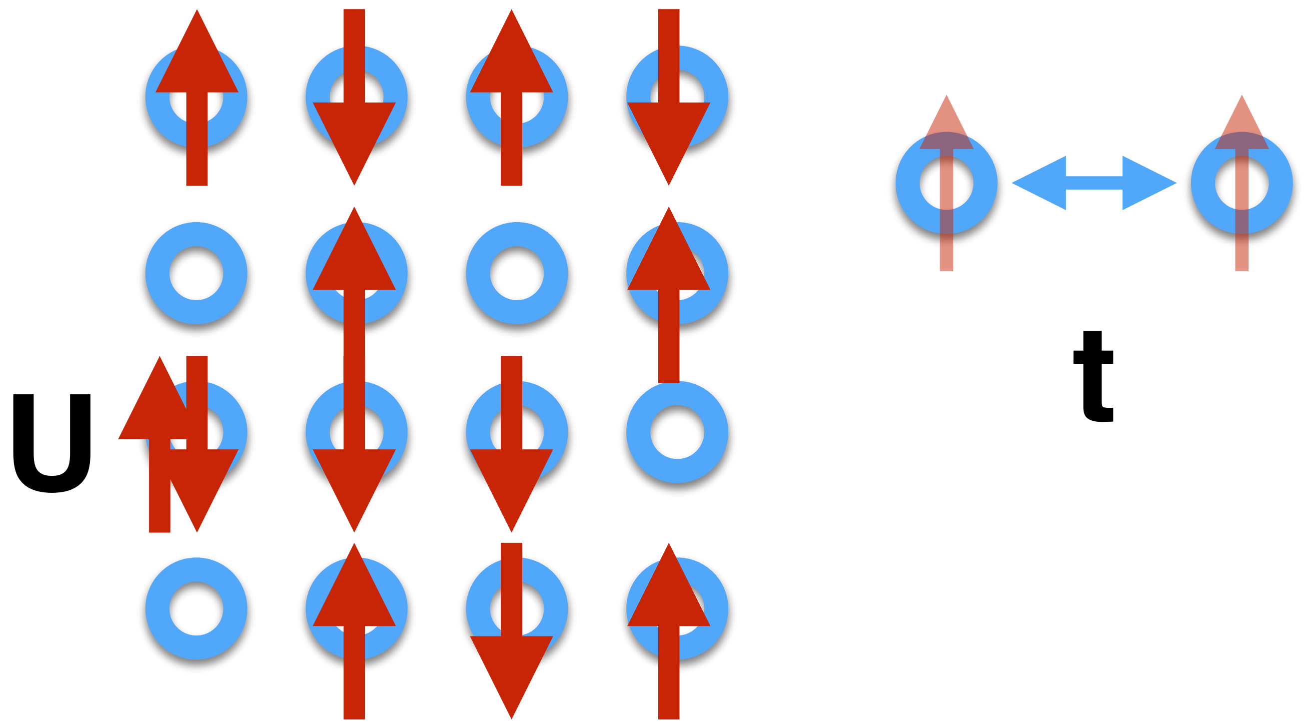
Ground state Phase diagram of the t-t'-J model

- Introduction: models for high Tc superconductivity and DMRG methods
- Phase diagram and new phases
- Comparison with experimental phase diagram
- Conclusions

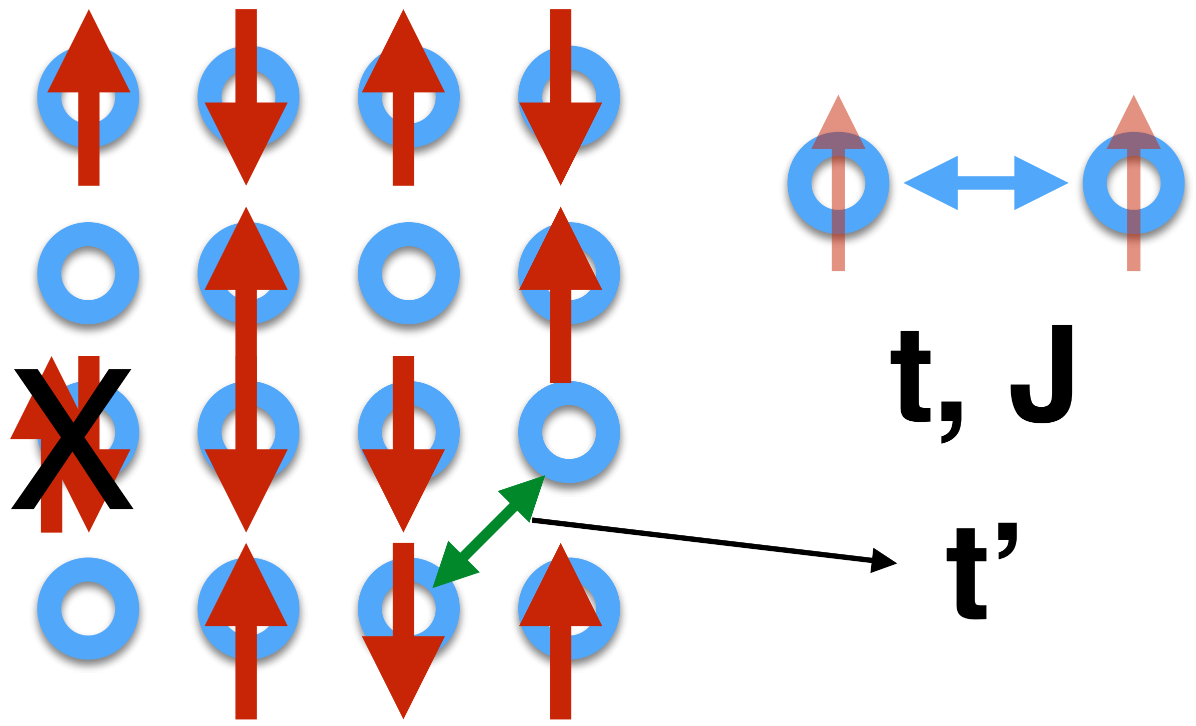
Shengtao Jiang

Steve White
UC Irvine

Doug Scalapino

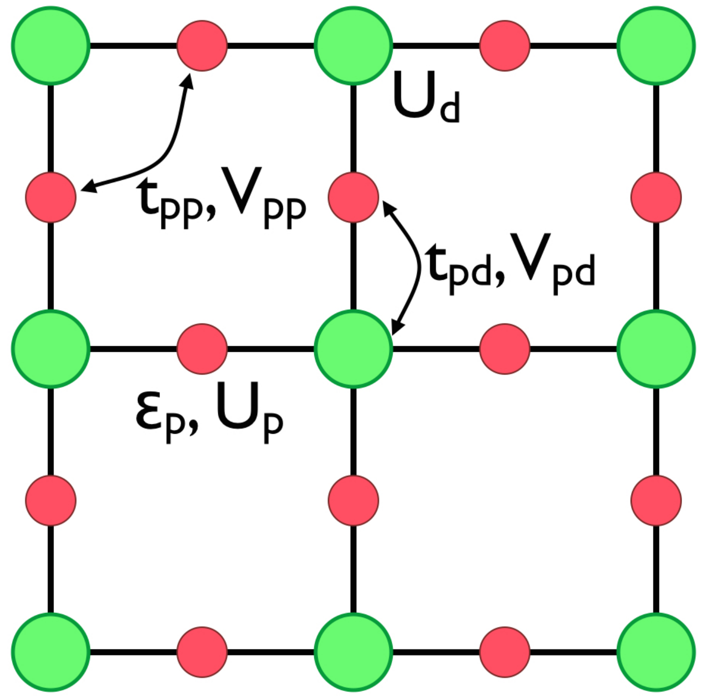


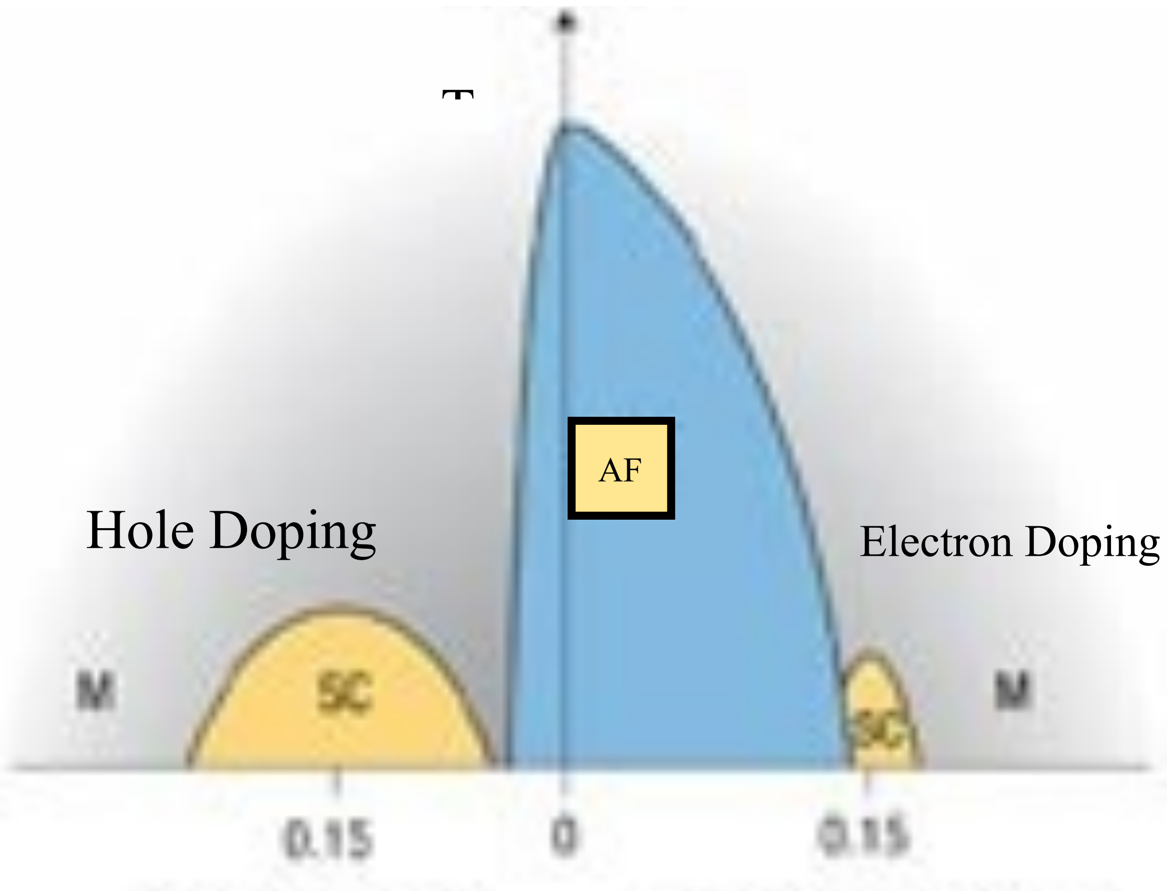
Hubbard Model



t-t'-J Model

The 2D Hubbard model and Family





<u>We are interested in a family of models:</u>

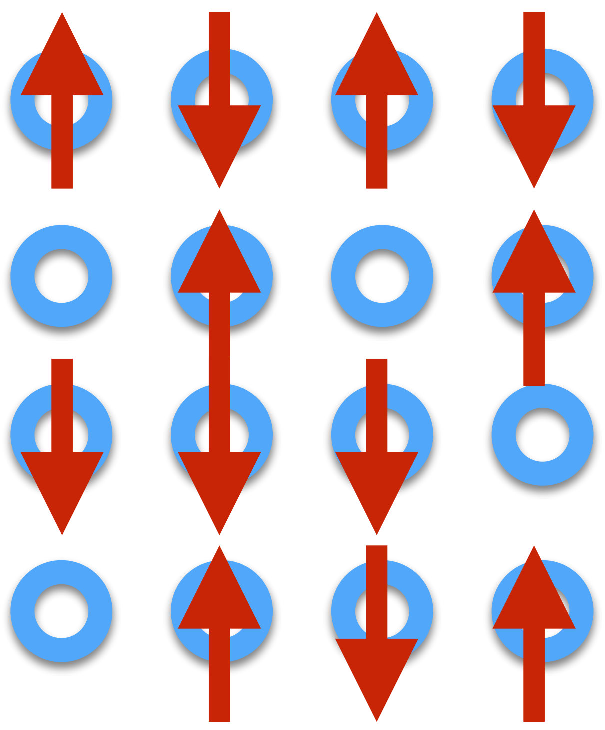
The **three band Hubbard model** has the most realistic description of the cuprates

The **one band Hubbard model** is simpler and more general, and has both weak and strong coupling regime.

The **t-J model** is simpler still, applying to the strong coupling regime only, more approximately.

A few notes on cuprates (experiments):

1. Always d-wave pairing
2. Hole doped has higher Tc. In one-band, t'<0 ~ hole doped, t'>0 ~ el doped
3. Stripes seen in many materials



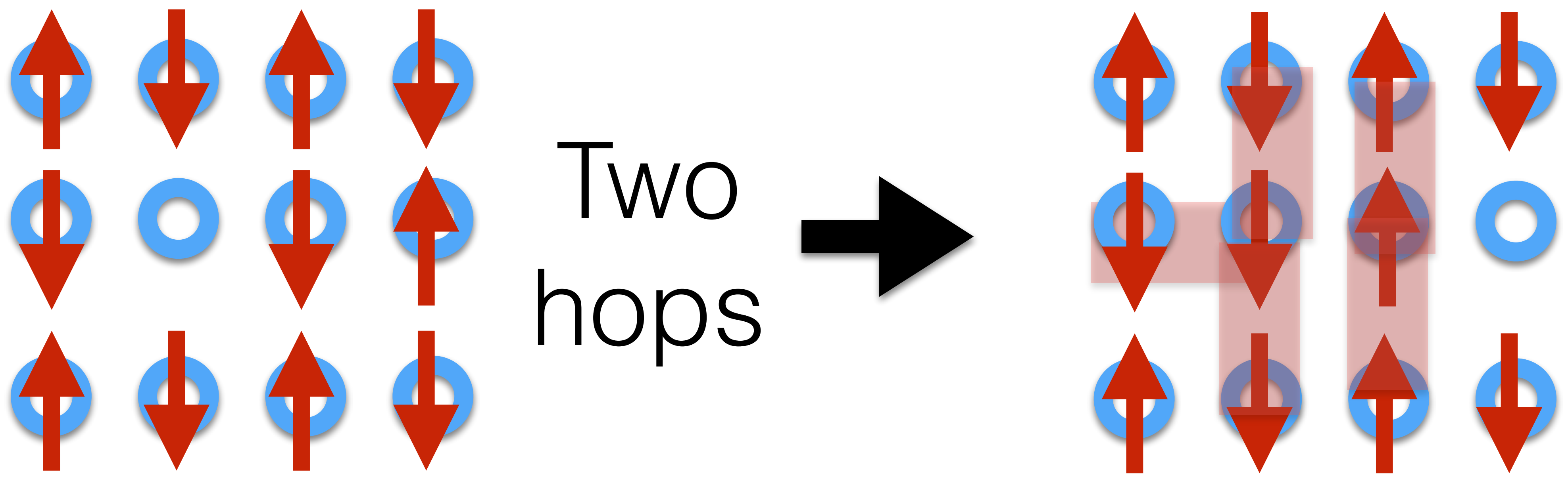
t=1: nearest neighbor

t': diagonal nnn

J=0.3-0.4

$$H = \sum_{ij,\sigma} - t_{ij}(c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + J \sum_{\langle ij \rangle} (S_i \cdot S_j - \frac{1}{4} n_i n_j)$$

Frustrated hole hopping is key to the physics

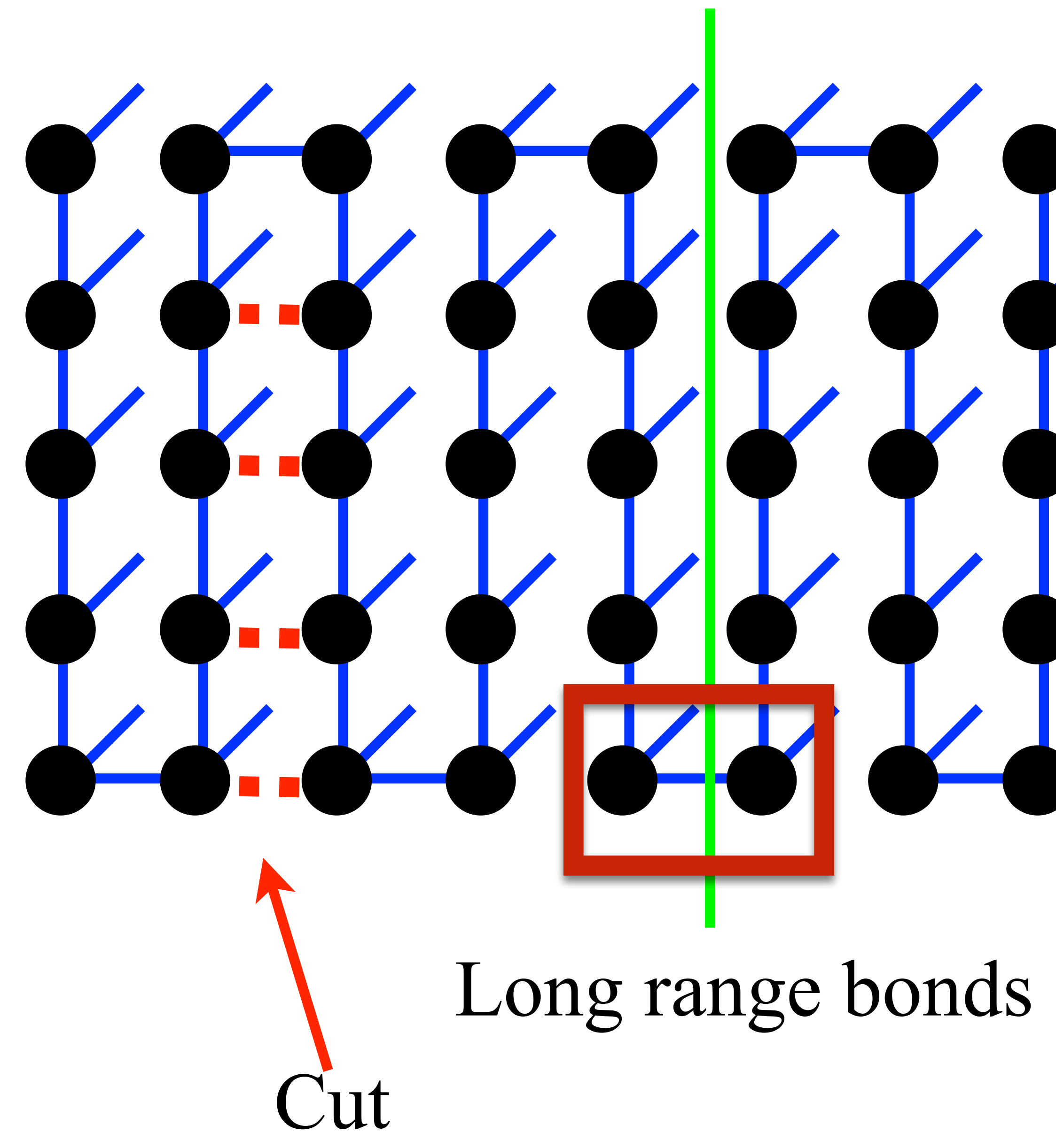


Tensor network methods for 2D systems

DMRG sweeping is essentially alternating least squares

Traditional DMRG method (MPS state)

Map finite 2D cluster onto 1D

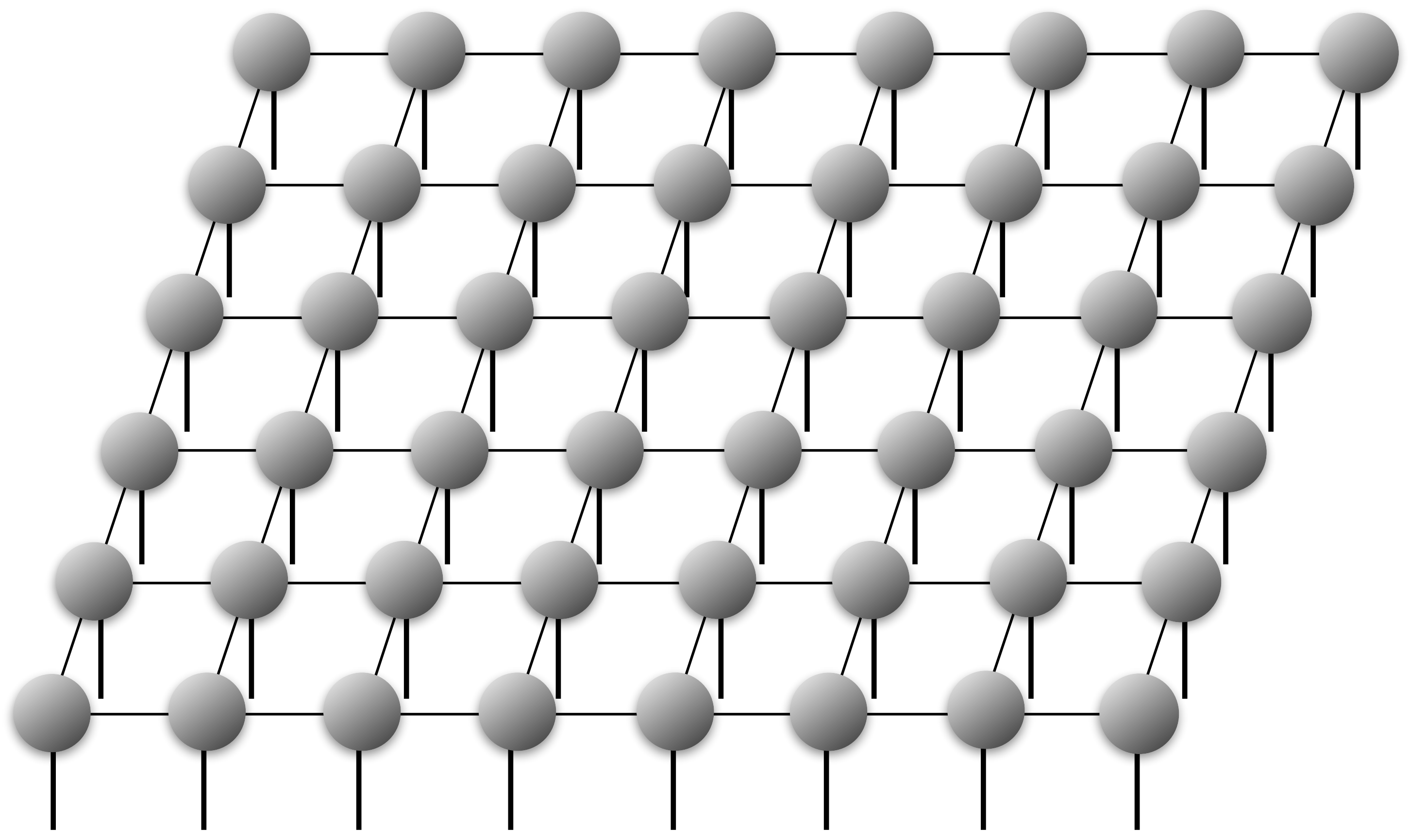


Entropy S $\sim L_y$ (area law)

Bond dimension $m \sim \exp(a\ L_y)$

$m \sim 10^4$, cpu time $\sim m^3$

Projected Entangled Pair State (PEPS)



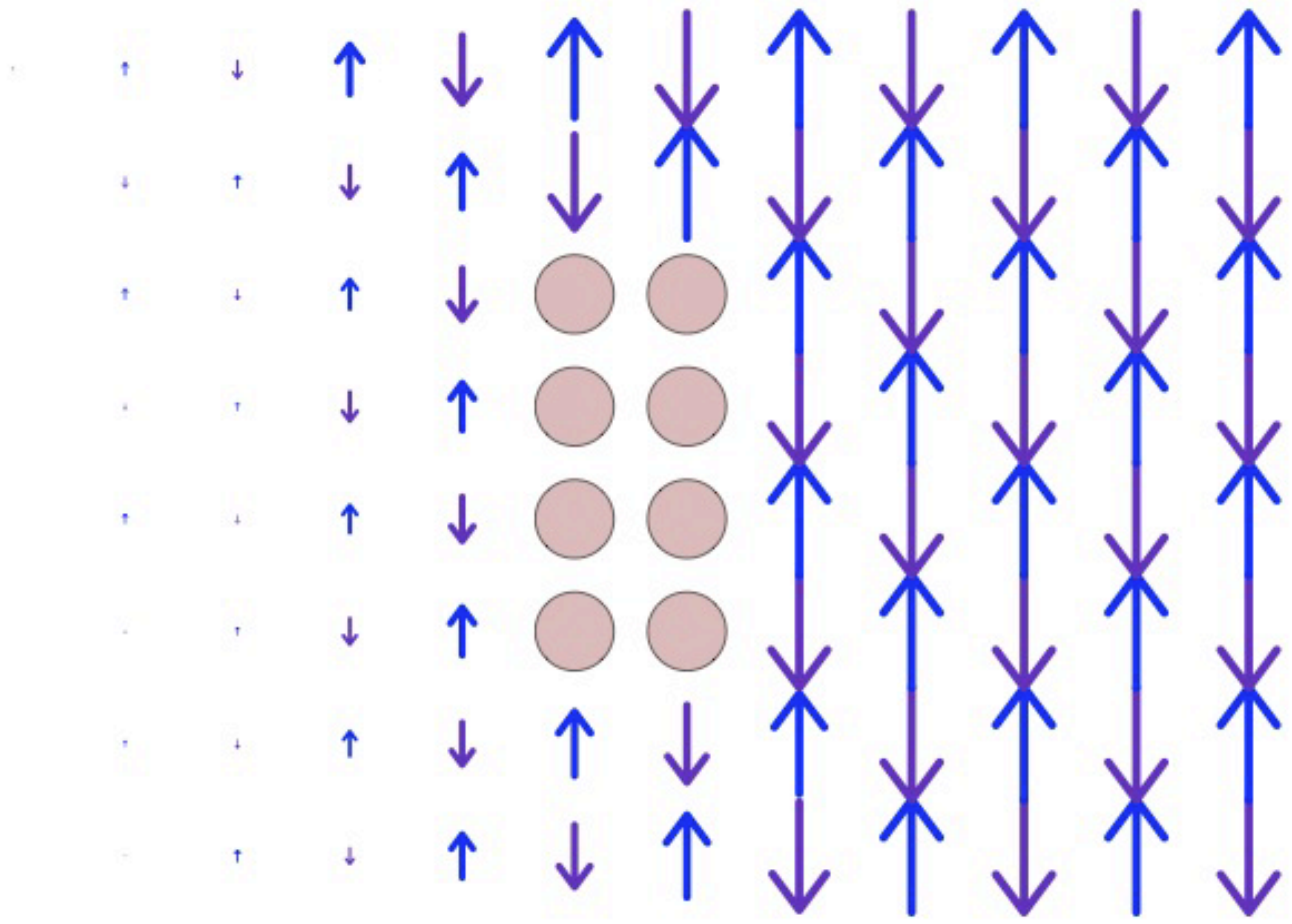
More natural representation

More efficient compression: m ~ 10-15 can provide high accuracy

Less efficient algorithms: $\sim m^{12}$

These two methods have reached approximate parity for 2D systems: high accuracy for smaller system versus less accuracy for very large systems. It is useful use them as complementary, along with certain types of quantum Monte Carlo

Early DMRG results: t-J Model (White and Scalapino, 1998–)



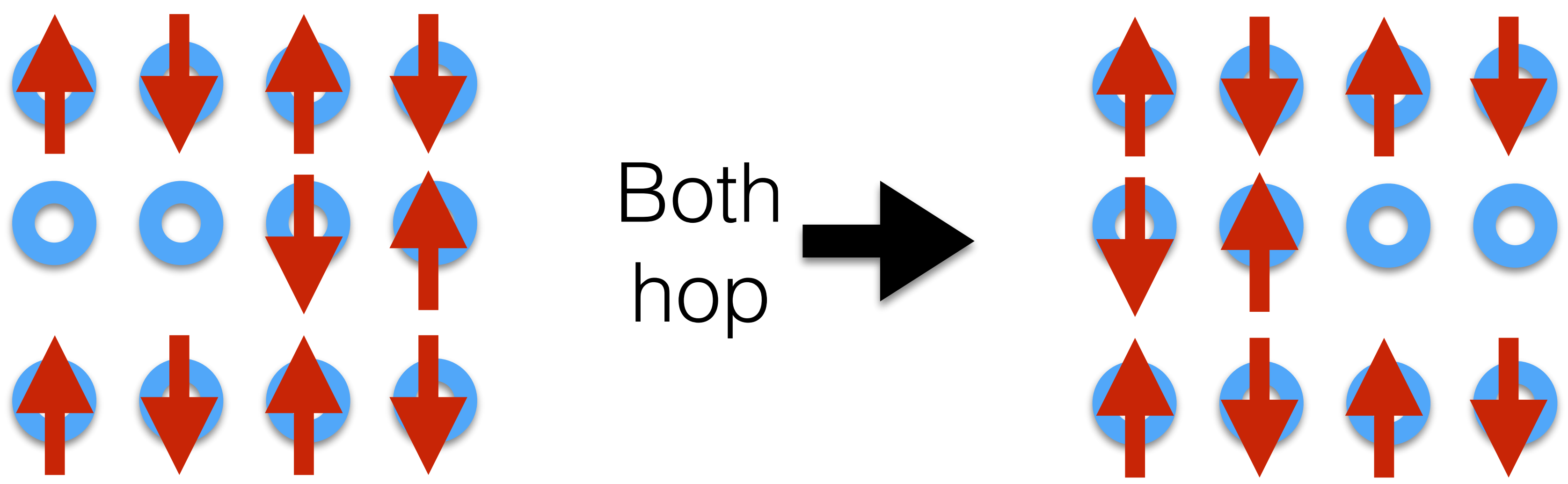
E = -31.7287   m = 70

(max size of matrices in MPS)

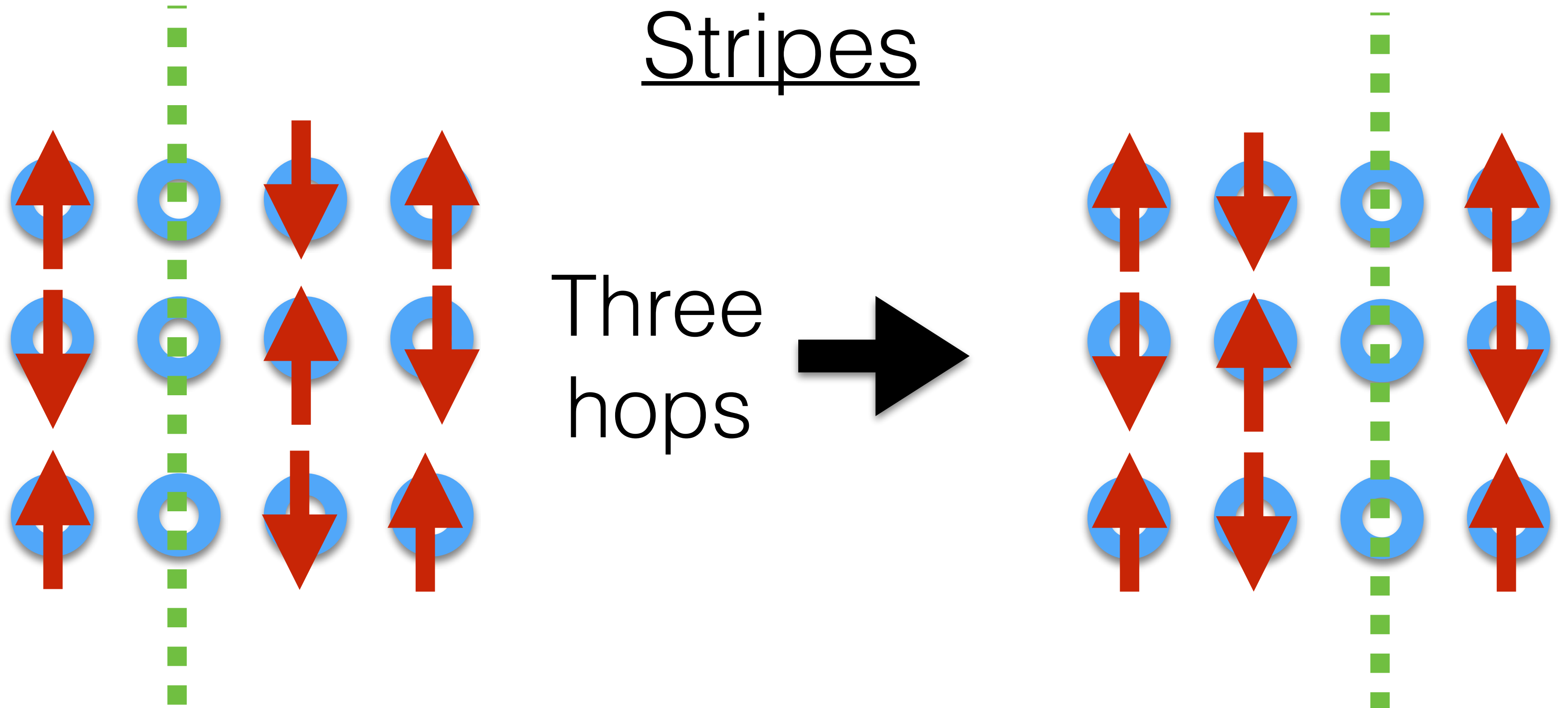
12x8   J=0.35
t'=0   8 holes

Diameter of circle proportional to hole probability
Length of arrows proportional to <Sz>. Color shows domains

Pairing



Stripes



Summary—early t-J

- The key unexpected feature we found was stripes in most of the phase diagram. These make robust AF domain walls.
- Stripes are caused by the same competition between hole motion and local AF order that causes pairing. Stripes and SC tend to compete, but they can also coexist. Overall, the pairing we saw seemed a little weak.
- The role of t' in pairing seems clear—but it is the opposite of what you would expect from experiments!

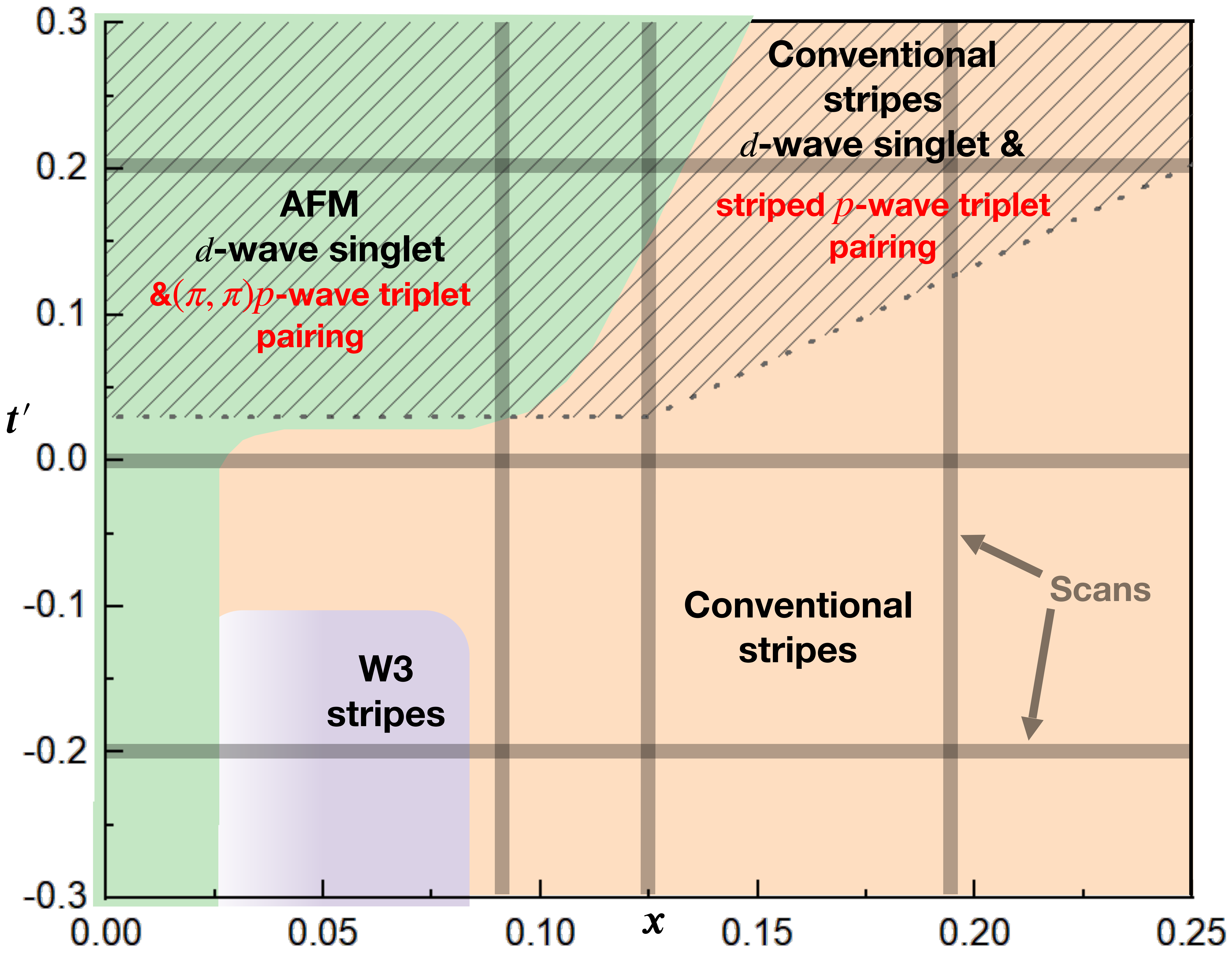
Subsequent work by many groups on Hubbard and t-J

- New approaches (iPEPS, DMET, …) and improvements to DMRG and QMC, DMFT methods have now made progress very rapid
- Frequent use of several methods together for complementary capabilities
- Many of the t-J features (stripes) solidly found in the Hubbard model
- Pairing features in Hubbard continue to be puzzling…

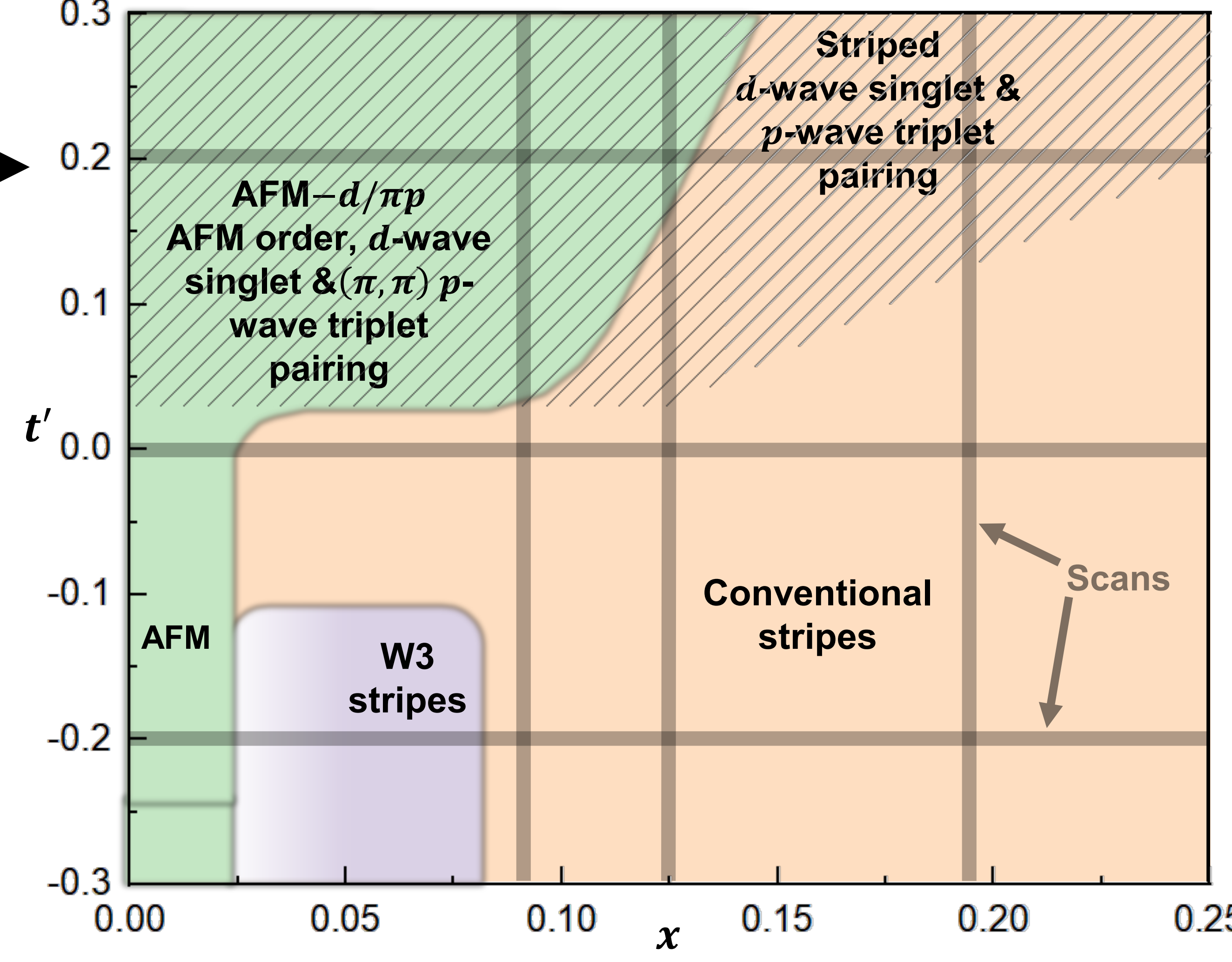
Phase diagram of t-t'-J model

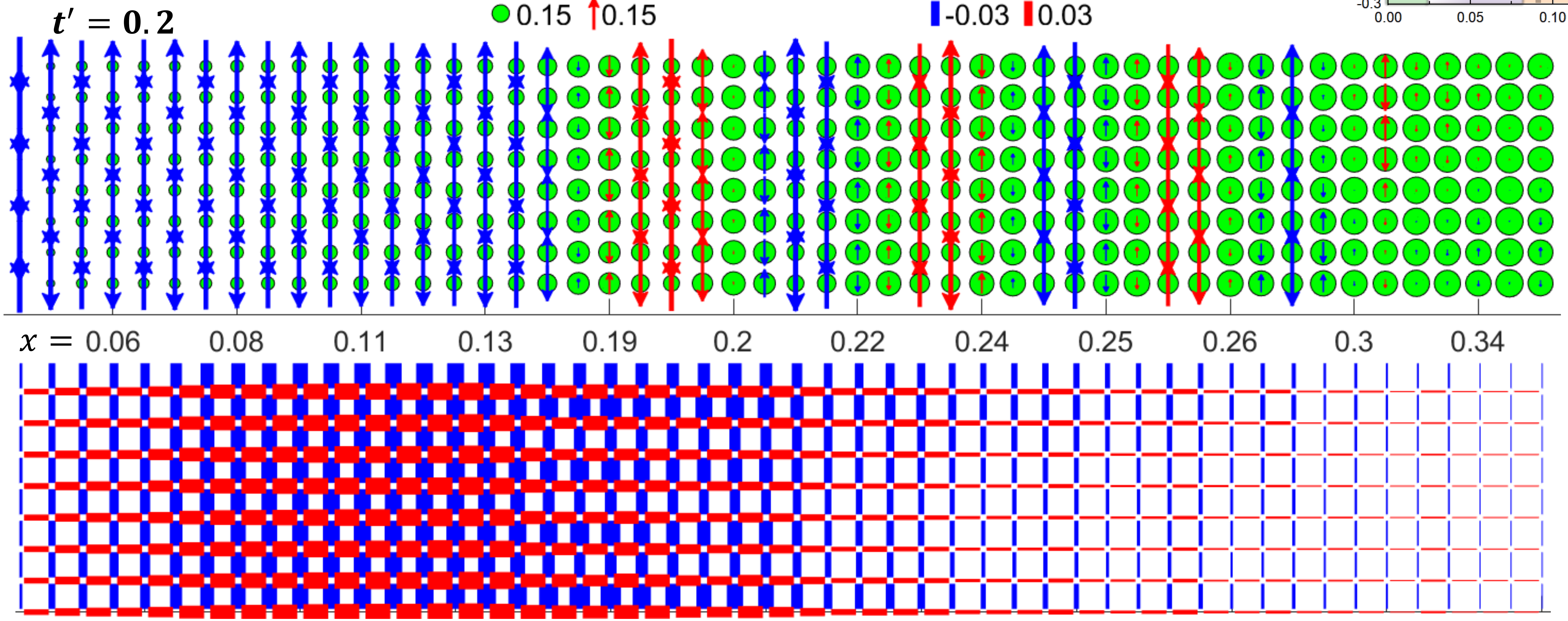
Jiang,Scalapino,White,
preprint will be out this week

J/t=0.4, based on width-8 cylinders



“Scan” simulation varying doping with position

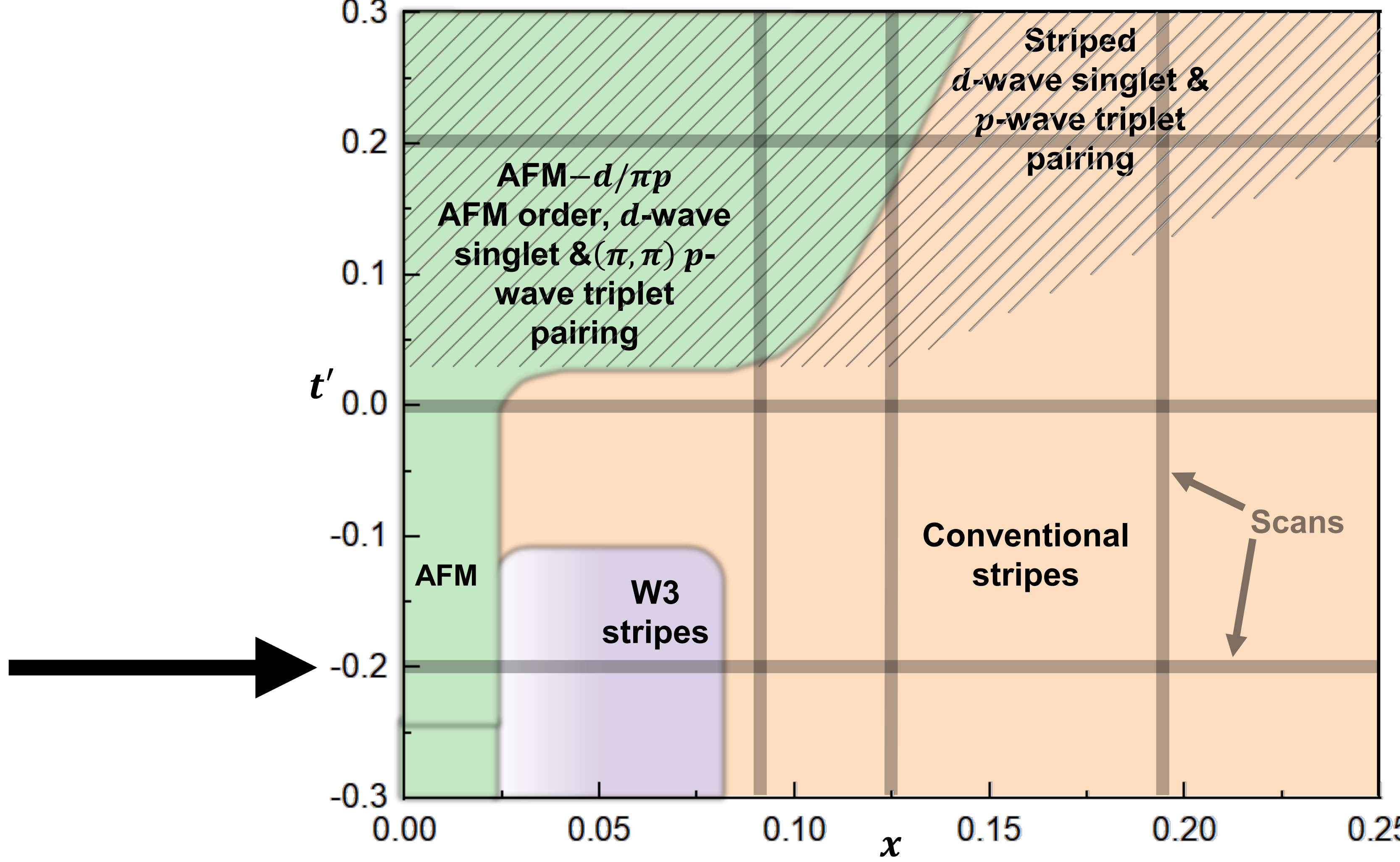


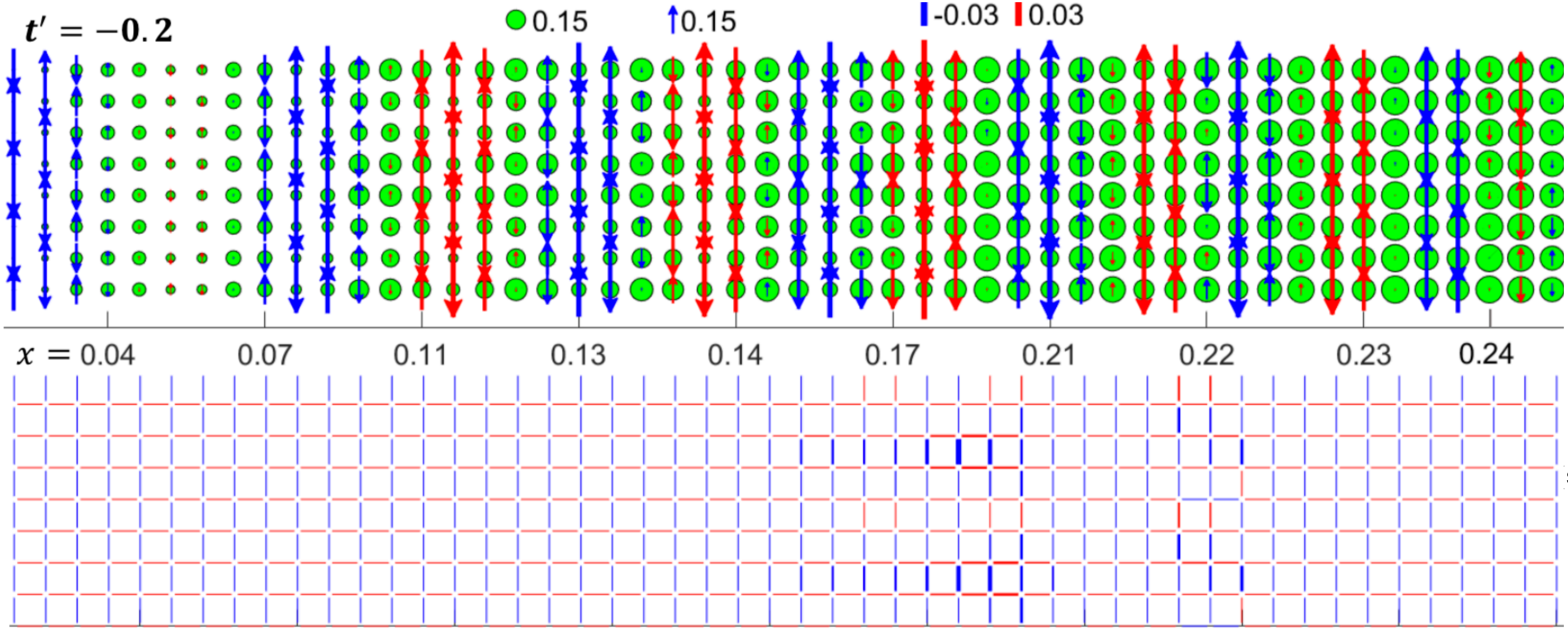


density, spin

pairing
(superconductivity)

“Scan” simulation varying doping with position

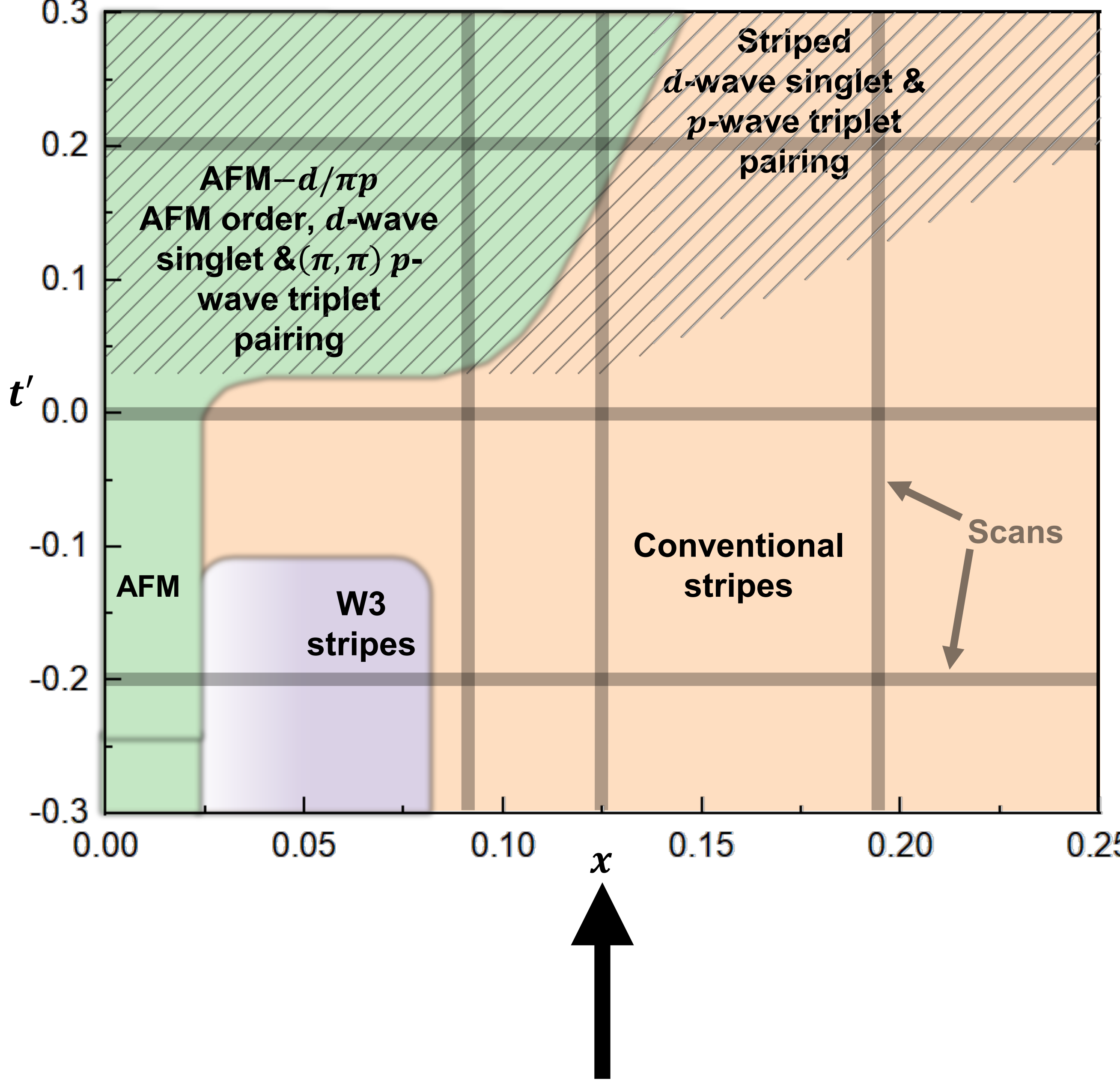


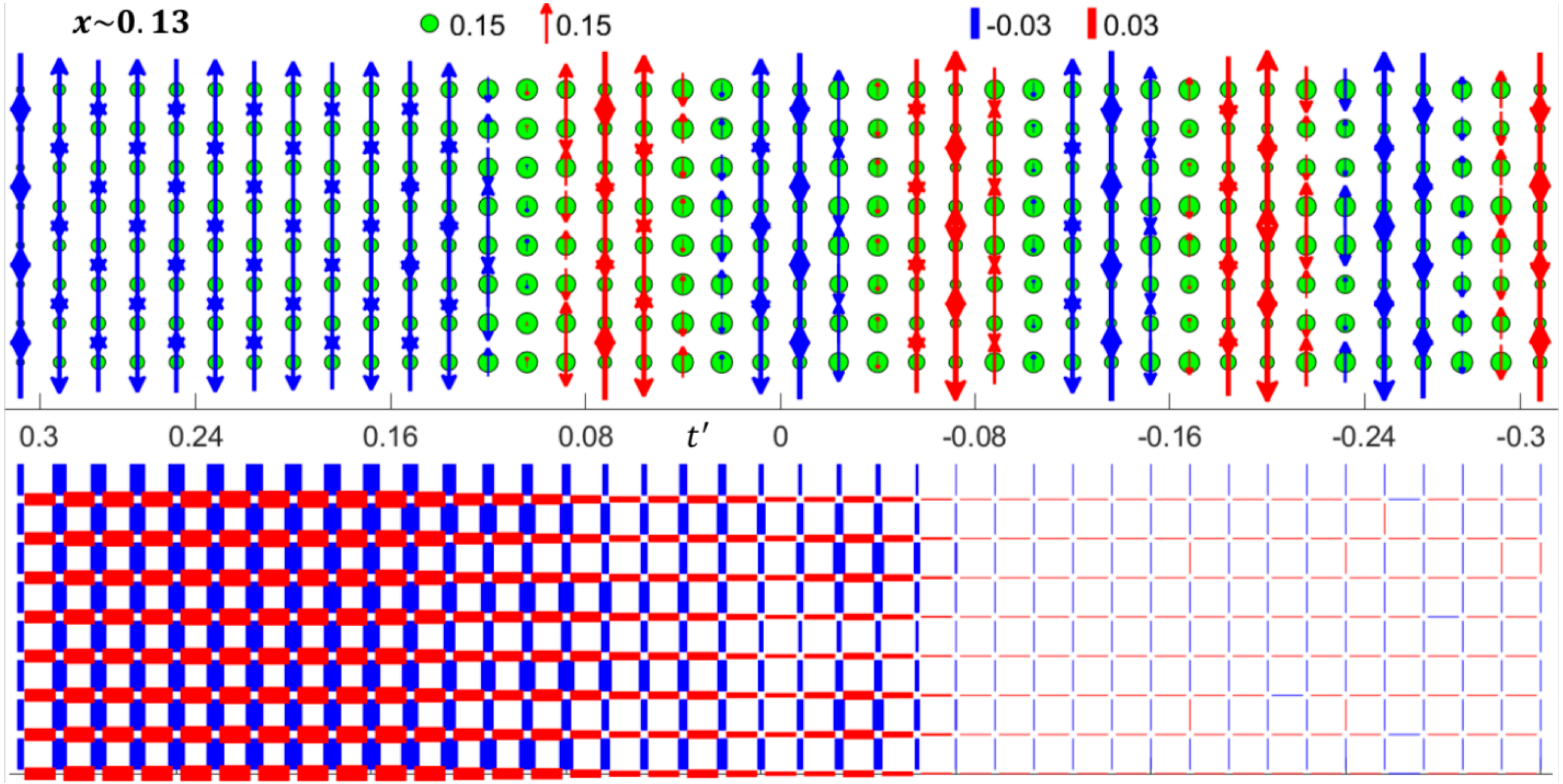


density, spin

pairing
(superconductivity)

“Scan” simulation varying t’ with x=0.13

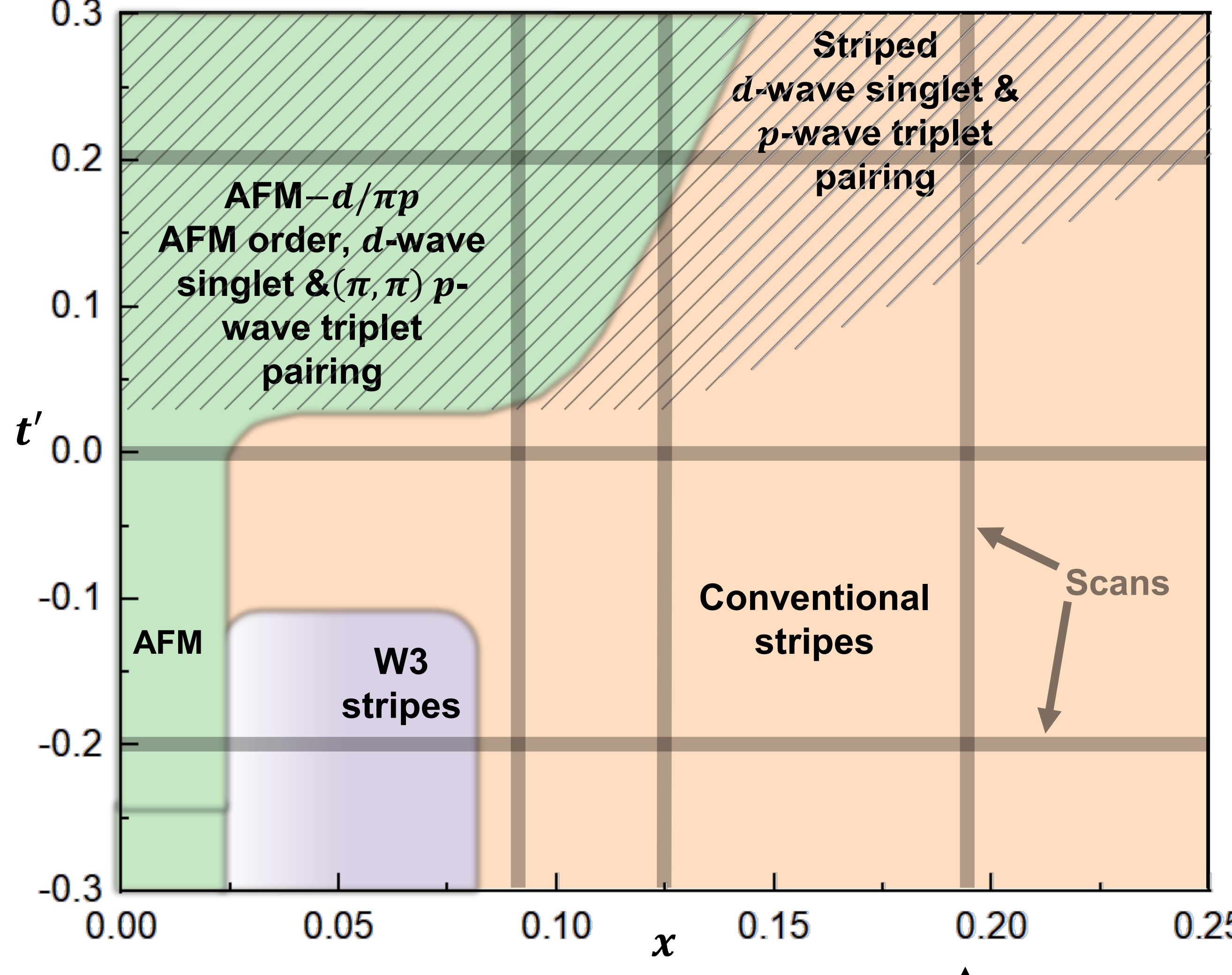


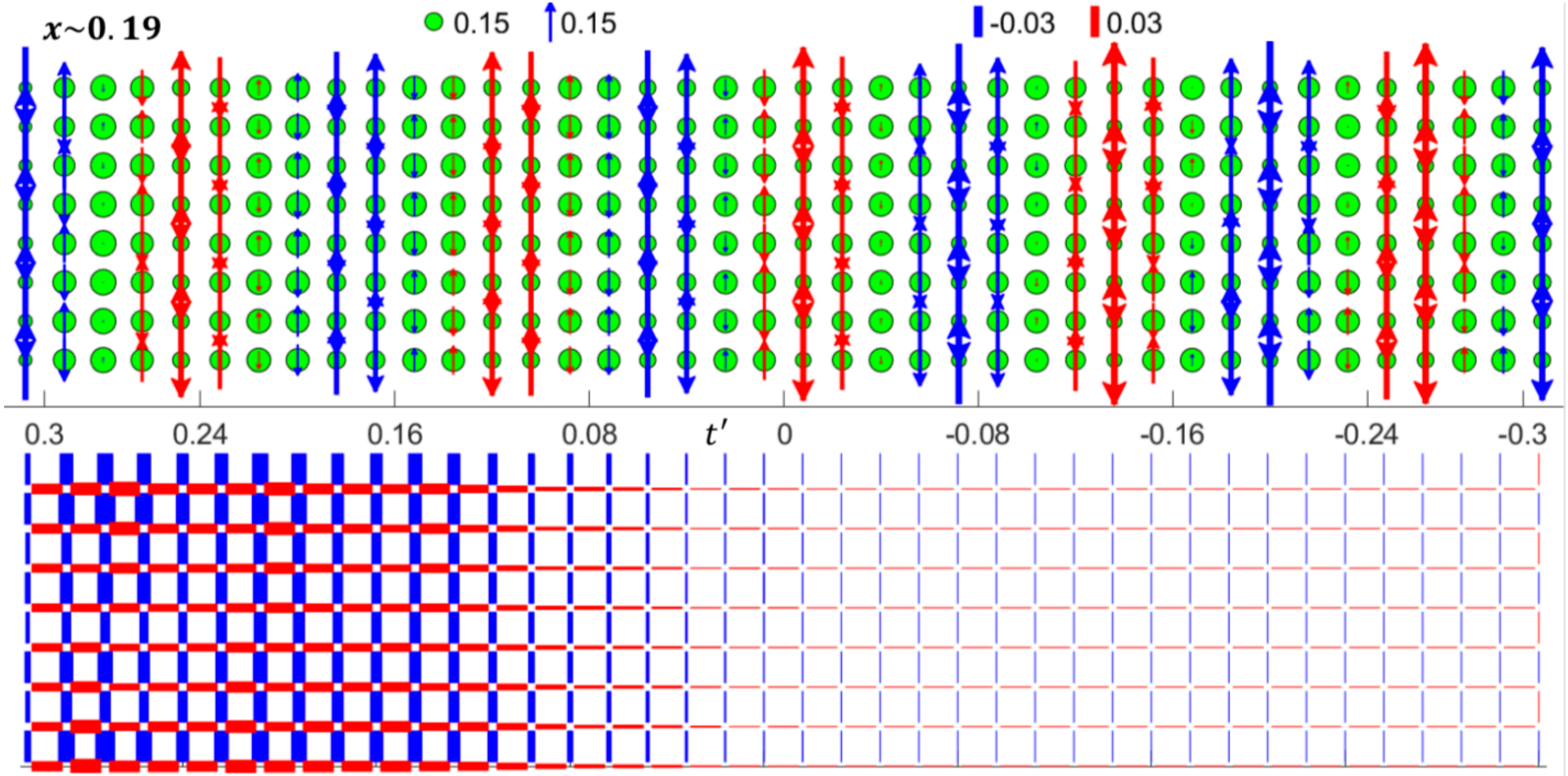


density,
spin

pairing
(superconductivity)

“Scan” simulation varying t’ with x=0.19



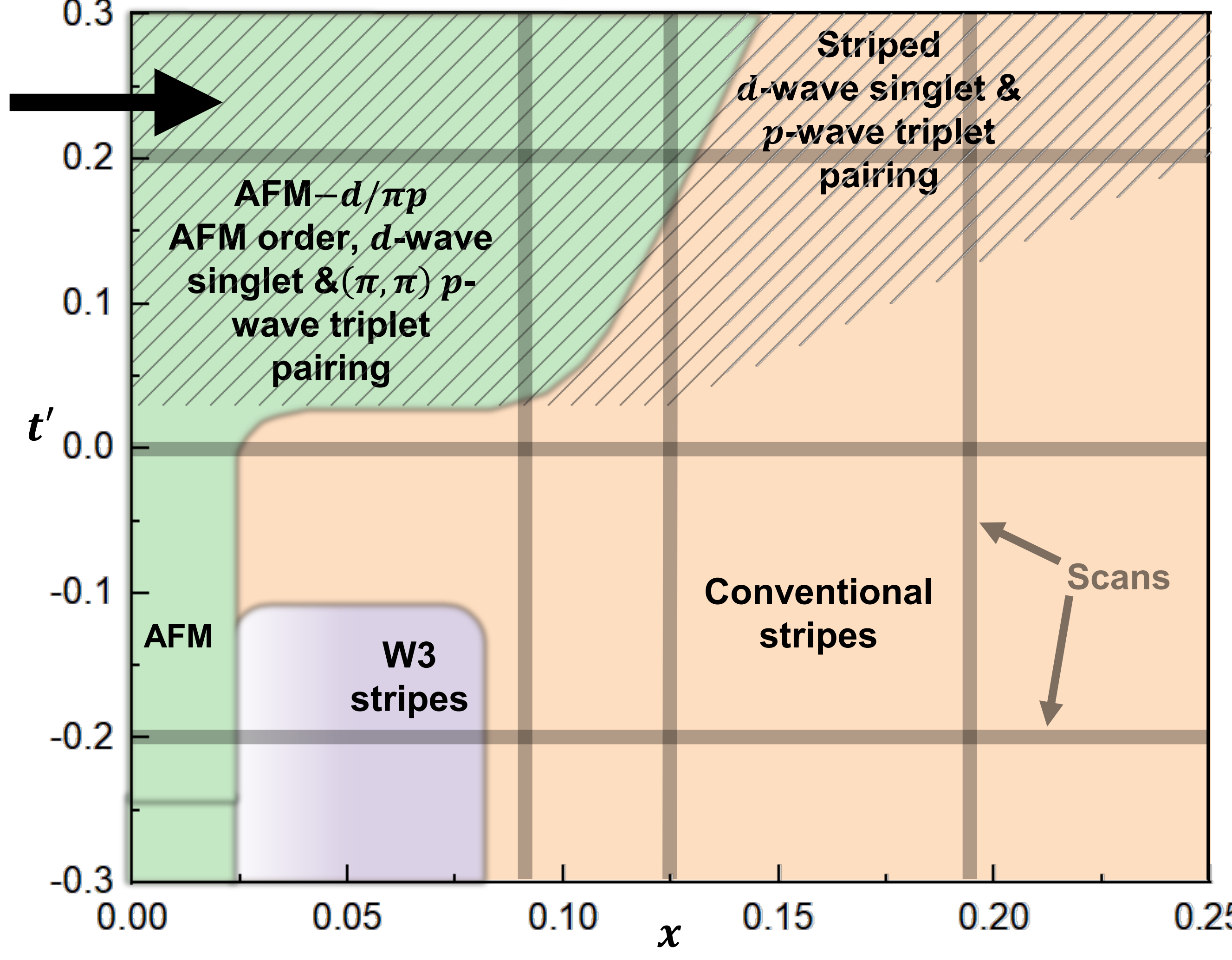


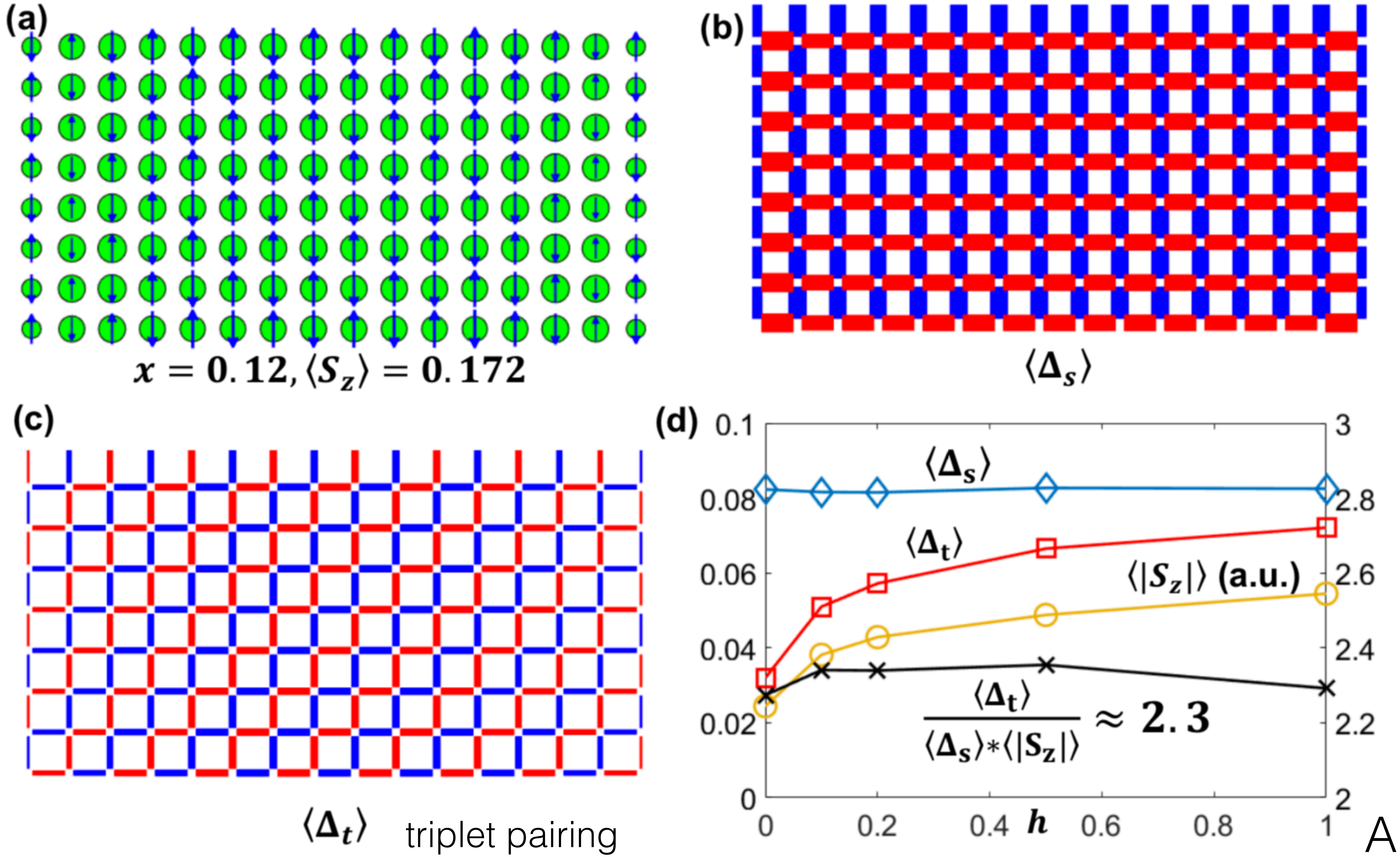
density, spin

pairing
(superconductivity)

Uniform AF/d/p-pi phase

Foley, et al PRB 99, 184510(2019); Almeida et al, (2017); Rowe, et al 2012
Robust d-wave in t-t'-J: Gong,Zhu,Sheng arxiv:2104.03758





$x = 0.12, \langle S_z \rangle = 0.172$

$\langle \Delta_s \rangle$

$\langle \Delta_t \rangle$ triplet pairing

$\frac{\langle \Delta_t \rangle}{\langle \Delta_s \rangle * \langle |S_z| \rangle} \approx 2.3$

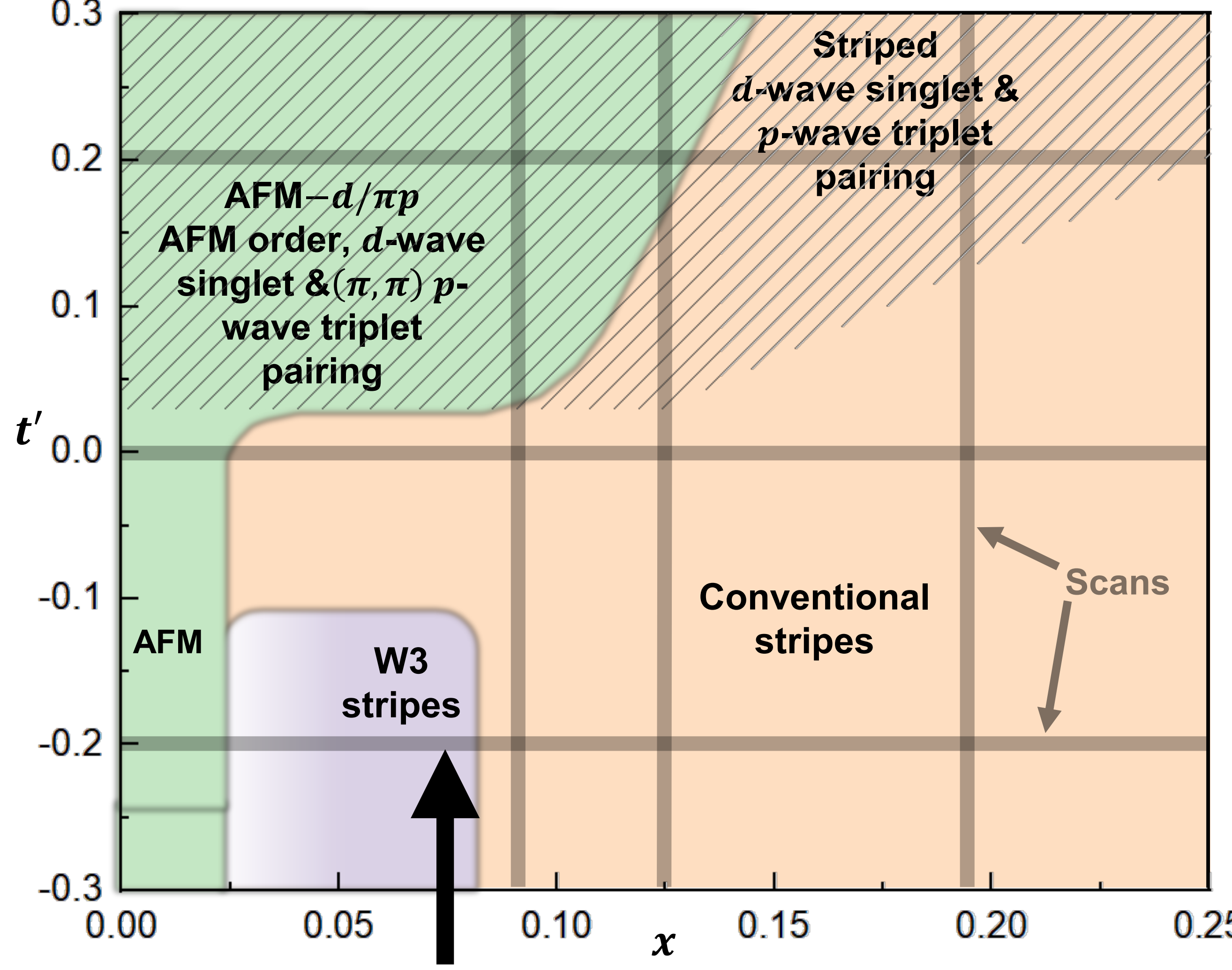
AF field h

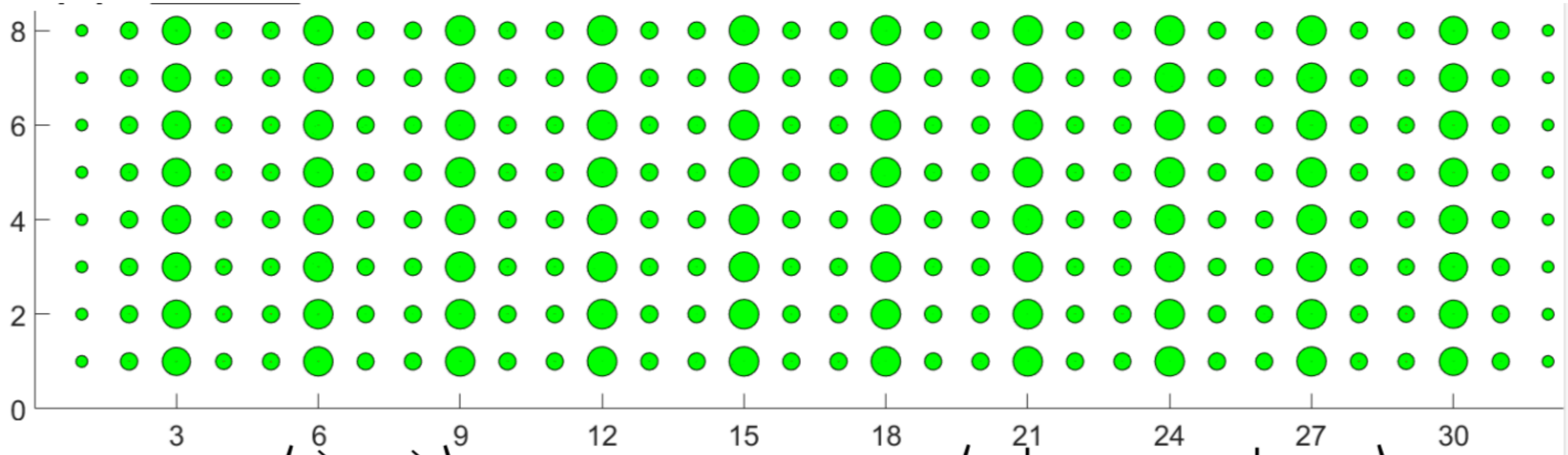
Artificially strengthening the AF order doesn't decrease the pairing

The momentum (π, π) triplet p-wave order is purely derivative from the combination of AF and d-wave

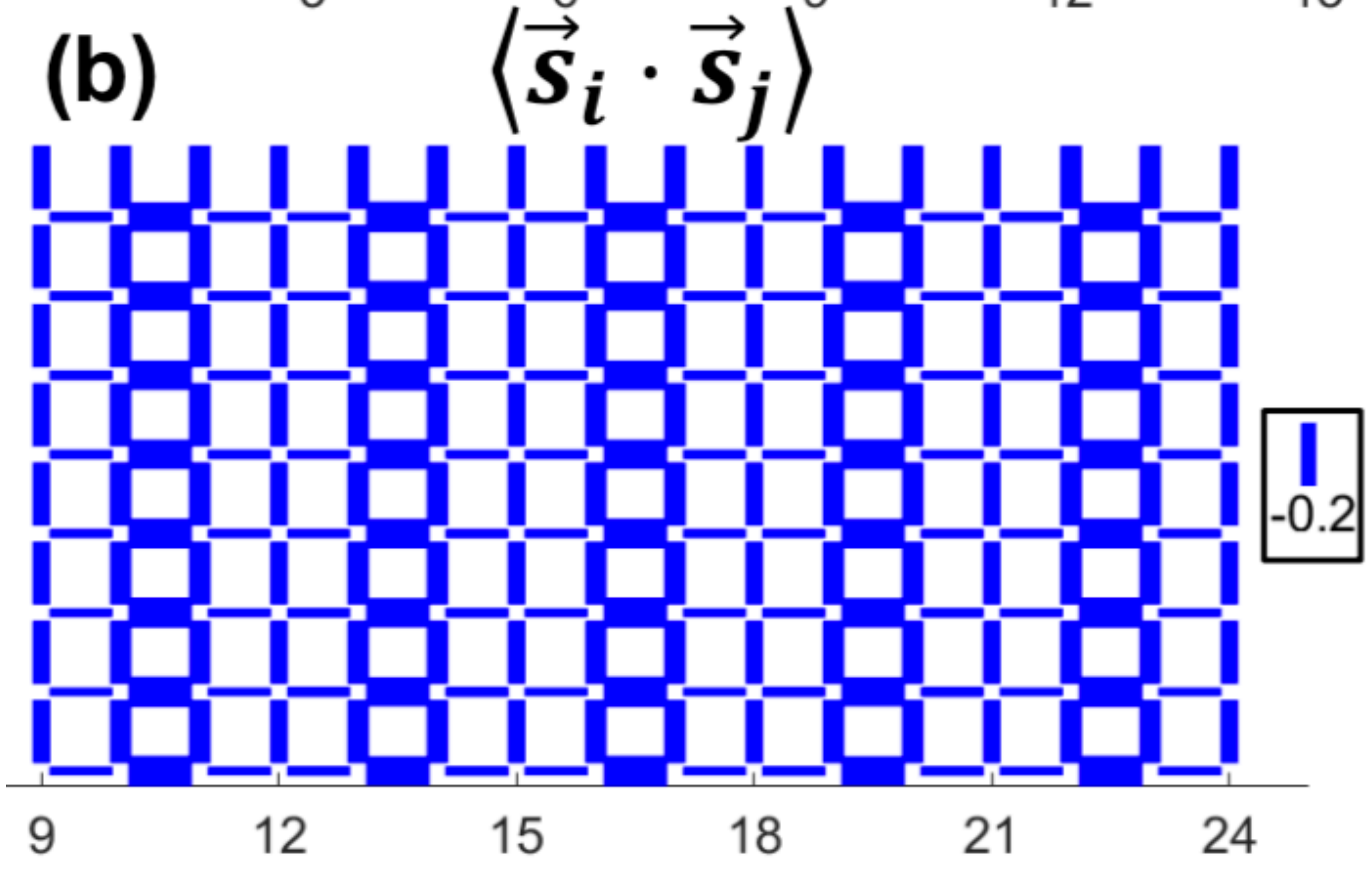
W3 stripes

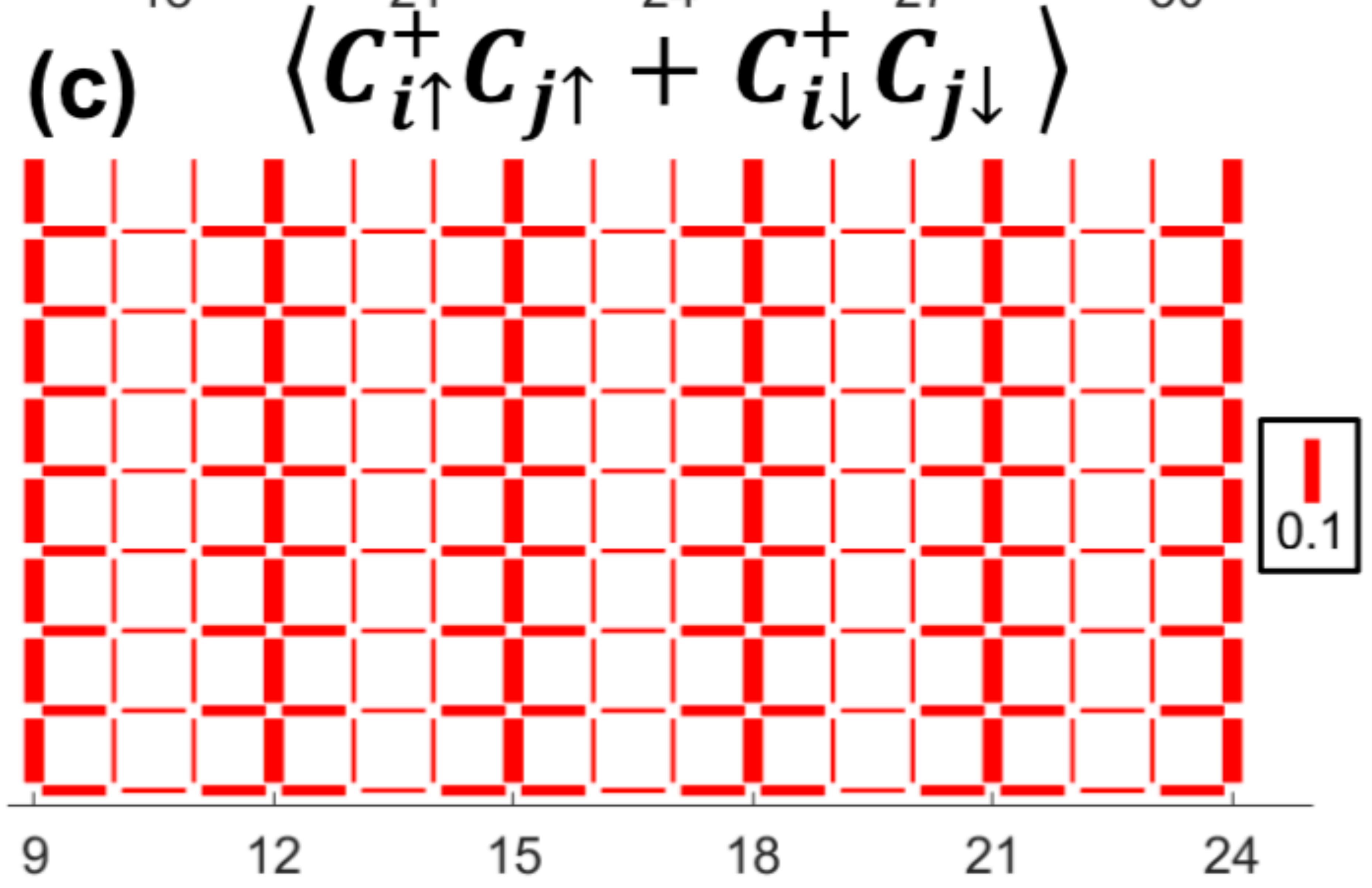
(Not previously seen)





density,
spin

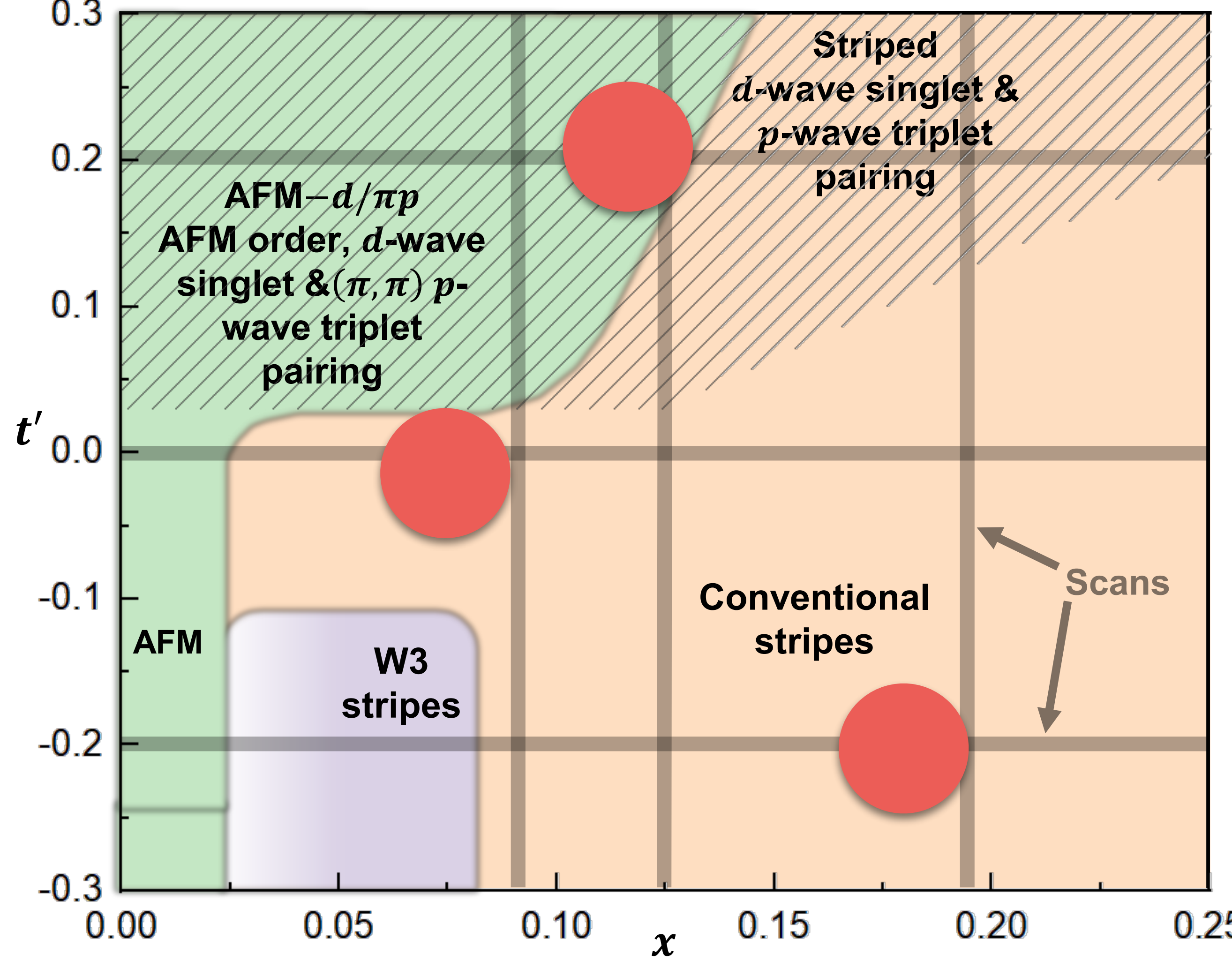




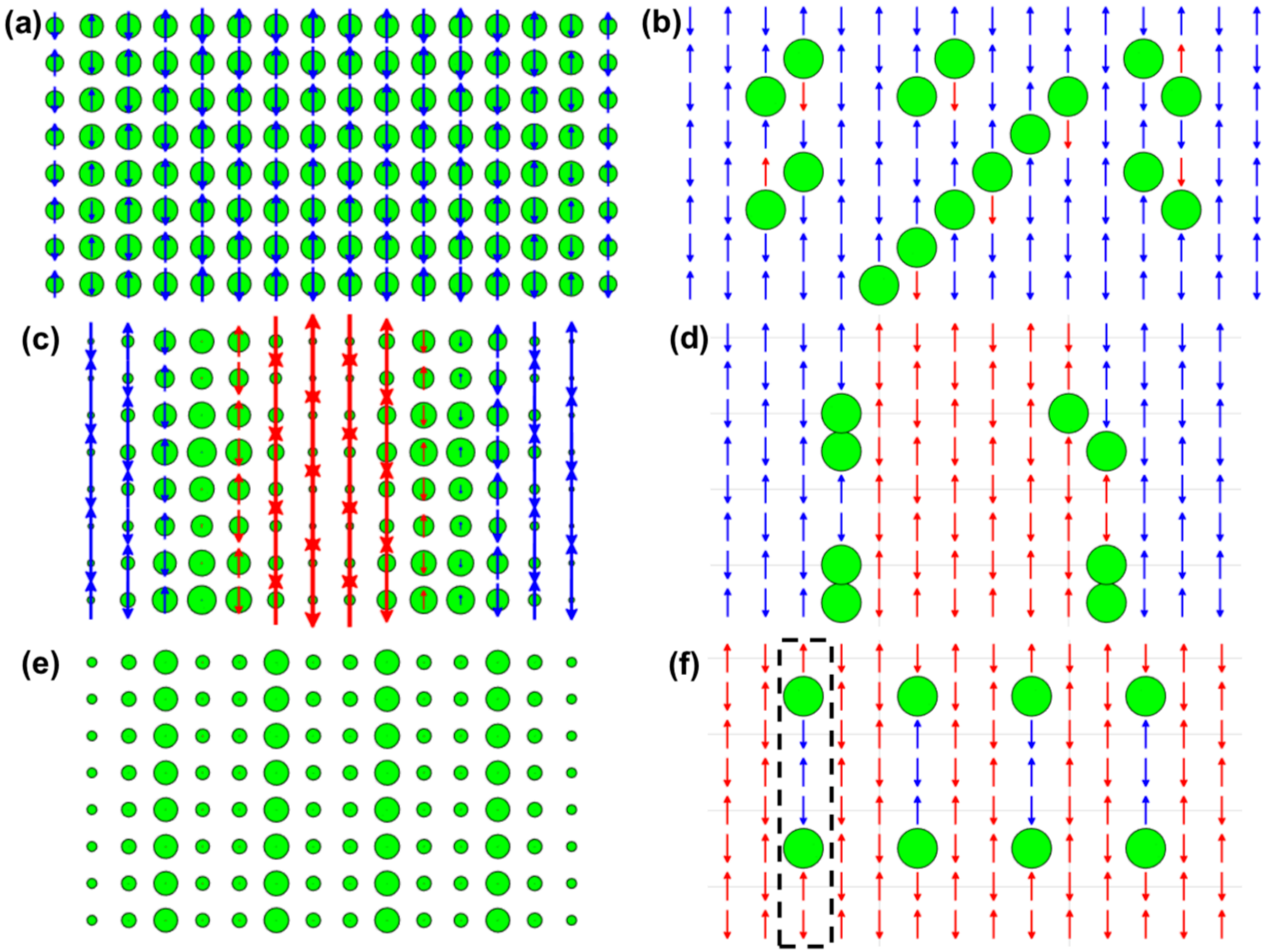
This novel phase looks like decoupled undoped ladders and doped chains

no
pairing

High probability product states



- The many-particle wavefunction can be decomposed as a sum of product states. Which is most probable? We don't know how to find it. But we can get high probability states with simple searches

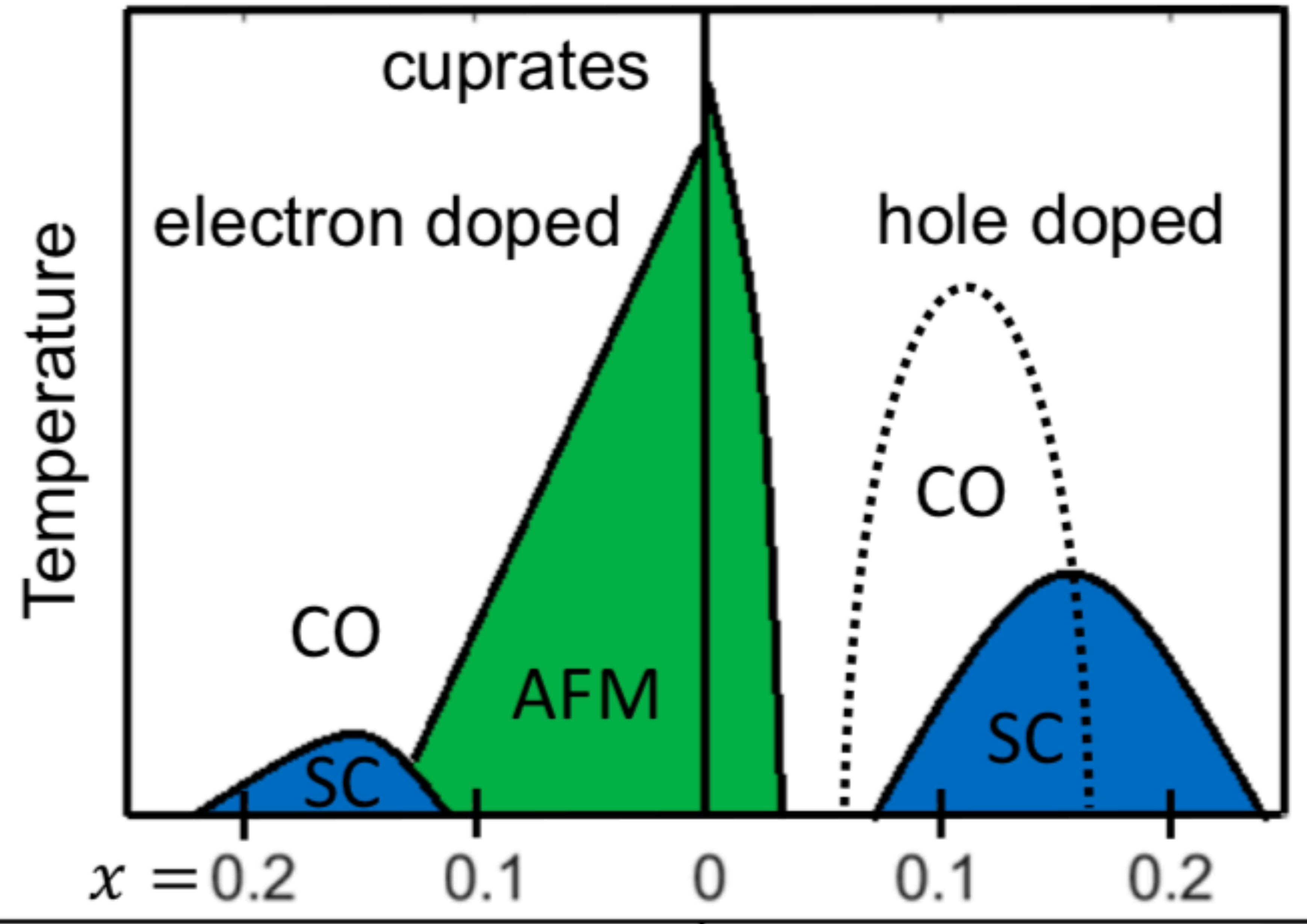


A gas of SC pairs

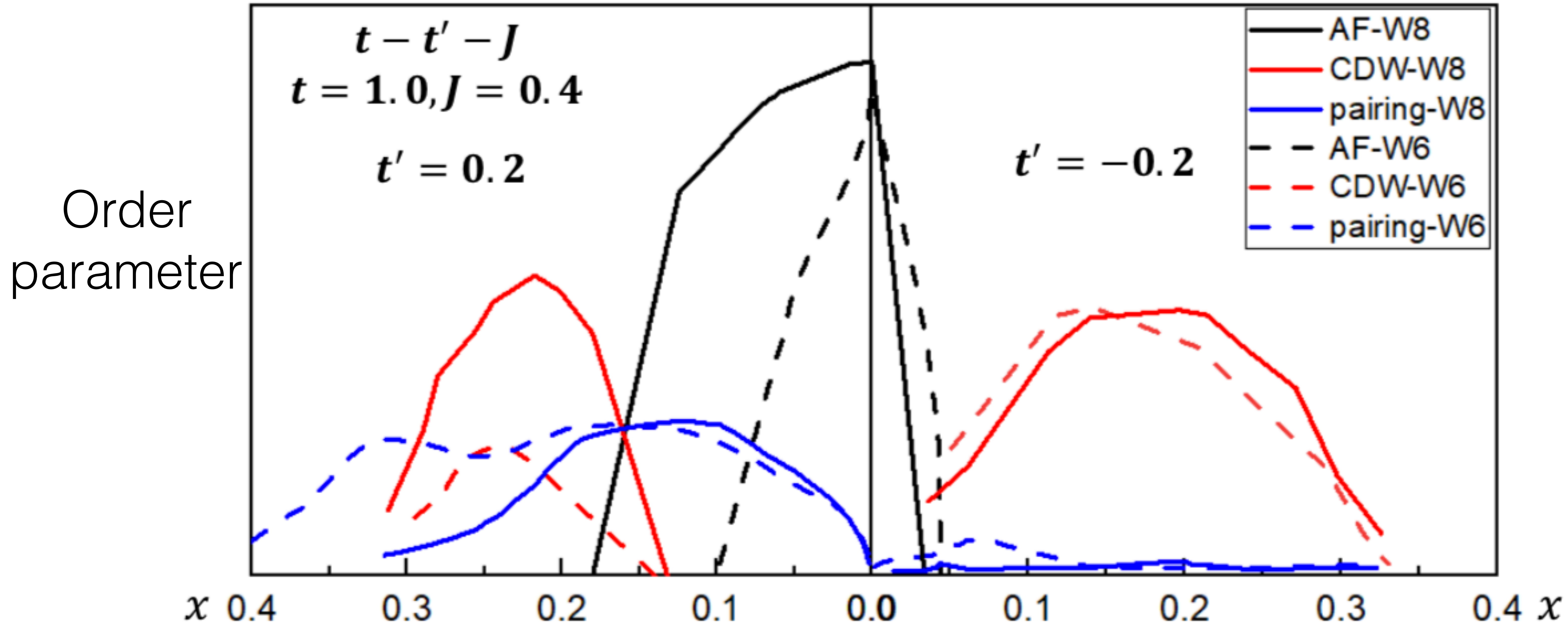
non-SC pairs locked in stripes

unpaired holes thinking they live in 1D

Comparison with the cuprates



“Typical” cuprate
$t' \approx -0.2$



The t-J model is constrained to hole-doping, but a particle hole-transformation maps electron-doped t’<0 to hole-doped t’>0

Magnetic, single particle, spin properties very similar! Superconductivity **is not**

Conclusions

- Tensor network simulations have improved enough to begin to resolve the phase diagrams of 2D strongly correlated model systems
- We have determined an approximate phase diagram of the t-t'-J model using DMRG on width 8 and 6 cylinders, finding small finite size effects for most properties.
- The t-t'-J model gives a qualitative description of the cuprates in terms of magnetism, stripe patterns, and single-particle properties. It fails in describing the superconductivity: electron doped systems appear to have much stronger SC in the t-t'-J model.
- How to fix the model is an open question.

Spontaneous broken symmetry in DMRG

- At bond dimension m=1, DMRG is a simple mean field theory. For a Heisenberg AF, it gives a Neel state. If you conserve Sz, it will be one of two Neel states. With no S conservation, it could point in any direction. With full SU(2) spin symmetry conserved—?? Probably a higher energy state than Neel.
- For infinite bond dimension, you get the exact ground state, which for a finite system with an even number of spins is a singlet, <Sz>=0 everywhere.
- For moderate bond dimension, you get broken symmetry, approximating the infinite 2D broken symmetry state.
- To determine the order parameter precisely, a strategy involving pinning the edges works best, playing with the aspect ration (about 2:1) to eliminate leading finite size effects (White&Chernyshev)
- For qualitative results, relying on spontaneous broken symmetry from DMRG is pretty good.