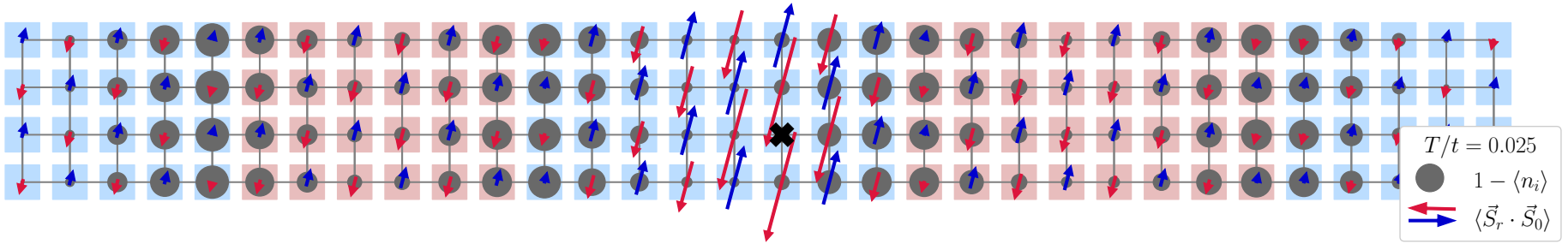
SPIN LIQUIDS, STRIPES, AND THE PSEUDOGAP IN THE HUBBARD MODEL AT FINITE TEMPERATURE

Collège de France



Alexander Wietek

06/03/2021

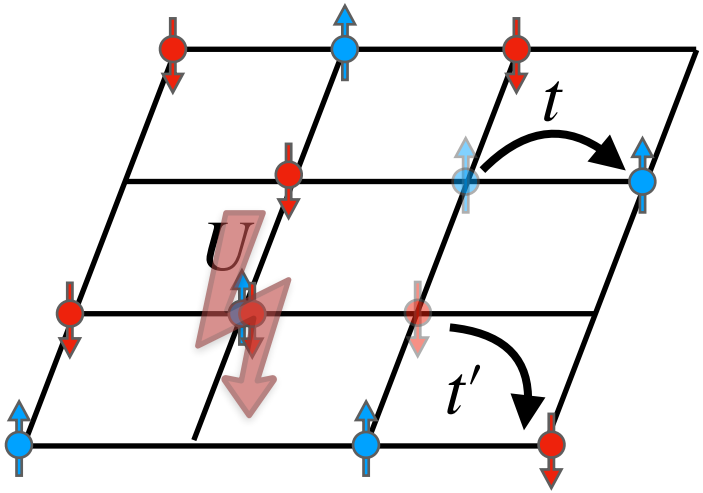
arXiv:2009.10736

Phys. Rev. X (2021)(to appear)

FLATIRON INSTITUTE
Center for Computational Quantum Physics

The Hubbard model at strong coupling

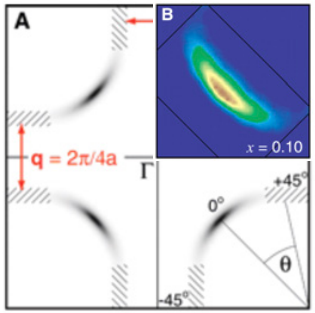
$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

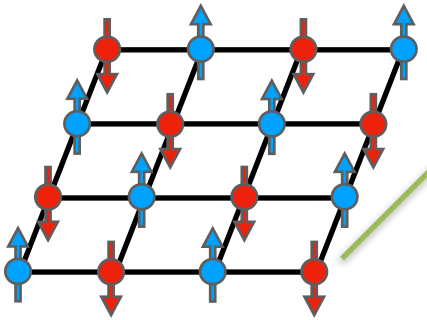


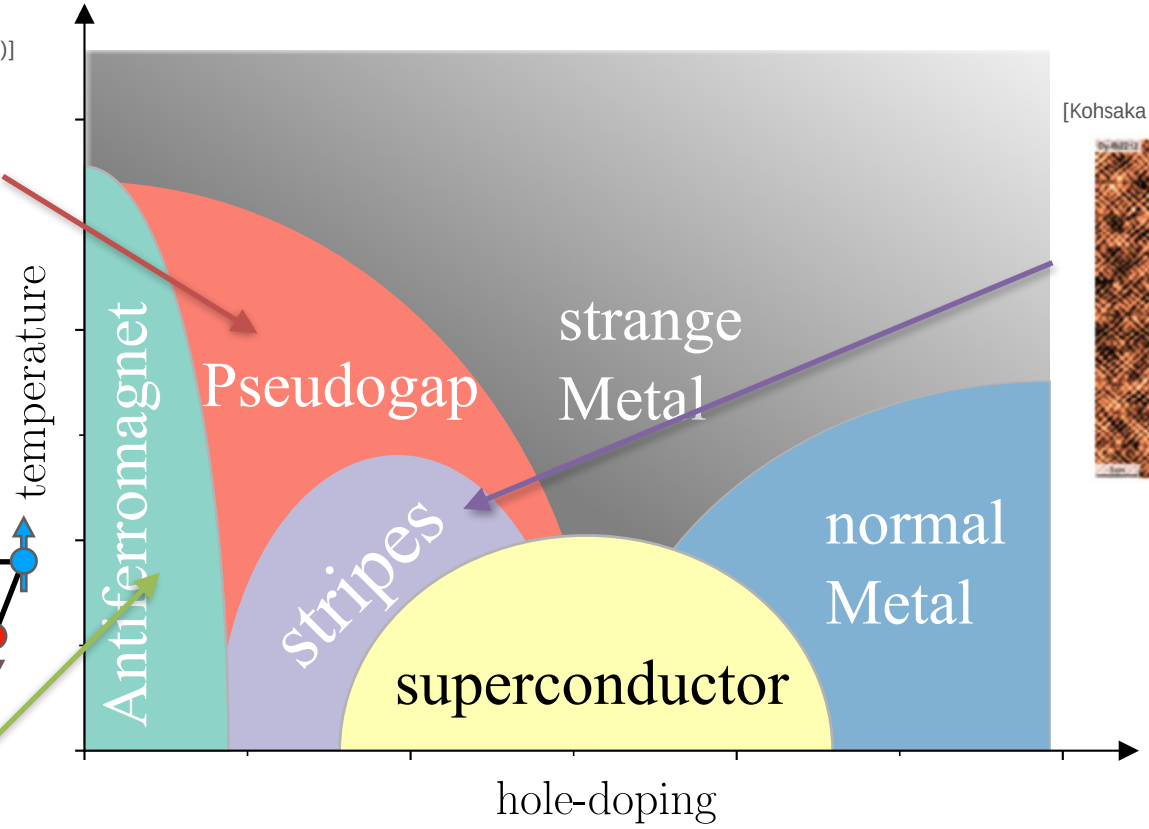
- Weak coupling: $U/t \lesssim 2$
  metals, Fermi liquids
- Strong coupling: $U/t \gtrsim 6$
  insulators, antiferromagnets

Cuprate phase diagram

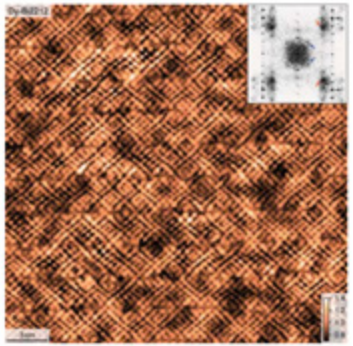
[Shen et al., Science, 307, 5711 (2005)]





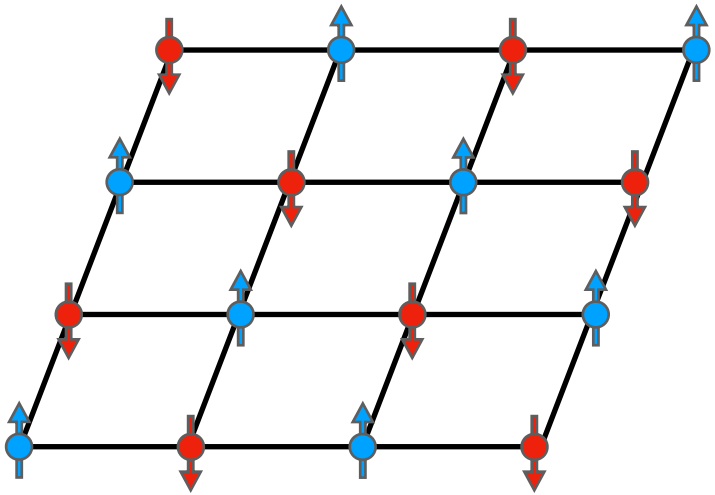


[Kohsaka et al., Science, 315, 1380 (2007)]



Stripe physics in hole-doped antiferromagnets

Antiferromagnetism at half-filling



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

$U/t \to \infty$

$$H_{\text{eff}} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

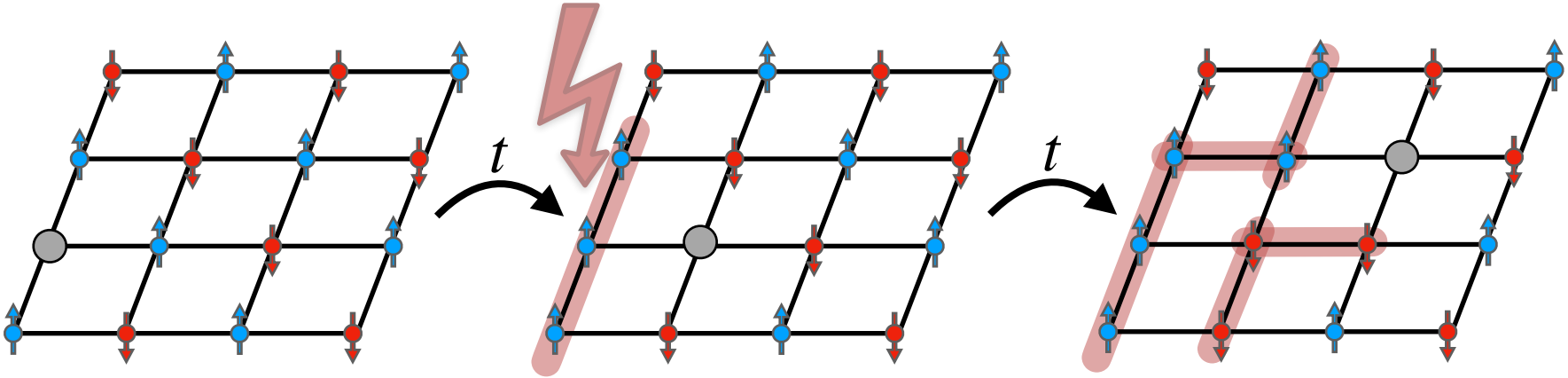
$$J = \frac{t^2}{U}$$

$$\vec{S}_i = (S_i^x, S_i^y, S_i^z)$$

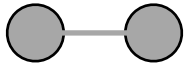
$$S_i^{\alpha} = \frac{1}{2} c^{\dagger}_{i\tau} \sigma^{\alpha}_{\tau\tau'} c_{i\tau'}$$

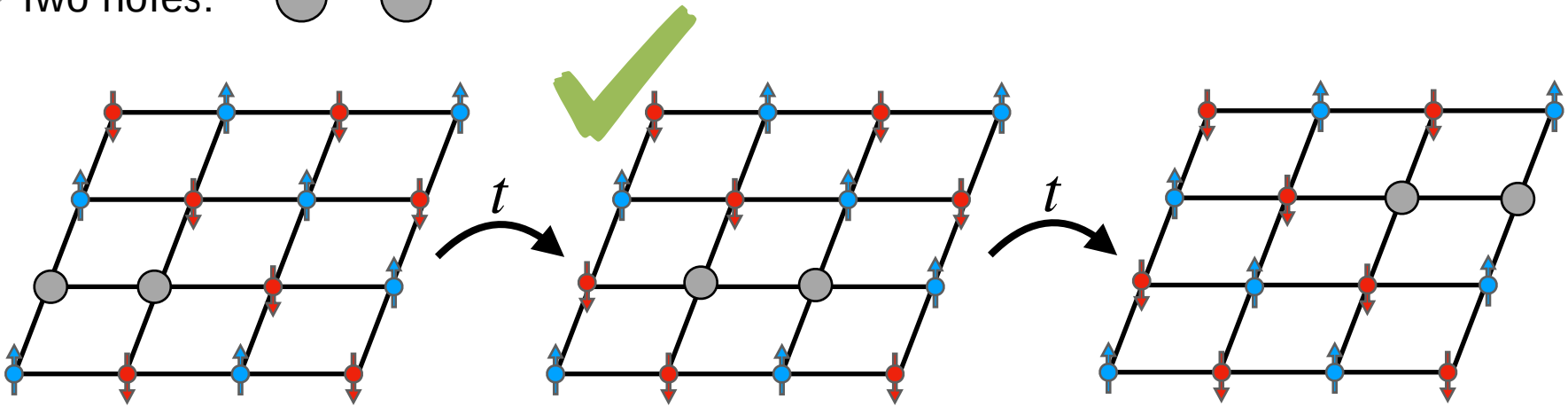
Hole-doping an antiferromagnet

- Single-hole: 



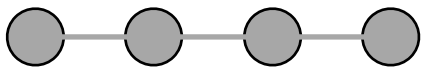
Hole-doping an antiferromagnet

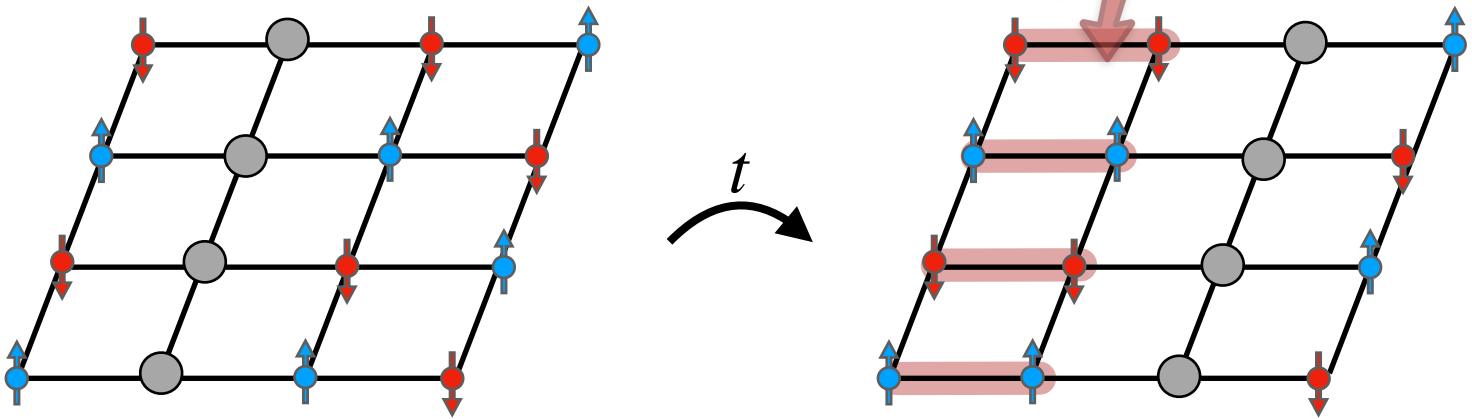
- Two holes: 



Stripe order

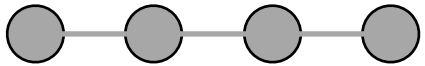
- More Holes:

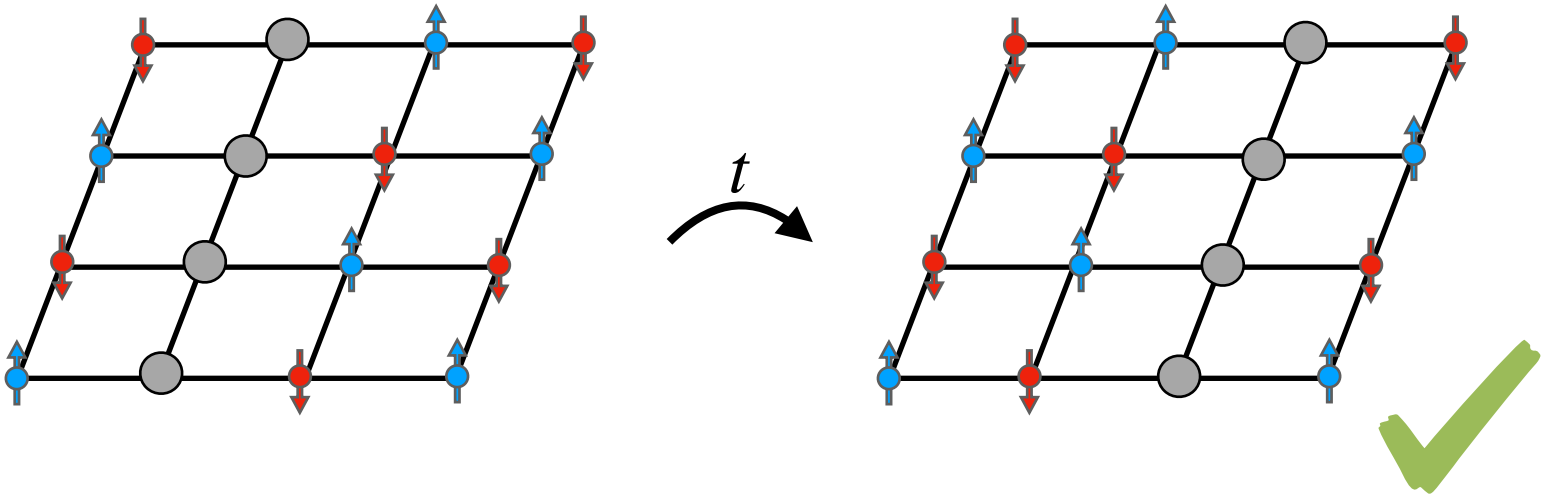




Stripe order

- More Holes:





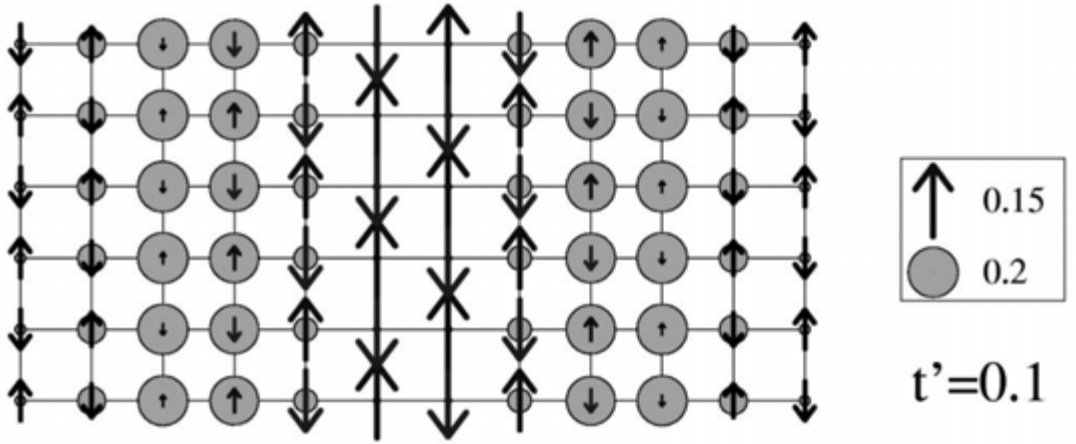
- Change of antiferromagnetic domain at maximum in hole density

Stripes in the Hubbard model

- Proposed within Hartree-Fock approximation

[D. Poilblanc and T. M. Rice, Phys. Rev. B 39, 9749(R), (1989)] [J. Zaanen and O. Gunnarsson, Phys. Rev. B 40, 7391(R) (1989)]

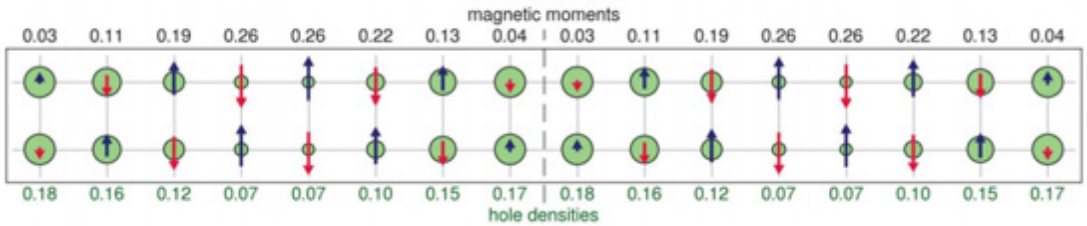
- Early evidence in DMRG simulations ($T = 0$) of the $t - J$ model ($U/t \to \infty$ limit)



[White, Scalapino, Phys. Rev. Lett. 80, 1272, (1998)] [White, Scalapino, Phys. Rev. B 60, R753(R), (1999)]

Stripes in the Hubbard model

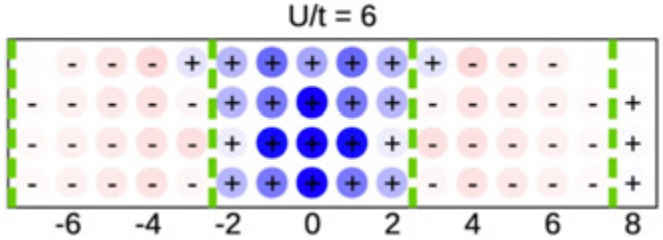
- Stripes at $T = 0$, $p = 1/8$, $U/t = 8$, $t'/t = 0$



[Zheng et al., Science 358, 6367 (2017)]

[White Scalapino, Phys. Rev. Lett. 91, 136403 (2003)]
[Ehlers et al., Phys. Rev. B 95, 125125 (2017)]
[LeBlanc et al., Phys. Rev. X 5, 041041 (2015)]
[Jiang et al., Phys. Rev. Research 2, 033073 (2020)]

- ... and at $T/t = 0.22$, $p = 1/8$, $U/t = 6$, $t'/t = -0.25$



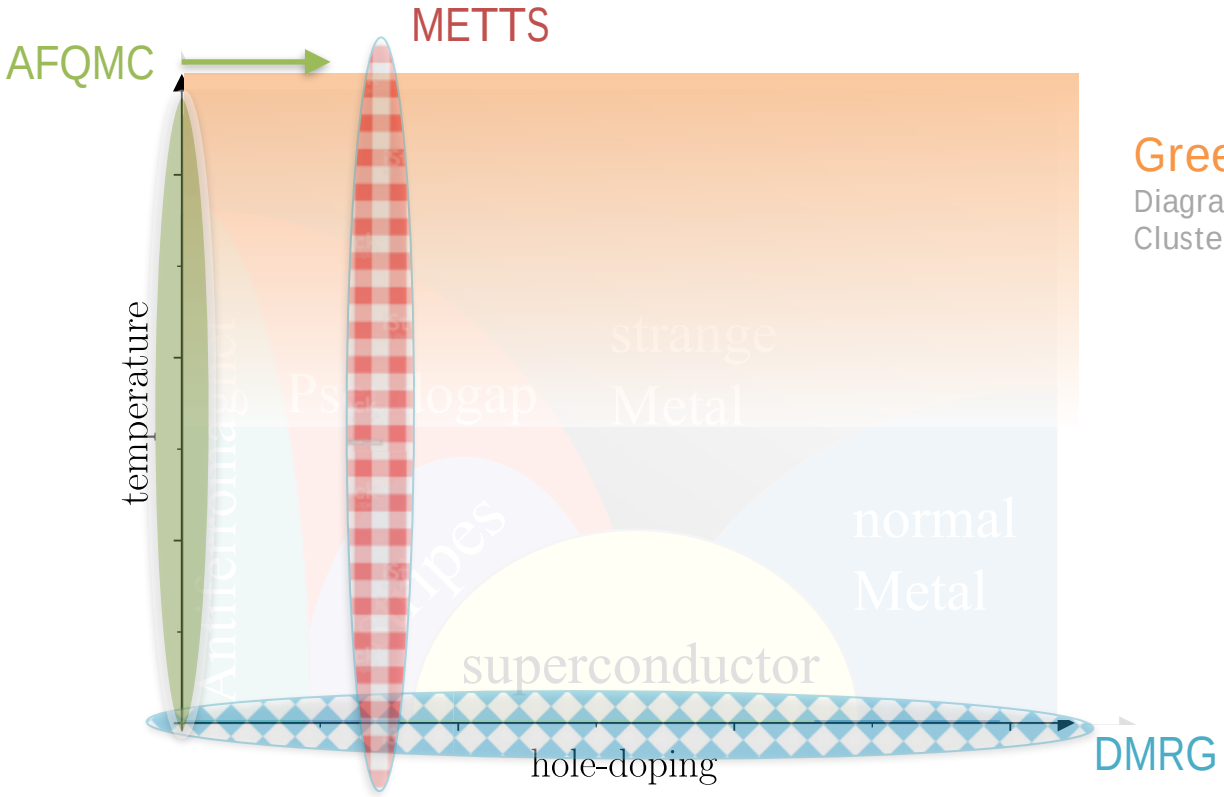
[Huang et al., npj Quant Mater 3, 22 (2018)]

Stripes, antiferromagnetism, and the pseudo gap in the doped Hubbard model at finite temperature

A. Wietek, Y.-Y. He, S. R. White, A. Georges, E. M. Stoudenmire

Phys. Rev. X (2021)(to appear)
arXiv:2009.10736

Numerical methods



Green's function methods

Diagrammatic QMC

Cluster DMFT

METTS

- Decomposition of density matrix into typical pure states

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}(\mathrm{e}^{-\beta H}\mathcal{O}) = \frac{1}{\mathcal{Z}} \sum_i p_i \langle \psi_i | \mathcal{O} | \psi_i \rangle \quad \text{with} \quad p_i \geq 0$$

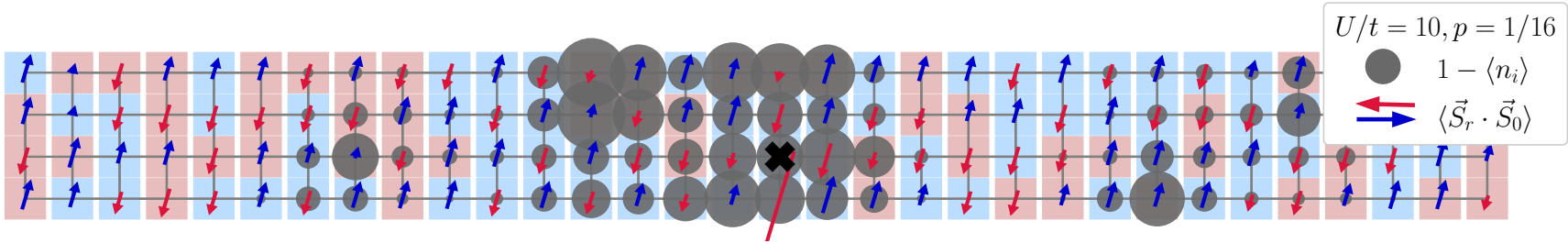
- Minimally-Entangled Typical Thermal State

[White, Phys. Rev. Lett. 102, 190601 (2009)]
[Stoudenmire, White, New J. Phys. 12, 055026 (2010)]

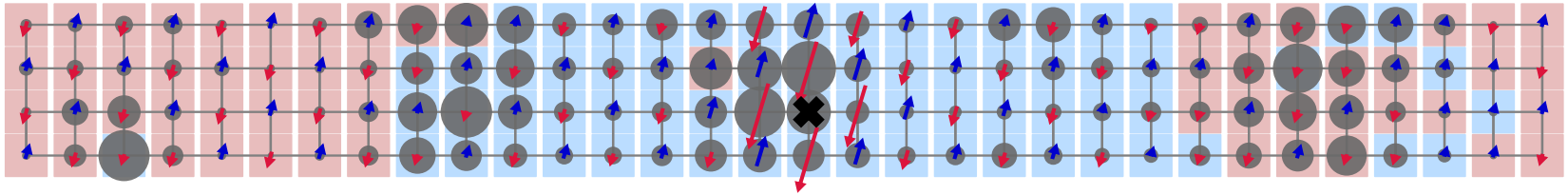
$$|\psi_i\rangle = \frac{1}{\sqrt{p_i}} \mathrm{e}^{-\beta H/2} |\sigma_i\rangle \ , \quad |\sigma_i\rangle = |\sigma_i^1\rangle \, |\sigma_i^2\rangle \ldots |\sigma_i^N\rangle \ , \quad p_i = \langle \sigma_i | \mathrm{e}^{-\beta H} | \sigma_i \rangle \geq 0$$

- Algorithm: random sampling of the states $|\psi_i\rangle$

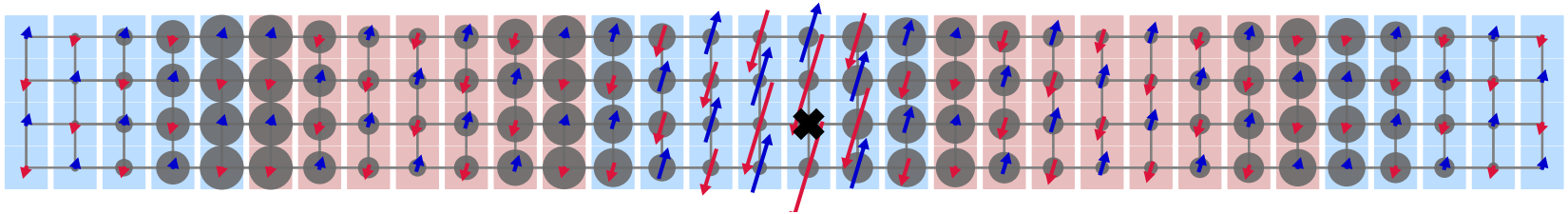
$T/t = 0.300$



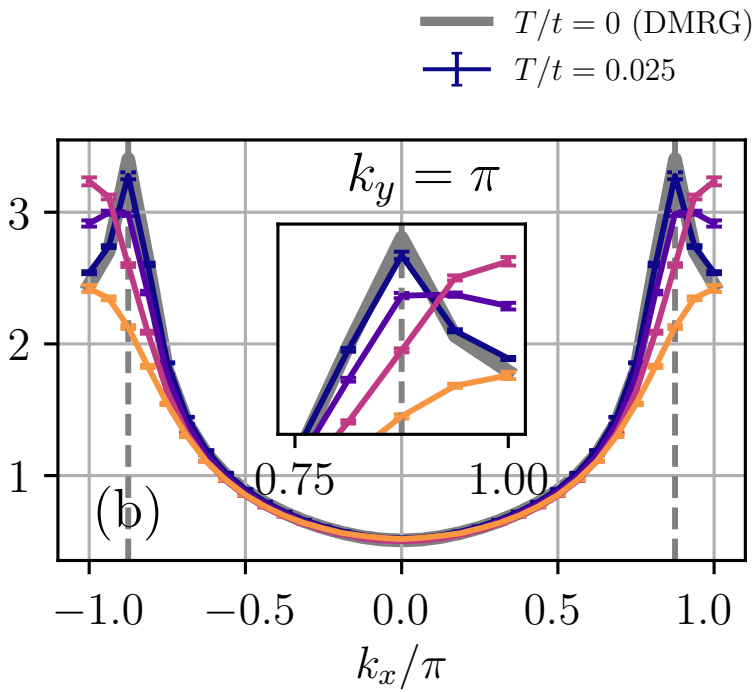
$T/t = 0.100$



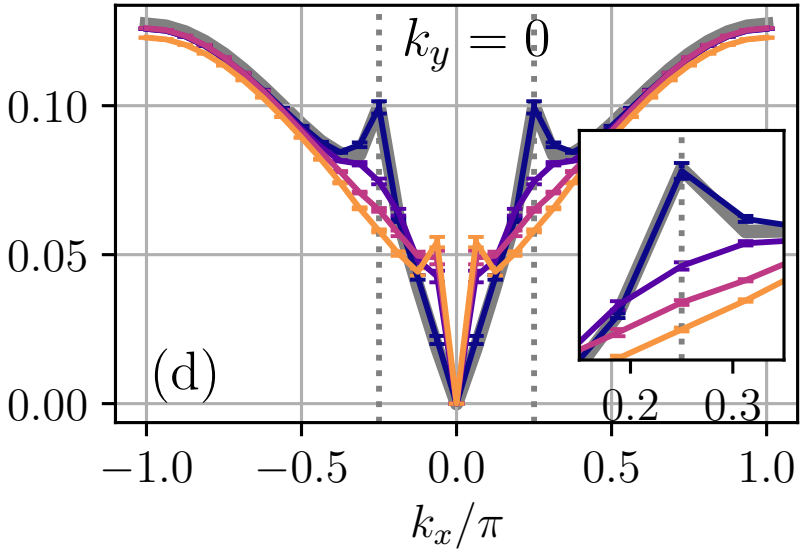
$T/t = 0.025$



Magnetic and Charge ordering

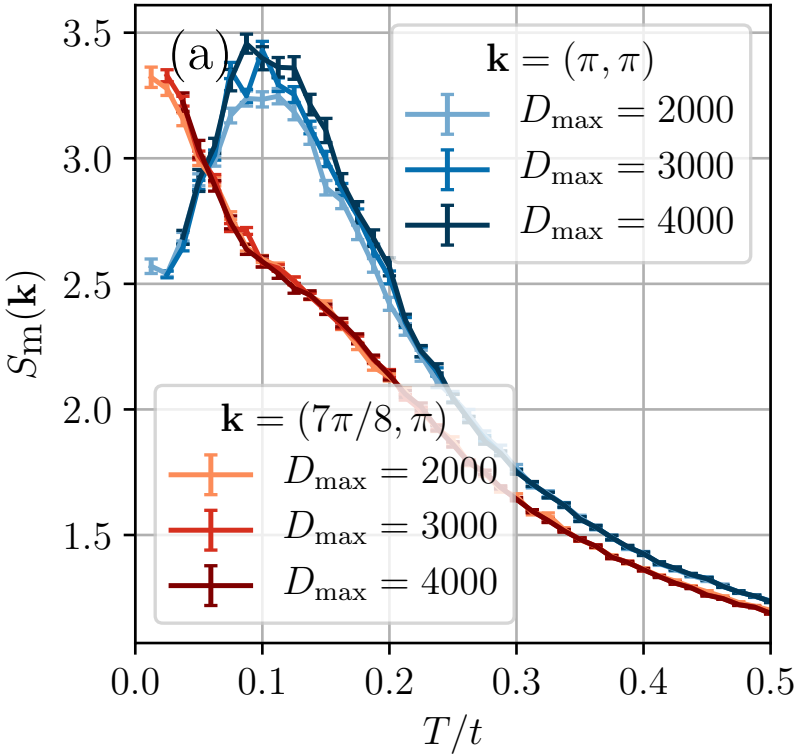


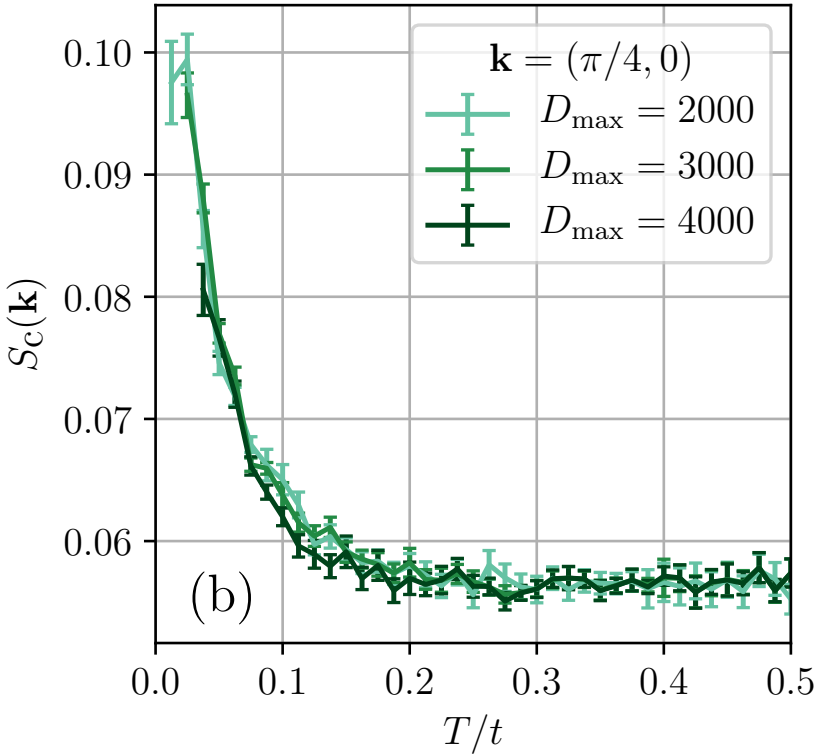
$$S_{\mathrm{m}}(\mathbf{k}) = \frac{1}{N}\sum_{l,m=1}^{N} e^{i\mathbf{k}\cdot(\mathbf{r}_l-\mathbf{r}_m)}\langle \vec{S}_l \cdot \vec{S}_m \rangle$$



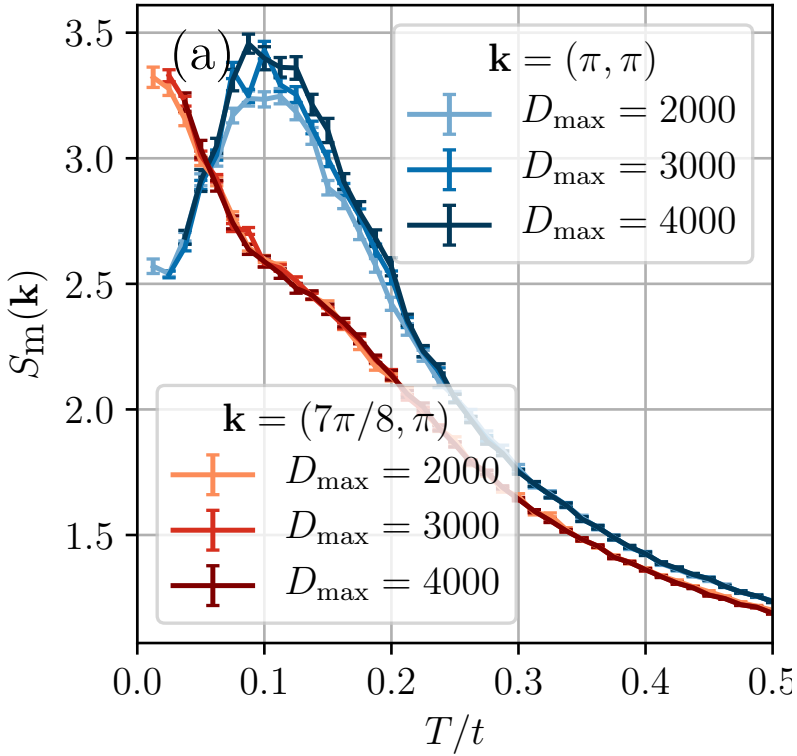
$$S_{\mathrm{c}}(\mathbf{k}) = \frac{1}{N}\sum_{l,m=1}^{N} e^{i\mathbf{k}\cdot(\mathbf{r}_l-\mathbf{r}_m)}\langle (n_l - n)(n_m - n) \rangle$$

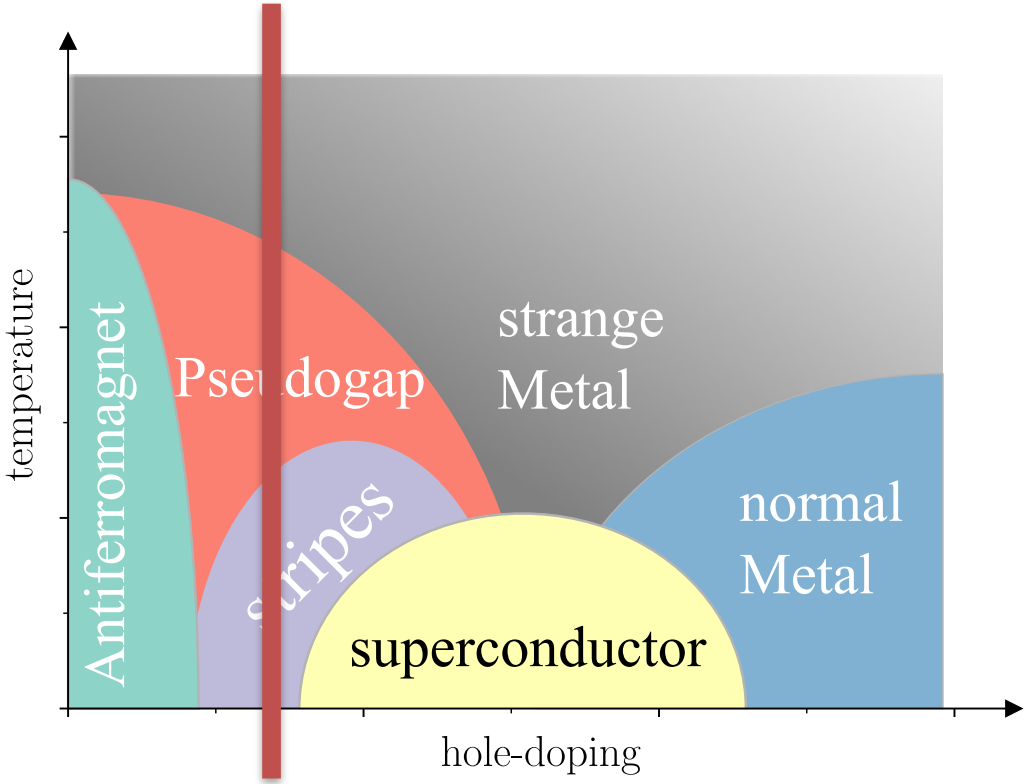
Magnetic and Charge ordering





Magnetic and Charge ordering





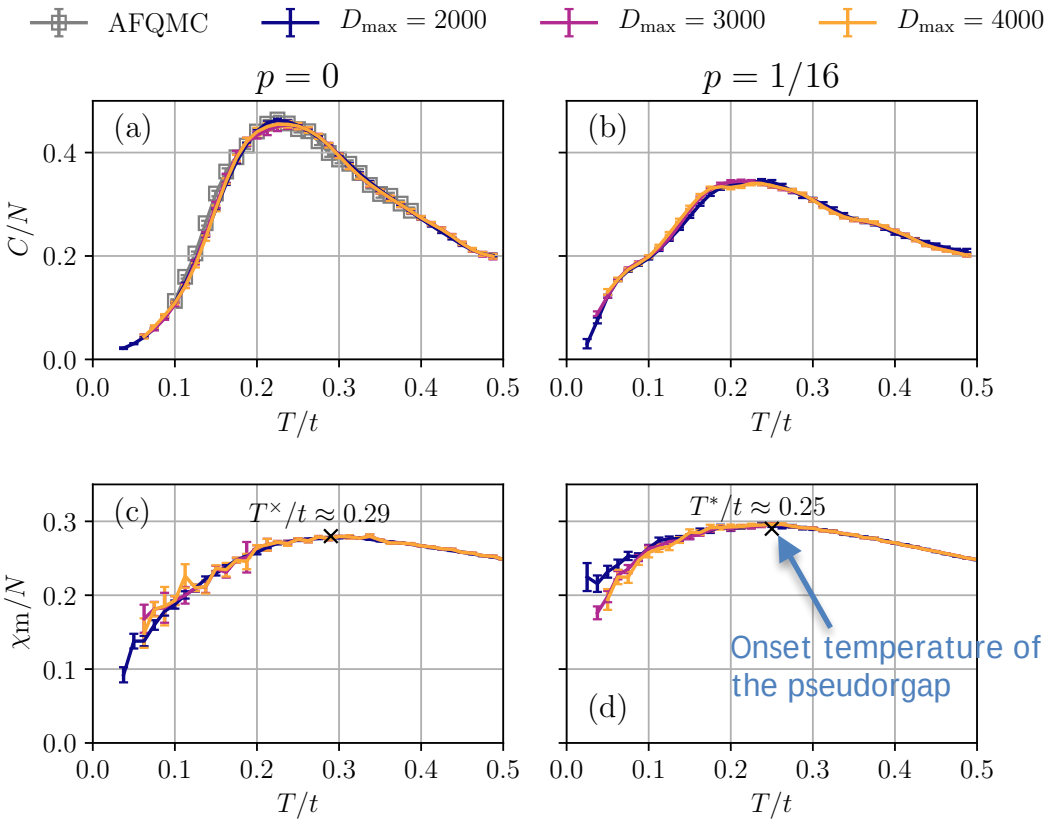
Thermodynamics

- Specific Heat

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

- Magnetic susceptibility

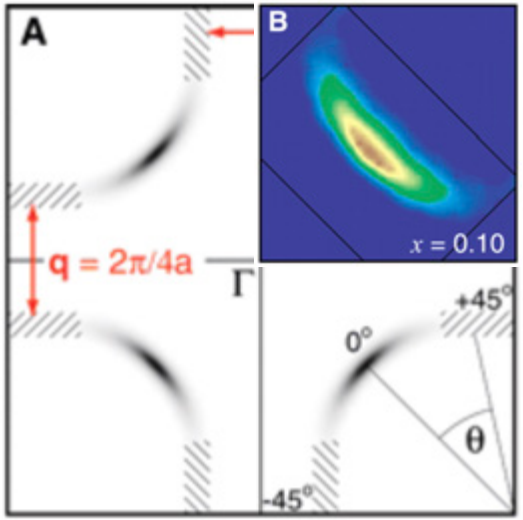
$$\chi_{\mathrm{m}} = \left.\frac{\mathrm{d}M}{\mathrm{d}H}\right|_{H=0}$$

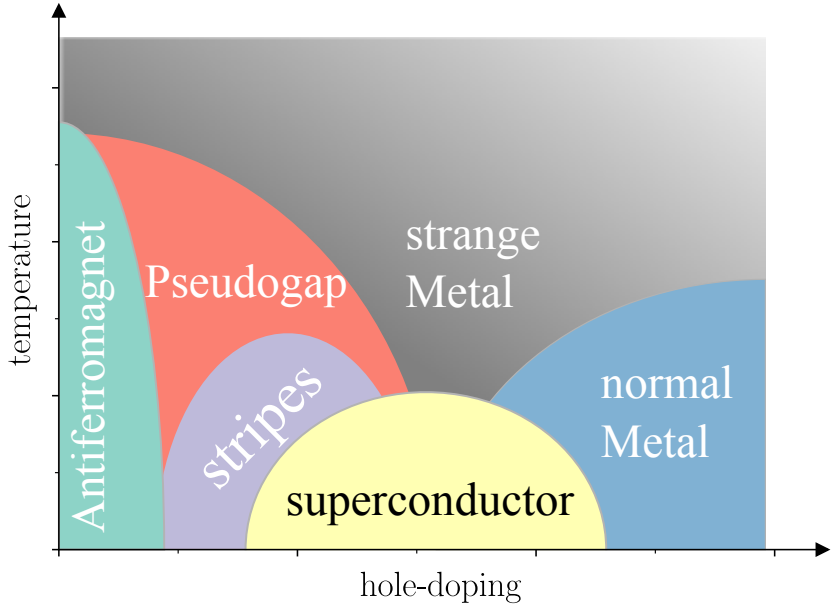


The pseudogap regime

- Region where Fermi surface is partially gapped

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

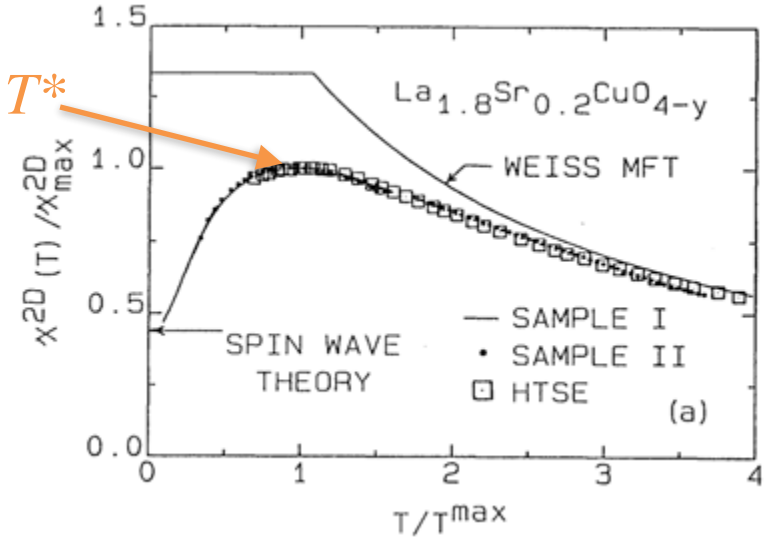


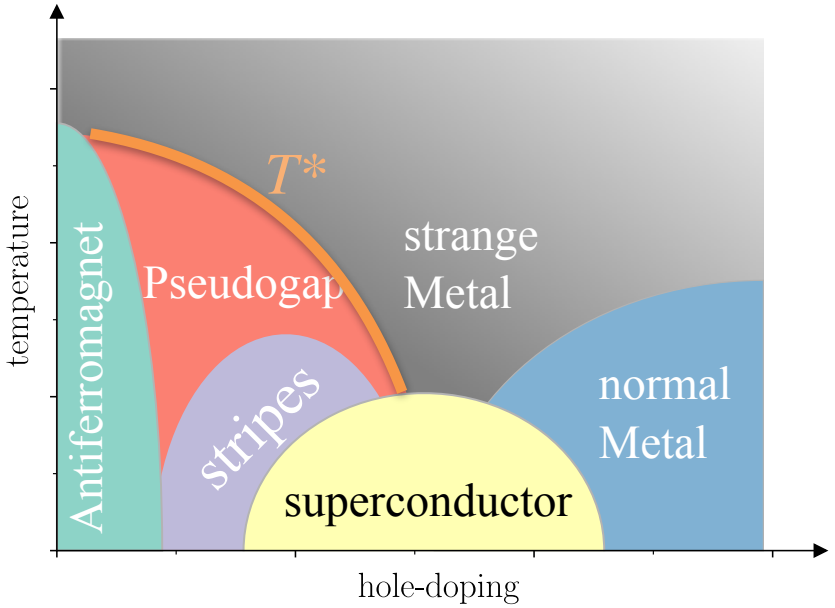


The pseudogap regime

- Onset temperature T^* as a maximum in the magnetic susceptibility

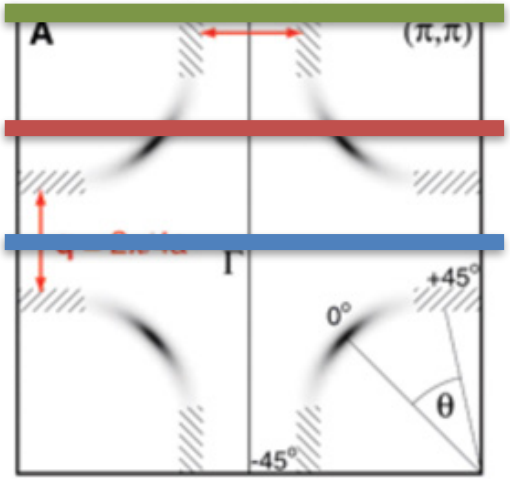
[Johnston, Phys. Rev. Lett., Phys. Rev. Lett. 62, 957 (1989)]



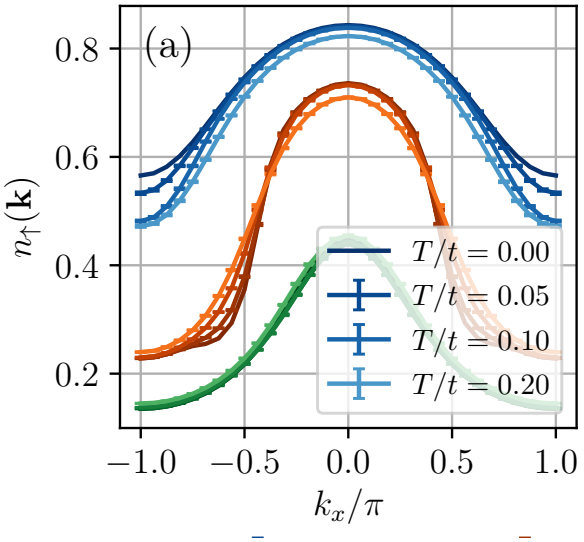


Momentum distribution function

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



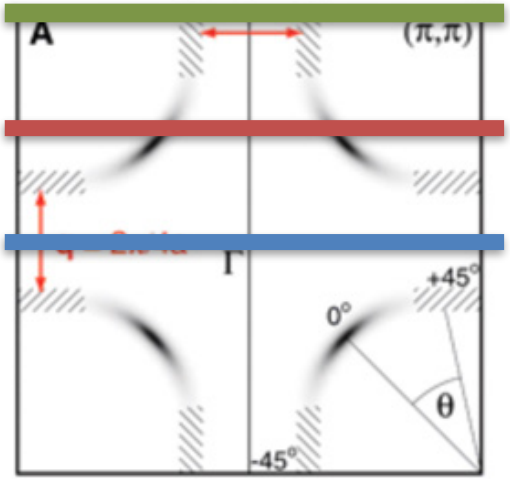
[Shen et al., Science, 307, 5711 (2005)]



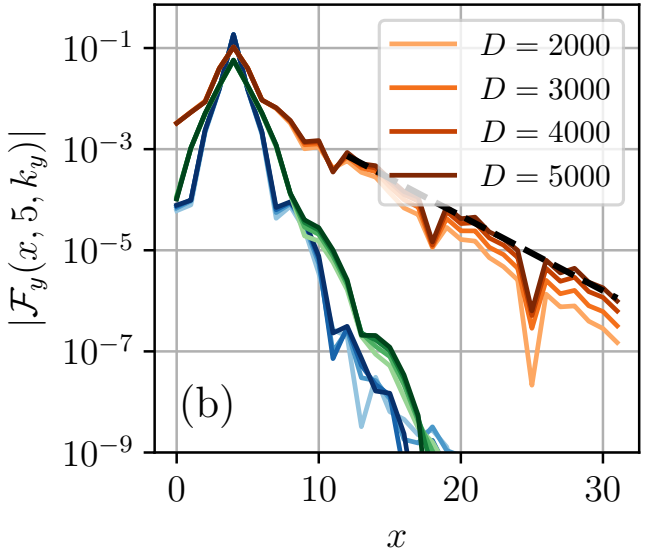
$k_y = 0$ $k_y = \pi/2$ $k_y = \pi$

Electron correlations

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



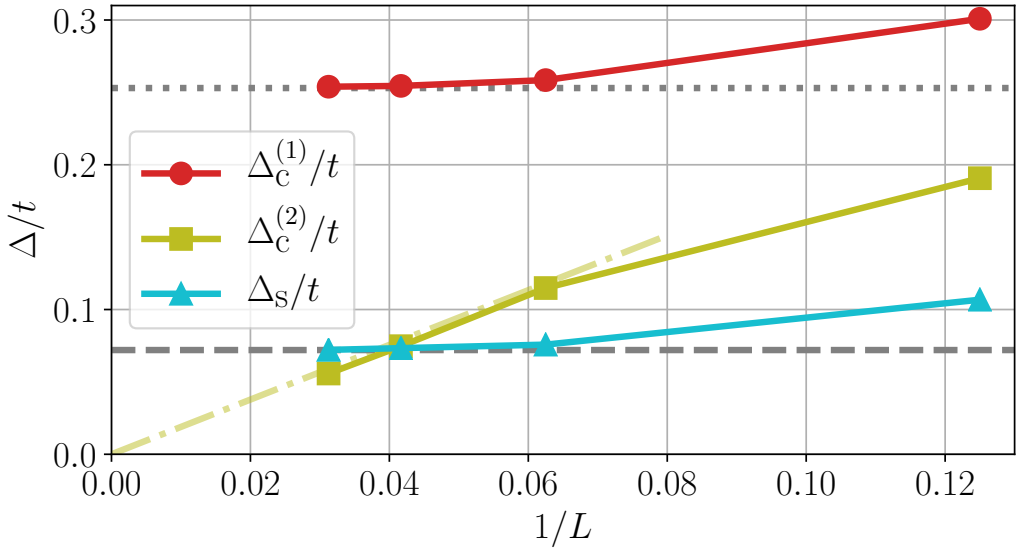
[Shen et al., Science, 307, 5711 (2005)]



$k_y = 0$ $k_y = \pi/2$ $k_y = \pi$

Energy gaps

- Spin gap $\Delta_s = E_0(m+1,m-1) - E_0(m,m)$
- Single particle gap $\Delta_c^{(1)}$
- Charge gap $\Delta_c^{(2)}$
- Computed using ground state DMRG
- Charge gap vanishes, spin and single particle gap remain finite



Computational technique:
Minimally entangled thermal typical states

Phys. Rev. X (2021)(to appear)
arXiv:2009.10736

METTS

- Decomposition of density matrix into typical pure states

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \mathrm{Tr}(\mathrm{e}^{-\beta H}\mathcal{O}) = \frac{1}{\mathcal{Z}} \sum_i p_i \, \langle \psi_i | \, \mathcal{O} \, | \psi_i \rangle \quad \text{with} \quad p_i \geq 0$$

- Minimally-Entangled Typical Thermal State

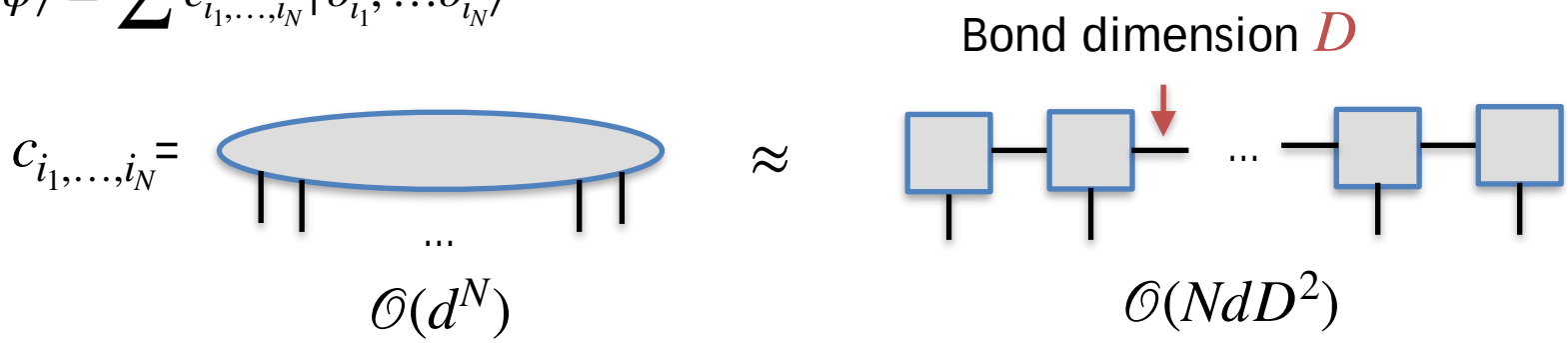
[White, Phys. Rev. Lett. 102, 190601 (2009)]
[Stoudenmire, White, New J. Phys. 12, 055026 (2010)]

$$|\psi_i\rangle = \frac{1}{\sqrt{p_i}} \mathrm{e}^{-\beta H/2} |\sigma_i\rangle \ , \quad |\sigma_i\rangle = |\sigma_i^1\rangle \, |\sigma_i^2\rangle \ldots |\sigma_i^N\rangle \ , \quad p_i = \langle \sigma_i | \, \mathrm{e}^{-\beta H} \, | \sigma_i \rangle \geq 0$$

- Algorithm: random sampling of the states $|\psi_i\rangle$

Tensor network methods

$$|\phi\rangle = \sum c_{i_1,\ldots,i_N} |\sigma_{i_1}, \ldots \sigma_{i_N}\rangle$$



- Density matrix renormalization group (DMRG) for studying ground states

[S. R. White, Phys. Rev. Lett. 69, 2863 (1992)] [S. R. White, Phys. Rev. B 48 (1993)]

- Finite-temperature calculations have been deemed challenging

Imaginary-time evolution

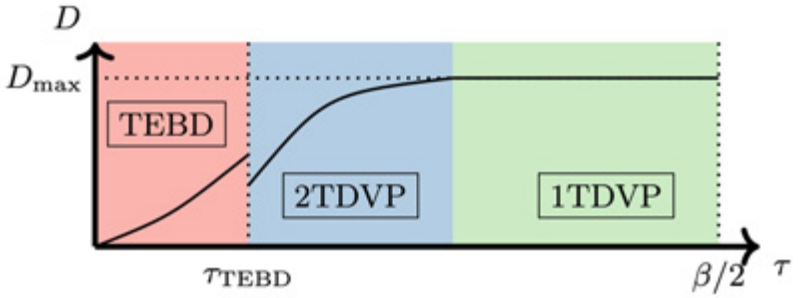
- Computing the imaginary-time evolution accurately is the key challenge

$$|\psi_i\rangle = \frac{1}{\sqrt{p_i}} e^{-\beta H/2} |\sigma_i\rangle$$

- Key algorithmic breakthrough: time dependent variational principle (TDVP)

[Haegemann et al., Phys. Rev. Lett. 107, 070601 (2011)]
[Haegemann et al., Phys. Rev. B 94, 165116 (2016)]
[Yang, White, Phys. Rev. B 102, 094315 (2020)]
[Paeckel et al., Ann. Phys. 411, 167998 (2019)]

- Imaginary-time evolution using TEBD + TDVP, together with accurate Lanczos-based exponential integrators.

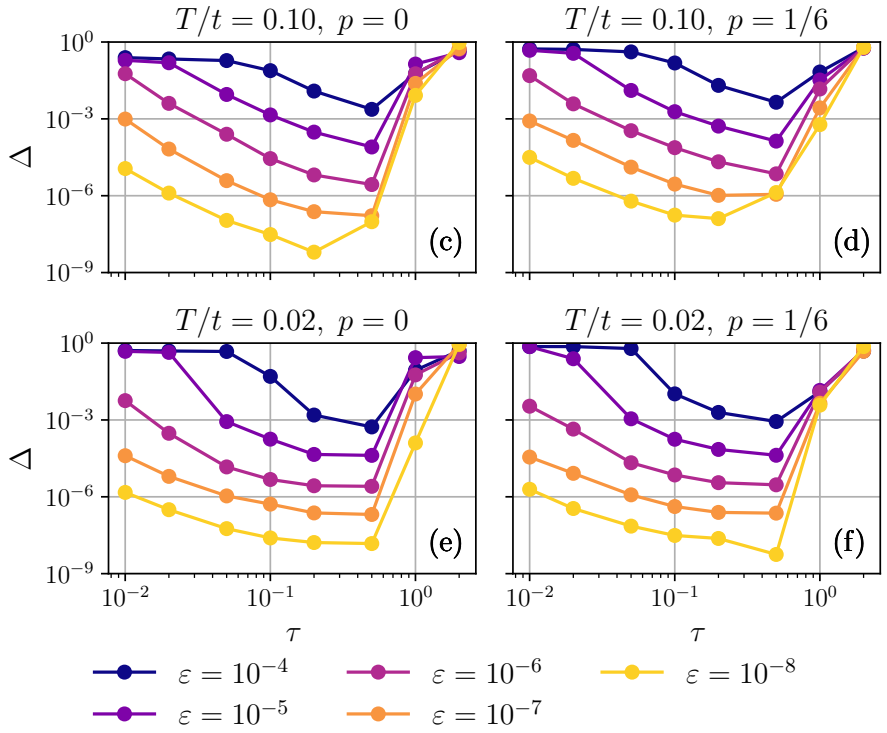


Imaginary-time evolution

- $|\psi_i\rangle \propto \mathrm{e}^{-\beta H/2}\,|\sigma_i\rangle$
- Time step size τ
- Cutoff ε in singular value decomposition (controls bond dimension)
- Comparison to Exact Diagonalization

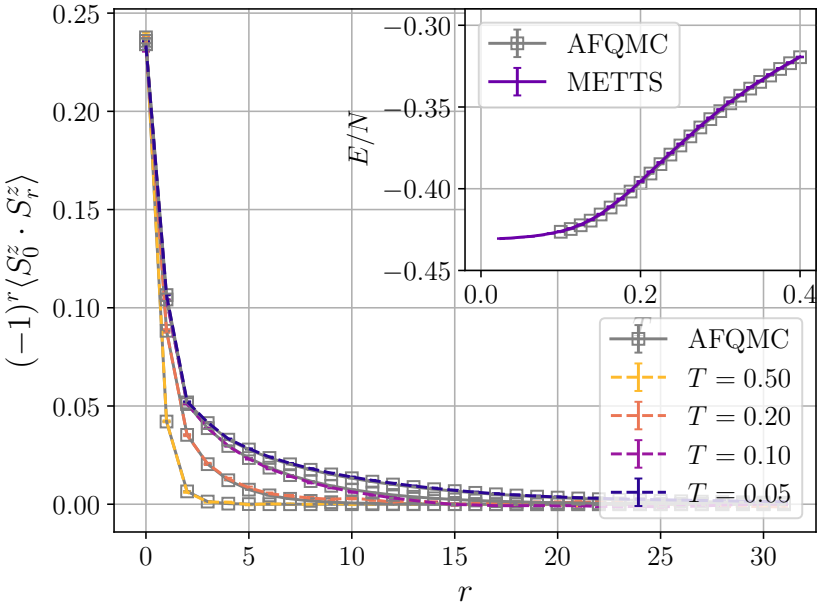
$$\Delta = 1 - \left|\langle\psi_{\mathrm{ED}}|\psi_{\mathrm{MPS}}\rangle\right|^2$$

$$|\sigma_{p=0}\rangle = \left|\uparrow\downarrow\;\downarrow\uparrow\;\uparrow\downarrow\;\downarrow\uparrow\right\rangle \quad \text{and} \quad |\sigma_{p=1/6}\rangle = \left|\uparrow\downarrow\;\downarrow\emptyset\;\uparrow\downarrow\;\uparrow\uparrow\right\rangle$$

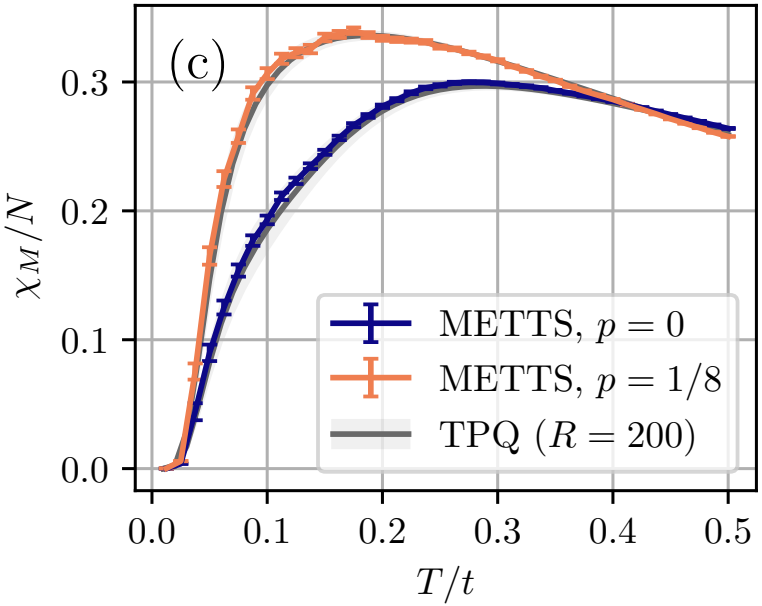


Validation with other methods

AFQMC, half-filling, $U/t = 10$

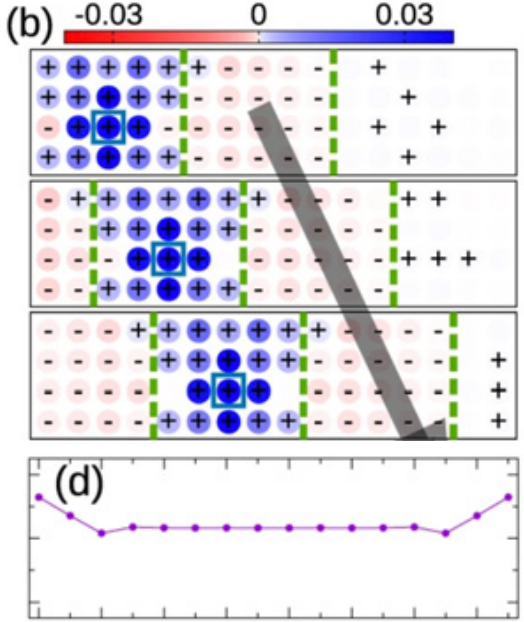


ED / TPQ, $U/t = 10$

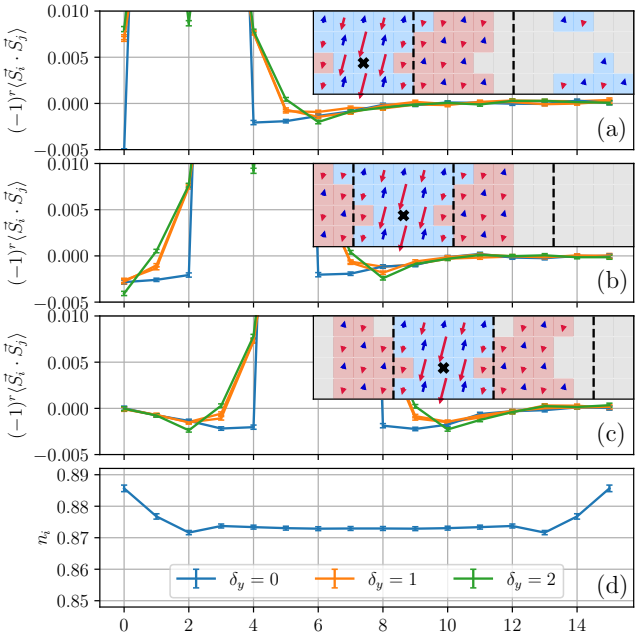


Validation with other methods

DQMC, $T/t = 0.22$, $p = 1/8$, $t'/t = -0.25$, $U/t = 6$

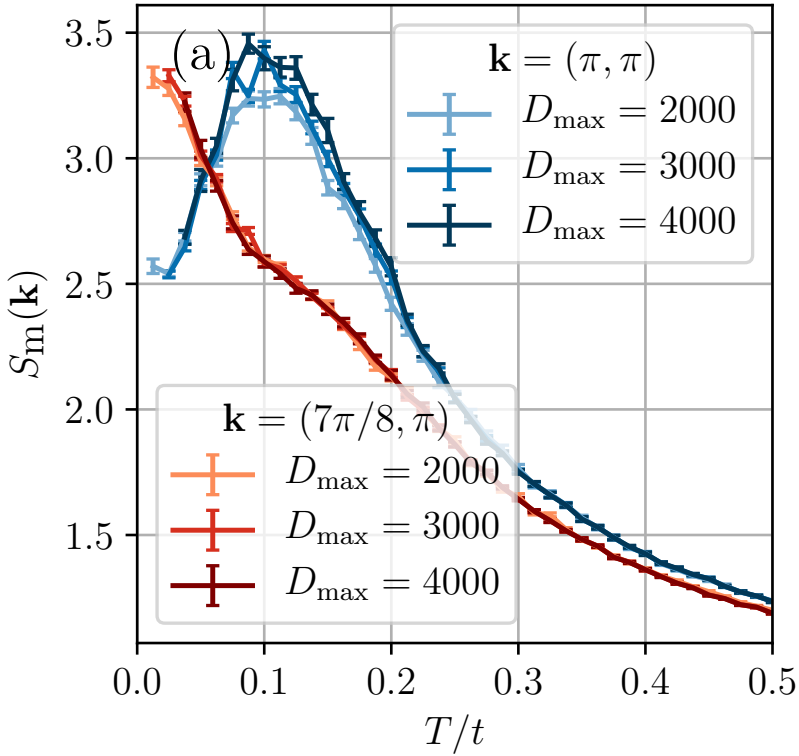


[Huang et al., npj Quant Mater 3, 22 (2018)]



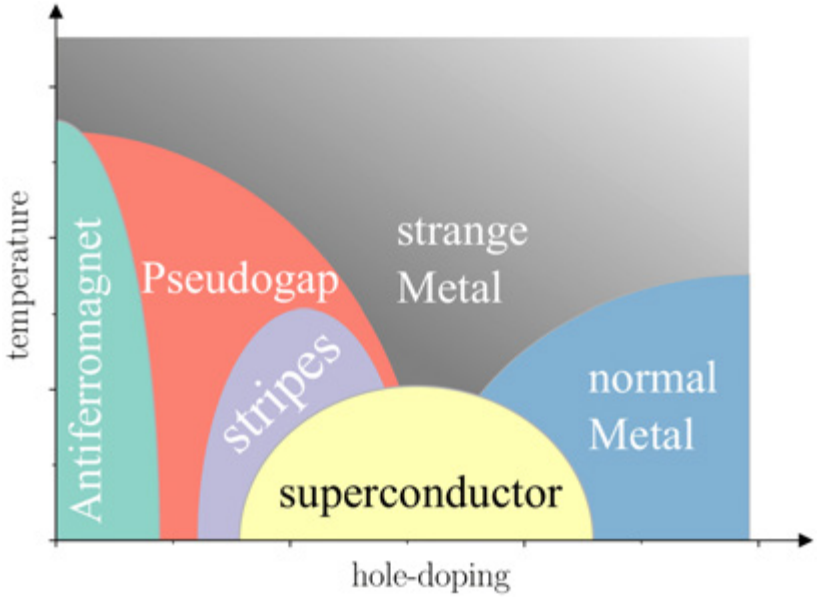
Summary

- First application of the METTS algorithm to simulate the 2D (1.5D) Hubbard model
- Access to a broad temperature regime
- Determine onset temperature of stripes
- Antiferromagnetism in the pseudogap regime
- Single-particle gap smallest at nodal point
- Vanishing charge gap



Outlook

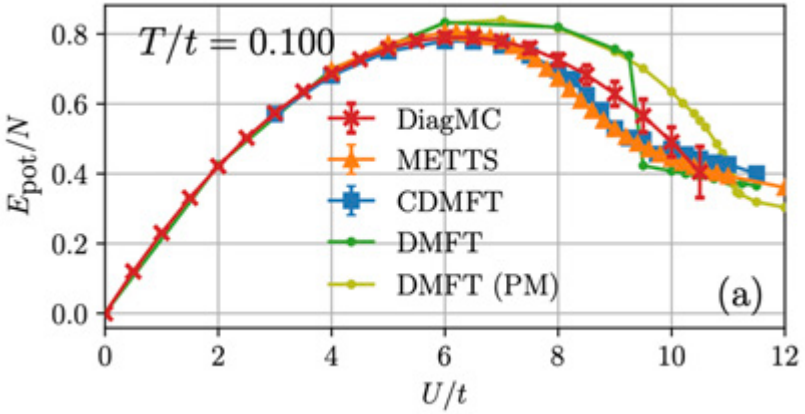
Exploring the cuprate phase diagram



"Handshake" with other methods

Mott insulating states with competing orders in the triangular lattice Hubbard model

A. Wietek, R. Rossi, F. Simkovic, M. Klett, P. Hansmann, M. Ferrero, E. M. Stoudenmire, T. Schäfer, A. Georges
arXiv:2102.12904



Collaborators:

arXiv:2009.10736

Steven R. White

Edwin M. Stoudenmire

Yuan-Yao He

Antoine Georges

Thank you for your attention!

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Center for Computational Quantum Physics

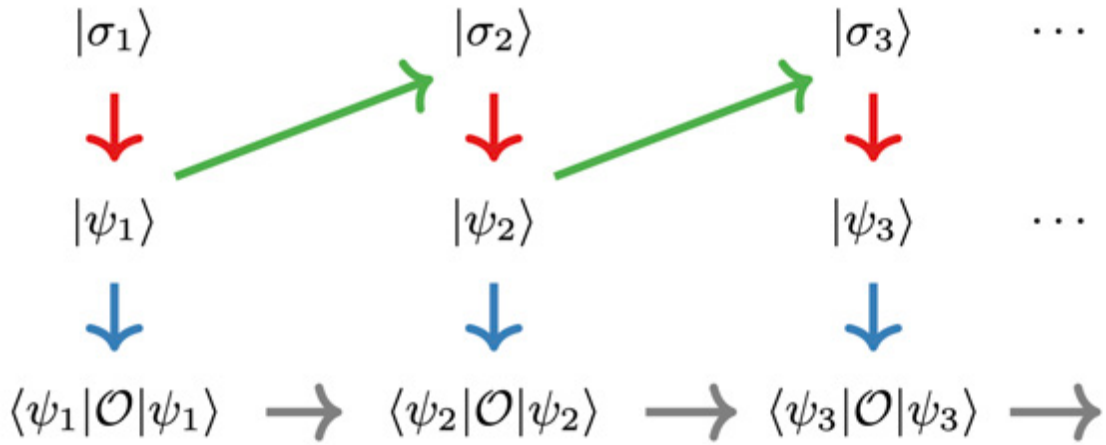
The METTS algorithm

- Step 1: compute

$$|\psi_i\rangle = \frac{1}{\sqrt{p_i}} \mathrm{e}^{-\beta H/2} |\sigma_i\rangle$$

- Step 2: measure

$$\langle \psi_i | \mathcal{O} | \psi_i \rangle$$

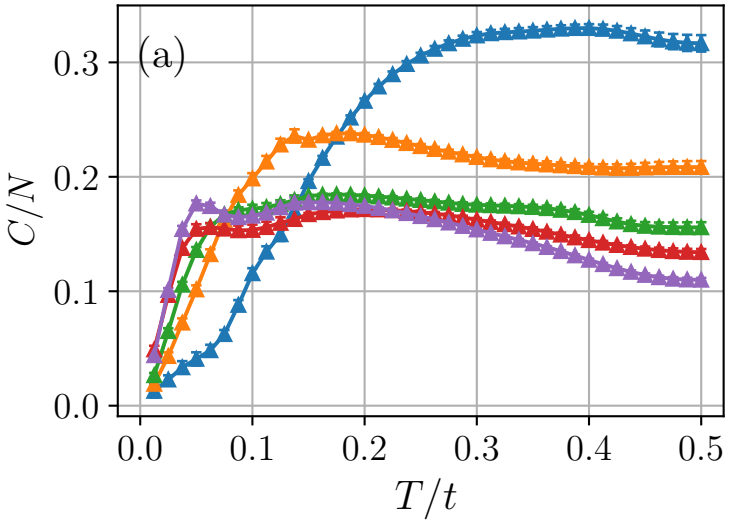


- Step 3: choose new product state $|\sigma_{i+1}\rangle$ according to probability $|\langle\psi_i|\sigma_{i+1}\rangle|^2$

Thermodynamics

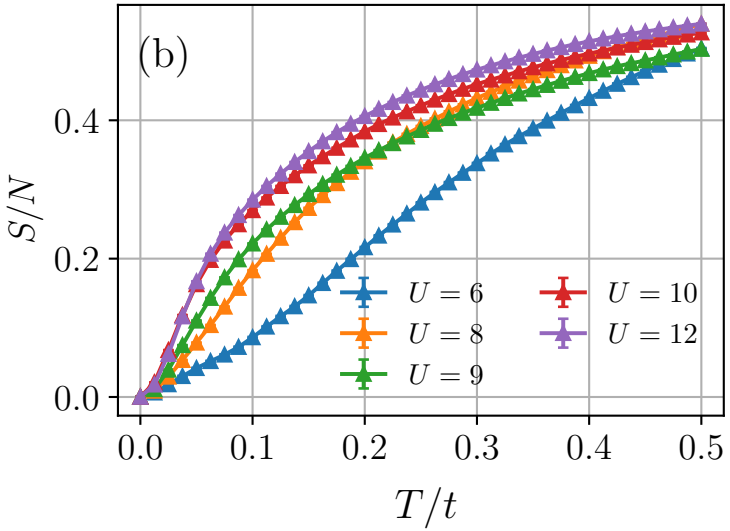
Specific heat:

$$C = \frac{\partial E}{\partial T}$$



Entropy:

$$S = \log(\mathcal{Z}) + \frac{E}{T}$$



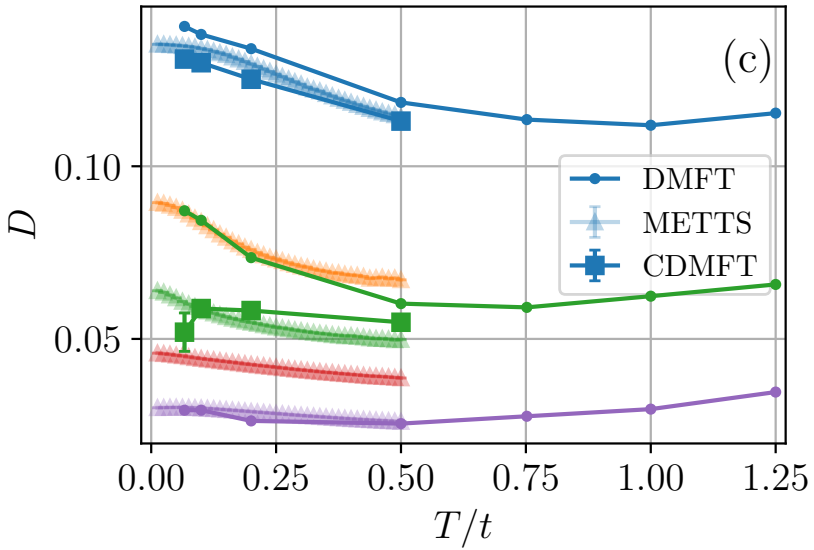
Thermodynamics

Maxwell relation:

$$\left.\frac{\partial S}{\partial U}\right|_T = -\left.\frac{\partial D}{\partial T}\right|_U$$

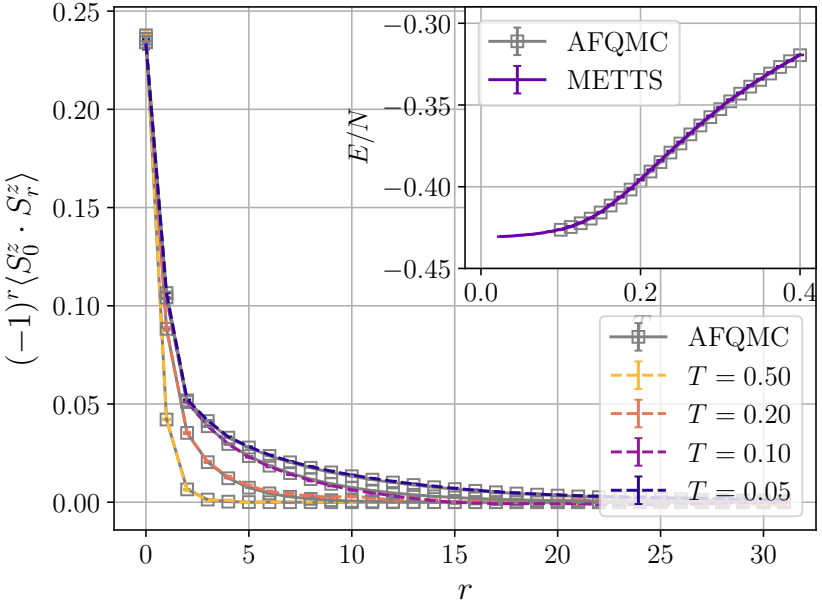
Double occupancy:

$$D = \frac{1}{N}\sum_{i=1}^{N}\langle n_{i\uparrow} n_{i\downarrow}\rangle$$

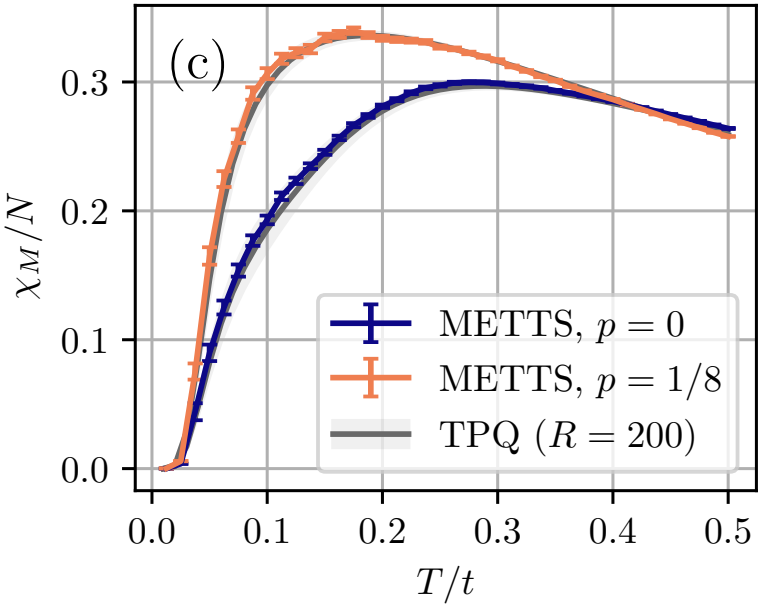


Validation with other methods

AFQMC, half-filling, $U/t = 10$

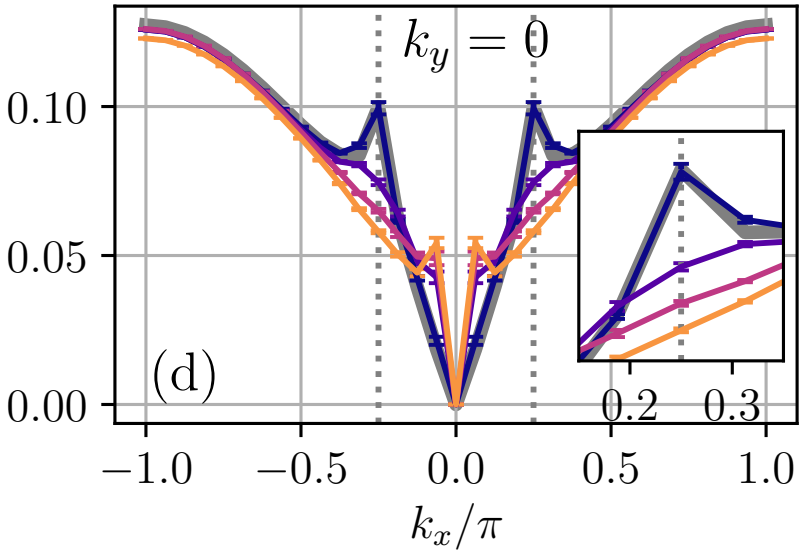


ED / TPQ, $U/t = 10$

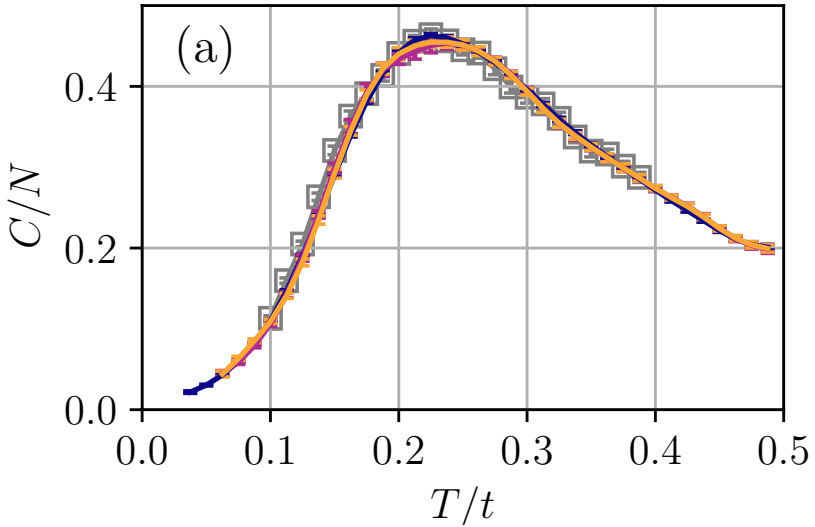


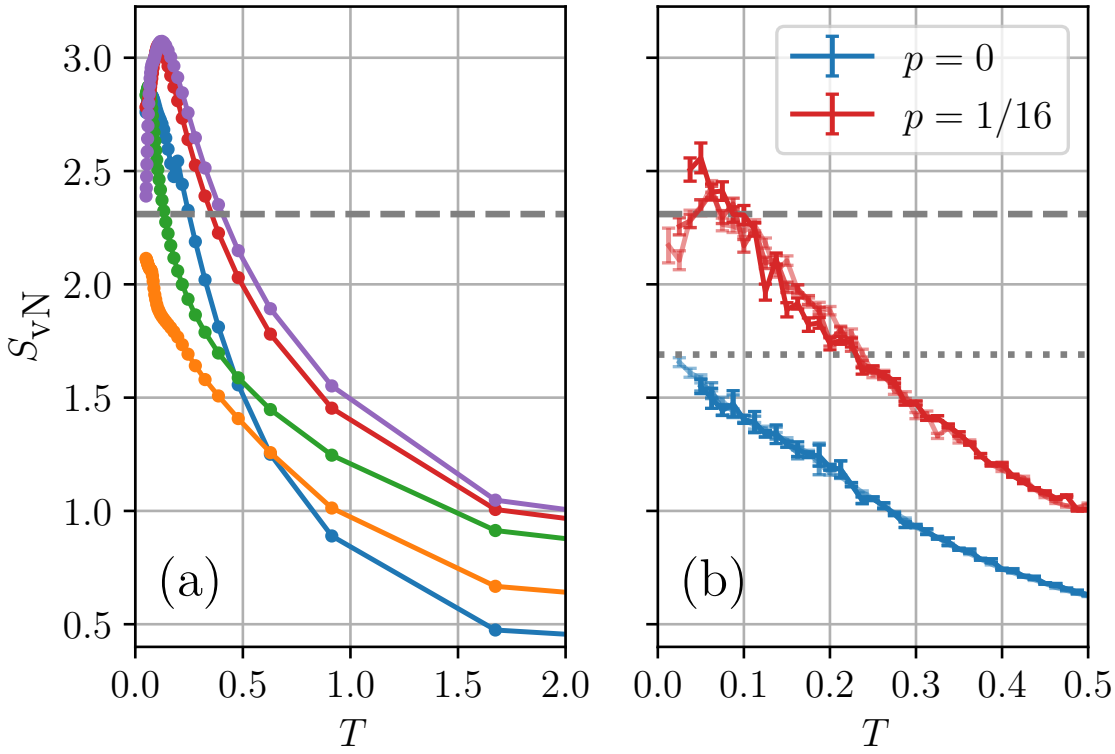
Validation with other methods

DMRG at $T = 0$, $p = 1/16$



AFQMC at half-filling




3.0
2.5
2.0
1.5
1.0
0.5
S_{vN}
(a)
0.0
0.5
1.0
1.5
2.0
T
$p = 0$
$p = 1/16$
(b)
0.0
0.1
0.2
0.3
0.4
0.5
T

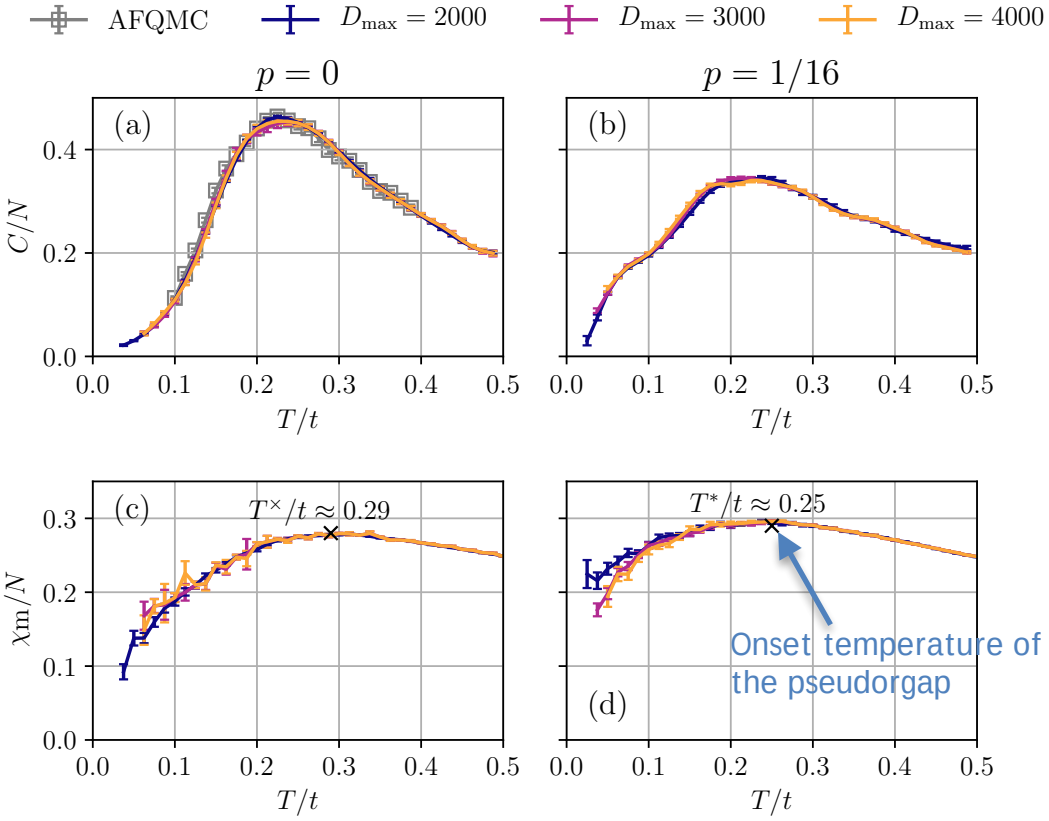
Thermodynamics

- Specific Heat

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

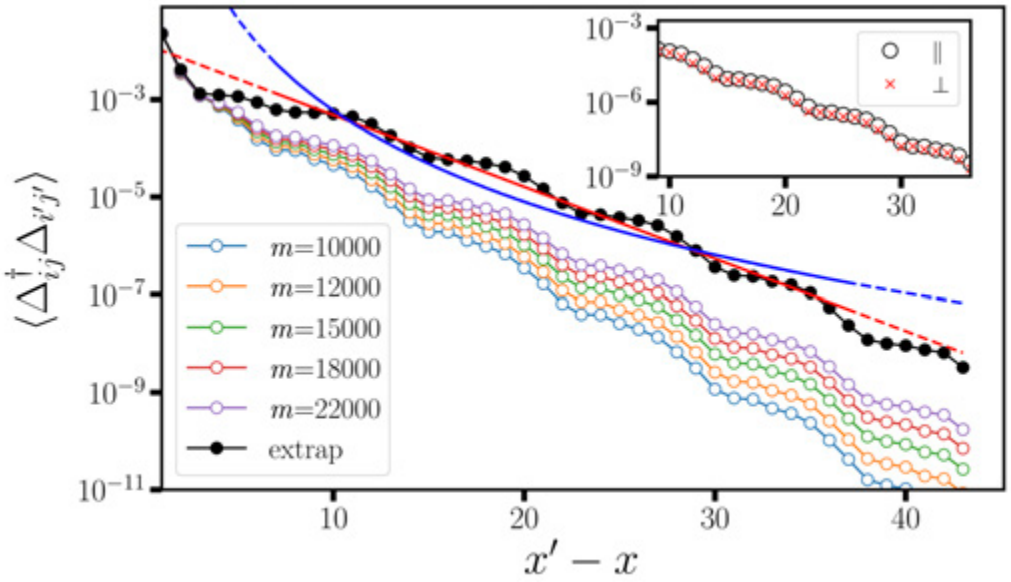
- Magnetic susceptibility

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



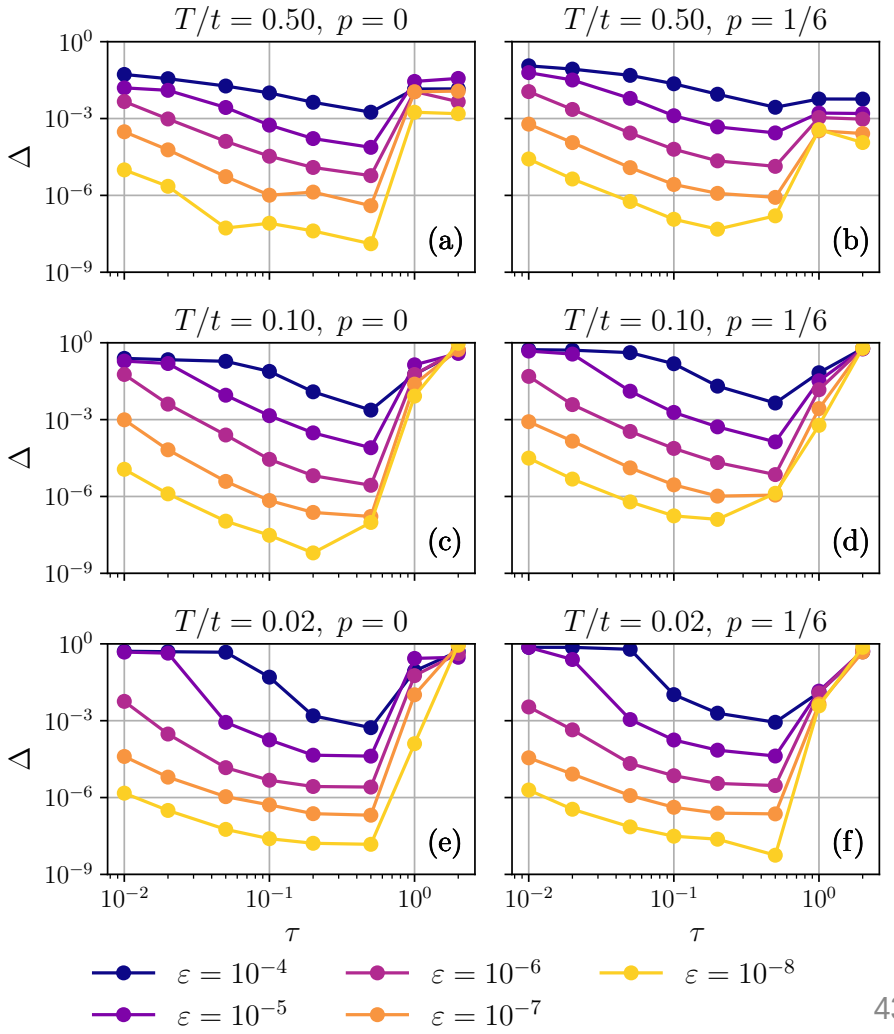
Superconductivity?

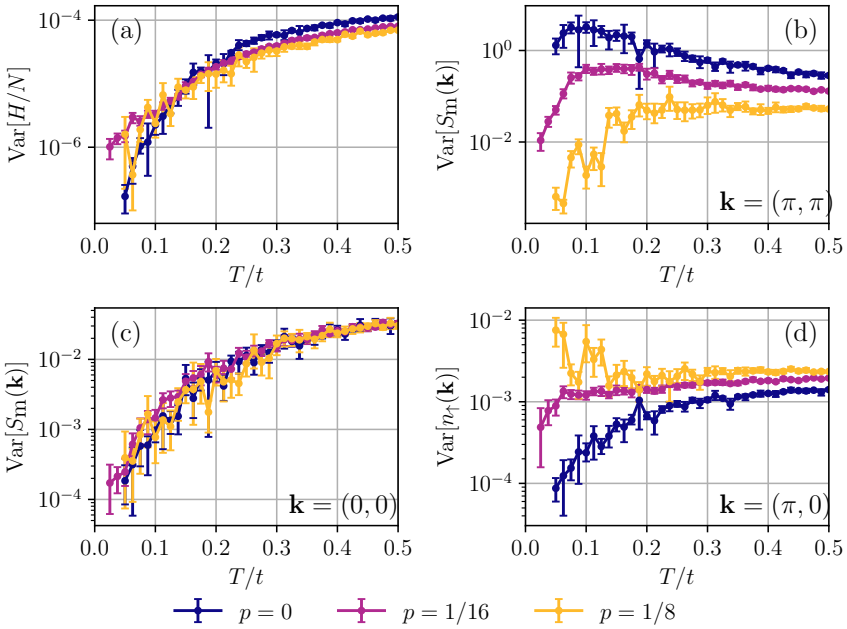
- No superconductivity at $T = 0$, $p = 1/8$, $U/t = 8$ from DMRG and AFQMC

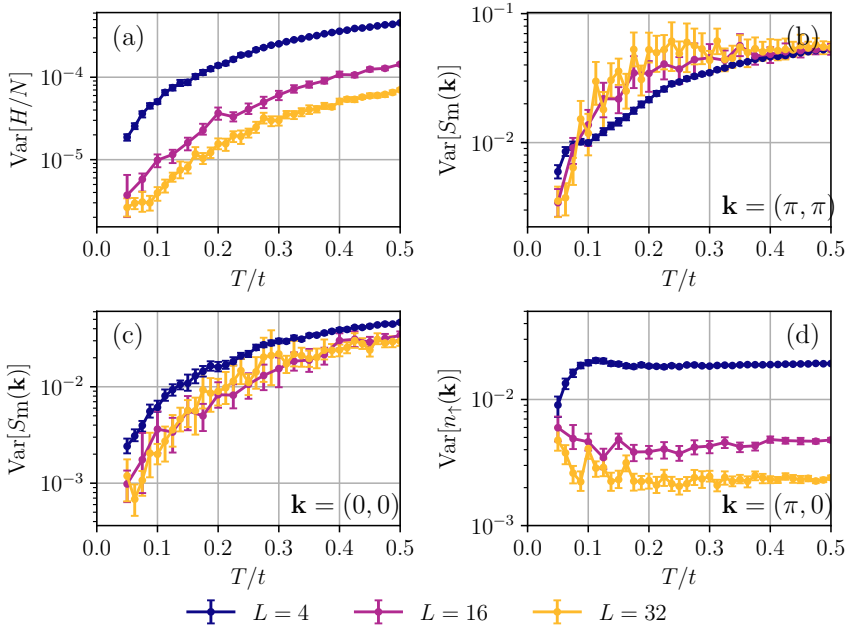


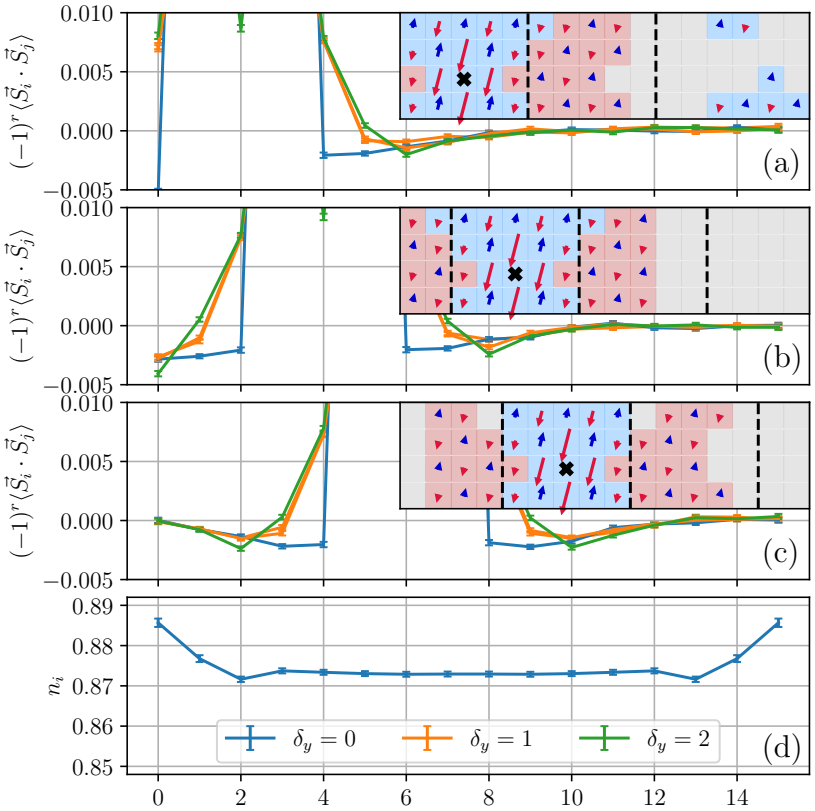
[Qin et al., Phys. Rev. X 10, 031016 (2020)]

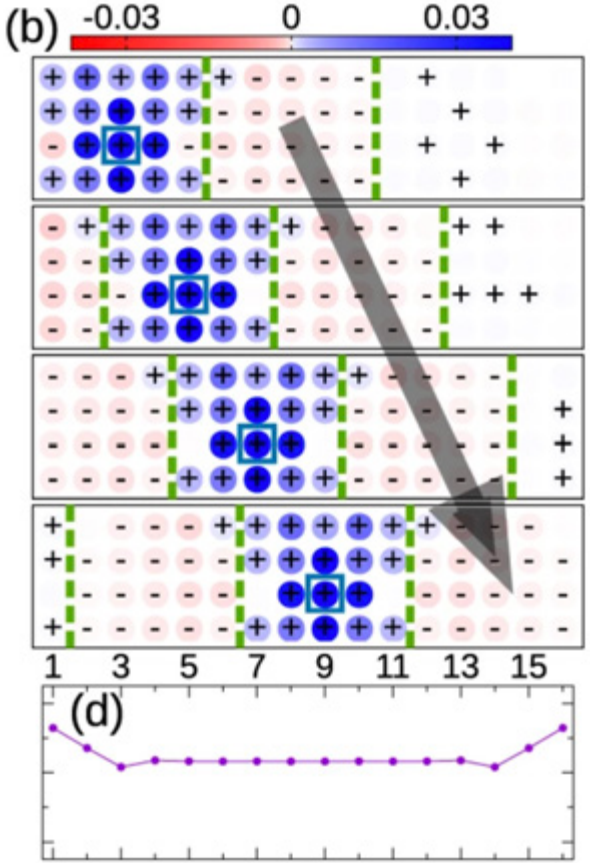
$$\Delta \equiv 1 - |\langle \psi^{\mathrm{MPS}} | \psi^{\mathrm{ED}} \rangle|^2,$$




(a)
(b)
(c)
(d)
$\mathrm{Var}[H/N]$
$\mathrm{Var}[S_{\mathrm{m}}(\mathbf{k})]$
$\mathrm{Var}[n_\uparrow(\mathbf{k})]$
T/t
$\mathbf{k} = (\pi, \pi)$
$\mathbf{k} = (0, 0)$
$\mathbf{k} = (\pi, 0)$
$p = 0$
$p = 1/16$
$p = 1/8$


(a)
(b)
(c)
(d)
$\mathrm{Var}[H/N]$
$\mathrm{Var}[S_{\mathrm{m}}(\mathbf{k})]$
$\mathrm{Var}[n_\uparrow(\mathbf{k})]$
T/t
$\mathbf{k} = (\pi, \pi)$
$\mathbf{k} = (0, 0)$
$\mathbf{k} = (\pi, 0)$
$L = 4$
$L = 16$
$L = 32$

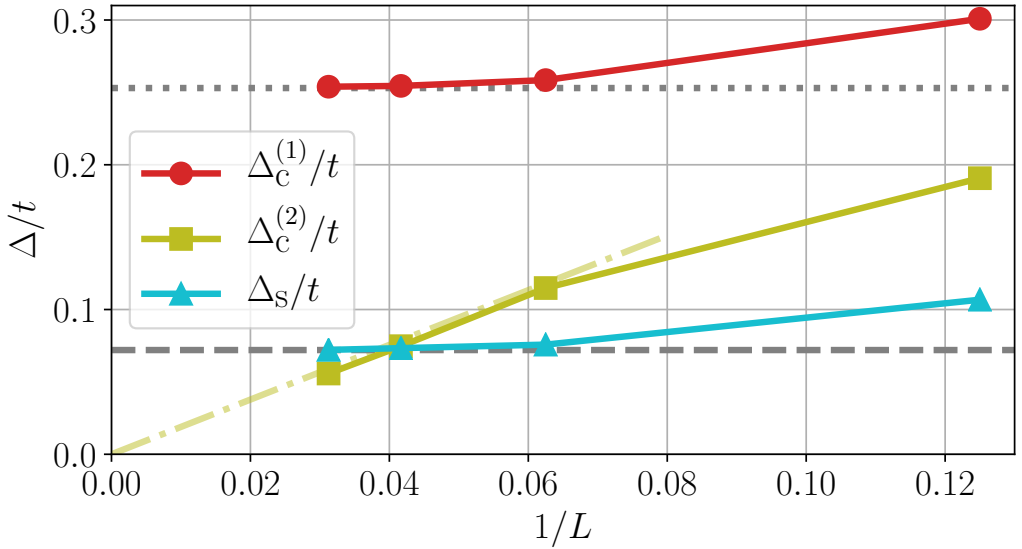


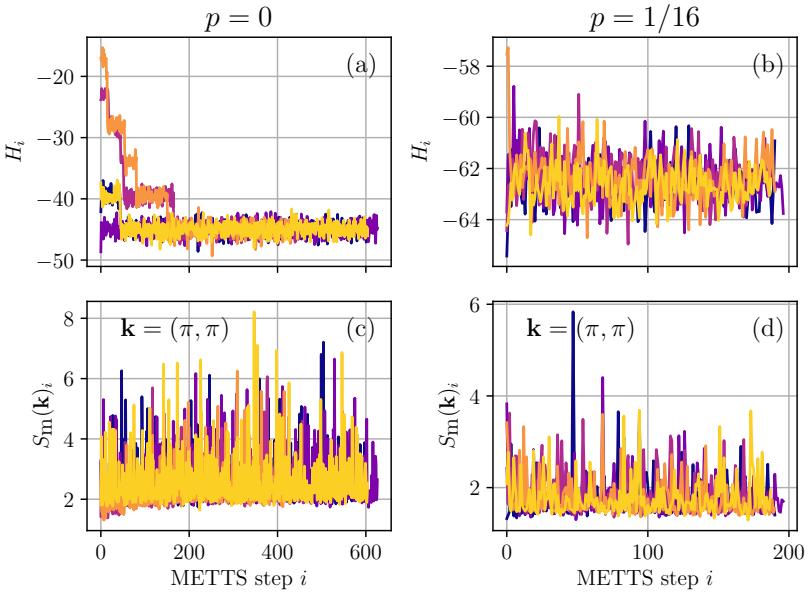


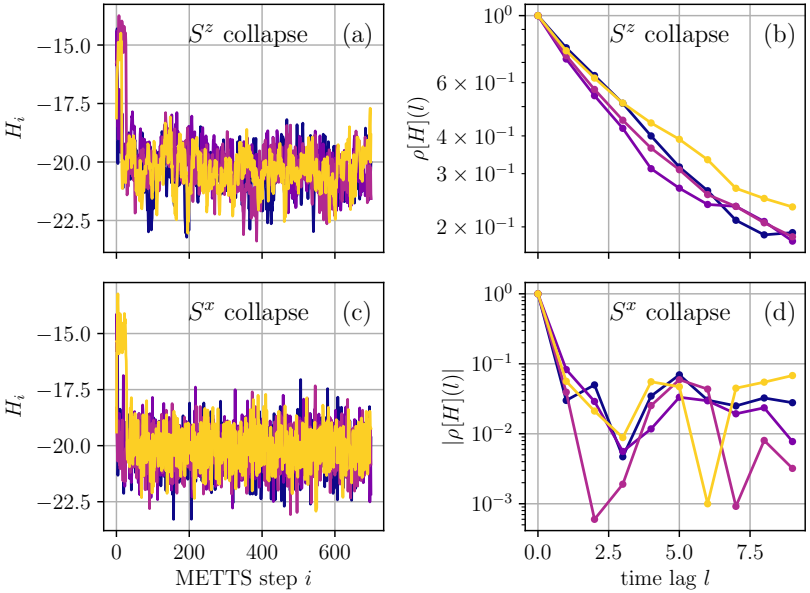
[Huang et al., npj Quant Mater 3, 22 (2018)]

Energy gaps

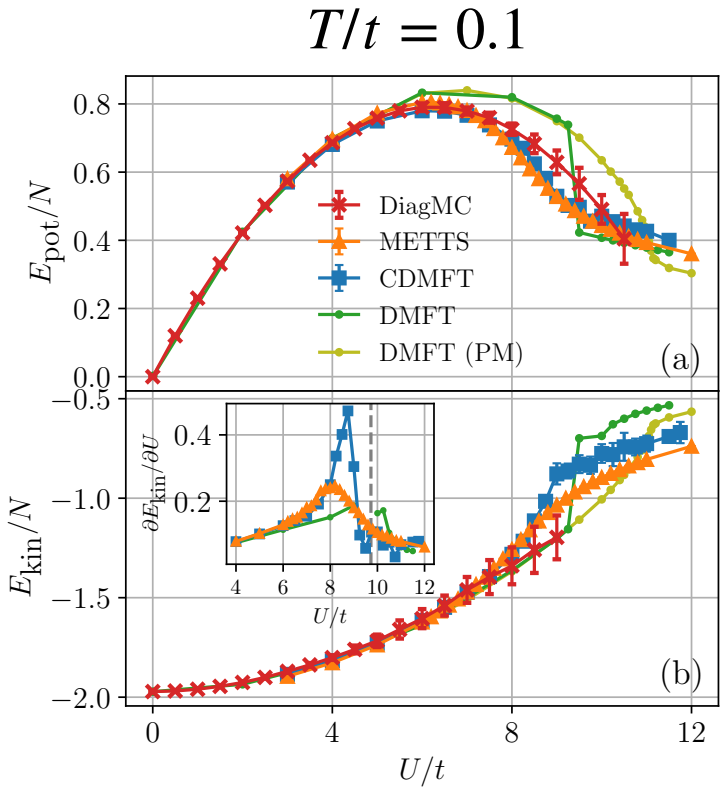
- Spin gap $\Delta_s = E_0(m+1,m-1) - E_0(m,m)$
- Single particle gap $\Delta_c^{(1)}$
- Charge gap $\Delta_c^{(2)}$
- Computed using ground state DMRG
- Charge gap vanishes, spin and single particle gap remain finite




$p = 0$
$p = 1/16$
(a)
(b)
(c)
(d)
H_i
$S_{\mathrm{m}}(\mathbf{k})_i$
$\mathbf{k} = (\pi, \pi)$
METTS step i


S^z collapse
S^x collapse
(a)
(b)
(c)
(d)
H_i
$\rho[H](l)$
$|\rho[H](l)|$
METTS step i
time lag l

“Handshake” among numerical methods



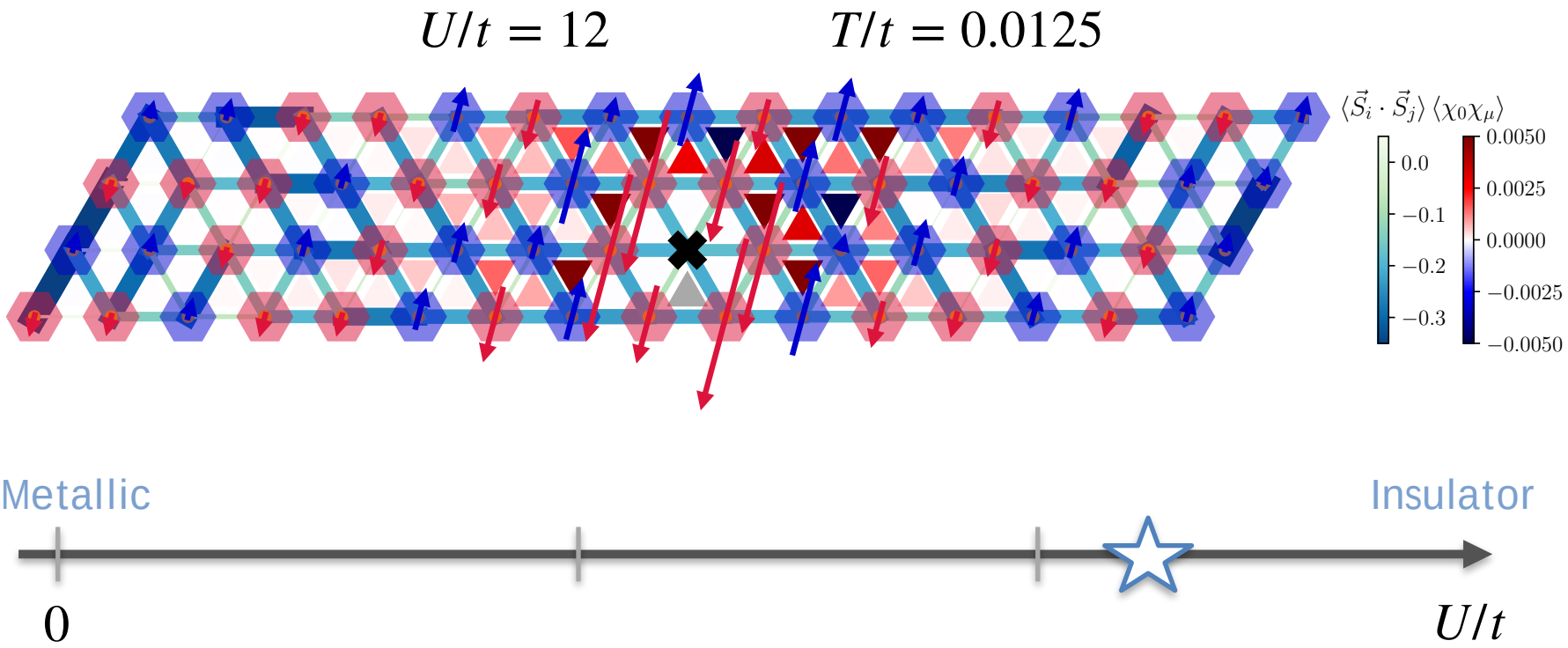
Potenial energy:

$$E_{\mathrm{pot}} = U \sum_i \langle \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \rangle$$

Kinetic energy:

$$E_{\mathrm{kin}} = -t \sum_{\langle i,j \rangle, \sigma} \langle \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma} \rangle \, .$$

The triangular lattice Hubbard model



Condensed Matter > Strongly Correlated Electrons

[Submitted on 22 Sep 2020]

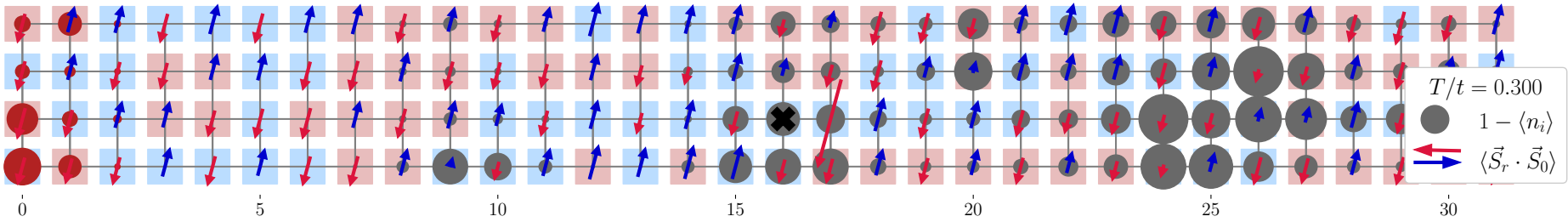
Stripes, Antiferromagnetism, and the Pseudogap in the Doped Hubbard Model at Finite Temperature

Alexander Wietek, Yuan-Yao He, Steven R. White, Antoine Georges, E. Miles Stoudenmire

$T/t = 0.300$

$U/t = 10$ and $p = 1/16$

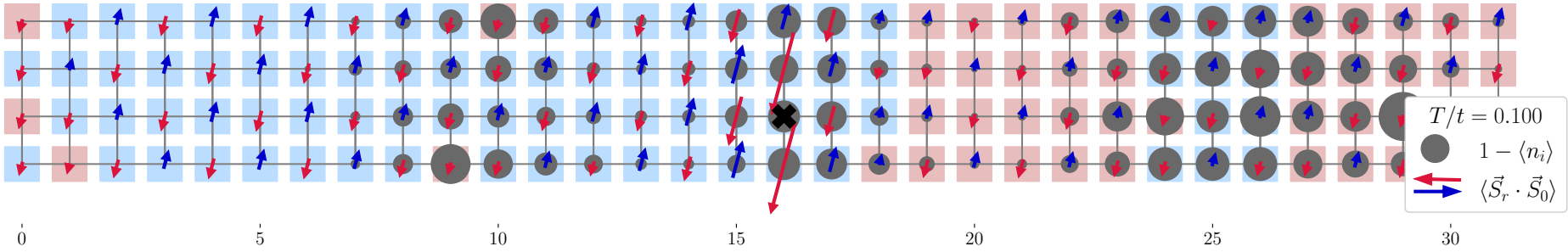
$|\psi_i\rangle =$



$T/t = 0.100$

$U/t = 10$ and $p = 1/16$

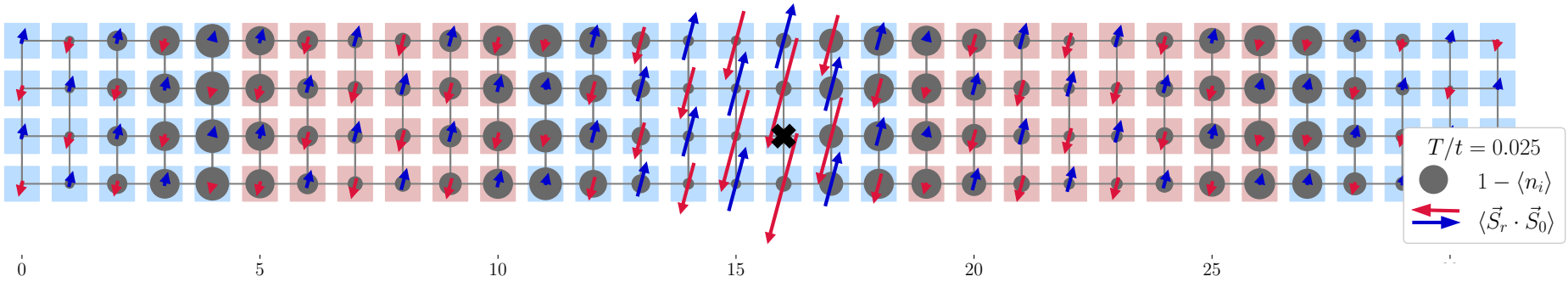
$|\psi_i\rangle =$



$T/t = 0.025$

$U/t = 10$ and $p = 1/16$

$|\psi_i\rangle =$

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