Title: Tackling old problems with new tools: from frustration to pairing in strongly correlated many body systems

Speakers: Annabelle Bohrdt

Series: Quantum Matter

Date: October 03, 2022 - 2:00 PM

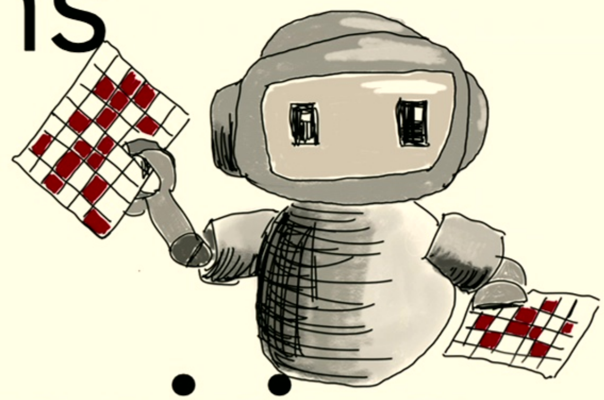
URL: https://pirsa.org/22100089

Abstract: New quantum simulation platforms provide an unprecedented microscopic perspective on the structure of strongly correlated quantum matter. This allows to revisit decade-old problems from a fresh perspective, such as the two-dimensional Fermi-Hubbard model, believed to describe the physics underlying high-temperature superconductivity. In order to fully use the experimental as well as numerical capabilities available today, we need to go beyond conventional observables, such as one- and two-point correlation functions. In this talk, I will give an overview of recent results on the Hubbard model obtained through novel analysis tools: using machine learning techniques to analyze quantum gas microscopy data allows us to take into account all available information and compare different theories on a microscopic level. In particular, we consider Anderson's RVB paradigm to the geometric string theory, which takes the interplay of spin and charge degrees of freedom microscopically into account. The analysis of data from quantum simulation experiments of the doped Fermi-Hubbard model shows a qualitative change in behavior around 20% doping, up to where the geometric string theory captures the experimental data better. This microscopic understanding of the low doping limit has led us to the discovery of a binding mechanism in so-called mixed-dimensional systems, which has enabled the observation of pairing of charge carriers in cold atom experiments.
Intriguingly, mixed-dimensional systems exhibit similar features as the original two-dimensional model, e.g. a stripe phase at low temperatures. At intermediate to high temperatures, we use Hamiltonian reconstruction tools to quantify the frustration in the spin sector induced by the hole motion and find that the spin background is best described by a highly frustrated J1-J2 model.

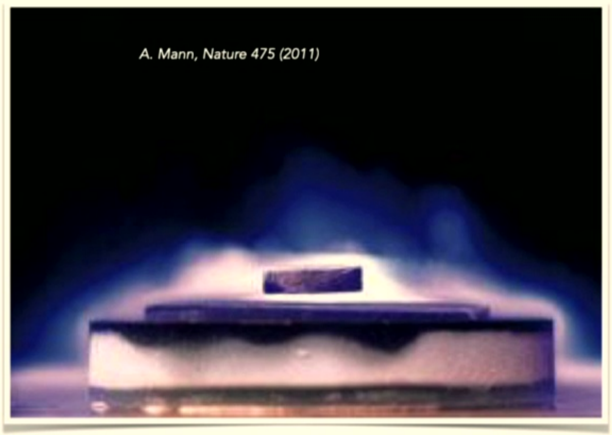
Zoom link: https://pitp.zoom.us/j/99449352935?pwd=cXdYYTJ2c1hVZ014SWRwZi9LRjQ3dz09

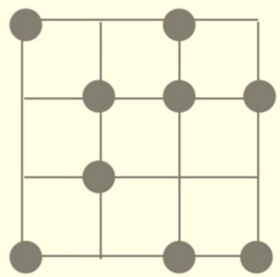
Annabelle Bohrdt

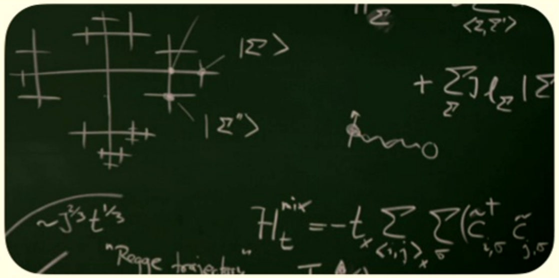
Tackling old problems with new tools: **from frustration to pairing**



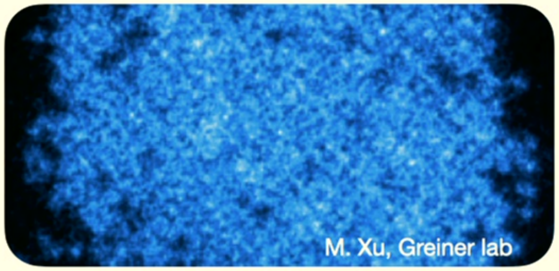
Perimeter, Oct 2022


A. Mann, Nature 475 (2011)



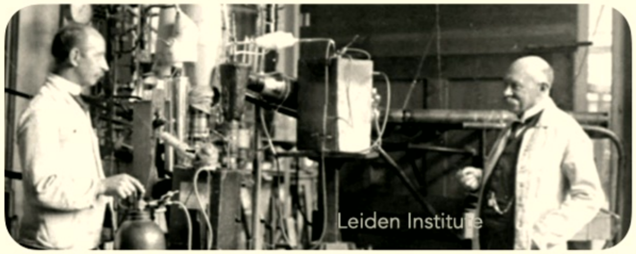



SUPERMUC-NG
Leibniz Rechenzentrum


M. Xu, Greiner lab

Annabelle Bohrdt

1911: Heike Kamerlingh Onnes discovers superconductivity



1957: BCS theory of conventional superconductivity

" the shame and despair of theoretical physics "

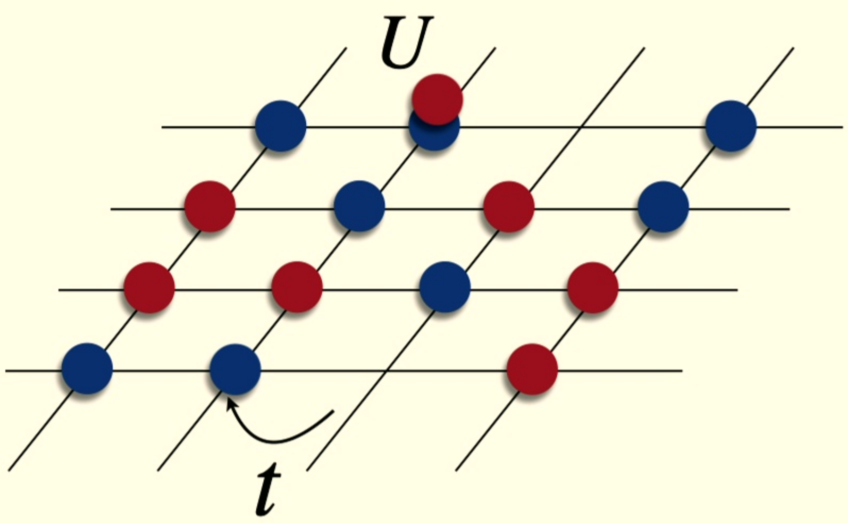
1986: Bednorz & Müller discover high temperature superconductivity

the shame and despair of theoretical physics?

J.M. Blatt, *Theory of Superconductivity* (Academic Press, New York, 1964)

Annabelle Bohrdt

Fermi-Hubbard model



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

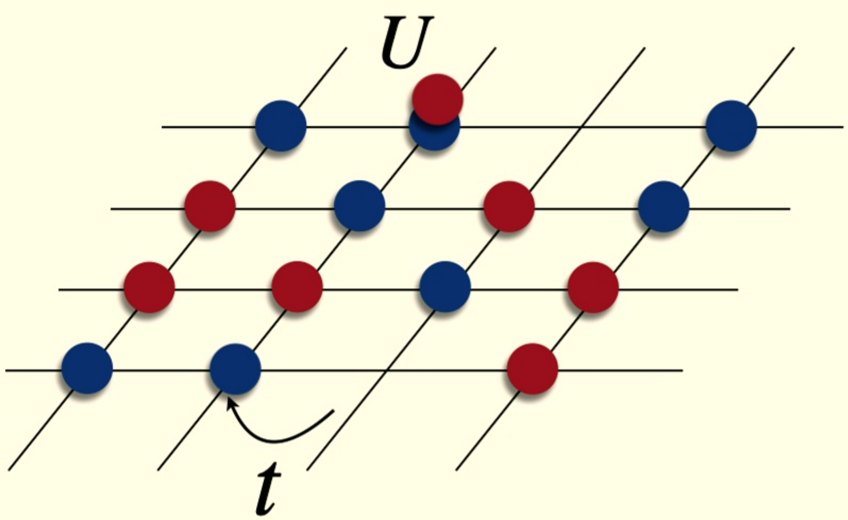
tunneling

interaction

Hilbert space dimension: $4^{16} = 4294967296$, using symmetries: $\sim 10^7$

Annabelle Bohrdt

Fermi-Hubbard model



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

tunneling — interaction

Hilbert space dimension: $4^{16} = 4294967296$, using symmetries: $\sim 10^7$

Annabelle Bohrdt

Quantum simulation & computation

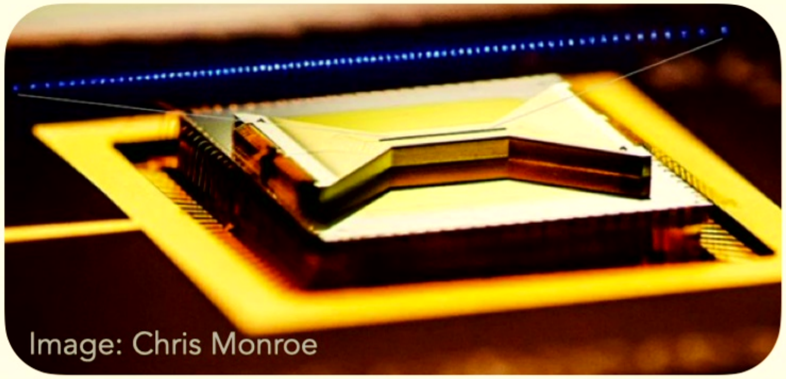


Image: Chris Monroe

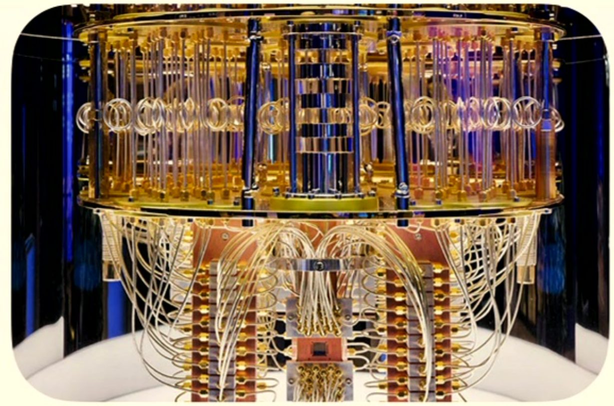
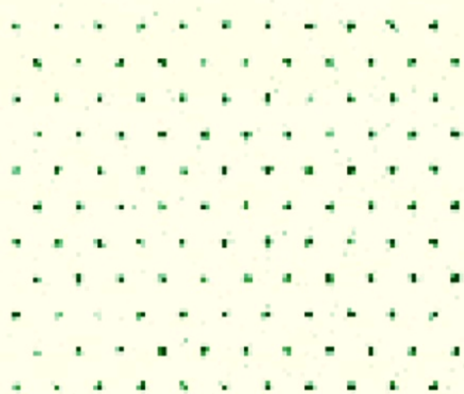


Image: IBM


Ebadi et al. (Lukin group), Nature 595 (2021)

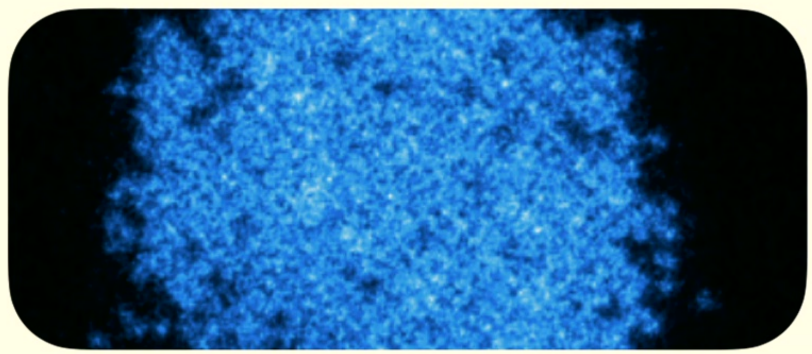
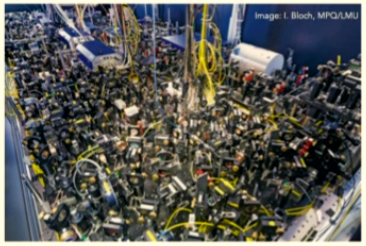
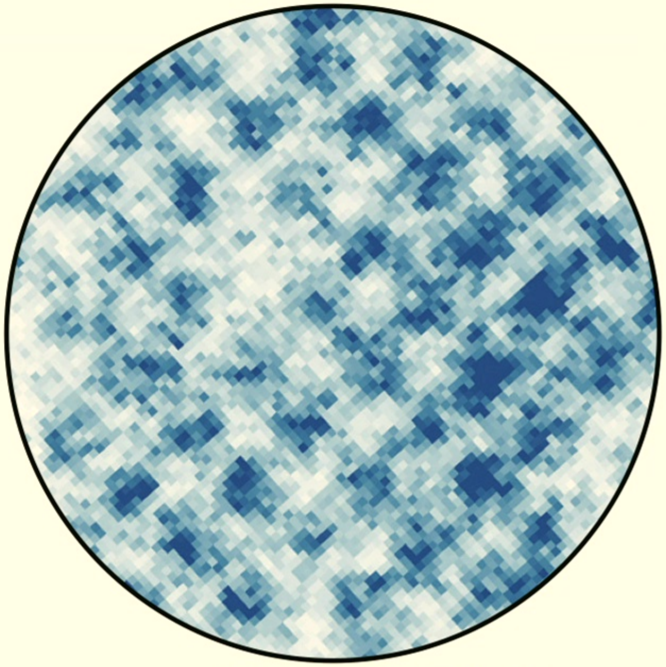


Image: Muqing Xu, Greiner lab

Annabelle Bohrdt

Quantum gas microscopy

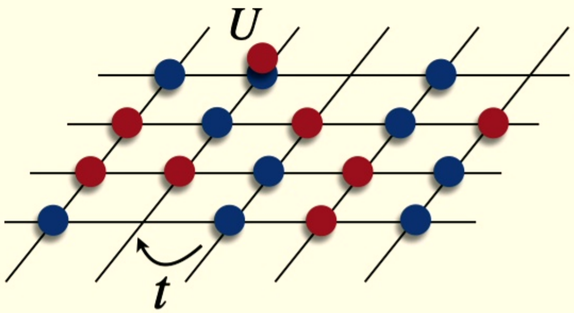




A. Mazurenko et al., Nature 545 (2017)

Annabelle Bohrdt

Fermi-Hubbard model



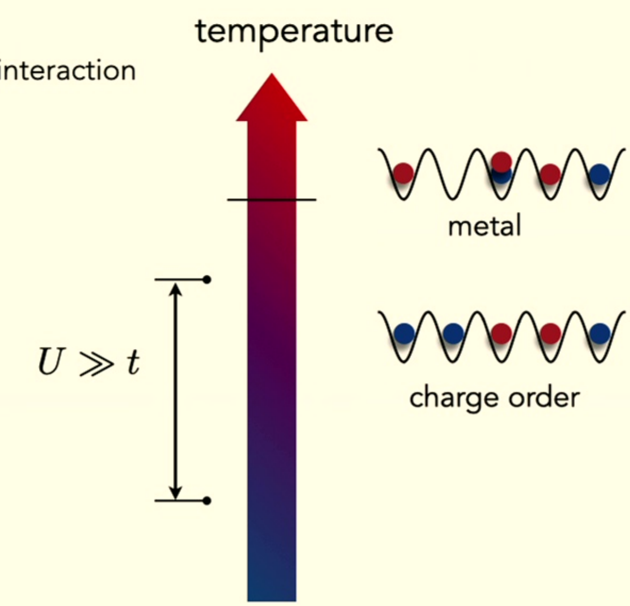
$$\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} \left(\hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} + h.c. \right) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}$$

tunneling — interaction

Large U limit: $t-J$ model

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

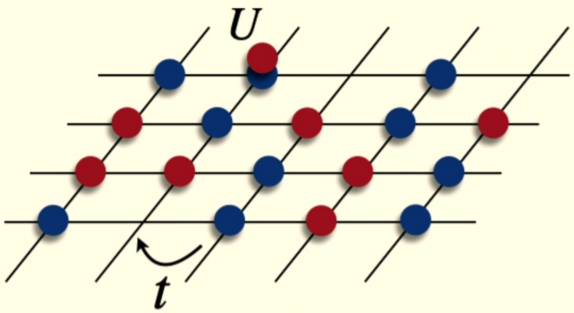
no double-occupancies — tunneling — spin-exchange



Imaging: see Kale et al., PRA 106 (2022)

Annabelle Bohrdt

Fermi-Hubbard model



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

tunneling

interaction

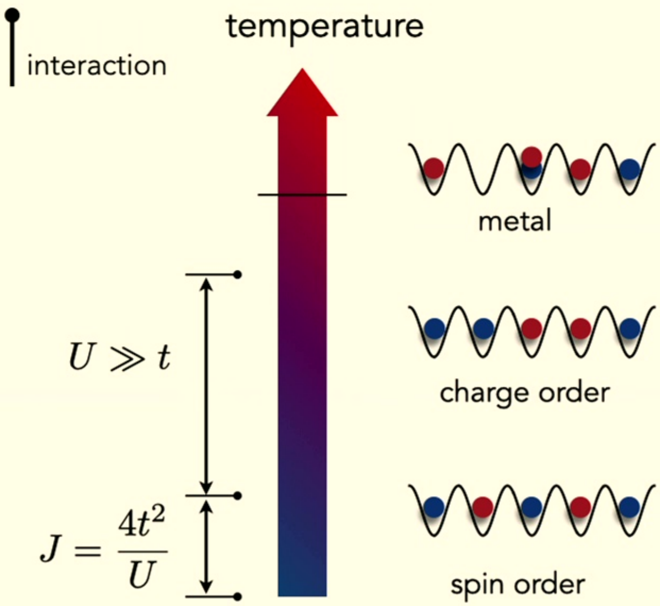
Large U limit: $t - J$ model

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

no double-occupancies

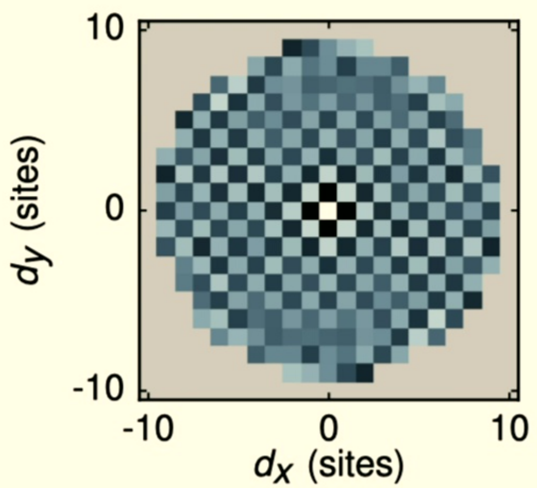
tunneling

spin-exchange



Fermi-Hubbard model

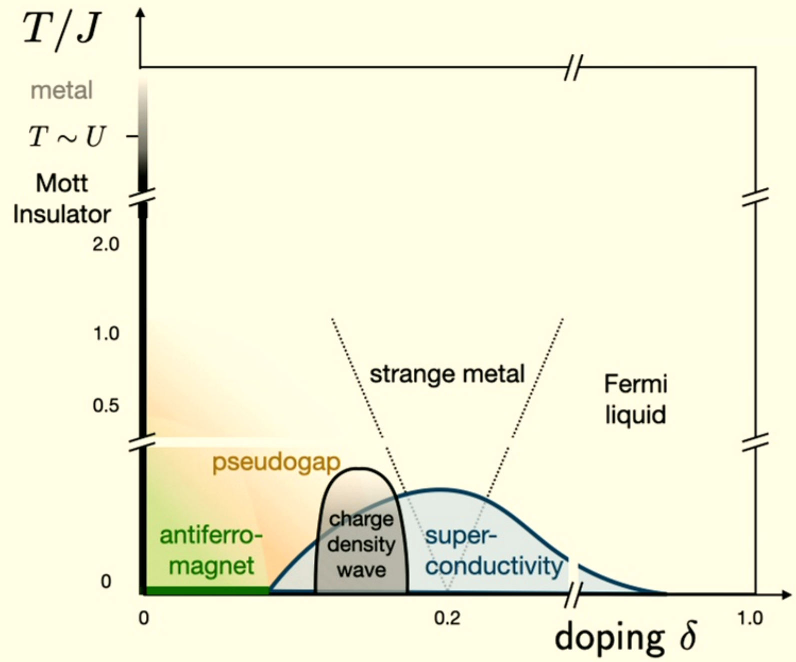
Annabelle Bohrdt



Mazurenko et al., Nature 545 (2017)

Review article: Fermi-Hubbard with cold atoms

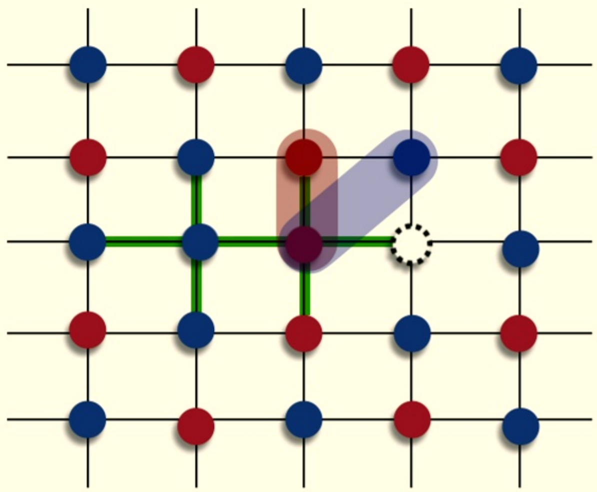
Bohrdt et al., Annals of Physics (2021)



Annabelle Bohrdt

Geometric string theory

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



$$\frac{dE}{dl} = 2J\left(C_{\mathbf{e}_x+\mathbf{e}_y} - C_{\mathbf{e}_x}\right)$$

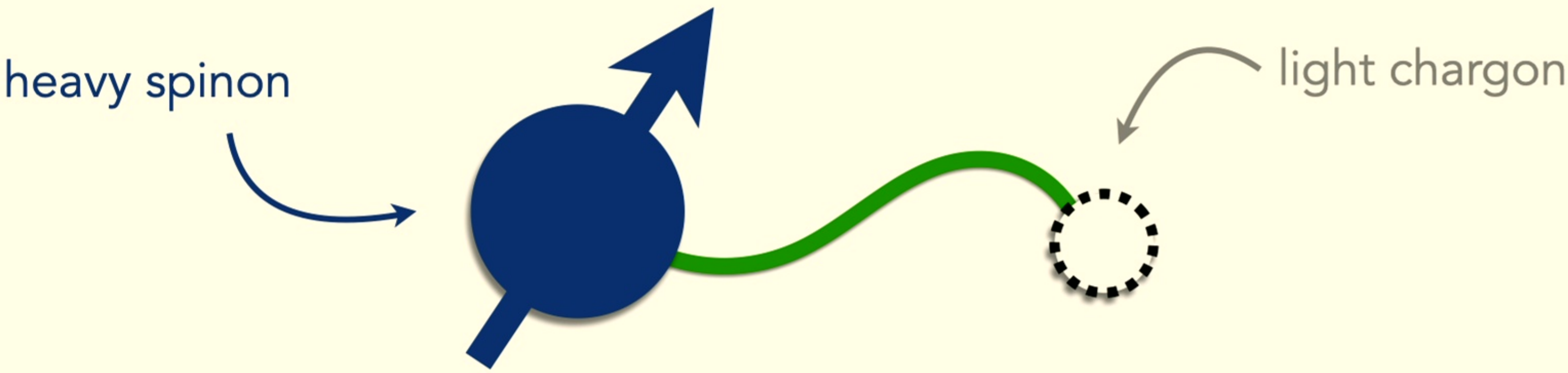
Grusdt et al., PRX 8 (2018), Grusdt et al., PRB 99 (2019), Bohrdt et al., NJP 22 (2020)

Early work: Bulaevskii et al., JETP 27 (1968), Trugman, PRB 37 (1988), Manousakis, PRB 75 (2007)

Annabelle Bohrdt

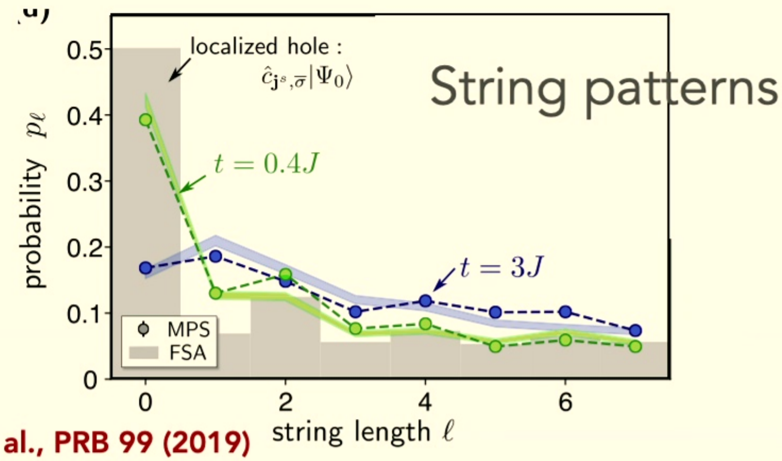
Geometric string theory

- Born-Oppenheimer approximation: $|\psi\rangle \simeq |\psi_{\mathrm{spinon}}\rangle \otimes |\psi_{\mathrm{string}}\rangle$

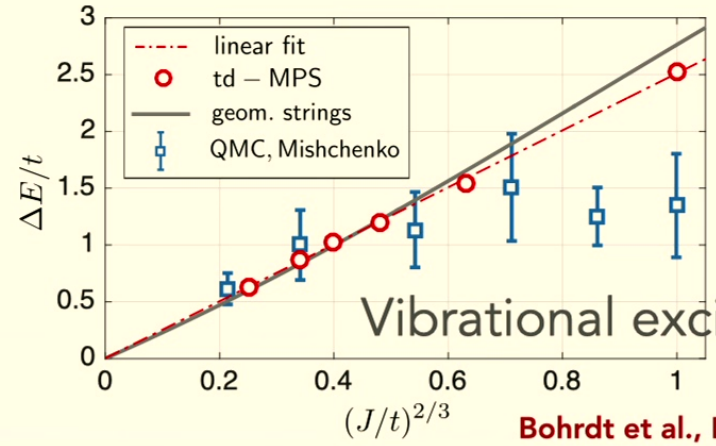


Annabelle Bohrdt

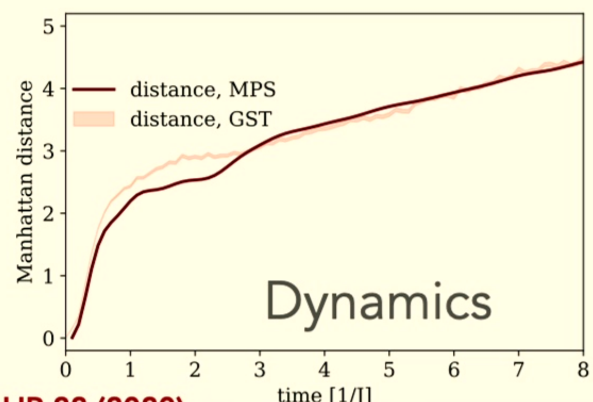
A single hole



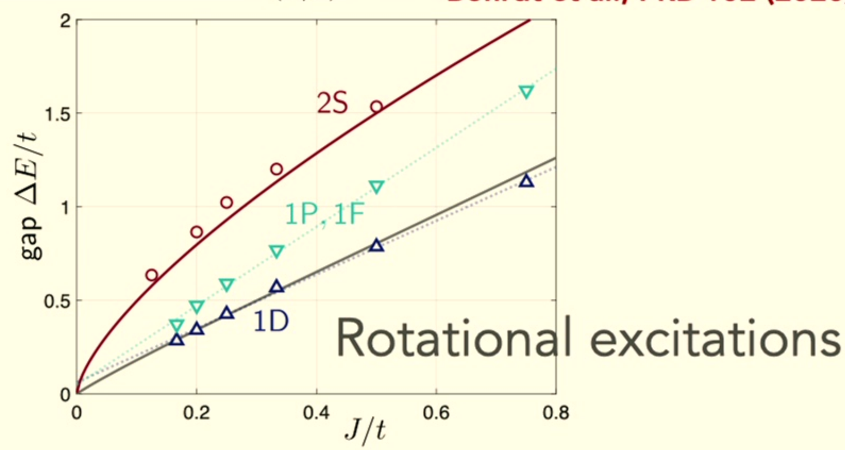
Grusdt et al., PRB 99 (2019)



Bohrdt et al., PRB 102 (2020)



Bohrdt et al., NJP 22 (2020)

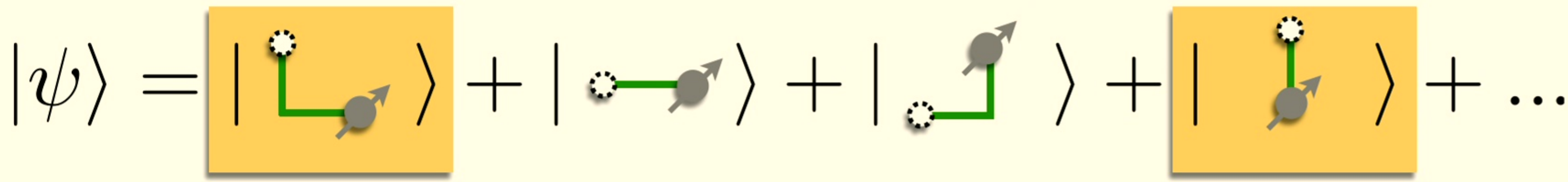


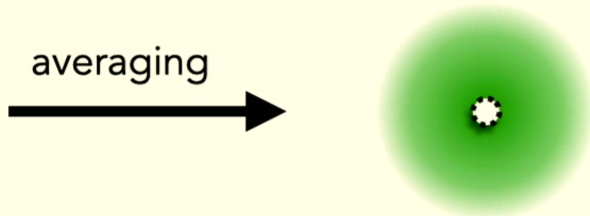
Bohrdt et al., PRL 127 (2021)

Perimeter, Oct 2022

Annabelle Bohrdt

Quantum projective measurements



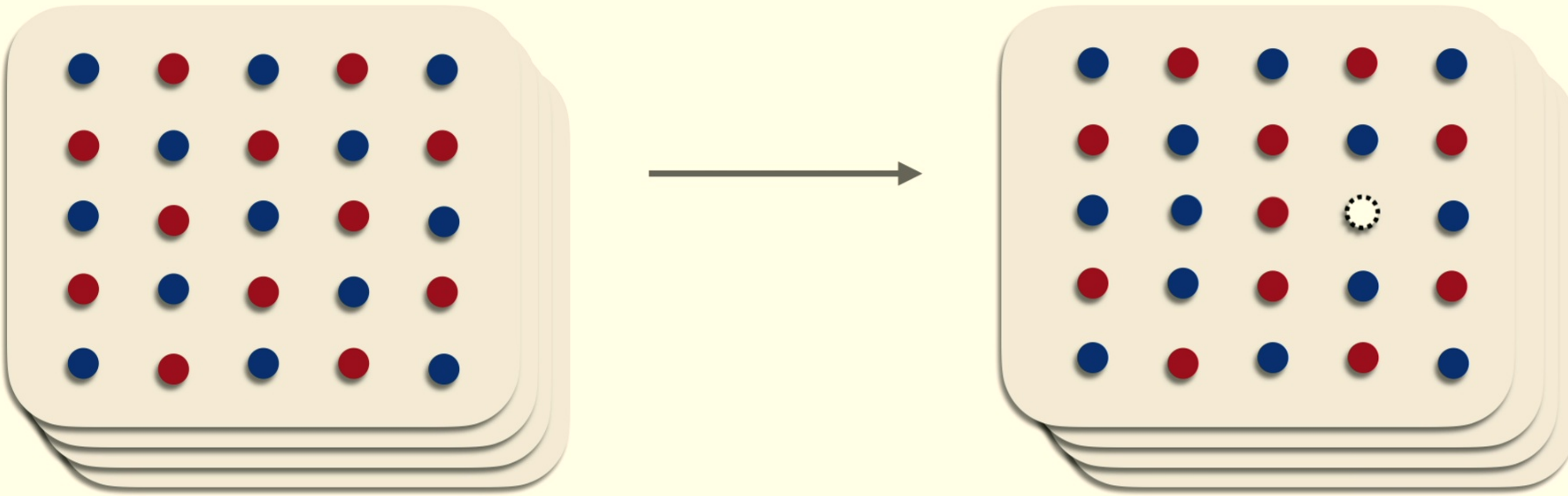


Geometric string theory snapshots

Annabelle Bohrdt

Snapshots at half-filling
(QMC, experimental data, …)

Geometric string theory snapshots
at finite doping

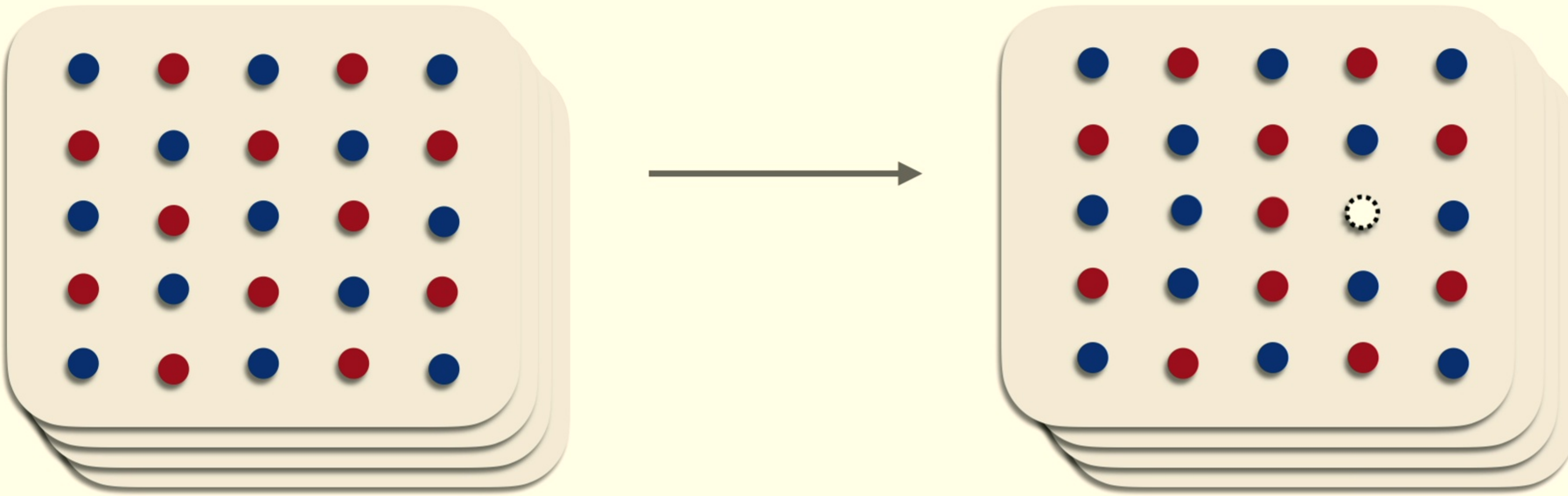


Geometric string theory snapshots

Annabelle Bohrdt

Snapshots at half-filling
(QMC, experimental data, …)

Geometric string theory snapshots
at finite doping



Resonating valence bond states

Annabelle Bohrdt

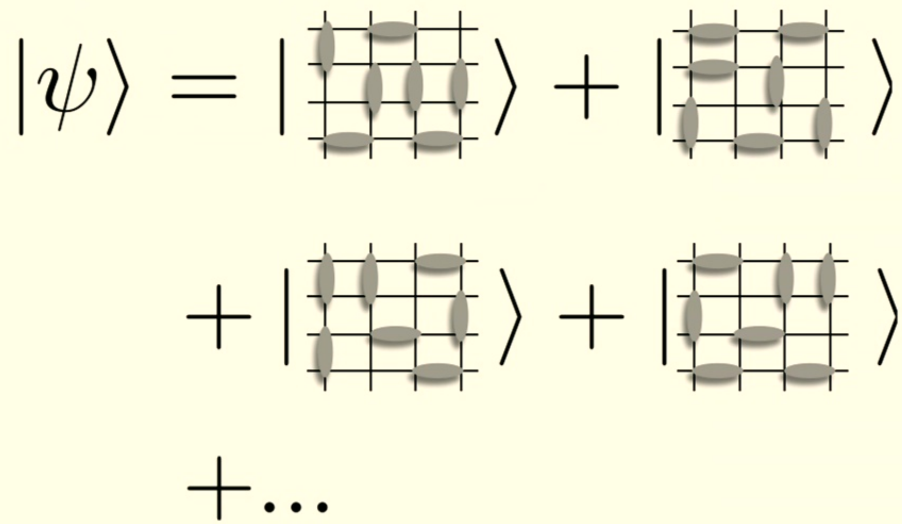
The Resonating Valence Bond State in La_2CuO_4 and Superconductivity

P. W. ANDERSON

RVB state.] It is our hypothesis that pure La_2CuO_4 is in an RVB state; this proposal is supported to some extent by the magnetic susceptibility data of Ganguly and Rao (*3*).

It is not easy to calculate with RVB states or to represent them. I want to give here a representation in terms of Gutzwiller-type projections of mobile-electron states, which is probably not particularly useful computationally but is suggestive. This representa-

Anderson, Science 235 (1987)



Resonating valence bond states

Annabelle Bohrdt

Trial wavefunction $$|\psi\rangle = \hat{P}_{GW}\,|\psi_0\rangle$$

Fermi sea

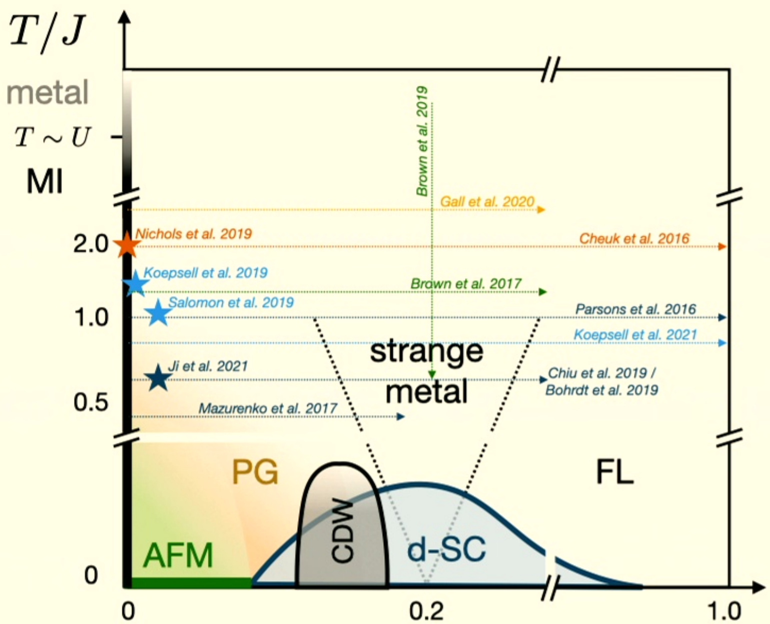
project out double occupancies

M. Gutzwiller, PRL 10 (1963); C. Gros, Annals of Physics 189 (1989)

Resonating valence bond states

Annabelle Bohrdt

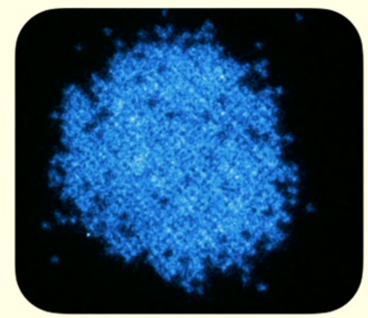
Review article: Fermi-Hubbard with cold atoms
Bohrdt et al., Annals of Physics (2021)



We want a finite temperature state

$$\hat{\rho} = \hat{P}_{GW} e^{-\hat{H}_{MF}/k_B T} \hat{P}_{GW}$$

We want snapshots

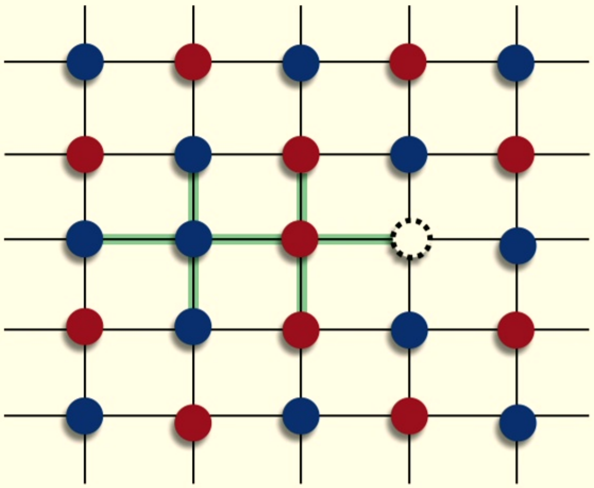


Metropolis Monte Carlo sampling with

$$p_\beta(\alpha_{\mathbf{r}}, \alpha_{\mathbf{k}}) = e^{-\beta E(\alpha_{\mathbf{k}})} \left|\langle \alpha_{\mathbf{r}} | \alpha_{\mathbf{k}} \rangle\right|^2$$

Candidate theories

Geometric string theory

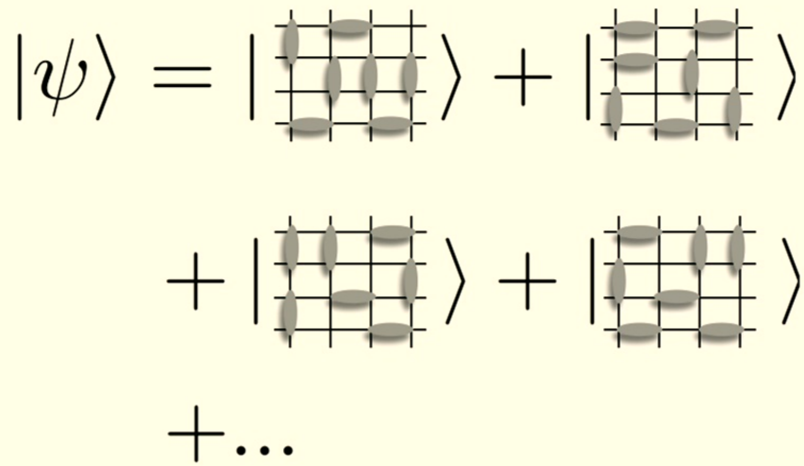


Grusdt et al., PRX 8 (2018), Grusdt et al., PRB 99 (2019), Bohrdt et al., NJP 22 (2020)

Early work: Bulaevskii et al., JETP 27 (1968), Trugman, PRB 37 (1988), Manousakis, PRB 75 (2007)

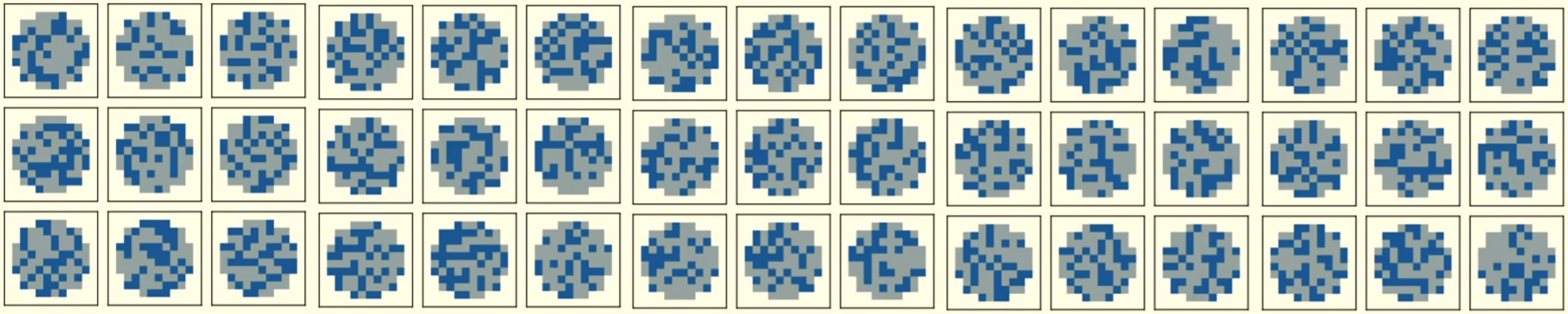
Resonating valence bond theory

(π-flux theory)



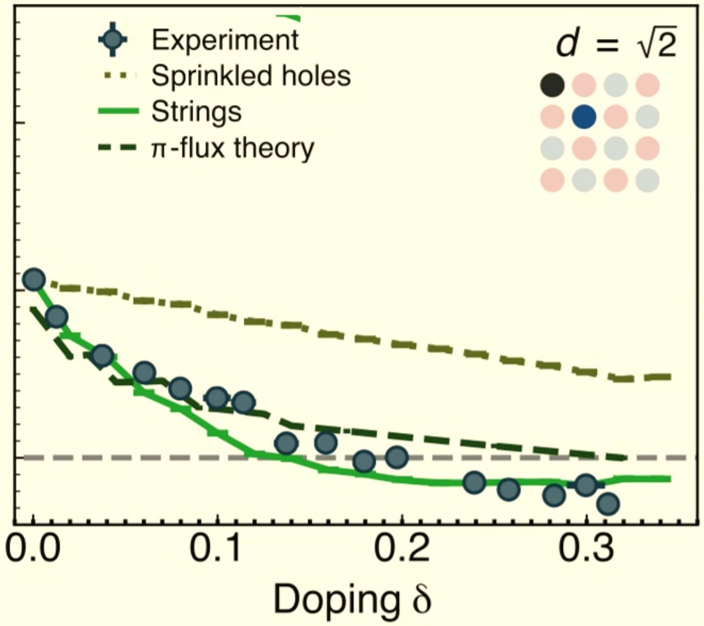
P. W. Anderson, Science 235, 1196 (1987)

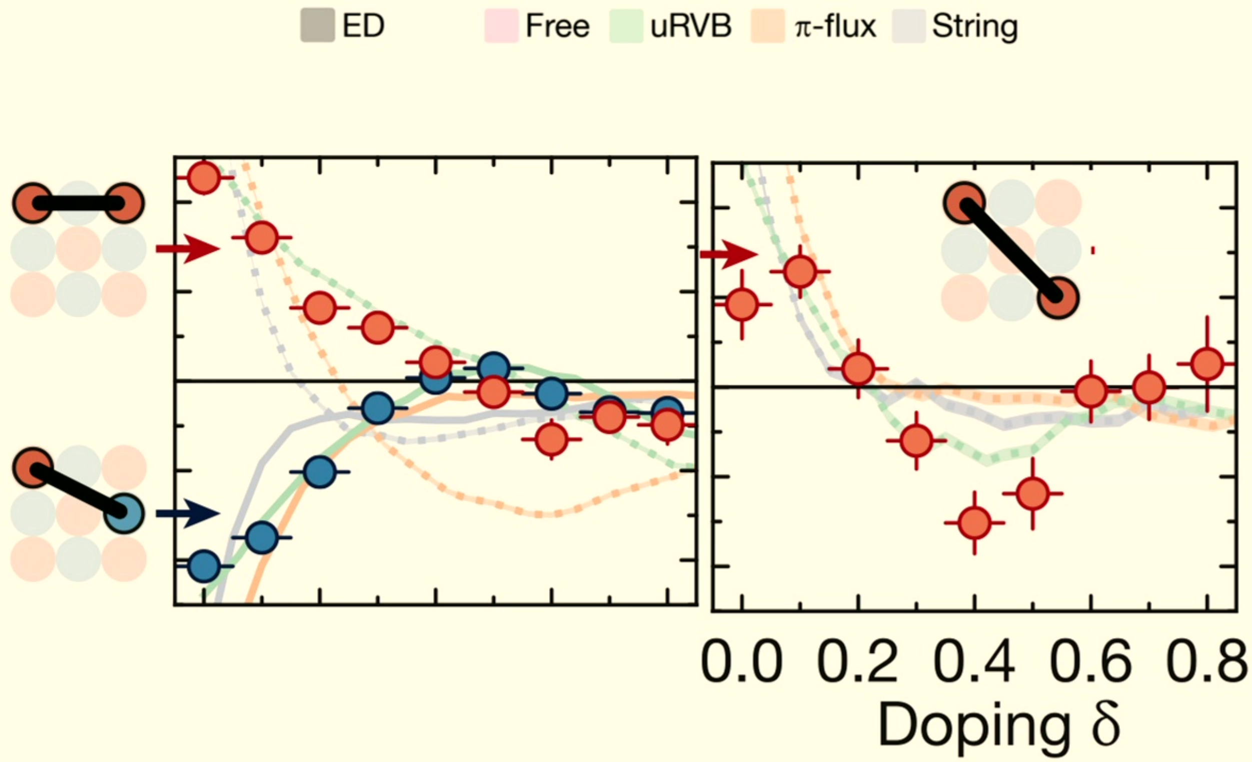
"The theoretical problem is so hard that **there isn't an obvious criterion for right.**"
— Steven Kivelson, Stanford University
Science 314 (2006)



Annabelle Bohrdt

What should we look for?



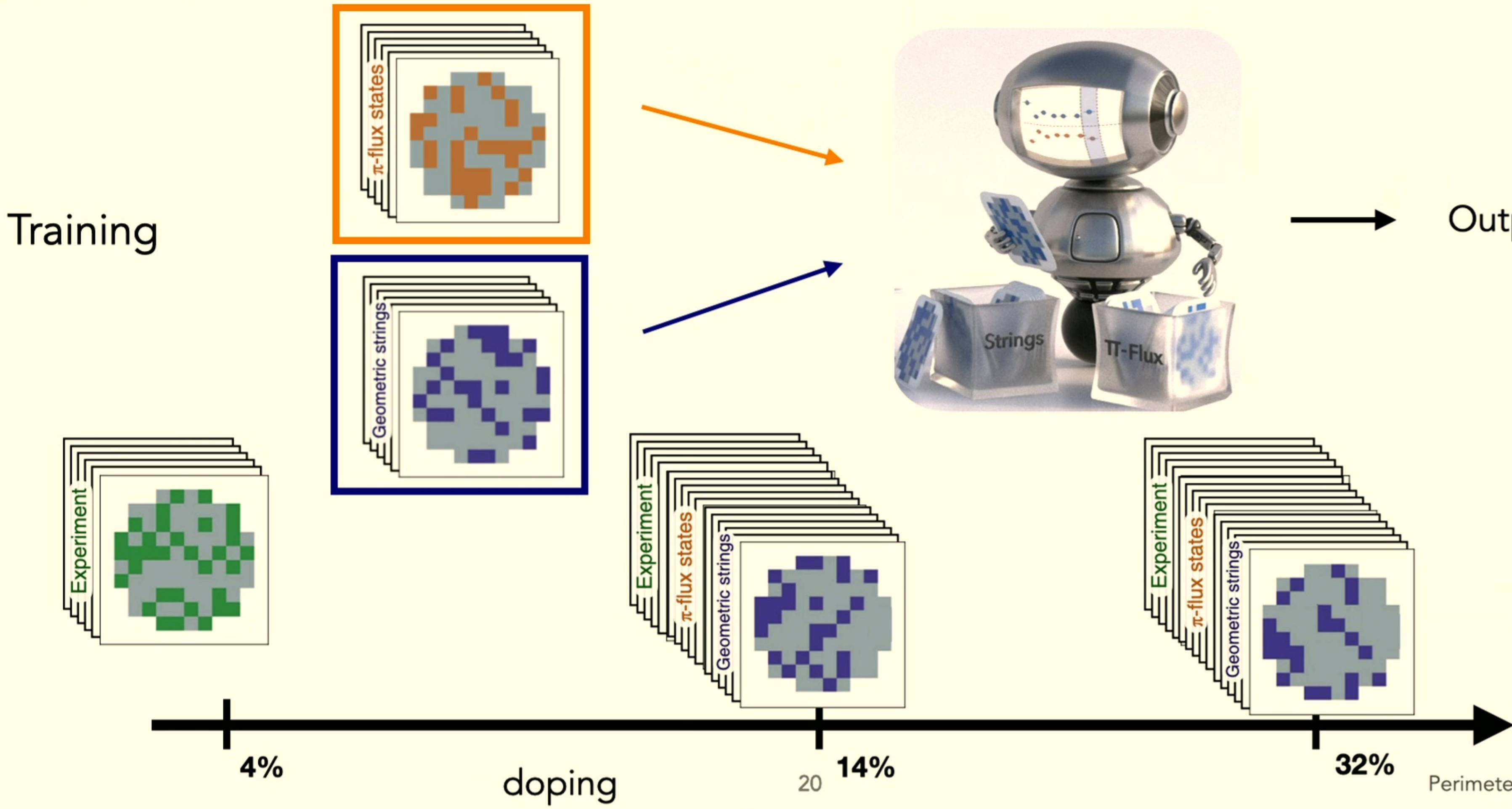


Chiu et al., Science 365, 6450 (2019)

Koepsell et al., Science 374 (2021)

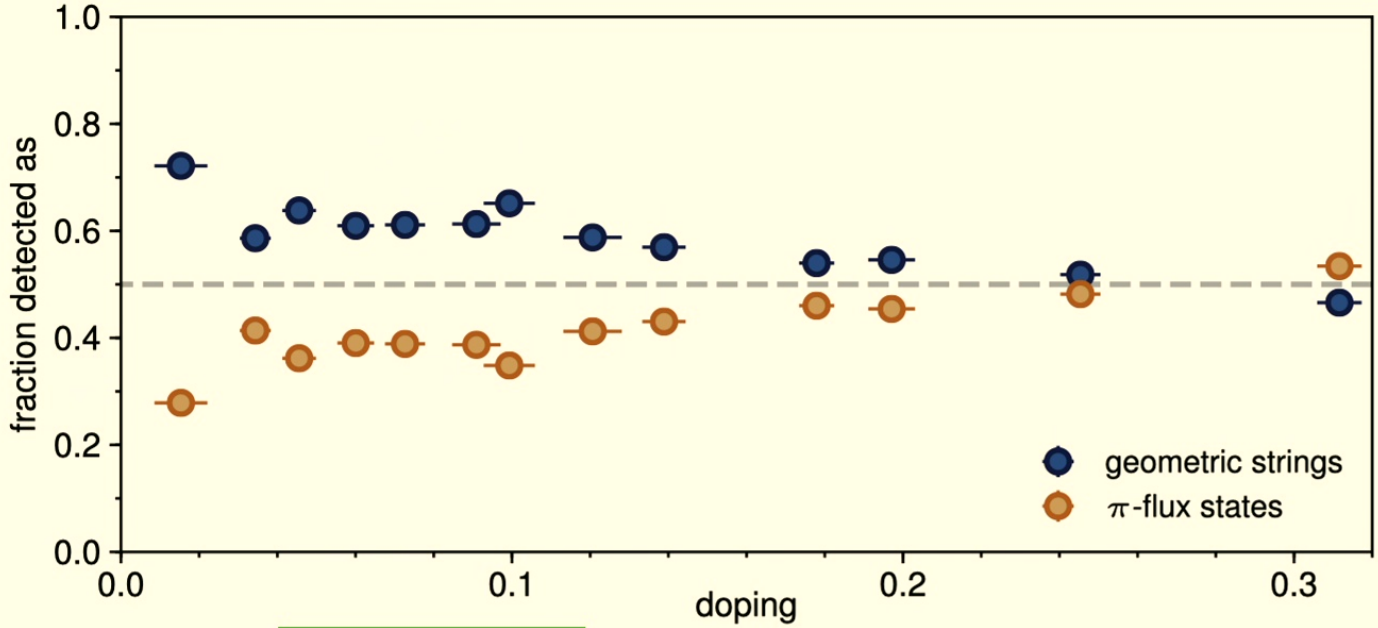
Machine learning snapshots

Annabelle Bohrdt

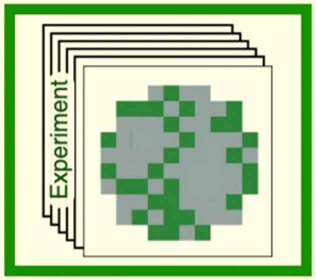


Annabelle Bohrdt

Machine learning snapshots



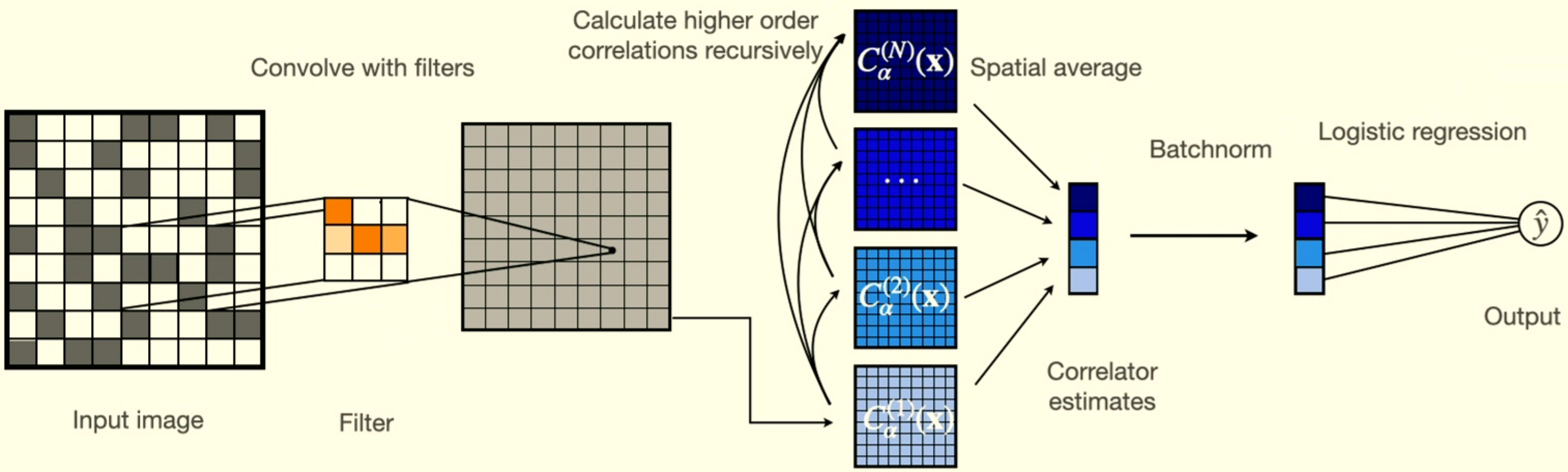
Classify



Output

Bohrdt et al., Nature Physics 15 (2019)

Interpretability



$$C_\alpha^{(1)}(\vec{x}) = \sum_{\vec{a},k} f_{\alpha,k}(\vec{a}) S_k(\vec{x}+\vec{a})$$

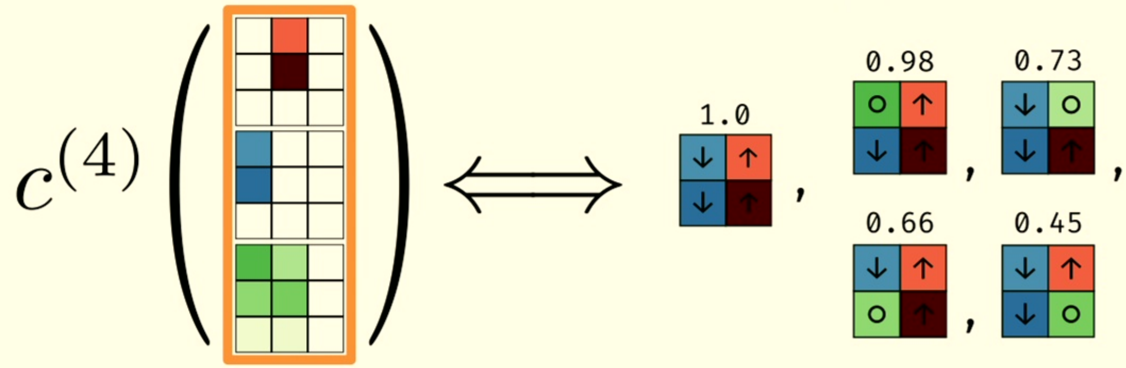
$$C_\alpha^{(2)}(\vec{x}) = \sum_{(\vec{a},k)\neq(\vec{b},k')} f_{\alpha,k}(\vec{a}) f_{\alpha,k'}(\vec{b}) S_k(\vec{x}+\vec{a}) S_{k'}(\vec{x}+\vec{b})$$

C. Miles, A. Bohrdt et al., Nature Communications 12 (2021)

See also: Wetzel & Scherzer, PRB 96 (2017)

Interpretability

Geometric String

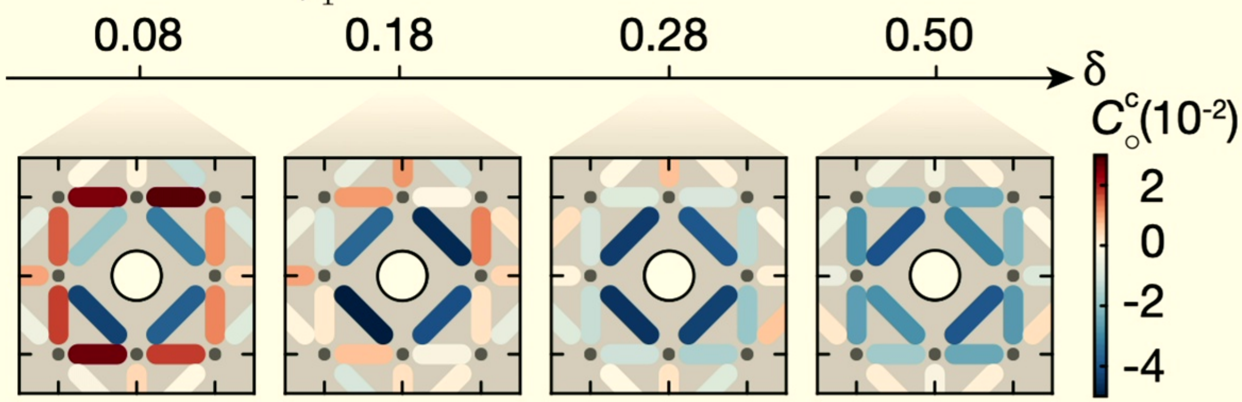


Miles, Bohrdt et al., Nature Communications 12, 3905 (2021)

Annabelle Bohrdt

Phase diagram

$$C^c_\circ(\boldsymbol{r},\boldsymbol{d}) = 4\sum_{\boldsymbol{r}_1}\left\langle \hat{S}^z_{\boldsymbol{r}_1}\hat{S}^z_{\boldsymbol{r}_1+\boldsymbol{d}}\hat{n}^h_{\boldsymbol{r}_1+\boldsymbol{d}/2+\boldsymbol{r}}\right\rangle - \left\langle \hat{S}^z_{\boldsymbol{r}_1}\hat{S}^z_{\boldsymbol{r}_1+\boldsymbol{d}}\right\rangle$$



Koepsell et al., Science 374 (2021)

Annabelle Bohrdt

What have we learned?

Geometric string theory is a good description! What about pairs?

- Strong pairing mechanism in mixed-dimensional bilayer systems
- Internal structure of pairs in 2D systems

RVB state doesn't capture spin-charge correlations correctly

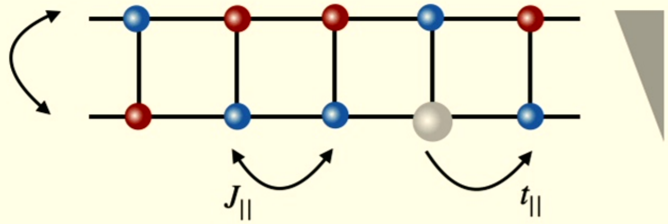
- What about the spin background?

Mixed dimensional systems

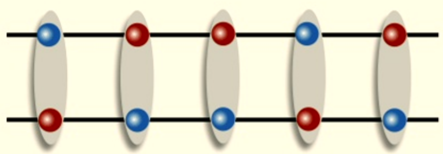
Annabelle Bohrdt

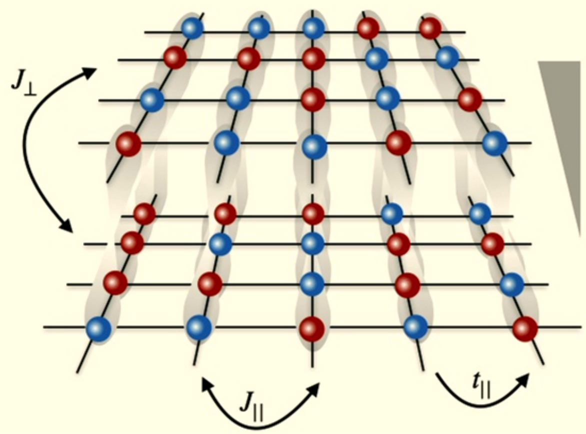
Mixed dimensional bilayer systems

$$J_\perp = \frac{4t^2 U}{U^2 - \Delta^2}$$



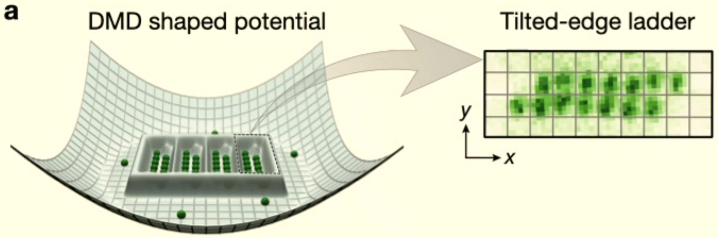
$$\hat{\mathcal{H}} = -t_\parallel \, \hat{\mathcal{P}} \sum_{ij} \sum_{\mu,\sigma=\pm} \left[\hat{c}^\dagger_{\vec{i},\mu,\sigma} \hat{c}_{\vec{j},\mu,\sigma} + h.c. \right] \hat{\mathcal{P}} + \sum_{\langle \vec{i}_\mu \vec{j}_{\mu'} \rangle} J_{\mu,\mu'} \left[\hat{\vec{S}}_{\vec{i}\mu} \cdot \hat{\vec{S}}_{\vec{j},\mu'} - \frac{1}{4} \hat{n}_{\vec{i},\mu} \hat{n}_{\vec{j},\mu'} \right]$$



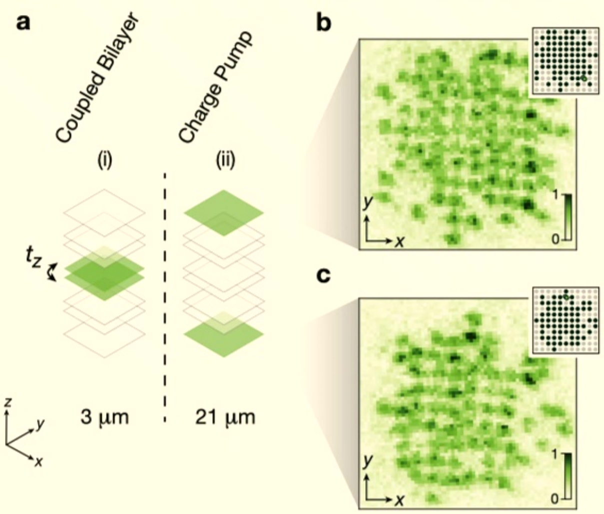


Ladder and bilayer systems

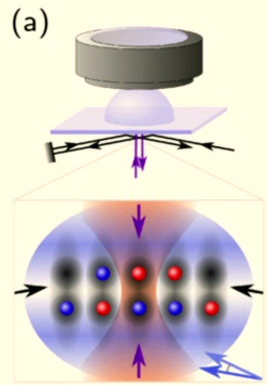
Annabelle Bohrdt



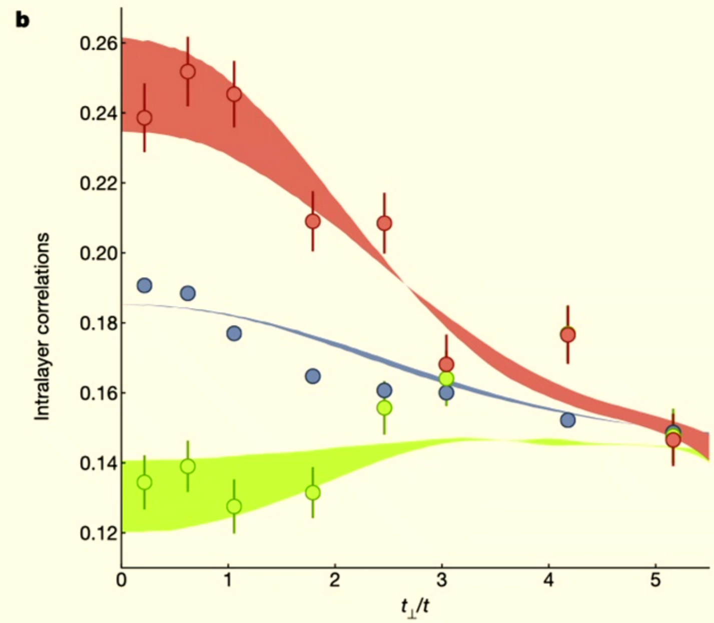
Sompet et al., Nature 606 (2022)



Koepsell et al., PRL 125, 010403 (2020)



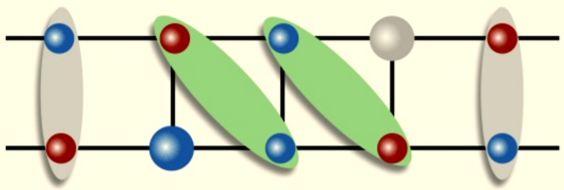
Hartke et al., PRL 125, 113601 (2020)

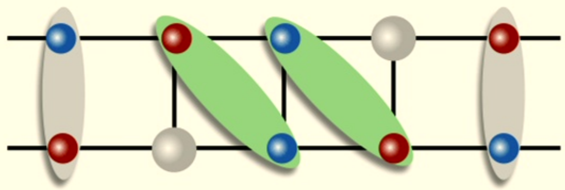


Gall et al., Nature 589, 40–43 (2021)

Annabelle Bohrdt

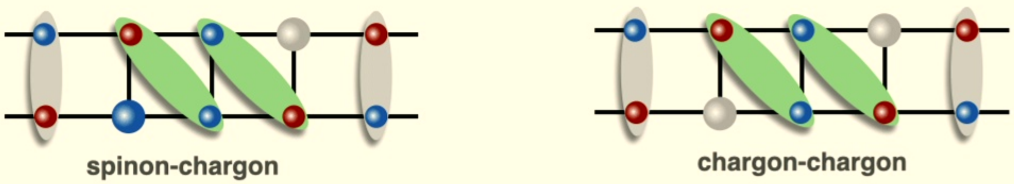
Pairing

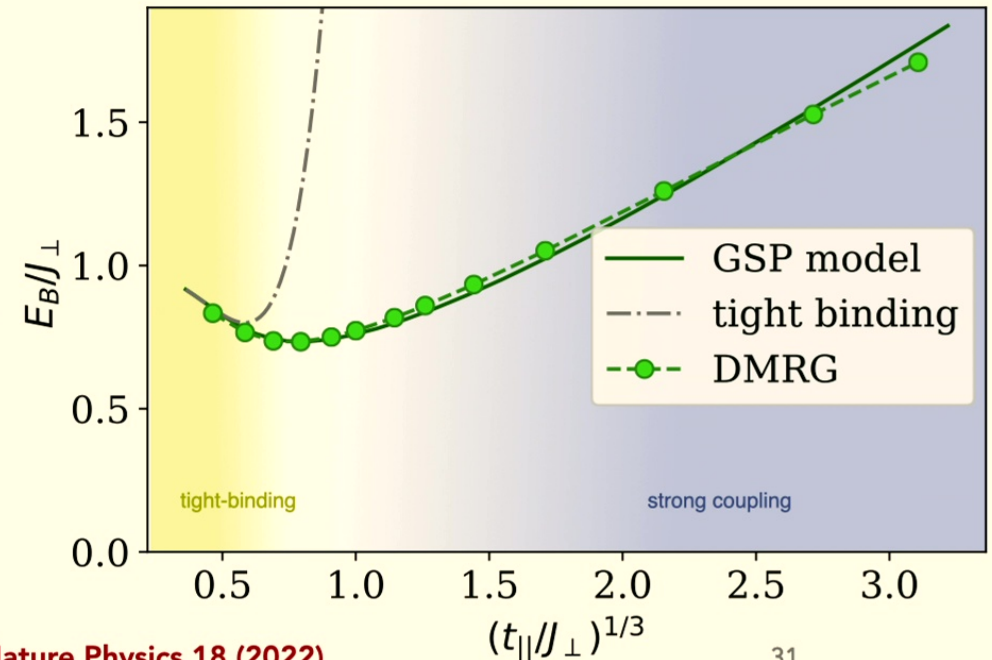




Annabelle Bohrdt

Binding energy





$$E_B = 2 \cdot E_1 - (E_0 + E_2)$$

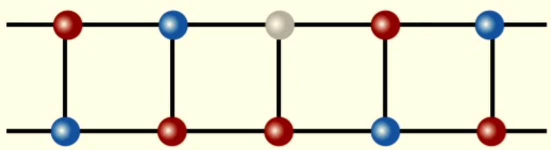
String theory prediction:

$$E_\mathrm{B} = \alpha \underbrace{(2 - 2^{1/3})}_{=0.740\ldots} t^{1/3}\sigma_0^{2/3} + \mathcal{O}(J)$$

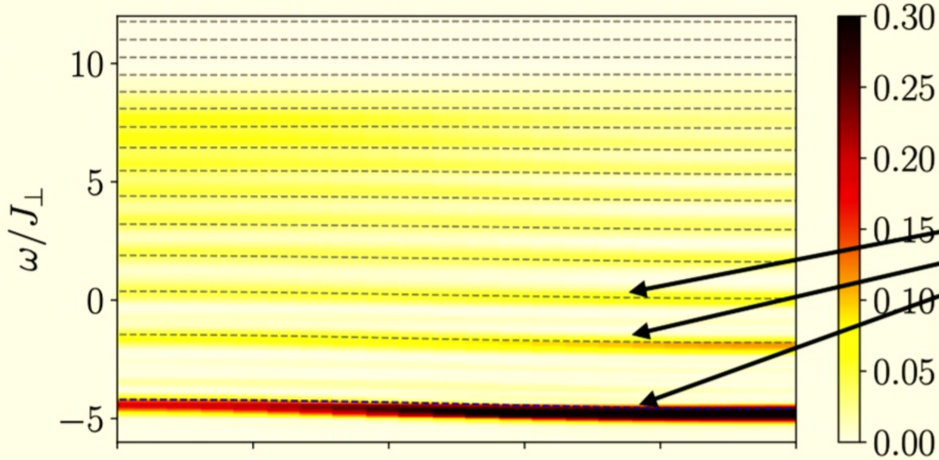
Bohrdt et al., Nature Physics 18 (2022)

Annabelle Bohrdt

Spectral function



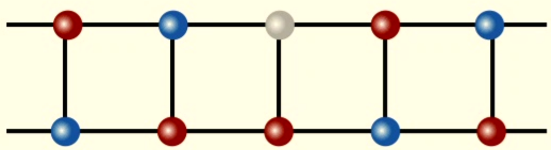
$$A_{1/2}(\vec{k},\omega) = \sum_n \delta(\omega - E_n^{(1)} + E_0) \left| \langle \psi_n \left| \hat{c}_{\vec{k}} \right| \psi_0 \rangle \right|^2$$



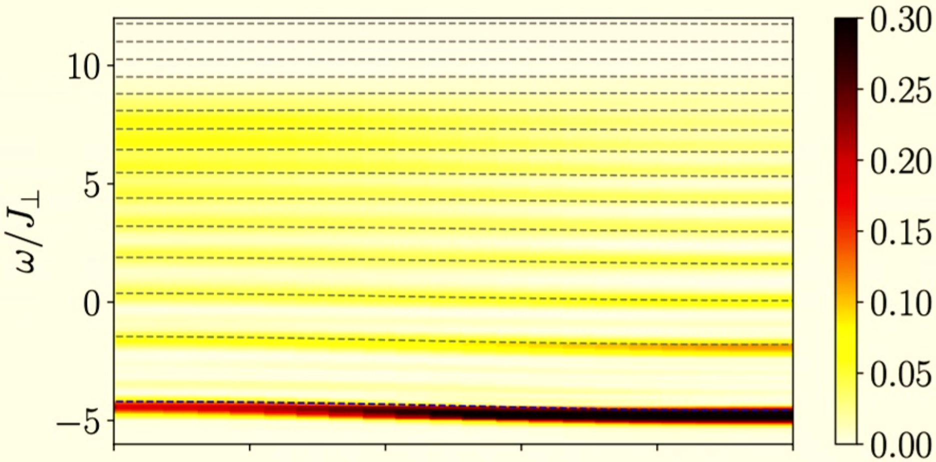
Parton model prediction

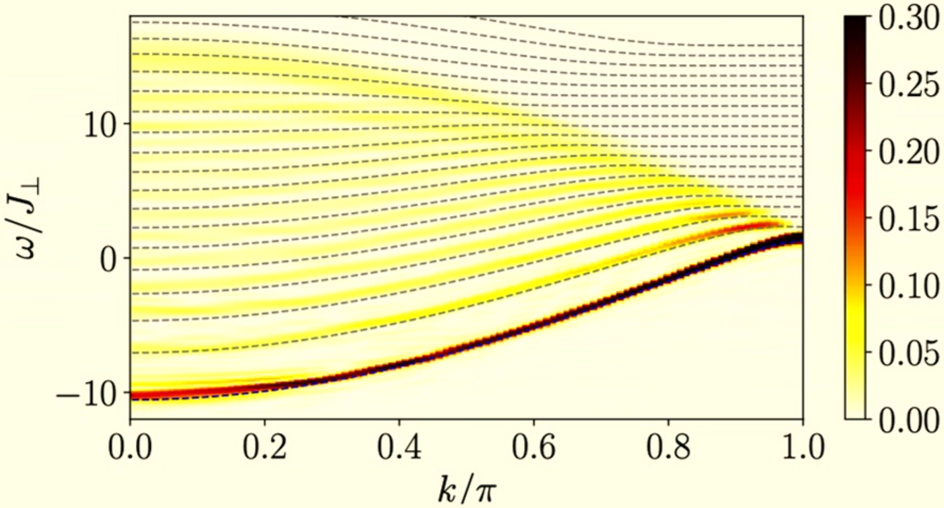
Annabelle Bohrdt

Spectral function



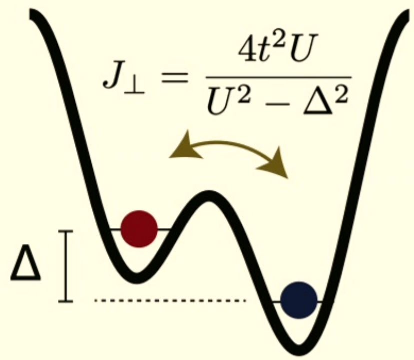
$$A_{1/2}(\vec{k},\omega) = \sum_n \delta(\omega - E_n^{(1)} + E_0) \left| \langle \psi_n \left| \hat{c}_{\vec{k}} \right| \psi_0 \rangle \right|^2$$

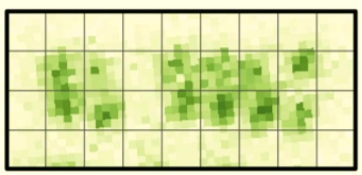




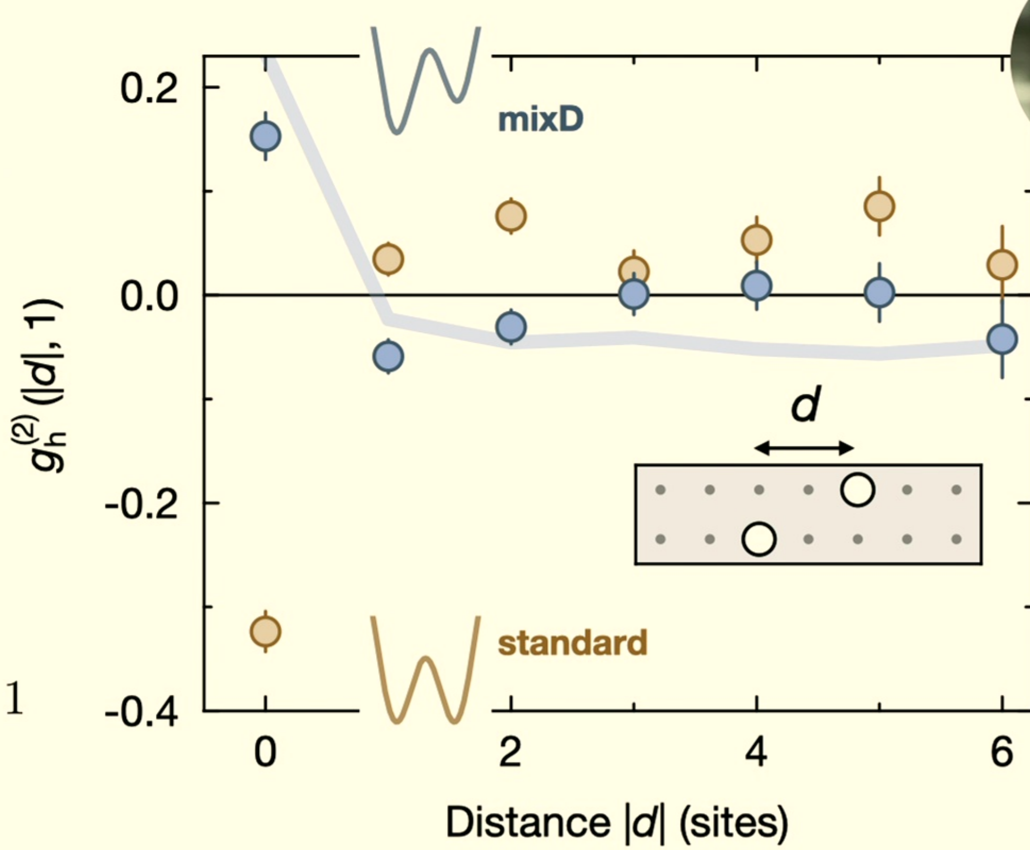
Pairing in mixed dimensions — experiments

Annabelle Bohrdt





$$g_h^{(2)}(\boldsymbol{r}) = \frac{1}{\mathcal{N}_{\boldsymbol{r}}} \sum_{\boldsymbol{i}-\boldsymbol{l}=\boldsymbol{r}} \frac{\langle \hat{n}^h_{\boldsymbol{i}} \hat{n}^h_{\boldsymbol{l}} \rangle}{\langle \hat{n}^h_{\boldsymbol{i}} \rangle \langle \hat{n}^h_{\boldsymbol{l}} \rangle} - 1$$

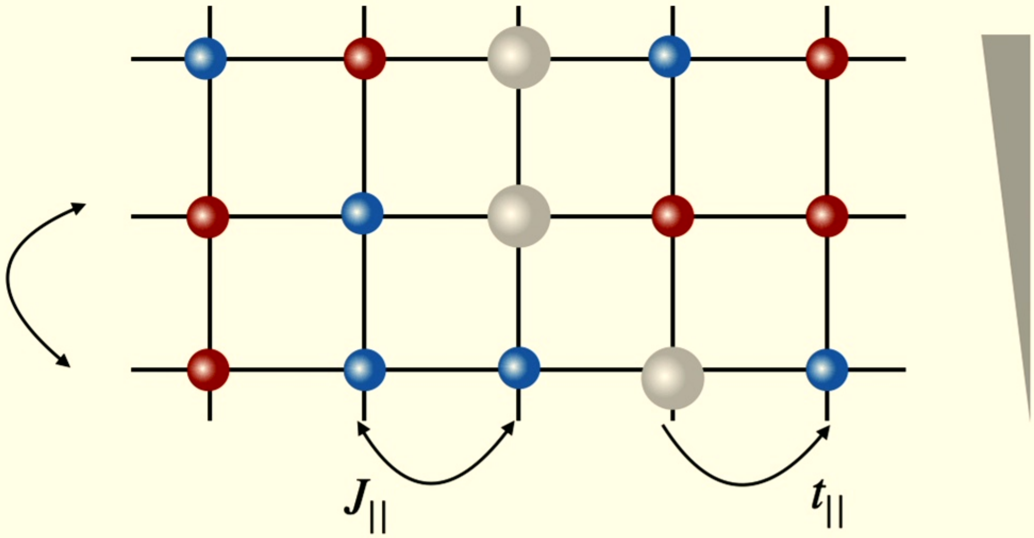


Hirthe et al., arXiv2203.10027

Mixed dimensional 2D systems

Annabelle Bohrdt

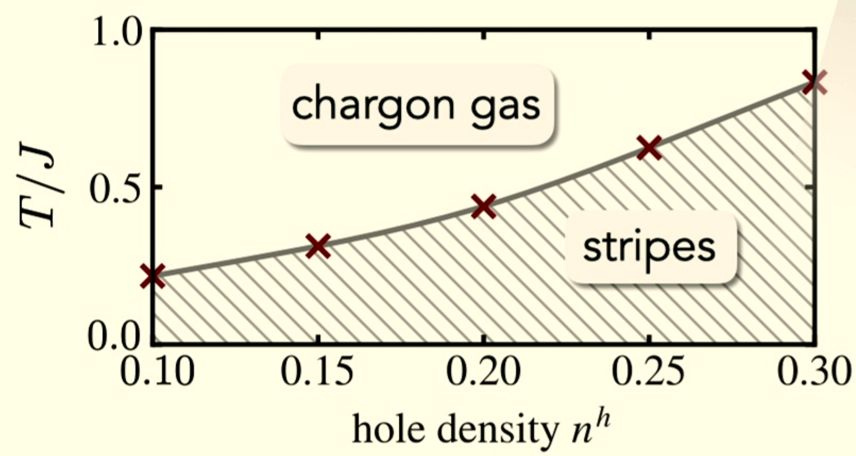
$$J_\perp = \frac{4t^2 U}{U^2 - \Delta^2}$$



$$\hat{\mathcal{H}} = -t_{\parallel}\, \hat{\mathcal{P}} \sum_{ij} \sum_{\mu,\sigma=\pm} \left[\hat{c}^\dagger_{\vec{i},\mu,\sigma} \hat{c}_{\vec{j},\mu,\sigma} + h.c. \right] \hat{\mathcal{P}} + \sum_{\langle \vec{i}_\mu \vec{j}_{\mu'} \rangle} J_{\mu,\mu'} \left[\hat{\vec{S}}_{\vec{i}\mu} \cdot \hat{\vec{S}}_{\vec{j},\mu'} - \frac{1}{4} \hat{n}_{\vec{i},\mu} \hat{n}_{\vec{j},\mu'} \right]$$

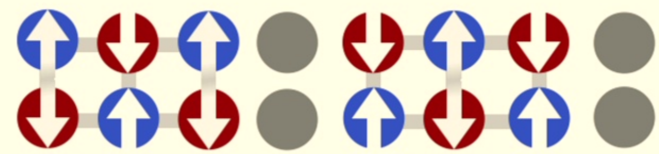
Phase diagram of the mixD $t-J$ model

Annabelle Bohrdt



stripes

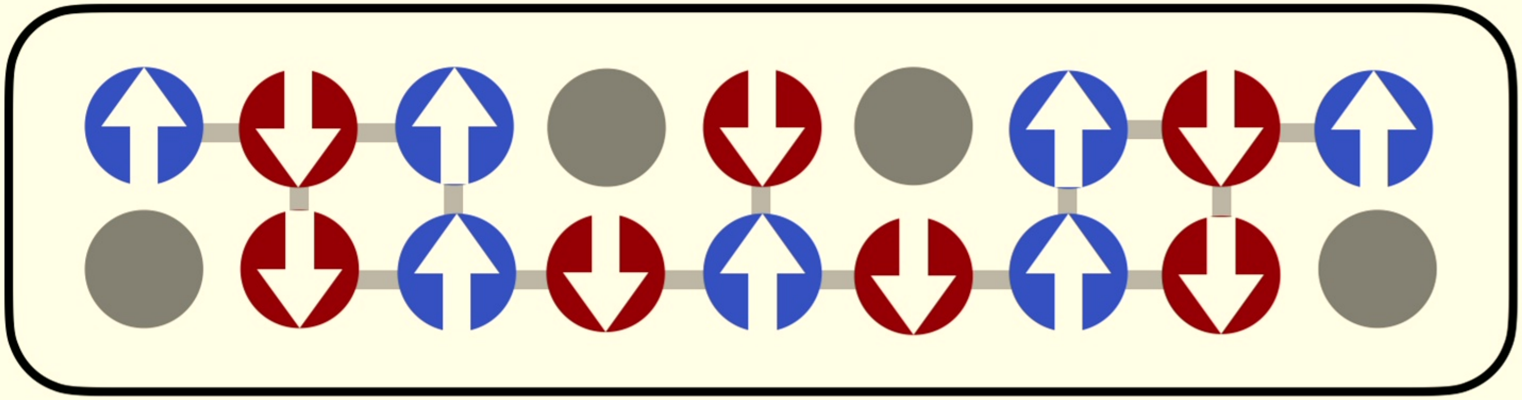
- Stable stripe phase → T_c of order J
- Hidden AFM correlations (long-range incommensurate order in ground state)



Schlömer et al., arXiv 2208.07366

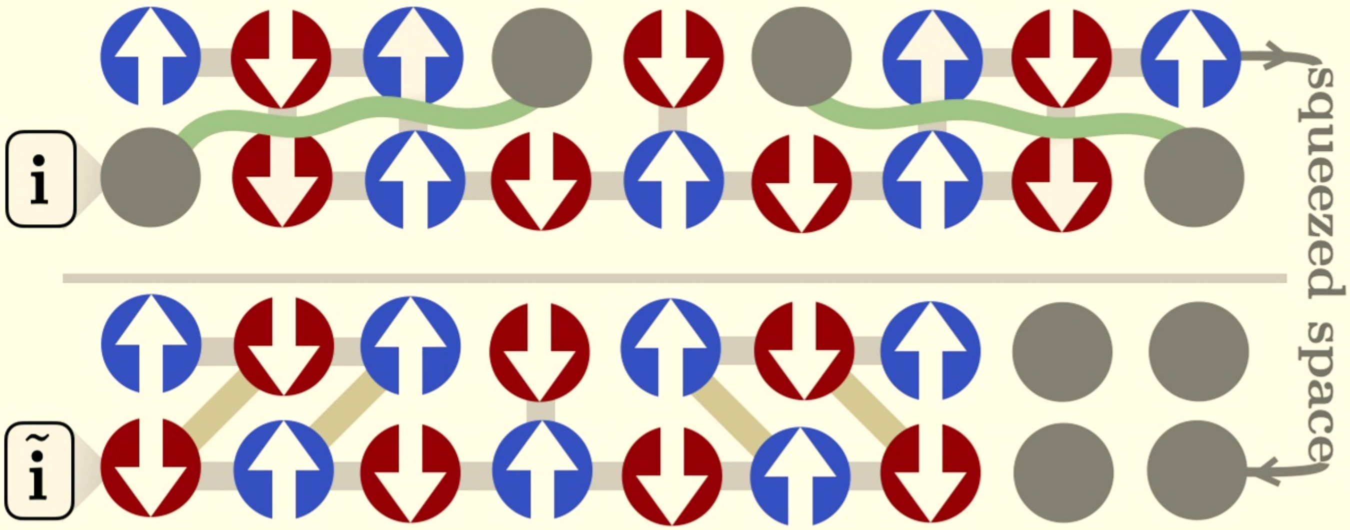
Hole motion induces frustration

Annabelle Bohrdt



Hole motion induces frustration

Annabelle Bohrdt



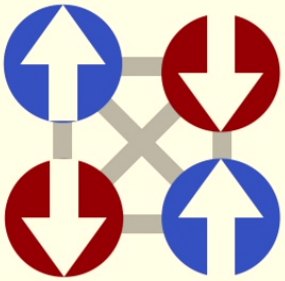
Squeezing

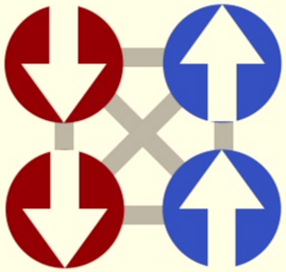
Effective diagonal, frustrating magnetic interactions

MixD setting: squeezed space well defined → ideal platform to quantify frustration

Annabelle Bohrdt

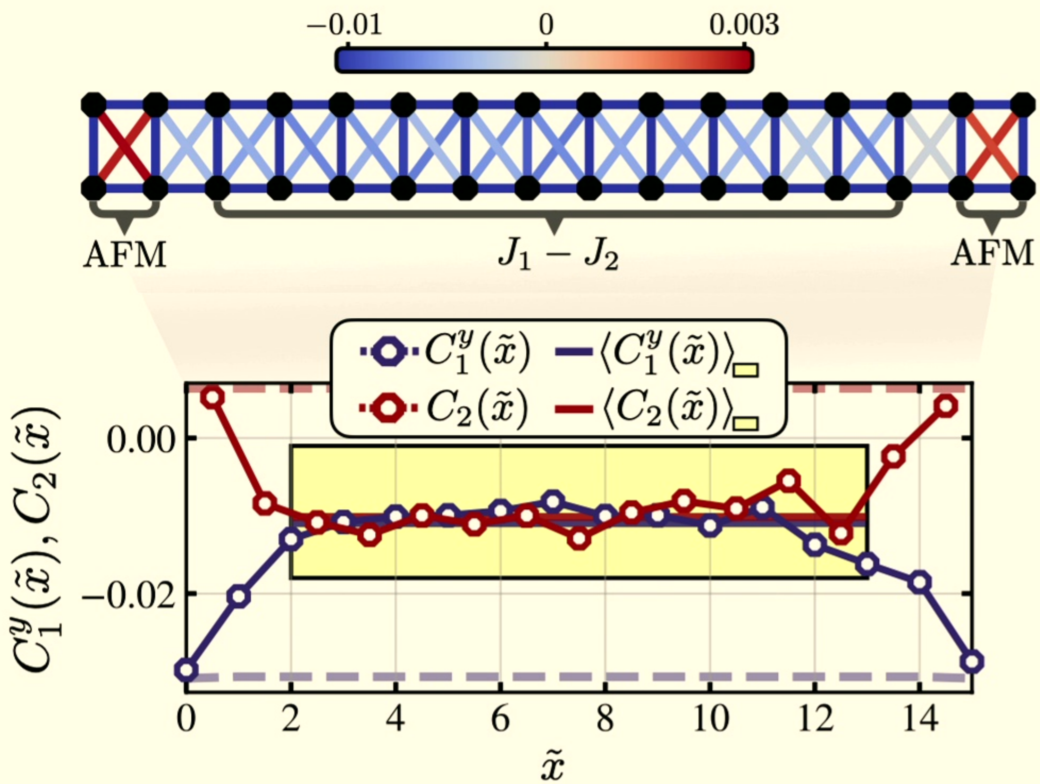
Frustration





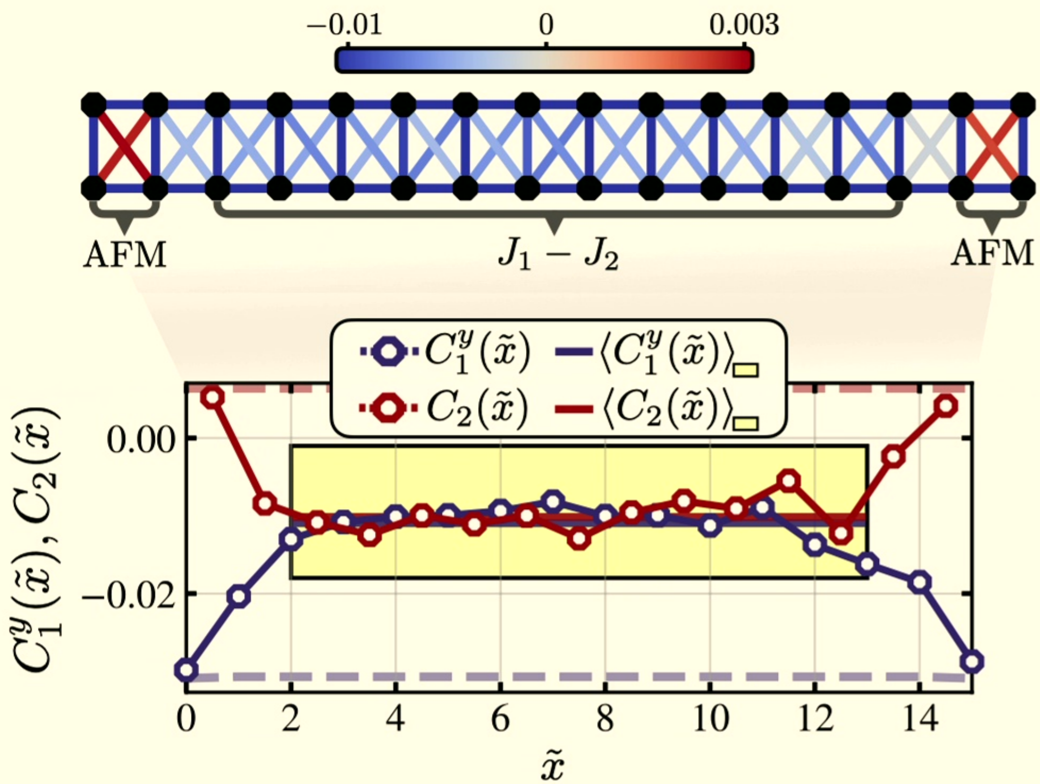
Annabelle Bohrdt

Correlations in squeezed space



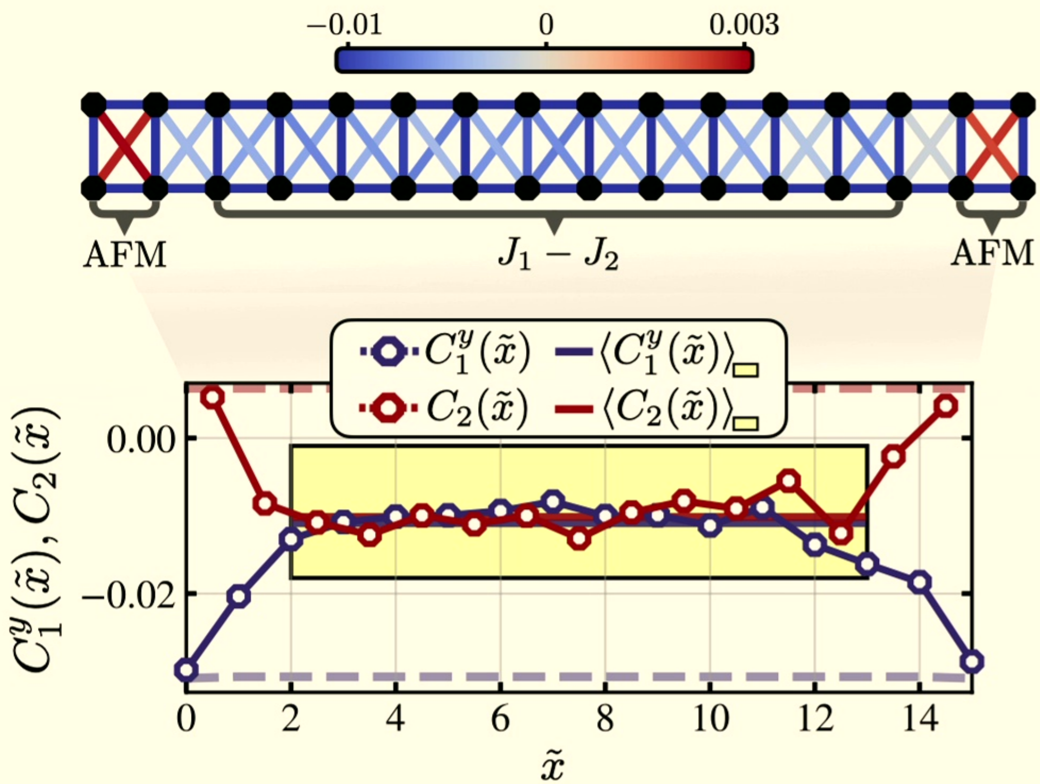
Schlömer,..., AB, arXiv2210.XXXX

Correlations in squeezed space



$$\hat{\mathcal{H}}_{\{J_H\}} = \sum_{\mu=x,y} J_1^\mu \sum_{\langle \tilde{\mathbf{i}},\tilde{\mathbf{j}}\rangle_\mu} \hat{\mathbf{S}}_{\tilde{\mathbf{i}}} \cdot \hat{\mathbf{S}}_{\tilde{\mathbf{j}}} + J_2 \sum_{\langle\langle \tilde{\mathbf{i}},\tilde{\mathbf{j}}\rangle\rangle_{\mathrm{diag}}} \hat{\mathbf{S}}_{\tilde{\mathbf{i}}} \cdot \hat{\mathbf{S}}_{\tilde{\mathbf{j}}}$$

Correlations in squeezed space



$$\hat{\mathcal{H}}_{\{J_H\}} = \sum_{\mu=x,y} J_1^\mu \sum_{\langle \tilde{\mathbf{i}},\tilde{\mathbf{j}}\rangle_\mu} \hat{\mathbf{S}}_{\tilde{\mathbf{i}}} \cdot \hat{\mathbf{S}}_{\tilde{\mathbf{j}}} + J_2 \sum_{\langle\langle \tilde{\mathbf{i}},\tilde{\mathbf{j}}\rangle\rangle_{\text{diag}}} \hat{\mathbf{S}}_{\tilde{\mathbf{i}}} \cdot \hat{\mathbf{S}}_{\tilde{\mathbf{j}}}$$

- SU(2) invariance — only need snapshots in z-basis!
- Only need to numerically simulate a spin Hamiltonian!

Schlömer,…, AB, arXiv2210.XXXX

Annabelle Bohrdt

Hamiltonian reconstruction scheme

Hamiltonian $H(\mu) = \sum_{l=1}^{m} \mu_l E_l$

E_l form a standard operator basis for local interactions

Thermal state $\rho_\beta(\mu) = \frac{e^{-\beta H(\mu)}}{Z_\beta(\mu)}$

Measure: $e_l = \mathrm{Tr}[\rho_\beta(\mu) E_l]$

Measurement of local expectation values sufficient for reconstruction

Find quantum state that fulfills $\mathrm{Tr}[\sigma E_l] = e_l$ and maximizes entropy $S(\sigma) = -\mathrm{Tr}[\sigma \log \sigma]$

Anshu et al., Nature Physics 17 (2021)

Hamiltonian reconstruction scheme

Annabelle Bohrdt

Hamiltonian $H(\mu) = \sum_{l=1}^{m} \mu_l E_l$

E_l form a standard operator basis for local interactions

Thermal state $\rho_\beta(\mu) = \frac{e^{-\beta H(\mu)}}{Z_\beta(\mu)}$

Measure: $e_l = \mathrm{Tr}[\rho_\beta(\mu) E_l]$

Measurement of local expectation values sufficient for reconstruction

Find quantum state that fulfills $\mathrm{Tr}[\sigma E_l] = e_l$ and maximizes entropy $S(\sigma) = -\mathrm{Tr}[\sigma \log \sigma]$

Anshu et al., Nature Physics 17 (2021)

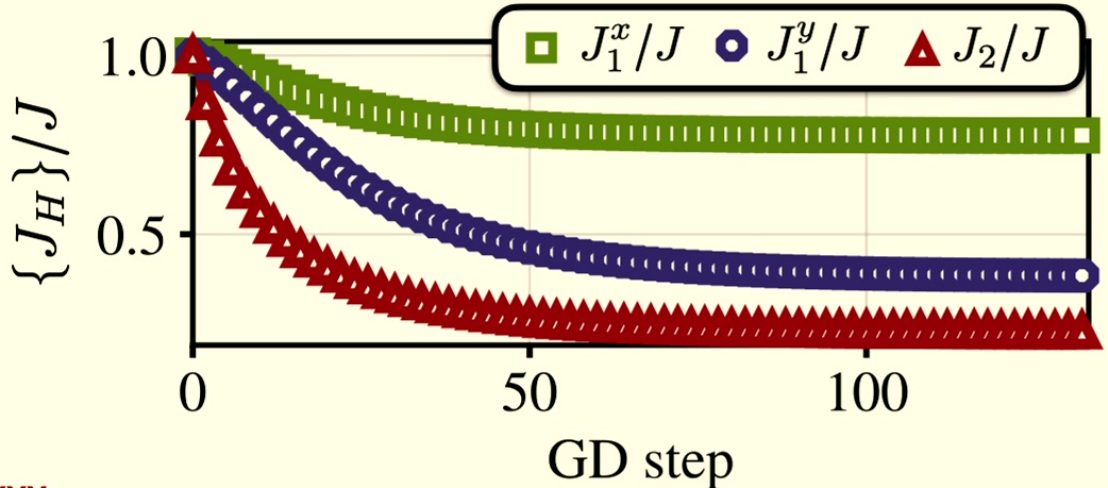
Hamiltonian reconstruction scheme

- Hamiltonian reconstruction via gradient descent

→ Minimize objective function $\mathcal{G} = \ln Z(\beta, \{J_H\}) + 3\beta \left(\sum_{\mu=x,y} J_1^\mu \mathcal{M}_1^\mu + J_2 \mathcal{M}_2 \right)$

Simulated, purely magnetic model

Measured correlations in squeezed space

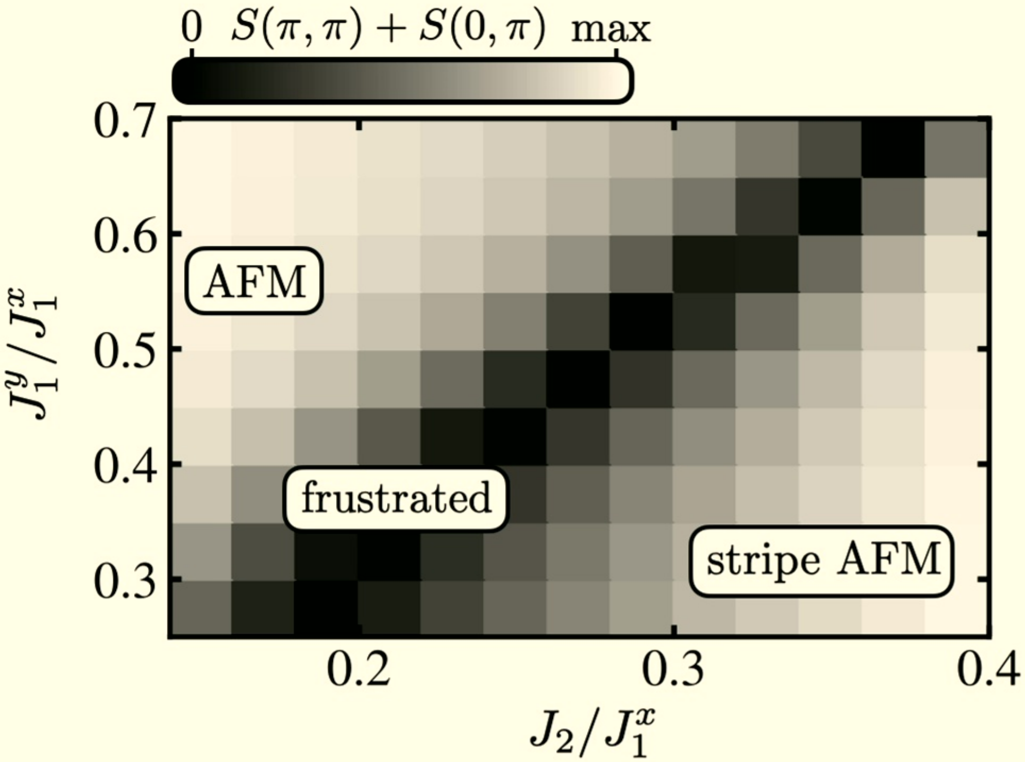


Schlömer et al., arXiv2210.XXXX

Quantifying frustration

Annabelle Bohrdt

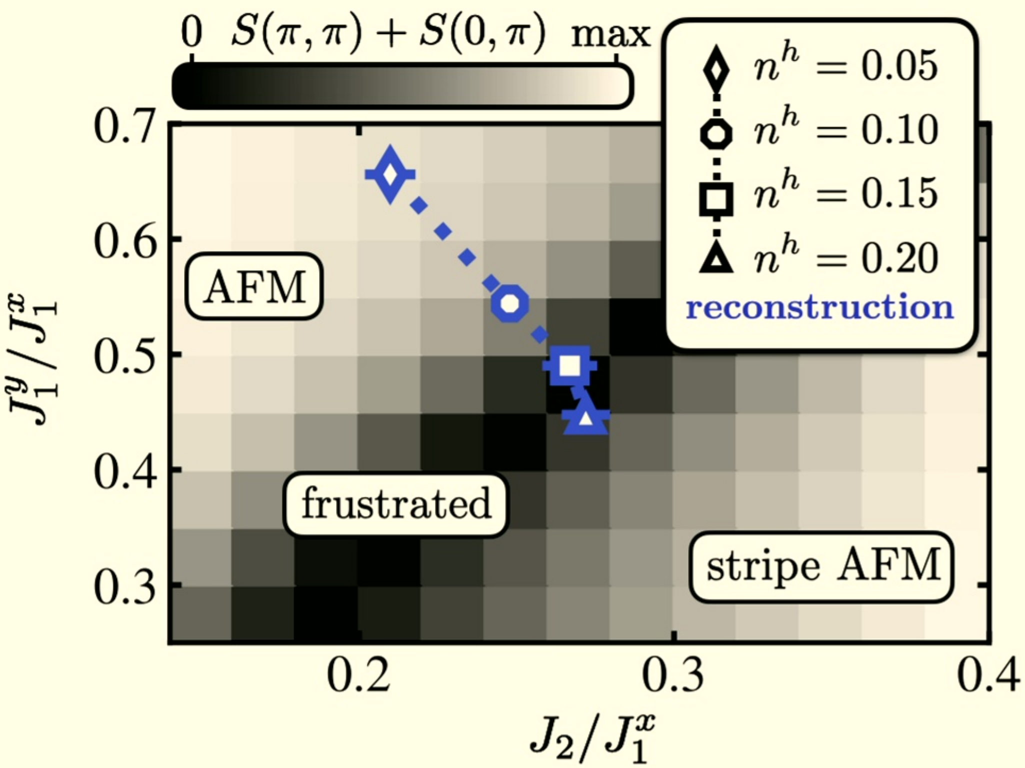
$T/J = 1.67,\ t/J = 3$



Schlömer et al., arXiv2210.XXXX

Quantifying frustration

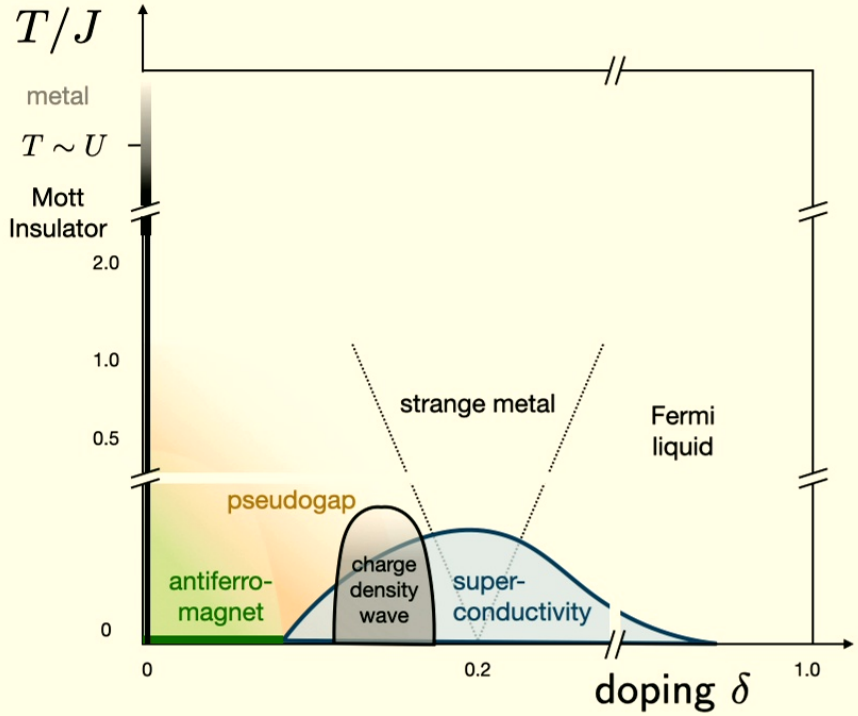
$T/J = 1.67,\ t/J = 3$

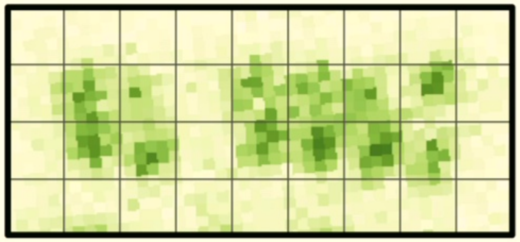


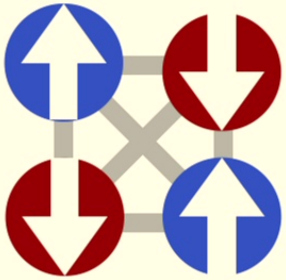
Schlömer et al., arXiv2210.XXXX

Annabelle Bohrdt

Summary







Perimeter, Oct 2022

Thank you for your attention!

Fabian Grusdt

Hannah Lange
Matjaz Kebric
Felix A. Palm
Maximilian Buser
Lukas Homeier
Christian Reinmoser

Henning Schlömer

Immanuel Bloch
Christian Gross
Joannis Koepsell
Jayadev Vijayan
Pimonpan Sompet
Guillaume Salomon
Dominik Bourgund
Petar Bojovic
Timon Hilker
Thomas Chalopin
Sarah Hirthe
Ulrich Schollwöck
Lode Pollet
Eugene Demler
Yao Wang
Cole Miles
Eun-Ah Kim
Michael Knap
Frank Pollmann
…

Markus Greiner
Daniel Greif
Christie Chiu
Geoffrey Ji
Muqing Xu
Martin Lebrat
Lev Kendrick
Justus Brüggenjürgen
Anant Kale
Julian Léonard
Sooshin Kim
Matthew Rispoli
Alex Lukin
Robert Schittko