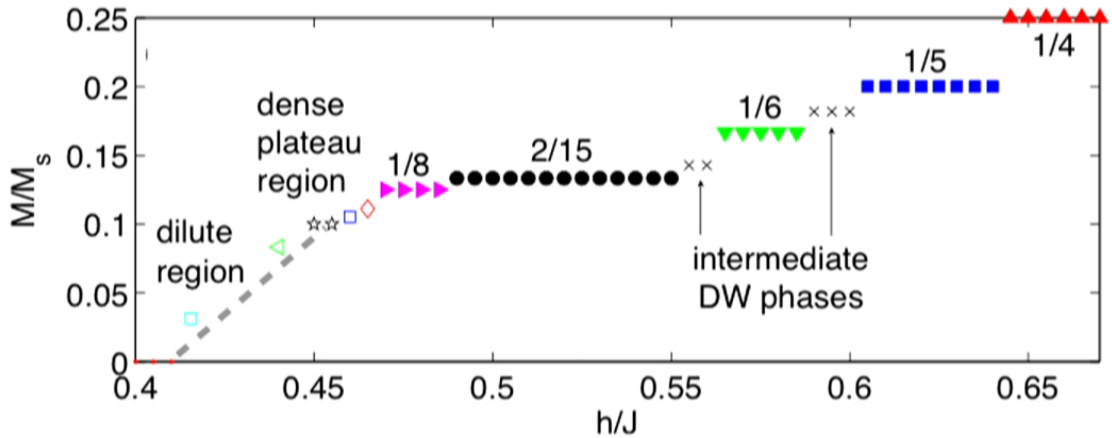


- There is a finite binding energy at sufficiently large D
- "higher-order" quantum fluctuations stabilize bound state


Binding energy
• Triplets repel each other (to lowest order) but can gain kinetic energy through resonating around a plaquette (correlated hopping process)
resonating

Magnetization curve obtained with iPEPS

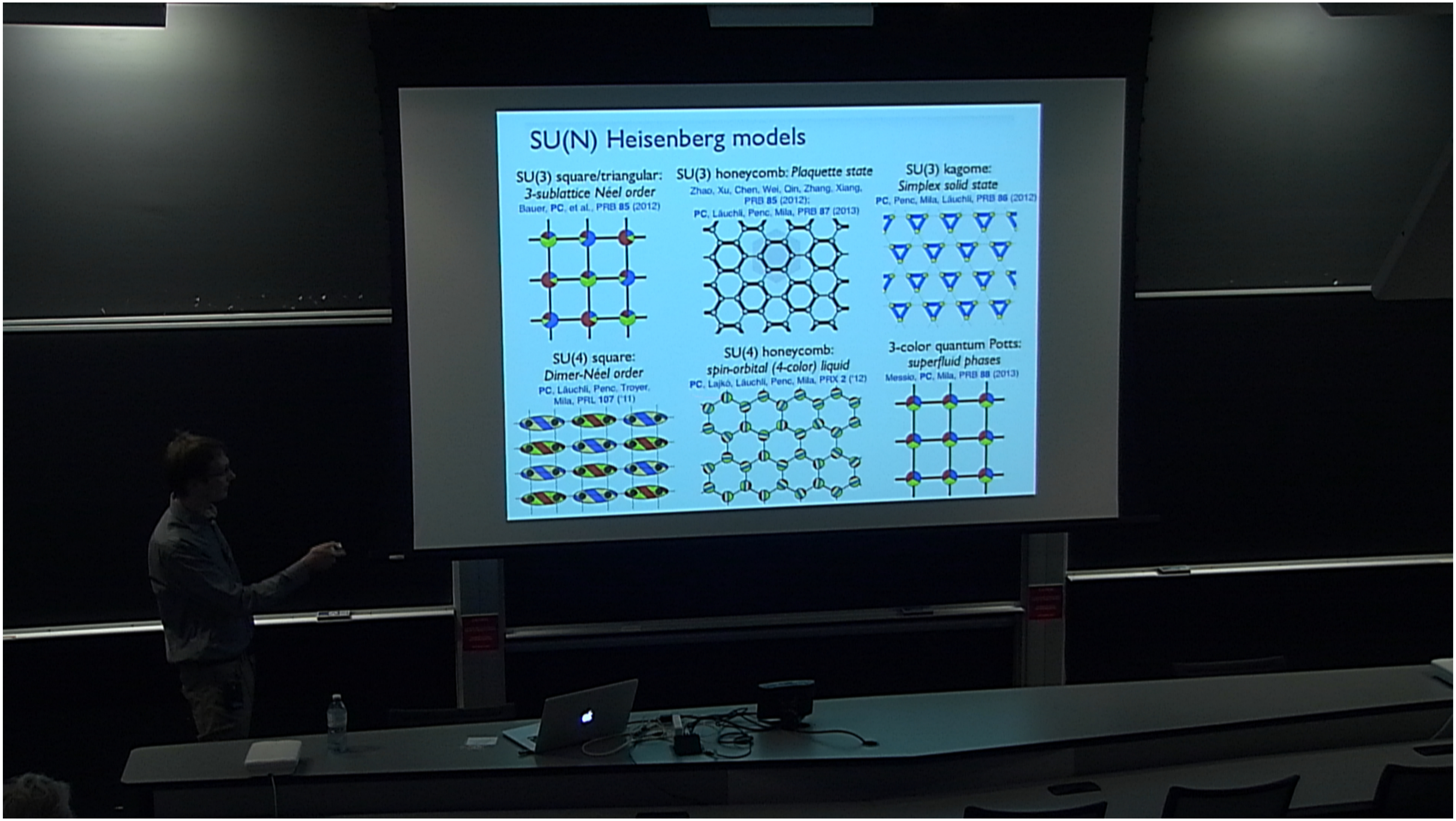
PC, F. Mila, PRL **112** (2014)

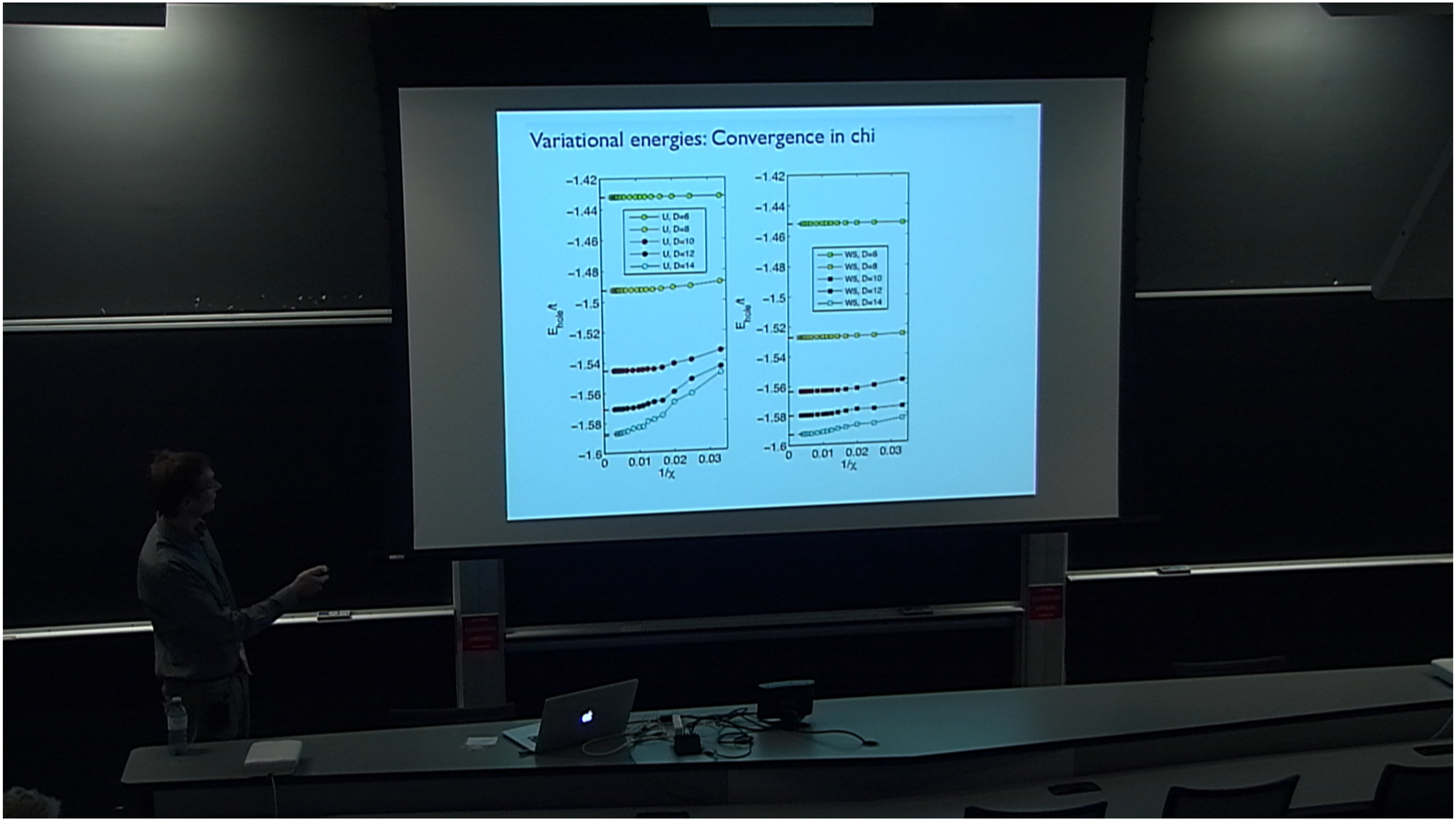


$J'/J = 0.63$

★ 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]


SU(N) Heisenberg models
SU(3) square/triangular:
3-sublattice Néel order
Bauer, PC, et al., PRB 85 (2012)
SU(3) honeycomb: Plaquette state
Zhao, Xu, Chen, Wei, Qin, Zhang, Xiang, PRB 85 (2012);
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)



Variational energies: Convergence in chi
U, D=6
U, D=8
U, D=10
U, D=12
U, D=14
WS, D=6
WS, D=8
WS, D=10
WS, D=12
WS, D=14
E_hole/t
1/χ