Dynamical Formation of a Magnetic Impurity

Michael Knap

Technical University of Munich

Collaborators:


A. Bohrdt


F. Grusdt


W. Kadow


F. Pollmann

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IAS TUM Institute for Advanced Study

MCQST

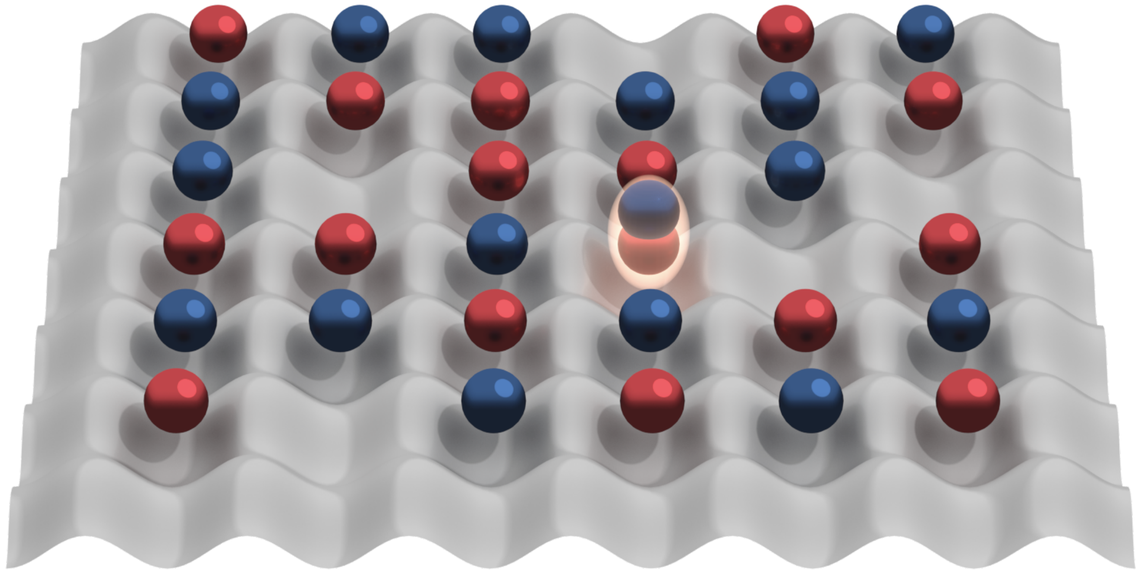
DFG

Fermi-Hubbard model

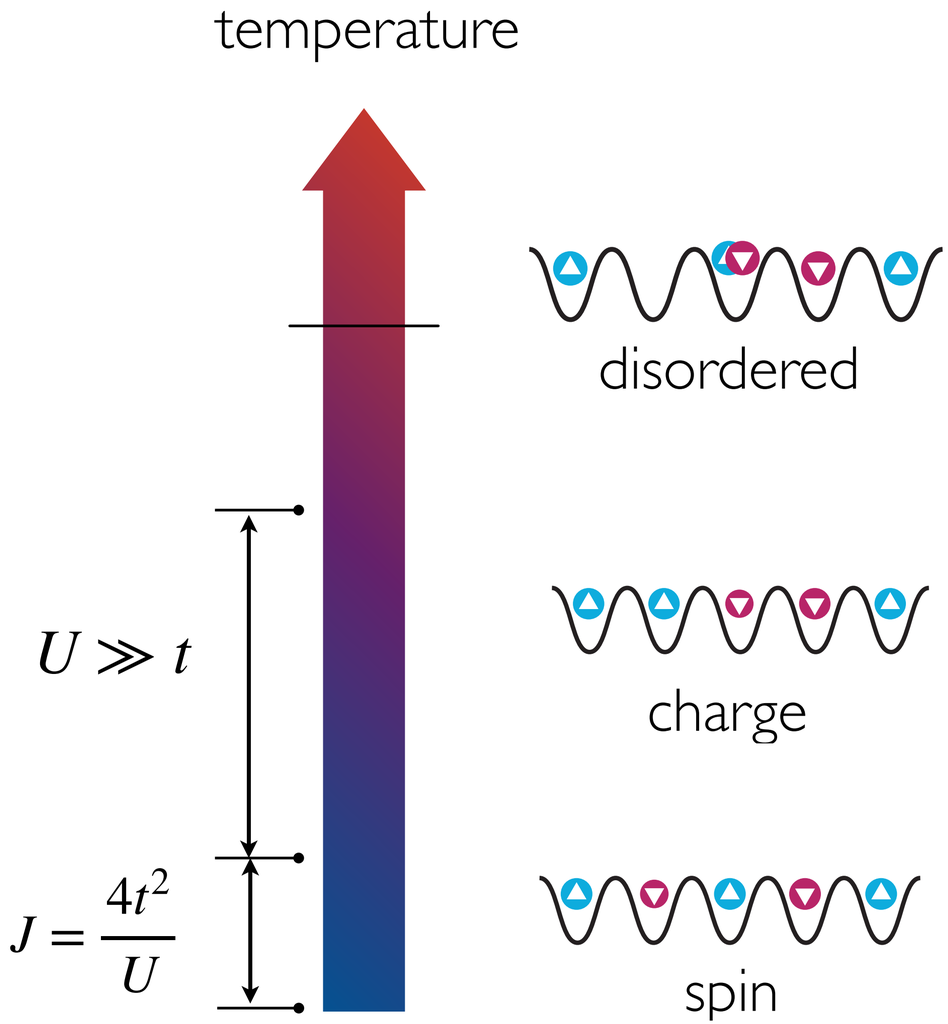
$$\hat{H} = -t \sum_{\langle i,j \rangle, \sigma} \left(c^{\dagger}_{i,\sigma} c_{i,\sigma} + h.c. \right) + U \sum_{i} \left(\hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} \right)$$

hopping

interactions



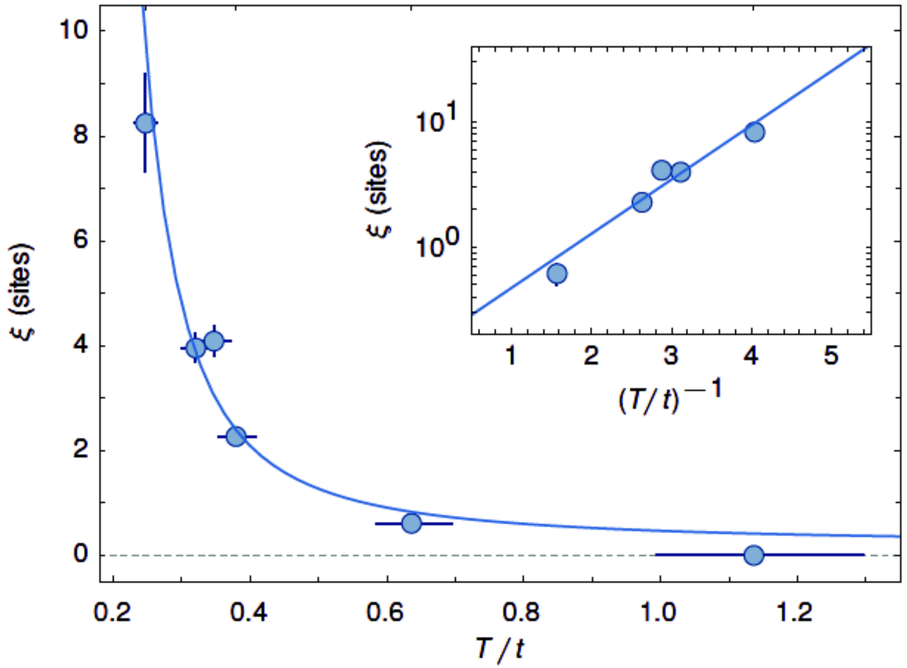
[Chiu et al., Science, 2019]

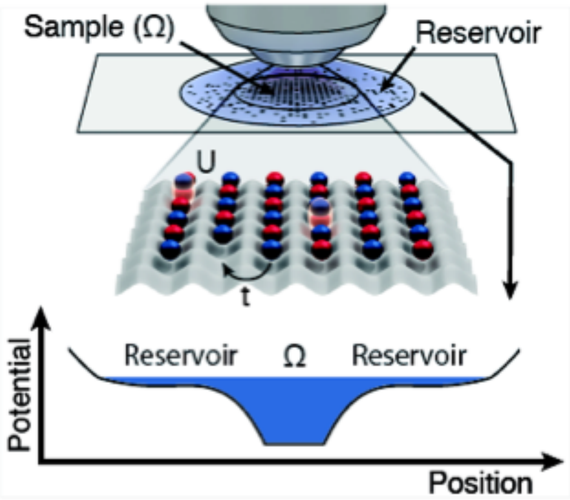


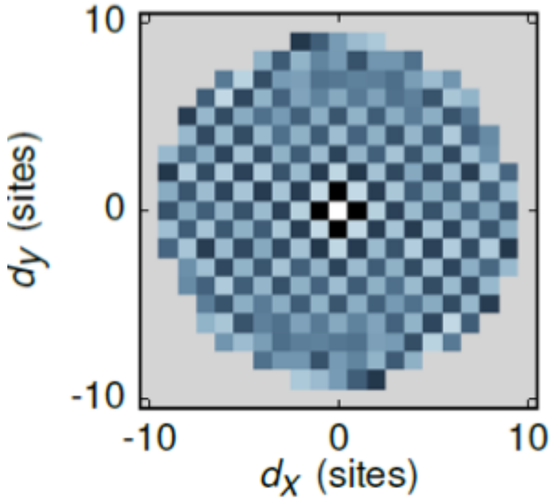
Anti-ferromagnetic correlations

Correlation length diverges with decreasing temperature

$$\xi(T) \sim e^{2\pi\rho_s/T}$$







[Mazurenko et al., Nature, 2017]

Strong Interactions

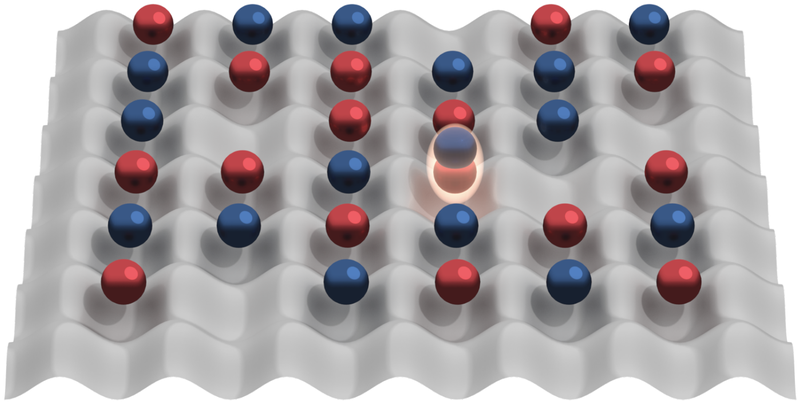
Strong interactions ($t \gg J = 4t^2/U$) ⟶ **tJ-Model**

Local configurations


spin down


spin up


hole



[Chiu et al., Science, 2019]

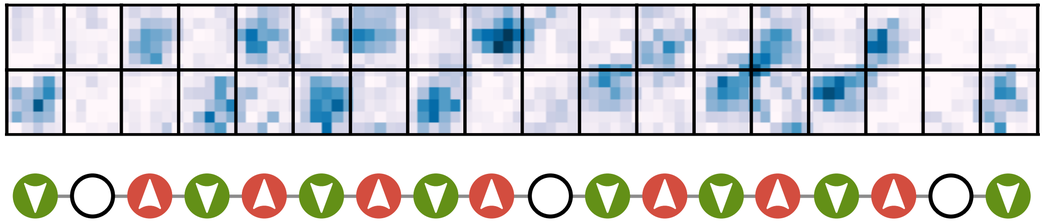
no double occupancies

$$\hat{\mathcal{H}}_{t-J} = -t\,\hat{\mathcal{P}}\Big[\sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} \hat{c}^{\dagger}_{\mathbf{i},\sigma}\hat{c}_{\mathbf{j},\sigma} + \text{h.c.}\Big]\hat{\mathcal{P}} + J\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\Big(\hat{\mathbf{S}}_{\mathbf{i}}\cdot\hat{\mathbf{S}}_{\mathbf{j}} - \frac{1}{4}\hat{n}_{\mathbf{i}}\hat{n}_{\mathbf{j}}\Big)$$

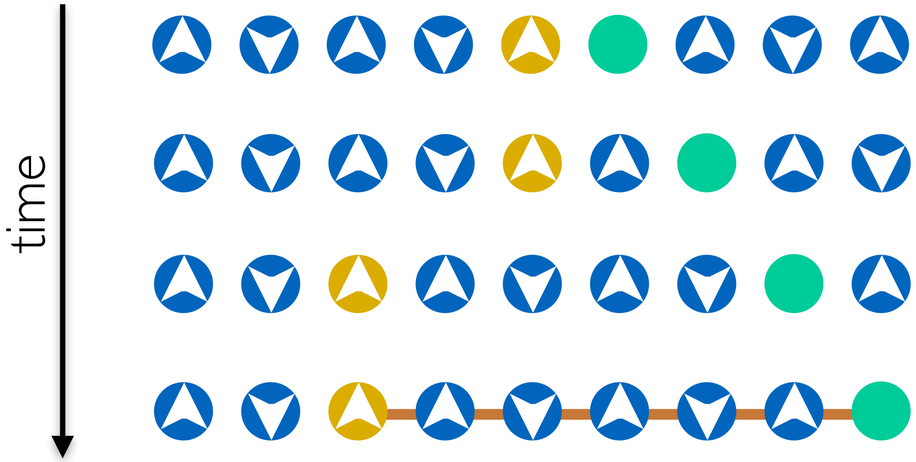
Hole doping in 1D - a parton picture

Spinon: fractional spin excitation $S = 1/2$

Chargon: keeps relative spin orientation



[Hilker et al., Science, 2017]



spinon

chargon

Spin-charge separation: deconfined spinons and chargons ($t \gg J = 4t^2/U$)

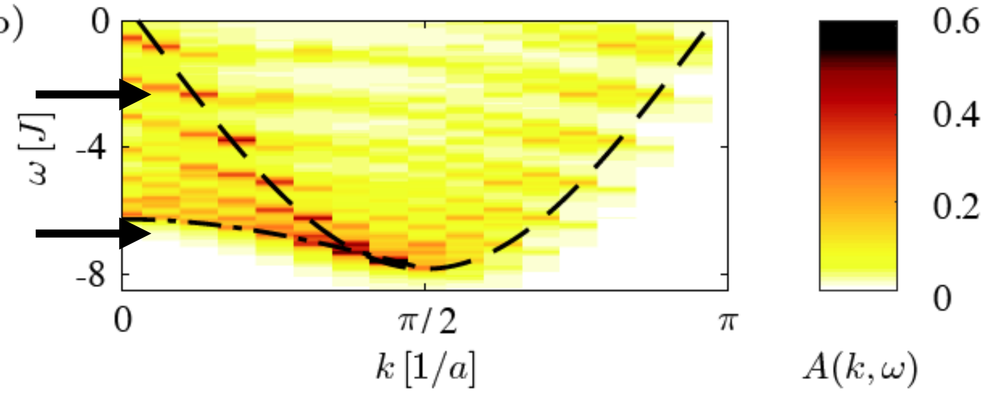
Manifestation of spin-charge separation

Single-hole spectral function (ARPES)

$$A(k,\omega) = A_{\text{spinon}} * A_{\text{holon}} = \int d\omega_{\text{h}} dk_{\text{h}}\ A_{\text{holon}}(k_{\text{h}},\omega_{\text{h}}) A_{\text{spinon}}(k-k_{\text{h}},\omega-\omega_{\text{h}})$$

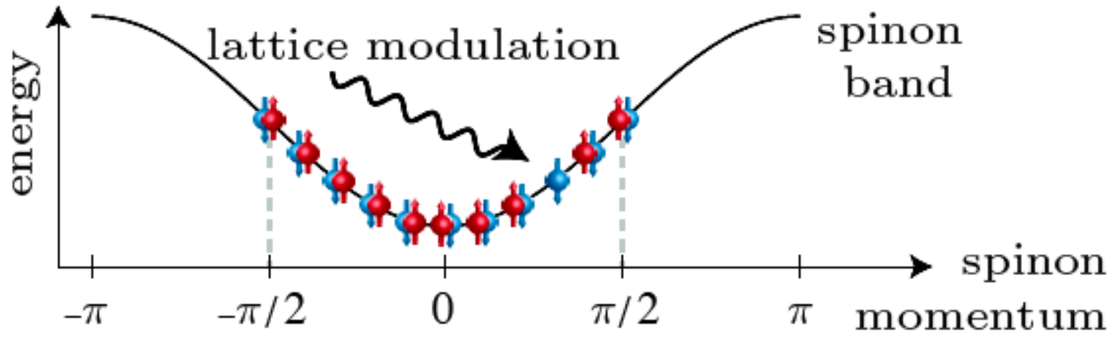
chargon

spinon



Asymmetry of spectral weight around $\pi/2$:

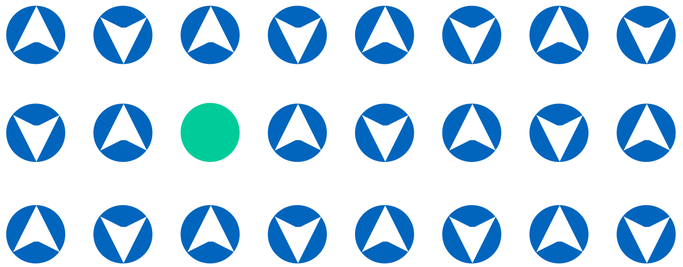
- Parton description of ground state
- Hole: create chargon and remove spinon

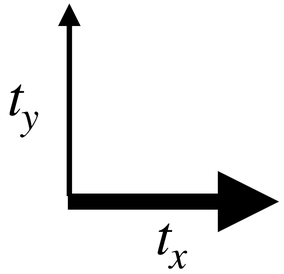


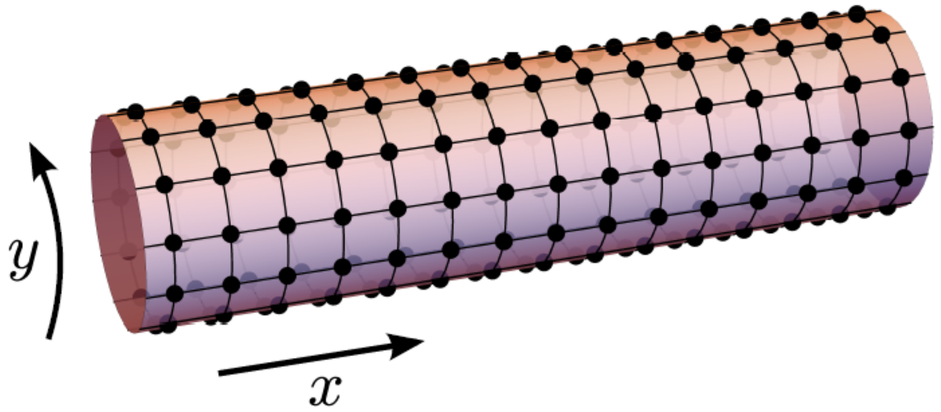
[**Bohrdt**, et al. Phys. Rev. B 2018]
cf. [Szczepanski, et al., Phys. Rev. B 1990], …

Dimensional crossover

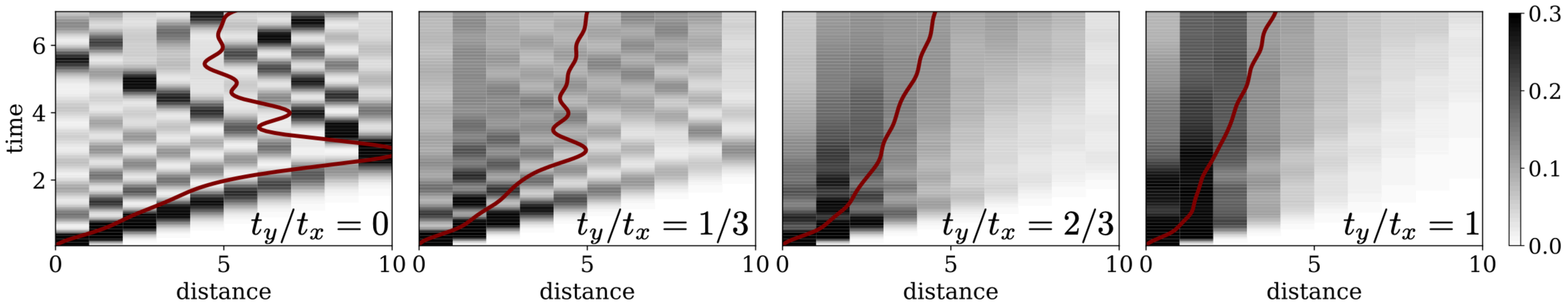
Numerical calculation: MPS on cylinders







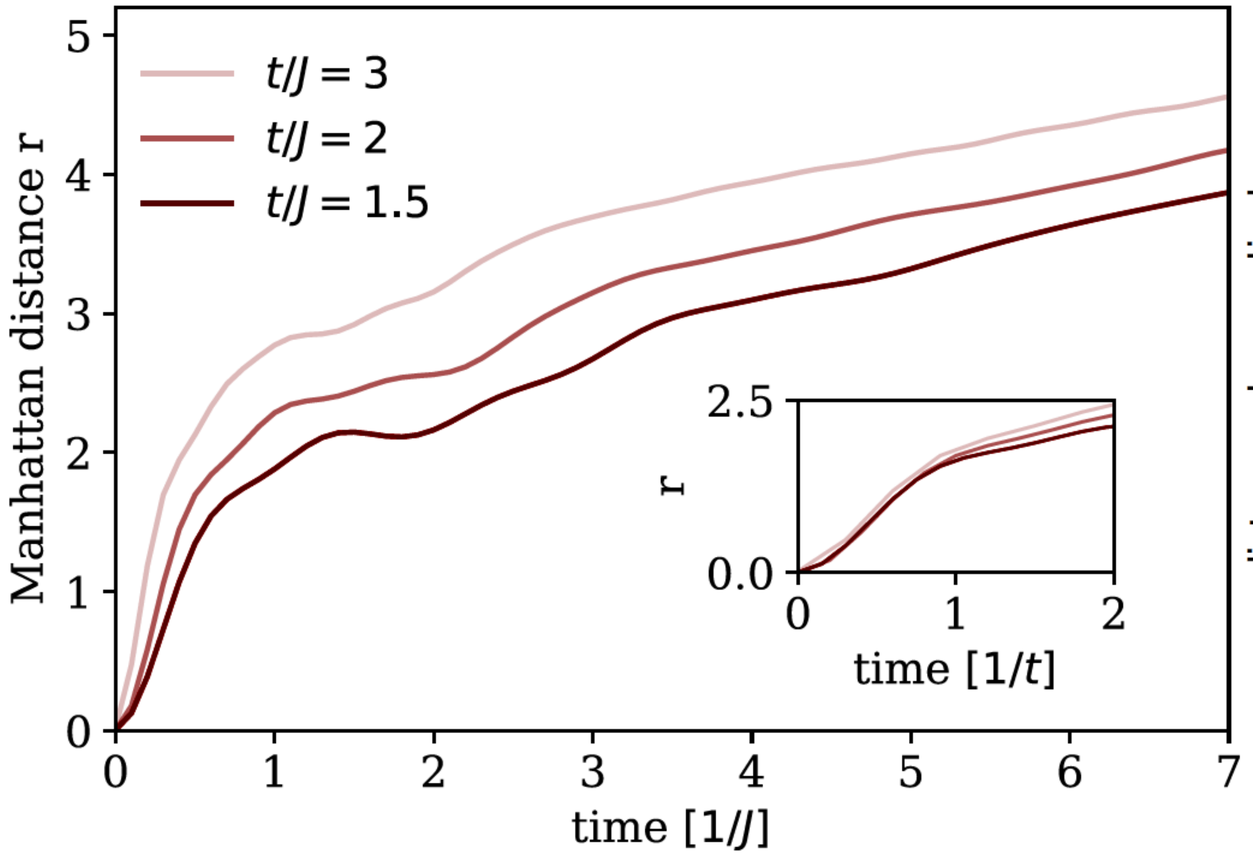
[2D DMRG: M. Zaletel et al., PRB 91 2015]



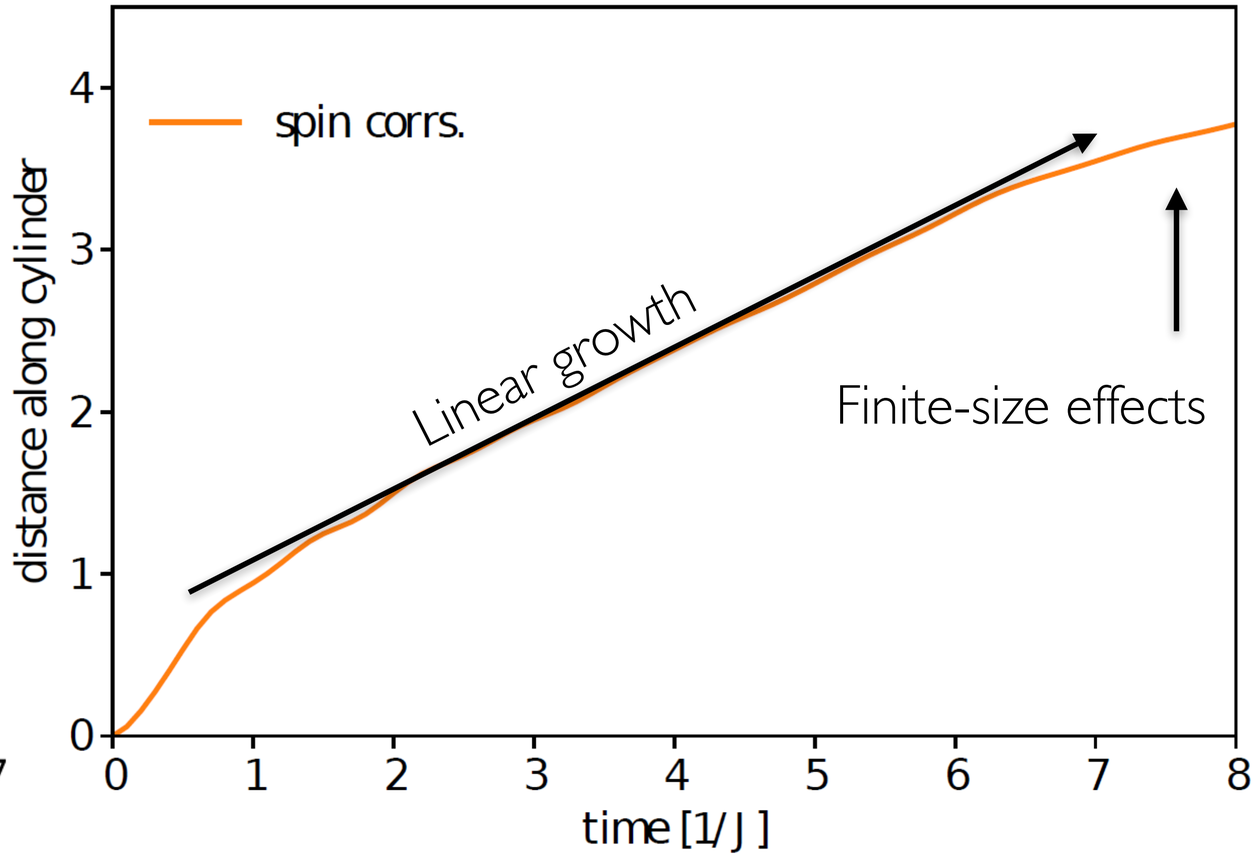
[**Bohrdt**, Grusdt, MK, NJP 2020]

Isotropic hopping $t_x = t_y$

Position of hole



Local spin-correlations

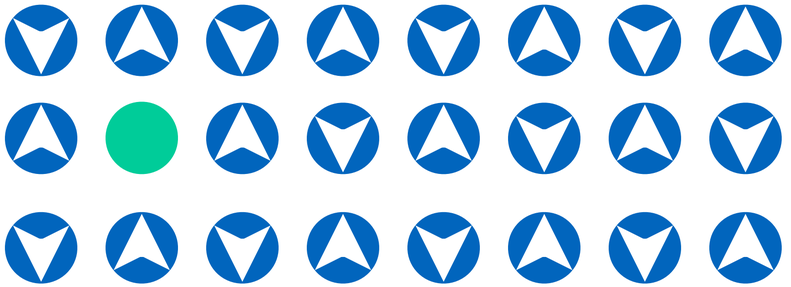


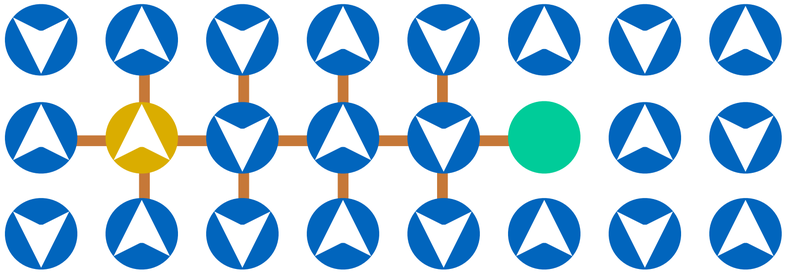
[**Bohrdt**, Grusdt, MK, NJP 2020]

Parton formalism in 2D

- Fractional spin excitation $S = 1/2$
- Chargon distorts 2D Néel state
- Chargon bound to spinon at the end of a string

$$E \sim J\ell$$

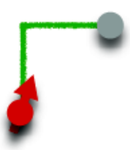
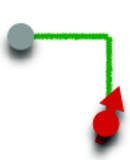
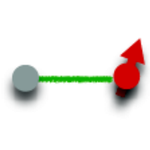




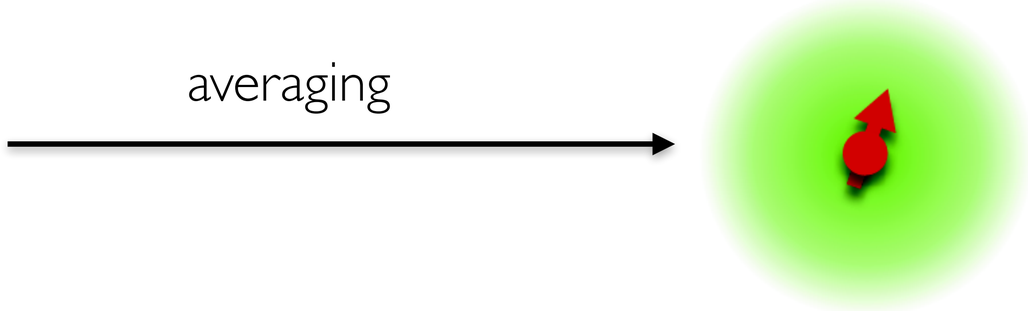
Competition: hopping vs. bound state energy
⟶ emergent length scale

[Beran, Poilblanc, Laughlin, Nucl. Phys. B, 1996]
[Grusdt, et al. PRX 2018]

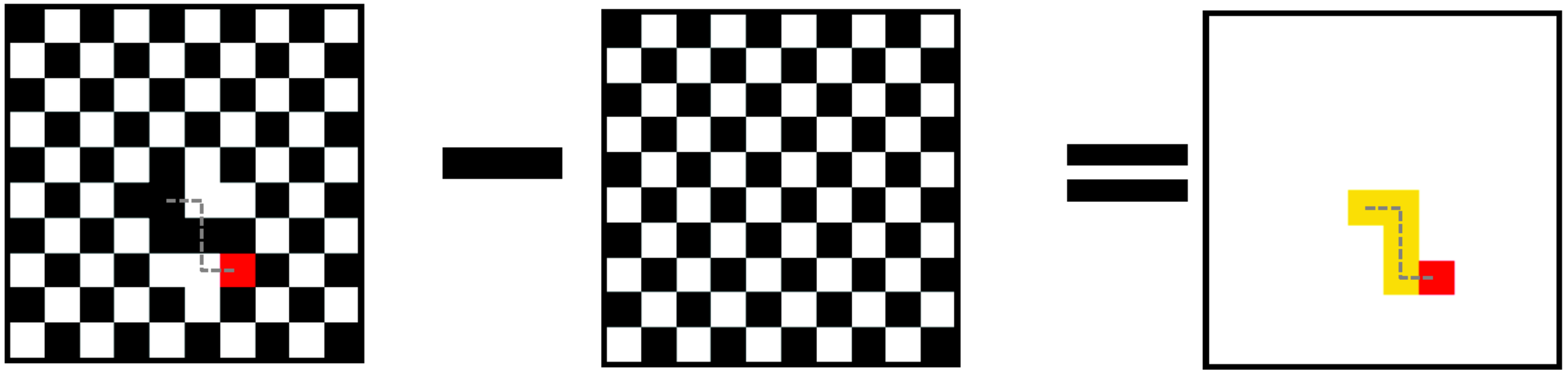
Quantum many-body wave function

$$|\Psi\rangle = |$$  $$\rangle + |$$  $$\rangle + |$$  $$\rangle + |$$  $$\rangle + \ldots$$

averaging



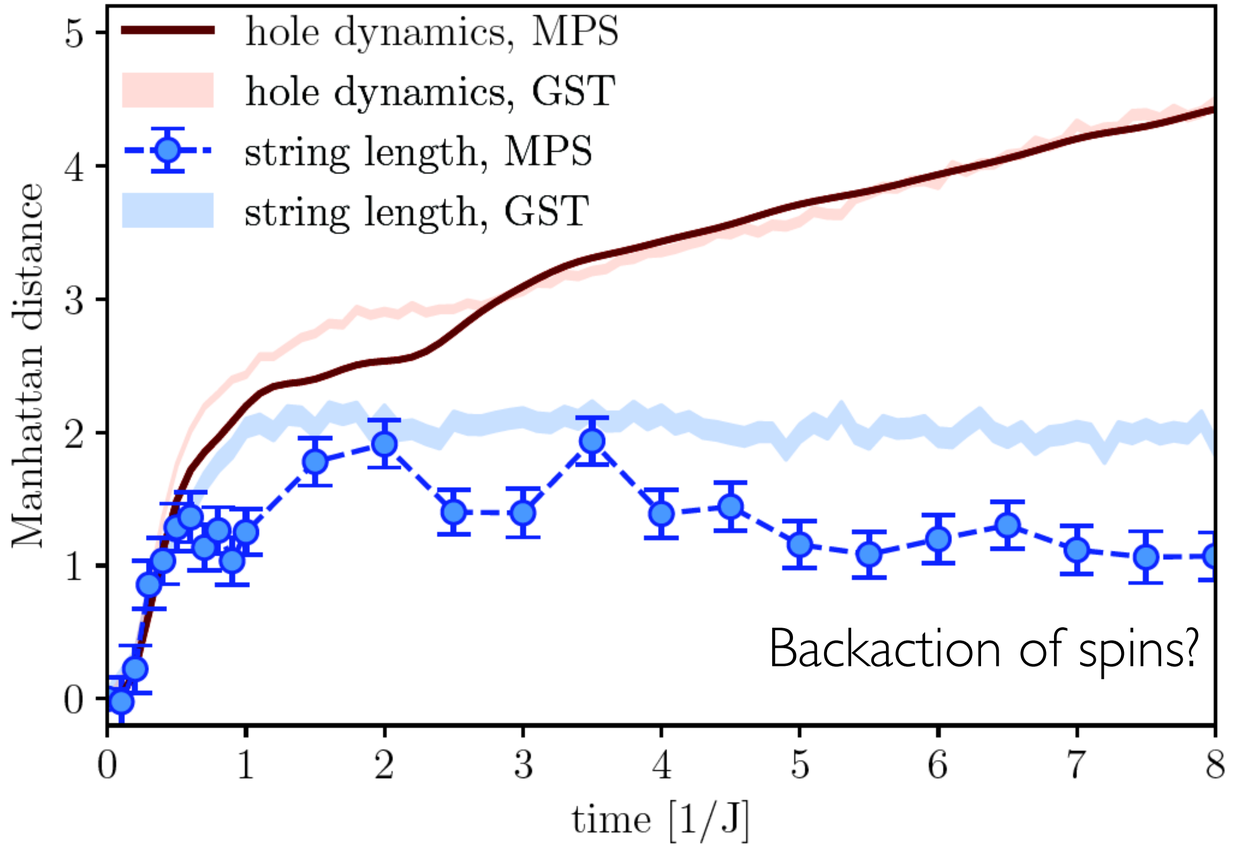
Detecting strings (approximately)



[**Chiu, Ji, Bohrdt**, et al. Science 2019]
c.f. [Ho, PNAS 2020]

Interpretation of our numerical results

1. Free chargon motion — creation of a string
2. Confinement — saturation of string length
3. Free center-of-mass motion by spinon



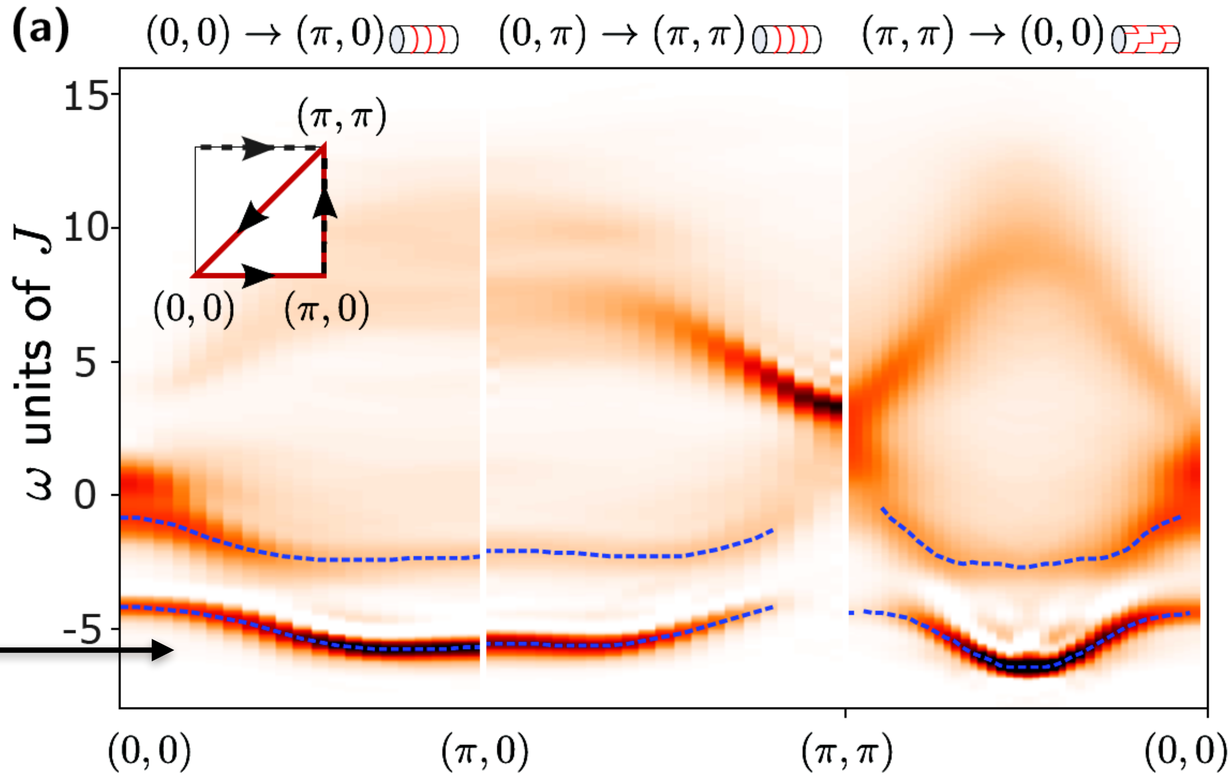
[**Bohrdt**, Grusdt, MK, NJP 2020]

Parton theory for ARPES

$$A(\omega, \boldsymbol{k})|_{\text{bound}} = \int d\nu \; A_{\text{s}}(\omega - \nu, \boldsymbol{k}) A_{\text{c}}(\nu).$$

- Momentum dependence due to spinon
- Structure factor: two spinons

magnetic polaron

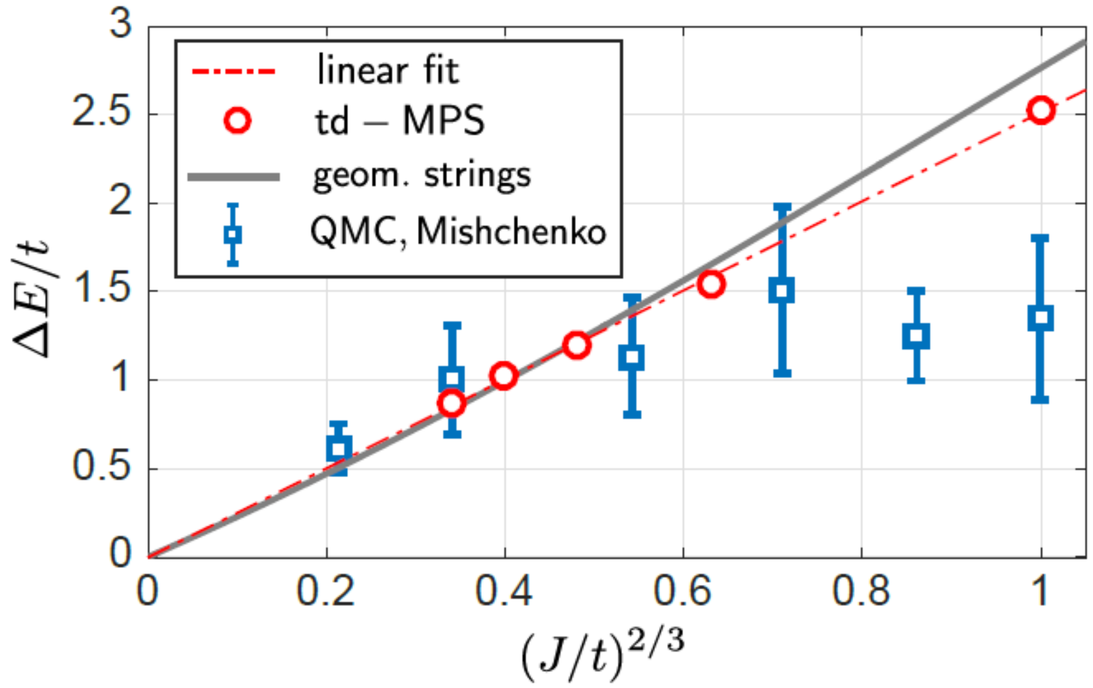


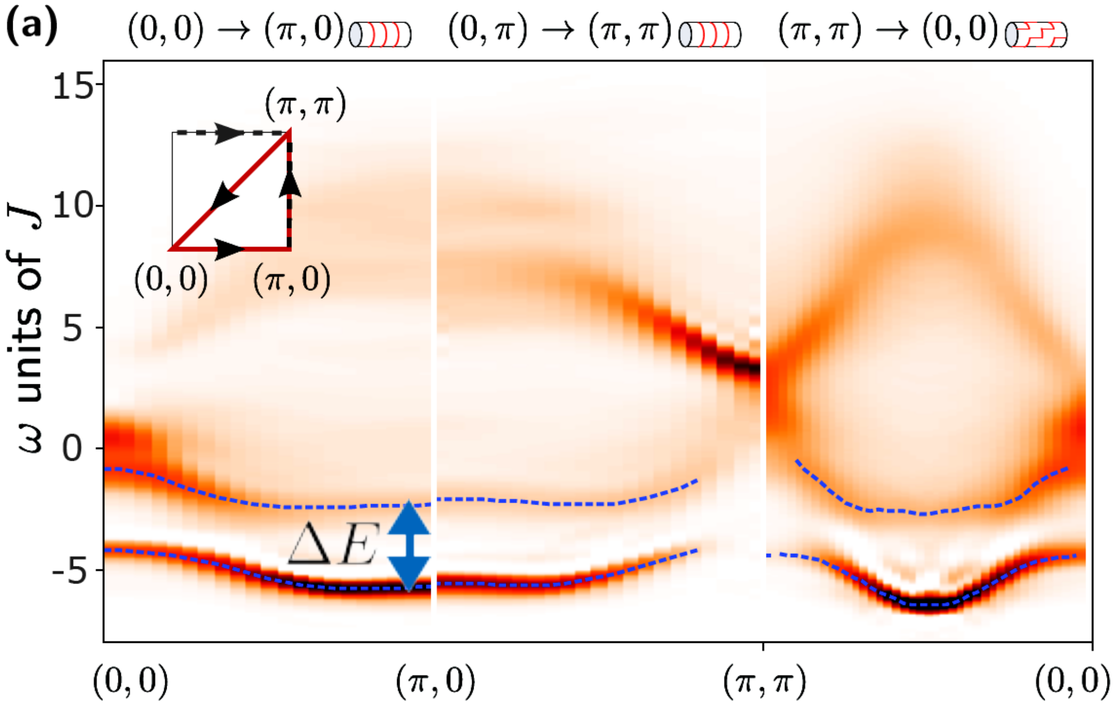
[**Bohrdt**, et al. PRB 2020]

Vibrational excitations

Geometric string leads to linear confinement

- Vibrational mode $\Delta E \sim (J/t)^{2/3}$
- Approximately constant gap for all k

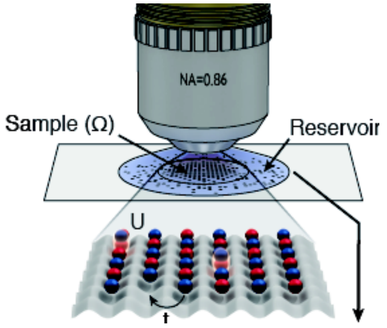


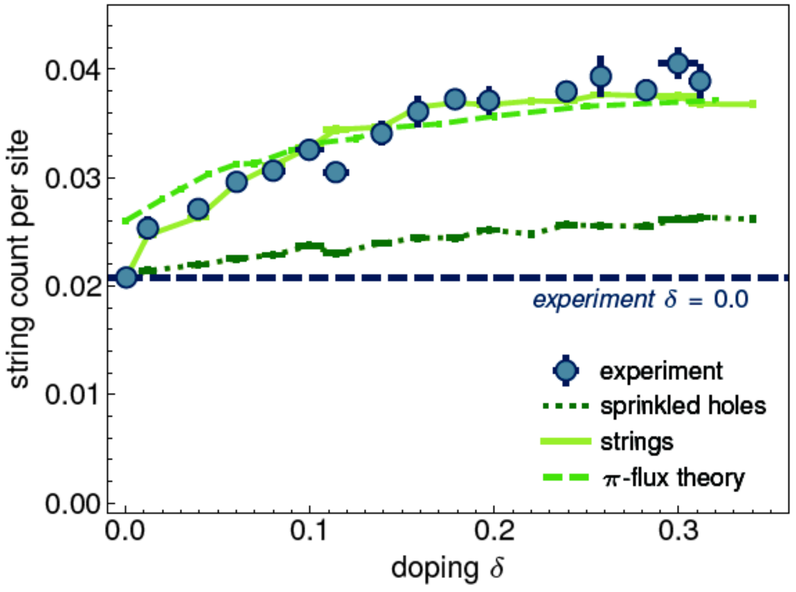


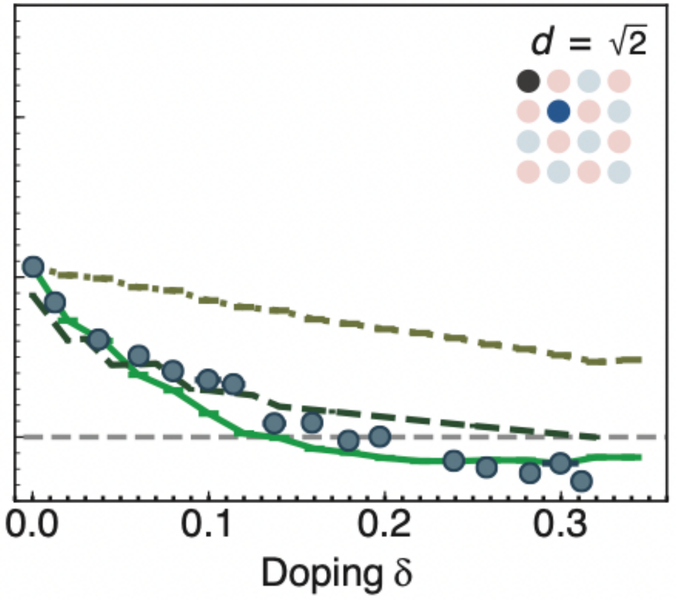
[**Bohrdt**, et al. PRB 2020]
c.f. [Bulaevskii et al. JETP 1968]

String patterns in the doped Hubbard model

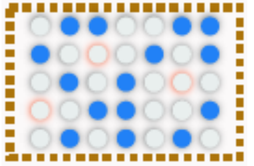
Christie S. Chiu[1], Geoffrey Ji[1], Annabelle Bohrdt[2,1,3], Muqing Xu[1], Michael Knap[2,3], Eugene Demler[1], Fabian Grusdt[1,3], Markus Greiner[1*], Daniel Greif[1]



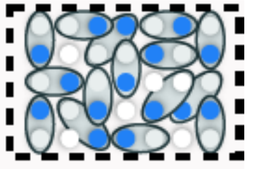




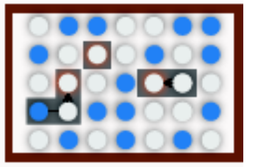
sprinkling



π-flux theory
(1 fit parameter)



geometric string theory
(**no** fit parameter)

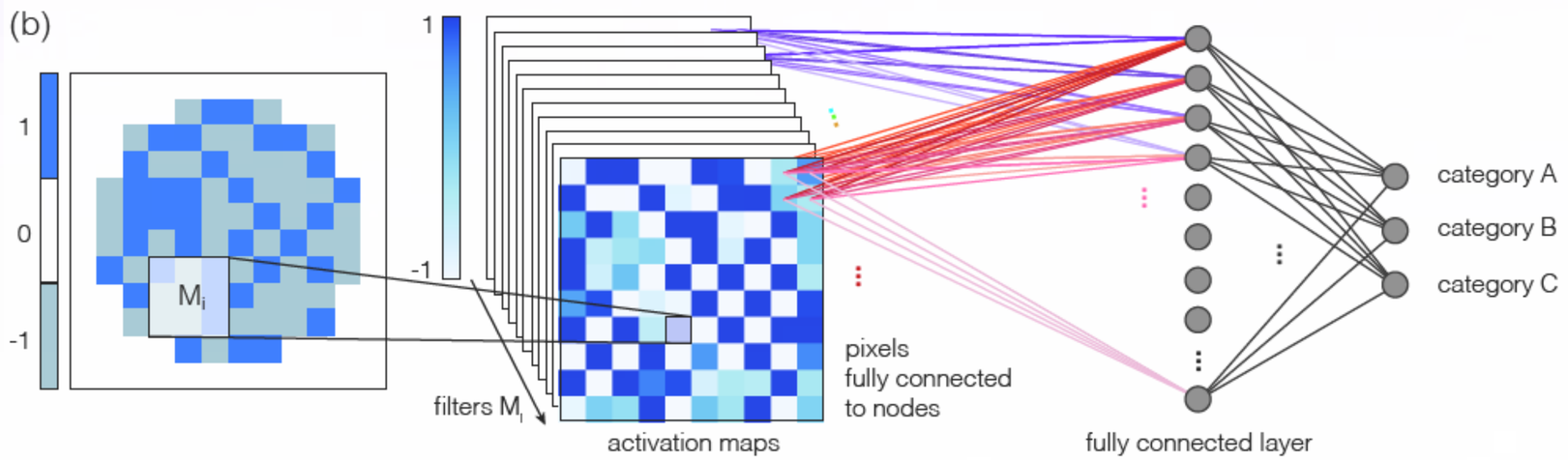


[**Chiu, Ji, Bohrdt**, et al. Science 2019]

"The theoretical problem is so hard
that there isn't an obvious criterion for right."

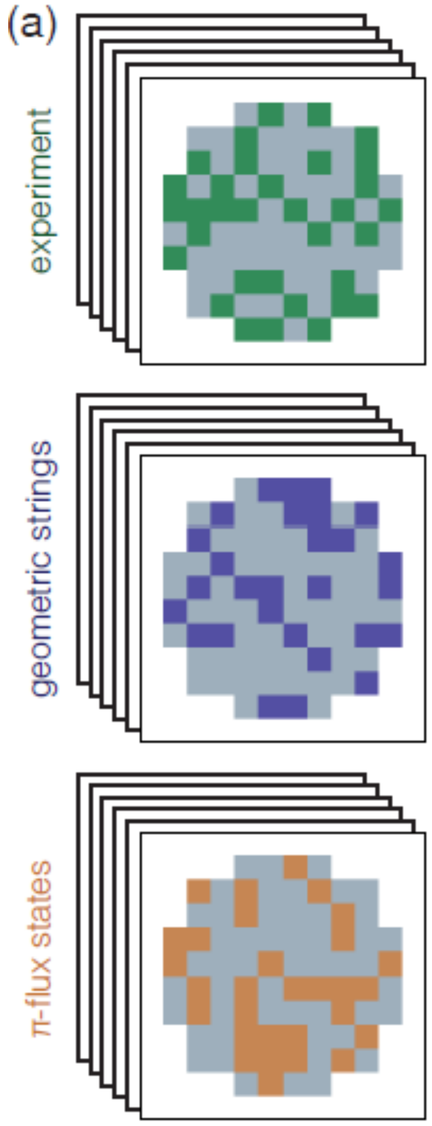
— Steve Kivelson, Science 314 (2006)

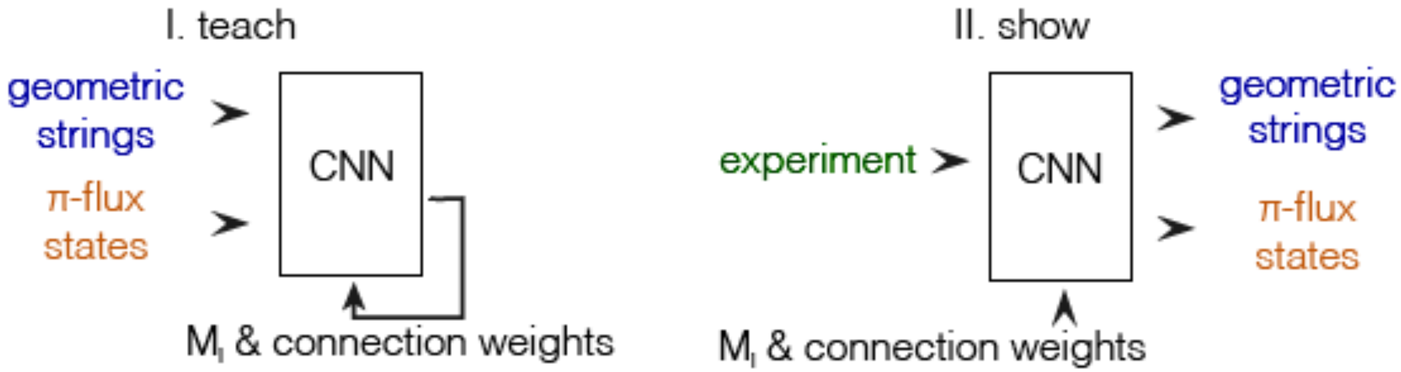
Which theory is more predictive?



[**Bohrdt**, et al. Nat. Physics 2019]

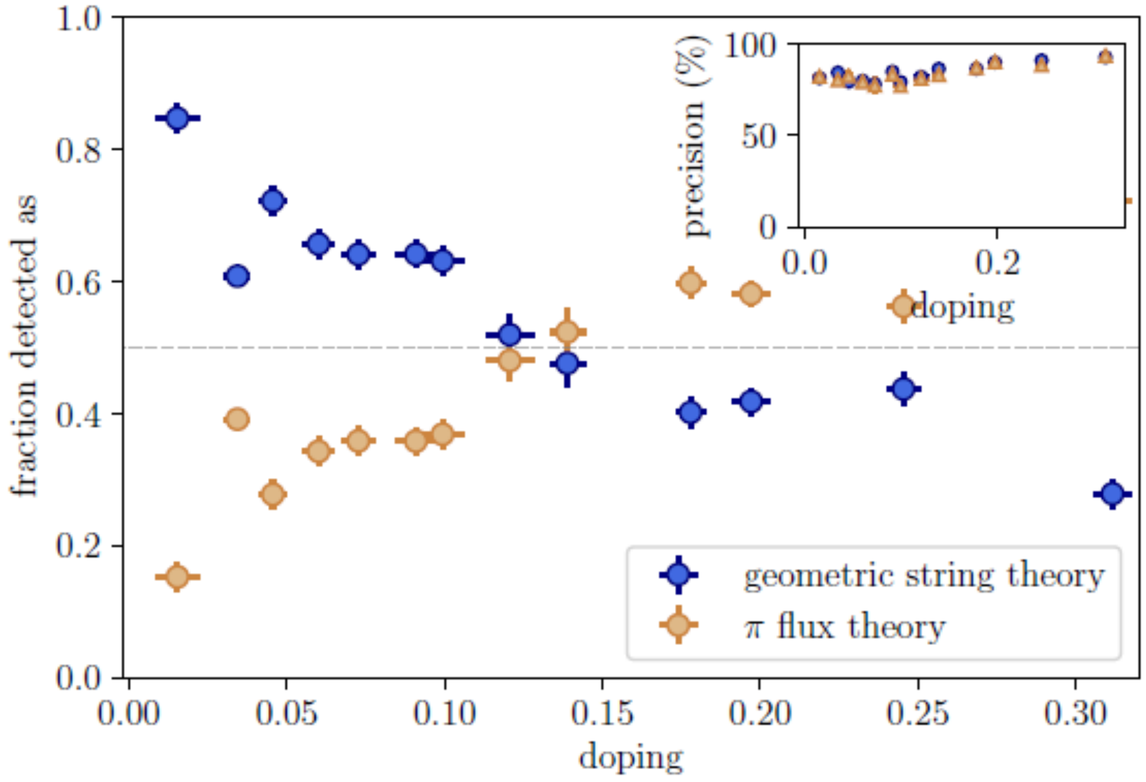
Learning from theoretical predictions





[**Bohrdt**, et al. Nat. Physics 2019]

Classifying experimental data



[**Bohrdt**, et al. Nat. Physics 2019]

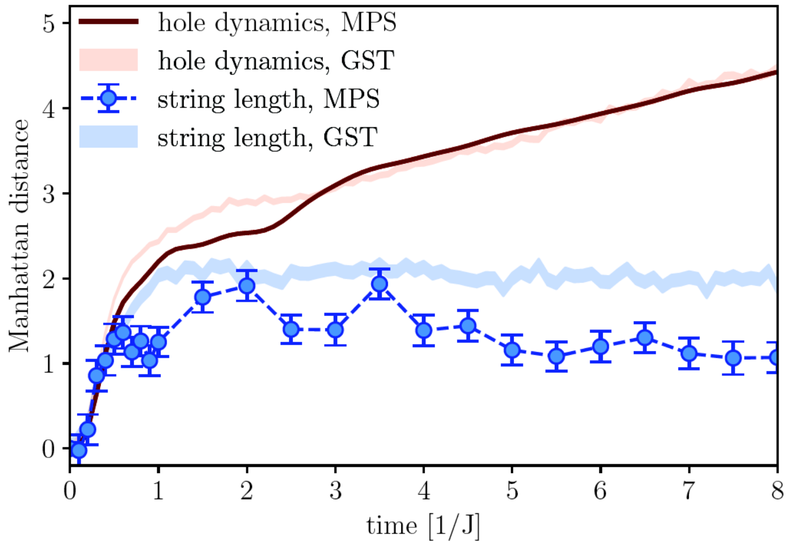
Summary and Outlook

Parton picture: useful interpretation of hole in AFM

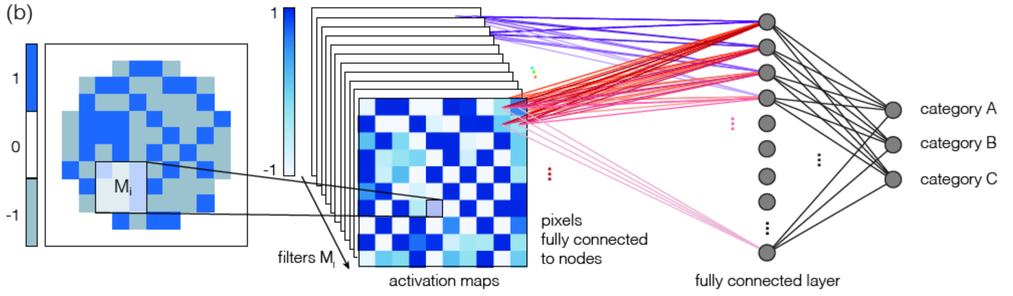
Neural Networks: a new route to analyze snapshots

Many open questions:

- Finite temperature?
- Dynamics of multiple holes?
- Frustrated quantum magnets?



[**Bohrdt**, Grusdt, MK, NJP 2020]
[**Bohrdt**, et al. PRB 2020]
[**Bohrdt**, et al. PRB 2018]



[**Bohrdt**, et al. Nat. Physics 2019]
[**Chiu, Ji, Bohrdt**, et al. Science 2019]