Diagrammatic Monte Carlo for the Hubbard model

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RPMBT 22, Tsukuba, Japan

26 September 2024

Plan

- How to compute lots of Feynman Diagrams (and why)
- Electrons interacting with AFM fluctuations
- Stripes signatures at intermediate temperature?
- Origin and fate of the pseudogap

Collaborators

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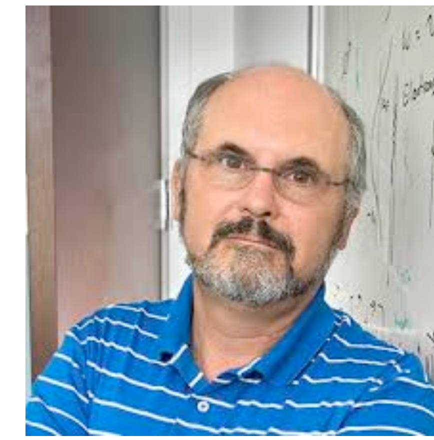

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Why computing (a lot of) Feynman diagrams?

Fermionic sign problem

- Traditional Quantum Monte Carlo

$$\langle \hat{Q} \rangle := \frac{Z_{\hat{Q}}}{Z}$$

$\mathbf{e}^{\#\beta\,\mathbf{N}_{\text{electrons}}}$

unphysical non-locality for fermions

Signal-to-noise-ratio $\sim e^{-\#\beta N_{\text{electrons}}}$

Fermionic sign problem

- Traditional Quantum Monte Carlo

$$\langle \hat{Q} \rangle := \frac{Z_{\hat{Q}}}{Z} \quad \leftarrow \mathbf{e}^{\# \beta\, \mathbf{N}_{\text{electrons}}}$$

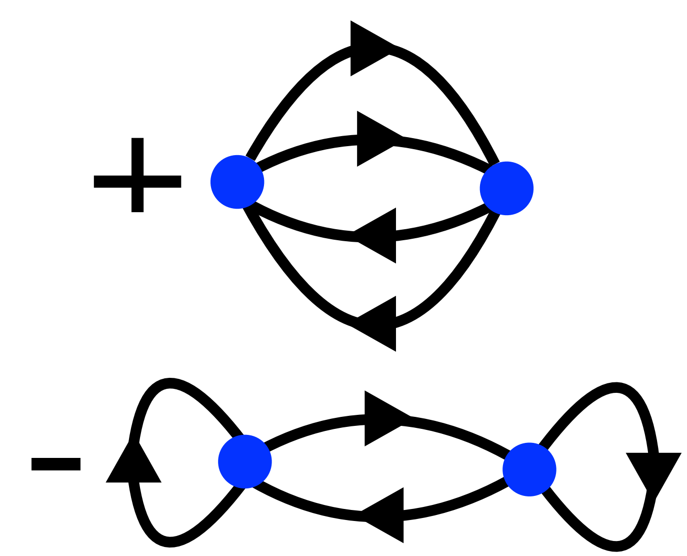
unphysical non-locality for fermions

Signal-to-noise-ratio $\sim e^{-\# \beta N_{\text{electrons}}}$

- Diagrammatic Monte Carlo

$$\langle \hat{Q} \rangle = Q_0 + g\, Q_1 + g^2 Q_2 + \ldots$$

Small signal $\Longleftrightarrow$ Small correction

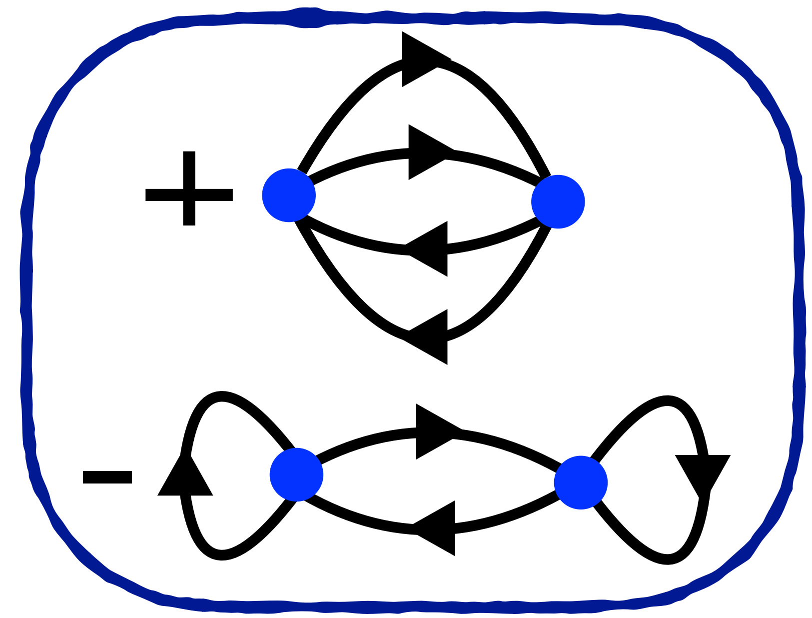


Diagrammatic Monte Carlo: cancellations are welcome

Analytics

$$\langle \hat{Q} \rangle = Q_0 + g\, Q_1 + g^2 Q_2 + \ldots$$

Monte Carlo



Bosons: $Q_n \sim n!$

Fermions on a lattice: $Q_n \sim (-R)^{-n}$

=> analytic continuation

Unitary Fermi Gas: $Q_n \sim (n!)^{1/5}$

=> conformal-Borel resummation

Factorial cancellations

Prokof'ev, Svistunov, PRL 2008

[RR, Ohgoe, Van Houcke, Werner, PRL 2018]

Bare series convergence: lattice fermions T>0

$$R_\beta := \lim_{L\to\infty} \min_n |z_{L,\beta;n}|$$

Theorem:

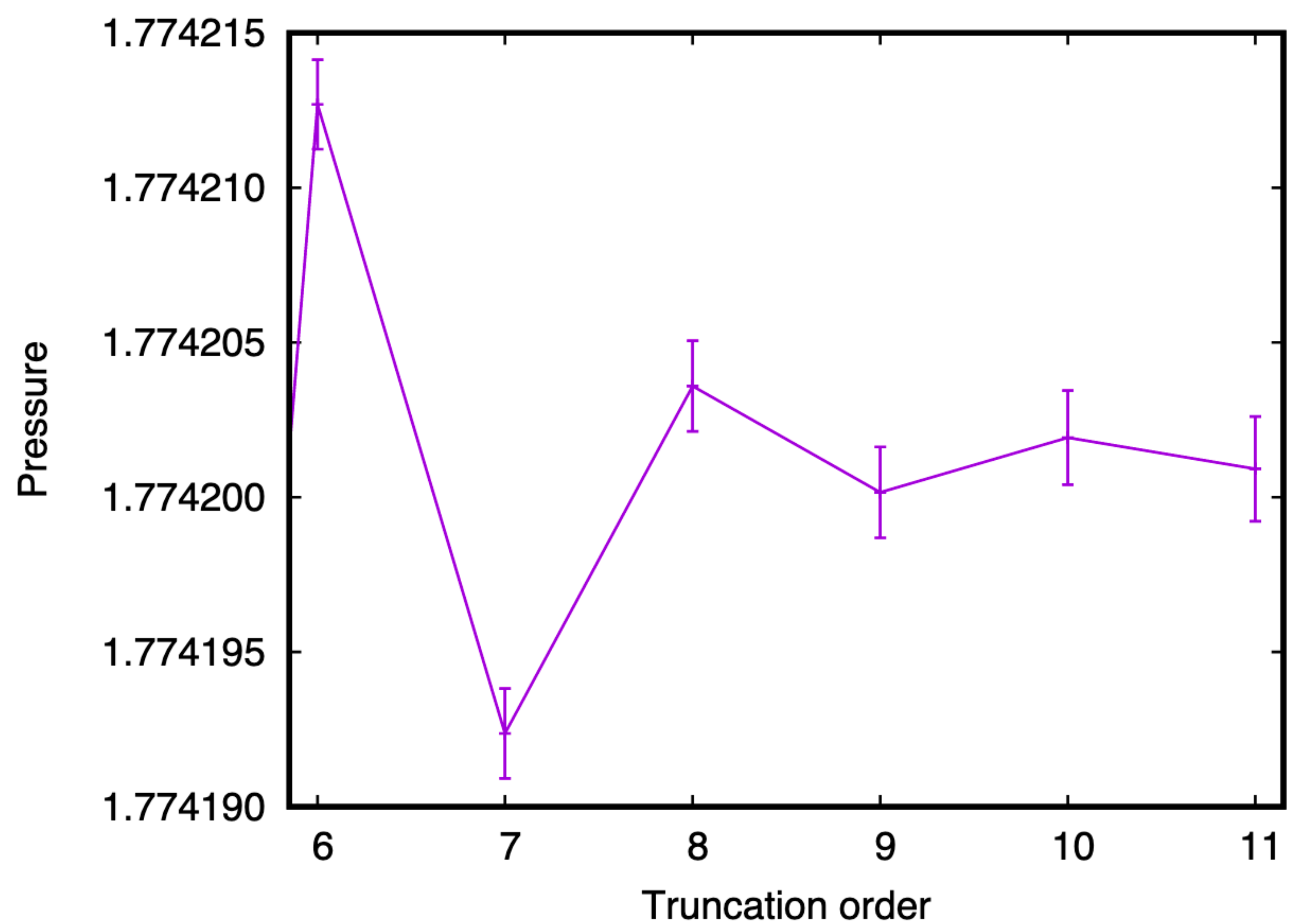
[Benfatto et al., Annales H. Poincaré 2006]:

$$R_\beta \underset{\beta\to\infty}{\gtrsim} \frac{1}{\log \beta}$$

<u>Dyson's argument:</u> $T > 0$ finite radius of convergence

Numerics:

$T/t = 1/8,\ U/t = 2,\ n = 0.87500(2)$

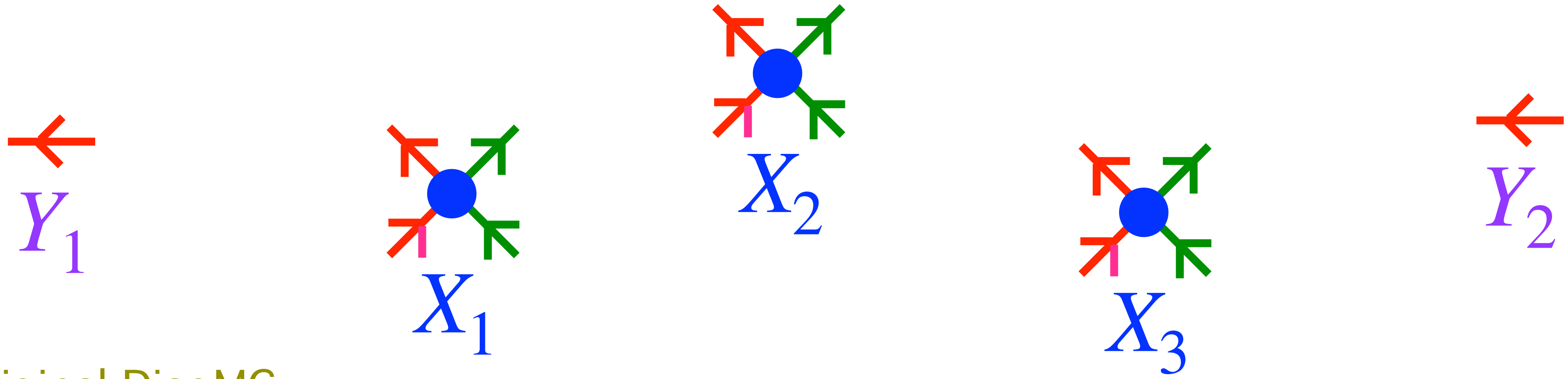


[RR, PRL 2017]

How to compute (a lot of) Feynman diagrams?

CDet main idea

O((n!)^2)



Original DiagMC
[Prokof'ev, Svistunov, PRL 1998]

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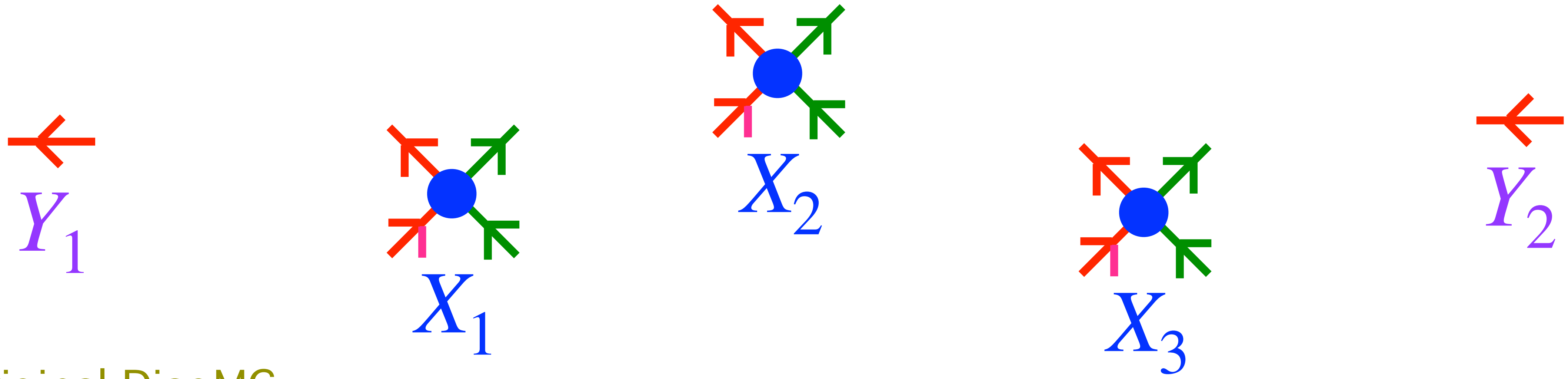

Original DiagMC
[Prokof’ev, Svistunov, PRL 1998]

$$A_{Y_1,Y_2}(\{X_1, X_2, X_3\}) := \det \begin{pmatrix} G(X_1,X_1) & G(X_1,X_2) & G(X_1,X_3) \\ G(X_2,X_1) & G(X_2,X_2) & G(X_2,X_3) \\ G(X_3,X_1) & G(X_3,X_2) & G(X_3,X_3) \end{pmatrix} \times$$

CT-INT
[Rubtsov, arXiv2003]
[Rubtsov, Savkin, Lichtenstein, PRB 2005]
[Bourovski, Prokof’ev, Svistunov, PRB 2004]

$$\det \begin{pmatrix} G(X_1,X_1) & G(X_1,X_2) & G(X_1,X_3) & G(X_1,Y_2) \\ G(X_2,X_1) & G(X_2,X_2) & G(X_2,X_3) & G(X_1,Y_2) \\ G(X_3,X_1) & G(X_3,X_2) & G(X_3,X_3) & G(X_1,Y_2) \\ G(Y_1,X_1) & G(Y_1,X_2) & G(Y_1,X_3) & G(Y_1,Y_2) \end{pmatrix}$$

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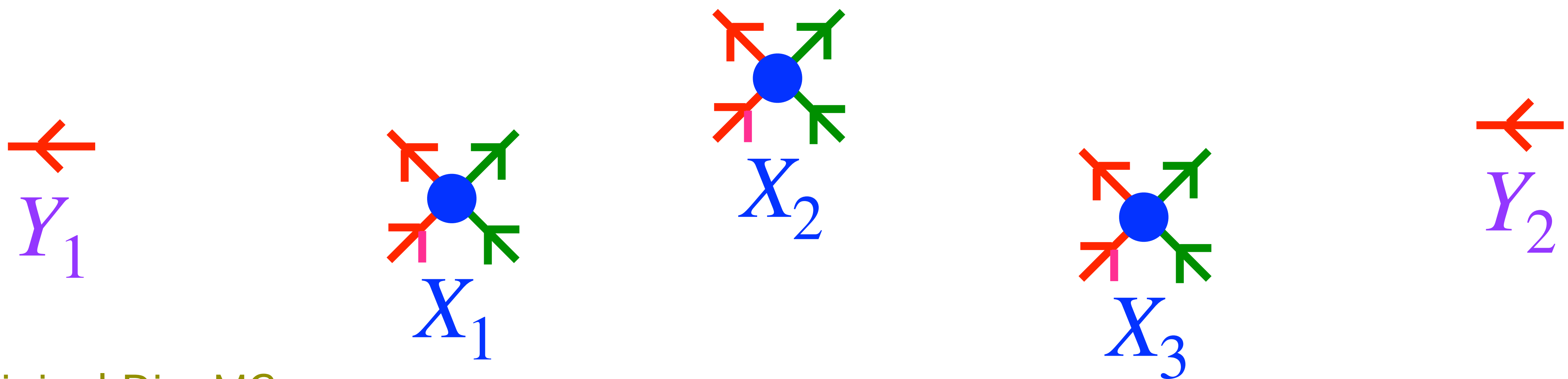

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CDet

$$C_{Y_1,Y_2}(\{X_1,X_2,X_3\}) := A_{Y_1,Y_2}(\{X_1,X_2,X_3\}) - \sum_{S\subsetneq\{X_1,X_2,X_3\}} C_{Y_1,Y_2}(S)\, A_{Y_1,Y_2}(\{X_1,X_2,X_3\}\backslash S)$$

[RR, PRL'17]

O(3^n)

Polynomial complexity of lattice fermions at non-zero T

CDet CPU time: $t_N \sim 3^N \times \left(\frac{|U|}{R_{A,\beta}} \right)^{2N}$

recursive formula

Monte Carlo variance

Exponential cost vs
Exponential convergence: $t(\epsilon) \sim \epsilon^{-\alpha}$

[RR et al, EPL'16]

[Troyer, Wiese, PRL'05]

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Exponential cost vs Exponential convergence: $$t(\epsilon) \sim \epsilon^{-\alpha}$$

[RR et al, EPL'16]

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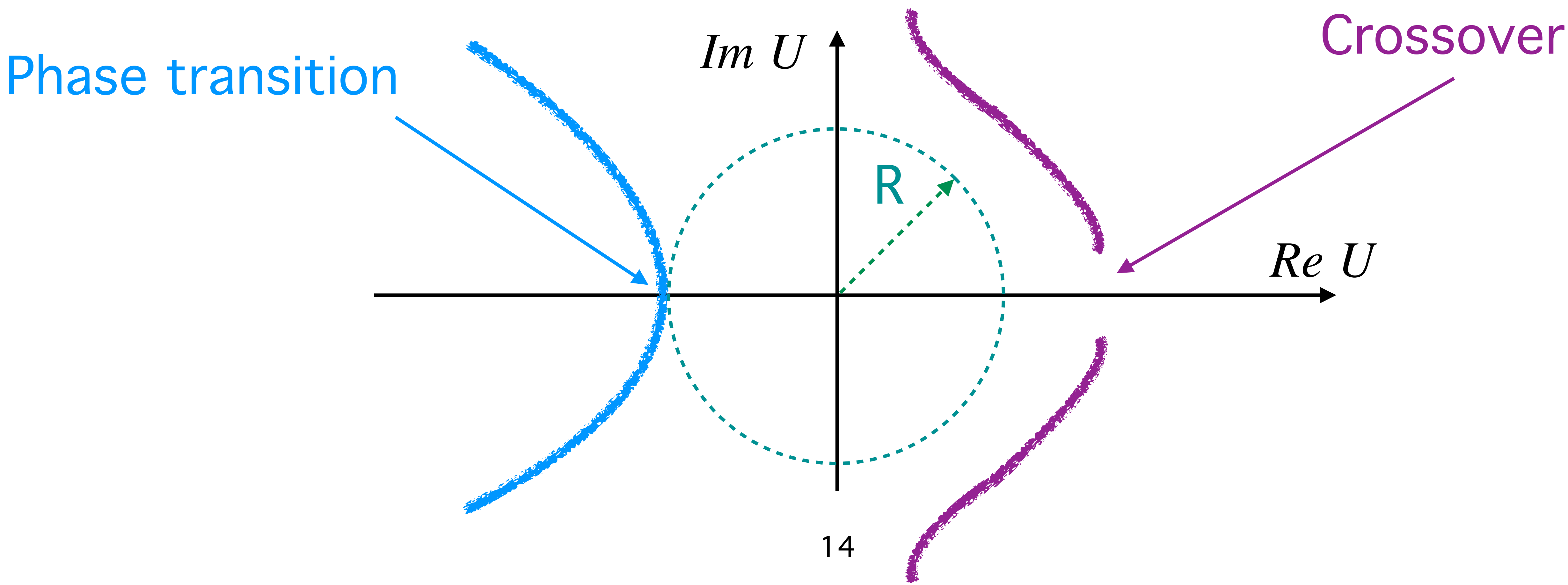


Algebraic renormalization

$$C[G_0, U] = \frac{A[G_0, U]}{Z[G_0, U]}, \qquad C(\{X_1, \ldots, X_n\}) := \frac{\delta^n}{\delta U(X_1) \ldots U(X_n)} C[G_0, U] \Big|_{U=0}$$

Nilpotent polynomials (aka hyperdual numbers)

$$U(z)(X) = \sum_{j=1}^{n} z_j \, \delta(X - X_j), \qquad [z_j, z_k] = 0, \quad z_j^2 = 0$$

$$C(z) := C[G_0, U(z)] = \frac{A[G_0, U(z)]}{Z[G_0, U(z)]} = \frac{A(z)}{Z(z)}, \qquad \frac{\partial^n}{\partial z_1 \ldots \partial z_n} C(z) = C(\{X_1, \ldots, X_n\})$$

$\Longrightarrow$ CDet is just a hyperdual-number polynomial division

Renormalization $\equiv [G_0(z), \Gamma_0(z)]$

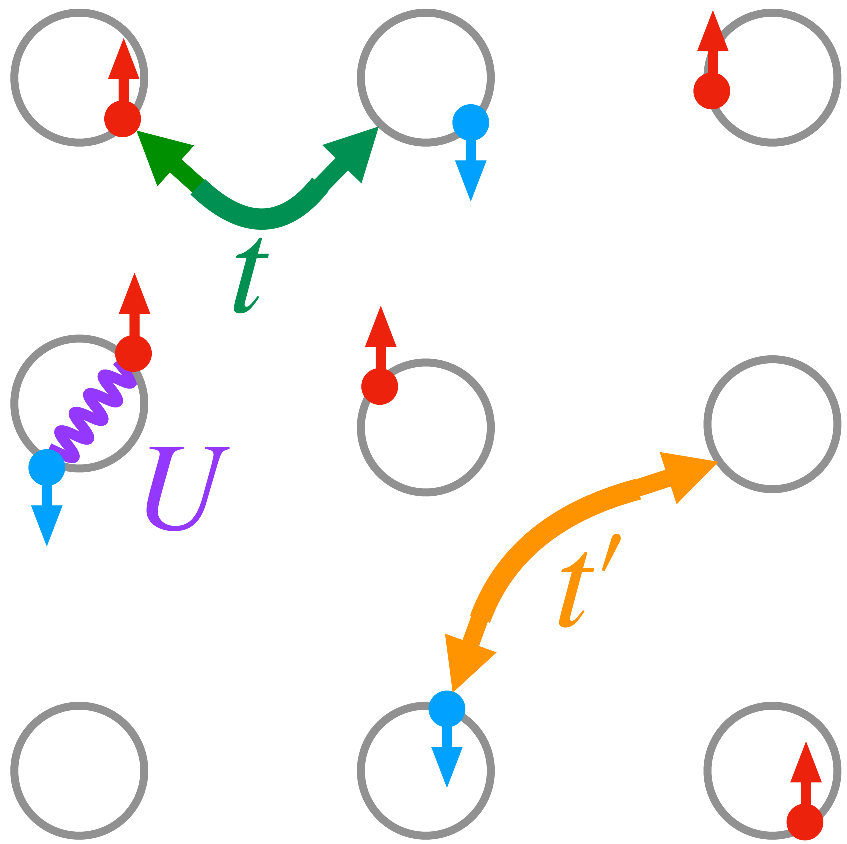
$\Longrightarrow$ „Bare“ CDet is all one needs

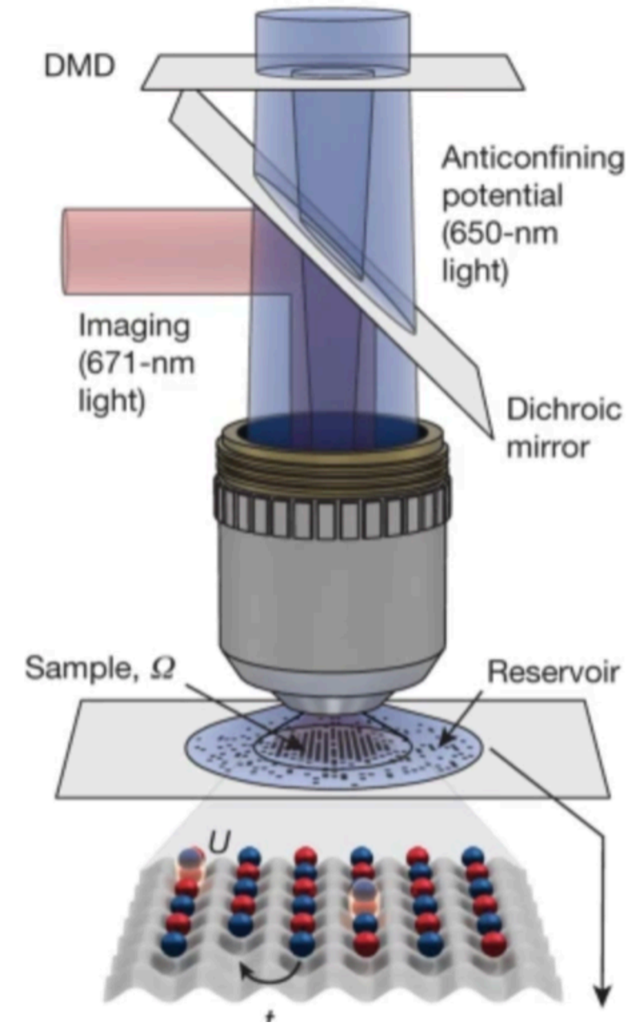
Application: fix density in g.c. ensemble by $\mu(w)$, where $w^{n+1} = 0$

[RR, Šimkovic, Ferrero, EPL 2020]

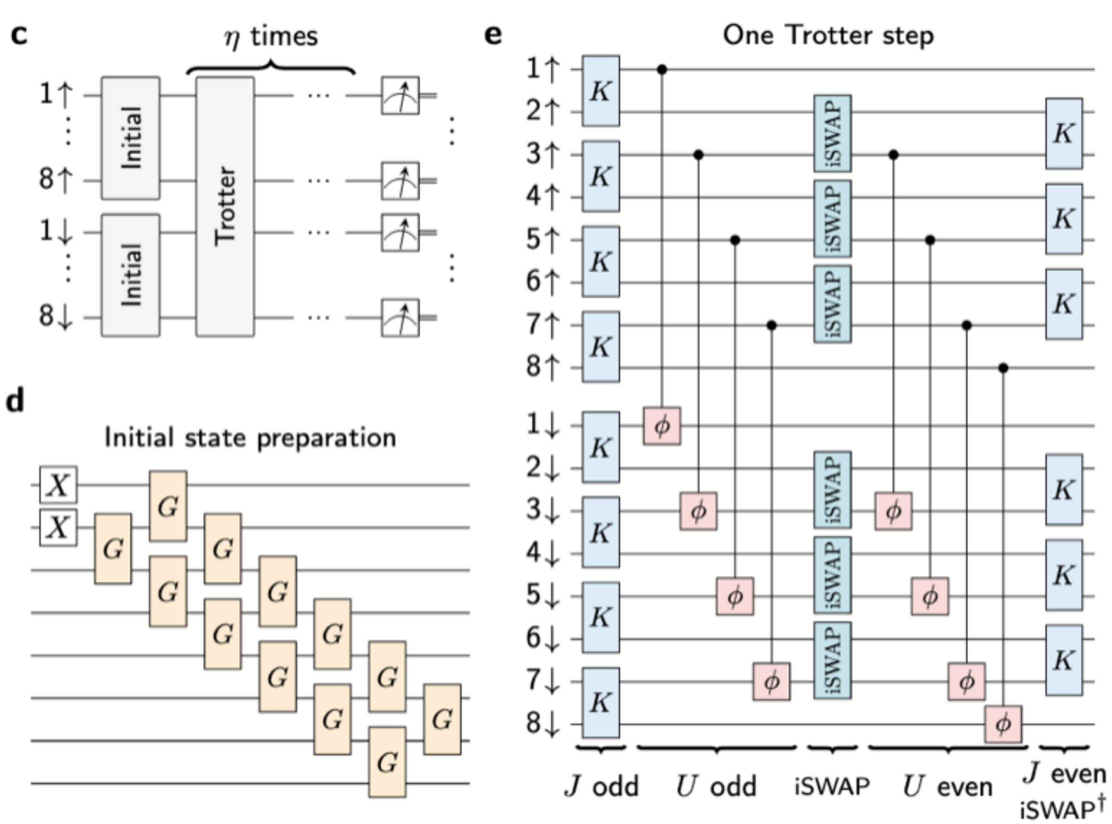
2D Hubbard model

Fermi-Hubbard model





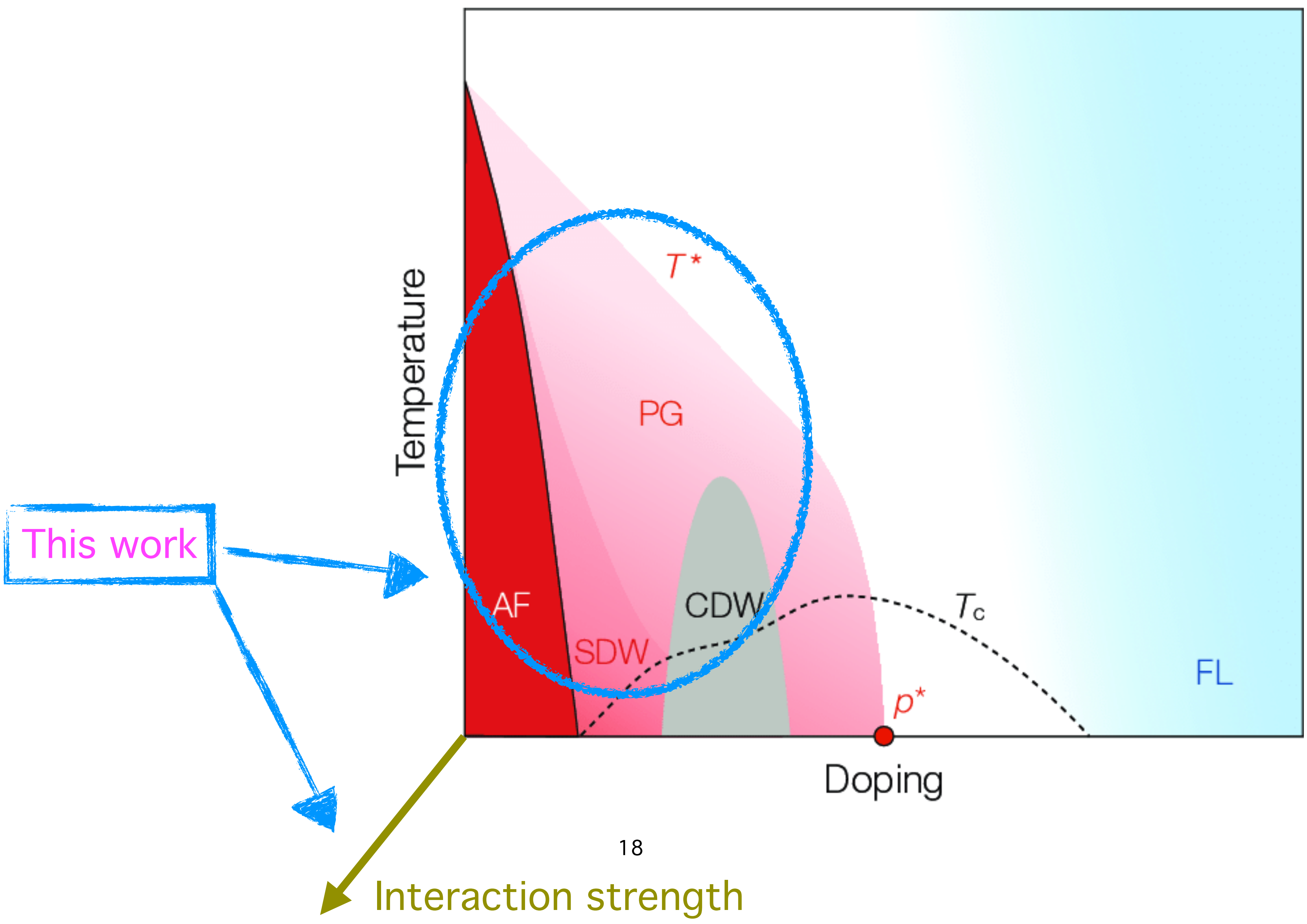
[Mazurenko et al, Nature 2017]



[Google AI Quantum, 2020]

Quantum simulators

Expected finite T situation in 2D (rough sketch)



Setting for the numerical experiment and probes

Square lattice

$$\hat{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + U \sum_{\mathbf{r}} \hat{n}_{\uparrow}(\mathbf{r}) \hat{n}_{\downarrow}(\mathbf{r}) - \mu \sum_{\mathbf{r}} \hat{n}(\mathbf{r})$$

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$$

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}\, e^{-\hat{H}/T}\, \hat{O}}{\mathrm{Tr}\, e^{-\hat{H}/T}}$$

$$\hat{O}(\tau) = e^{\tau \hat{H}}\, \hat{O}\, e^{-\tau \hat{H}}$$

Self-energy

$$G(\mathbf{r},\tau) = -\langle \hat{c}_{\uparrow}(\mathbf{r},\tau) \hat{c}^{\dagger}_{\uparrow}(\mathbf{0}) \rangle$$

$$G^{-1} = G_0^{-1} - \Sigma$$

Spectral function proxy

$$A(\mathbf{k}) = \frac{-1}{\pi} \mathrm{Im}\, G_{k,i\omega_0}$$

Spin susceptibility

$$\chi_{sp}(\mathbf{r}) = \int_0^{1/T} d\tau\, \langle \hat{S}_z(\mathbf{r},\tau) \hat{S}_z(\mathbf{0},\tau) \rangle$$

Charge susceptibility

$$\chi_{ch}(\mathbf{r}) = \int_0^{1/T} d\tau\, [\langle \hat{n}(\mathbf{r},\tau) \hat{n}(\mathbf{0},0) \rangle - \langle \hat{n}(\mathbf{r}) \rangle \langle \hat{n}(\mathbf{0}) \rangle]$$

Strong-coupling probes

$D = \langle \hat{n}_{\uparrow}(\mathbf{r}) \hat{n}_{\downarrow}(\mathbf{r}) \rangle$ $\quad\quad$ $\langle \hat{n}(\mathbf{r}) \rangle$ versus μ

Alternatives

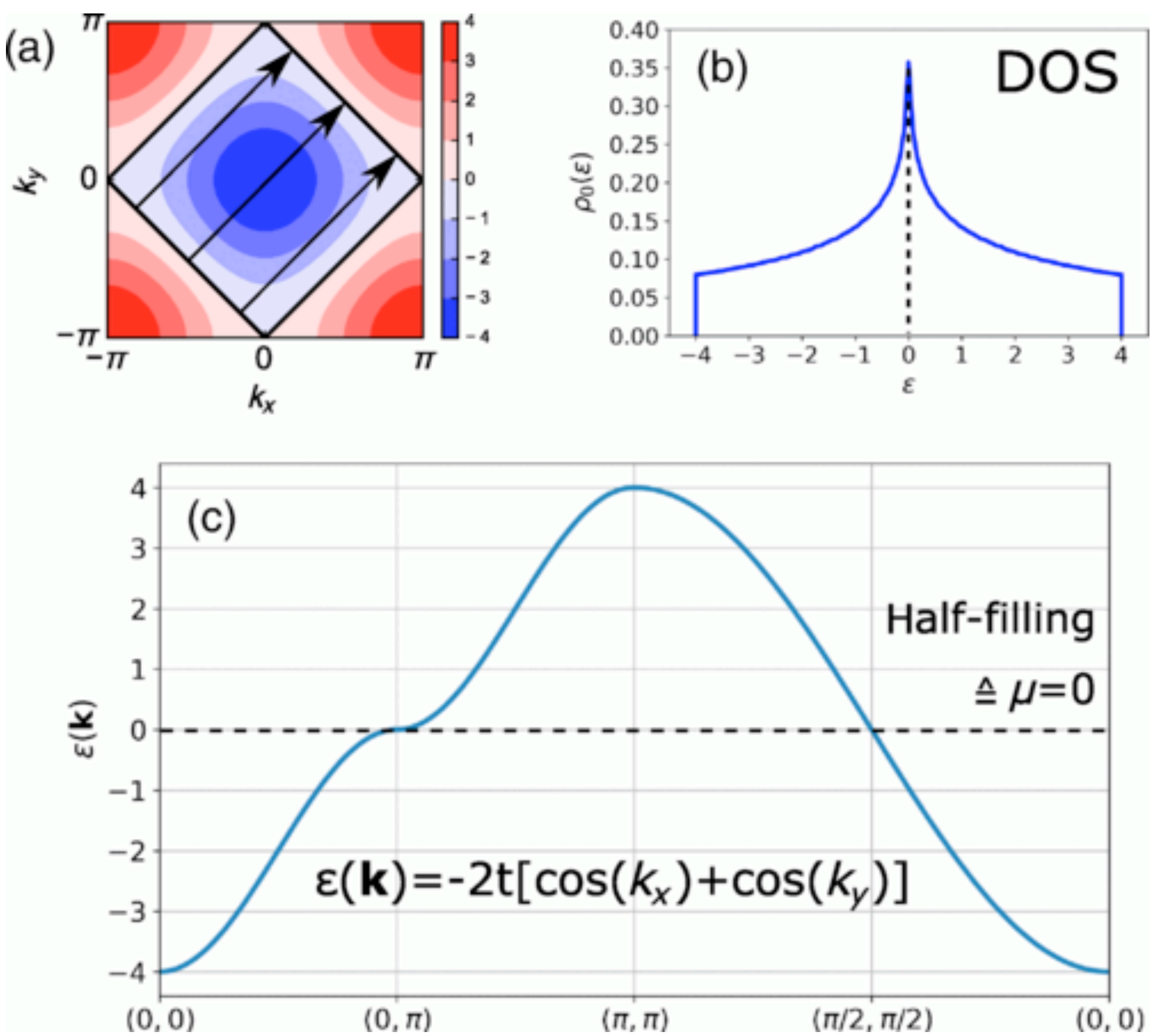
$$S_{\mathrm{sp}}(\mathbf{r}) = \langle \hat{S}_z(\mathbf{r}) \hat{S}_z(\mathbf{0}) \rangle$$

$$S_{\mathrm{ch}}(\mathbf{r}) = \langle \hat{n}(\mathbf{r}) \hat{n}(\mathbf{0}) \rangle$$

Fermions interacting with AFM fluctuations

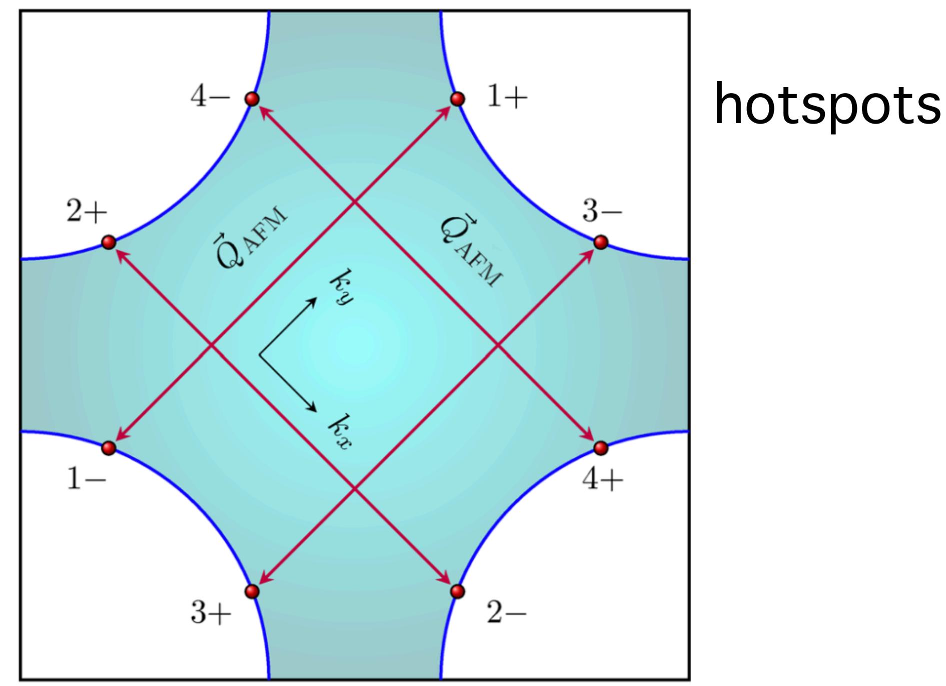
Previous works

Half-filled Hubbard with ph sym: Perfect nesting

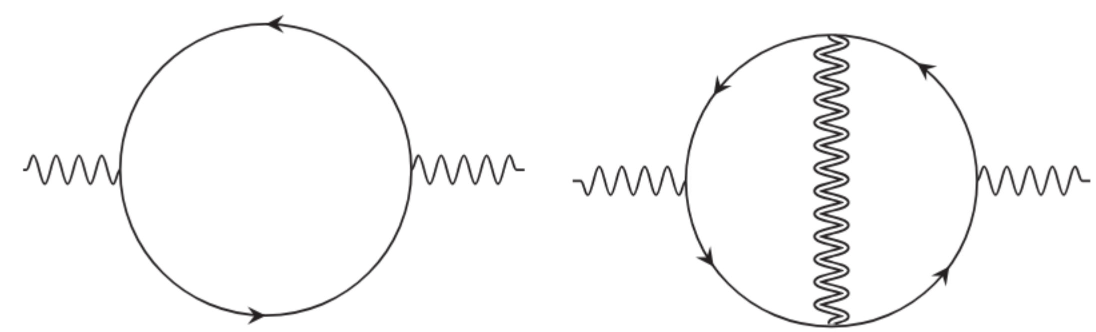


[Simkovic et al, PRL 2020]

[Schafer et al, PRX 2021]



Exact RG fixed point?



$$D(q)^{-1} = |q_0| + c(v)[|q_x| + |q_y|]$$

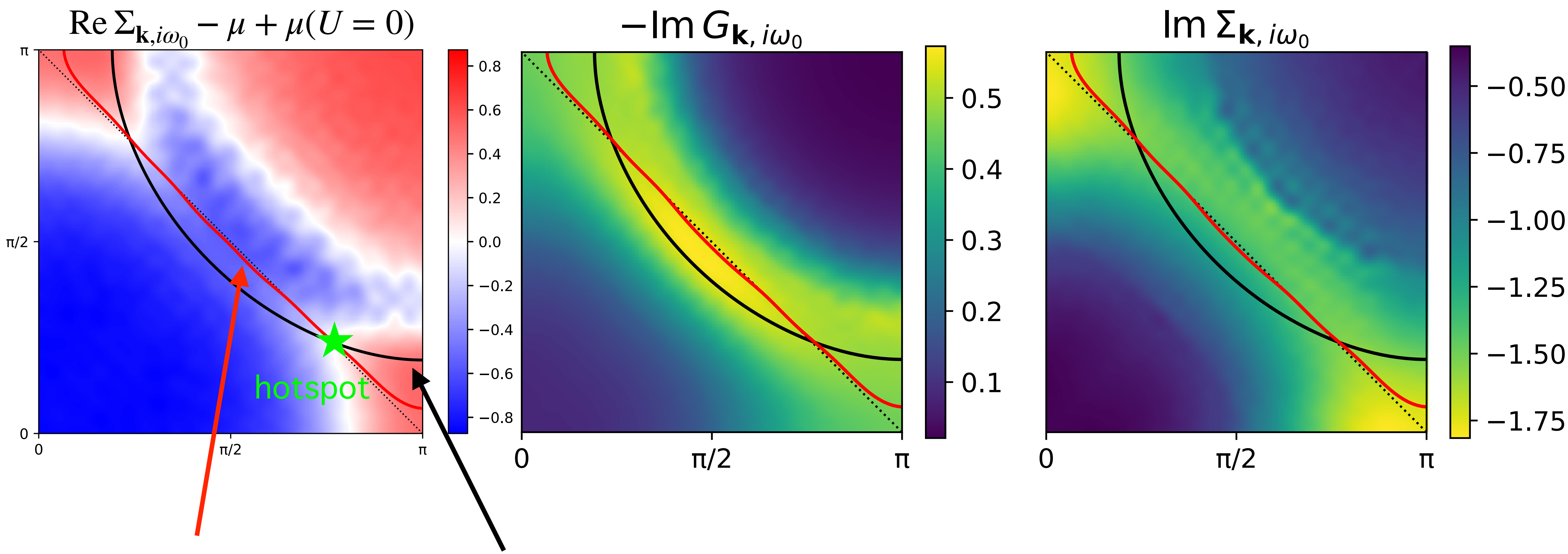
[Schlief et al, PRX 2017]

Our numerical experiment: Half-filled Hubbard model with t’

[RR, Šimkovic, Ferrero, Georges, Tsvelik, Prokofiev, Tupitsyn, PRR’24]

Flowing toward nesting? Hotspots?

Half filling, $U/t = 5.75, \quad t'/t = -0.3, \quad T/t = 1/7$



Line of zeros of renormalized dispersion relation

Non interacting Fermi surface

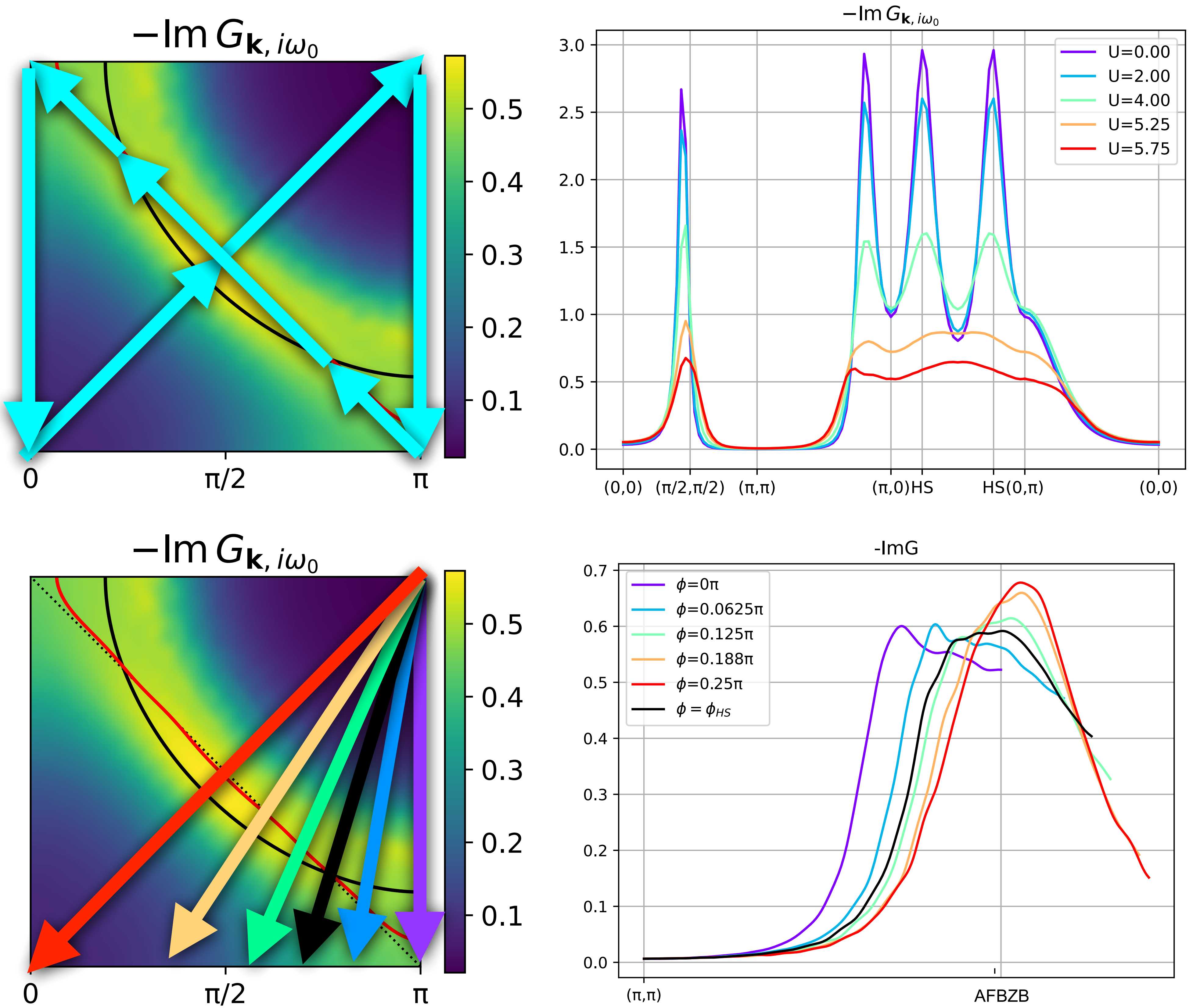
AFM spin fluctuations $\Sigma_{\mathbf{k},i\omega_n} \sim \dfrac{1}{i\omega_n - \xi_{\mathbf{k+Q}}}$

$\epsilon_{\mathbf{k}} + \mathrm{Re}\,\Sigma_{\mathbf{k},i\omega_0} - \mu = 0 \neq \mathrm{FS} = \mathrm{argmax}[-\mathrm{Im}G_{\mathbf{k},i\omega_0}]$

Σ pole developing at antinodes, not at the hotpots!

[RR, Šimkovic, Ferrero, Georges, Tsvelik, Prokofiev, Tupitsyn, PRR’24]

Fermi surface reconstruction tendencies



Spectral intensity is minimal at the hotspots

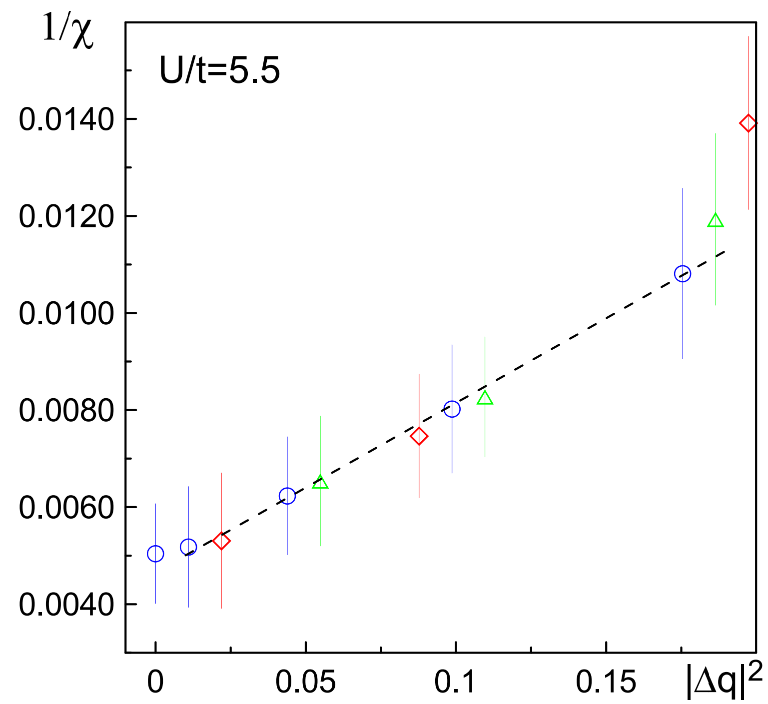
-> Signature of FS reconstruction without magnetic order

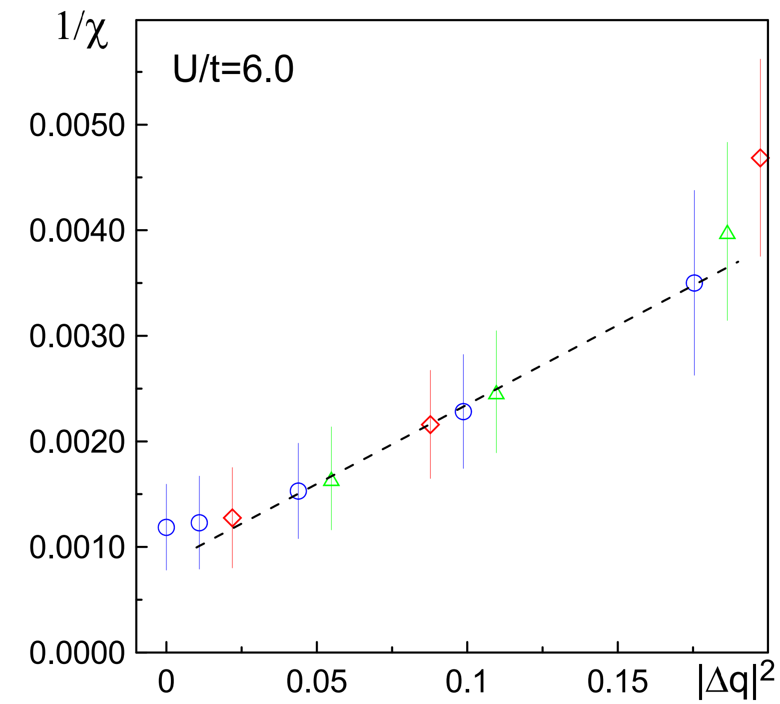
[RR, Šimkovic, Ferrero, Georges, Tsvelik, Prokofiev, Tupitsyn, PRR'24]

Exact RG fixed point of Schlief-Lunts-Lee?

$\chi_{sp}^{-1}(\mathbf{k}, \omega = \mathbf{0}) = \mathbf{c}(|\mathbf{k_x}| + |\mathbf{k_y}|)$ [Schlief et al, PRX 2017]

Hubbard model:
<u>no sign of linear scaling</u>
for as low as $T/t = 1/10$



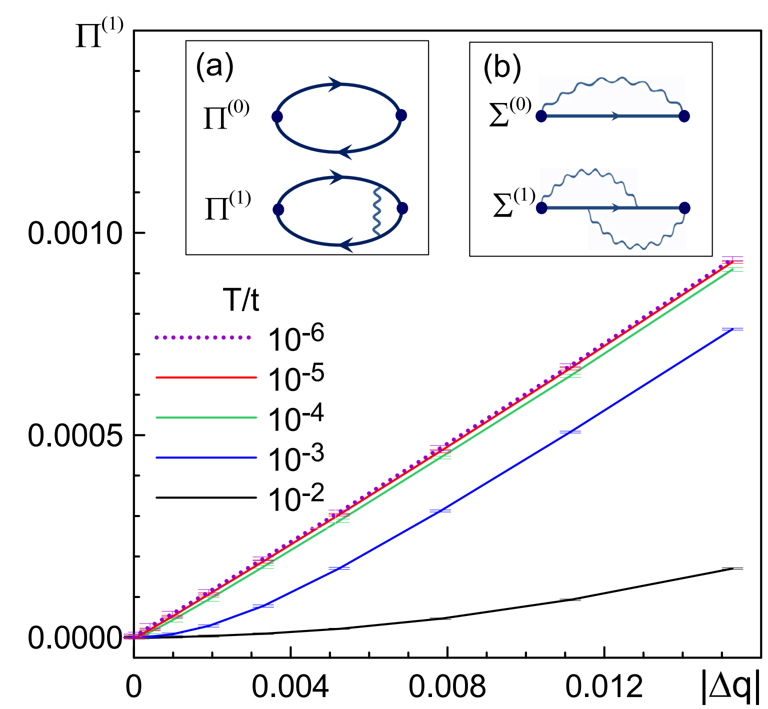


Spin-Fermion model:

$$\hat{H} = \sum_{\mathbf{k},\alpha} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\alpha} c_{\mathbf{k},\alpha} + \sum_{\mathbf{k}} \chi_0^{-1}(\mathbf{k})\ \mathbf{S}(\mathbf{k}) \cdot \mathbf{S}(-\mathbf{k}) + g \sum_{\mathbf{k},\mathbf{q},\alpha,\beta,i} c^{\dagger}_{\mathbf{k+q},\alpha} \sigma^i_{\alpha,\beta} c_{\mathbf{k},\beta} S^i_{-\mathbf{q}}$$

<u>No trace of linear scaling</u> for as low $T/t = 10^{-4}$

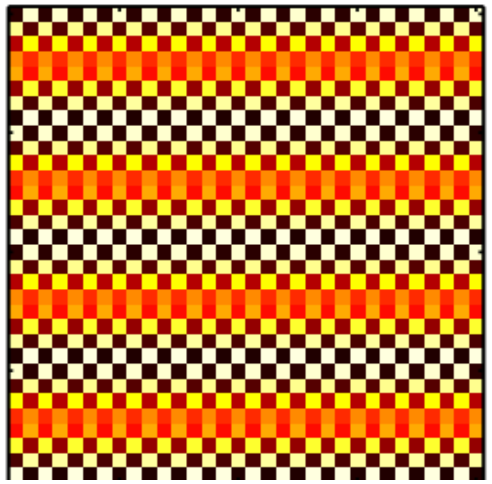
See also
[Bauer et al, PRR 2020]



[RR, Šimkovic, Ferrero, Georges, Tsvelik, Prokofiev, Tupitsyn, PRR’24]

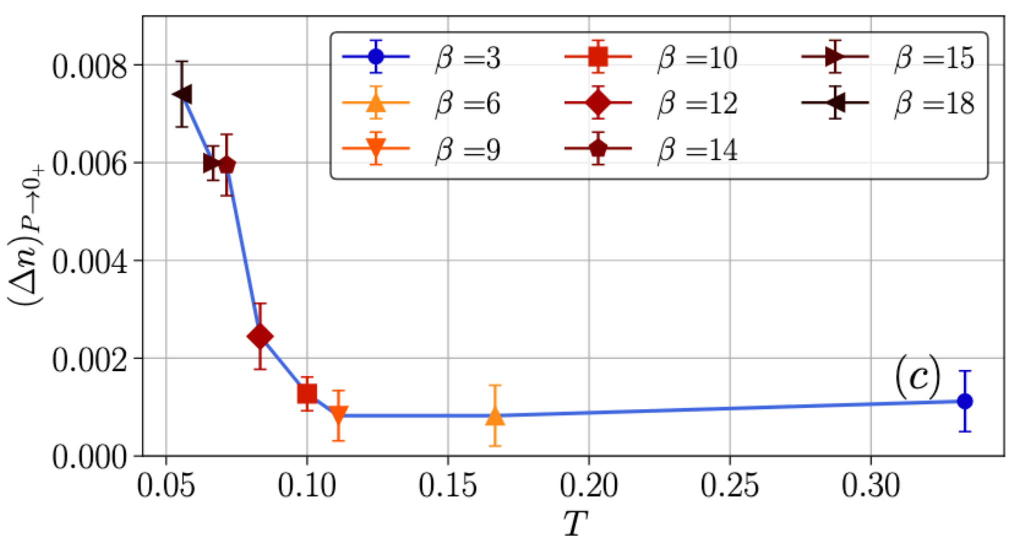
Stripe precursors at intermediate temperature?

Stripes in the Ground state of the HM (t'=0)



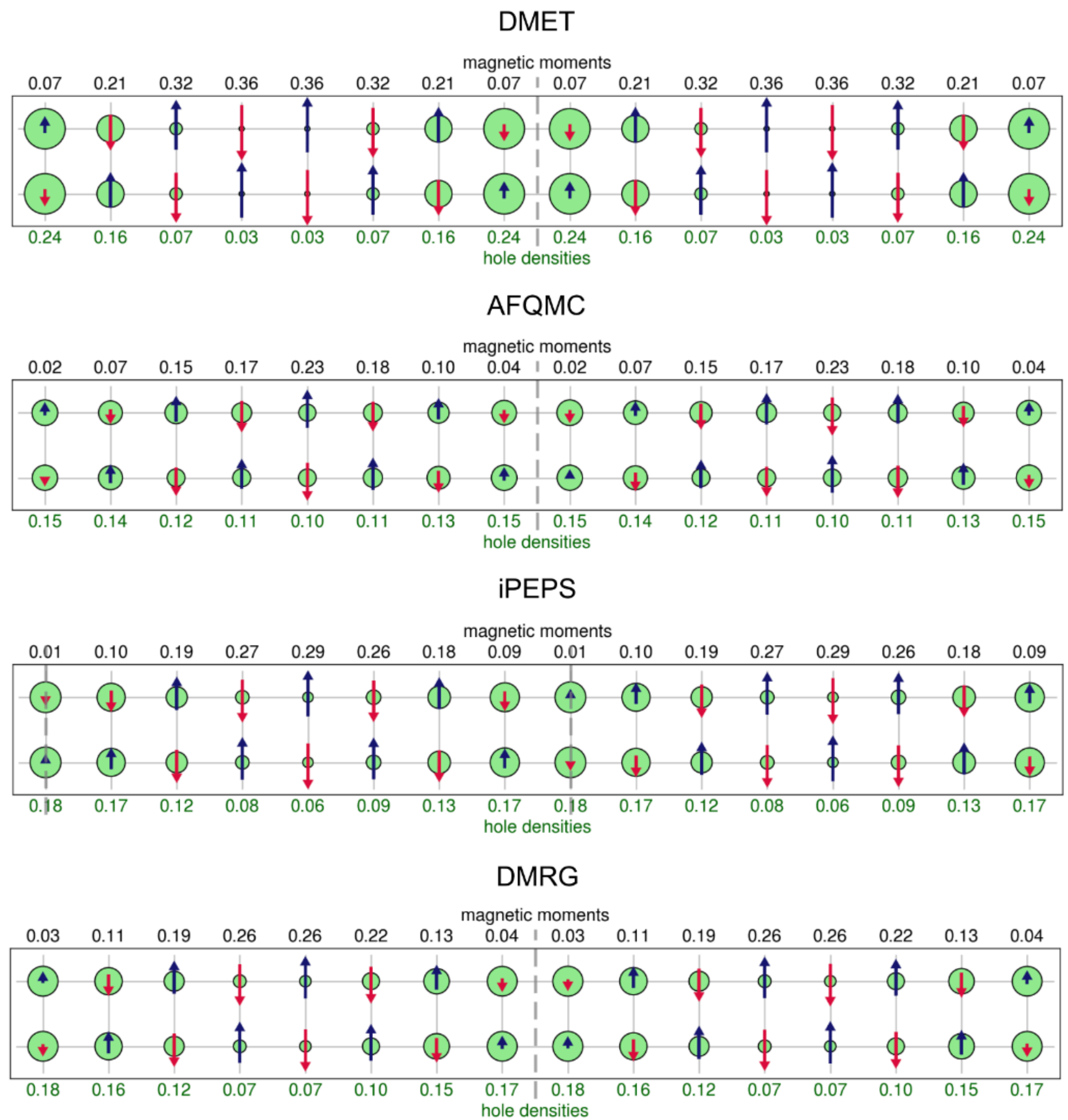
[Xu et al, J. Phys.: Condens. Matter 2011]

Also $T > 0$



[Xiao et al, PRX 2023]

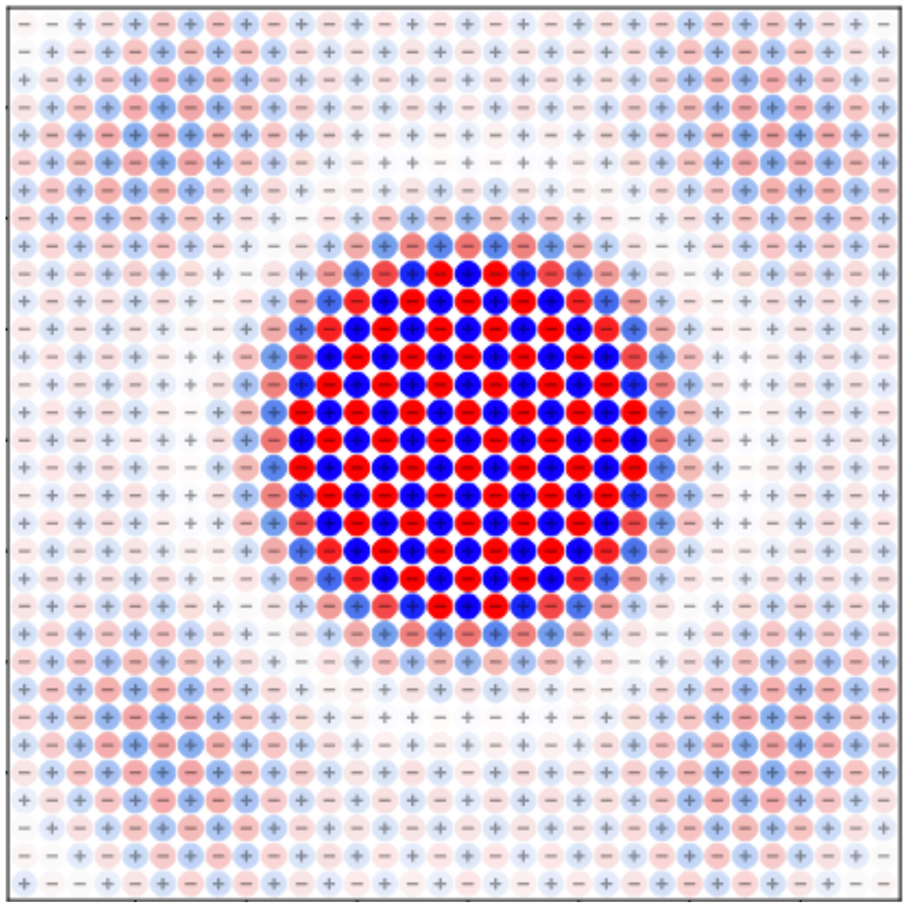
with pinning+external fields



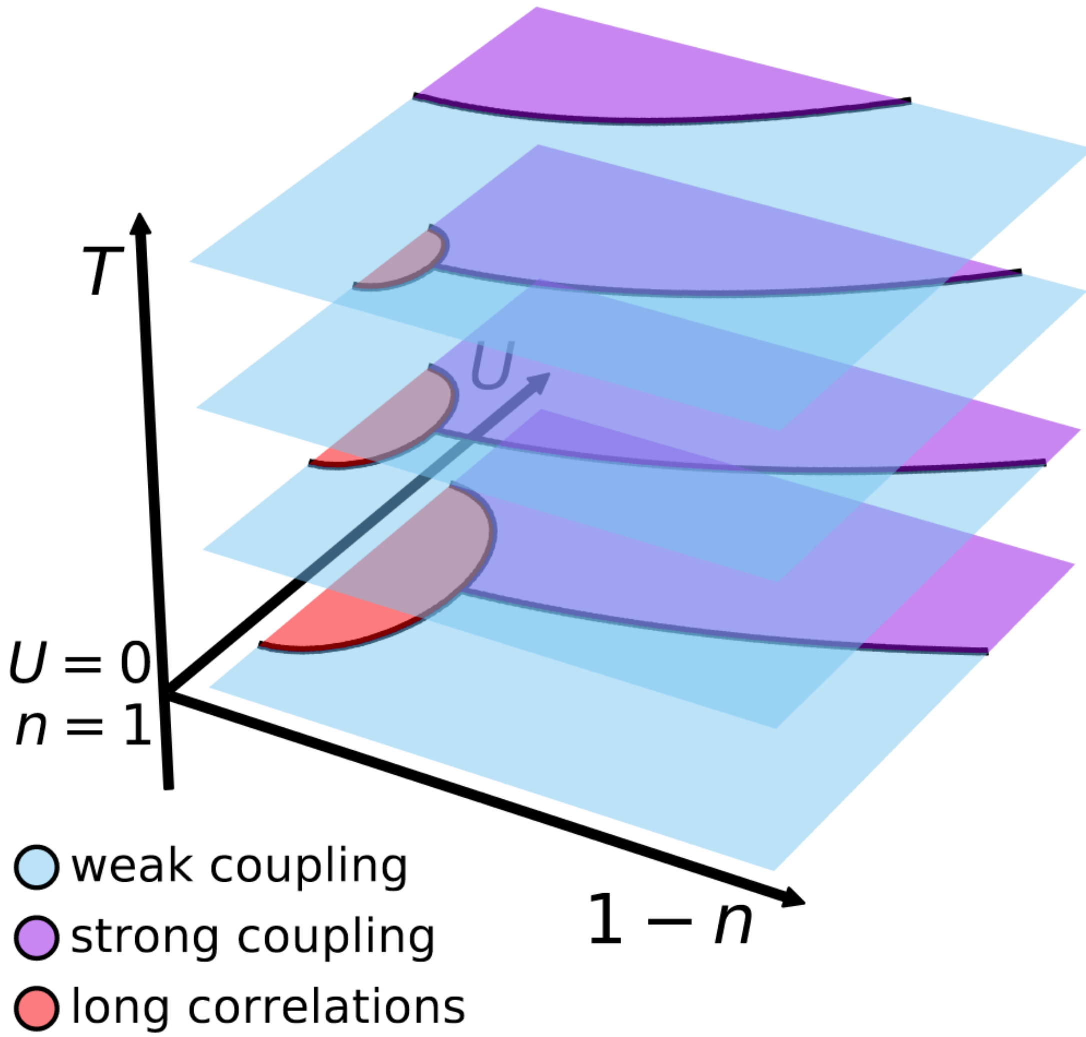
[Zheng et al, Science 2017]

The Weak, the Long, and the Strong

U/t=4, T/t=0.1, n=0.925



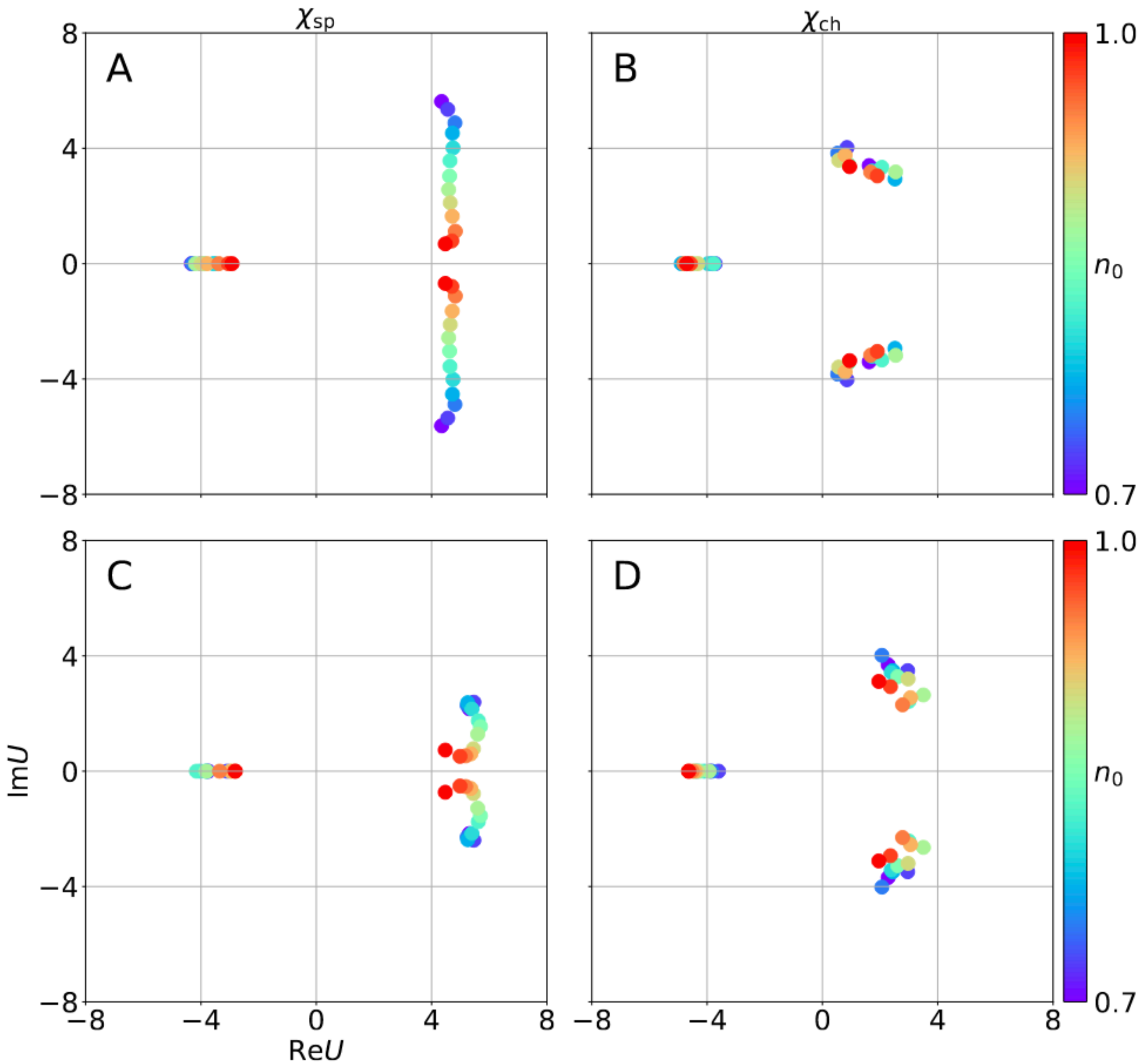
$\chi_{sp}(\mathbf{r})$

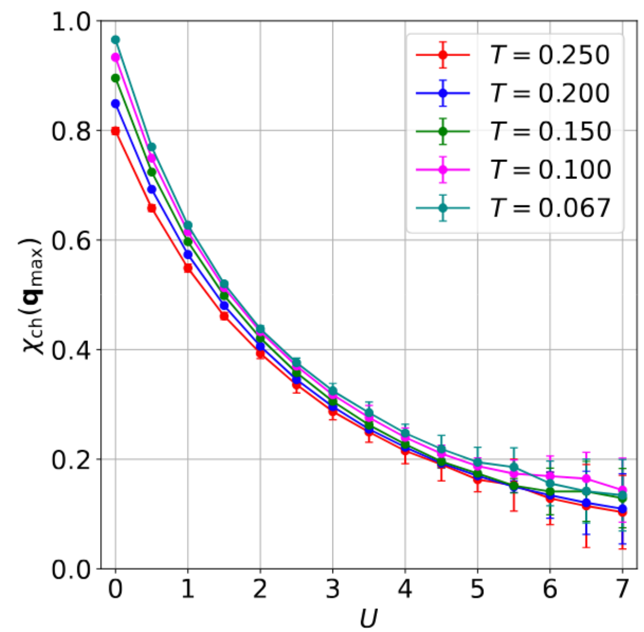


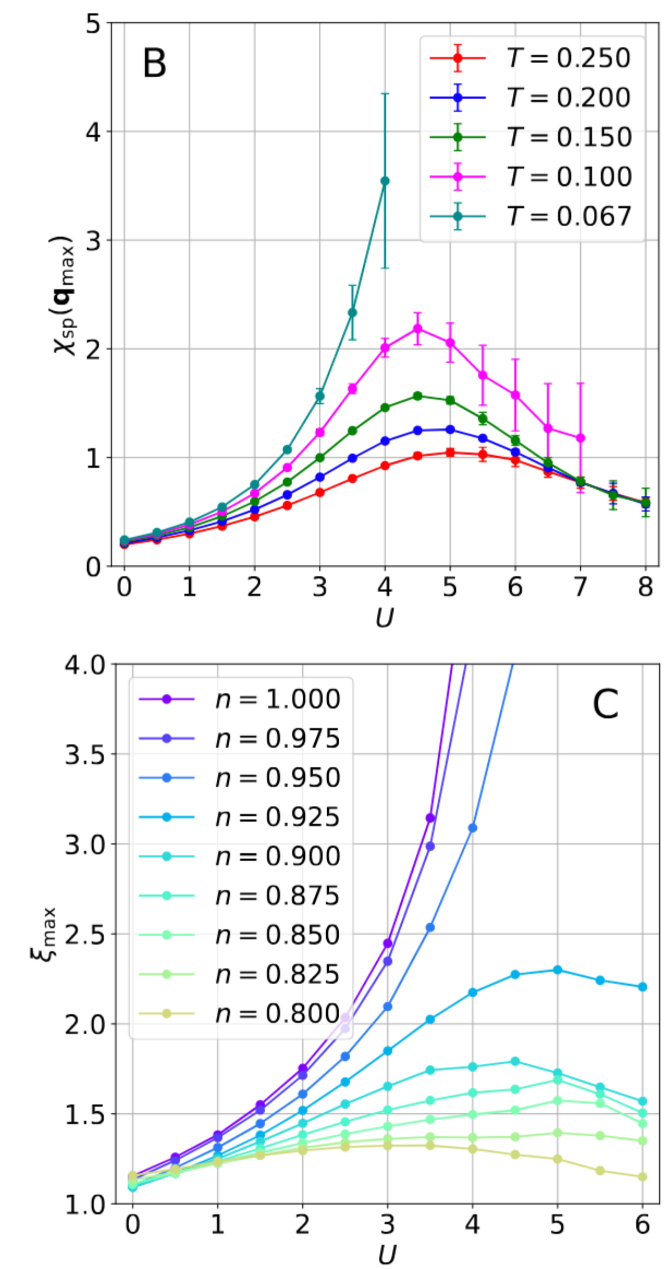
But no signature of stripe precursors!

[F. Simkovic, RR, M. Ferrero, PRR 2022]

Spin and charge decoupling from analytic structure







Singularity hitting the real positive U axis as $T \to 0$
for spin susceptibility $\Longrightarrow$ SDW crossover

No such thing happening for charge!

[Šimkovic, RR, Ferrero, PRR 2022]

Origin and fate of the pseudogap phase

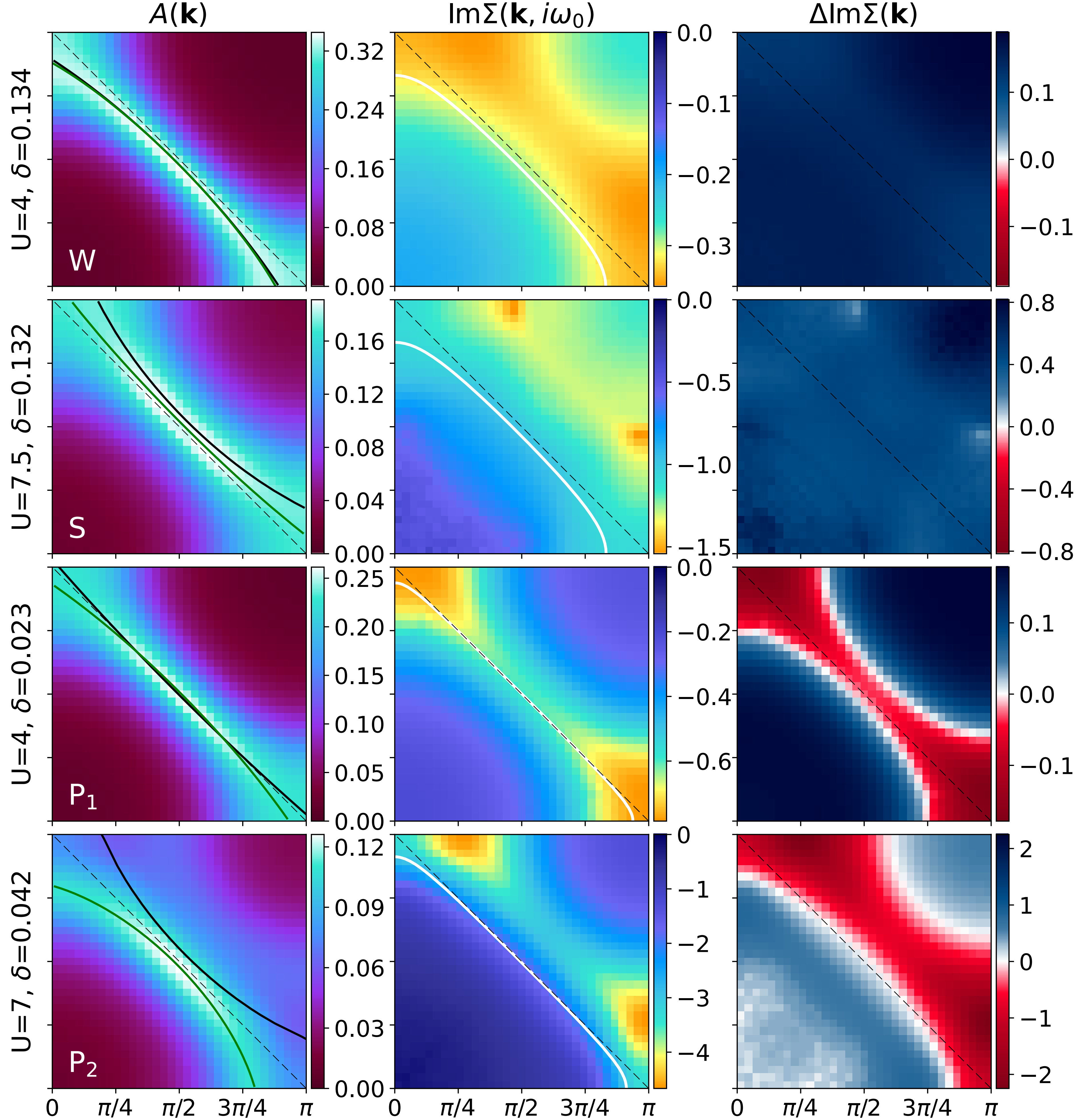
Pseudogap regimes

Pseudogap: momentum-dependent destruction of quasiparticles

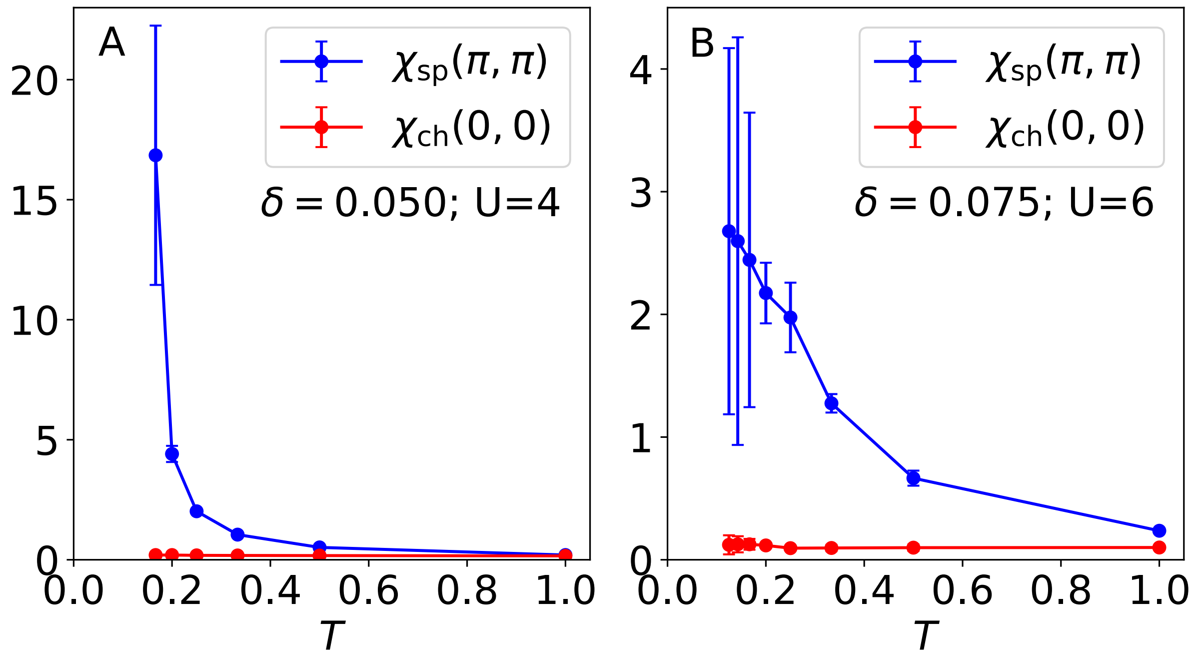
Weak-coupling pseudogap: long spin correlation length

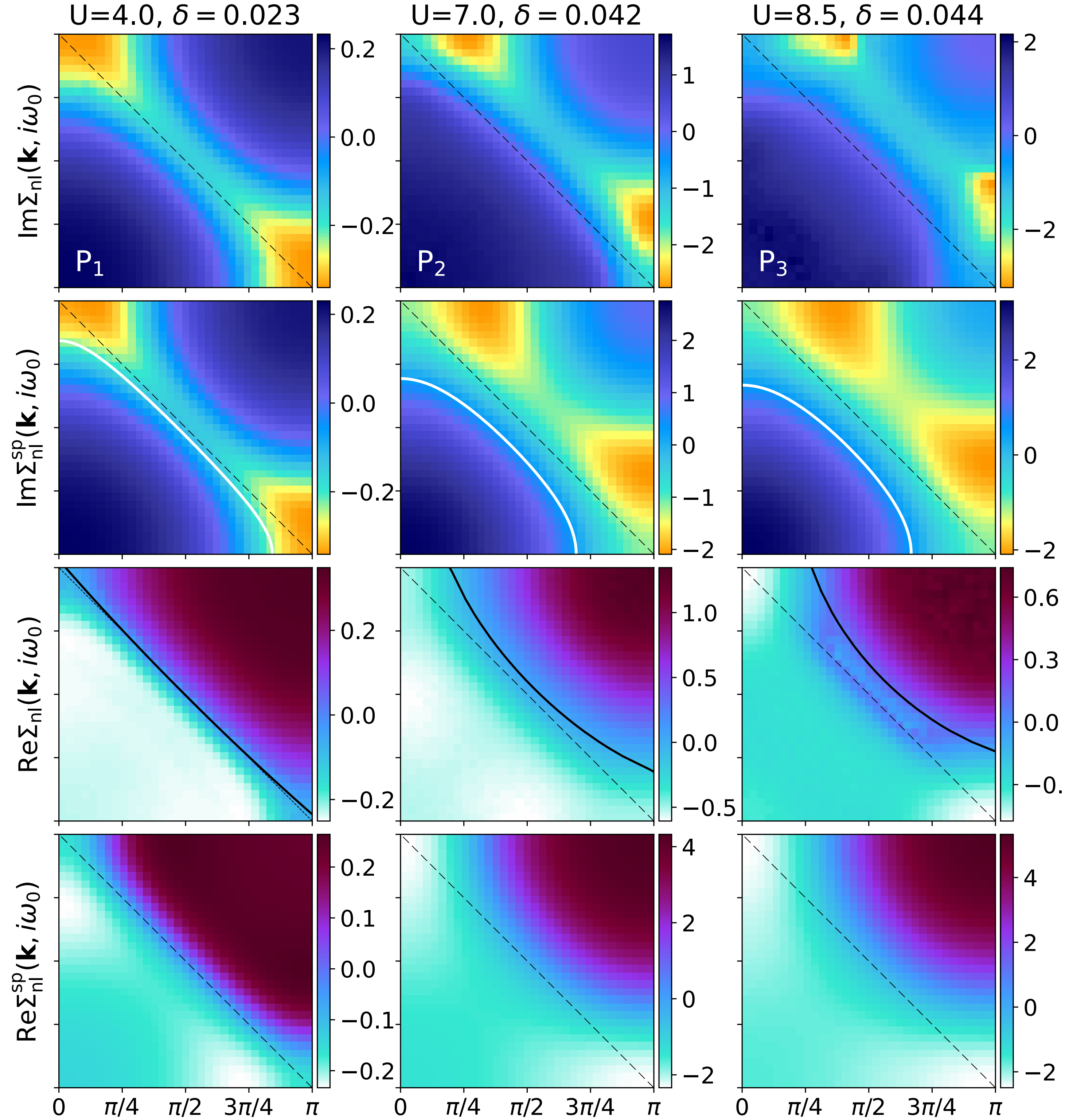
Strong-coupling pseudogap: short-range spin correlations

[Šimkovic, RR, Georges, Ferrero, Science 2024]



Pseudogap: origin





Modified Spin Fluctuaction Theory

$$\Sigma = \Sigma_{loc} + \Sigma_{nl}$$

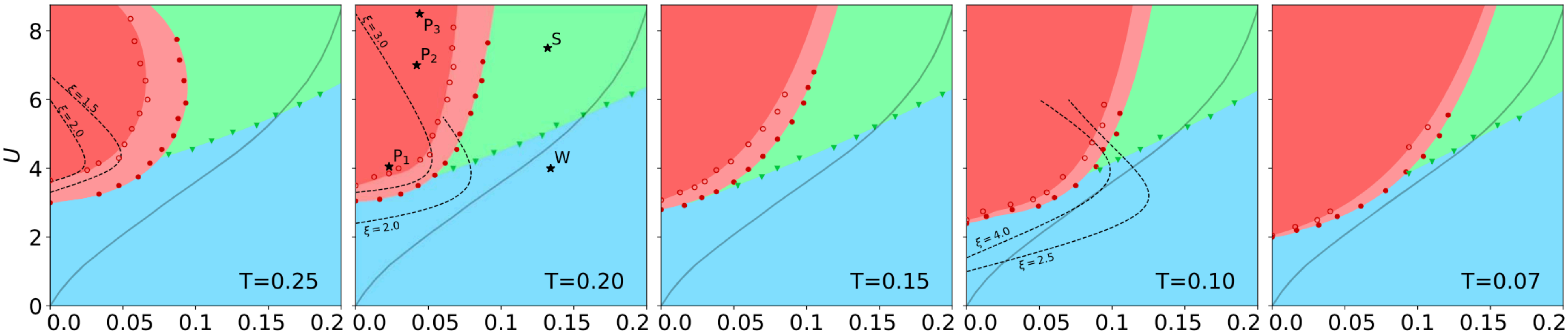
$$\Sigma = -G \star W \star \Gamma \qquad W = U - U^2 \chi_{sp} \qquad \Gamma = \bar{\gamma}$$

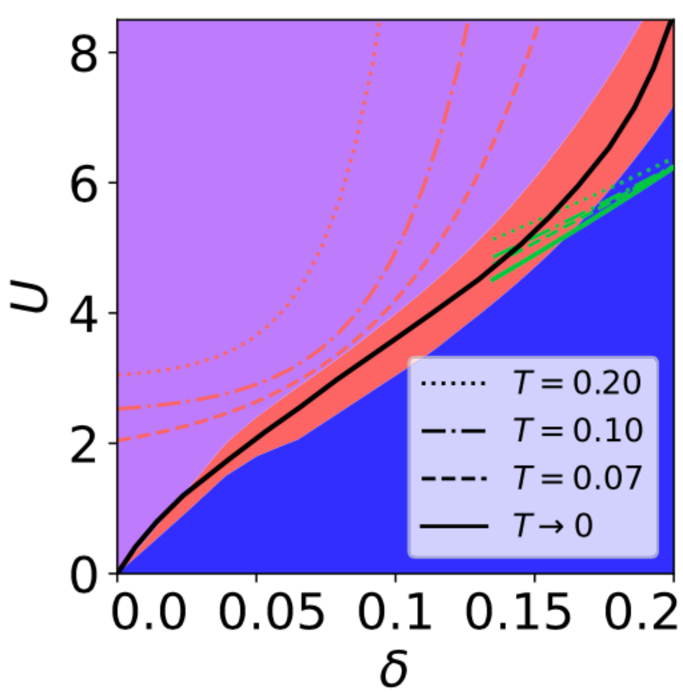
$$\Sigma^{sp}_{nl}(\mathbf{k}, i\omega_0) = \bar{\gamma}\, U^2\, T \frac{1}{N} \sum_{\mathbf{q}} \frac{G_0(\mathbf{k}+\mathbf{q}, i\omega_0, \bar{\mu})}{|\mathbf{Q}-\mathbf{q}|^2 + \bar{\xi}^{-2}}$$

Quantitative agreement not possible
in the strong-coupling pseudogap region

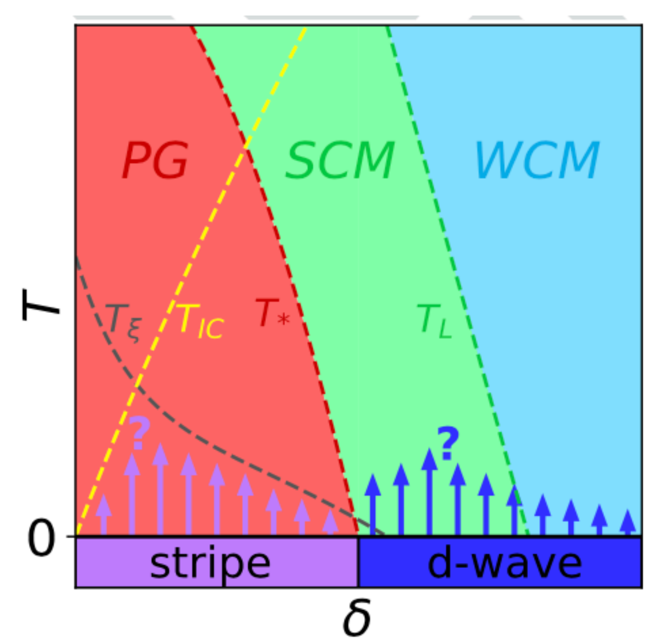
[Šimkovic, RR, Georges, Ferrero, Science 2024]

Pseudogap: Fate?





[Xu et al, PRR 2022]



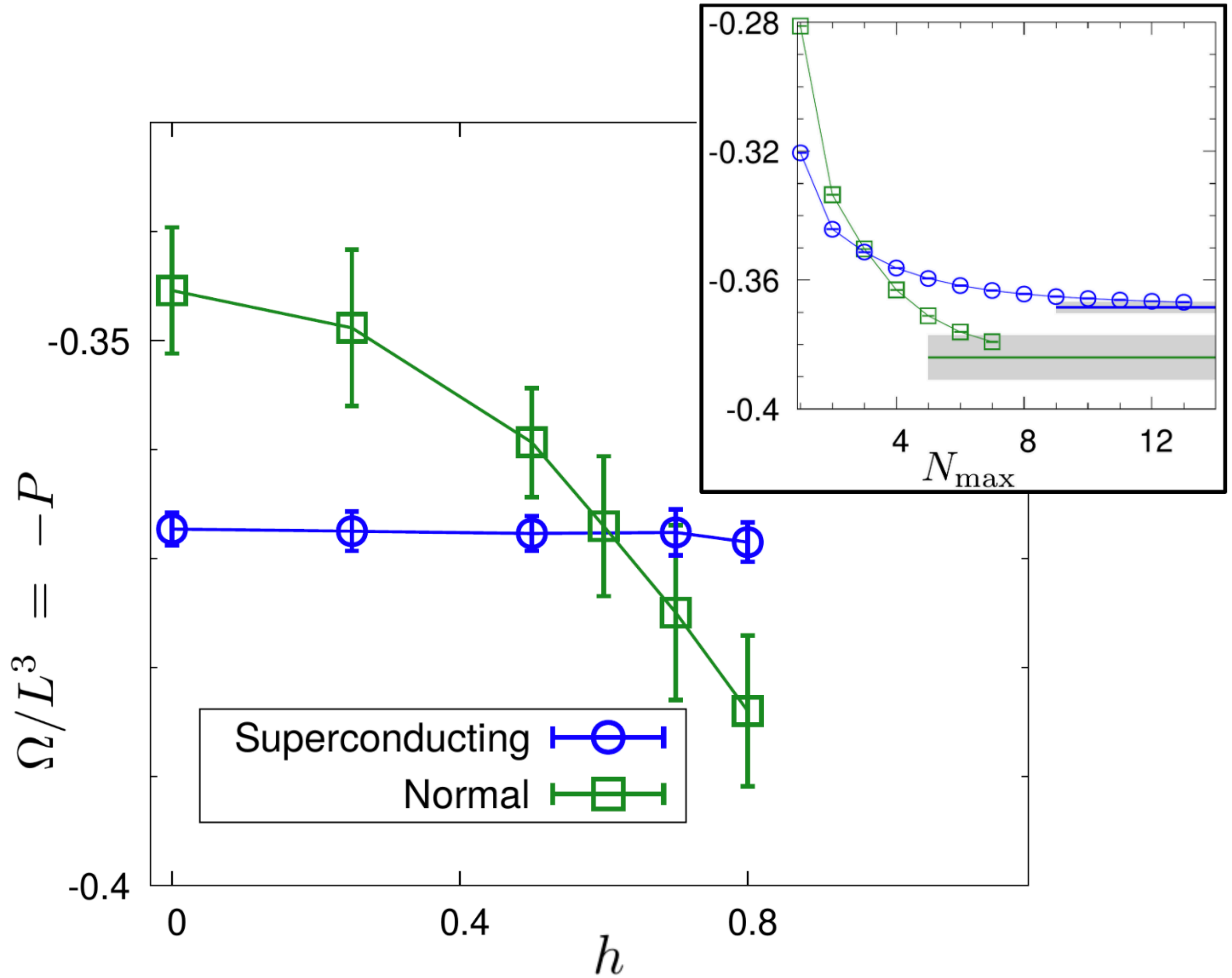
Pseudogap phase exactly extrapolates to stripe ground state!

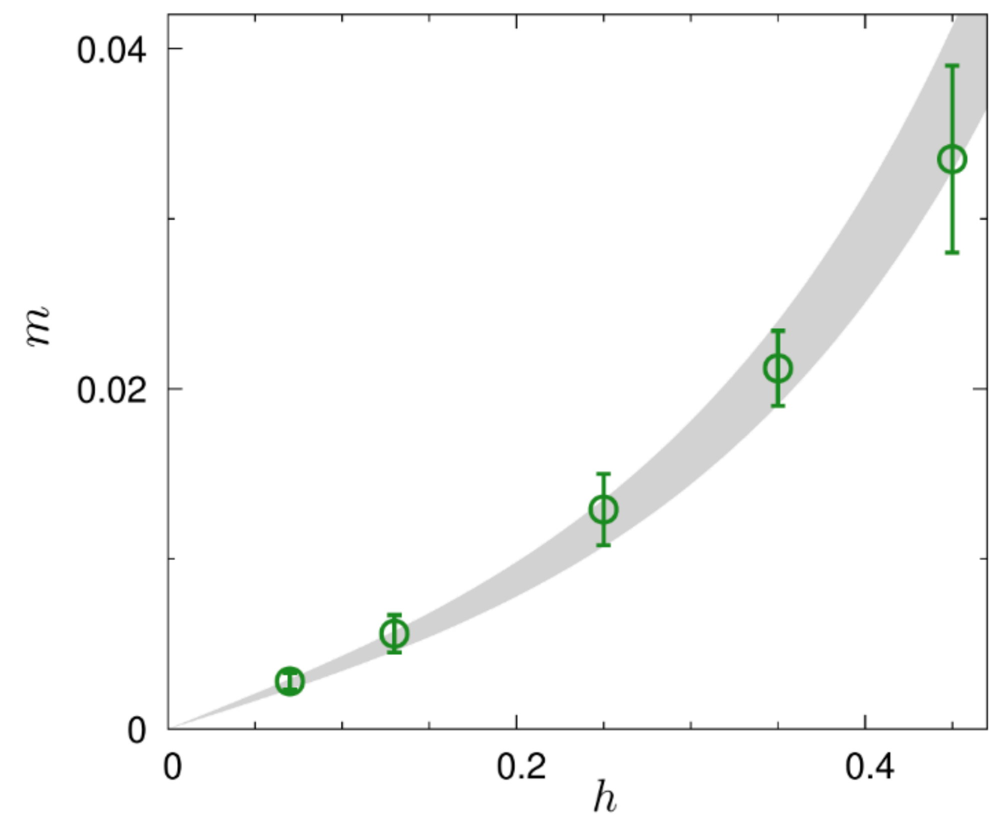
[Šimkovic, RR, Georges, Ferrero, Science 2024]

Conclusion

- We can compute unprecedented number of Feynman diagrams, and it is useful for fermions (poly-time method)
- AFM fluctuations in the HM: Hotspots, ~nesting
- No stripe precursor at intermediate temperature
- Origin and fate of the pseudogap in the HM

Outlook





- d-wave and stripe-order SB high-order expansions for the 2D model
- Renormalized expansions to reach lower T
- C++ code at https://github.com/FastFeynmanDiagrammatics, Julia code under development

[Spada, RR, Šimkovic, Garioud, Ferrero, Van Houcke, Werner, arXiv:2021]

[Garioud, Šimkovic, RR, Spada, Schäfer, Werner, Ferrero, PRL 2022]