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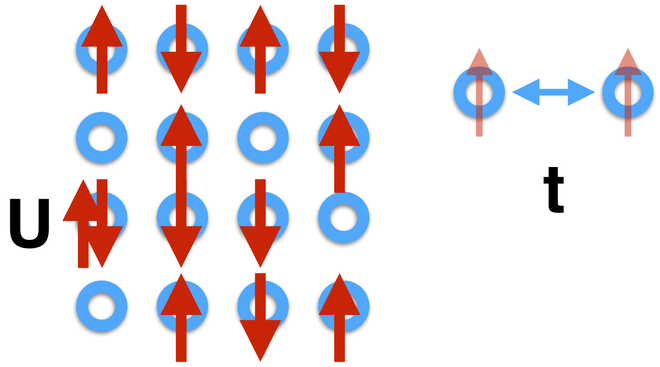
The Simons Collaboration on the Many Electron Problem

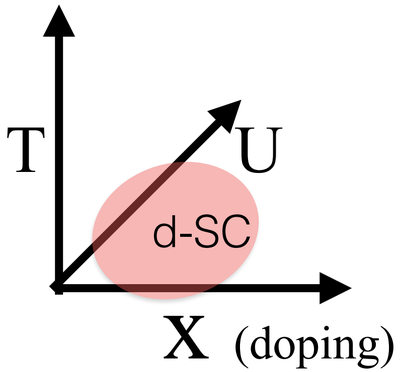
- Brief Intro to the Hubbard model
- Four powerful simulation methods
- Results for U=8, 1/8 doping:
  - Consensus on the phase of the ground state
  - Stripes with nearly degenerate wavelengths

The 2D Hubbard model



$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}.$$

Perhaps the most important model in condensed matter physics—widely regarded as the starting point for understanding the high-Tc superconductors



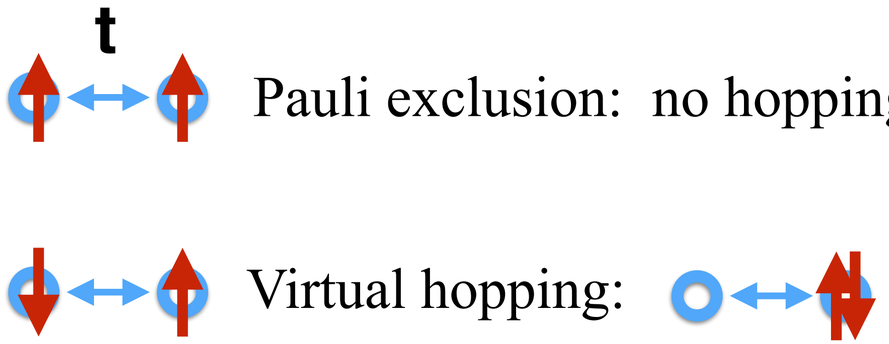
t sets the energy scale, so only one parameter in H
You can also vary the temperature and doping.
The phase diagram specifies: phase(T,x,U)

For the high-Tc cuprates:
U/t ~ 8, 0 < x < 0.3,
T_{sc} < ~J/12 ~ t/40
T_{ps} < ~J ~ t/3

The t and U terms compete.
Bandwidth W = 8t, maximal competition W ~ U, or U=8t (cuprates!)

The model is more easily understood for small U or large U.
Small U: quasiparticles, Fermi surfaces, diagrams, self energies….
Large U: exchange, mapping to Heisenberg and t-J models (which are still hard to solve!)

The 2D Hubbard model—large U/t



Pauli exclusion: no hopping

Virtual hopping:

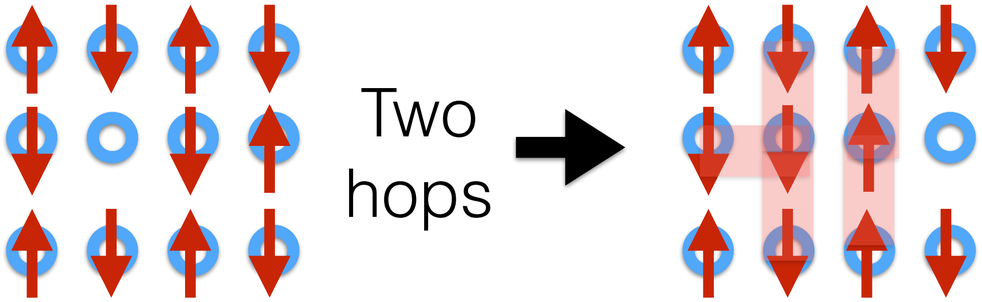
Perturbative effect: new exchange interaction

$$J\vec{S}_i \cdot \vec{S}_j \qquad J \approx 4t^2/U$$

favoring antiferromagnetism

t-J model: keep original hopping for holes, replace U term by $J\vec{S}_i \cdot \vec{S}_j$

Frustrated hole hopping in an antiferromagnet:

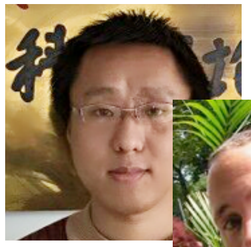
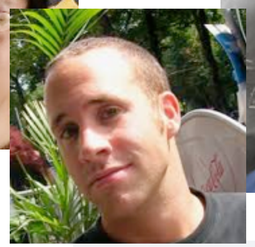
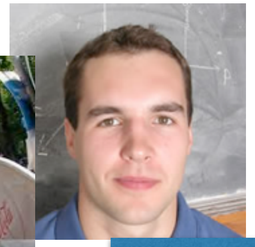


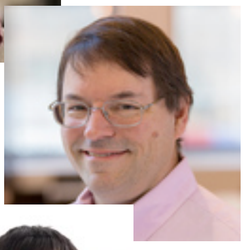
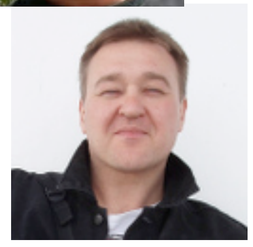
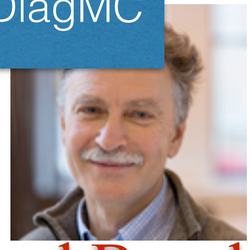
Single hole hopping is highly "frustrated"

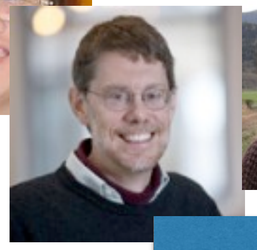
Pairing: one hole can follow the other, erasing ferromagnetic bonds

Stripes: a vertical line of holes can hop together without frustration

Generic feature of frustrated systems: new states can appear that are not directly favored by H, if they relieve frustration



DMRG
DiagMC
DCA





DF


First Hubbard Benchmark paper
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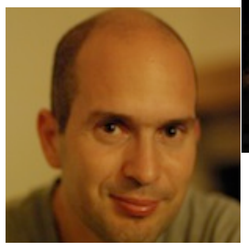
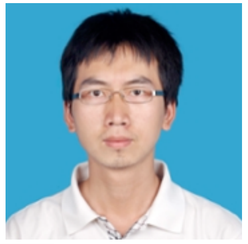
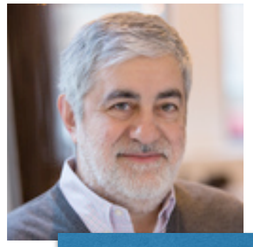
MRPHF
VMC & Fixed Node DMC





UCCSD
UCCSDT(Q)
DMET


AFQMC

Solutions of the Two Dimensional Hubbard Model: Benchmarks and Results from a Wide Range of Numerical Algorithms

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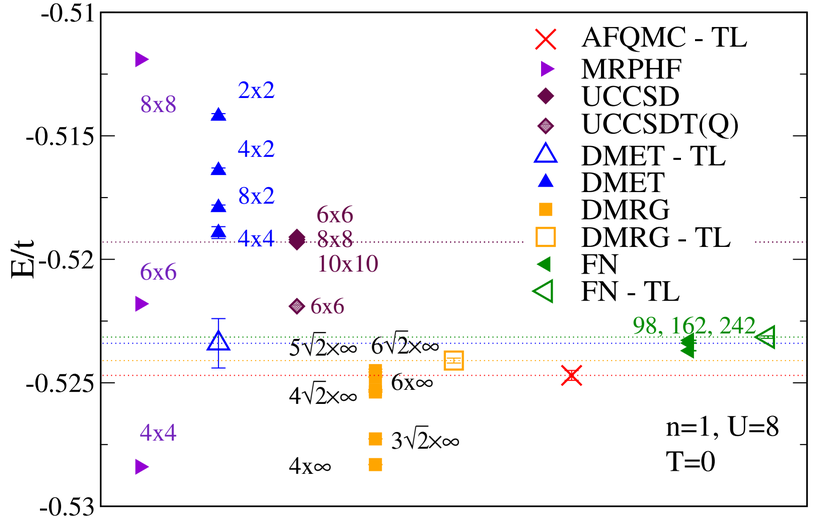
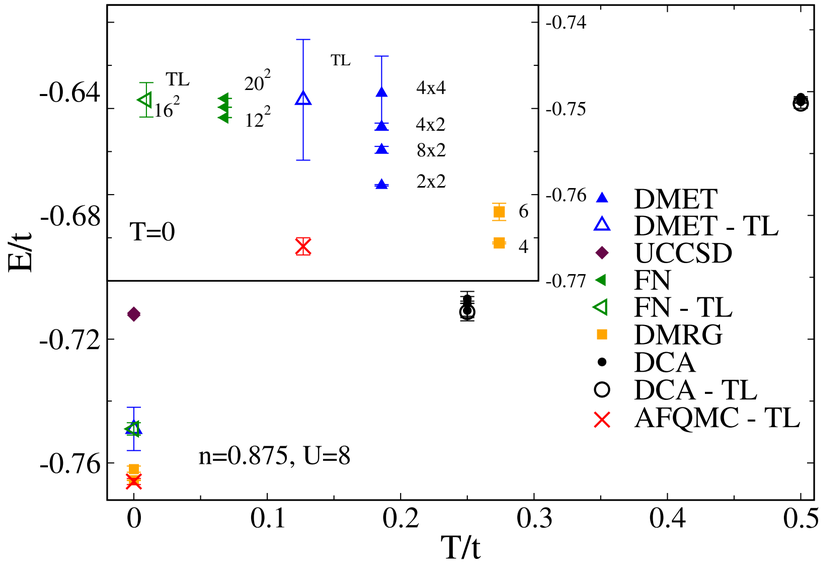


Ground state energies, **half-filling**, U=8



Energies vs T, **1/8 doping**, U=8

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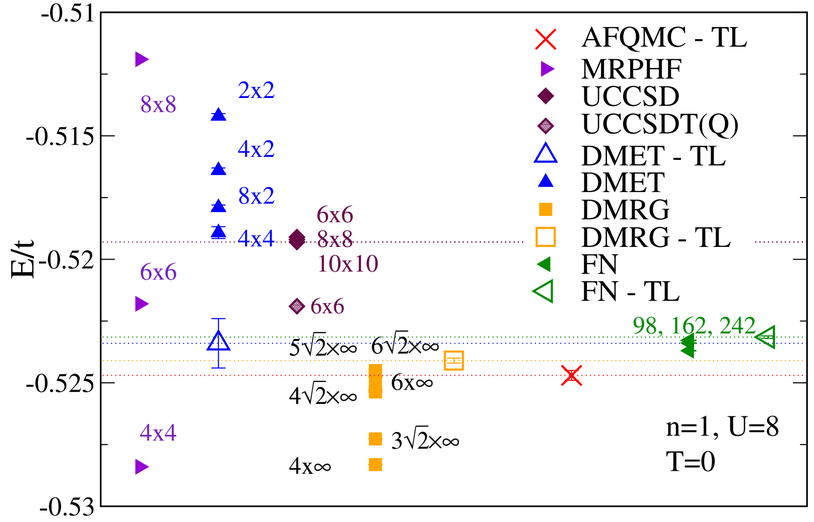

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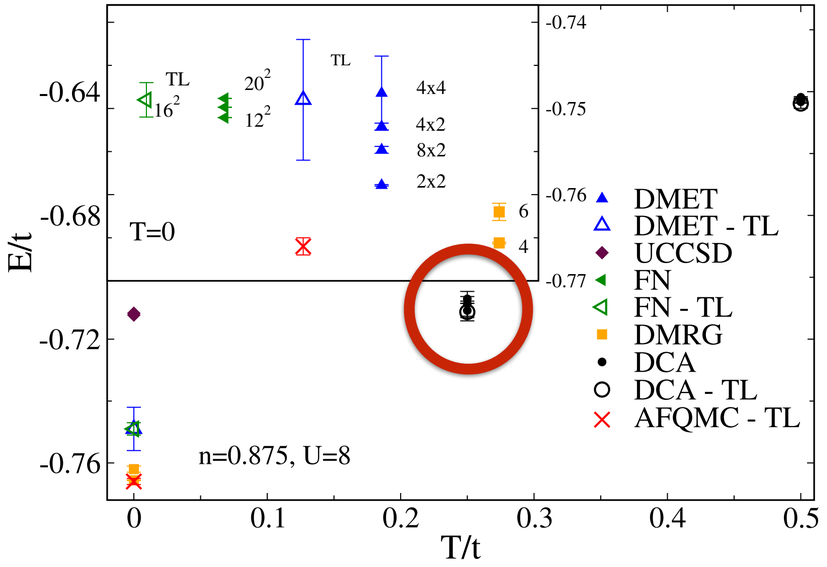

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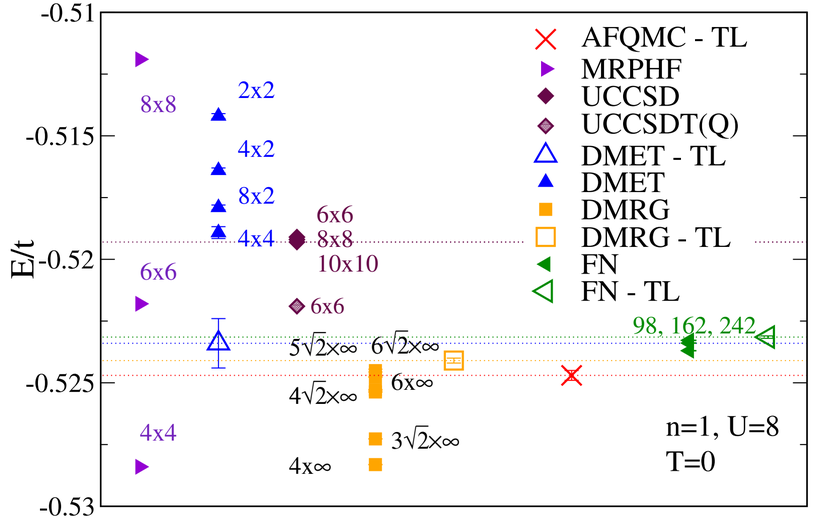

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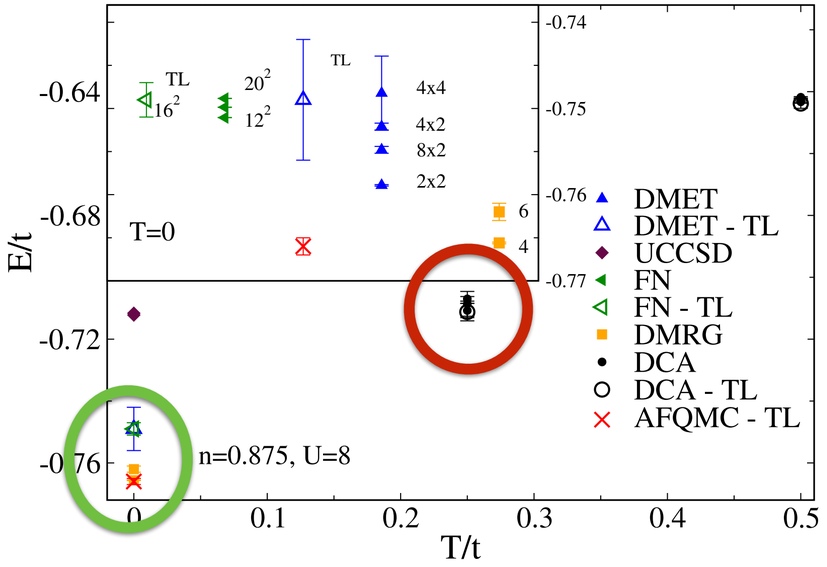

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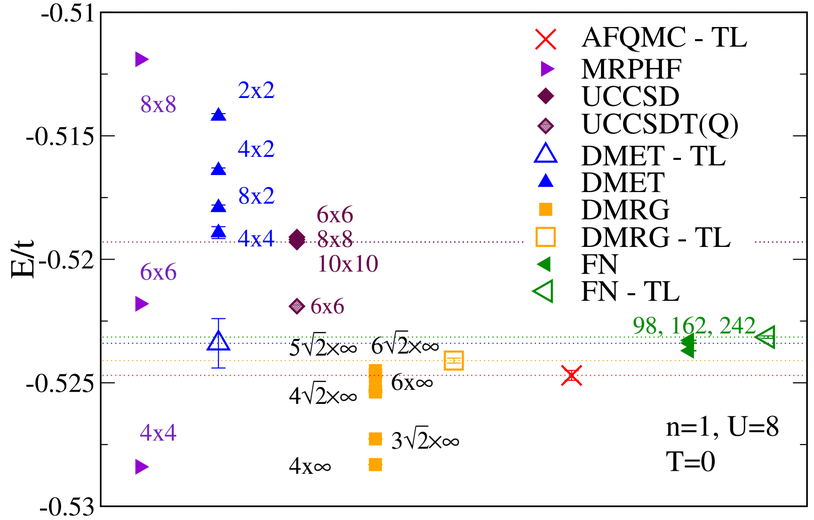

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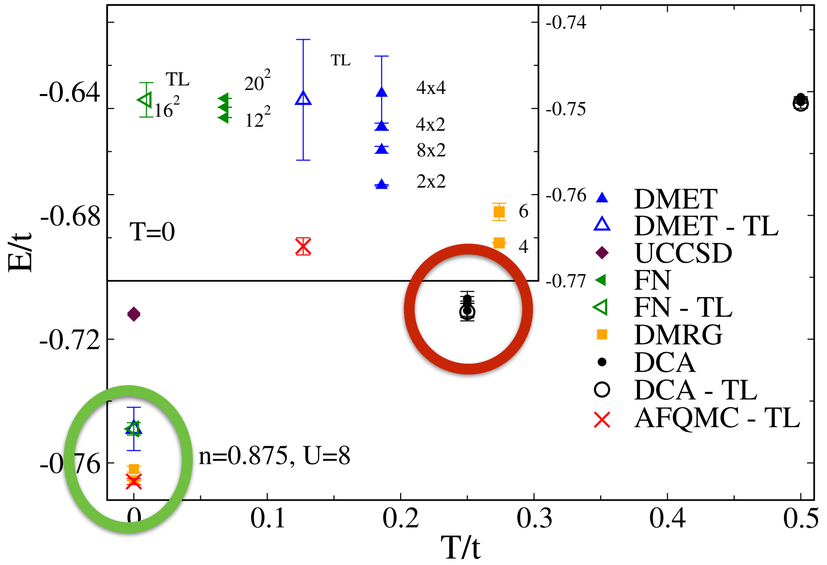


Energies vs T, **1/8 doping**, U=8

A smaller group of us then decided to focus on this toughest region to see if we could resolve differences

Stripe order in the underdoped region of the two-dimensional Hubbard model

Bo-Xiao Zheng[1,2], Chia-Min Chung[3], Philippe Corboz[4], Georg Ehlers[5], Ming-Pu Qin[6], Reinhard M. Noack[5], Hao Shi[6], Steven R. White[3], Shiwei Zhang[6], Garnet Kin-Lic Chan[1*]

To appear in ***Science***

T=0, U=8, 1/8 doping

maximum uncertainty in the phase, maximum inhomogeneity

What is the ground state phase?

- Density matrix renormalization group (DMRG) (real-space and hybrid real/momentum space)
  - Uncontrolled errors: finite cylinder size
- Density Matrix Embedding theory (DMET)
  - Uncontrolled errors: finite cluster size
- Infinite projected entangled pair states (IPEPS)
  - Uncontrolled errors: finite bond dimension and extrapolation
- Constrained Path Monte Carlo (CPMC, AFQMC)
  - Uncontrolled errors: Constraint based on trial wavefunction

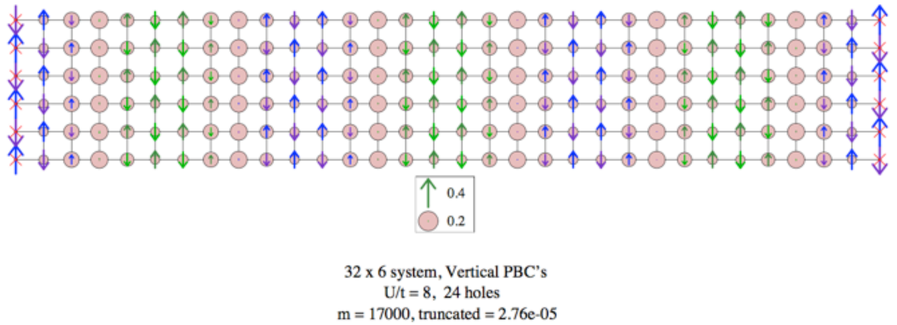
Like cluster DMFT but entanglement-based, not frequency-based. Cluster solved with DMRG (Garnet Chan)

By focusing one one point in the phase diagram, we were all able to improve our results substantially—longer runs, better techniques, new techniques.

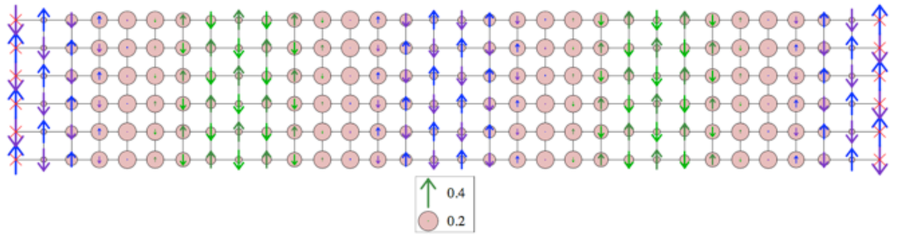
A key aspect of the work is that the uncontrolled errors are very different. Thus, if multiple methods agree, we can have high confidence we have the right answer.

Cross Validation: example

- DMRG: performed on cylinders; difficulty increases exponentially with cylinder width w. w=4: nearly exact, w=6, highly precise, w=8: out of reach
- CPMC: The constraint error is surprisingly small even with a noninteracting trial state. But no internal determination of size of error; hard to improve systematically.
- Cross validation: check CPMC error with DMRG on w=4, 6 (very small). Then we can trust CPMC on w=8-12. We can also estimate an energy correction from DMRG
- Both methods were initially giving stripes, but with different wavelengths. We were able to trace this to a problem in the DMRG analysis: filled stripes were metastable but higher energy at small bond dimension, but dropped below for large m! After fixing the DMRG, excellent agreement (all four methods).



32 x 6 system, Vertical PBC's
U/t = 8, 24 holes
m = 17000, truncated = 2.76e-05



32 x 6 system, Vertical PBC's
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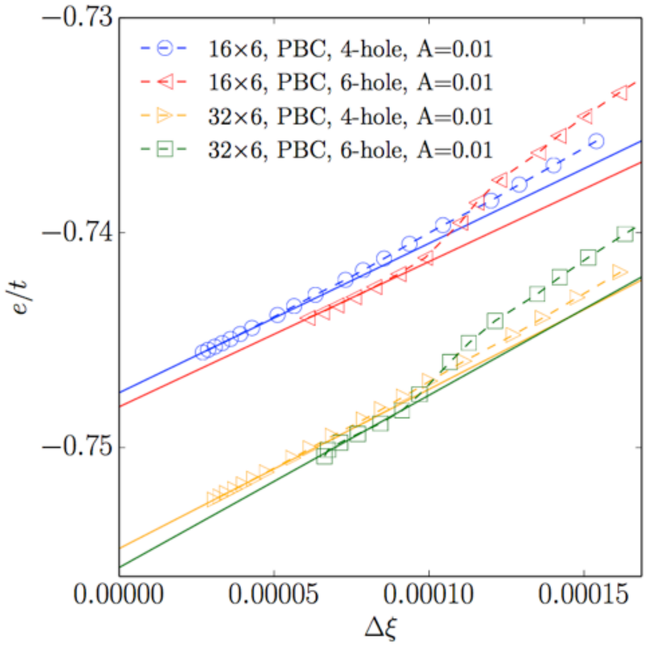
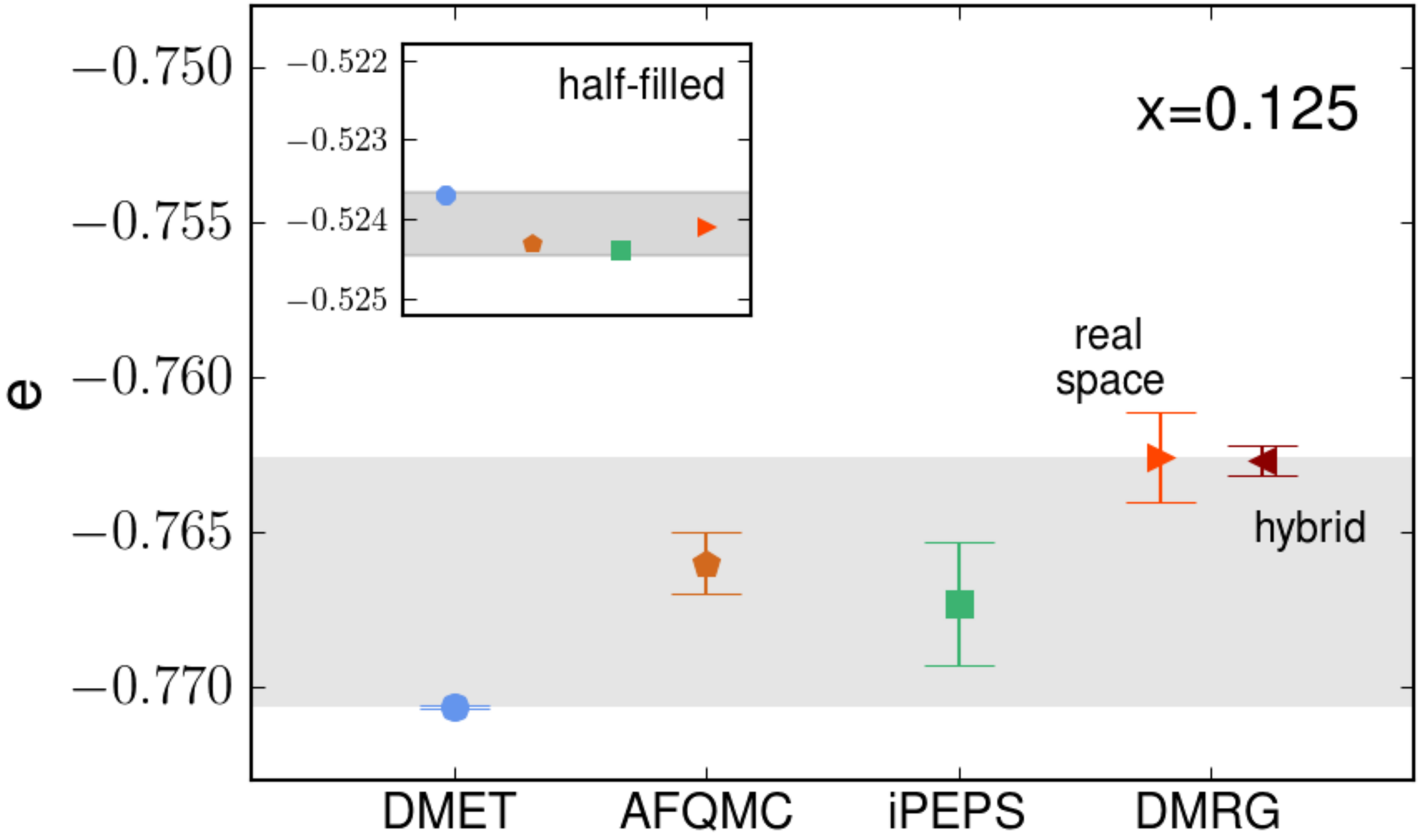




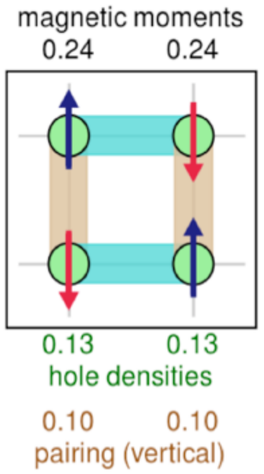
Energy extrapolated to thermodynamic limit

Overall uncertainty almost an order of magnitude reduced from previous benchmark

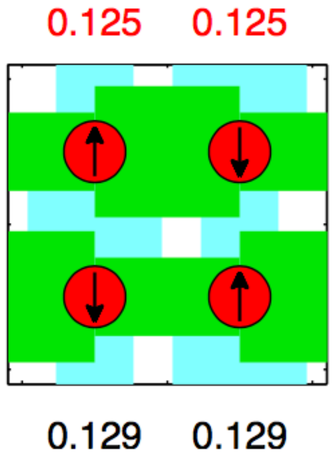
Error bars neglect systematic errors—that is what we need the comparison for.

Uniform state versus stripes

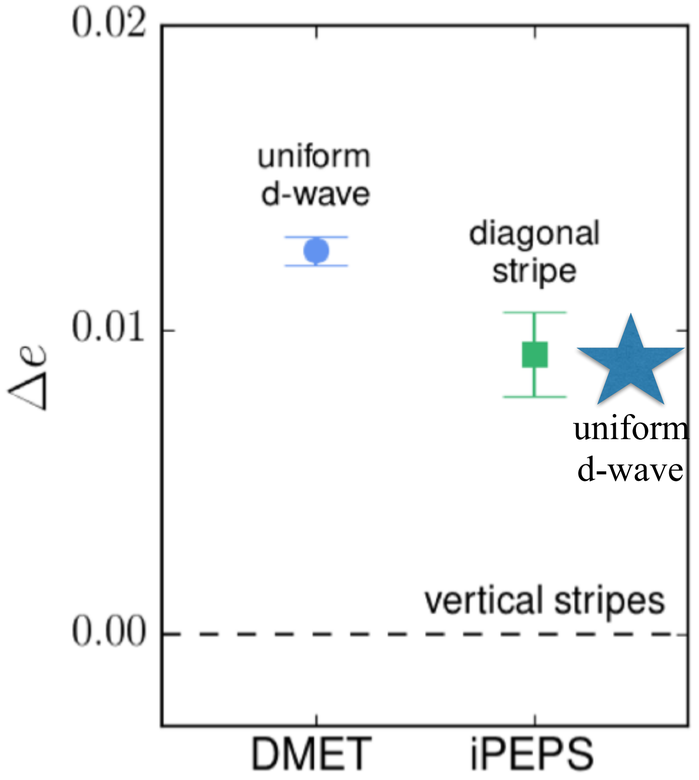
- DMET and iPEPS both can be forced to give uniform states:
  - DMET has a cluster size. For a 2x2 cluster, no stripe patterns can form
  - iPEPS similarly has a cluster that is repeated to infinity. A 2x2 cluster cannot have stripes
- DMRG always gives stripes. Currently no way to force a uniform state. CPMC also gives stripes as lowest energy state.



DMET



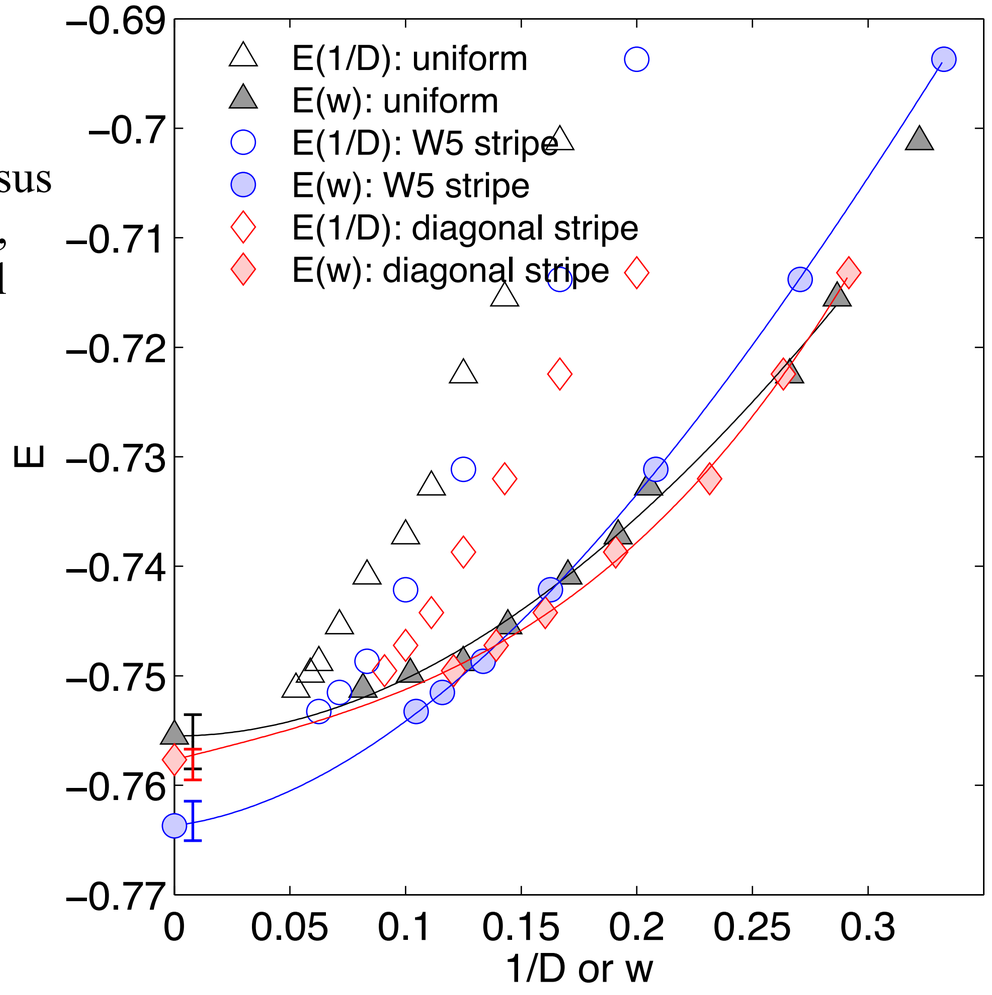
iPEPS

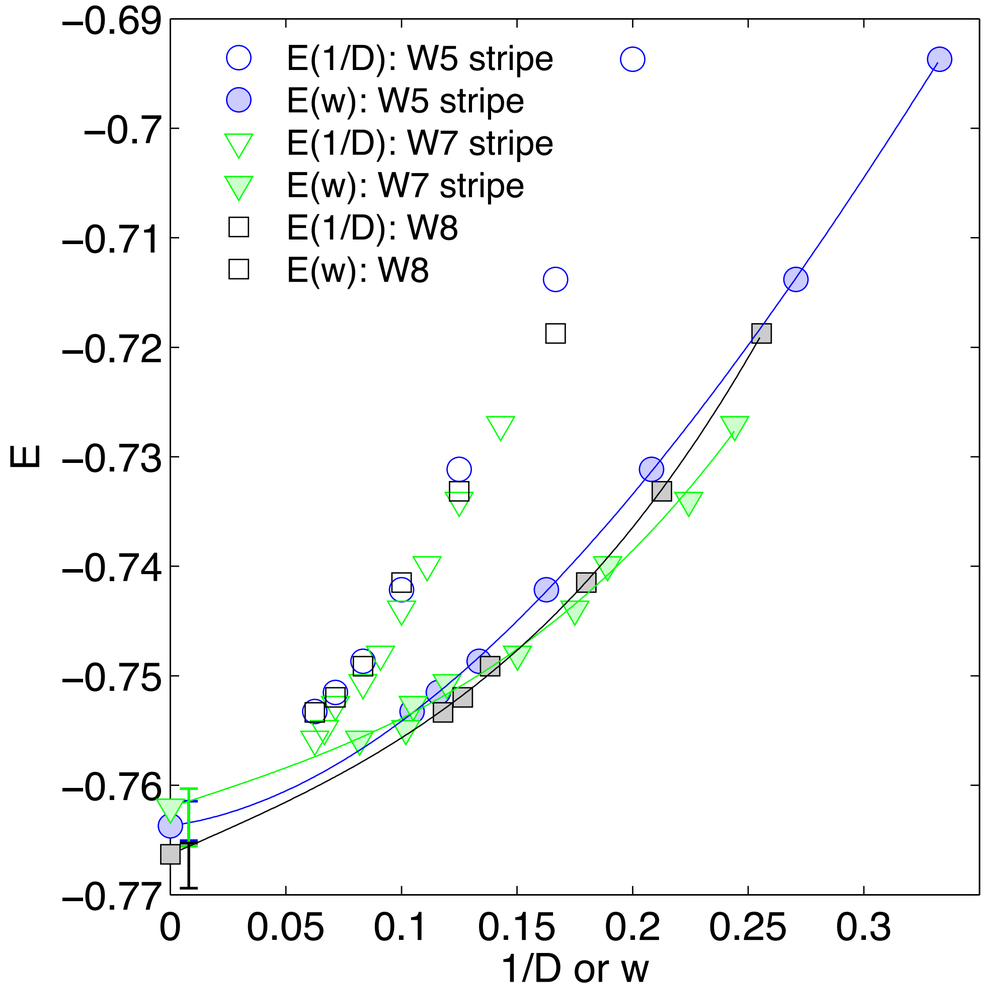


Both uniform states from DMET and iPEPS show d-wave pairing

New iPEPS Energy Extrapolation method (Corboz)

Vertical stripes versus uniform, diagonal stripes



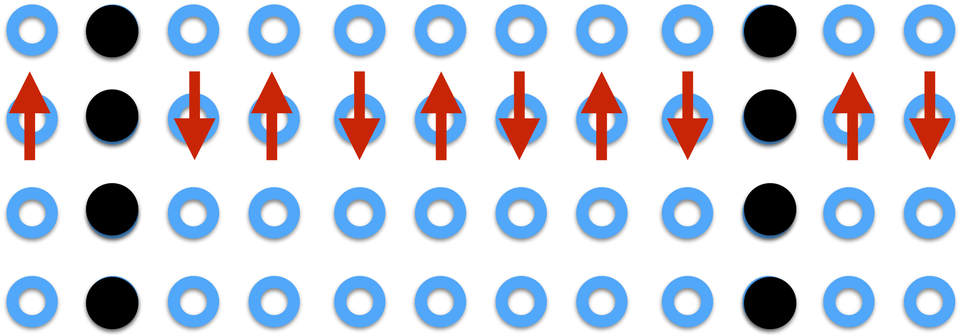


Vertical stripes with different spacings

Uniform, diagonal stripes higher in energy

Near degeneracy for vertical stripes with different spacings

Vertical stripes: filling, wavelength

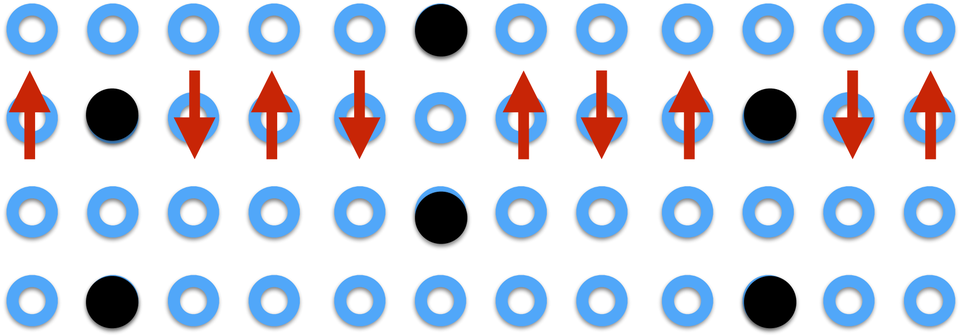


Filled Stripe

f = 1

λ = 8

The magnetic wavelength is 2 λ



Half filled Stripe

f = 1/2

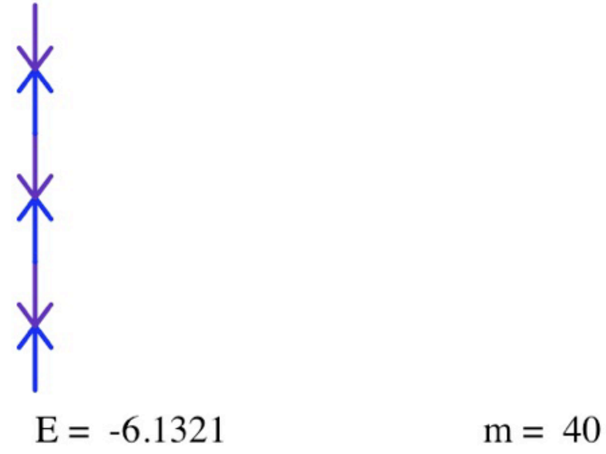
λ = 4

Filled stripes were found with Hartree Fock in late 80's—but HF may not be not accurate

Zaanen

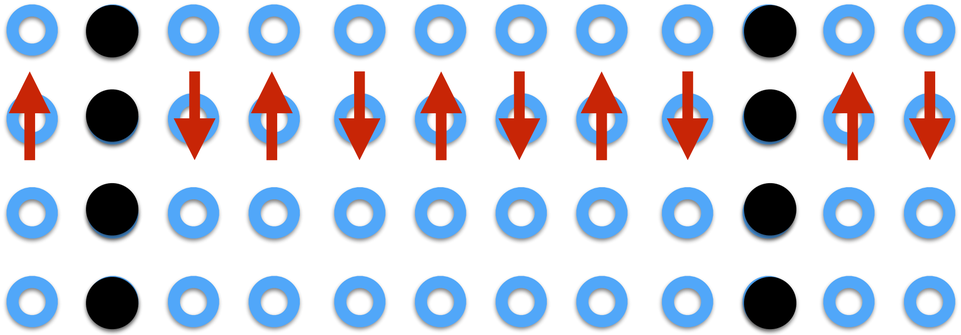
Half-filled stripes were found in some cuprates in the mid 90's. A few years later, DMRG on the t-J model showed half-filled stripes (White & Scalapino)

Tranquada



DMRG on the t-J model—formation of two half-filled stripes

Vertical stripes: filling, wavelength



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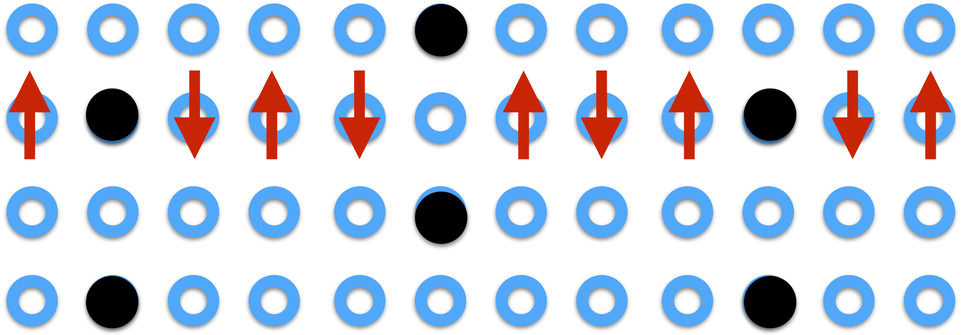

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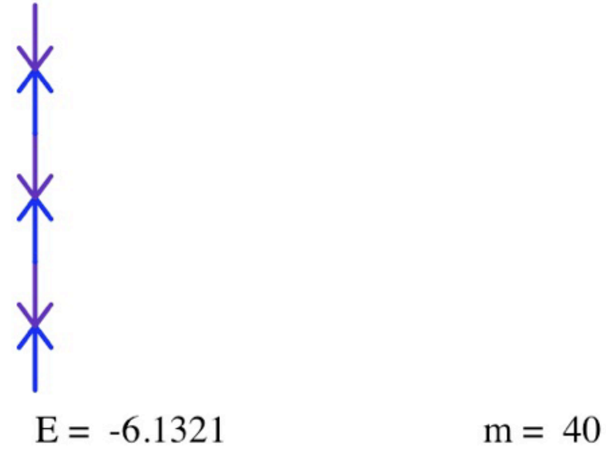
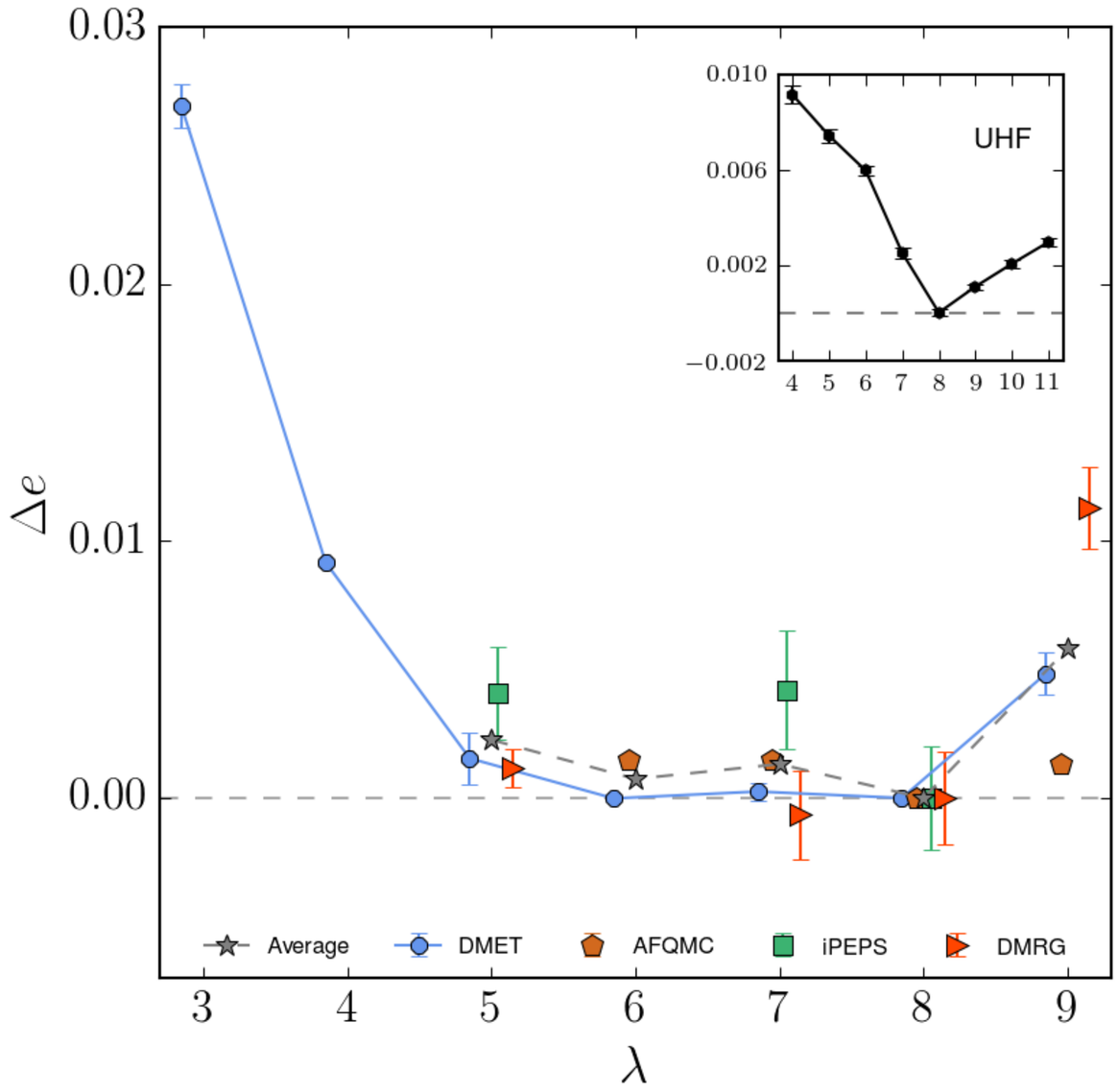


DMRG on the t-J model—formation of two half-filled stripes

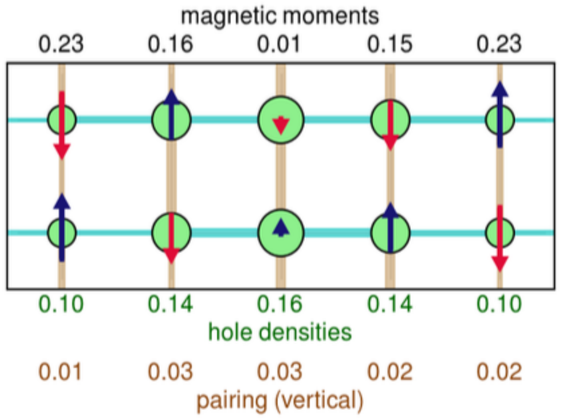
Vertical stripes: Energy versus wavelength



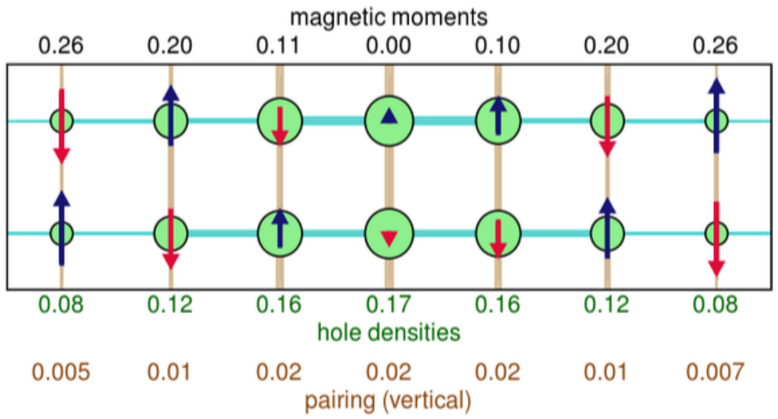
We find a remarkable near-degeneracy for states with different stripe wavelengths, with λ=8 very slightly lower in energy, and λ=4 significantly higher.

The near degeneracy likely points towards disordered stripes and/or fluctuating stripes.

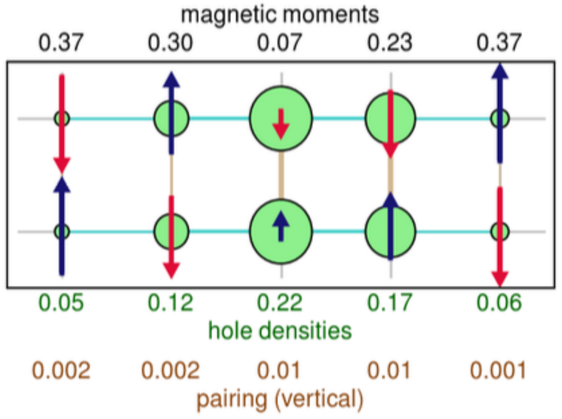
Pairing with partially filled stripes



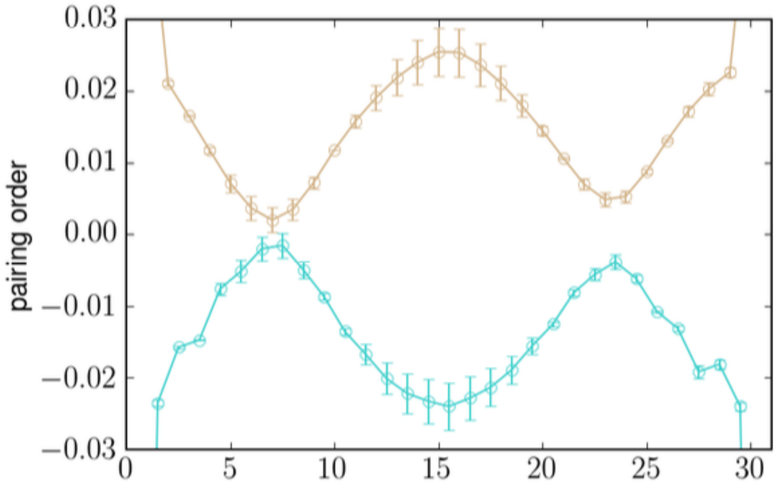
(a) iPEPS $\lambda = 5$



(b) iPEPS $\lambda = 7$



(c) DMET metastable $\lambda = 5$



(d) DMRG pairing order parameters.

32x4, edge pairing fields, stripes smeared

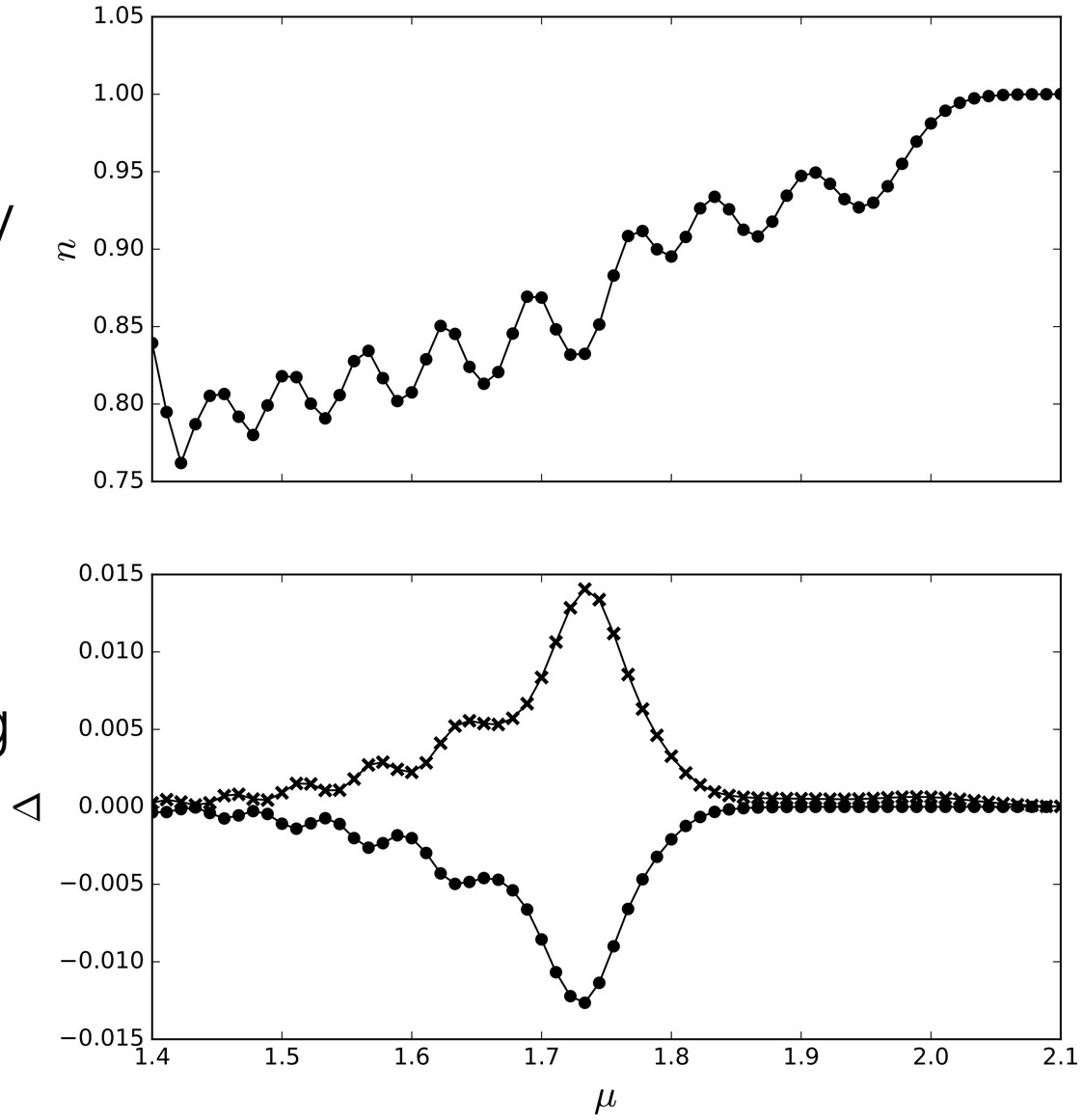
For <u>filled</u> stripes, no d-wave pairing

For partially filled stripes, d-wave pairing is seen but not consistently

Pairing and stripes “intertwined” on Lx4 cylinders (DMRG)

density

pairing



position along cylinder

Grand canonical simulation so pairing order parameter could be measured locally.

This was a long cylinder with the chemical potential linearly varying with position.

We see a peak in pairing near optimal doping but coexisting with stripes

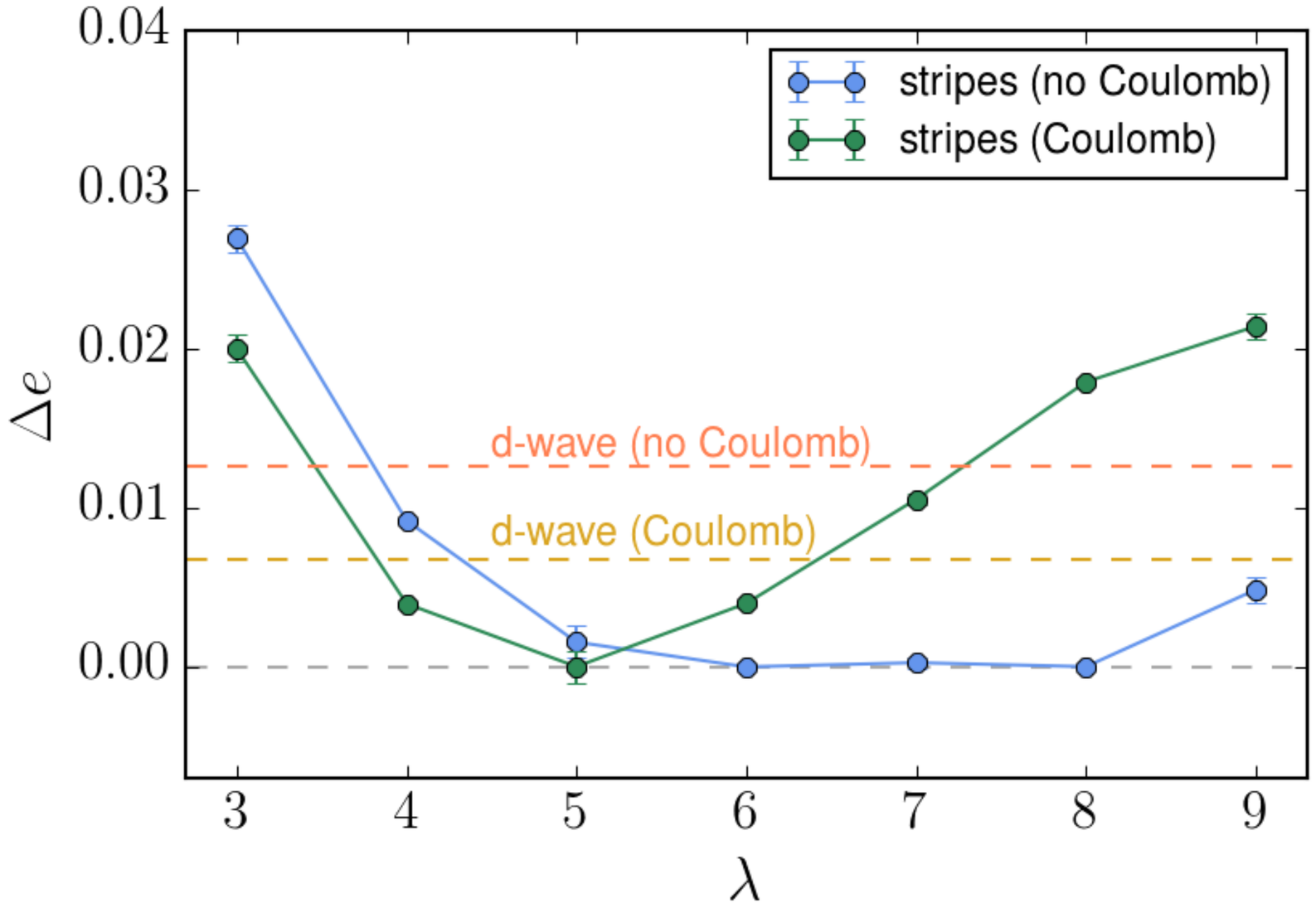
Chia-Min Chung

Solving the Hubbard model: where do we stand?

- Our energy resolution of 0.004t corresponds ±10K per site. Since superconductivity occurs ~100K in the cuprates, this should be enough to understand high-Tc SC!
- Using four different methods with very different uncontrolled errors, we have converged to a consistent general picture of the Hubbard ground state at perhaps the most difficult, important point in the phase diagram
- In applying this to the cuprates, the uncertainty in the *Hamiltonian* is now central. Small changes to the Hamiltonian from additional terms can change the competition between different phases

Extra Slides

Static corrections from long-range Coulomb



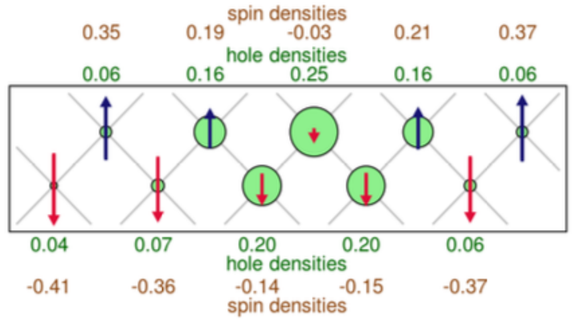
Assume a substantial dielectric constant inducing screening

Calculate energy correction by integrating up the Coulomb contribution from each density pattern. Coulomb favors lower-filled stripes, and favors uniform states

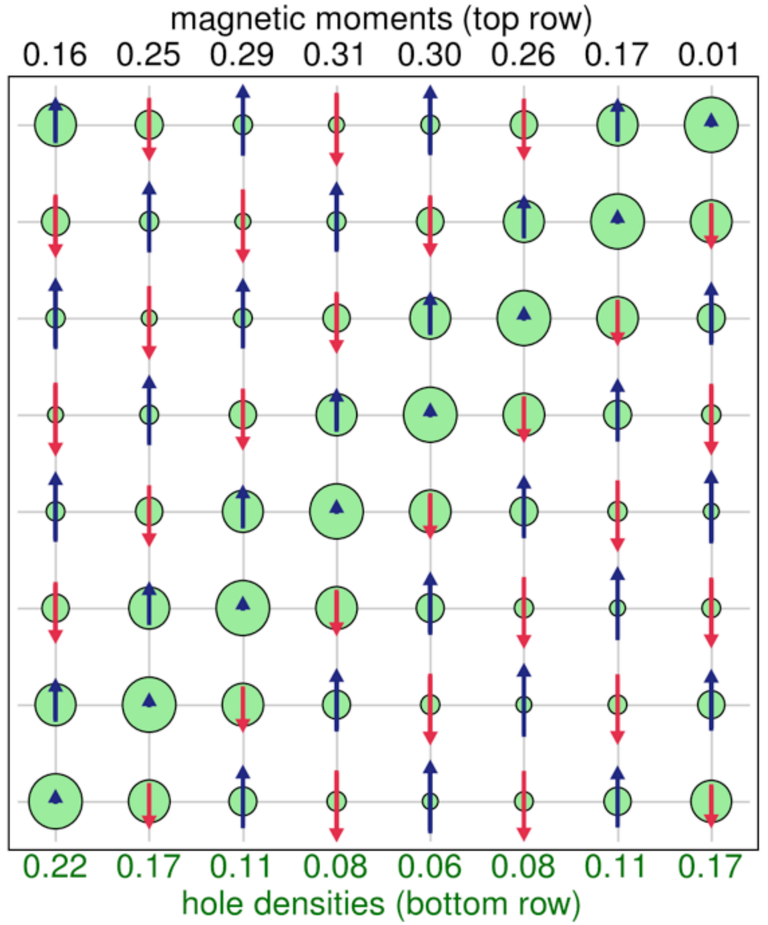
This correction drives our results closer to the cuprates.

Vertical versus diagonal stripes

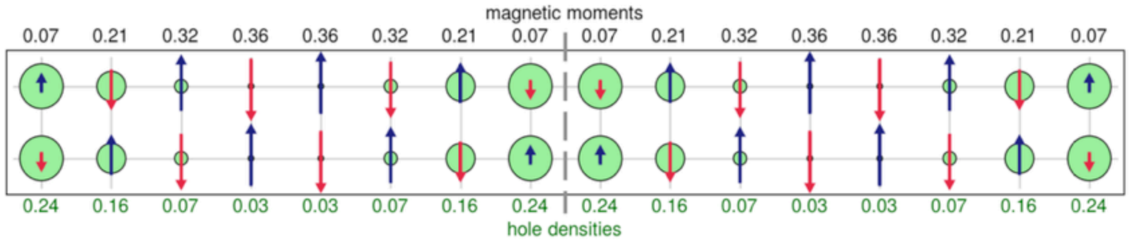
- DMET and iPEPS both can be forced to give diagonal striped states
- Both give higher energies, by ~0.005 t
- The diagonal stripes are “filled”: one hole per root-2 distance
- Boundary conditions on the cylinders used by DMRG and CPMC frustrate diagonal stripes, and they were not seen.



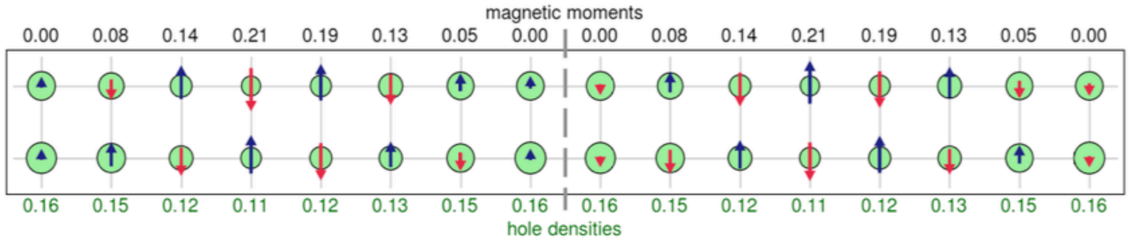
DMET



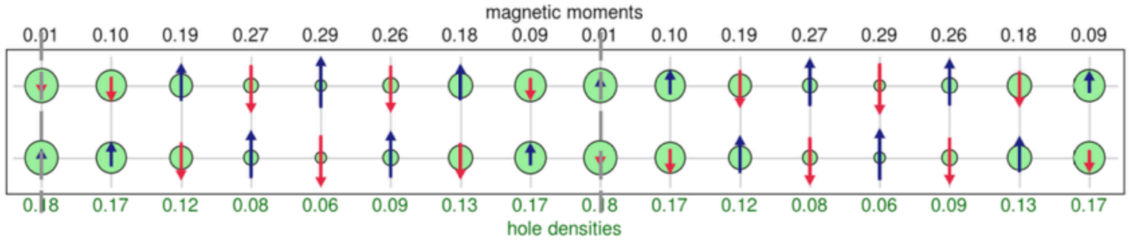
iPEPS



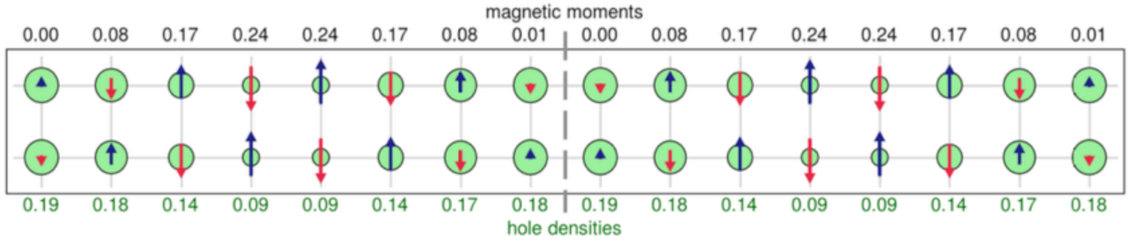
(a) DMET



(b) AFQMC



(c) iPEPS



(d) DMRG

Filled stripes as seen by all four methods