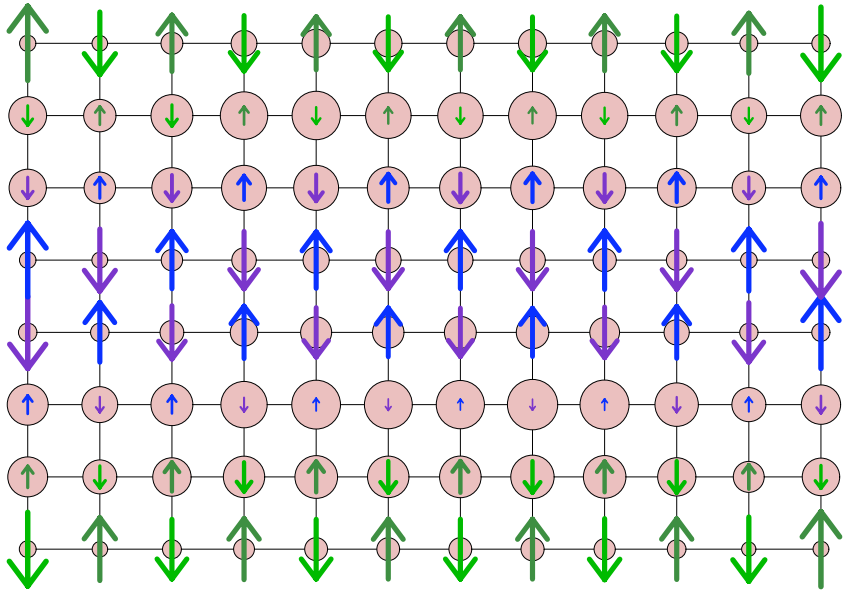
DMRG results for the 2D t-J model



main collaborator:

Doug Scalapino

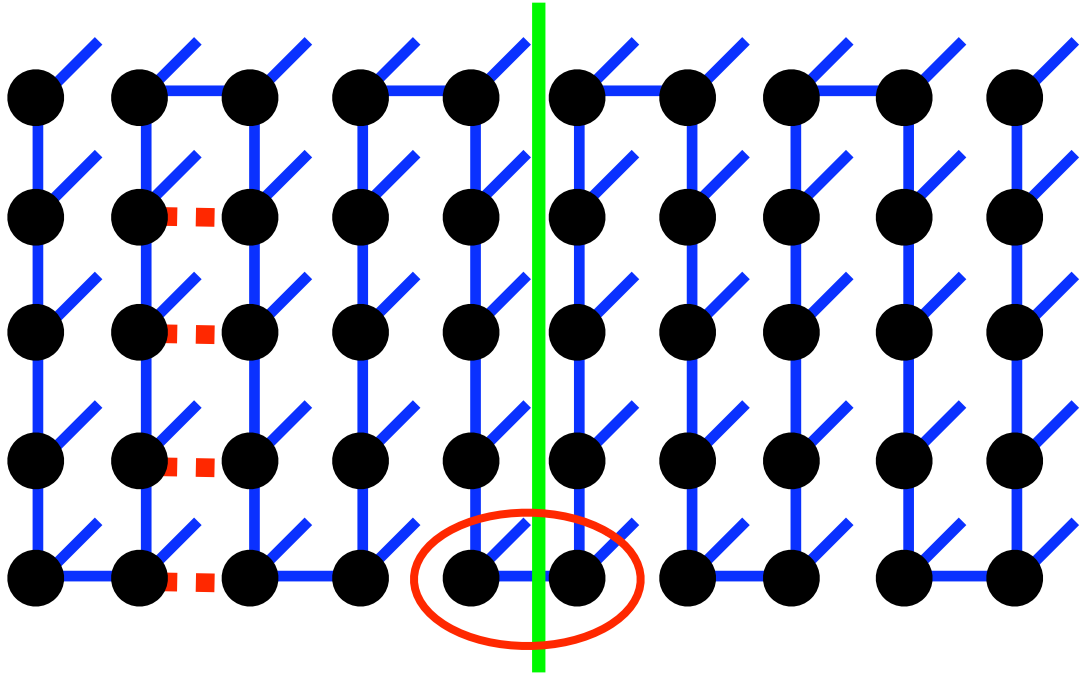
UCIrvine
University of California, Irvine

Outline

- In the Wednesday afternoon tradition, this is a discussion oriented talk focused on the numerical results
- Questions to focus on:
  - Can we do large enough systems, control errors and boundary conditions, to say with reasonable certainty what the ground state phase is?
  - Does the t-J model with the standard values of J, t', t" adequately describe the cuprates?
  - Do stripes and pairing compete, cooperate, or just tolerate each other?
  - Does the t-J model support anti-phase pairing?

Brief notes on the calculations

- DMRG represents the wavefunction as a 1-D matrix product state with matrix dimension m
- The state is optimized with sweeps through the lattice, becoming exact with more sweeps and $m \rightarrow \infty$
- Computational effort is linear in length, exponential in width



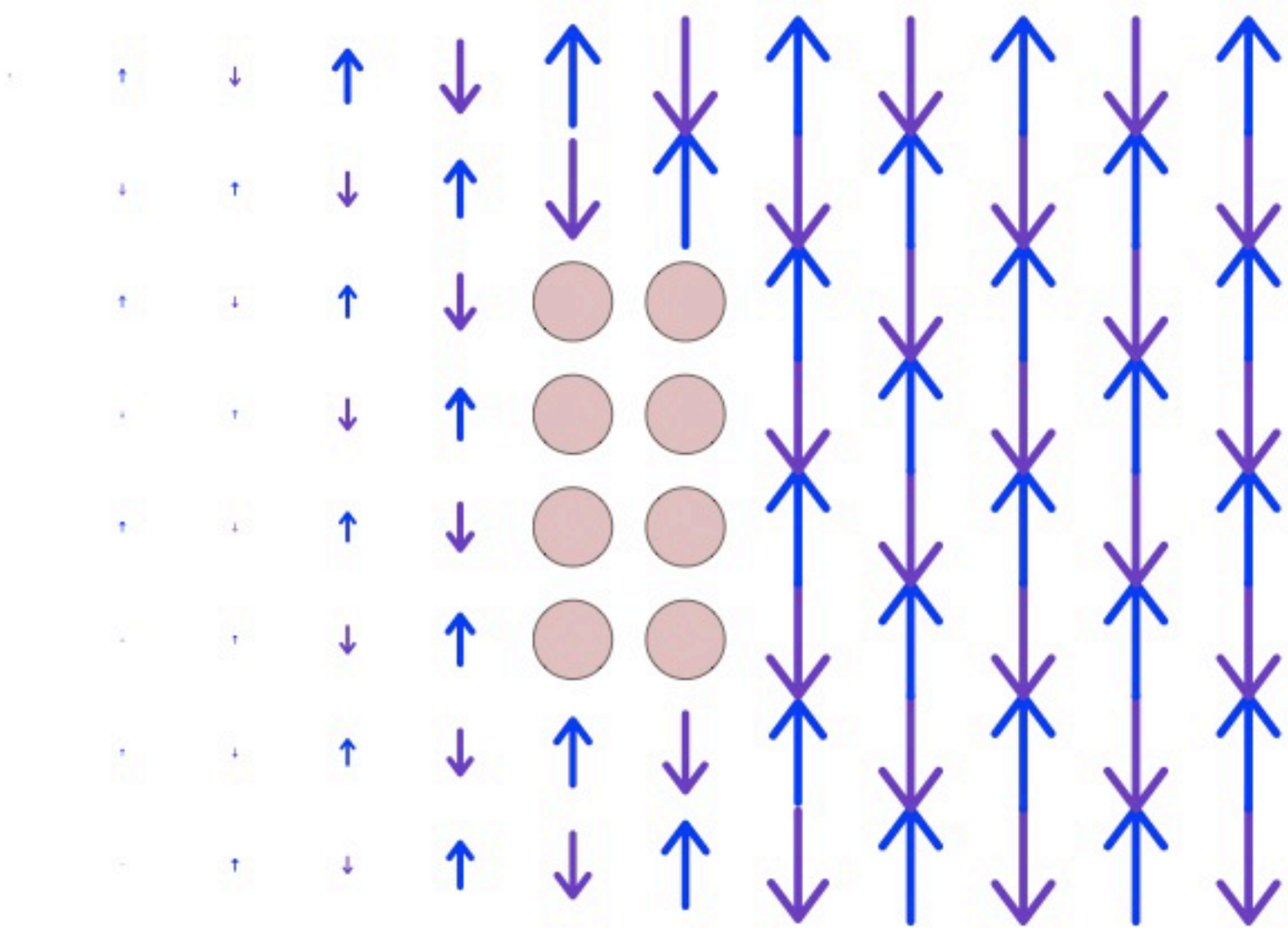
First question

- Can we do large enough systems, control errors and boundary conditions, to say with reasonable certainty what the ground state phase is?
  - Answer: in many cases, mostly yes
  - We will examine the convergence, etc for one simple case, J/t=0.35, t'=t"=0, near 1/8 doping

Stripes forming from a blob of 8 holes

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

Stripes forming from a blob of 8 holes



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

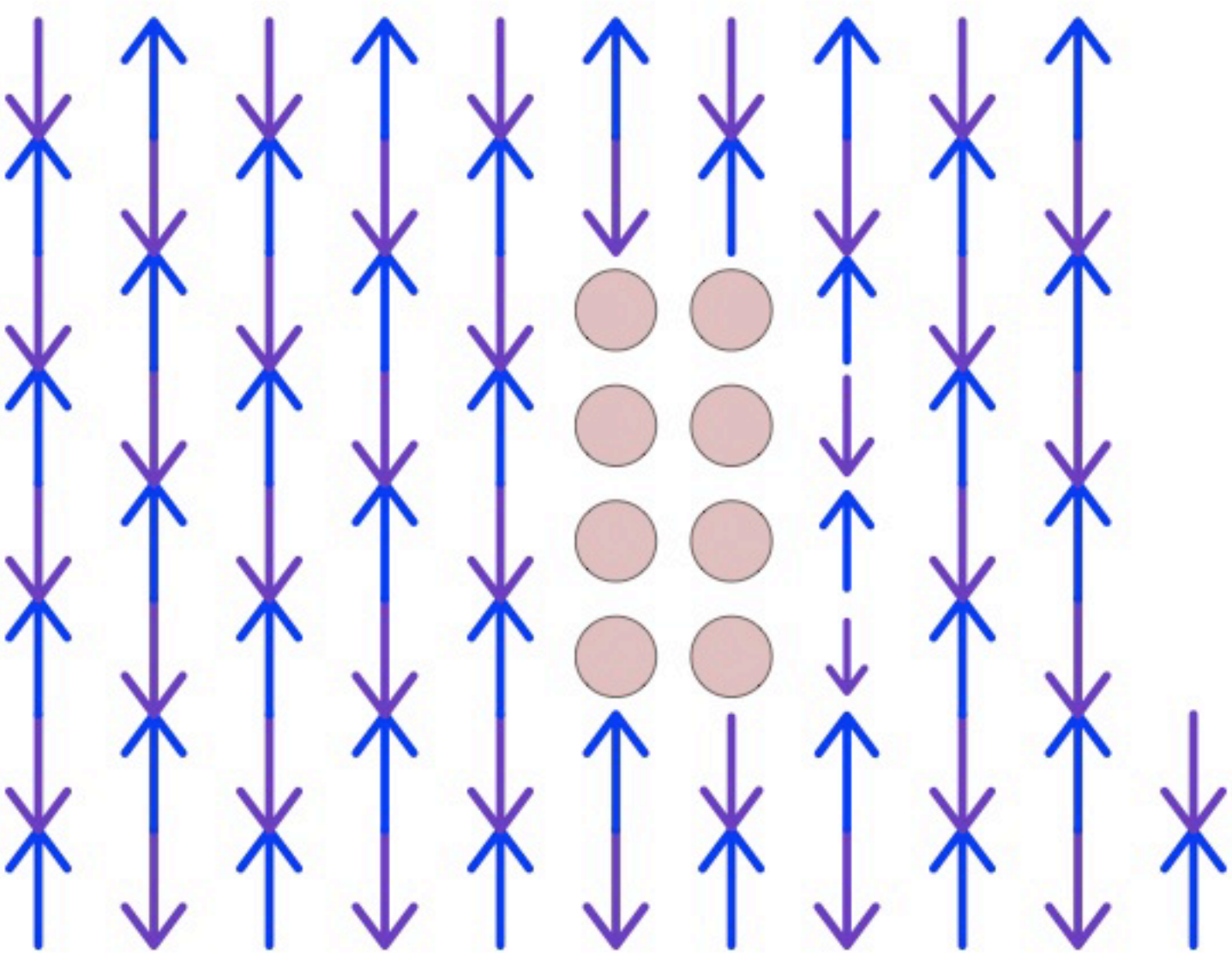
E = -31.7287

m = 70

Stripes forming from a blob of 8 holes

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



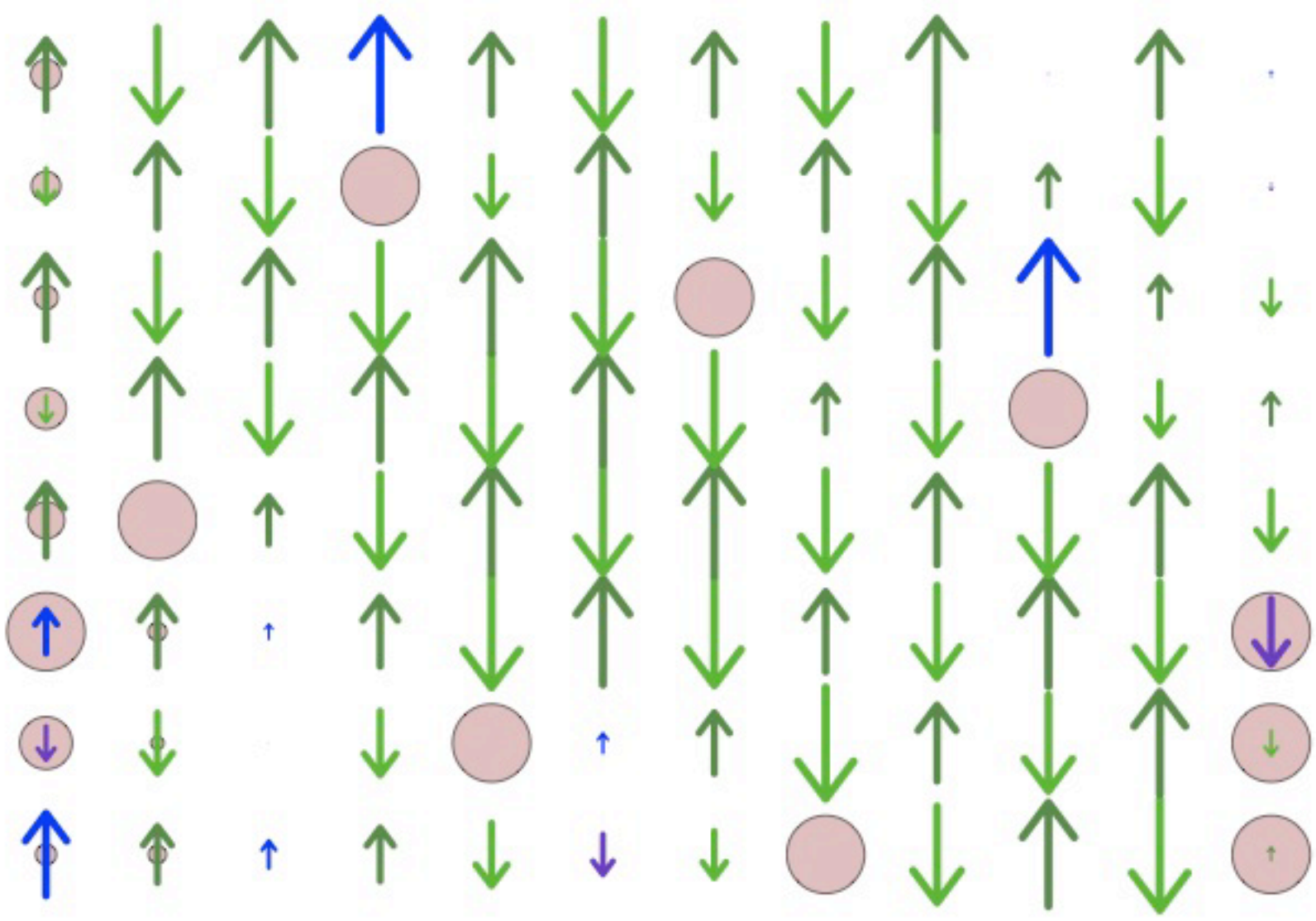
E = -30.7350 m = 40

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 not forming from a bad initial state

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.

Stripes not forming from a bad initial state



E = -30.6370

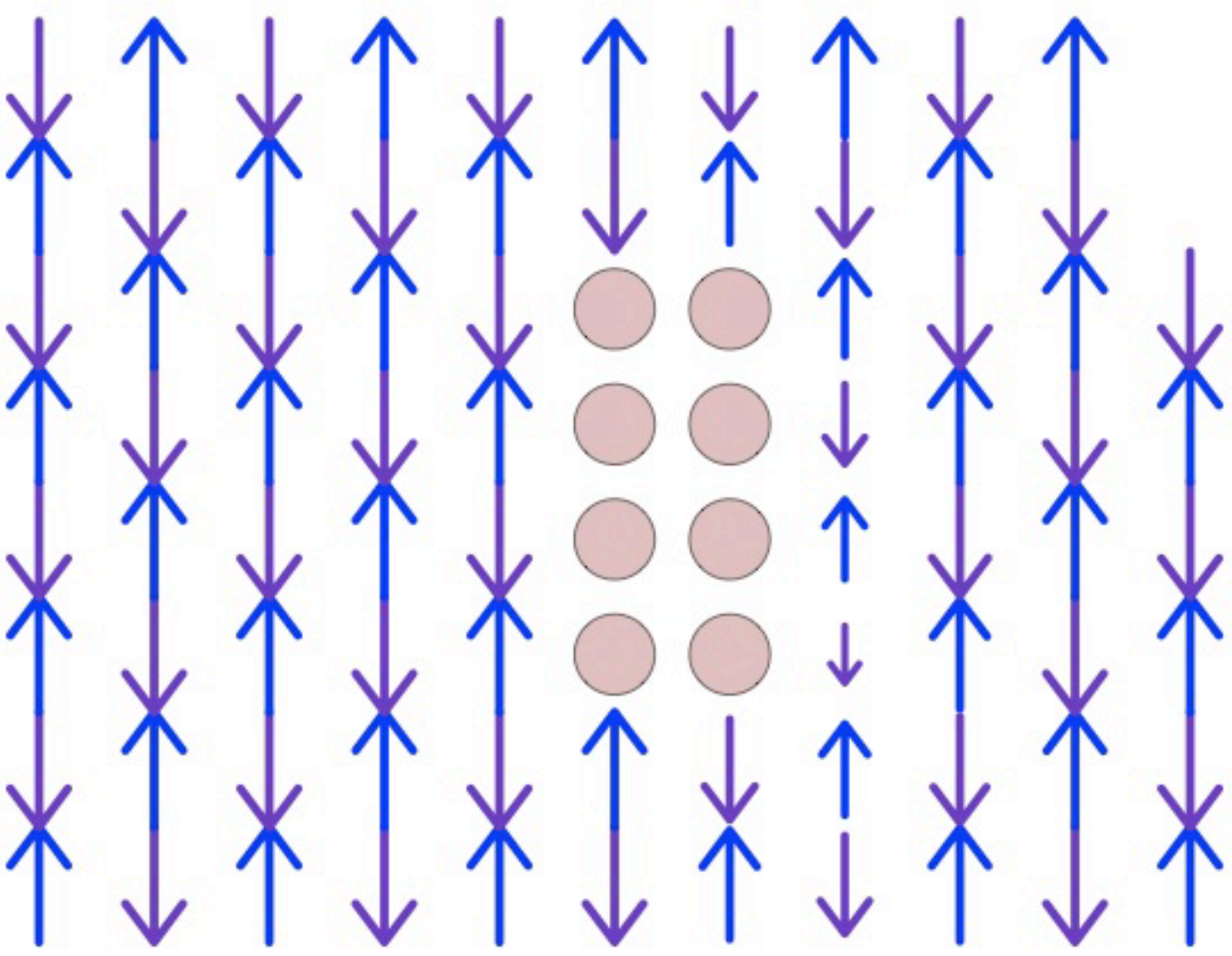
m = 70

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

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

Curved Stripe forms due to open BCs

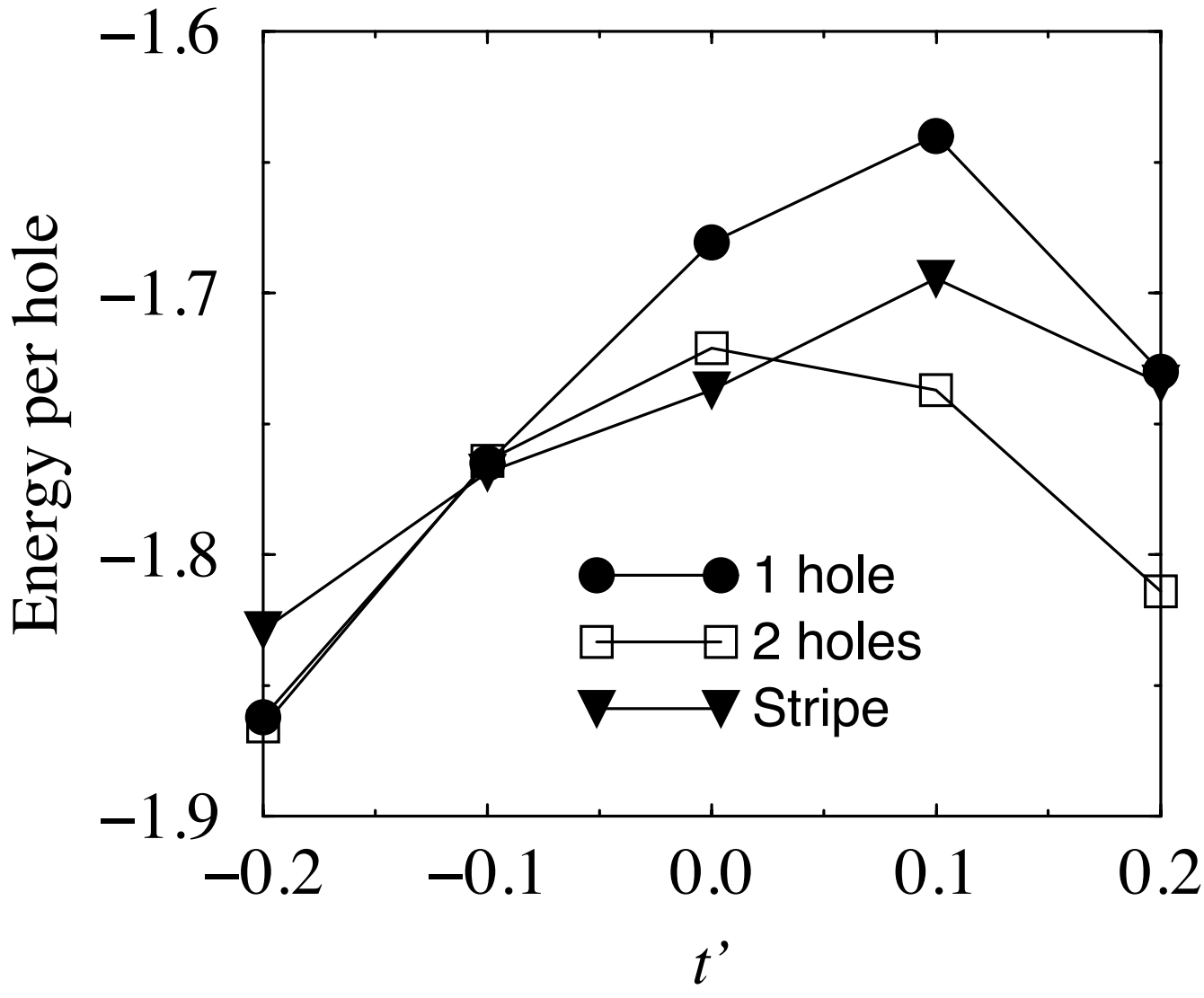


E = -30.8532 m = 40

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

How universal are stripes?

- Key parameter which affects stripes: t'



Systems: 1 or 2 holes on an 8x8, J=0.35

Half-filled stripe on a 16x6 with pinning to force stripe

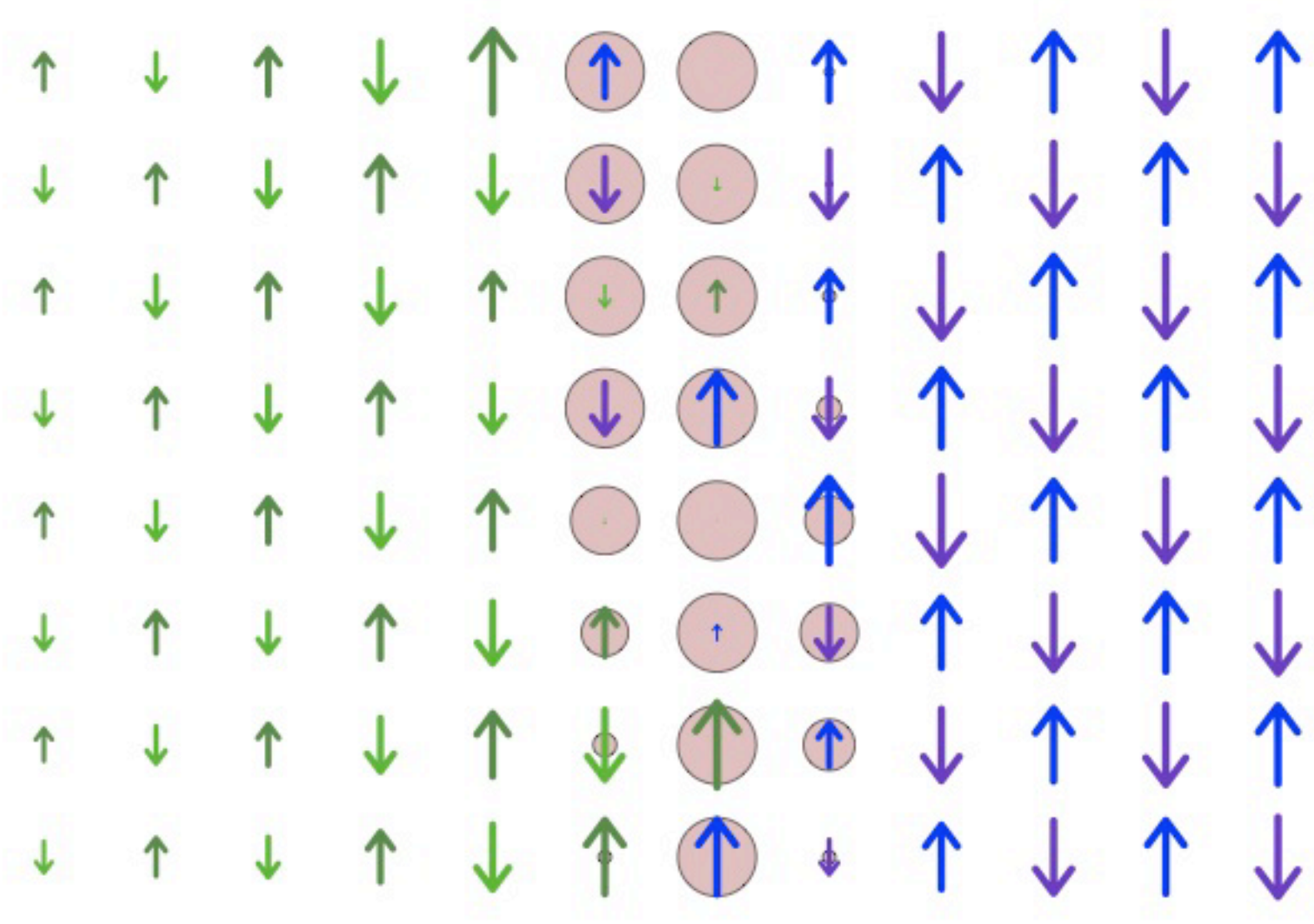
Comparison valid only for low doping

PRB 60, R753 (1999)

t'=0.2: stripe plus pair from a blob of 8 holes

12x8
Cylindrical BCs
t=1, J=0.35
t'=0.2
8 holes
No pinning
fields

t'=0.2: stripe plus pair from a blob of 8 holes



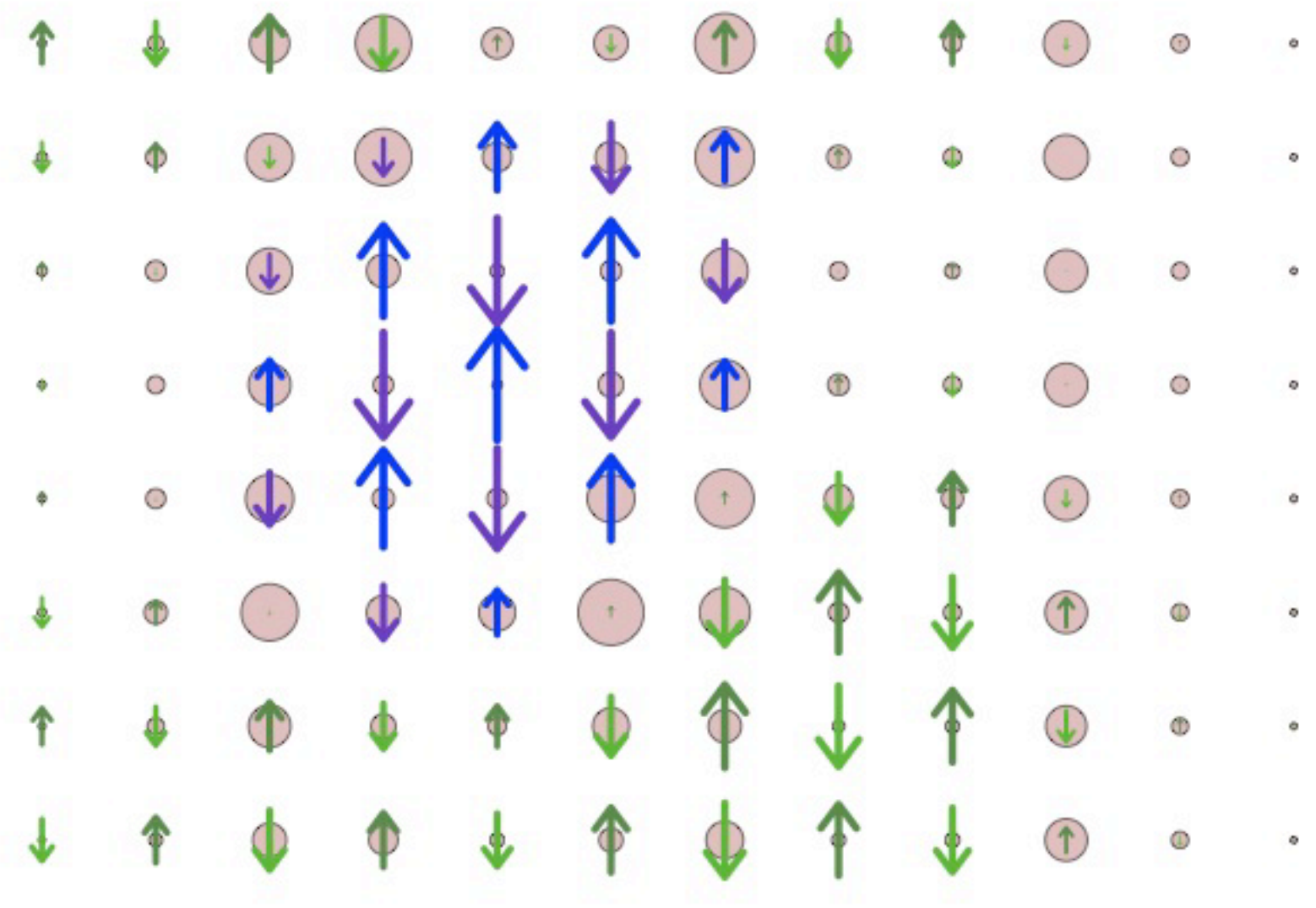
E = -41.7350 m = 100

12x8
Cylindrical BCs
t=1, J=0.35
t'=0.2
8 holes
No pinning
fields

t'=-0.2: Inhomogeneous mystery state forms

12x8
Cylindrical BCs
t=1, J=0.35
t'=-0.2
8 holes
No pinning
fields

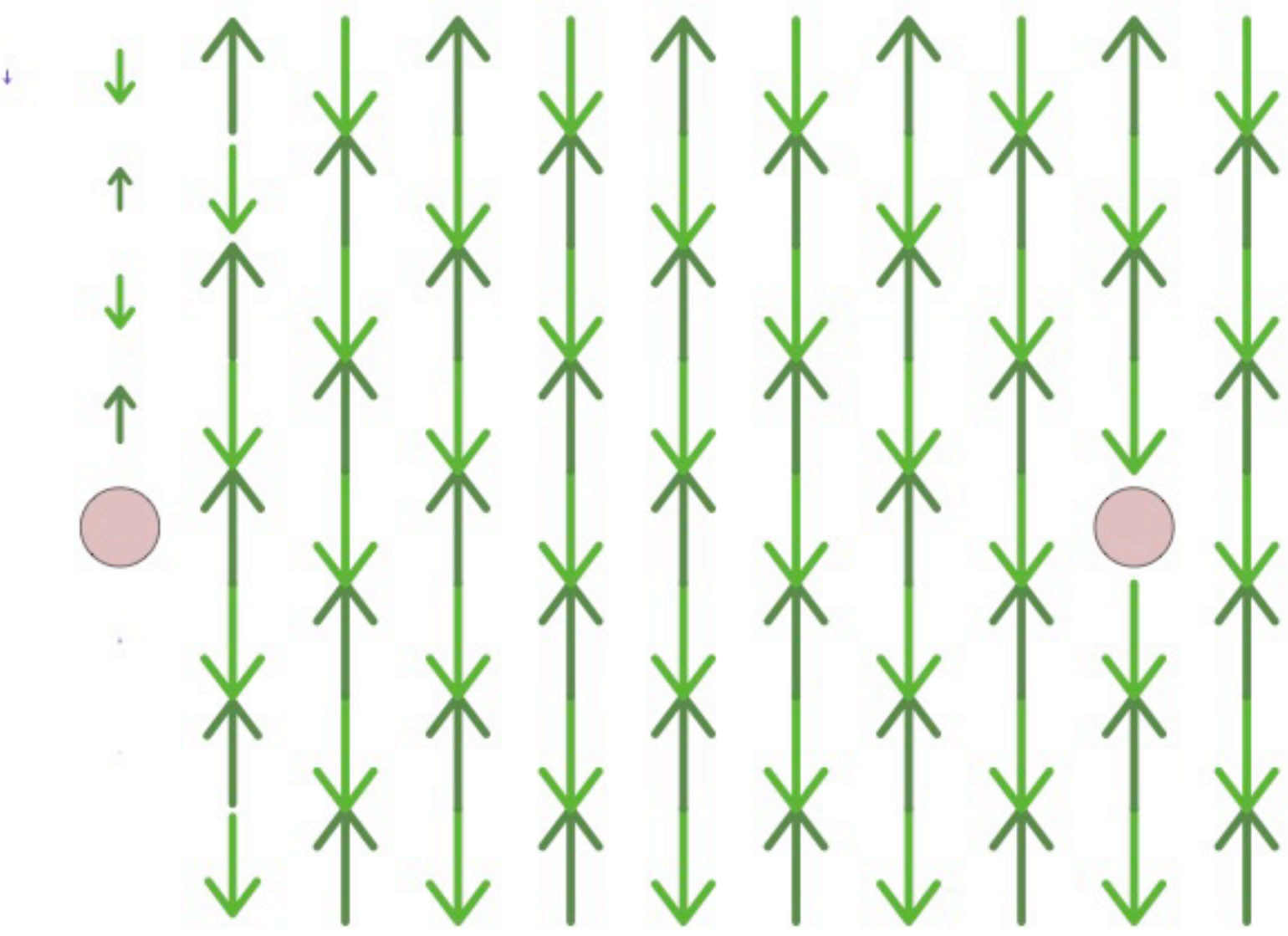
t'=-0.2: Inhomogeneous mystery state forms



E = -52.8438 m = 3000

12x8
Cylindrical BCs
t=1, J=0.35
t'=-0.2
8 holes
No pinning
fields

t'=0.3: two holes attract



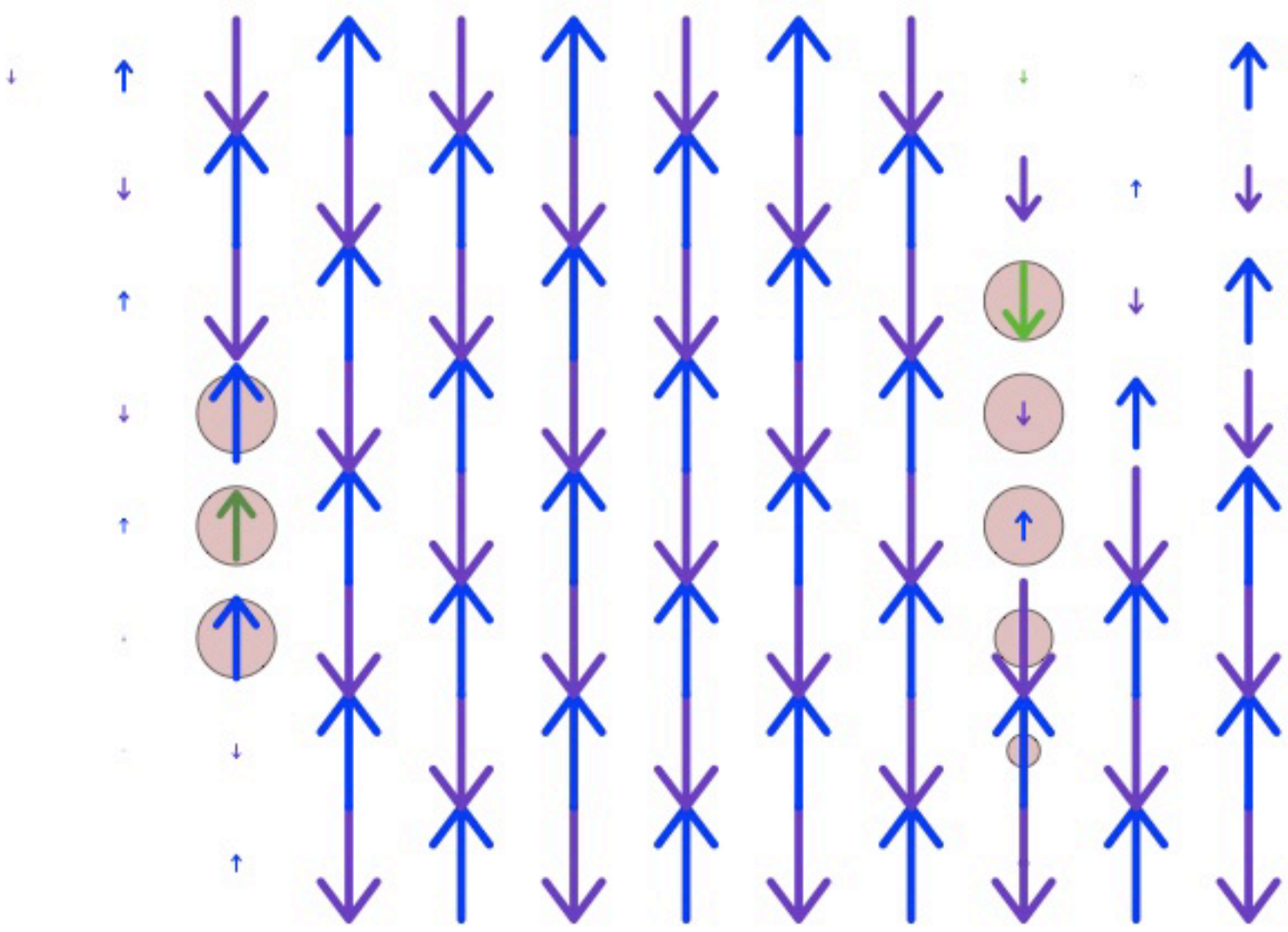
E = -31.0529 m = 40

12x8
Open BCs
t=1, J=0.35
t'=0.3
2 holes
No pinning
fields

t'=-0.3: two holes repel

12x8
Open BCs
t=1, J=0.35
t'=-0.3
2 holes
No pinning fields

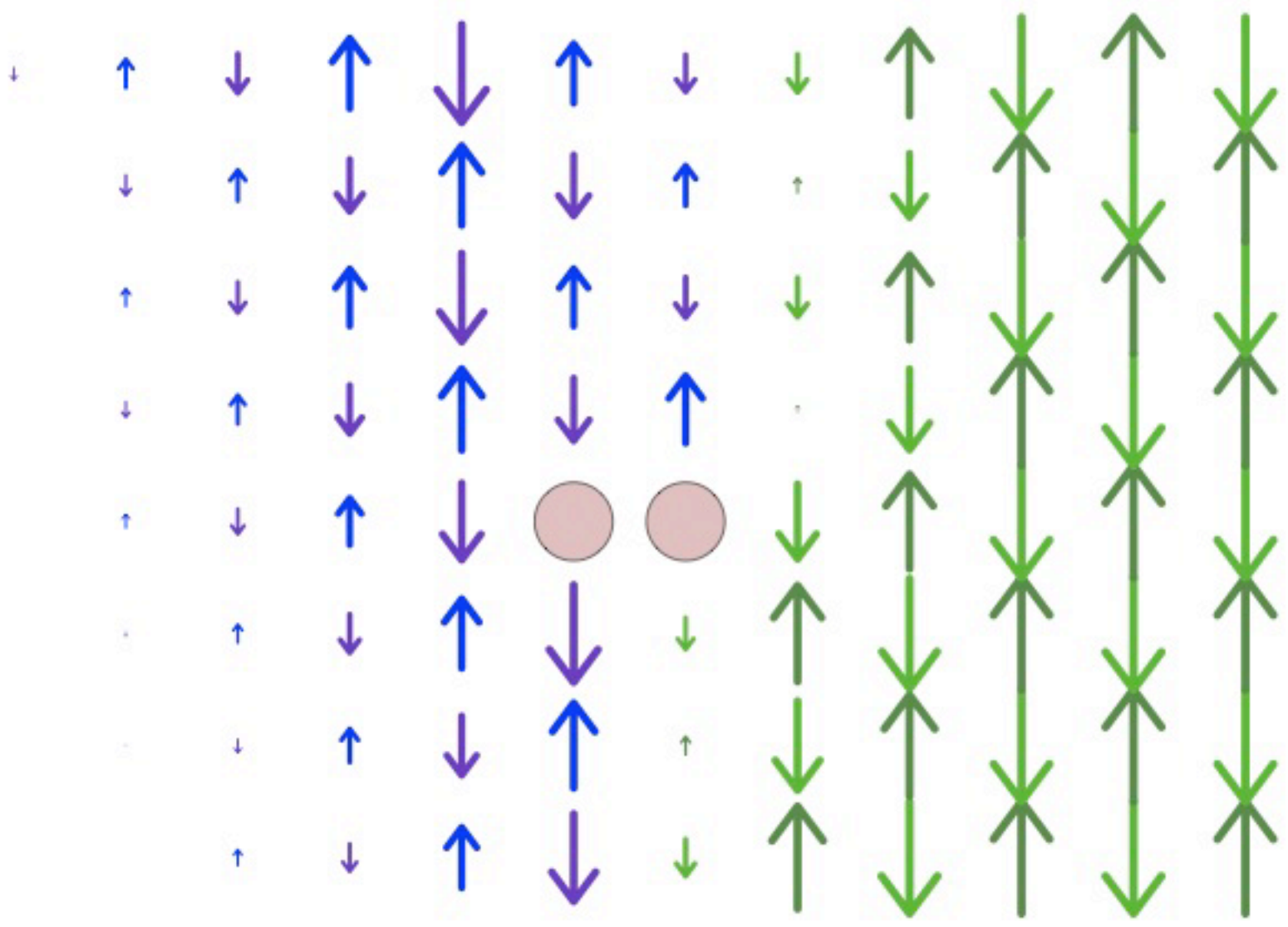
t'=-0.3: two holes repel



E = -35.9676 m = 70

12x8
Open BCs
t=1, J=0.35
t'=-0.3
2 holes
No pinning fields

t'=-0.3: two holes repel



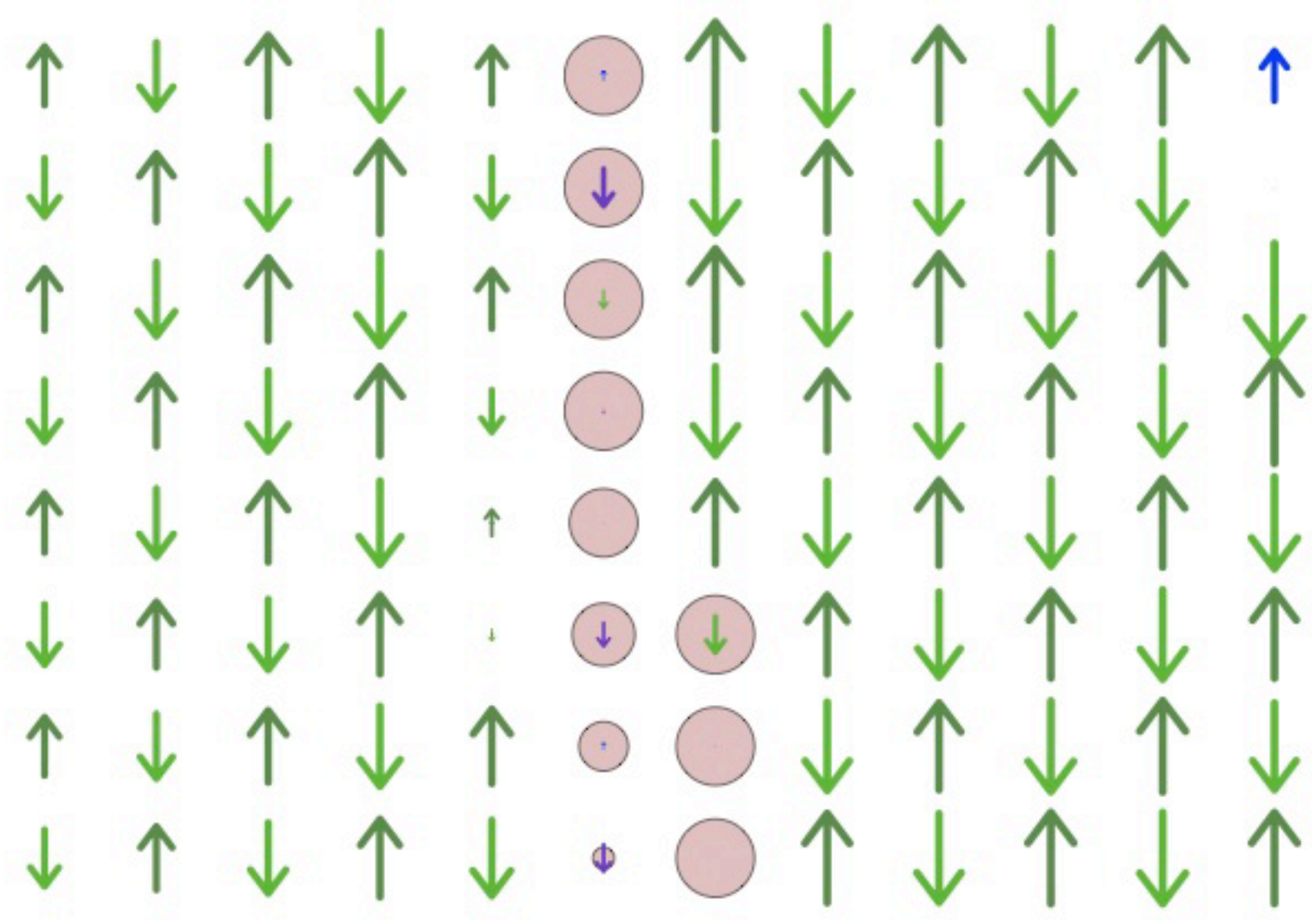
E = -30.5980 m = 40

12x8
Open BCs
t=1, J=0.35
t'=-0.3
2 holes
No pinning fields.
Energy higher by 0.08t

t'=0.2 : 4 holes split into two pairs

12x8
Cylindrical BCs
t=1, J=0.35
t'=0.2
4 holes
No pinning
fields

t'=0.2 : 4 holes split into two pairs



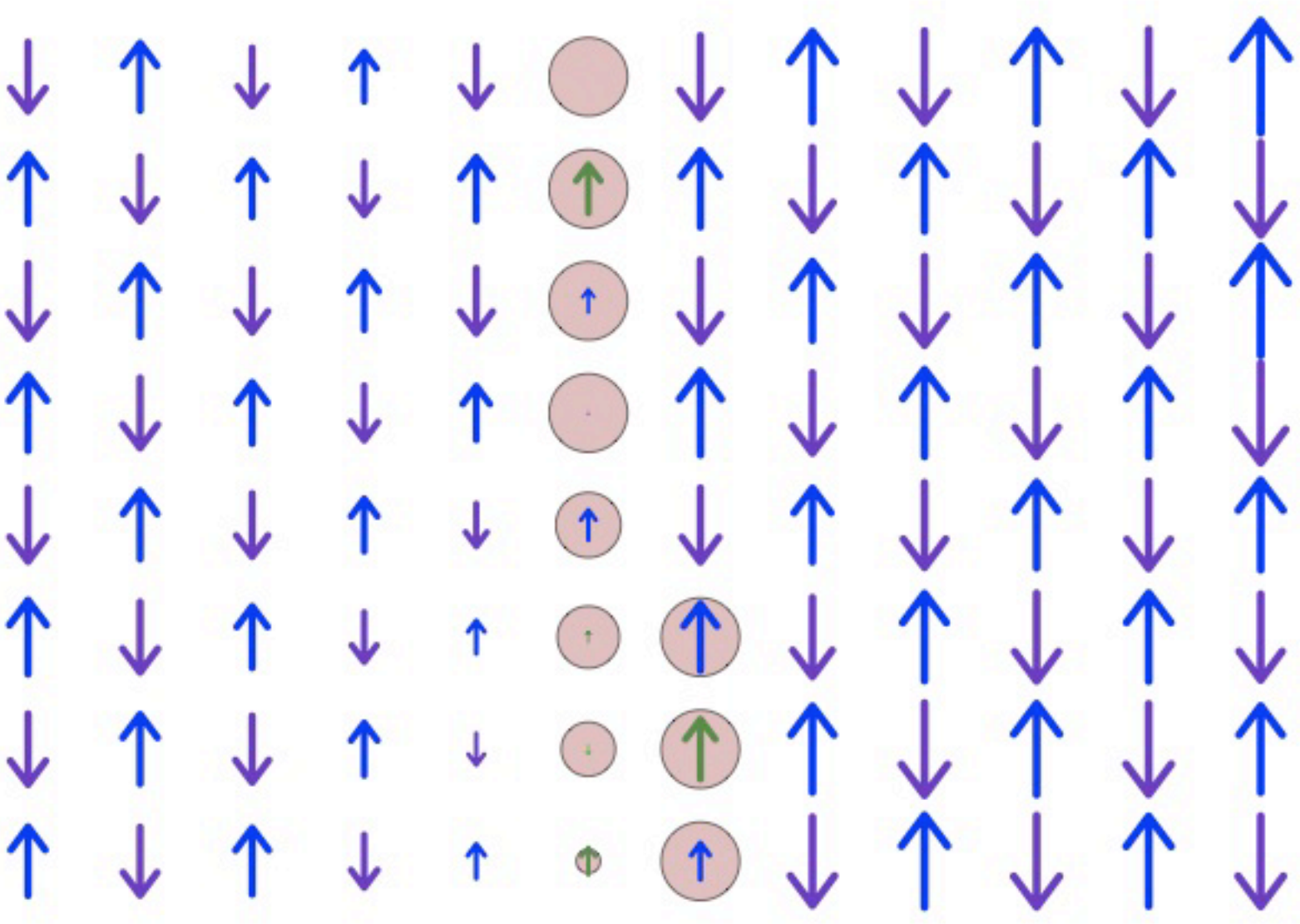
E = -36.5673 m = 50

12x8
Cylindrical BCs
t=1, J=0.35
t'=0.2
4 holes
No pinning
fields

t'=0 : 4 holes barely split into two pairs

12x8
Cylindrical BCs
t=1, J=0.35
t'=0.0
4 holes
No pinning
fields

t'=0 : 4 holes barely split into two pairs



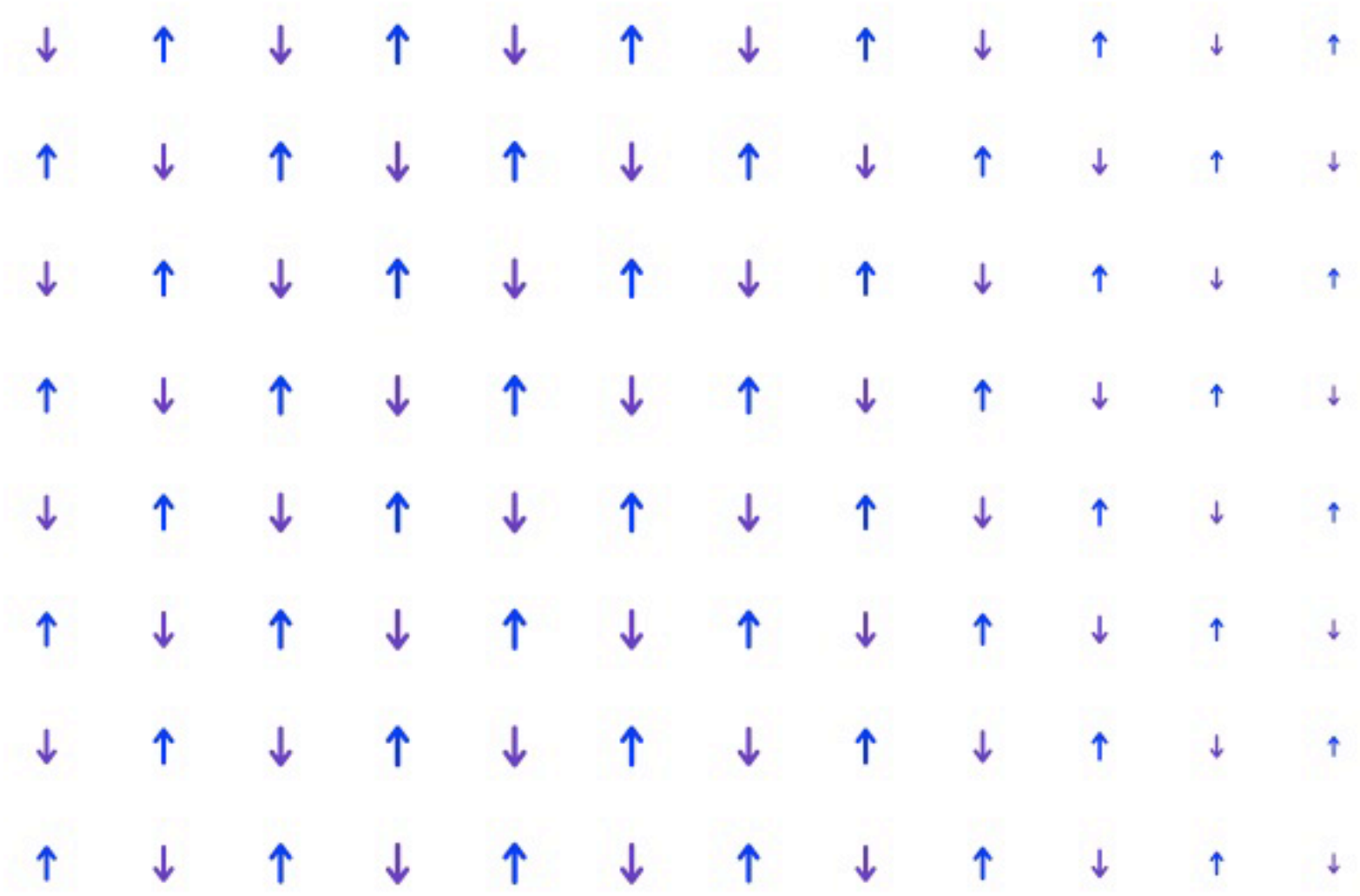
E = -36.2225 m = 50

12x8
Cylindrical BCs
t=1, J=0.35
t'=0.0
4 holes
No pinning
fields

Undoped system: Restoration of SU(2) symmetry

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

Undoped system: Restoration of SU(2) symmetry

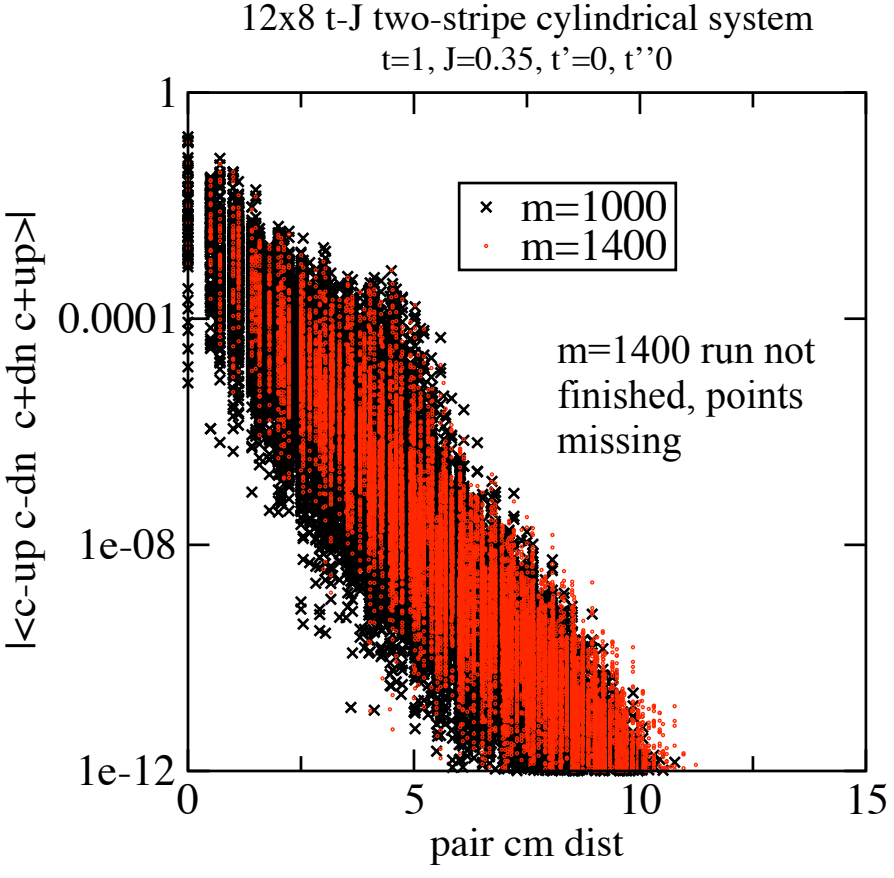


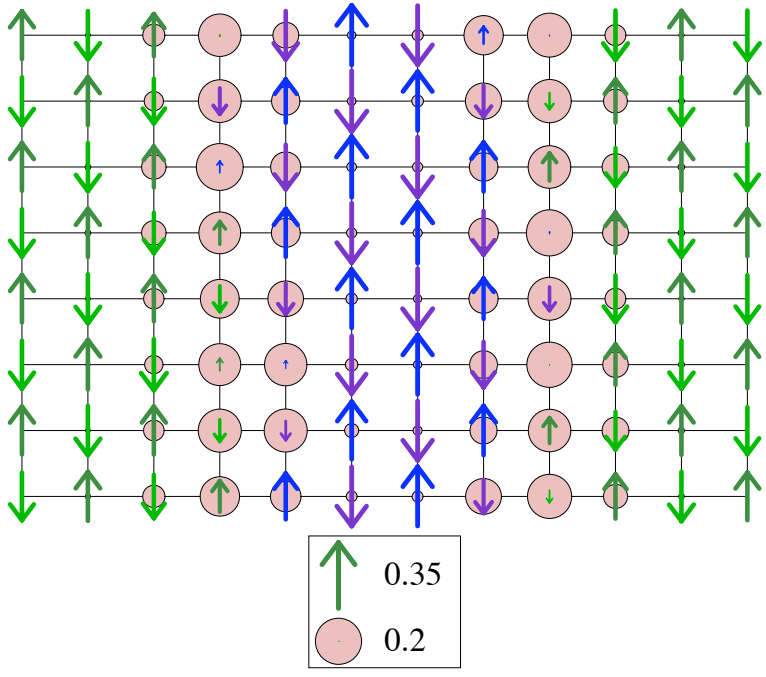
12x8
Cylindrical BCs
J=0.35
0 holes
No pinning fields

E = -38.0681 m = 600

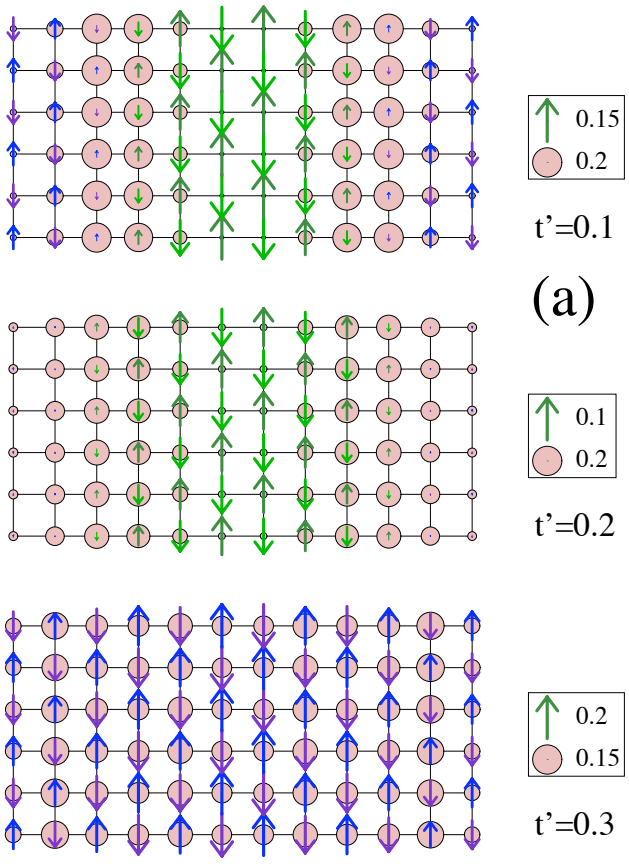
What about pairing?

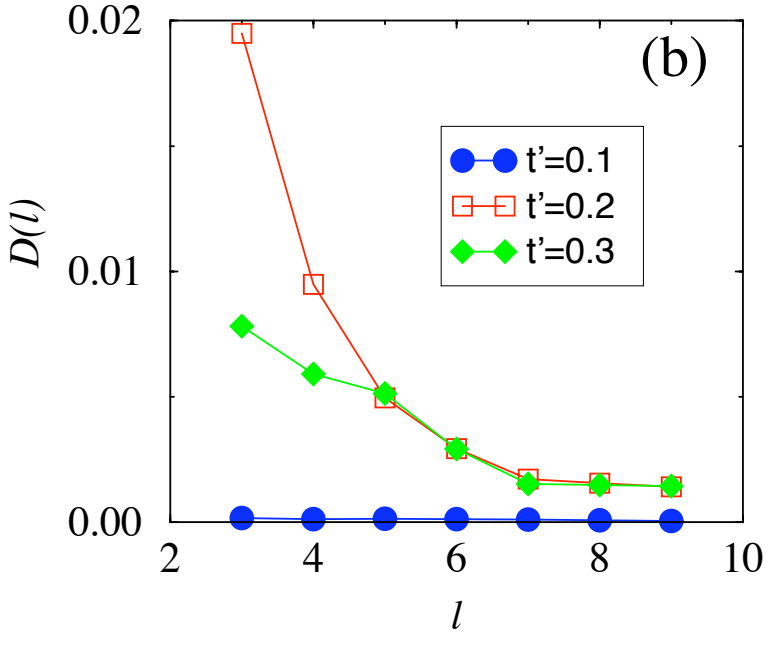
- Are their pairing correlations in a stripe?
- Is a striped phase superconducting?
- Can we find a phase with sensible model parameters with superconductivity but no stripes?





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





The energy for 2 extra or 2 less holes in a stripe is high, suppressing pairing in this geometry.

Increasing positive t' melts the stripes and leads to pairing.

But: positive t' corresponds to electron-doped cuprates, lower Tc!

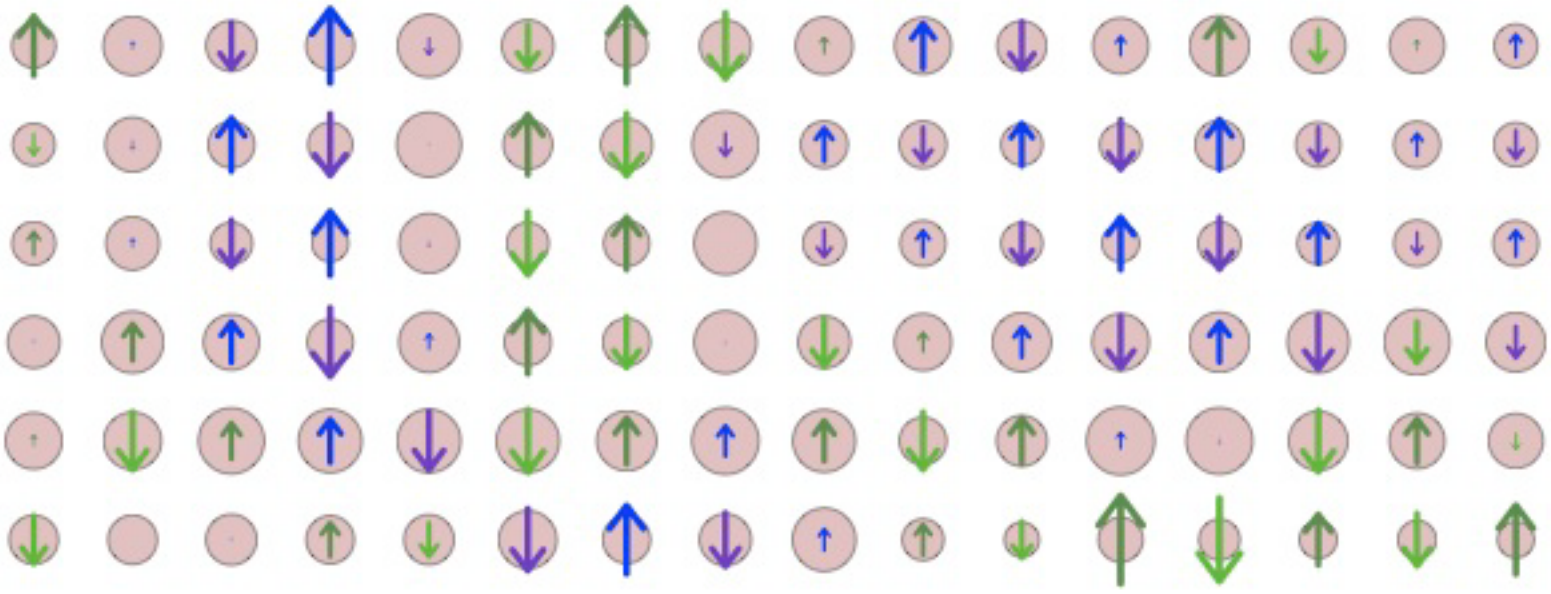
What about negative t'?

“Realistic” parameters on an open 16x6

16x6
Open BCs
t=1, J=0.35
t’=-0.25,
t”=0.12
18 holes, x=0.19
No pinning
fields

See T. Tohyama, PRB 70, 174517 (2004)--20 site Lanczos seeing some enhanced pairing for these parameters at x=0.3

“Realistic” parameters on an open 16x6

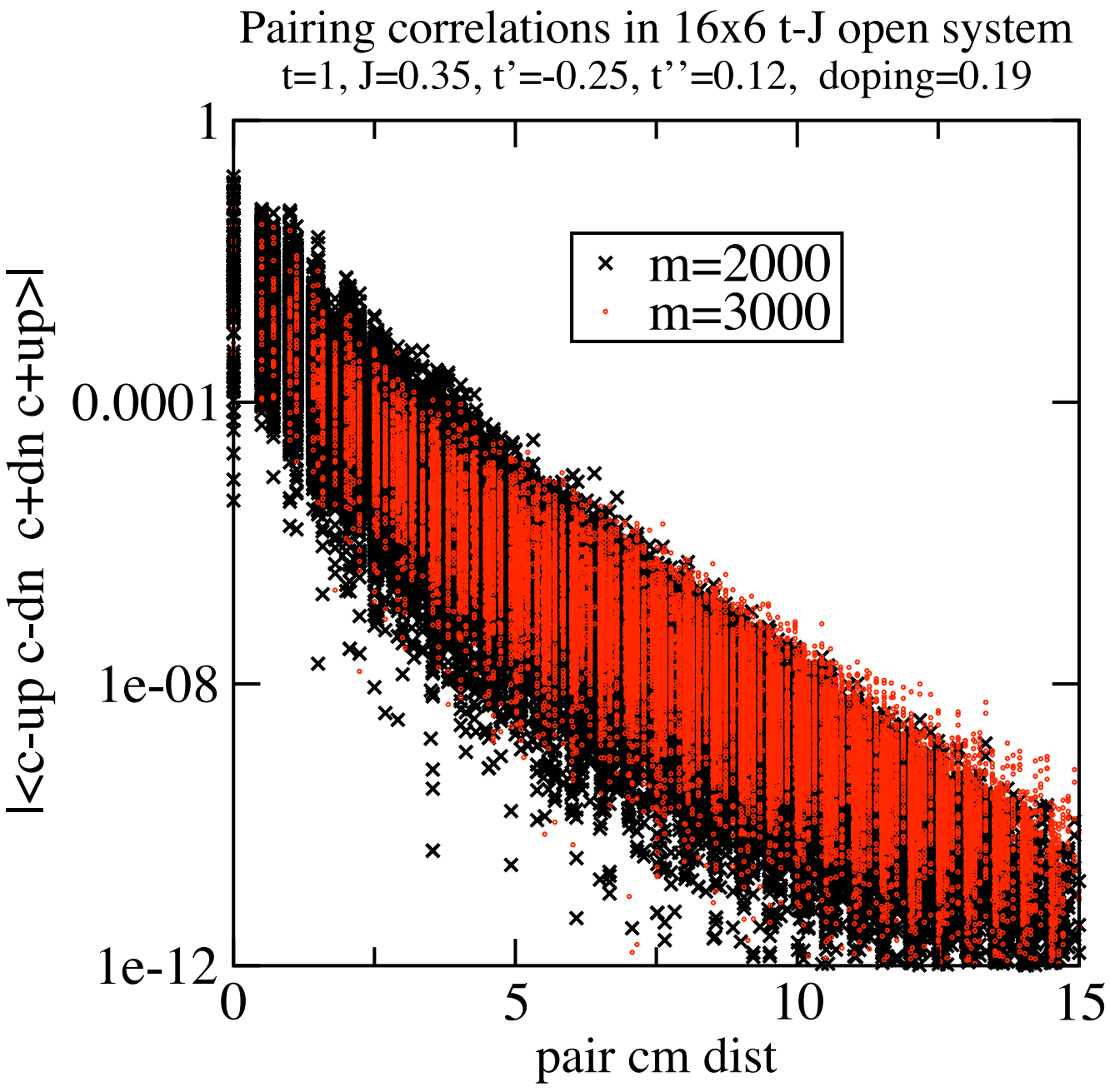


E = -66.7073 m = 3000

16x6
Open BCs
t=1, J=0.35
t’=-0.25,
t”=0.12
18 holes, x=0.19
No pinning
fields

See T. Tohyama, PRB 70, 174517 (2004)--20 site Lanczos seeing some enhanced pairing for these parameters at x=0.3

“Realistic” parameters on an open 16x6



16x6
Open BCs
t=1, J=0.35
t’=-0.25,
t”=0.12
18 holes, x=0.19
No pinning fields

Note: m=3000 run not finished, points missing

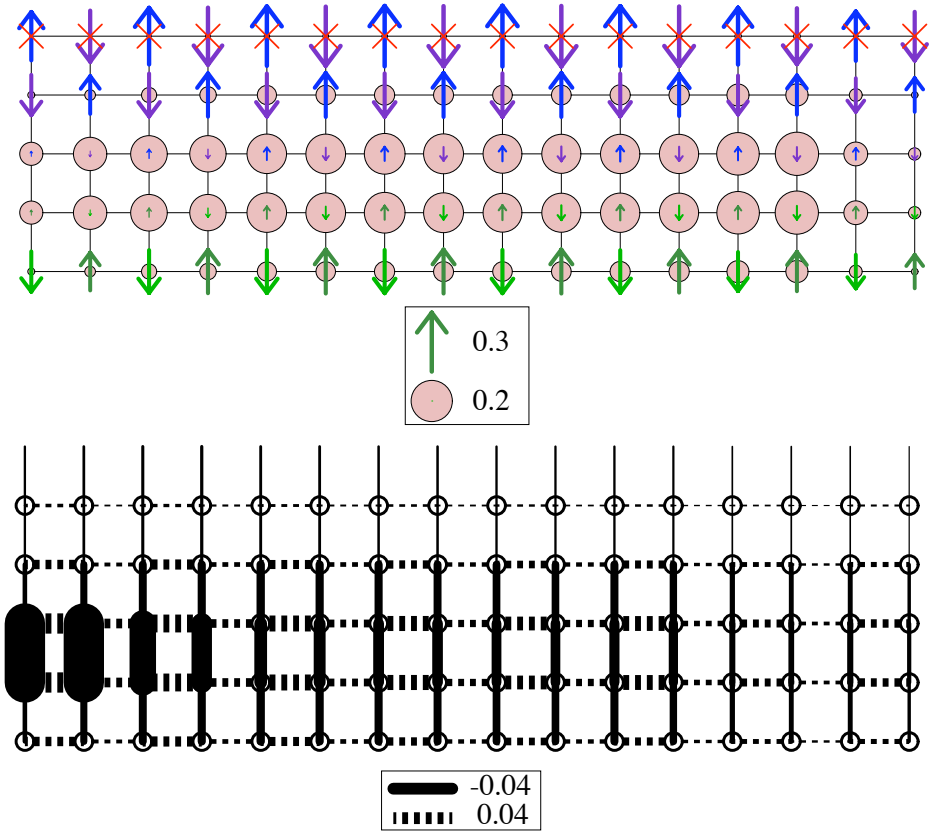
Pairing and t': summary so far

- t'>0, "Electron doped": strong pairing, stripes mostly melt into pairs
- t'<0, "Hole doped": pairing suppressed, stripes destabilize into strange state

- Thus we find that the t-t'-t"-J with the usual parameter ranges fails to capture the behavior of the hole doped cuprates!

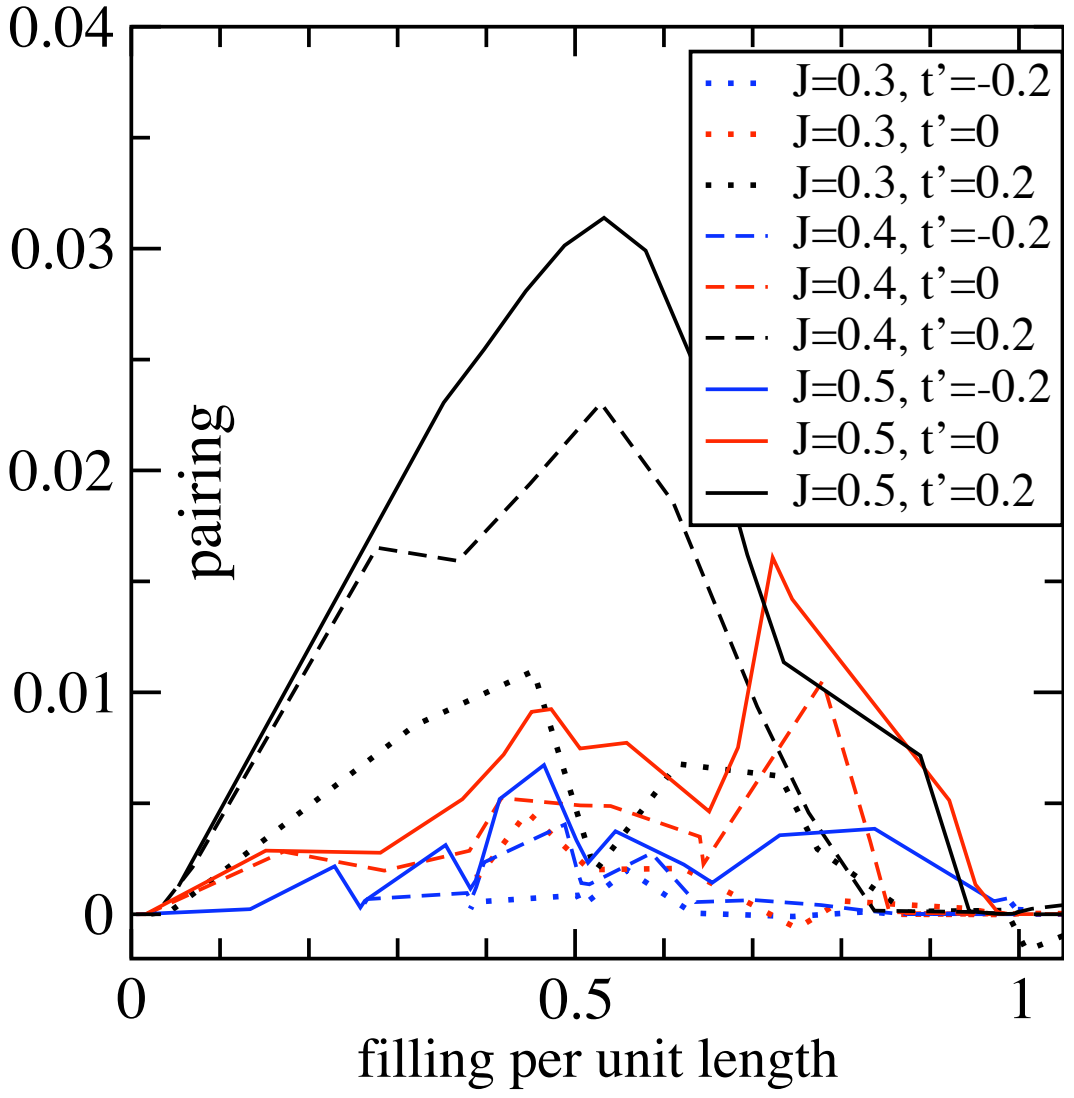
- Are there states with both stripes and pairing if we vary the parameters to be a little less "realistic"? We have already seen the other three combinations.

Longitudinal stripes with proximity effect



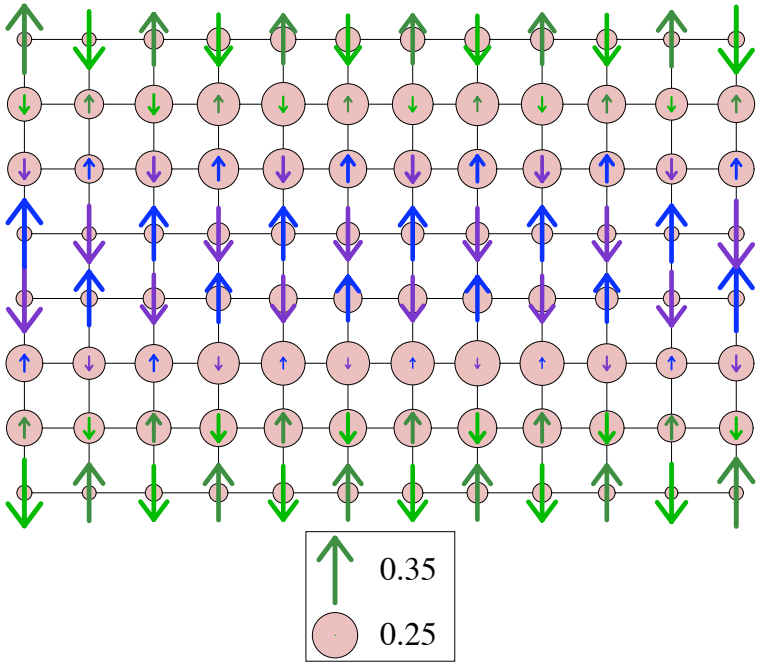
16 x 5 system, Vertical PBC's
J/t = 0.5, t'=0.2, mu=1.41,doping=0.1065

$\Delta + \Delta^+$ applied on links

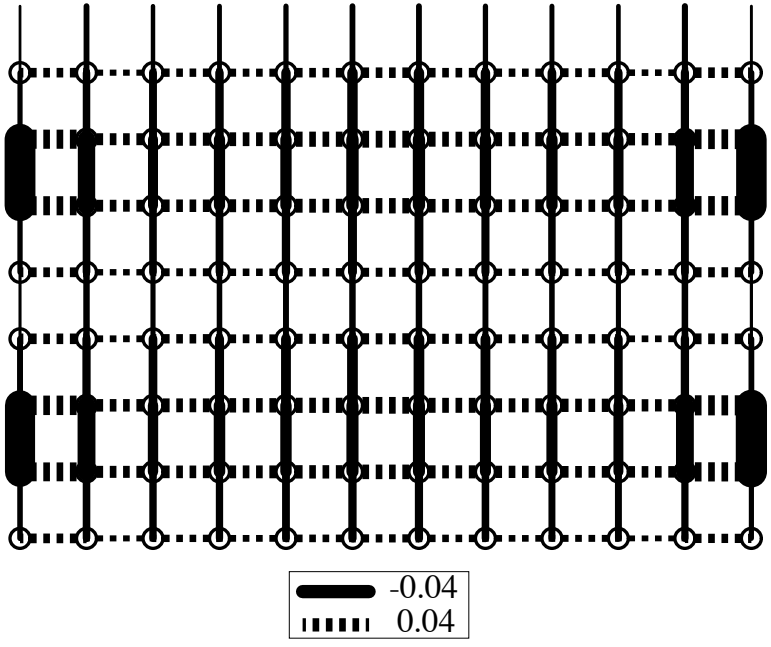


See PRB 79, 220504(R) (2009)

Longitudinal stripes with proximity effect



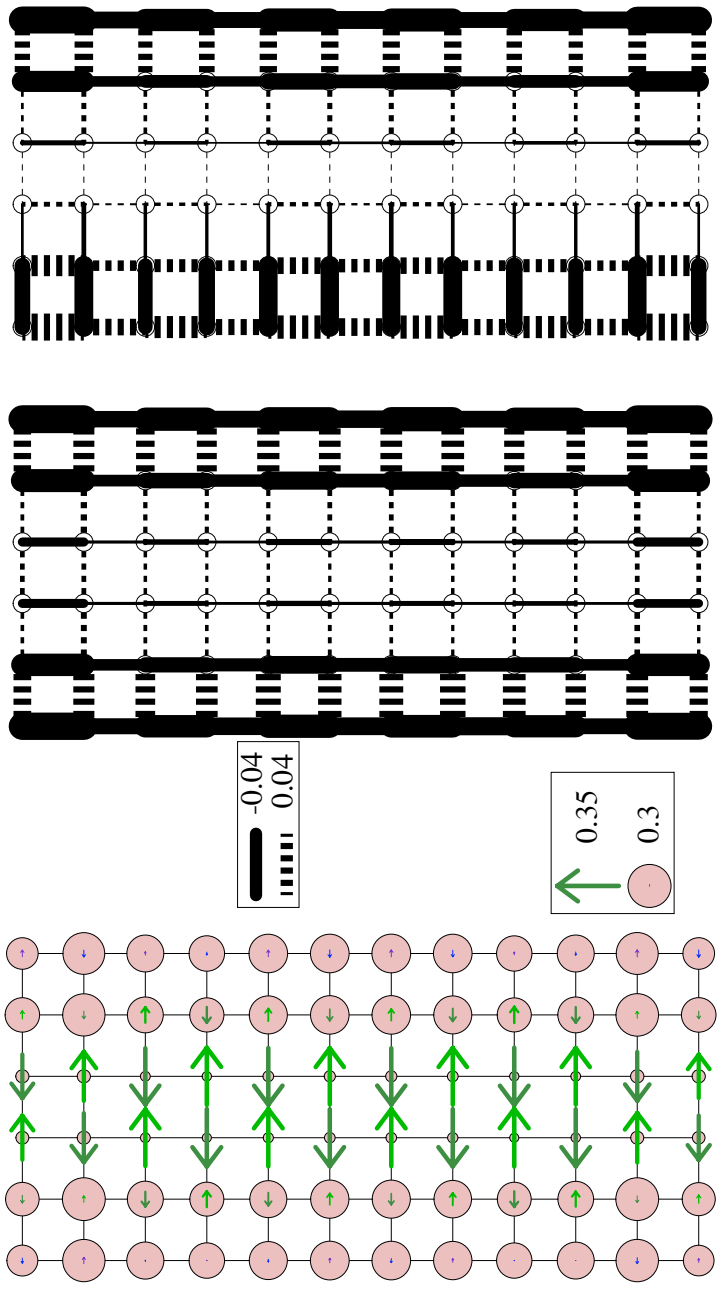
12 x 8 system, Vertical PBC's
Jx/t= 0.55,Jy/t=0.45, mu=1.165,doping=0.1579

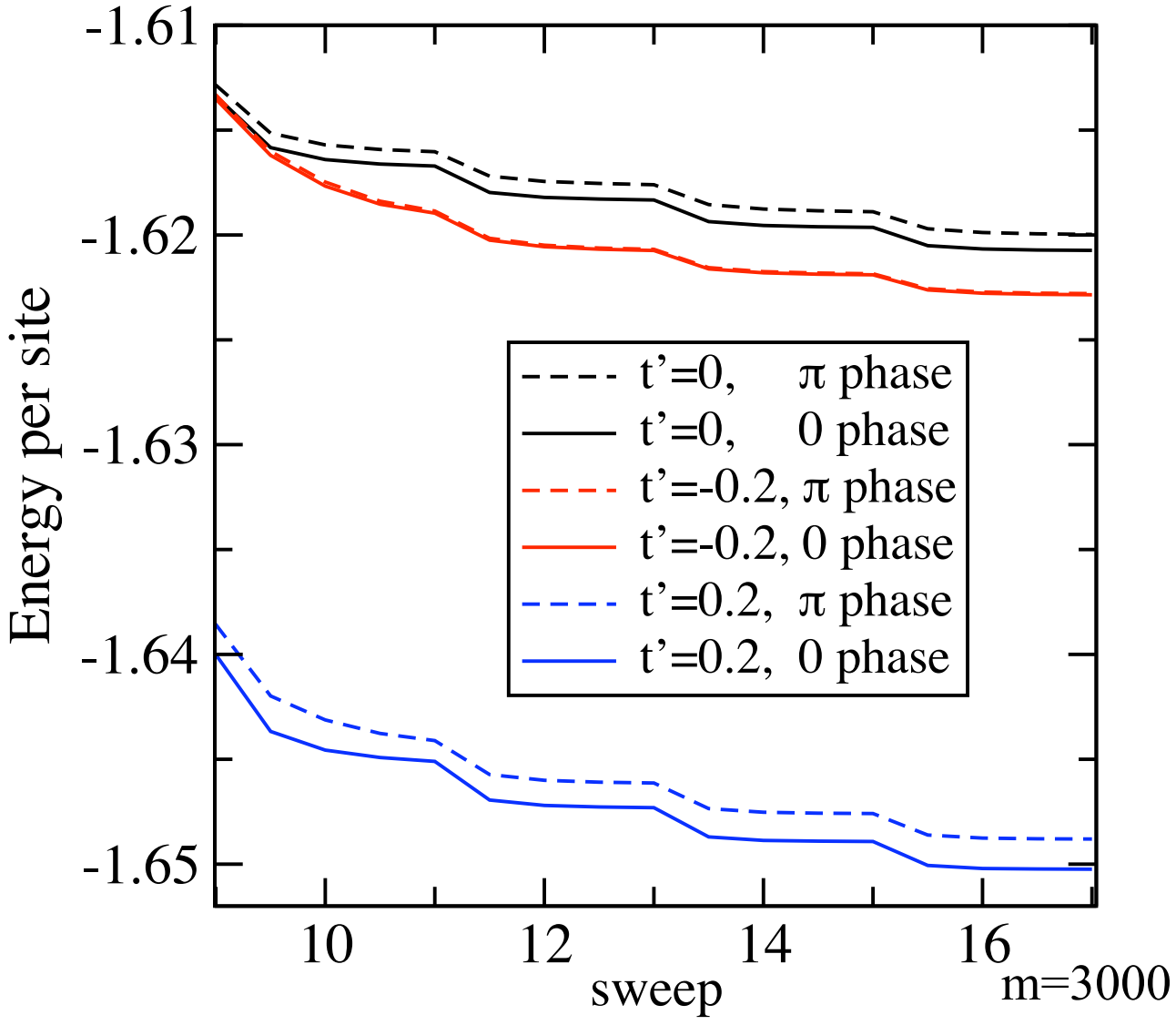


12 x 8 system, Vertical PBC's
Jx/t= 0.55,Jy/t=0.45, mu=1.165,doping=0.1579

AF pinning & Prox effect on left and right sides

Looking for antiphase striped pairing





Conclusions

- For the 2D t-J model we can answer many questions about the ground state phases
- The biggest issue is that the model doesn't adequately describe the cuprates
  - Do we need a multiband model, or
  - Can we fix the model with the right additional terms?
- Generally speaking, stripes and pairing are like brothers and sisters: they have the same cause, they tolerate each other, sometimes they like each other, sometimes they don't.
- The t-t'-J model doesn't seem to produce antiphase pairing.