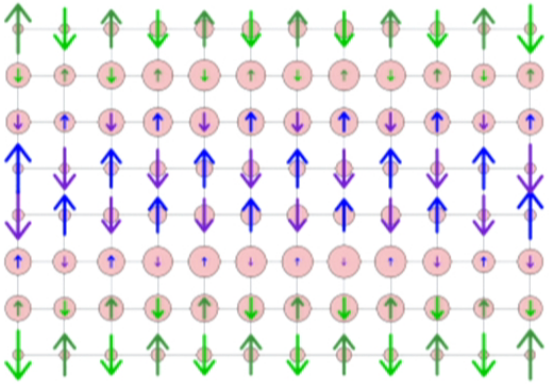
Title: Stripes and pairing in t-J and Hubbard models

Date: Sep 11, 2014 02:00 PM

URL: http://pirsa.org/14090074

Abstract: This has been a leading question in condensed matter physics since the discovery of the cuprate superconductors. In this talk I will review some of the DMRG and tensor network results for the ground states of these models. A key question I'll address is the issue of stripes: are the ground states striped? Do stripes compete with or induce d-wave superconductivity? Another question I'll address is: how well does 2D DMRG do in comparison with iPEPS and quantum Monte Carlo. I will also show recent results for a standard 3-band Hubbard model for the cuprates. The asymmetry between hole and electron doped systems which is seen in the cuprates arises naturally from this model.

Stripes and Pairing in t-J and Hubbard models



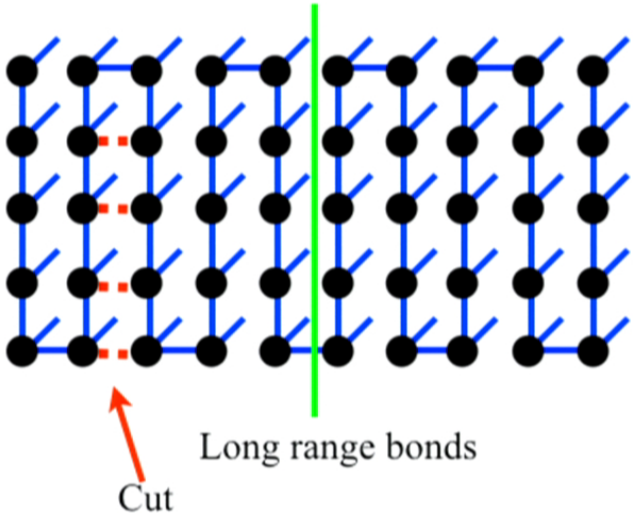
With:
Doug Scalapino

Outline

- DMRG in 2D: quick introduction
- t-J model: Stripes, strong coupling physics
  - Stripes
  - Superconducting stripes
- Hubbard model, 3 band model

Tensor network methods for 2D systems

Traditional DMRG method (MPS state)

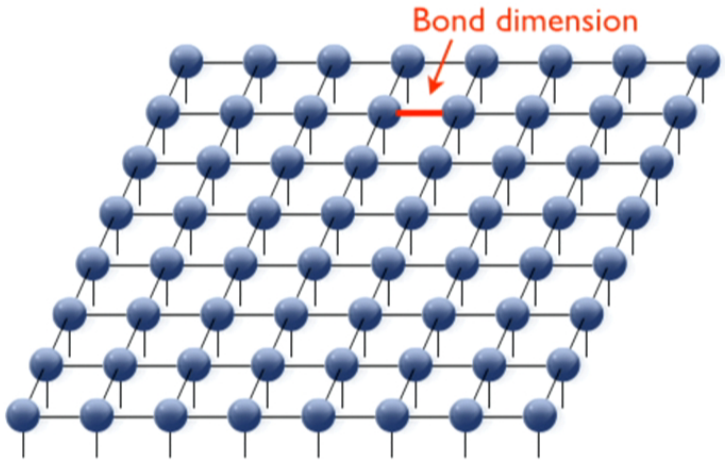


Entropy S ~ L_y ("area law")
Bond dimension m ~ exp(a L_y)

Calc time: $L_x L_y^2 m^3$;
Practical calculations: m ~ 10000,
L_y ~ 12-14 for S=1/2 Heisenberg

PEPS

projected entangled-pair state

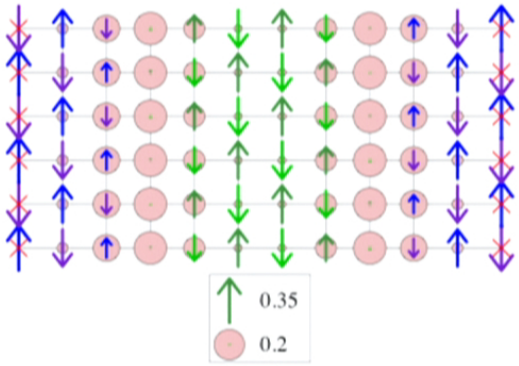


Verstraete and Cirac, cond-mat/0407066

Naturally obeys Area Law
Can work directly with L_x ,$L_y \to \infty$
Calc time: ~m^{12};
Practical calculations: m ~ 15,
S=1/2 Heisenberg

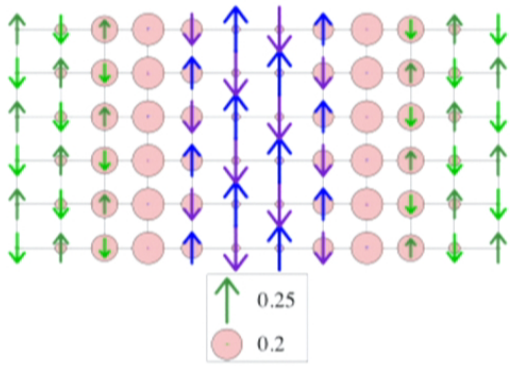
Crossover in accuracy as a function of width for DMRG, L_y ~ 10

t-J model: stripes on width 6 cylinders



12 x 6 system, Vertical PBC's
J/t = 0.35, 8 holes

Pinning AF fields

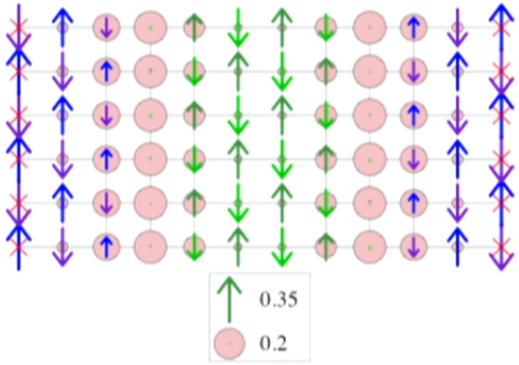


12 x 6 system, Vertical PBC's
J/t = 0.35, 8 holes

No Pinning AF fields
m=1600

- Issues: How well converged are the results with m?
- Are these just finite size artifacts? (i.e. are they just Friedel oscillations?)
- Do the stripes destroy pairing?

t-J model: stripes on width 6 cylinders



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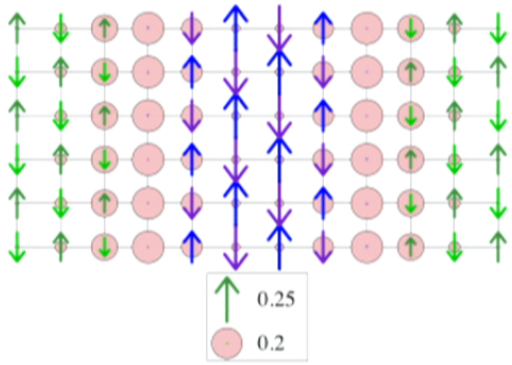

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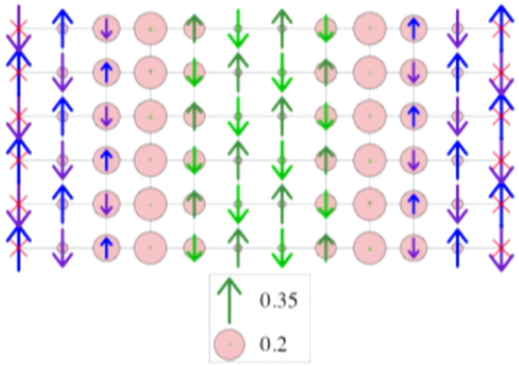

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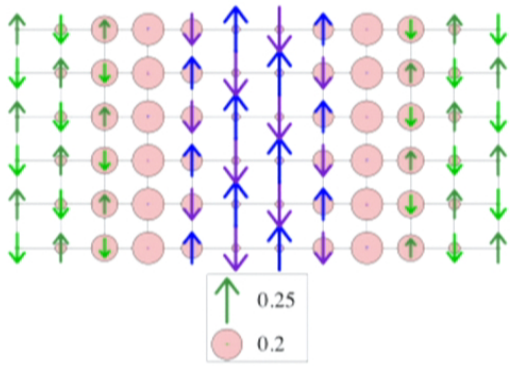

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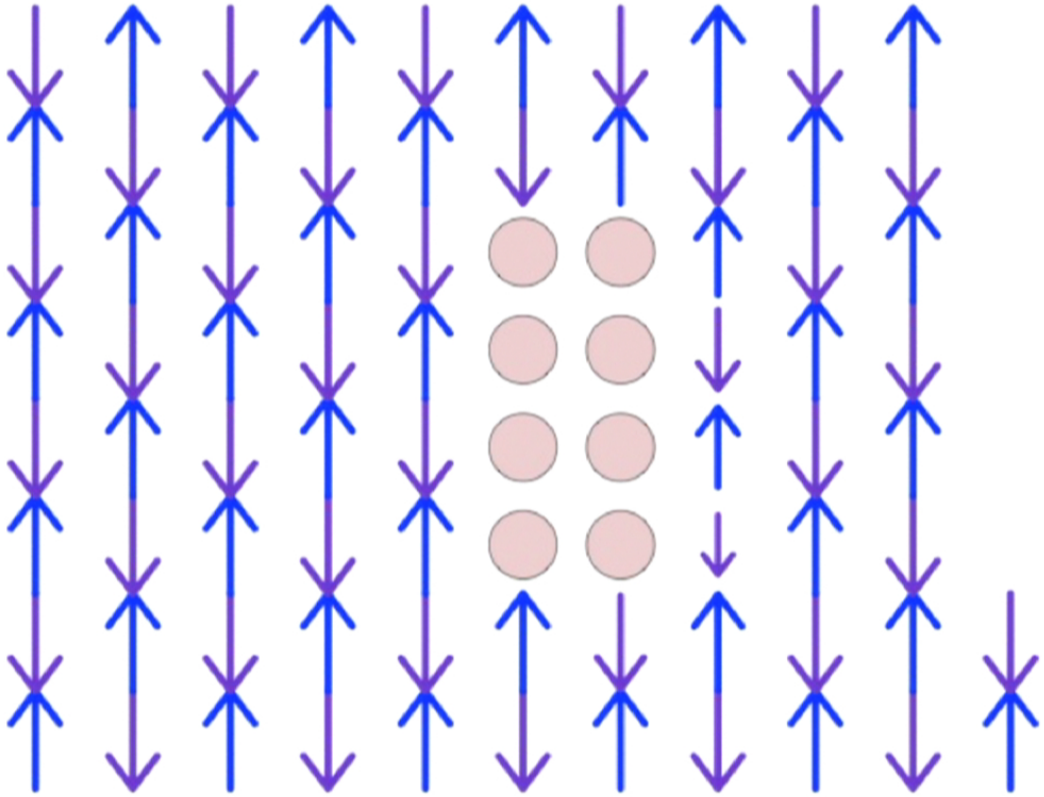
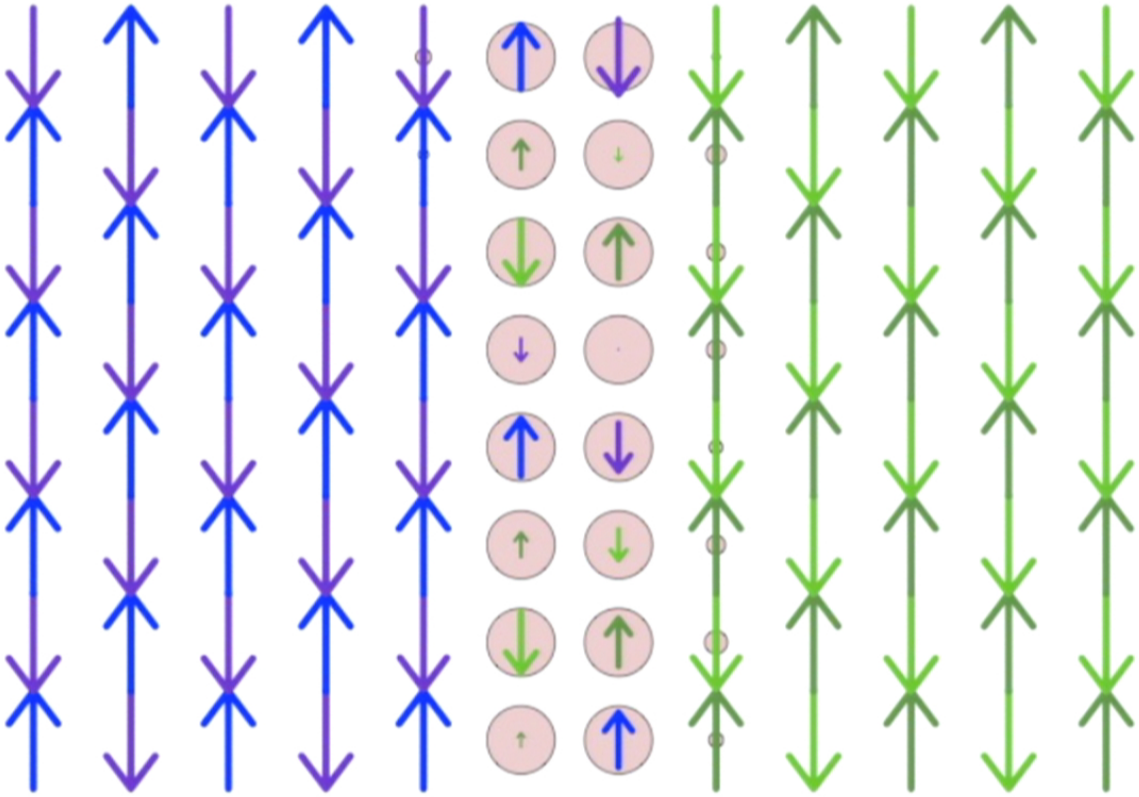
Stripes forming from a blob of 8 holes



E = -30.7350 m = 40

12x8
Cylindrical BCs
t=1, J=0.35
t'=t''=0
8 holes
AF edge pinning fields applied for two sweeps to favor one stripe

Stripes forming from a blob of 8 holes



E = -48.6539

m = 70

12x8
Cylindrical BCs
t=1, J=0.35
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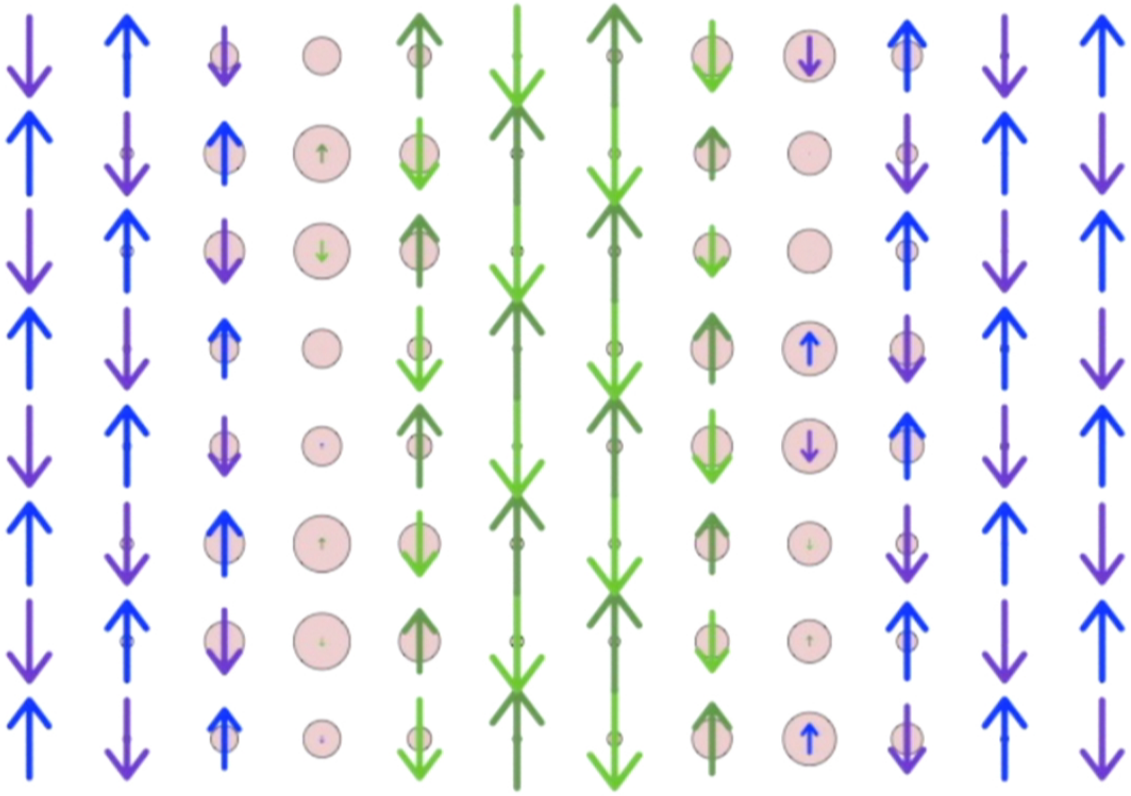

E = -51.6272

m = 1850

12x8
Cylindrical BCs
t=1, J=0.35
t'=t''=0
8 holes
AF edge pinning fields applied for two sweeps to favor one stripe

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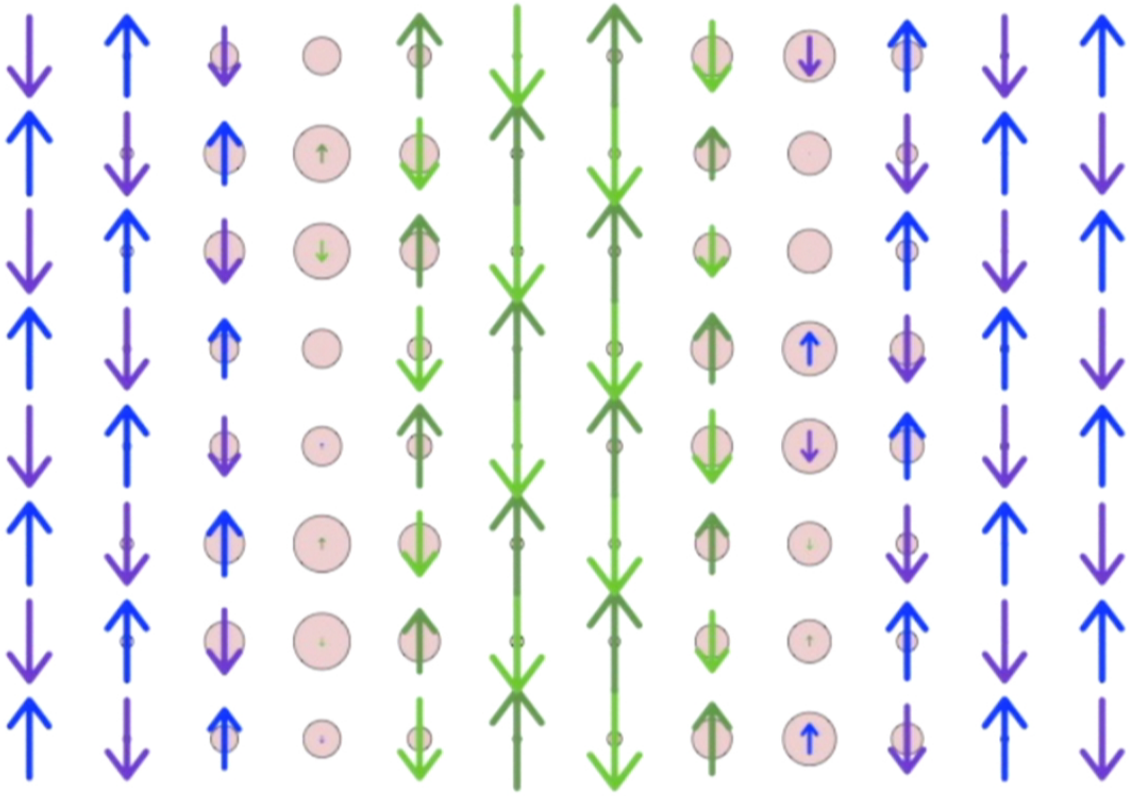

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Cylindrical BCs
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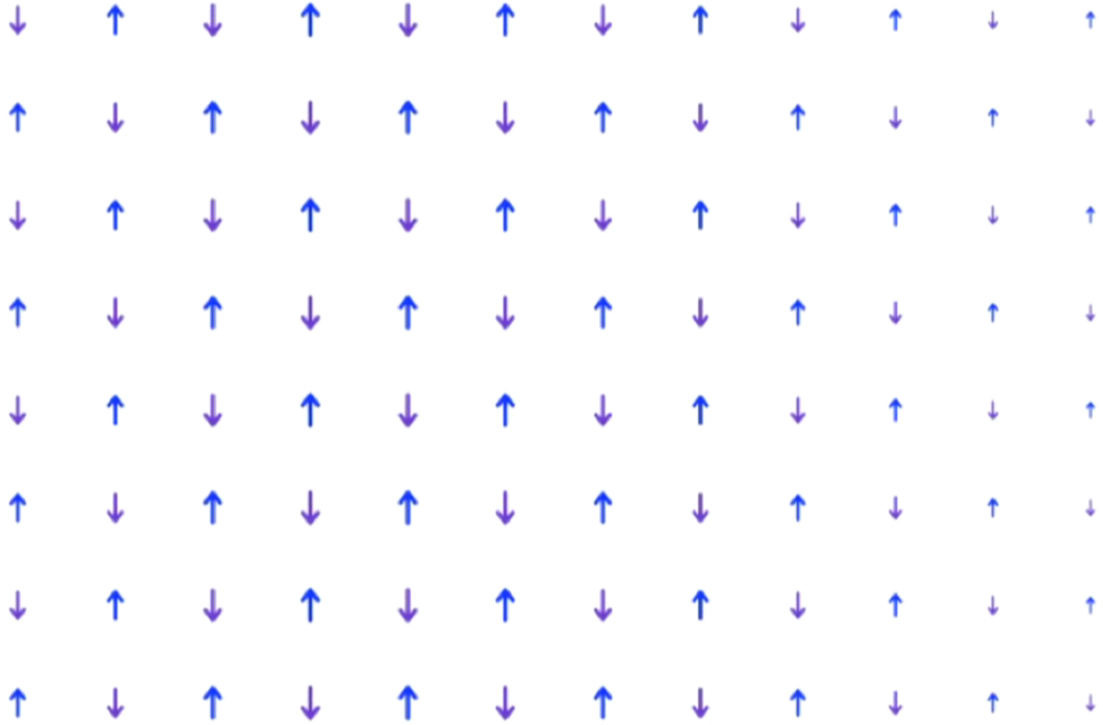
Undoped system: Restoration of SU(2) symmetry



12x8
Cylindrical BCs
J=0.35
0 holes
No pinning fields

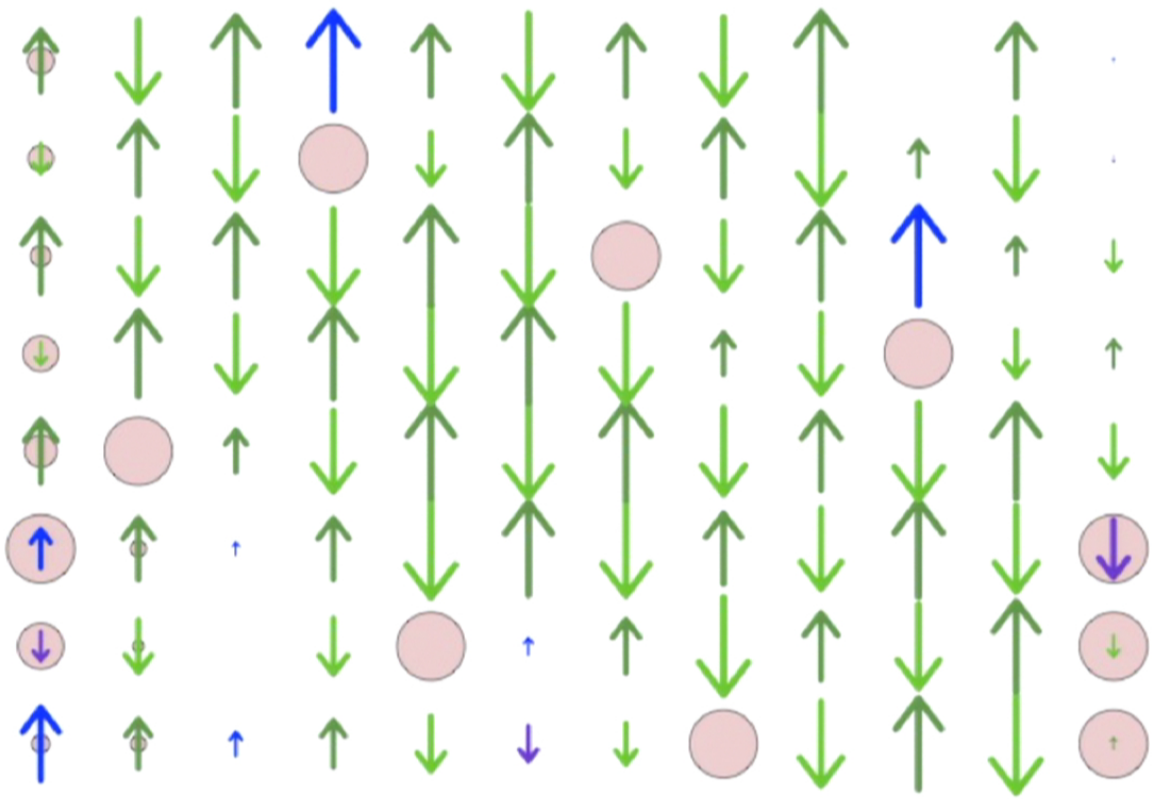
E = -38.0681 m = 600

Undoped system: Restoration of SU(2) symmetry

12x8
Cylindrical BCs
J=0.35
0 holes
No pinning
fields

E = -38.0810 m = 2000

Stripes not forming from a bad initial state

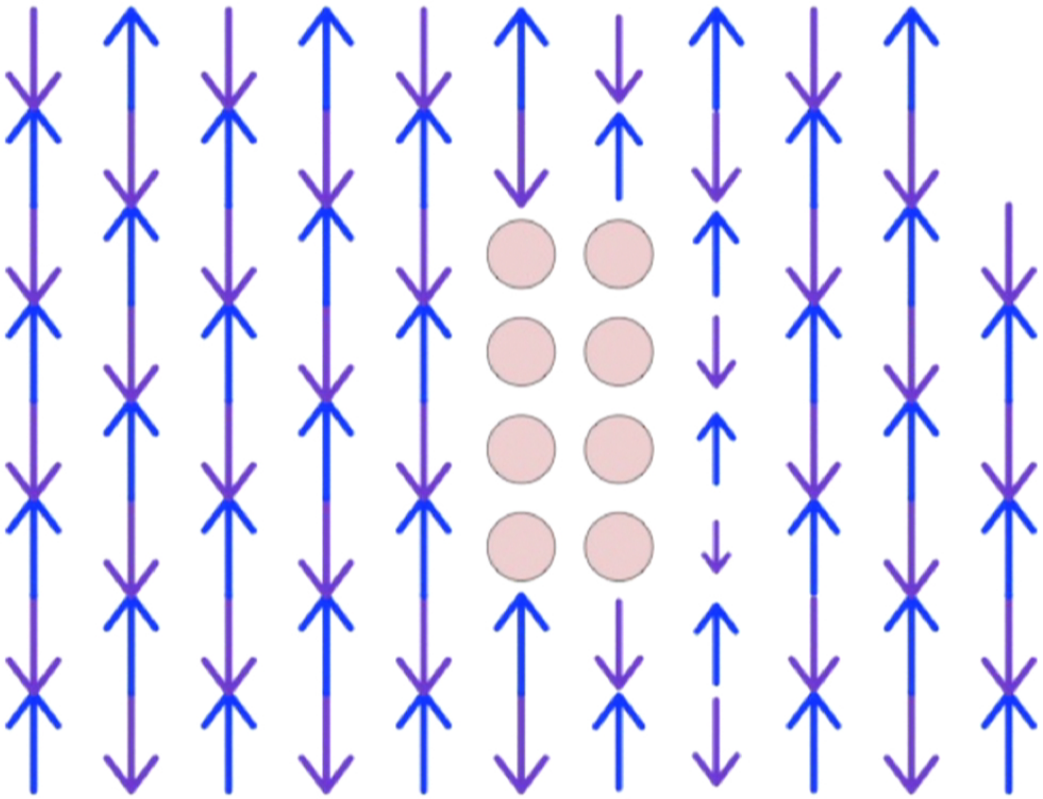


E = -30.6370

m = 70

12x8
Cylindrical BCs
t=1, J=0.35
t'=t''=0
8 holes
No pinning fields.
Initial state has holes spread out so favored striped state is hard to find.
Energy higher by ~0.3 t.

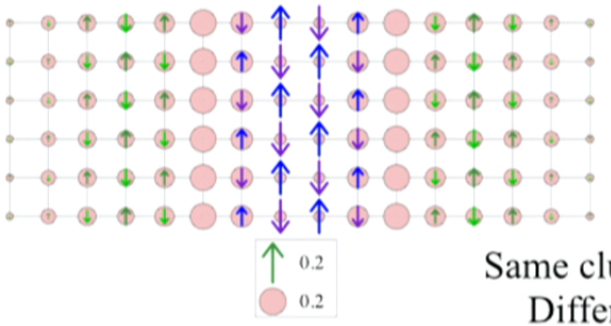
Curved Stripe forms due to open BCs



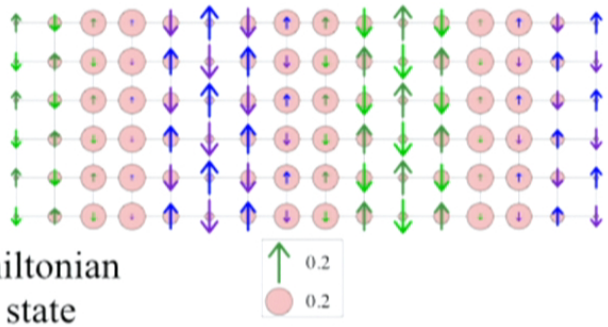
E = -30.8532 m = 40

12x8
Open BCs
t=1, J=0.35
t'=t''=0
8 holes
No pinning
fields

t-J model: stripes on width 6 cylinders



Same cluster, Hamiltonian
Different initial state



16 x 6 system, Vertical PBC's
J/t = 0.35, 12 holes

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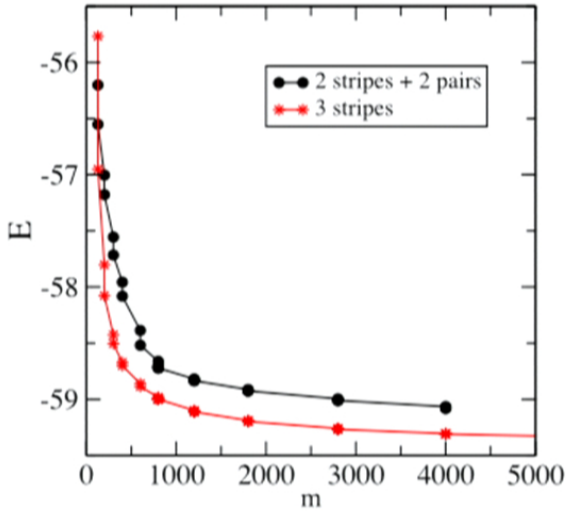
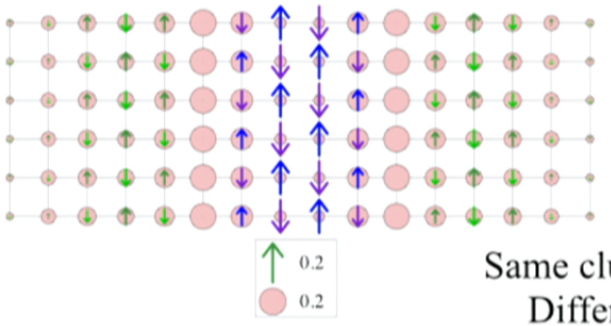


Convergence to metastable state: excellent

Tunneling between metastable states: can be very hard—need to try many initial states

t-J model: stripes on width 6 cylinders



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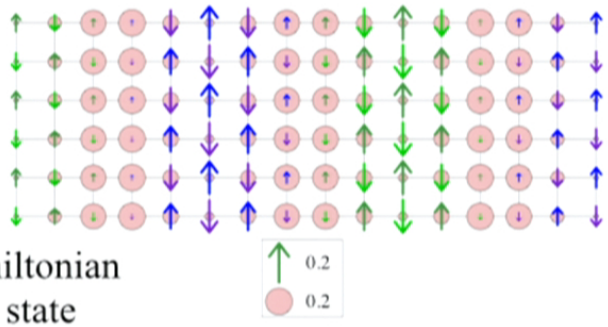

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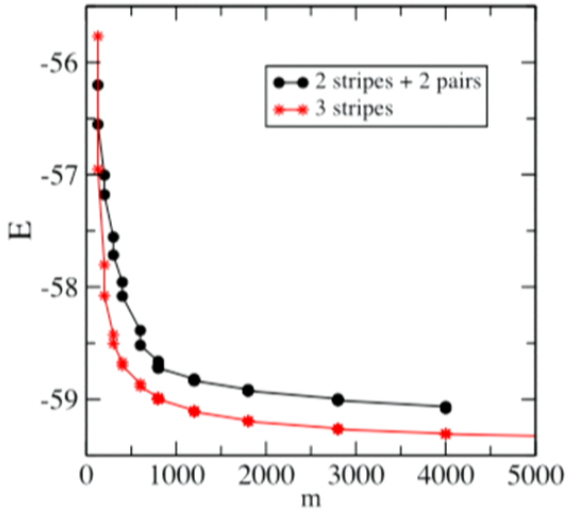

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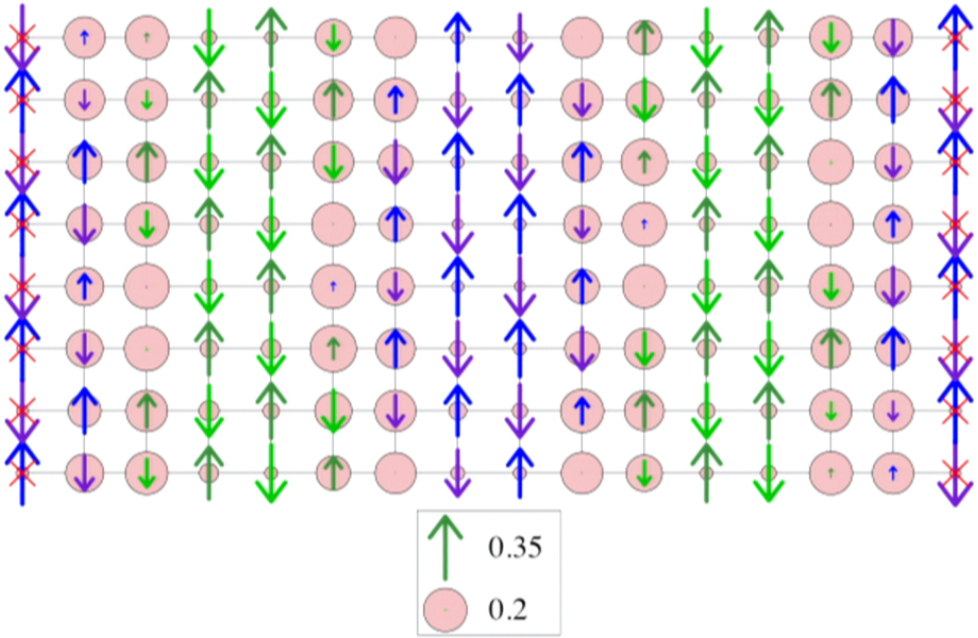
Stripes on 8 leg ladders



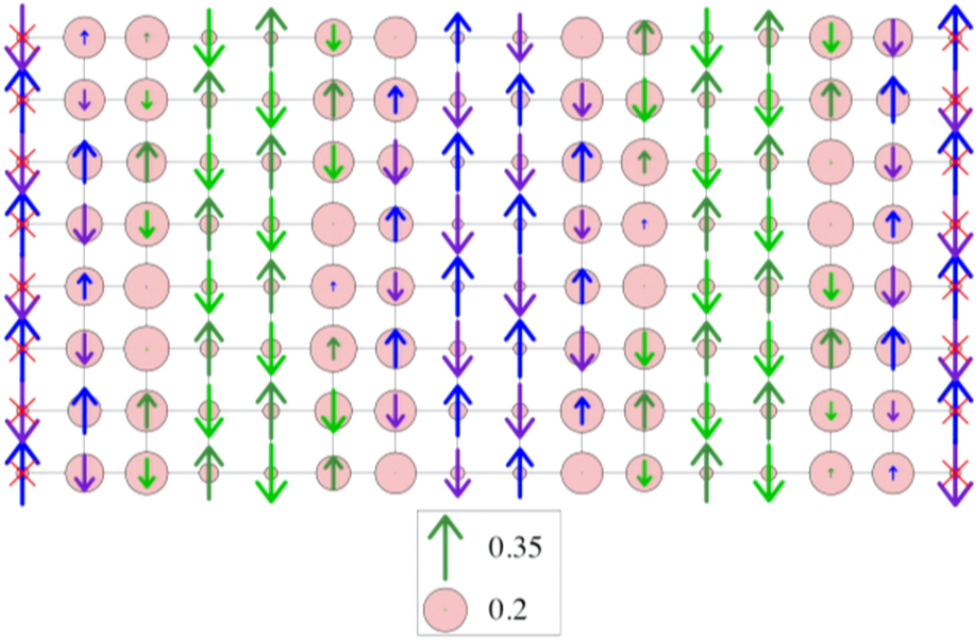
16 x 8 system, Vertical PBC's

J/t = 0.35, 16 holes

White and Scalapino,PRL '98

m ~ 2000 → m ~ 10000-15000 still striped

Stripes on 8 leg ladders



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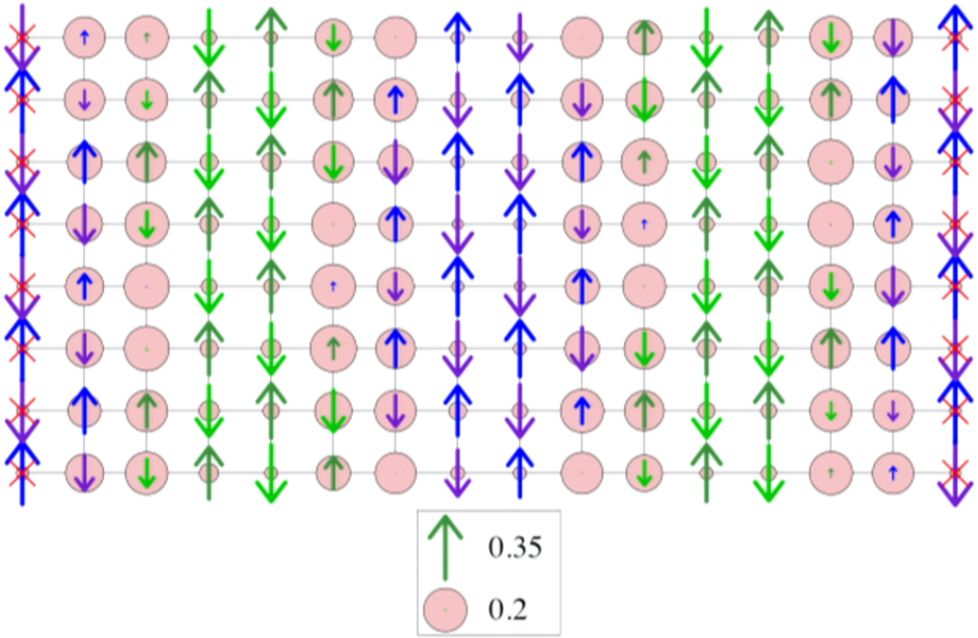

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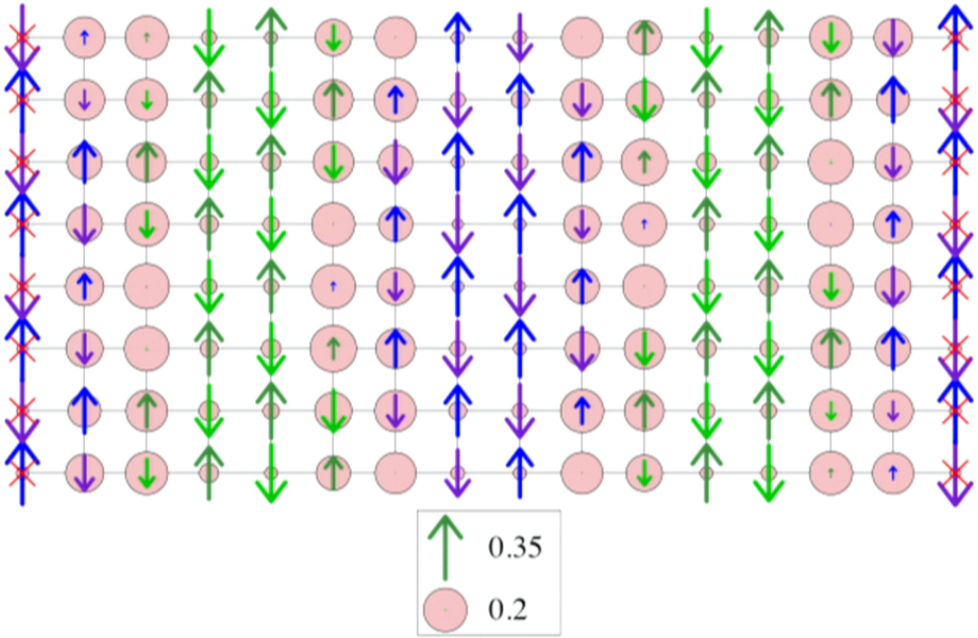

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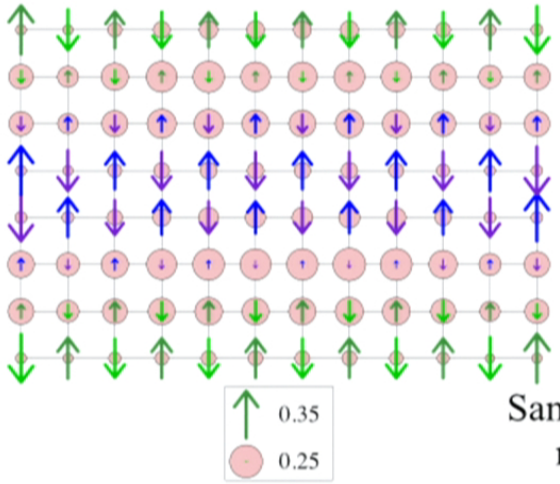
J/t = 0.35, 16 holes

White and Scalapino,PRL '98

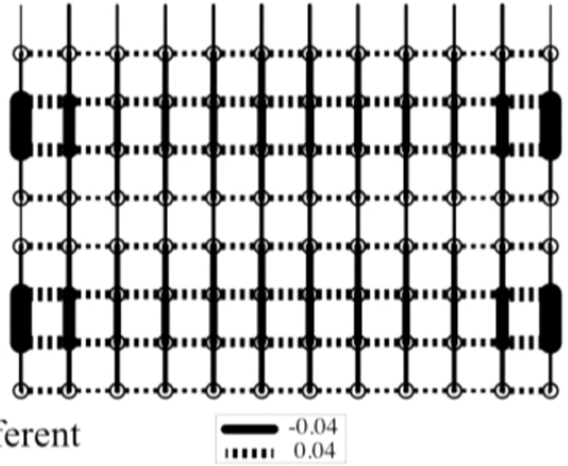
m ~ 2000 → m ~ 10000-15000 still striped

Pairing and stripes, 2 stripes, cylindrical BCs
Particle numbers not conserved



12 x 8 system, Vertical PBC's
Jx/t= 0.55,Jy/t=0.45, mu=1.165,doping=0.1579

Same state, different measurements

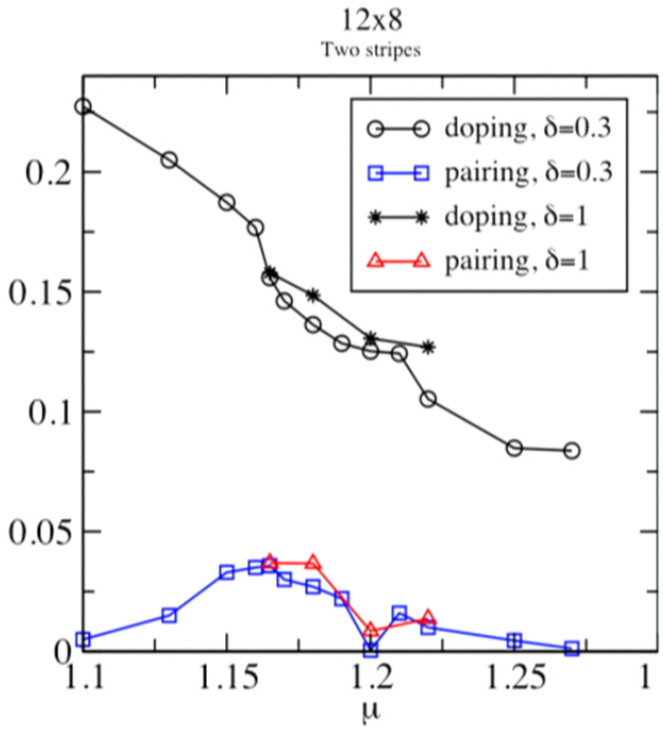


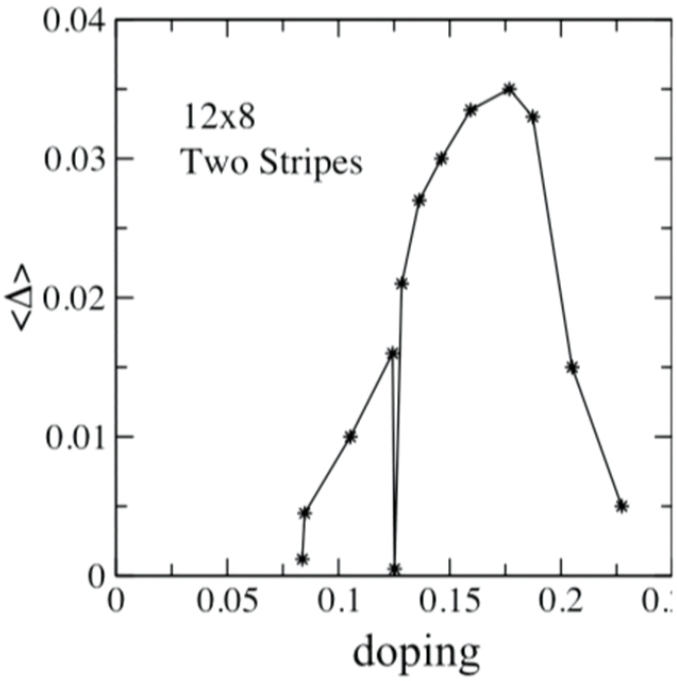
12 x 8 system, Vertical PBC's
Jx/t= 0.55,Jy/t=0.45, mu=1.165,doping=0.1579

Bond thickness shows pairing strength (dashed = negative)

- To orient the stripes longitudinally, we use Jx>Jy.
- Larger J gives stronger pairing.
- Local measurements of response converge much more quickly than correlations, especially for pairing.

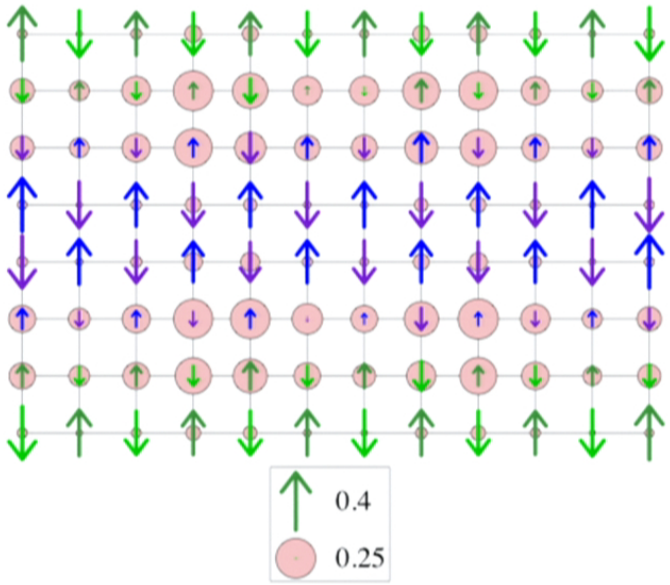
Pairing response in center, two stripes



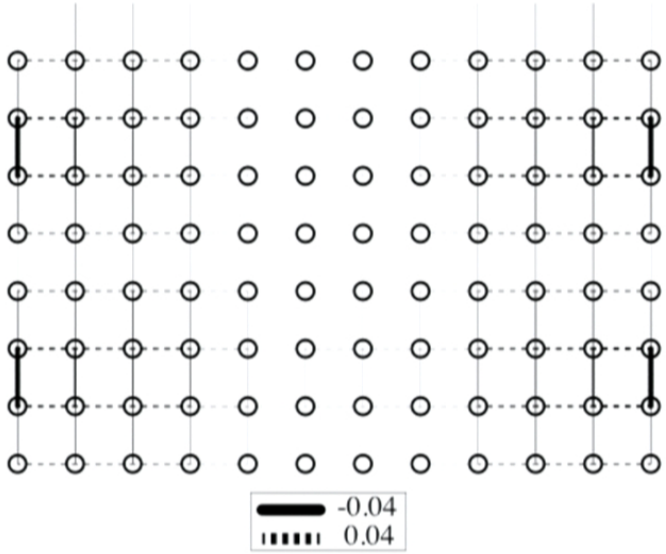


Very similar to some of the cuprates

Pairing suppression at 0.125



12 x 8 system, Vertical PBC's
Jx/t= 0.55,Jy/t=0.45, mu=1.2,doping=0.1252



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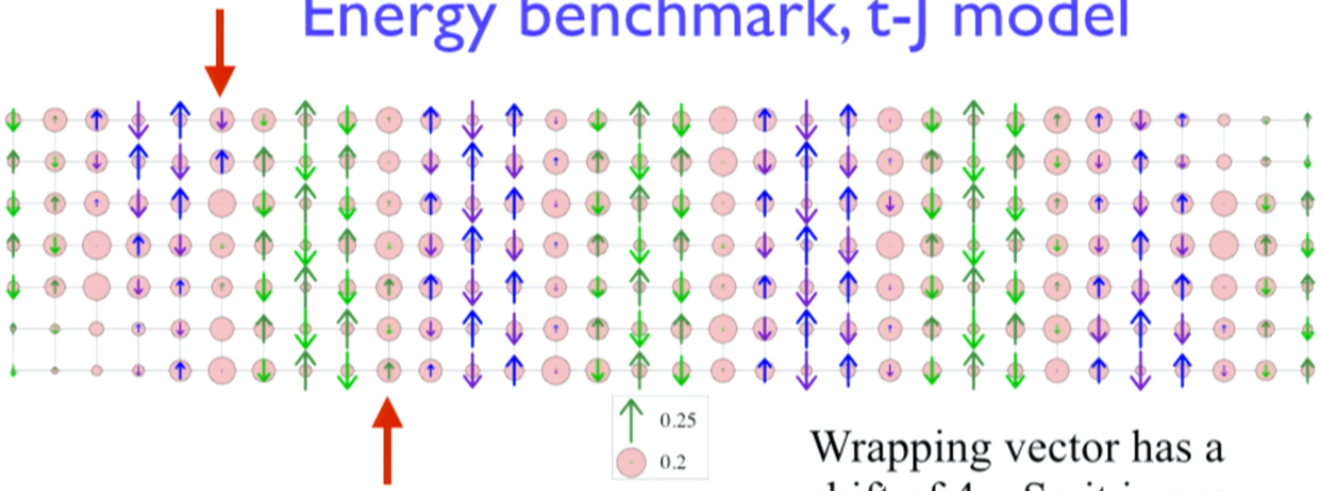
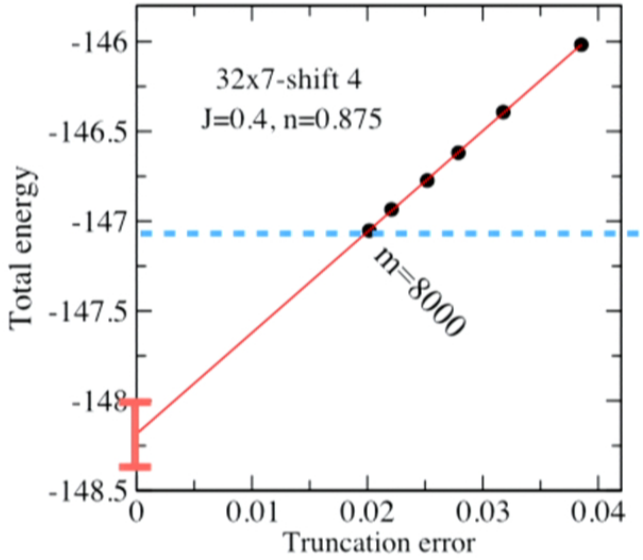
Jx/t= 0.55,Jy/t=0.45, mu=1.2,doping=0.1252

Energy benchmark, t-J model



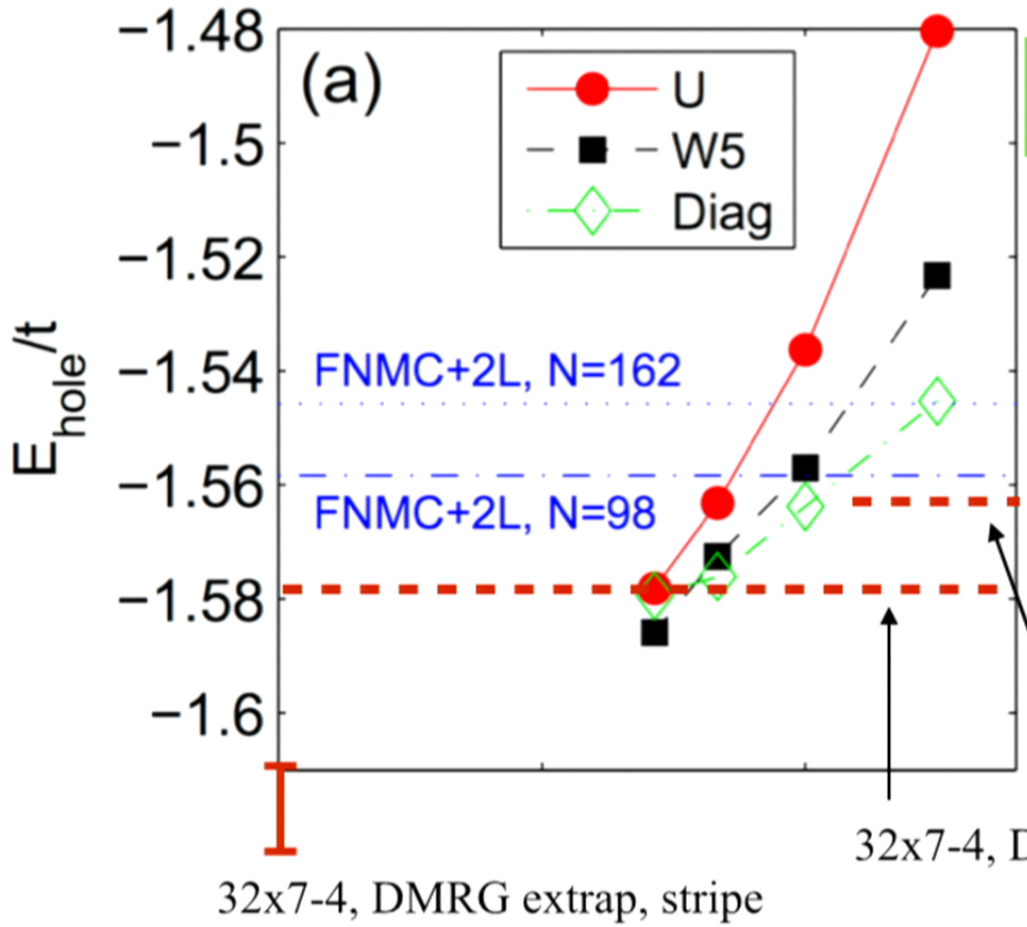
Wrapping vector has a shift of 4—So it is one long stripe



Variational result

Energy per hole: subtract off the energy of the similar undoped cluster (32x7-shift 3, same number of bonds)
Result: -1.618(8) per hole
Variational: -1.577

Energy benchmark, t-J model



Corboz, Rice, Troyer, iPEPS
PRL 113, 046402 (2014)

U = Uniform d-wave
W5 = vertical stripe, d-wave
Diag = Diagonal stripe

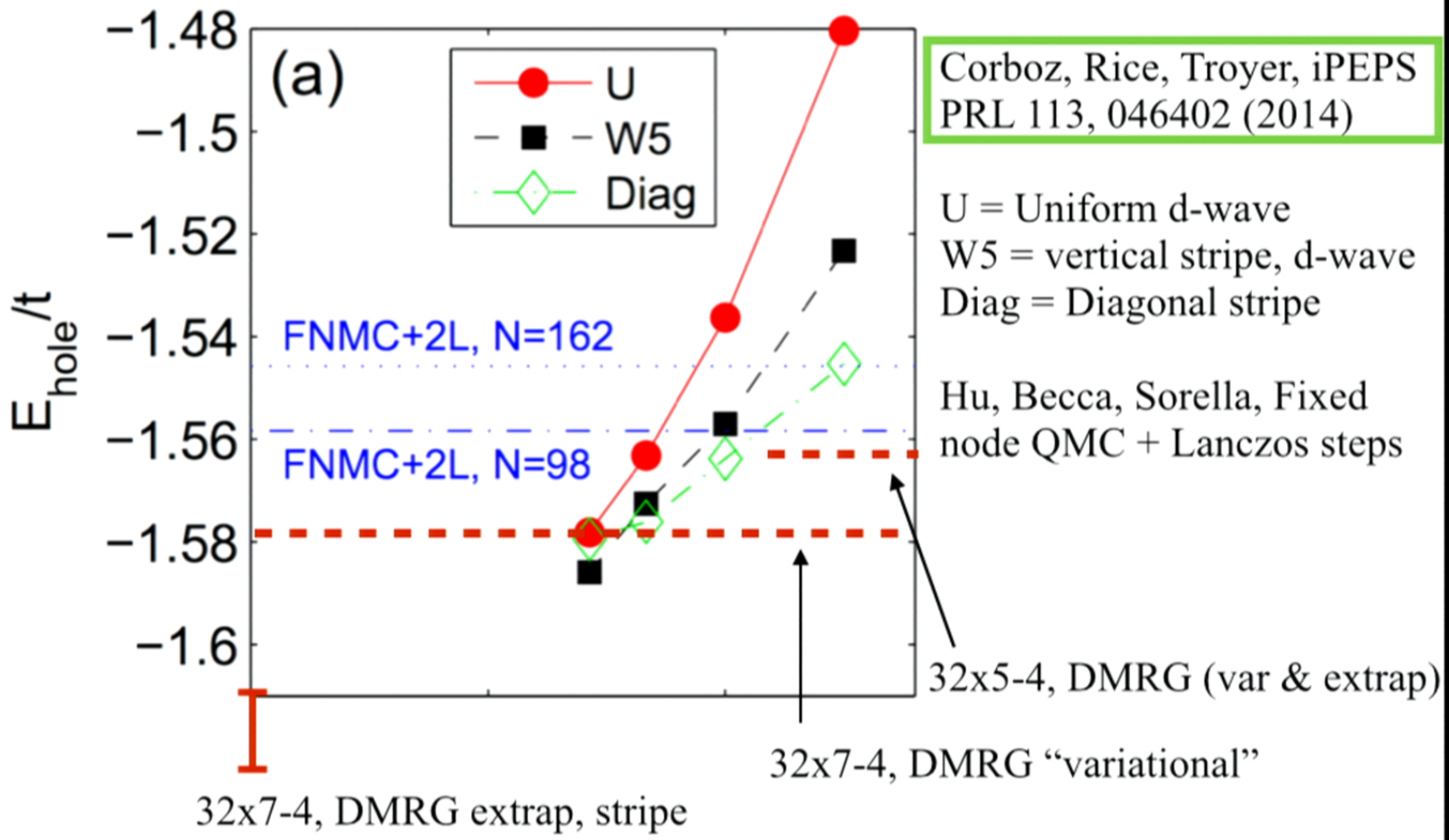
Hu, Becca, Sorella, Fixed node QMC + Lanczos steps

32x5-4, DMRG (var & extrap)

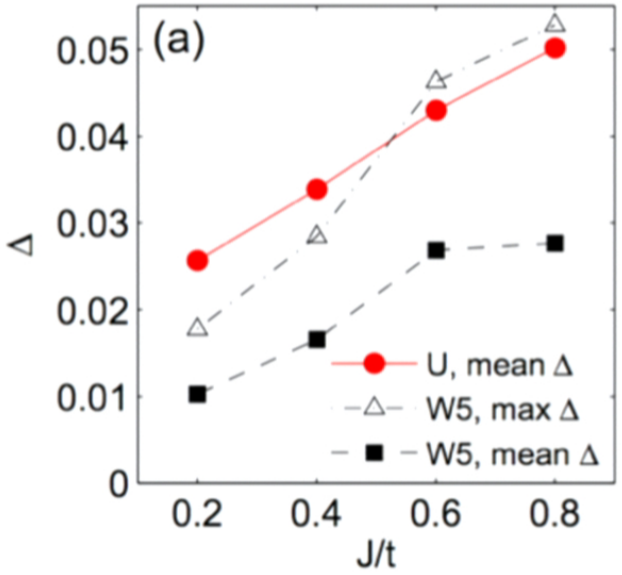
32x7-4, DMRG "variational"

32x7-4, DMRG extrap, stripe

Energy benchmark, t-J model



Why the close competition between the striped and d-wave states?



Corboz, et al:
Pairing and Energy competition track closely as a function of J/t: Why??

Could it be that the two states are almost the same?
stripe = modulated d-wave state??
uniform d-wave = fluctuating stripe??

Note: as D gets large in iPEPS, we expect the exact ground state energy regardless of the shape of the unit cell: U, W5, Diag curves must meet at large D

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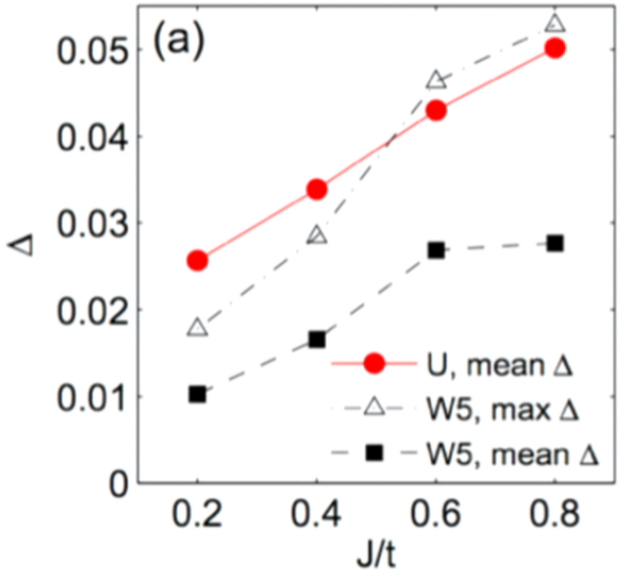

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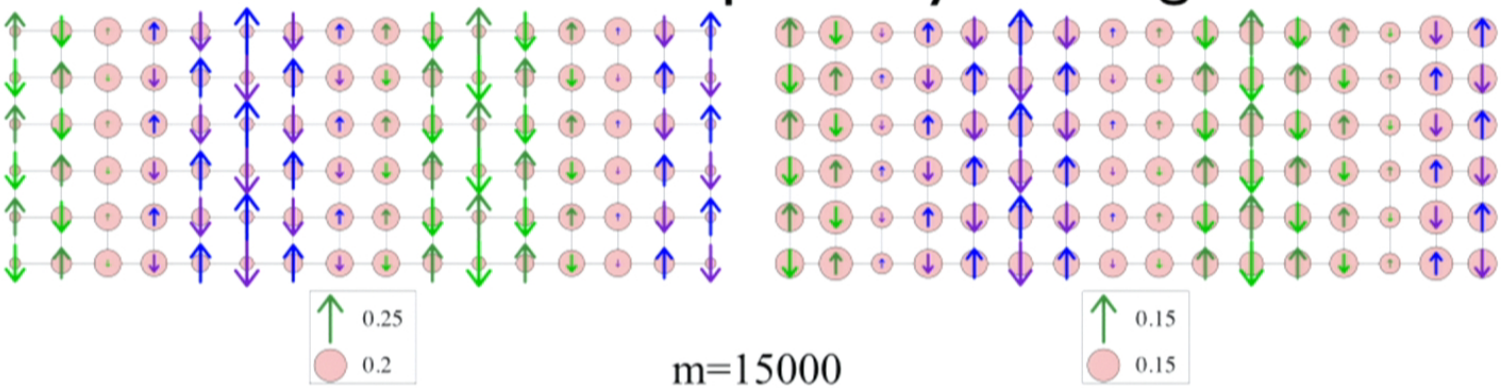
Hubbard model: stripes only for larger U/t



16 x 6 system, Vertical PBC's
U/t = 8, 12 holes

Energy accuracy ~ 0.05%
Variational: 0.25%

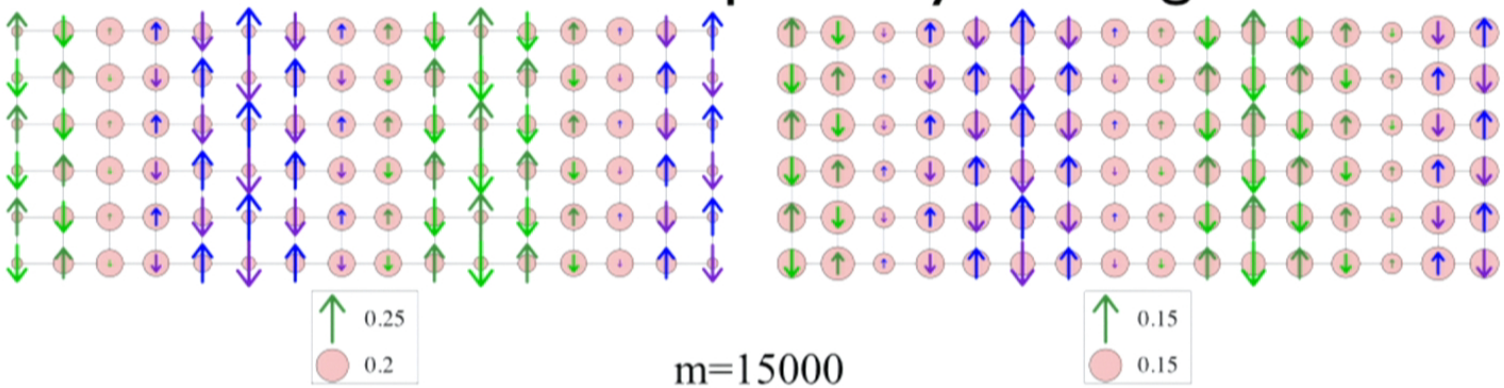
16 x 6 system, Vertical PBC's
U/t = 3, 12 holes

Energy accuracy ~ 0.07%
Variational: 0.3%

Qualitatively different behavior for small versus large U/t, but no sign of a sharp transition in local properties as a function of U

Both regimes appear to support d-wave pairing

Hubbard model: stripes only for larger U/t



16 x 6 system, Vertical PBC's
U/t = 8, 12 holes

Energy accuracy ~ 0.05%
Variational: 0.25%

16 x 6 system, Vertical PBC's
U/t = 3, 12 holes

Energy accuracy ~ 0.07%
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Qualitatively different behavior for small versus large U/t, but no sign of a sharp transition in local properties as a function of U

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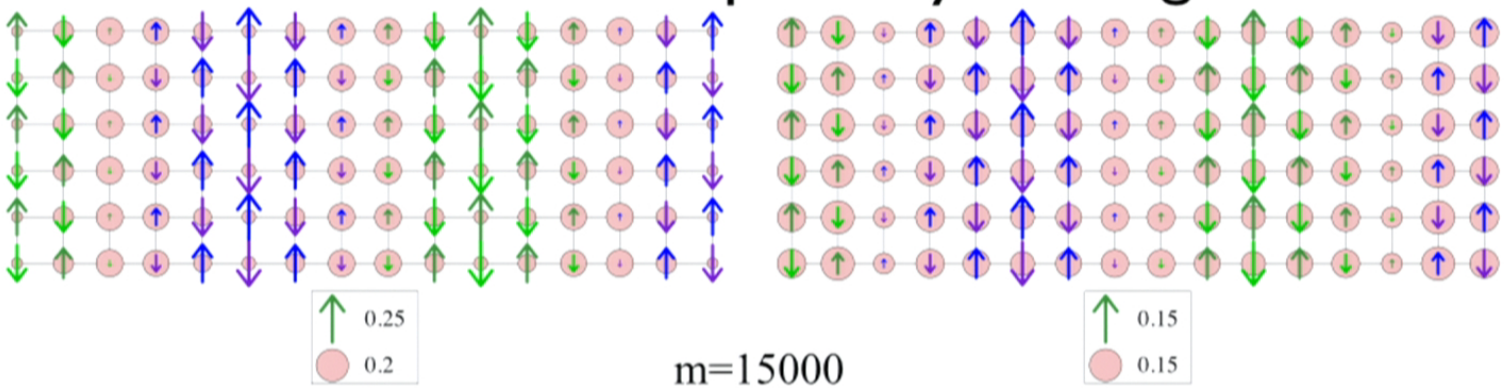

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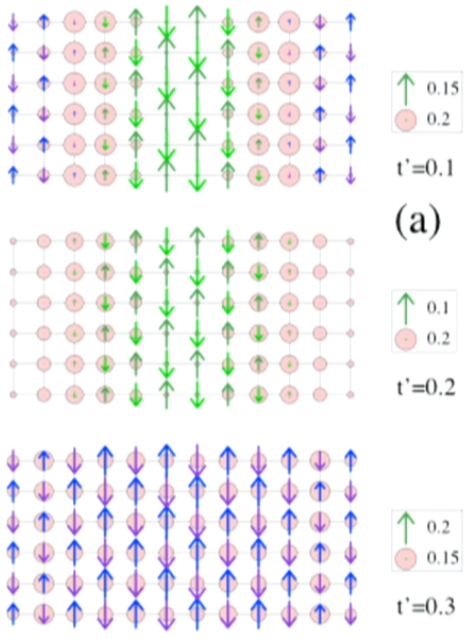
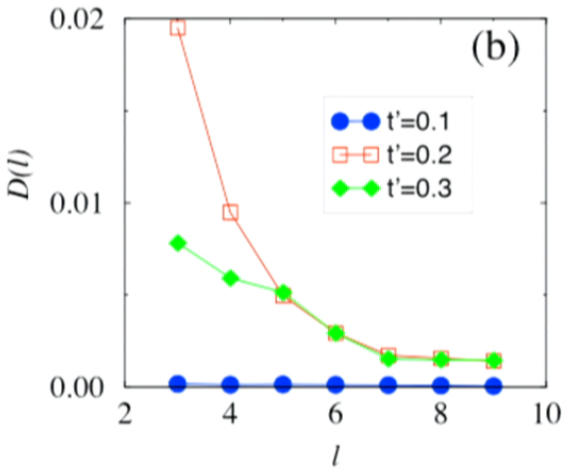
t'>0 strongly enhances pairing, eventually killing stripes.

The problem: t'>0 is thought to correspond to electron doped cuprates,
t'<0 to hole doped!

t'=0: pairing killed by holes being locked up in transverse stripes



t-J only



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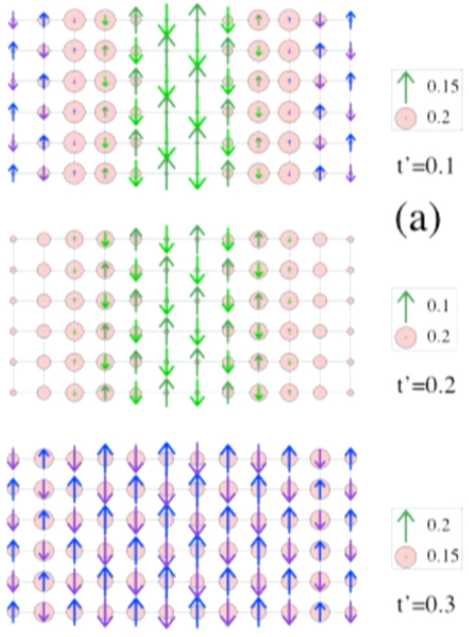

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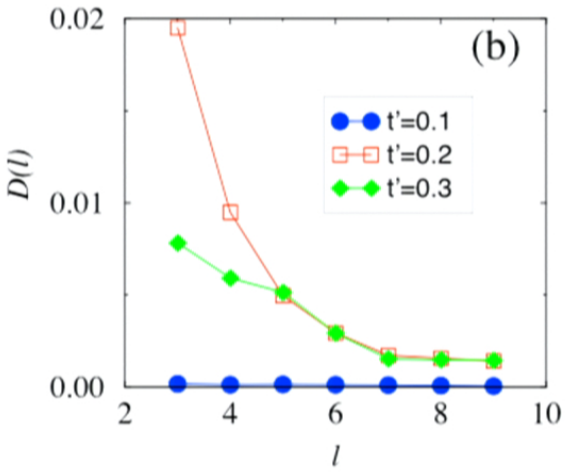
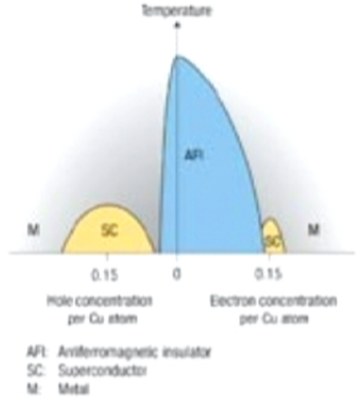
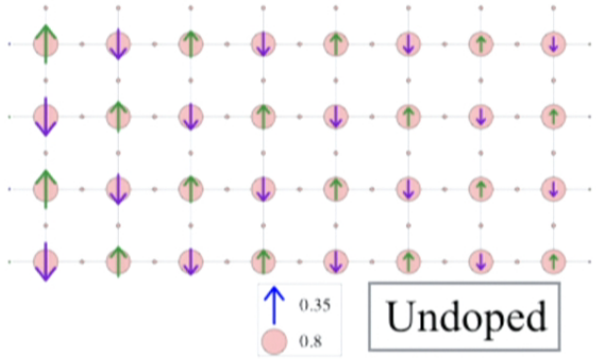
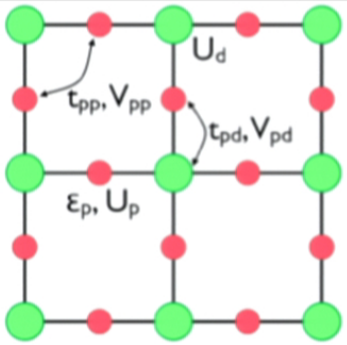


3 Band Hubbard (Emery) model



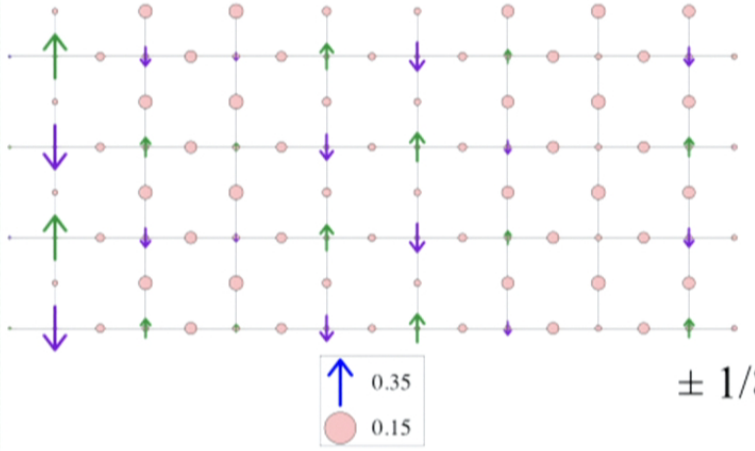


Undoped

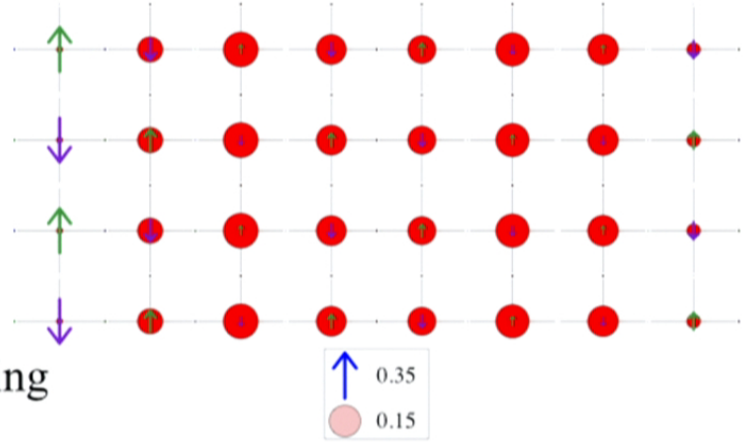


$t_{pd}=1$, $t_{pp}=0.5$, $U_d=8$, $U_p=3$
$\varepsilon_p-\varepsilon_d = 3$, $V_{pd}=1$, $V_{pp}=0.75$

Difference in densities relative to undoped



± 1/8 doping



Hole doped, showing 2 “stripes”

Electron doped, showing commensurate AF

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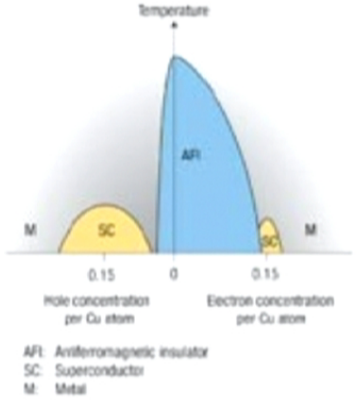
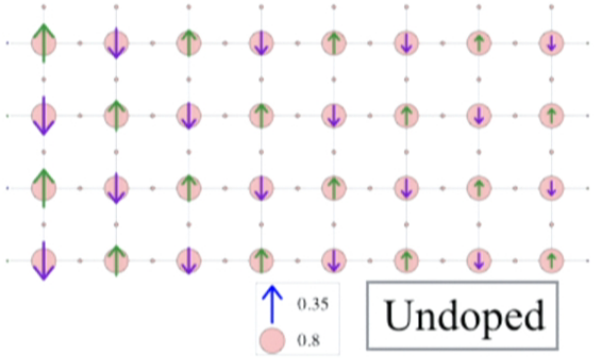
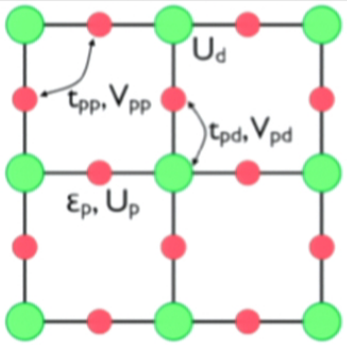




Undoped



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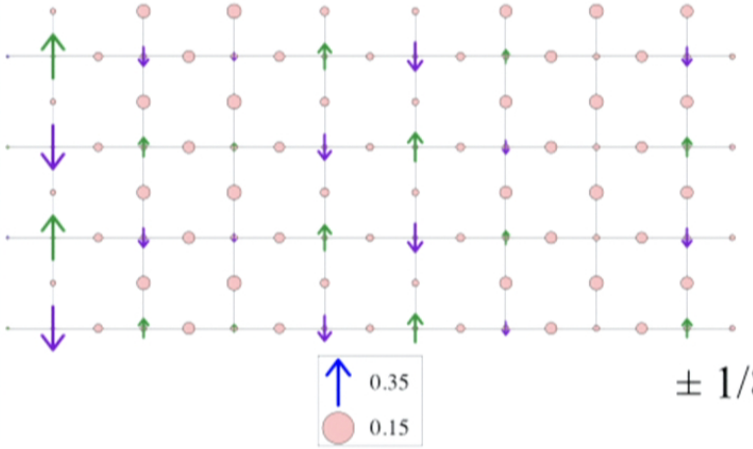

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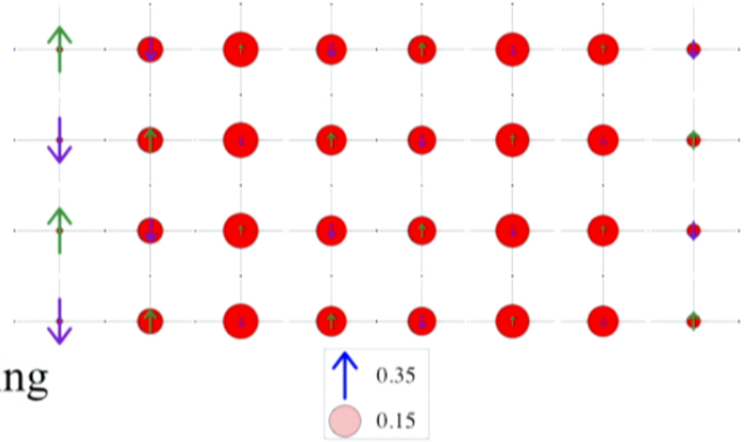

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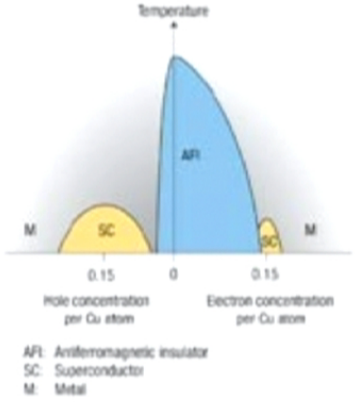
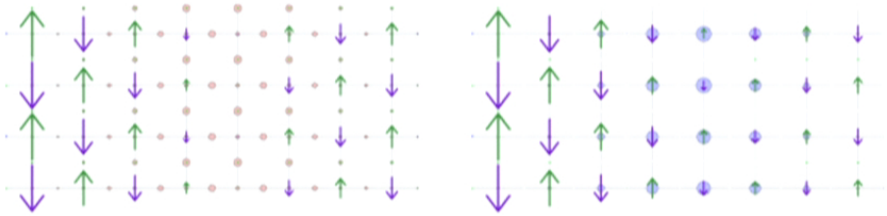
3 Band Hubbard

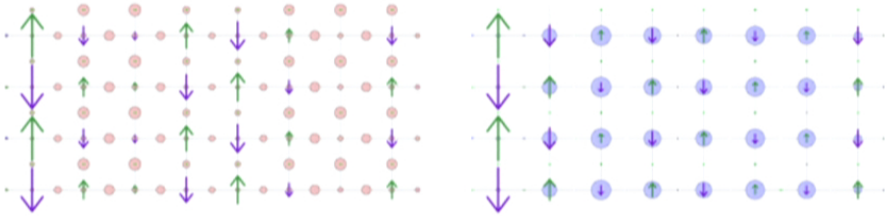


Doping:

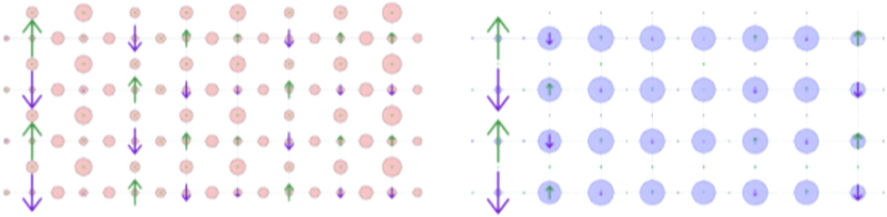
2 ptles



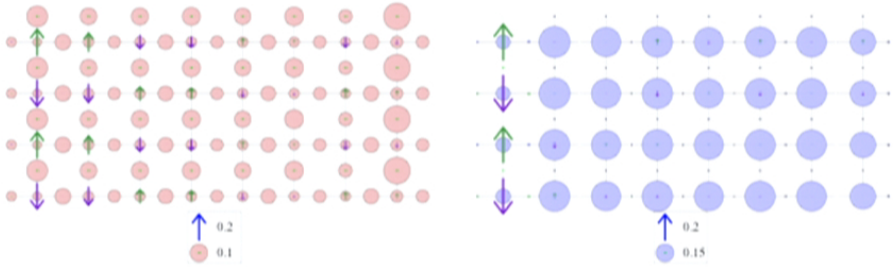
4 ptles



6 ptles

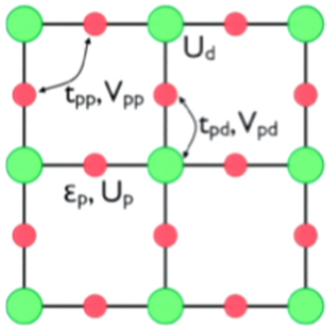


8 ptles

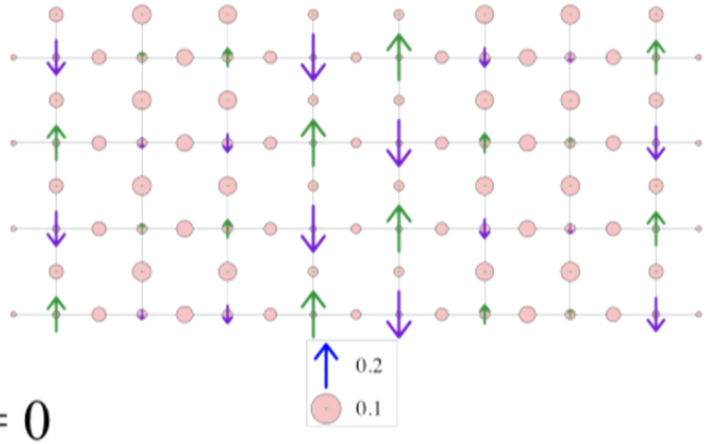


3 Band Hubbard

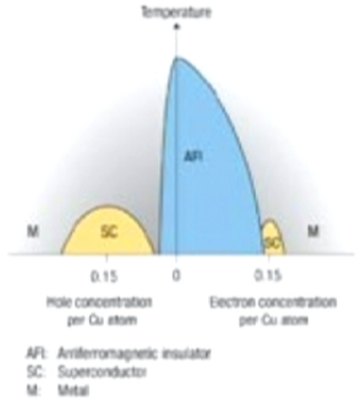
Origin of the asymmetry between hole and electron doped stripes: t_{pp}



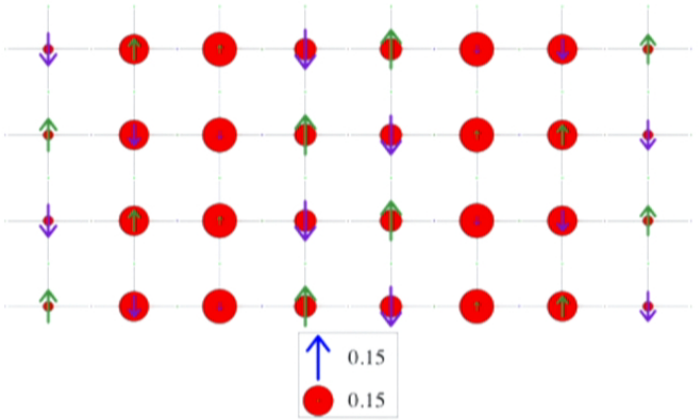
$t_{pp} = 0$ has little obvious effect on the hole doped system: still striped



$t_{pp} = 0$



$t_{pp} = 0$ makes the electron doped system have stripes



Conclusions

- With DMRG, we can study small to moderate width cylinders with good accuracy for t-J and Hubbard models
- The key issue is the presence of stripes, and their relationship to superconductivity
- The strength of pairing and stripe formation depends sensitively on model parameters
- J/t=0.5, t'=0: now see robust "superconducting stripes"
- Hubbard model: large U/t, similar to t-J
- CuO model: electron/hole doped asymmetry as seen in cuprates comes out with standard model parameters