Finite temperature METTS study of Hubbard cylinders

- What is the METTS method?
- Full temperature range study of 4-leg Hubbard cylinders

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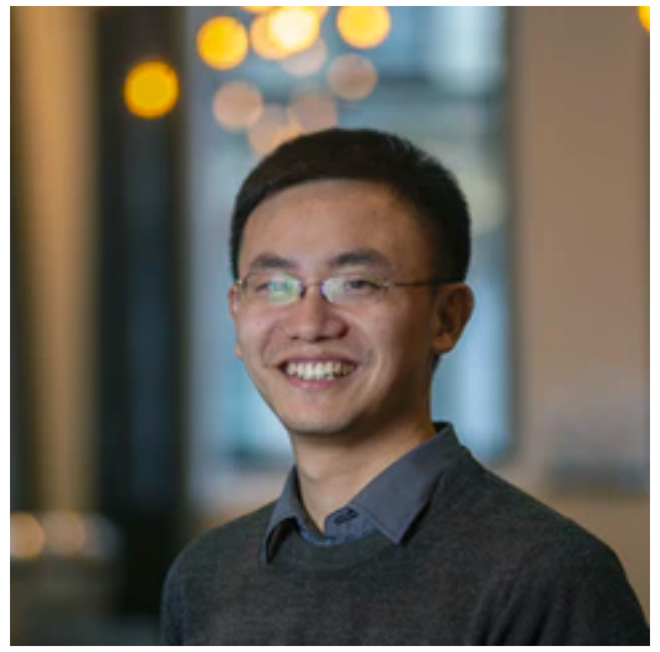
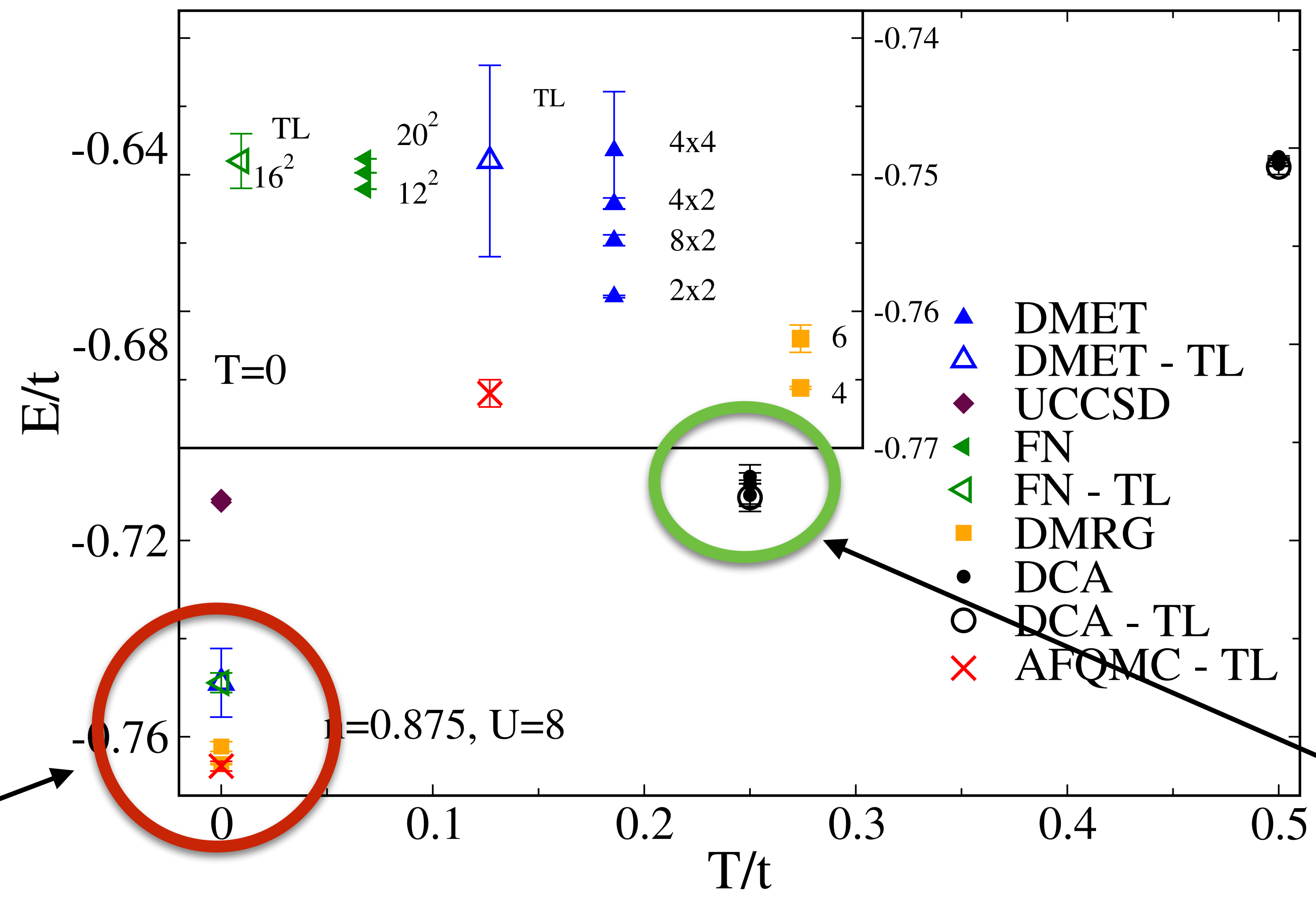


Yuan-Yao
He

All at CCQ

Simulating the Hubbard model: where are we?



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

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T=0

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

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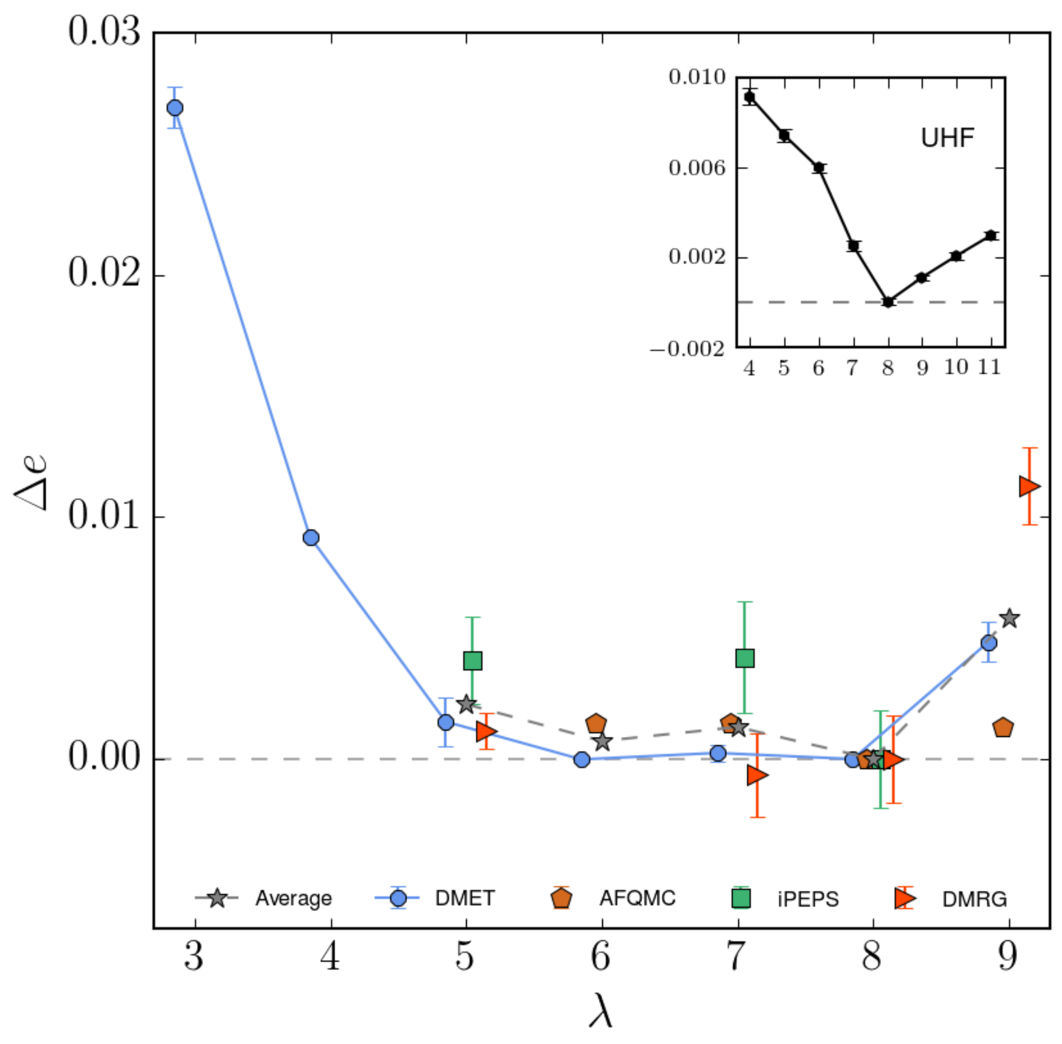
DMRG, AFQMC, PEPS, DMET

- Much progress has been made in the last 5 years on the ground state of the Hubbard model—competition/coexistence between stripes and superconductivity



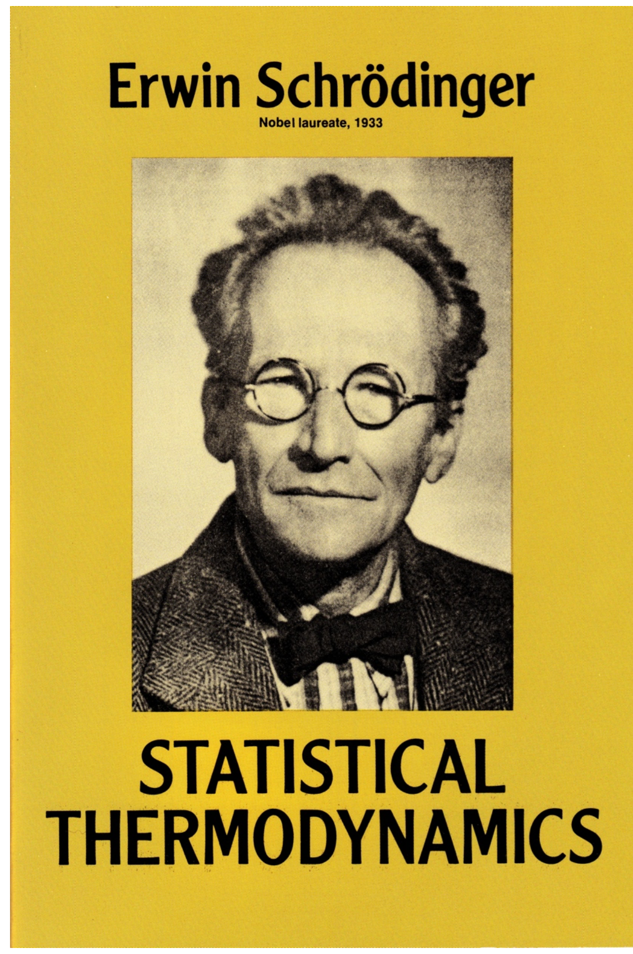
Stripe wavelength

- Finite temperature: good agreement between methods, QMC, cluster DMFT, diagrammatic MC, …development of short range AF order, pseudogaps, change of FS topology, … (pairing)…
- **<u>But unable to reach low enough T to connect to the T=0 results</u>**

Finite Temperature Tensor Network methods

- Probably the most well-known methods are:
  - 1) Matrix product operator representation of $e^{-\beta H}$ (Zwolak and Vidal, 2004)
  - 2) Ancilla method (a.k.a. purification, thermofield-double) (Verstraete, Garcia-Ripoll, Cirac, 2004)
  - Both these methods work well at moderate temperature or chains. But near T=0, both methods *double* the entanglement of the ground state (two copies) [Some recent progress in unitary-rotating away much of the extra entanglement (Hauschild, et al 2017)]
- An alternative approach is to use an ensemble of pure states. In fact, the first version of quantum stat mech we all learned uses the ensemble of eigenstates of H with Boltzmann probabilities $e^{-\beta E_i}$
  - But eigenstates have volume-law entanglement, exponentially small energy gaps (so takes exponentially long to prepare them), and physically, they are fragile against decoherence
  - Why did we learn stat mech this way?? Schrödinger, in his 1946 Stat mech book, on whether systems are really ensembles of eigenstates: "this assumption is irreconcilable with the very foundations of quantum mechanics", "...the attitude is altogether wrong", <u>"We yet decided to adopt it ... very convenient ... same results ..."</u>

TN methods are based on low entanglement



Minimally Entangled Typical Thermal States

(SRW, PRL 102, 190601(2009), Stoudenmire and White, 2010)

- An ensemble of pure states reproducing thermodynamics is obtained from *any* orthonormal complete set of states $\{\,|\,i\rangle\}$:

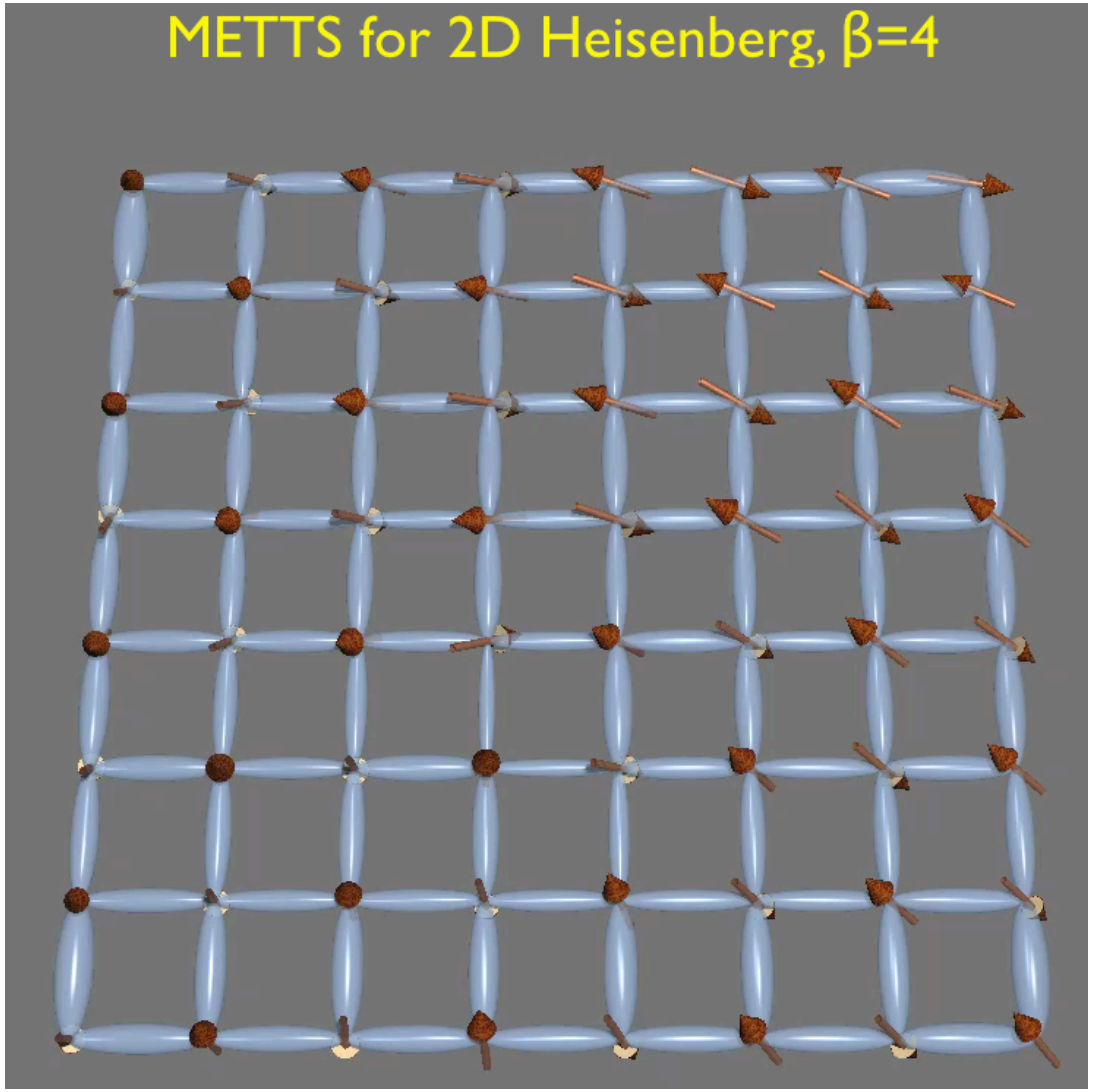
  $$\rho = e^{-\beta H/2} \sum_i |\,i\rangle\langle i\,|\,e^{-\beta H/2}$$

  Define $|\,\phi(i)\rangle = P(i)^{-1/2} e^{-\beta H/2}\,|\,i\rangle$ with $P(i) = \langle i\,|\,e^{-\beta H}\,|\,i\rangle$ (normalization)

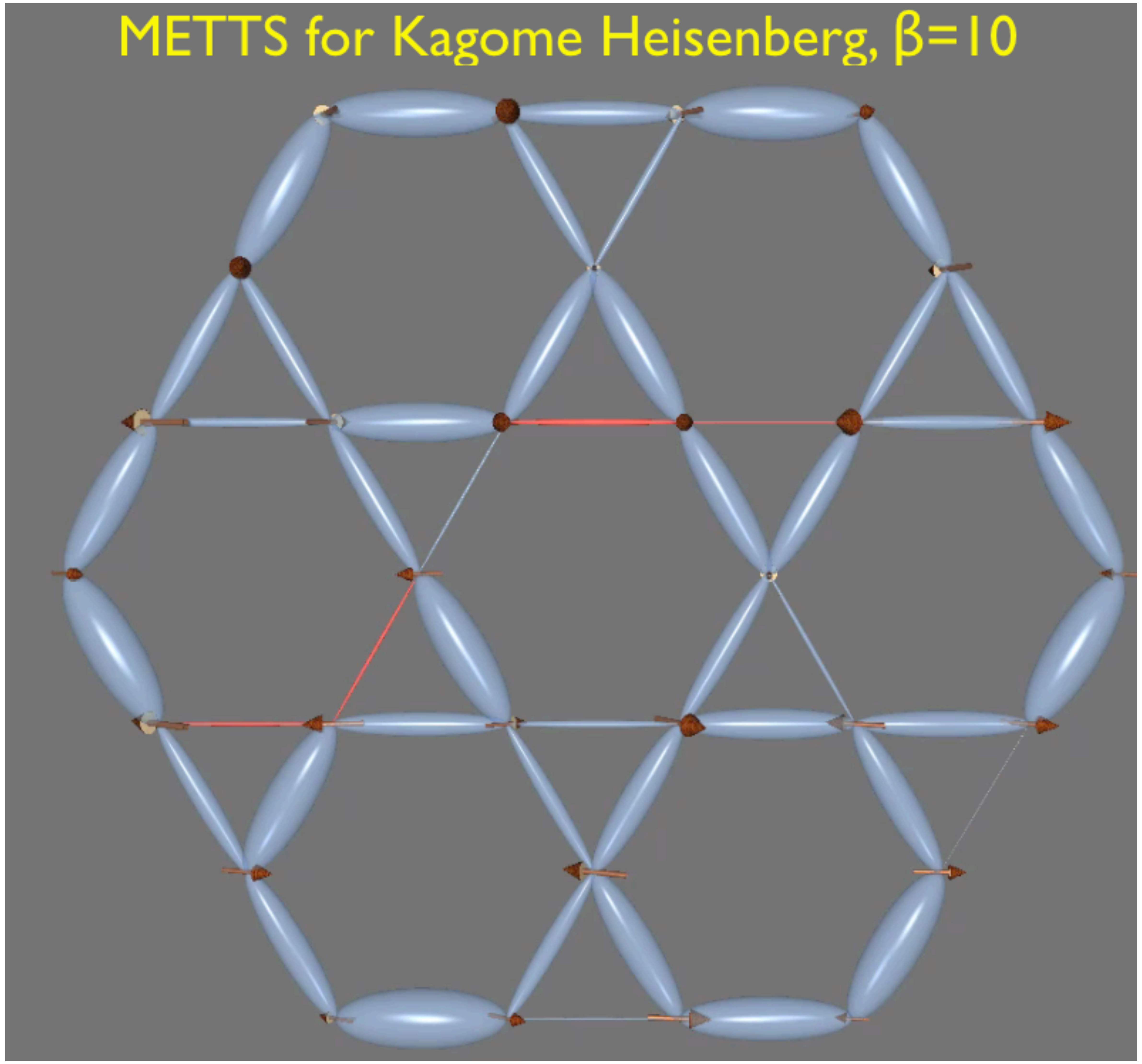
  Then $\rho = \sum_i P(i)\,|\,\phi(i)\rangle\langle\phi(i)\,|$

- A METTS is one of the set $\{\,|\,\phi(i)\rangle\}$ with $|\,i\rangle$ = the set of trivial product states, e.g. $|\uparrow\uparrow\downarrow\uparrow\downarrow\ldots\rangle$ for spins (zero entanglement)
- How are METTS "typical"?
  - Mathematically, expectation values are diagonal, so just average over them: $\langle A\rangle = \sum_i P(i)\langle\phi(i)\,|\,A\,|\,\phi(i)\rangle$ QMC sampling is not typical!
  - Physically, they seem to resemble the experimental world…

At T=0, all METTS are the ground state



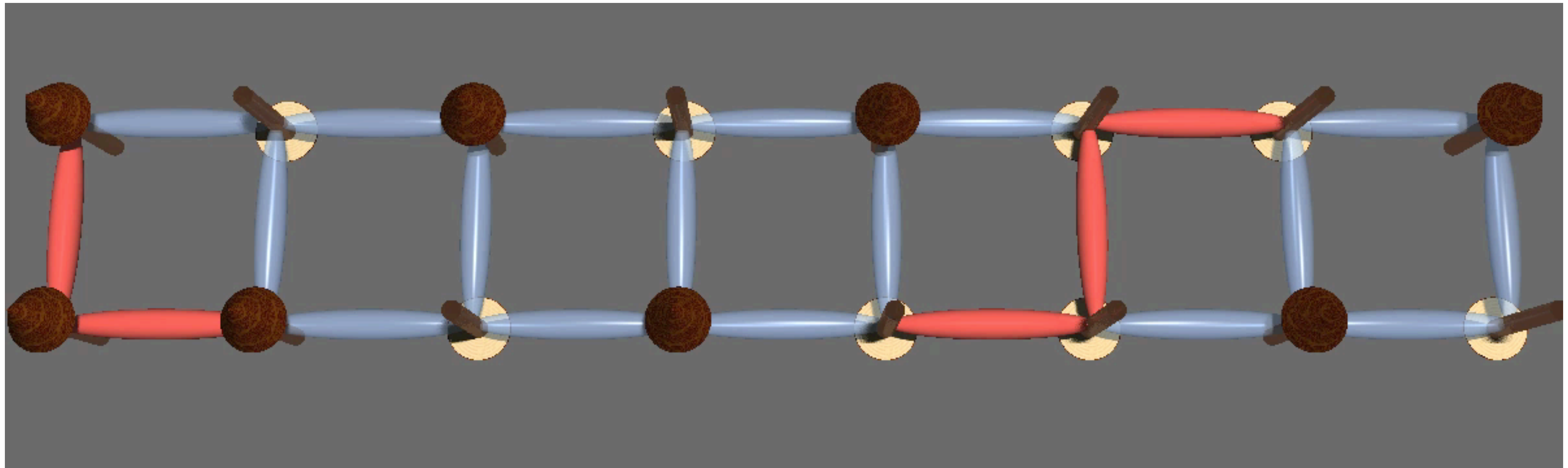
Looks like the nonlinear σ model!



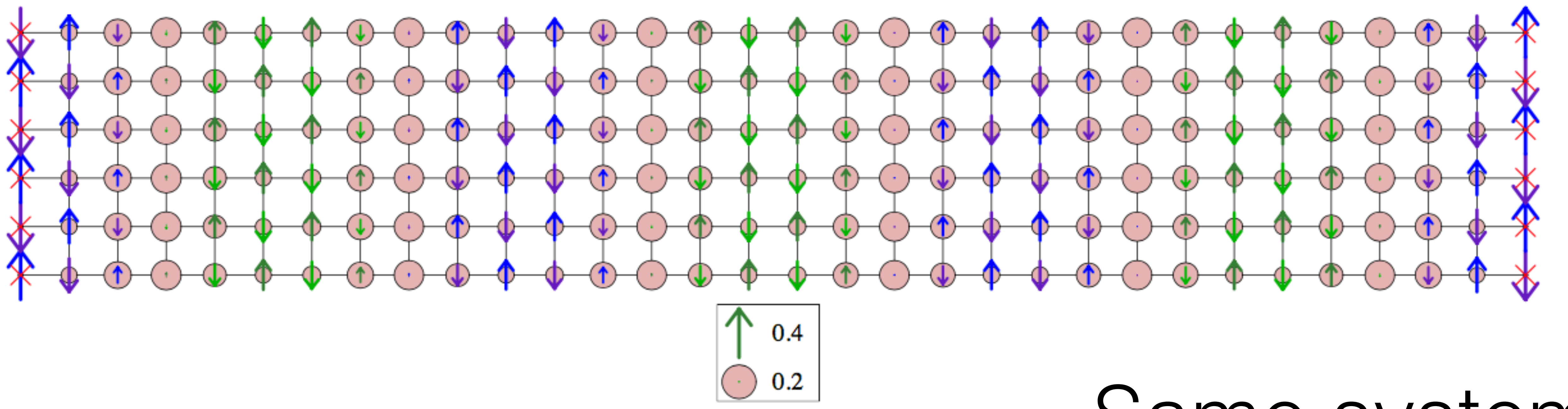
Looks like RVB!

The METTS Algorithm

- Start with a random product state $|i\rangle$
- Evolve in imaginary time to $\beta/2$ to get $|\phi(i)\rangle$ (first METTS) (Measure properties here)
- Perform a "Measurement" to get a new product state $|i'\rangle$ (calculate probabilities, roll the dice with random numbers, one site at a time)
- Repeat.
- The probability of going from $|i\rangle$ to $|i'\rangle$ and back satisfies detailed balance: evolves to exact thermo equilibrium $P(i)$, subject to ergodicity

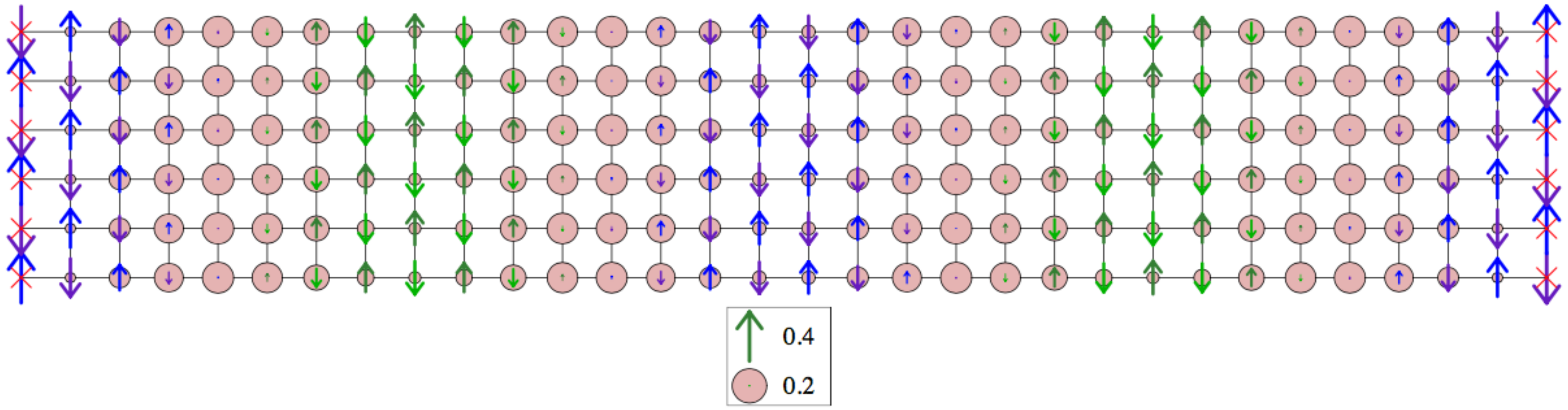


T=0: Striped states, pairing…



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

Same system, different states



32 x 6 system, Vertical PBC's
U/t = 8, 24 holes
m = 17000, truncated = 6.1e-05

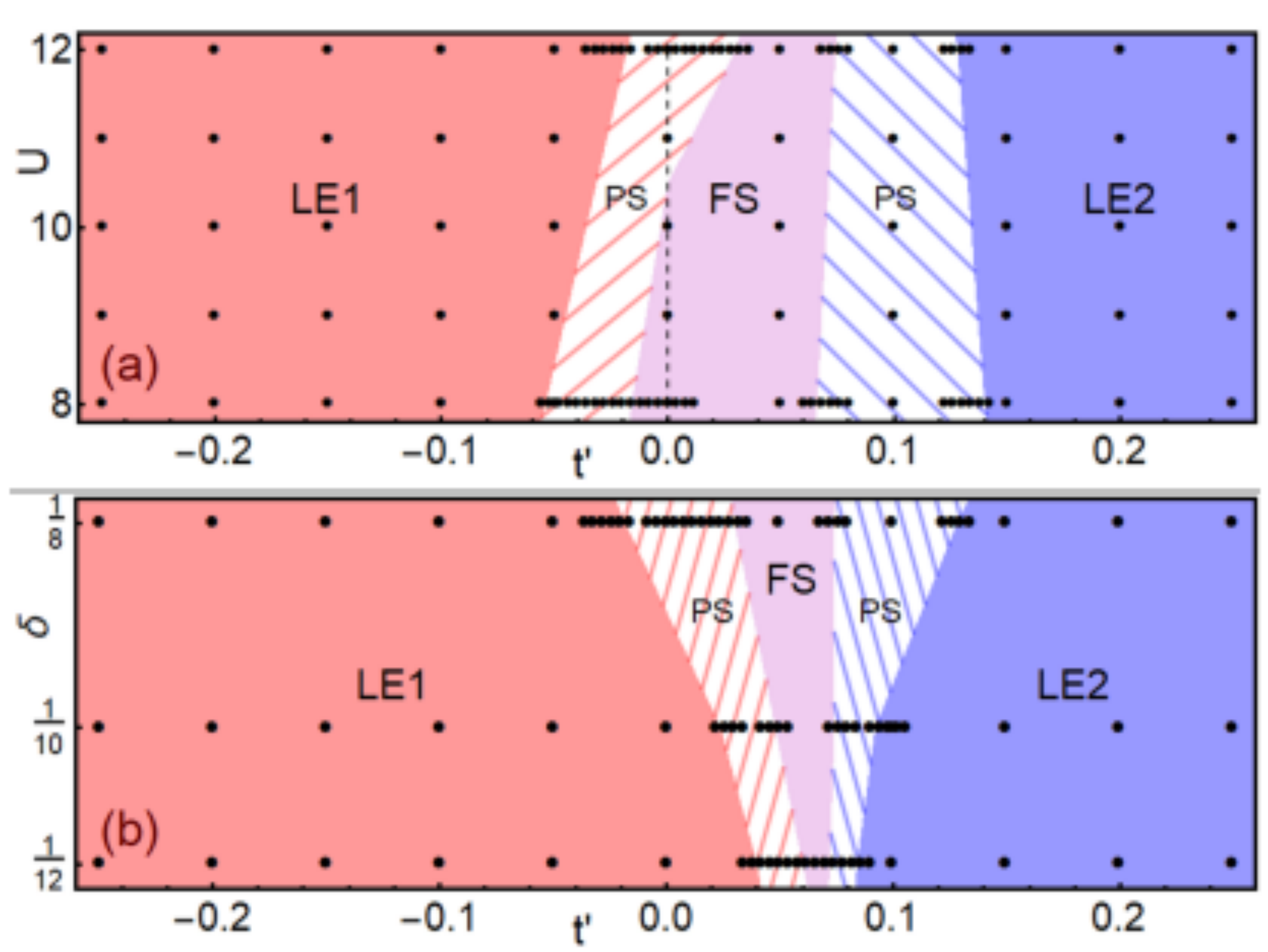


FIG. 1. (Color online) Ground state phase diagram of the Hubbard model in Eq.(1) in (a) as a function of U and t' at hole doping concentration $\delta = 12.5\%$ where the dashed line labels $t' = 0$, and in (b) as a function of δ and t' at $U = 12$. Here $t = 1$ and the black dots are the data points.

Ground state phase diagram of the doped Hubbard model on the 4-leg cylinder

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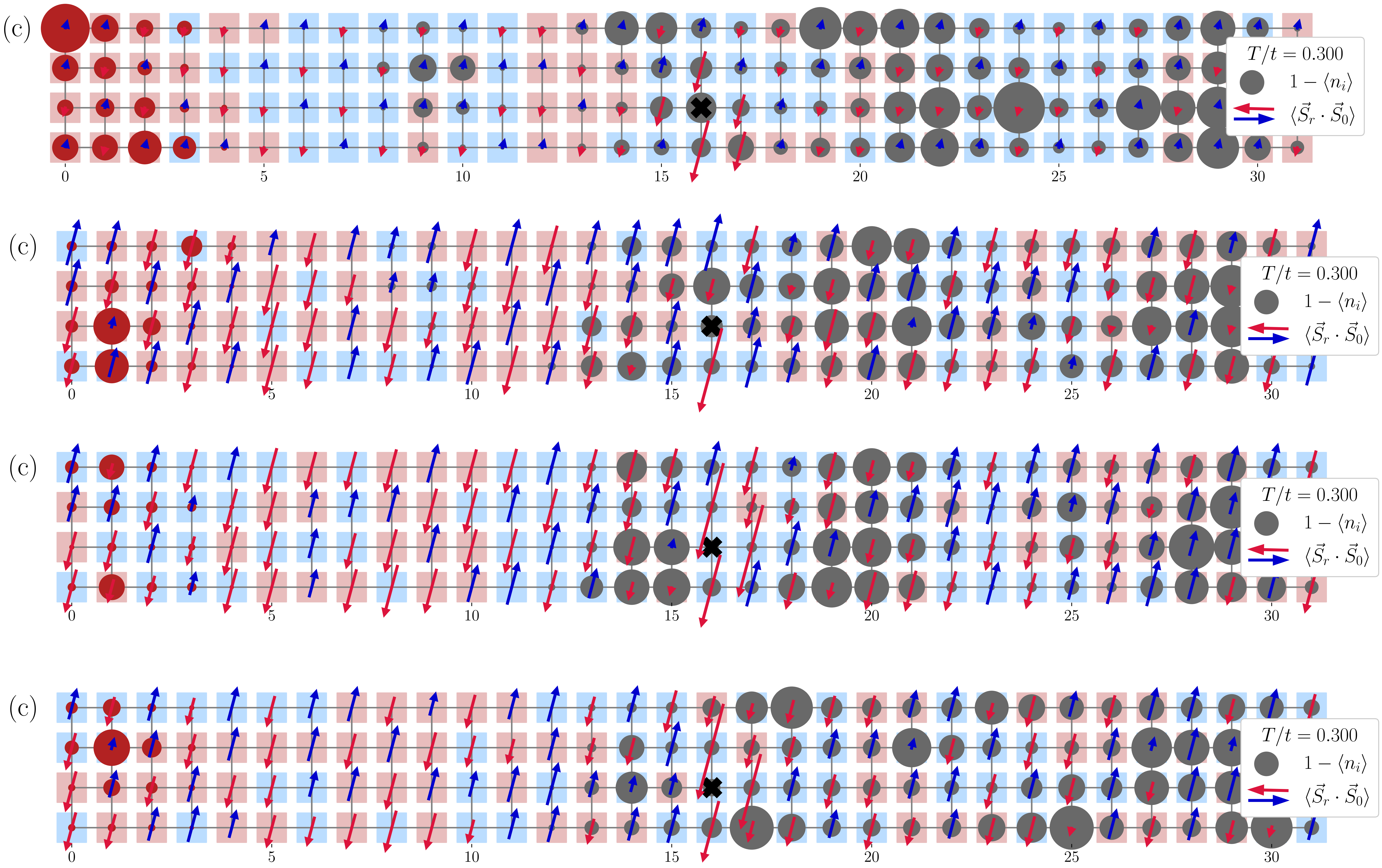
FS = filled stripe
LE (Luther Emery) have half-filled stripes competing with pairing

METTS

Doublons

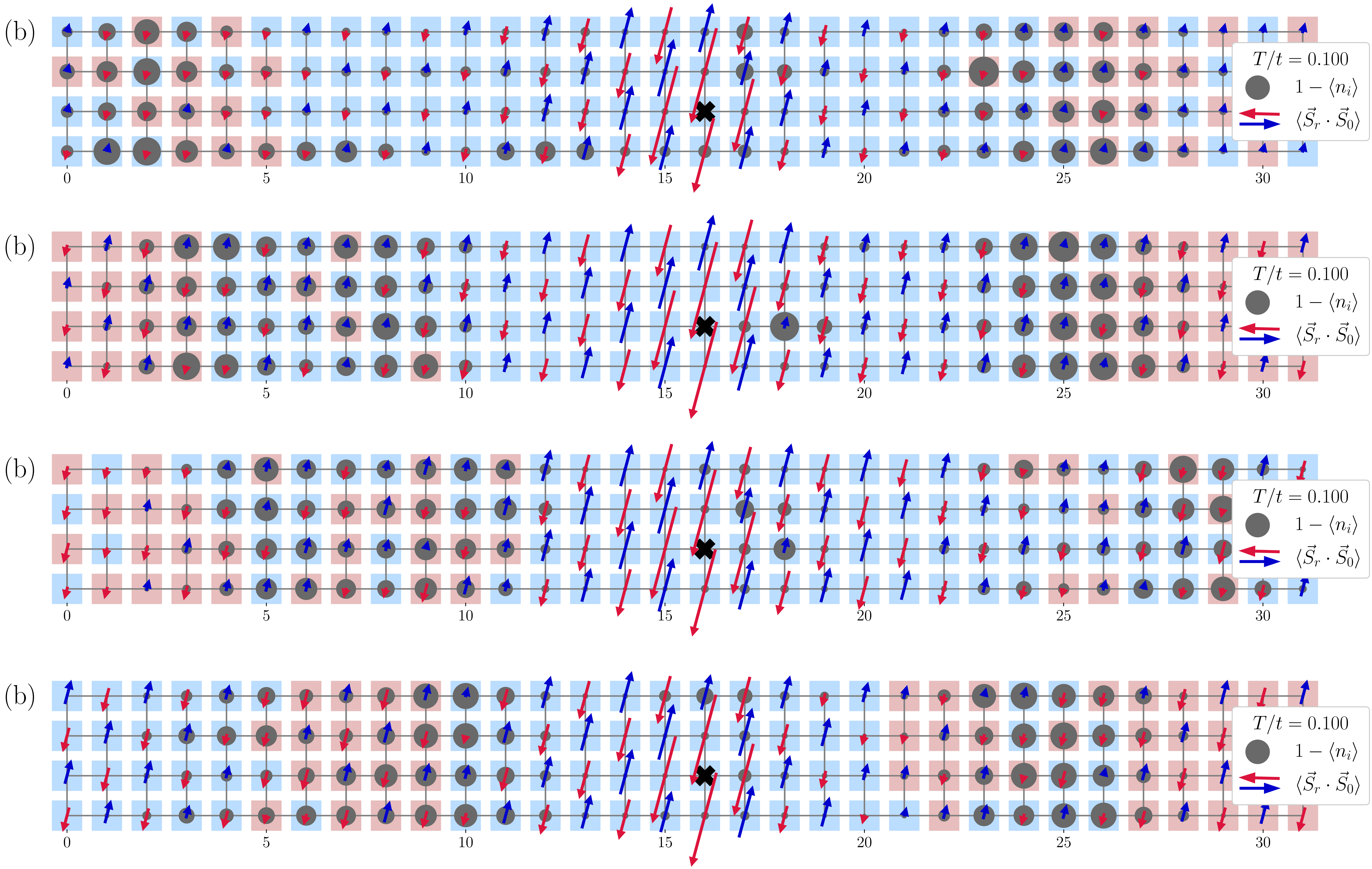


U/t=10
doping=1/16
<u>T/t=0.3</u>

Very local, fluctuating AF correlations
Apparent tendency for hole attraction, but strong fluctuations
Some doubly occupied sites

These are four successive METTS: short autocorrelationt time, but some slow modes

METTS



U/t=10

doping=1/16

<u>T/t=0.1</u>

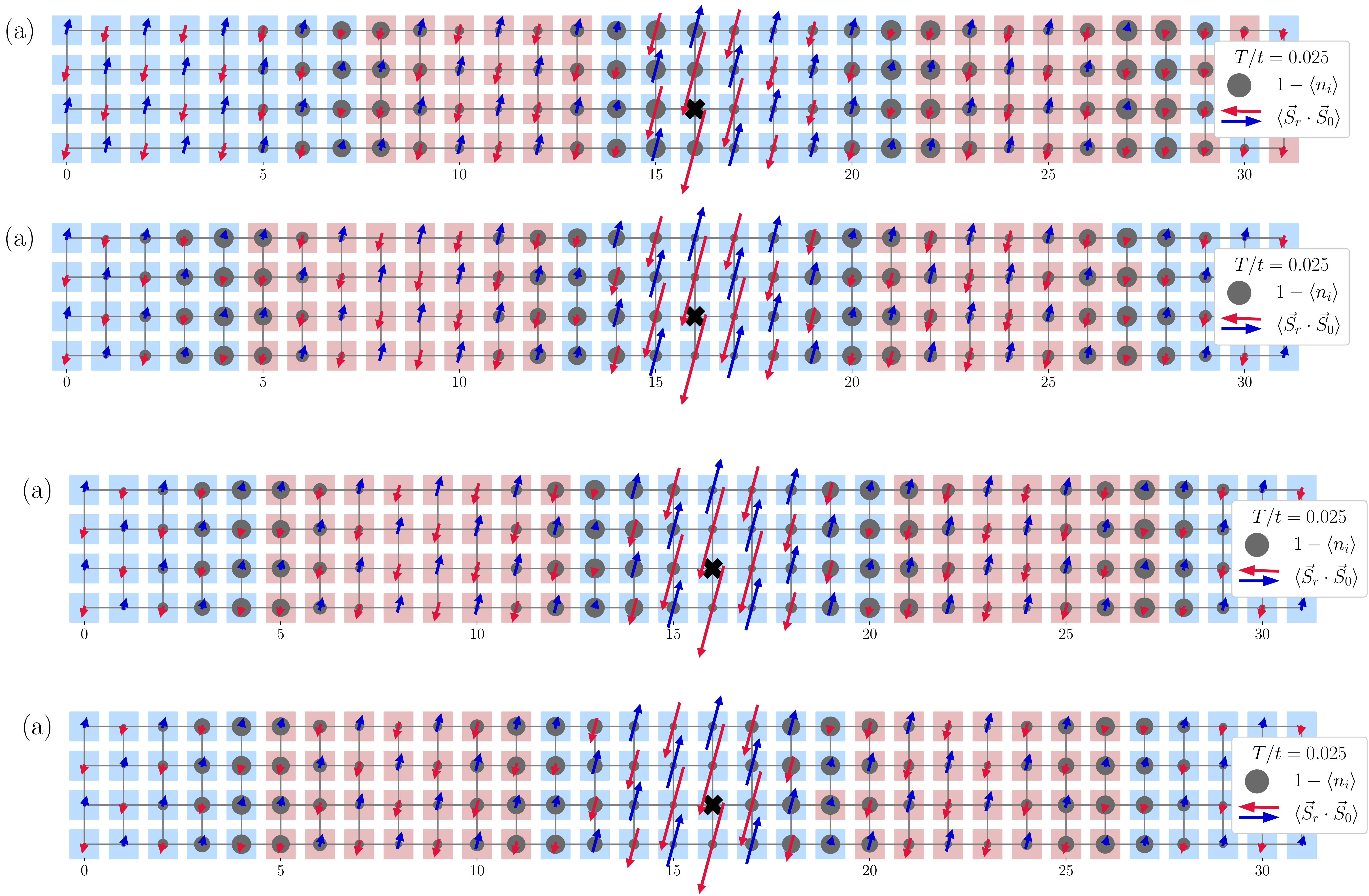
Medium ranged fluctuating AF correlations

Stronger tendency for hole clustering, but strong fluctuations

Tendency for “stripes” to mediate a domain wall in the local AF order

Fluctuating filled stripes?

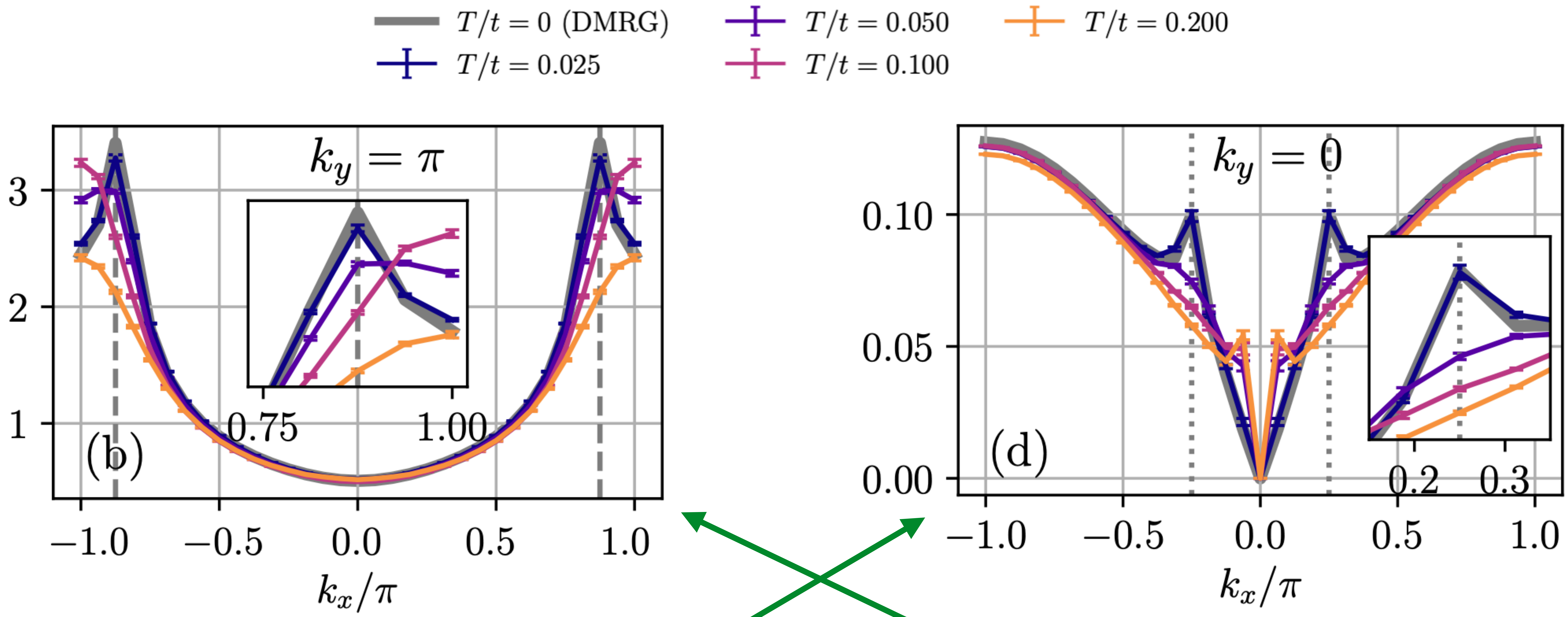
METTS



U/t=10
doping=1/16
T/t=0.025

Clear striped state with fluctuations (looks like sloshing of stripe positions)

Charge and Magnetic ordering



$$S_{\mathrm{c}}(\mathbf{k}) = \frac{1}{N}\sum_{l,m=1}^{N} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}_l-\mathbf{r}_m)}\langle (n_l - n)(n_m - n)\rangle$$

$$S_{\mathrm{m}}(\mathbf{k}) = \frac{1}{N}\sum_{l,m=1}^{N} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}_l-\mathbf{r}_m)}\langle \vec{S}_l \cdot \vec{S}_m\rangle$$

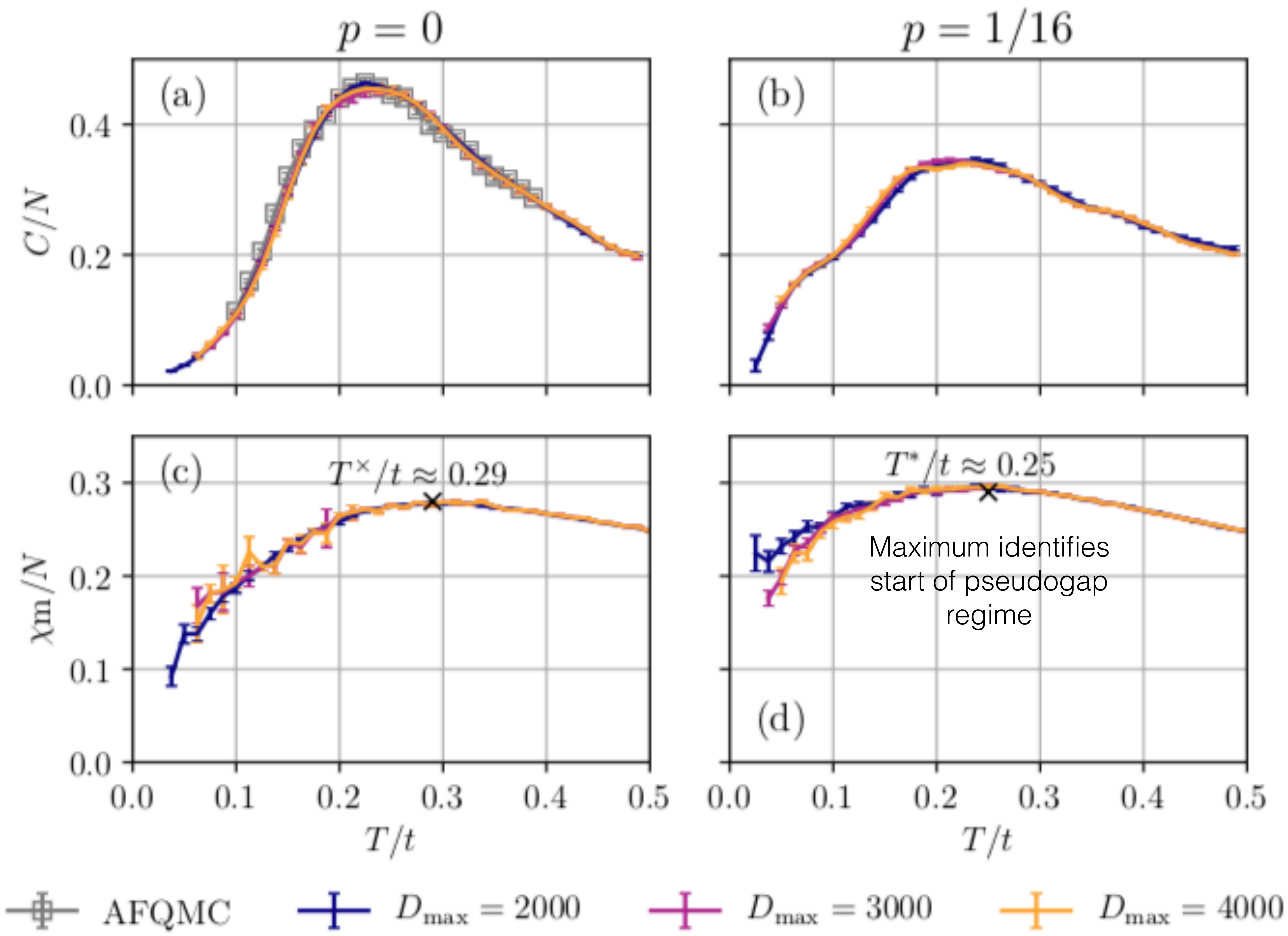
Thermodynamics

- Specific Heat

$$C = \frac{\mathrm{d}E}{\mathrm{d}T}$$

- Magnetic susceptibility

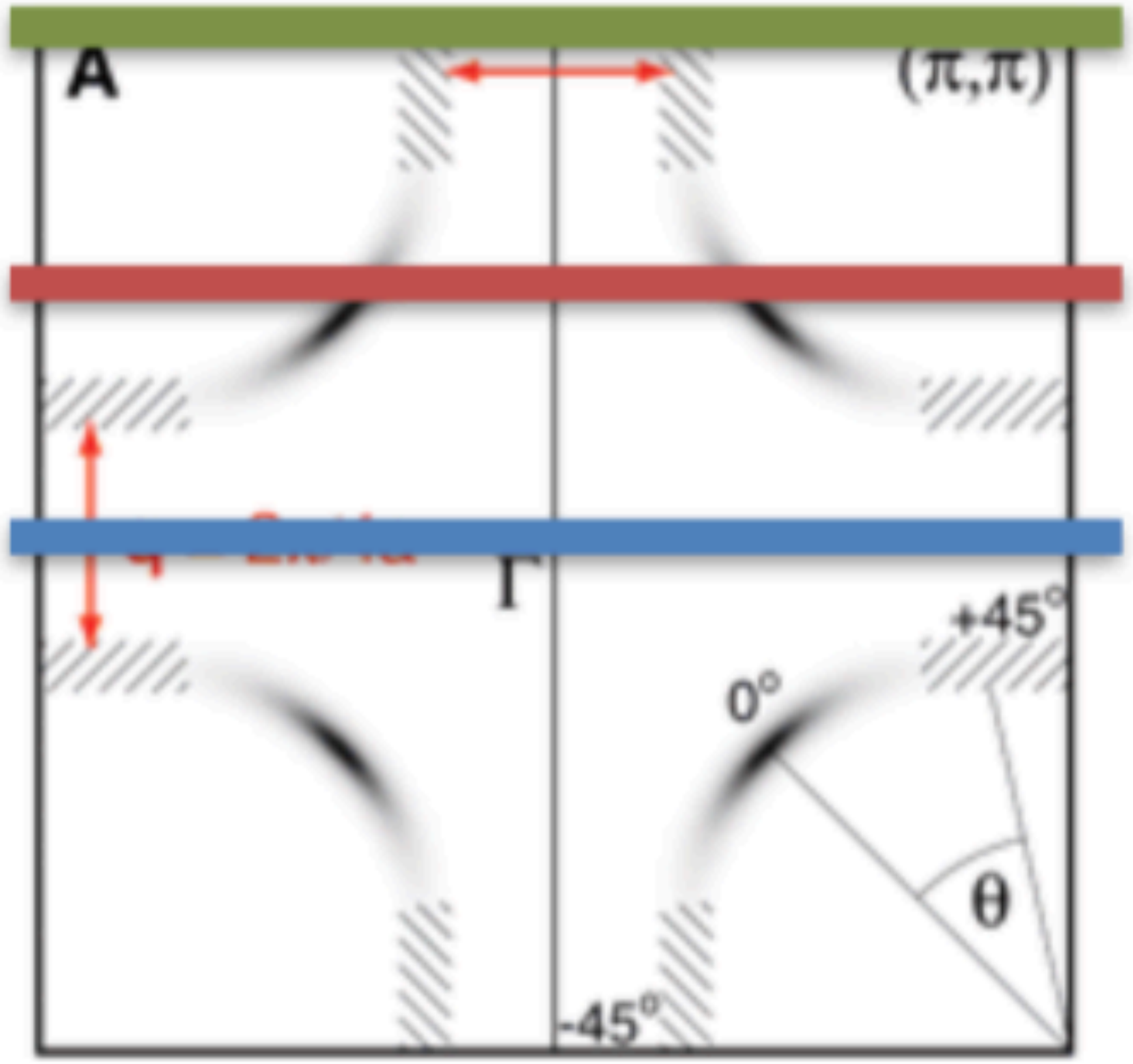
$$\chi_{\mathrm{m}} = \left.\frac{\mathrm{d}M}{\mathrm{d}H}\right|_{H=0}$$



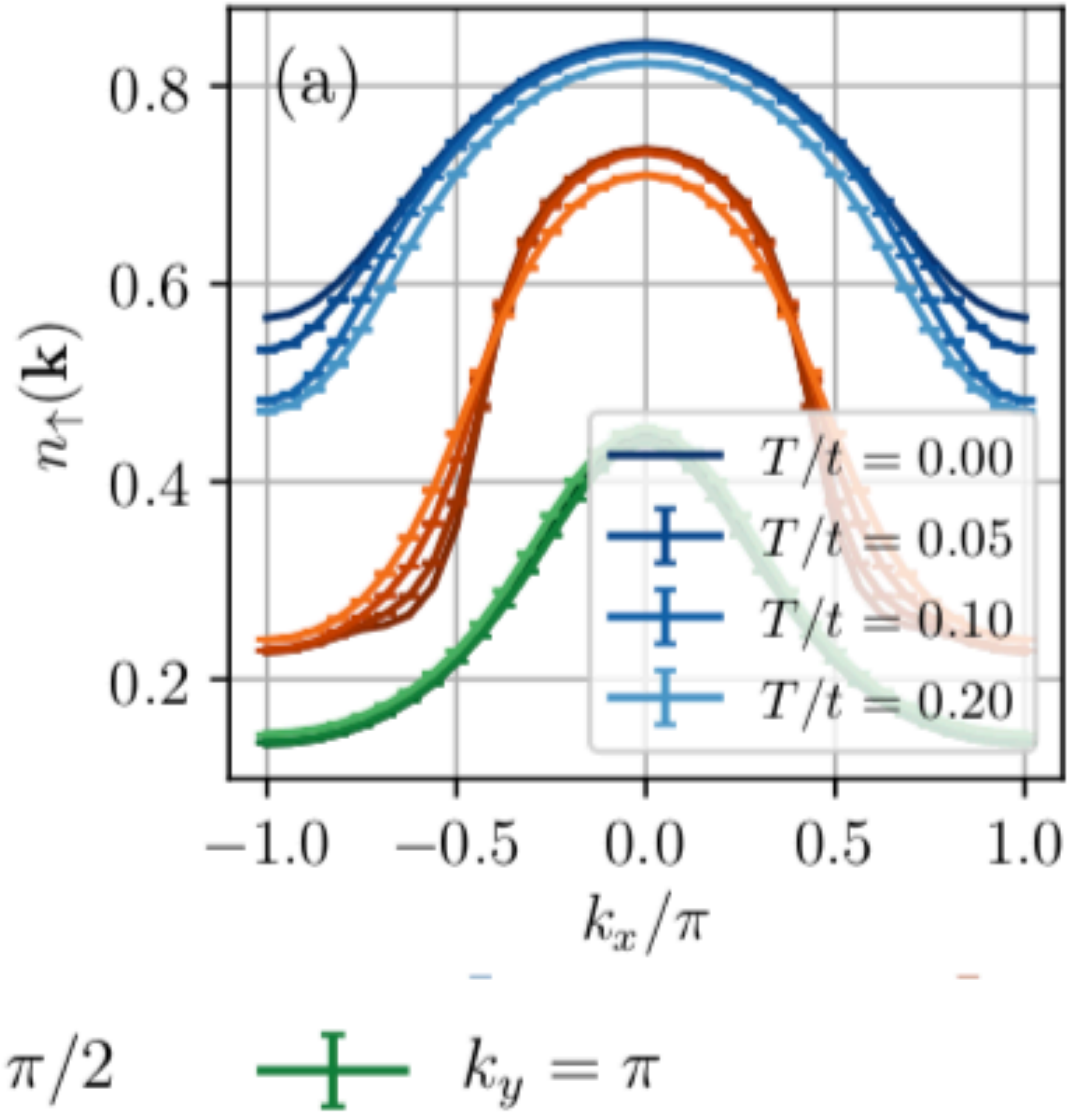
Momentum distribution function

$$n_\sigma(\mathbf{k}) = \frac{1}{N}\sum_{l,m=1}^{N} e^{i\mathbf{k}\cdot(\mathbf{r}_l-\mathbf{r}_m)}\langle c^\dagger_{l\sigma}c_{m\sigma}\rangle$$

Is most of the "Fermi Surface" gapped except near the nodal region?

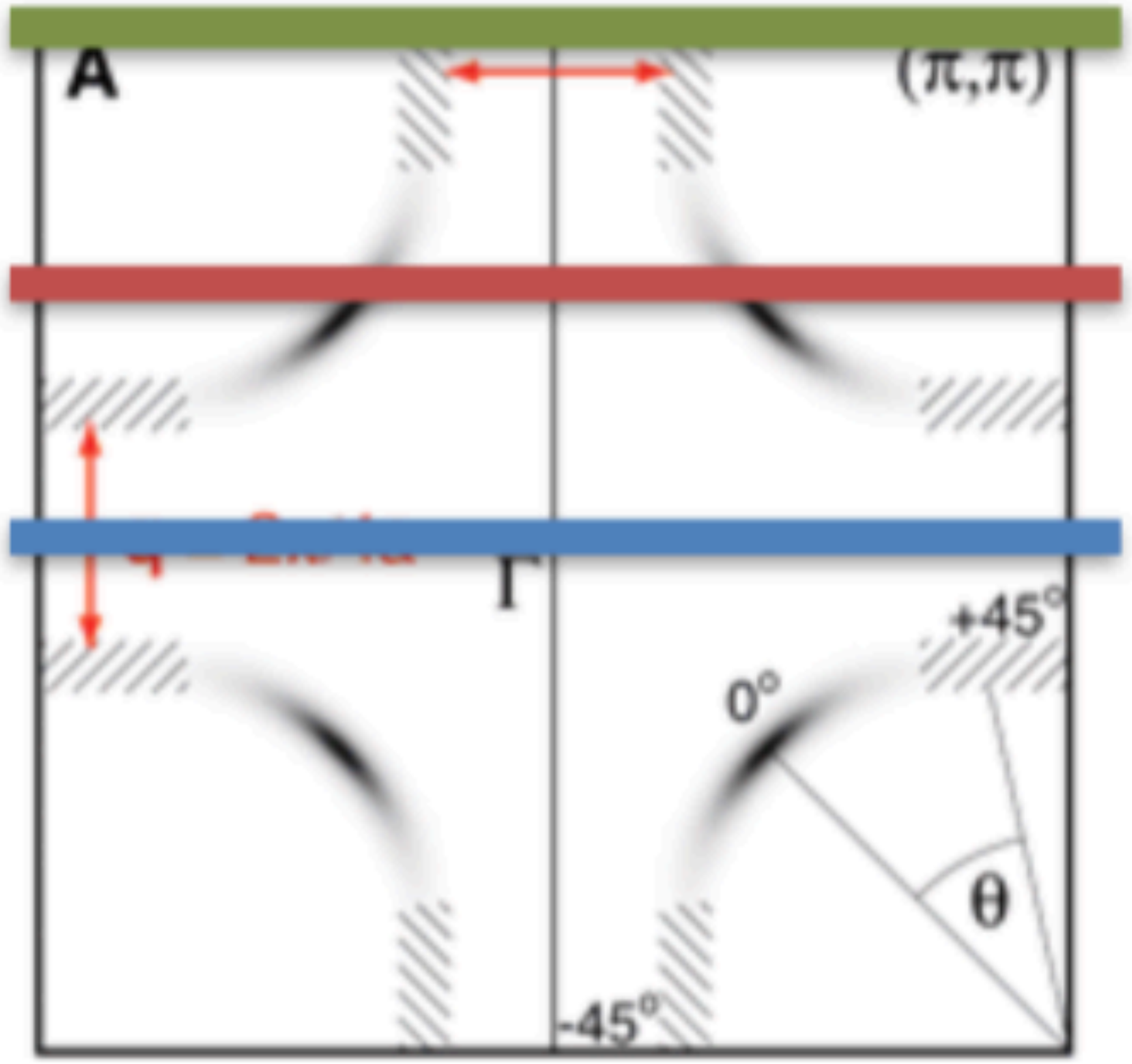


[Shen et al., Science, 307, 5711 (2005)]

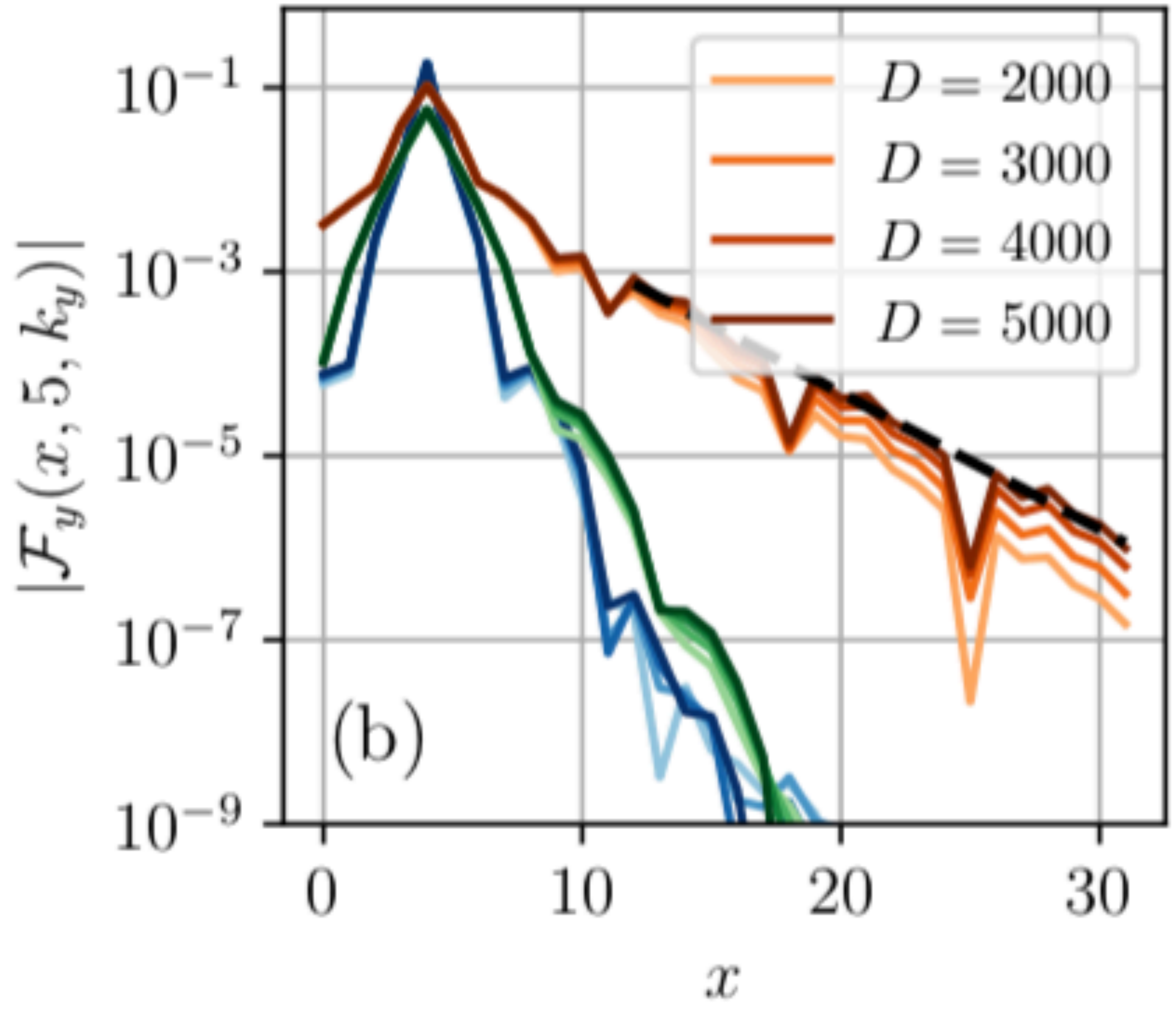


Electron correlations

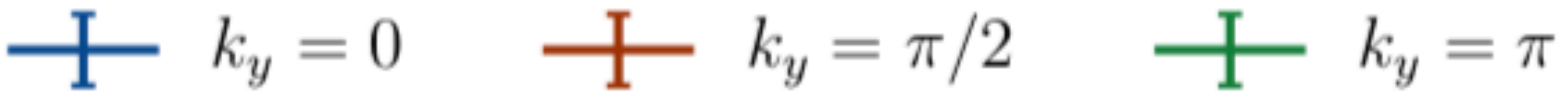
$$\mathscr{F}_y(x_l, x_m, k_y) = \frac{1}{W}\sum_{n=1}^{W} \mathrm{e}^{ik_y y_n}\langle c^\dagger_{(x_l,y_n)} c_{(x_m,y_n)}\rangle$$



[Shen et al., Science, 307, 5711 (2005)]



Finite correlation length even near the nodes



Energy gaps

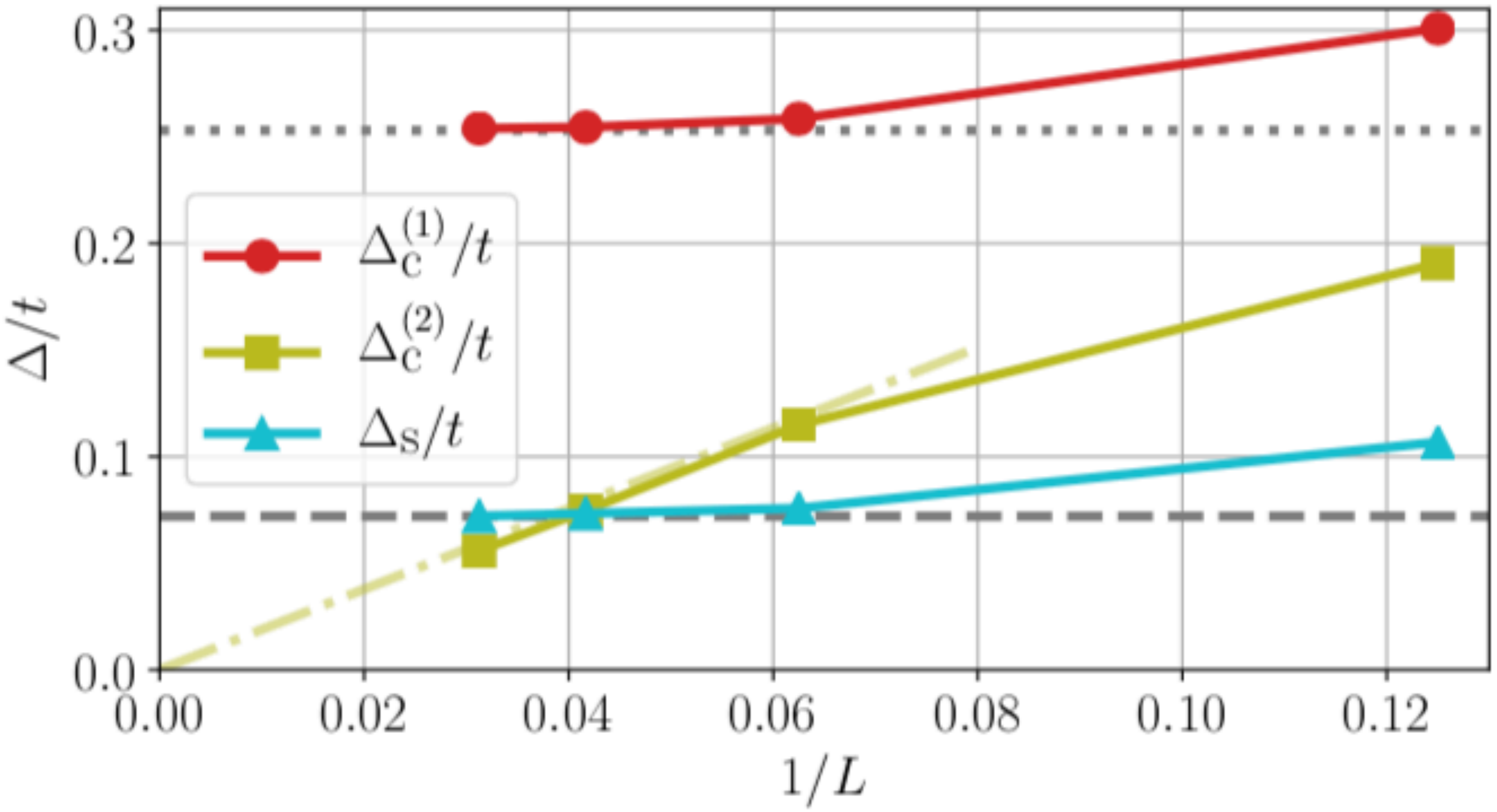
- Spin gap $\Delta_s = E_0(m+1, m-1) - E_0(m, m)$
- Single particle gap $\Delta_c^{(1)}$

$E(N+1) + E(N-1) - 2E(N)$

- Charge gap $\Delta_c^{(2)}$

$\frac{1}{2}[E(N+2) + E(N-2) - 2E(N)]$

- Computed using ground state DMRG
- Charge gap vanishes, spin and single particle gap remain finite



Consistent with a SC w/o nodal qps—does Δ_c^1 vanish on wider cylinders??

Summary

- METTS is finally proving itself capable of doing low T in difficult quasi-2D systems. The same techniques could be applied to frustrated magnets and other systems where DMRG can be useful
- We have finally been able to connect the finite T and T=0 regimes in Hubbard simulations. In this system, stripes melt near $T = 0.05t$ and the magnetic peak shifts between commensurate and incommensurate at this temperature.
- Details still to be figured out: nodal gaps, temperature dependence of pairing, and at T=0, pairing versus t'
- The reason METTS is proving itself now rather than a few years ago is mostly due to improvements in time evolution methods (TDVP), plus very impressive development by Alex. See also our new ancillary Krylov improvement of TDVP (Yang and White, arXiv:2005.06104)