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Quantum interacting particles on a ring: binary Tree Tensor Networks studies

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Benasque - 19.02.2016

OUTLINE

- Motivation: why periodic boundaries?
- Tree Tensor Networks & adaptive gauge picture
- Some benchmark data
- Disordered Bose-Hubbard model
- Summary & Future perspectives

Periodic Boundaries: numerical tool

- generally easier for analytical treatments
(Fourier transform & co.)

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(e.g., better and longer reliable correlations)
- faster and cleaner scaling to thermodynamic limit
(useful to study phase transitions) Fisher, Barber, PRL 28, 1516 (1972)

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- avoid undesired edge effects in observables (e.g., better and longer reliable correlations)
- faster and cleaner scaling to thermodynamic limit (useful to study phase transitions) Fisher, Barber, PRL **28**, 1516 (1972)
- access phase stiffnesses and topological invariants via twisting the boundaries $\Psi(0) = e^{i\phi} \Psi(L)$

$$I \propto \partial E / \partial \phi$$

$$\rho_s \propto \partial^2 E / \partial \phi^2$$

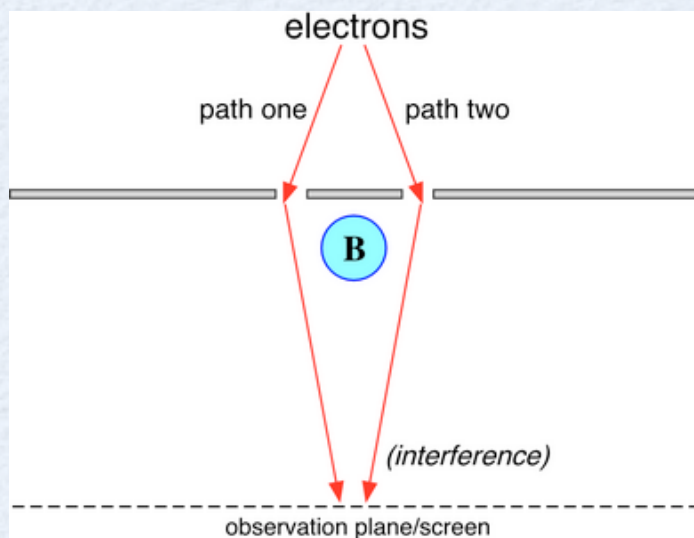
$$\phi_{\text{Zak}} = \int_{-\pi}^{\pi} \langle \Psi | \partial_{\phi} | \Psi \rangle$$

Periodic Boundaries: physical consequences

- In a doubly-connected system, pierced by a flux Φ , all quantities are periodic in the flux by a period $\Phi_0 = h/q$ (q = effective particle charge)

Byers, Yang, PRL 7, 46 (1961)

- AHARANOV-BOHM EFFECT



$$\vec{\nabla} \times \vec{A} = \vec{B}$$

$$\Phi = \oint \vec{A} \cdot d\vec{l}$$

$$\vec{p} \longrightarrow \vec{p} - q\vec{A} \quad \Rightarrow \quad \phi_{L/R} = \int_{L/R} \frac{q\vec{A}}{\hbar} \cdot d\vec{l}$$

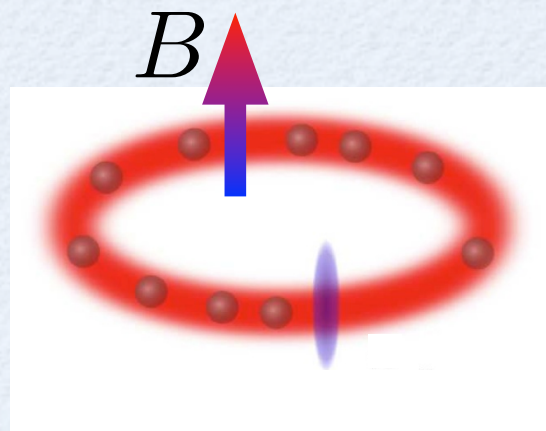
$$\phi = \phi_L - \phi_R = 2\pi\Phi/\Phi_0$$

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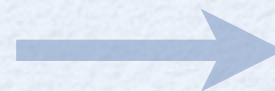
Byers, Yang, PRL 7, 46 (1961)

- PERSISTENT CURRENTS



$$\frac{dF}{dt} = I V \quad V = -\frac{\partial \Phi}{\partial t}$$

$$\frac{dF}{dt} = \frac{\partial F}{\partial \Phi} \frac{\partial \Phi}{\partial t}$$



Bloch, PRB 2, 109 (1970)

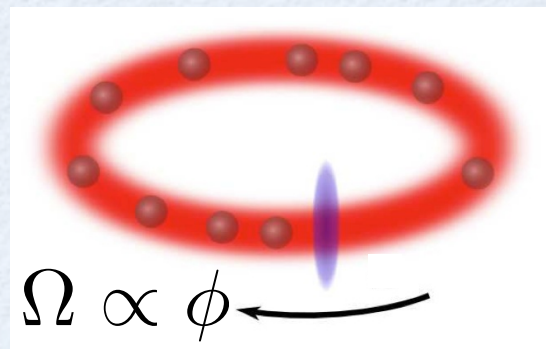
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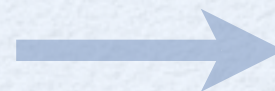
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Periodic Boundaries: physical systems

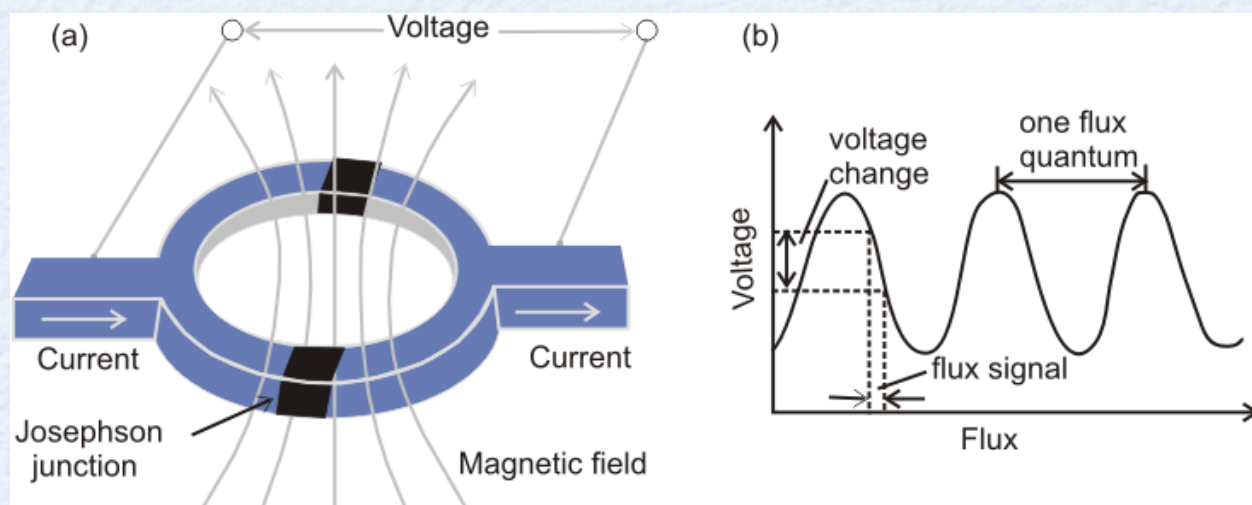
- bulk superconductors

B. S. Deaver and W. M. Fairbank, PRL 7, 43 (1961)

N. Byers and C. N. Yang, PRL 7, 46 (1961)

L. Onsager, PRL 7, 50 (1961)

- SQUID = superconducting quantum interference device



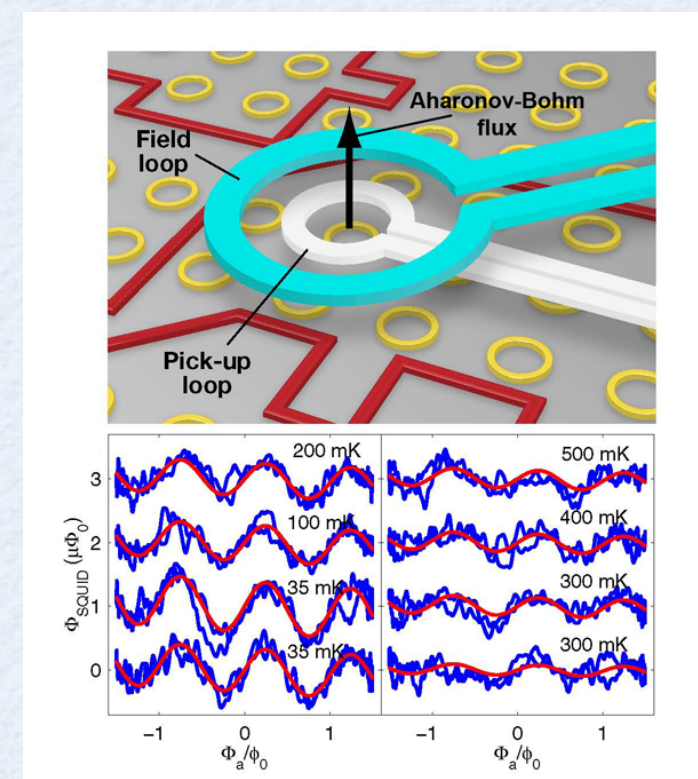
- normal metallic rings

L. P. Levy, et al., PRL 64, 2074 (1990)

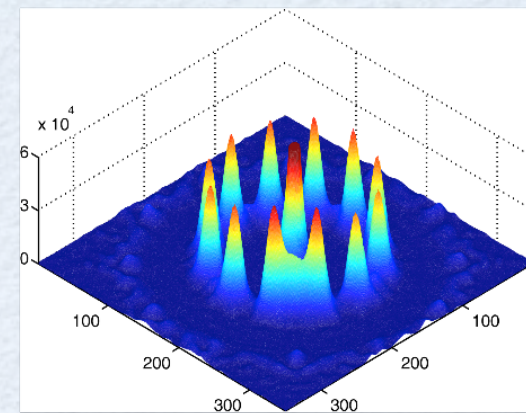
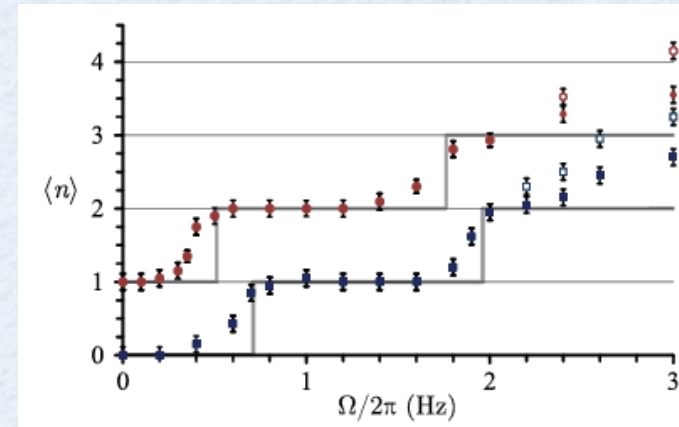
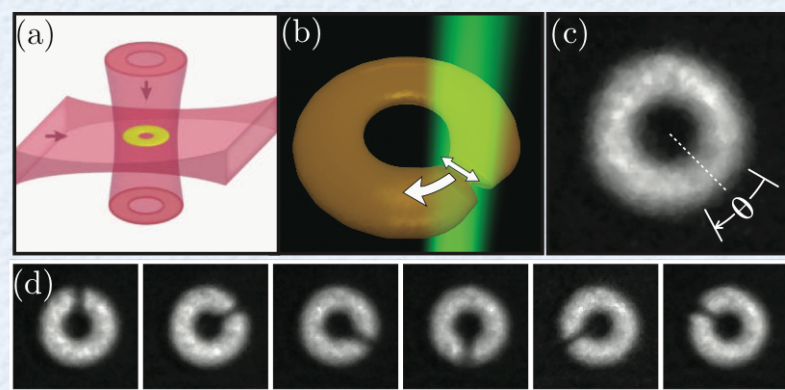
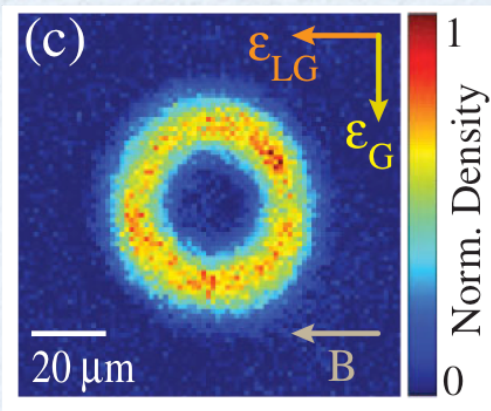
D. Mailly, et al., PRL 70, 2020 (1993)

H. Bluhm et al., PRL 102, 136802 (2009)

A. C. Bleszynski-Jayich, et al., Science 326, 272 (2009)



Periodic Boundaries: physical systems

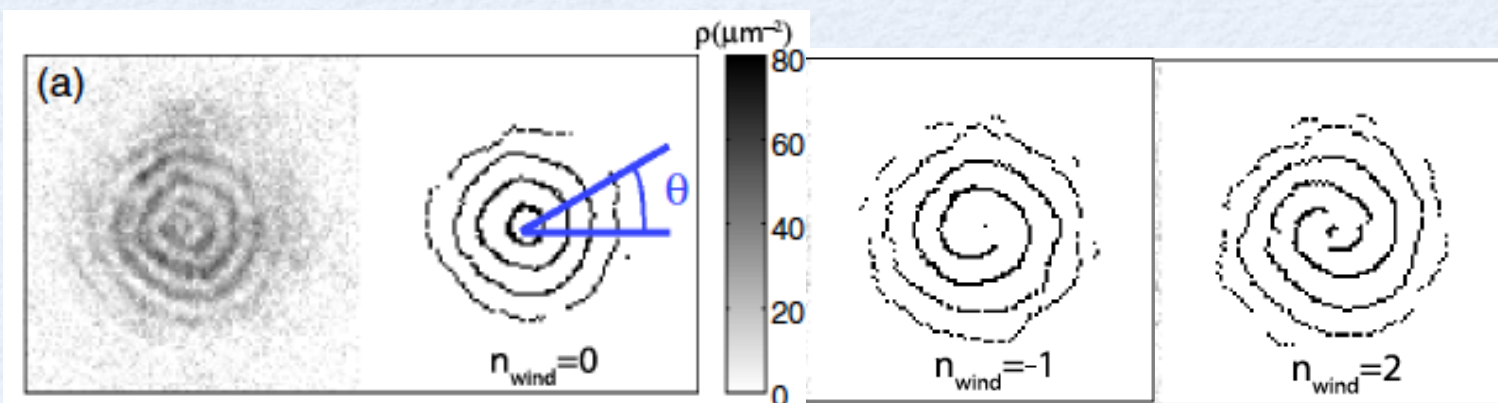


Ramanathan et al., PRL 106, 130401 (2011); Wright et al., PRL 110, 025302 (2013); Moulder et al., PRA 86, 013629 (2012); Beattie, et al., PRL 110, 025301 (2013); C. Ryu, et al., PRL 111, 205301 (2013); and many more

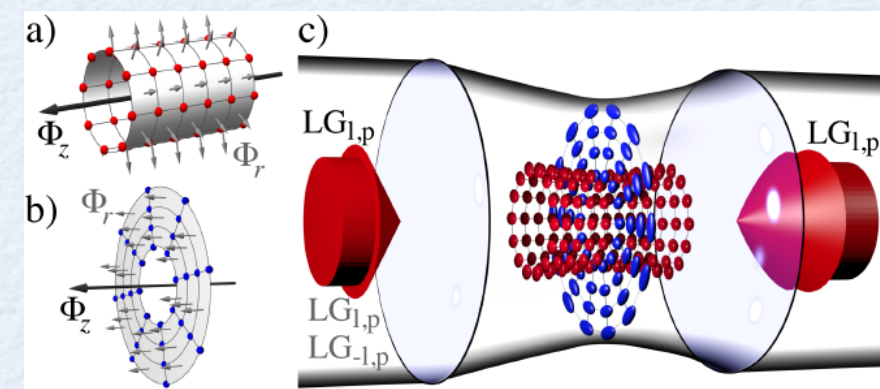
Amico et al., Sci. Rep. 4, 4298 (2014)

- persistent currents flowing > 2 mins !
- diverse starting & measuring protocols
- multi-species setups (i.e., spin currents)

- ★ long coherence qubits
- ★ precise interferometry
- ★ fractional QHE states

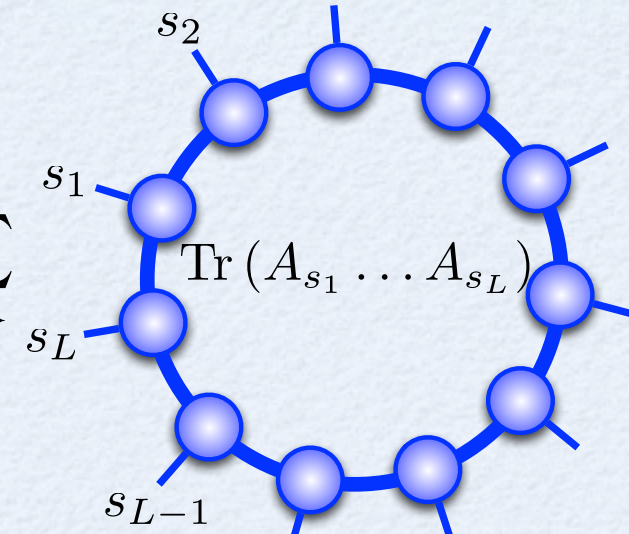


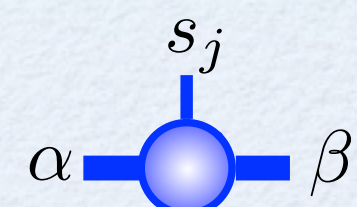
L. Corman, et al., PRL 113, 135302 (2014)



M. Łącki, et al., arXiv:1507.00030

Periodic Boundaries: tensor networks

$$|\psi\rangle = \sum_{\{s\}} \text{Tr}(A_{s_1} \dots A_{s_L}) |s_1 s_2 \dots s_L\rangle$$




$$A_{s_j \alpha \beta}^{[j]}$$

$$s_j \in \{0, \dots, n_j^{\max}\}$$

$$\alpha, \beta = 1 \dots m$$

Verstraete, et al.,
PRL 93, 227205 (2004);

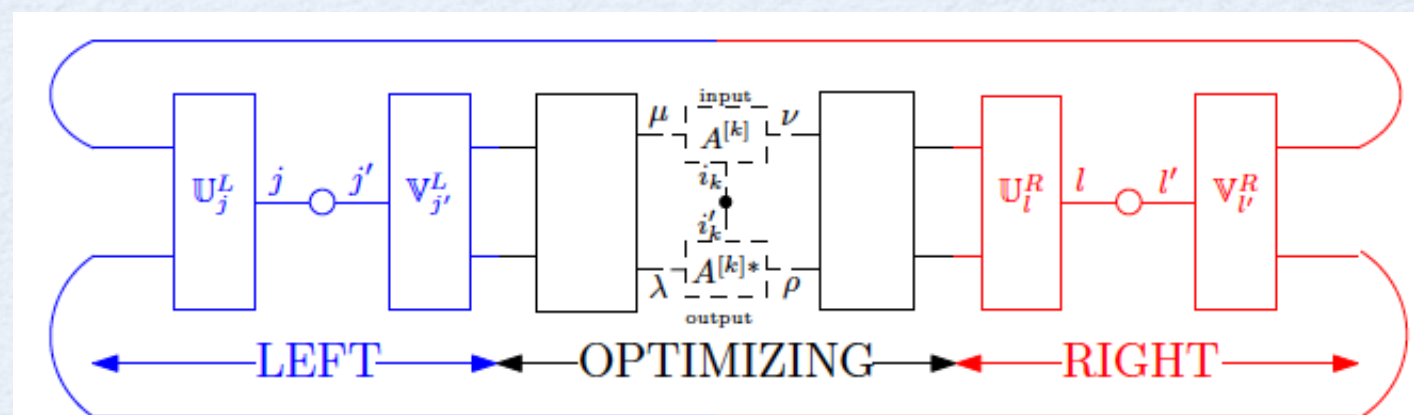
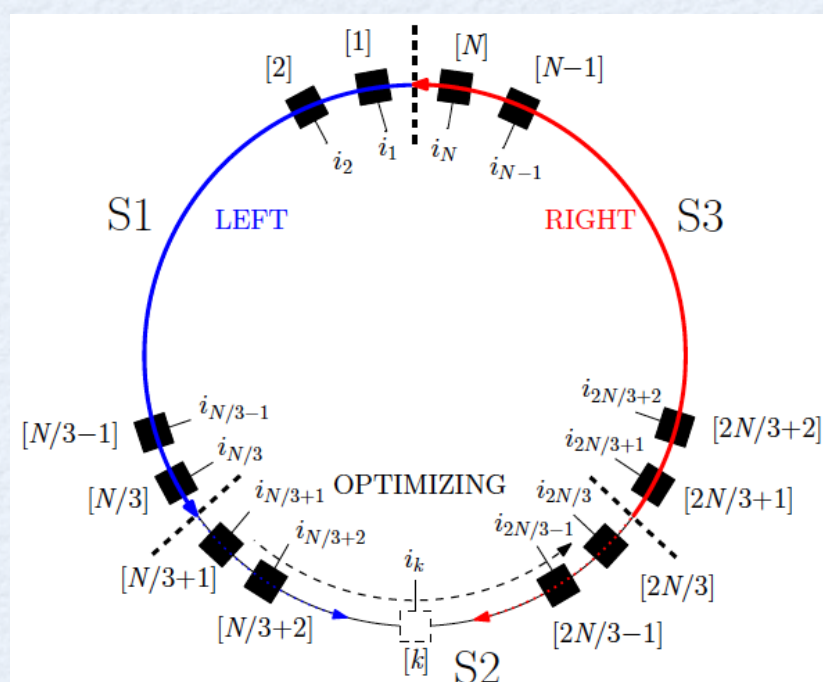
Pippan, et al.
PRL 81, 081103(R) (2010);

Pirvu, et al.,
PRL 83, 125104 (2011)

Weyrauch, et al.,
arXiv:1303.1333

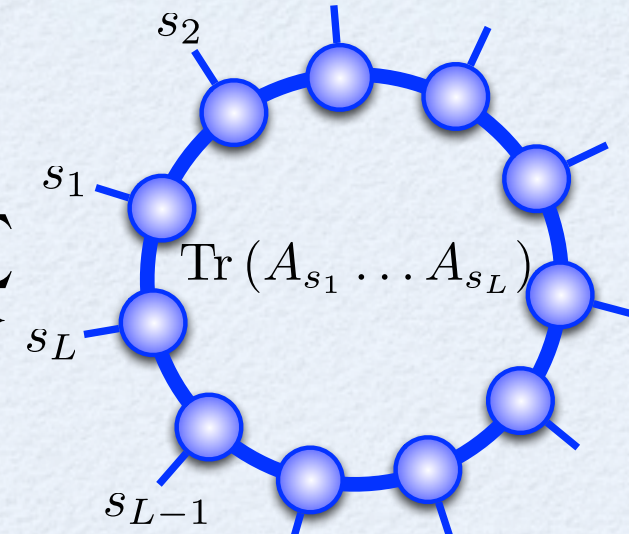
- Periodic MPS suffer from:
 - higher contraction costs $O(m^5)$ vs. $O(m^3)$
 - absence of a isometric gauge

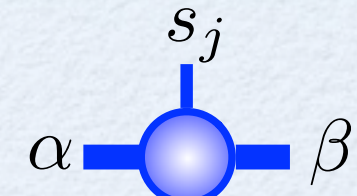
- tricks based on transfer matrices of long homogeneous chains may help



Rossini, et al., *J. Stat. Mech.* (2011) P05021

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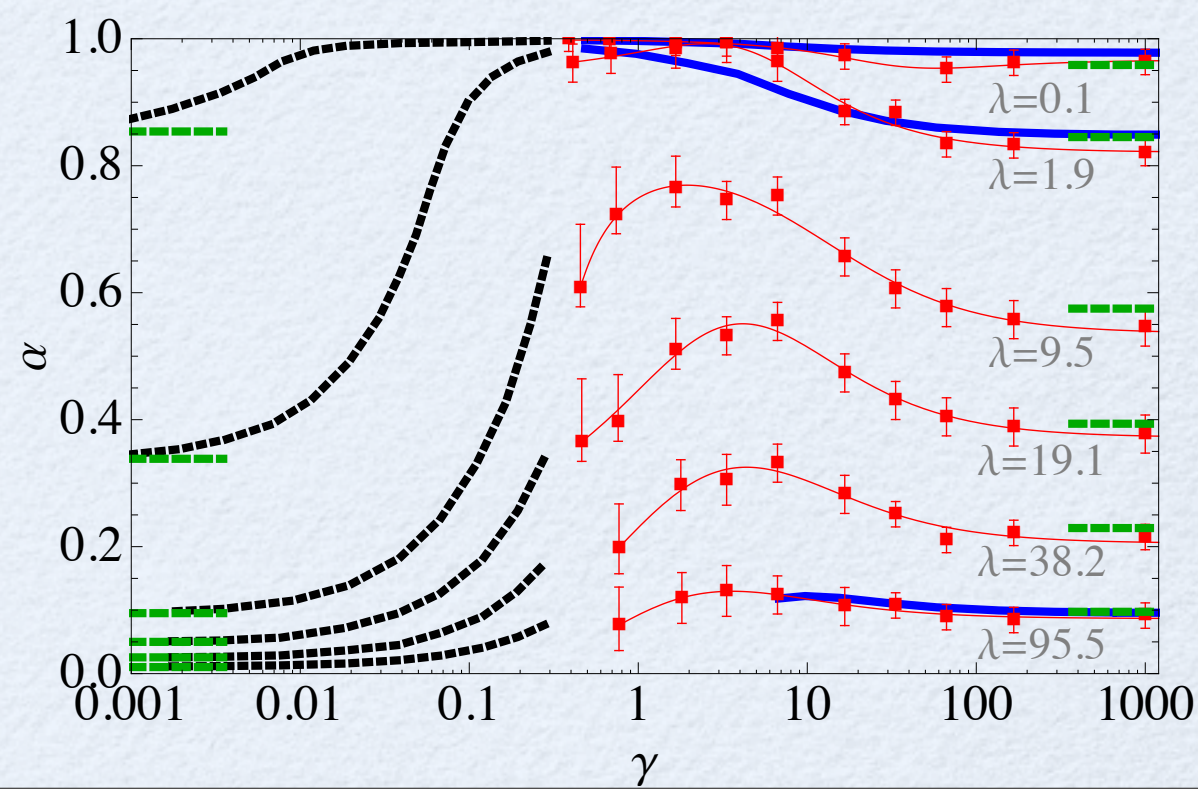
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- EXAMPLE:

Bose-Hubbard model at low filling
+ Peierls substitution + impurity

Cominotti, MR, et al., PRL 113, 025301 (2014)

alternative: cMPS for Lieb-Liniger
ongoing with D. Draxler, J. Haegeman



OUTLINE

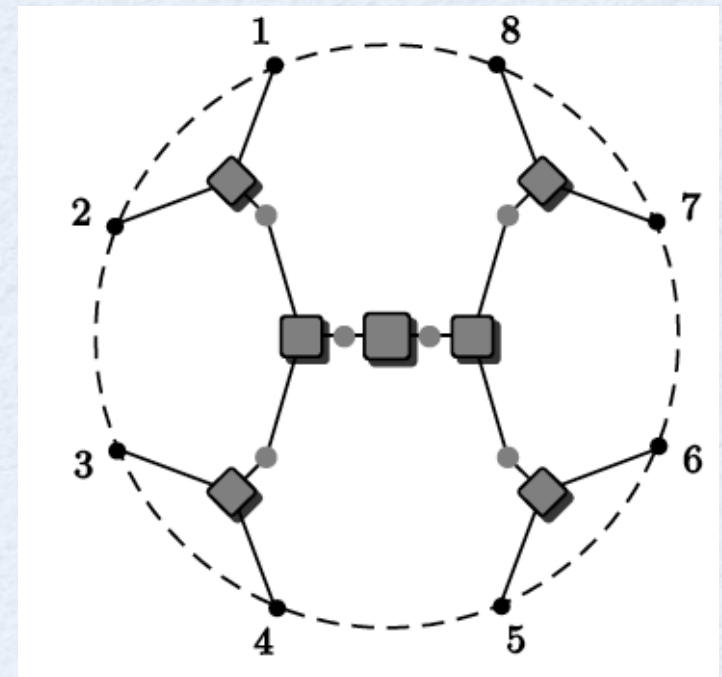
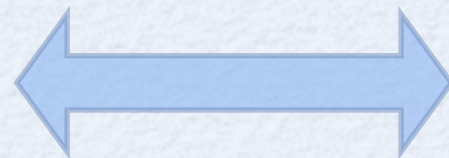
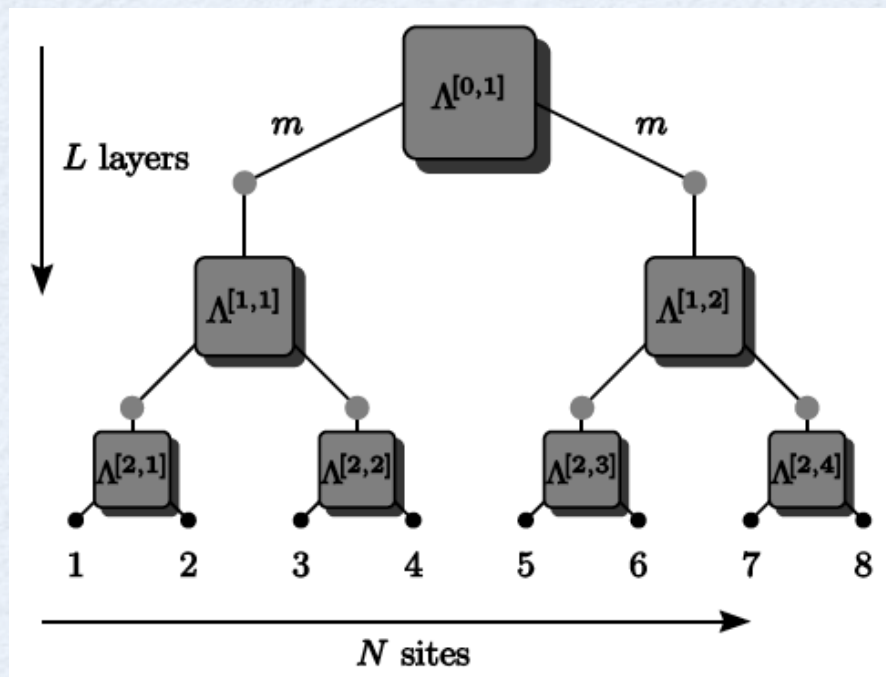
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Tree Tensor Networks (TTN)

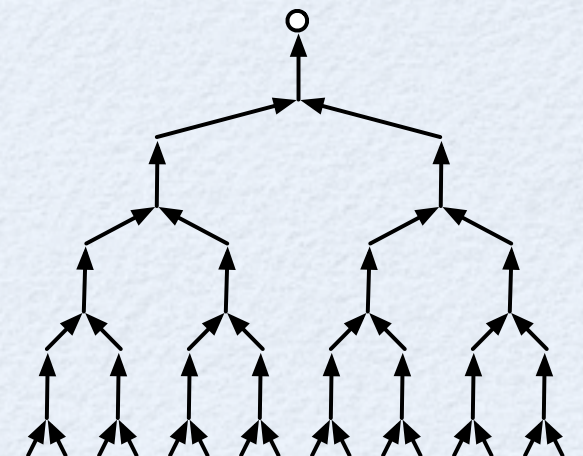
- loop-free, hierarchical, structure treating PBC on the same footing of OBC



- set of $(N-1)$ tensors $\left\{ \Lambda^{[l,n]} \right\}_{n=1,\dots,2^l}^{l=0\dots \log_2(N/2)}$

bond dimension **m**

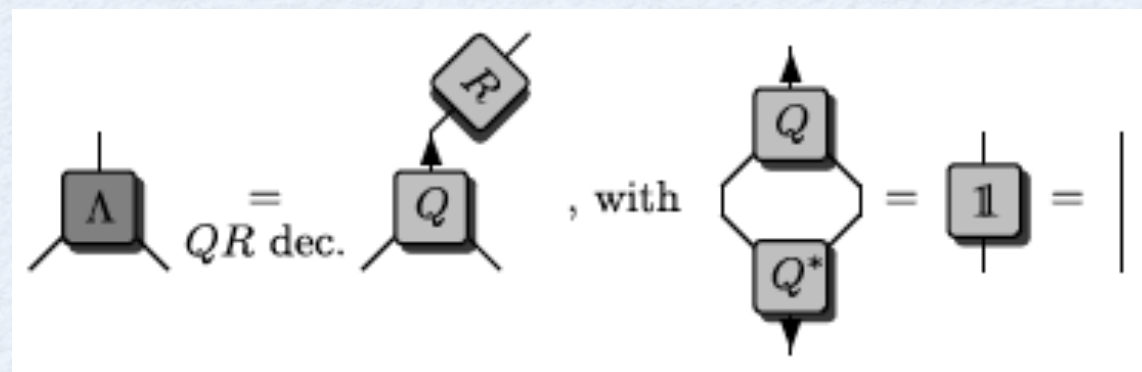
- storage $O(Nm^3)$; computation $O(Nm^4)$
- standard interpretation: RG flow from L towards 0 [i.e., a MERA without disentanglers ...]



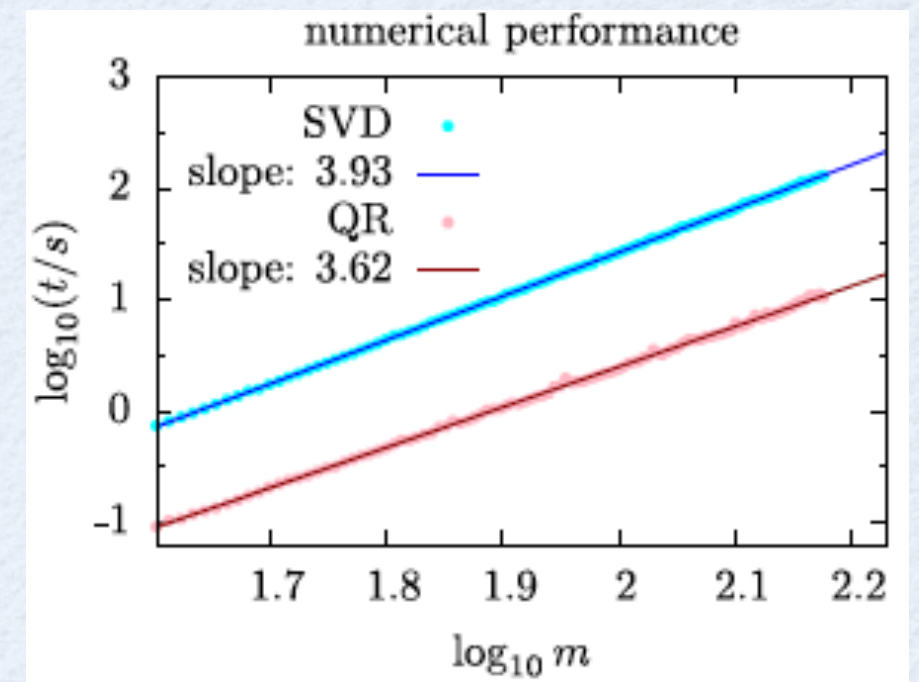
M. Gerster, MR, et al. Phys. Rev. B 90, 125154 (2014)

Adaptive gauging of a TTN

- loop-free structure allows for more ! *Central gauge* towards any tensor !
- INGREDIENT: Isometrization of a single tensor via QR decomposition

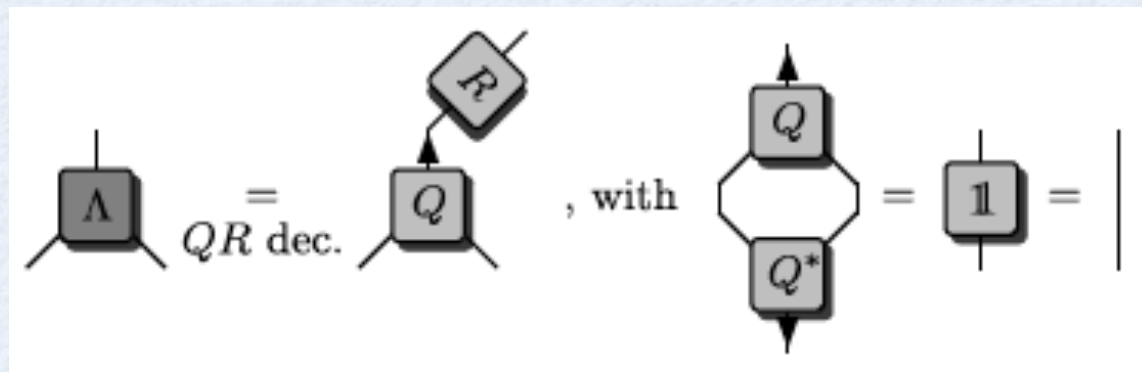


(feasible on all legs ...)



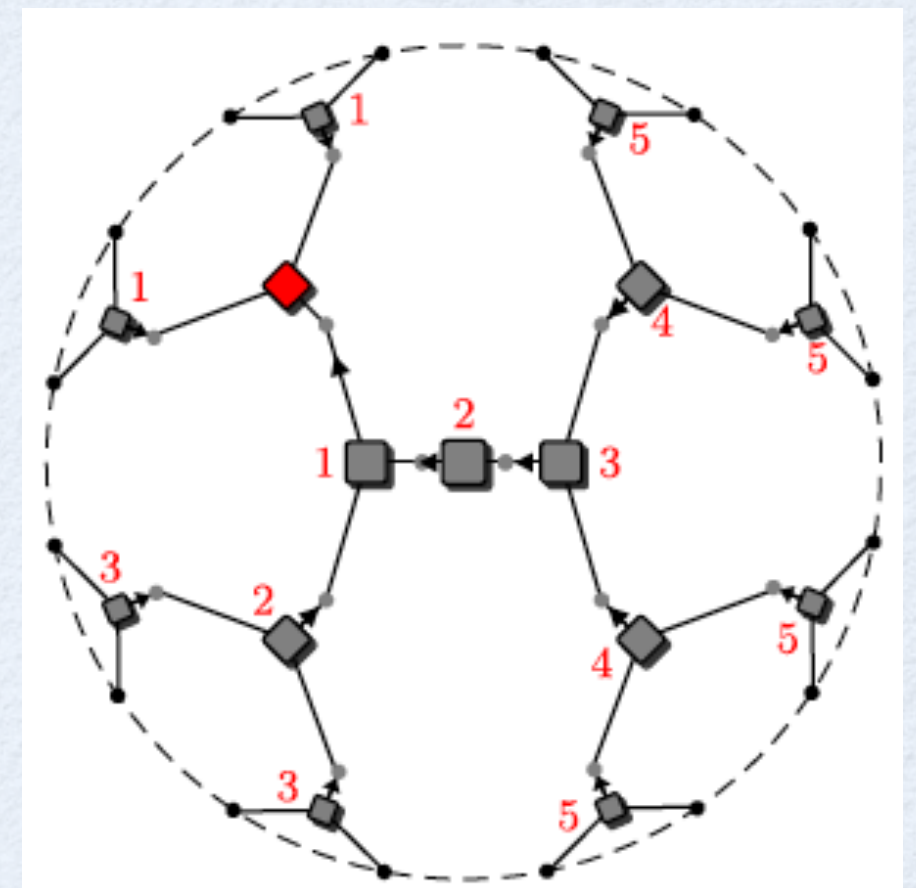
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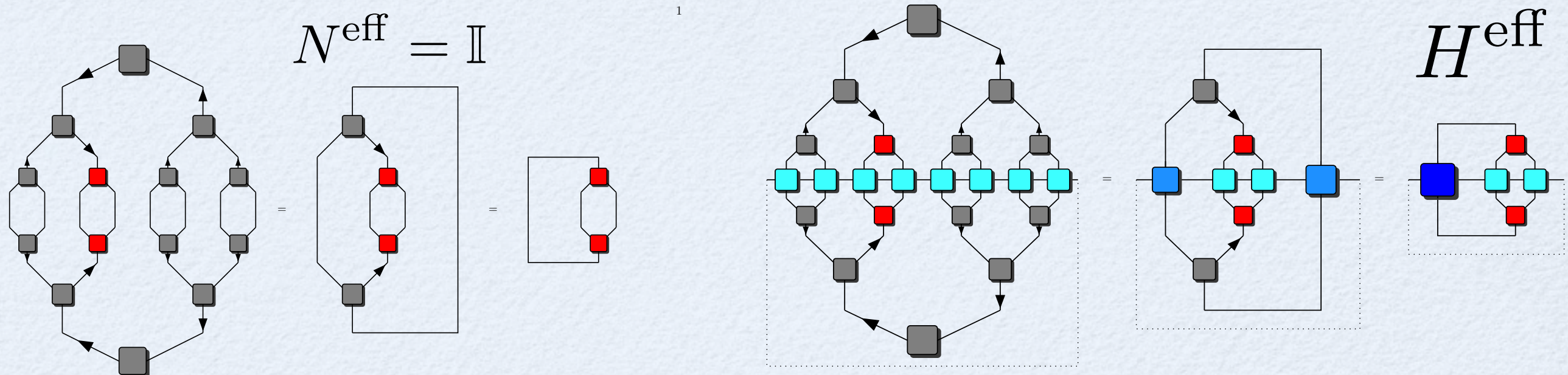
- **RECIPE:**
 - a) for each tensor determine distance from “nucleus”
 - b) perform QR in order & direction of decreasing distance
 - c) adsorb the R remainder in the not yet isometrized tensors



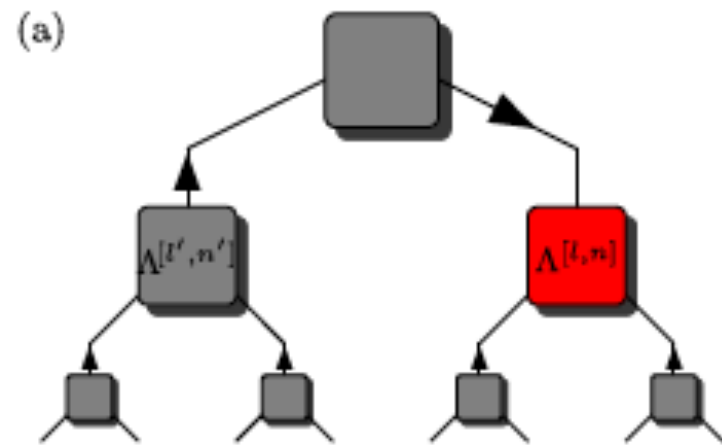
Ground state variational algorithm

- **loop-free structure** allows for more ! *Central gauge* towards any tensor !
- ADVANTAGE: effective norm operator disappears in the secular problem
i.e., no need for less stable generalized eigenvalue problem solver !

$$\min_{|\Psi\rangle \in \text{TN}} \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle \quad \rightarrow \quad H_j^{\text{eff}} A_{[j]} = \varepsilon N_j^{\text{eff}} A_{[j]} \quad (\text{cycle on } j)$$

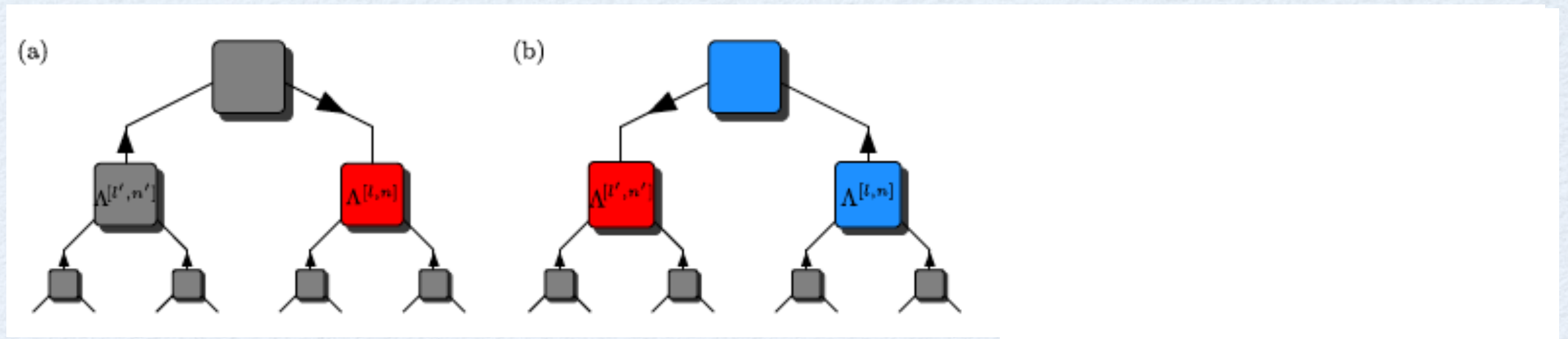


Ground state variational algorithm



(a) optimize $\Lambda^{[l,n]}$, i.e., solve the secular problem $H_{[l,n]}^{\text{eff}} \Lambda_{[l,n]} = \varepsilon \Lambda_{[l,n]}$

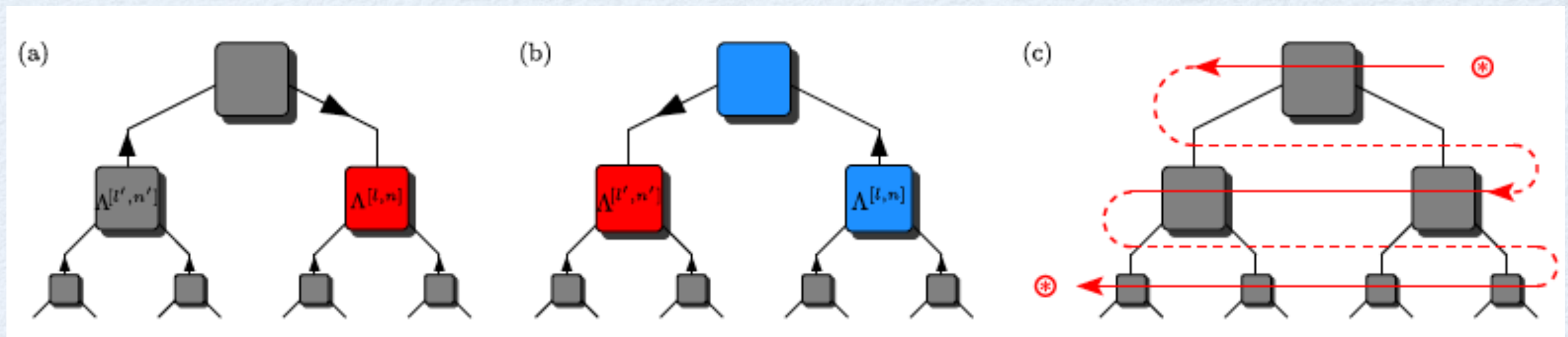
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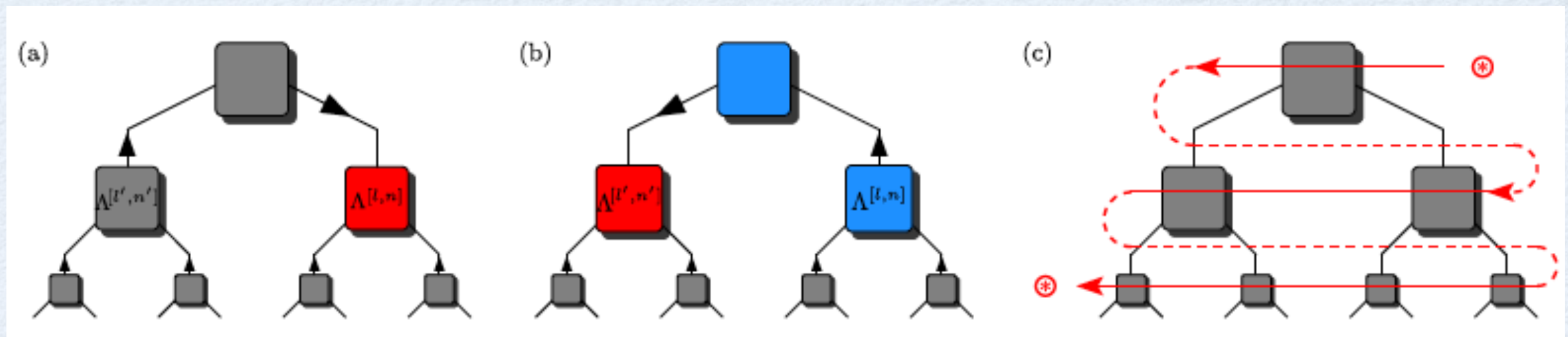
(b) target the next tensor $\Lambda^{[l',n']}$ by adjusting isometrization and updating effective Hamiltonian terms

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- (c) repeat for each tensor (= “sweep”) and stop when converged
- **Numerically stable!** Only ingredients needed:
 QR + eigensolver (Arnoldi/Lanczos) + tensor contraction routines
 (+ SVD in case of two-tensor optimization)
- ternary tensors + loop-free ==> **easily implemented symmetries !**

Effective Hamiltonian Construction

- Particularly simple with nearest-neighbor terms only
(and easily generalizable also to MPOs)

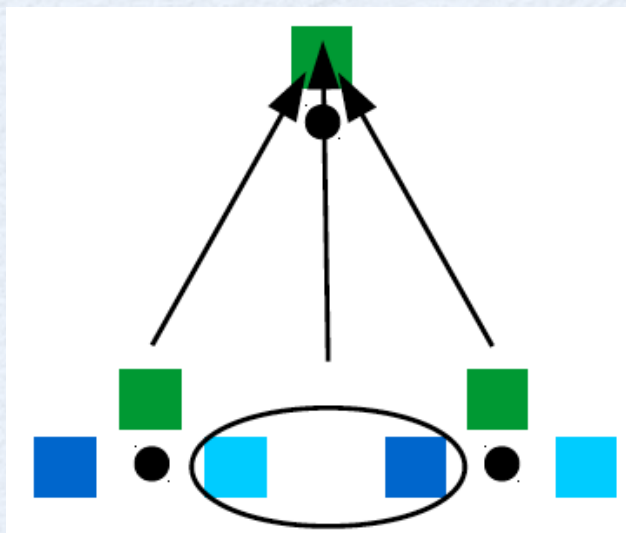
$$H = \sum_i H_{\text{loc}}^i + \sum_i H_A^i H_B^{i+1}$$

■
■
■

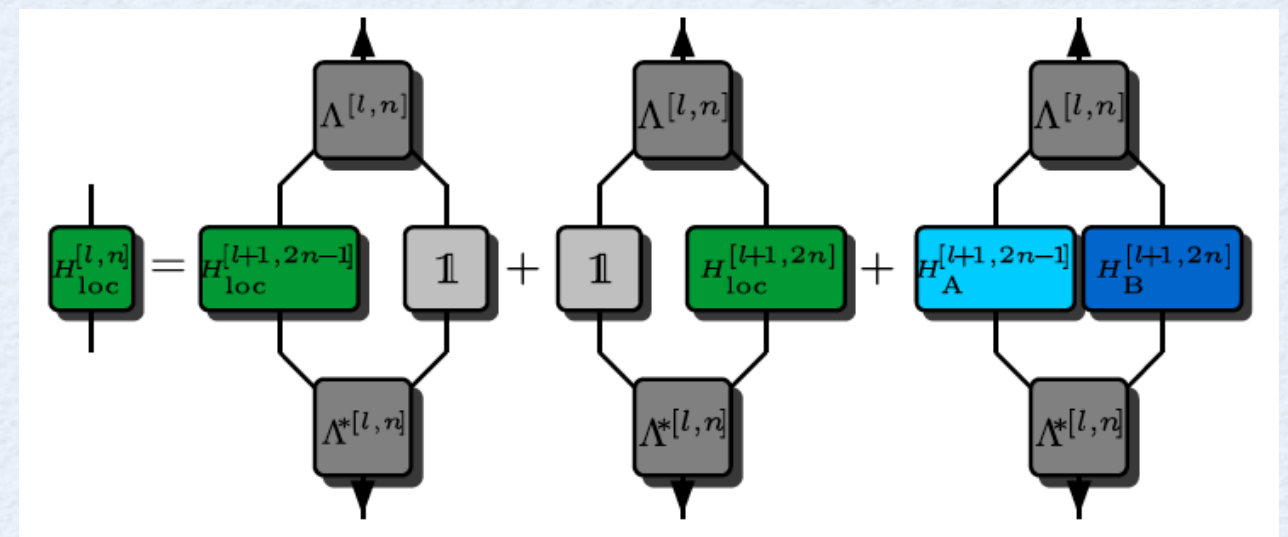
- Mapping from one level to the next:

l

 $l + 1$



≡



Effective Hamiltonian Construction

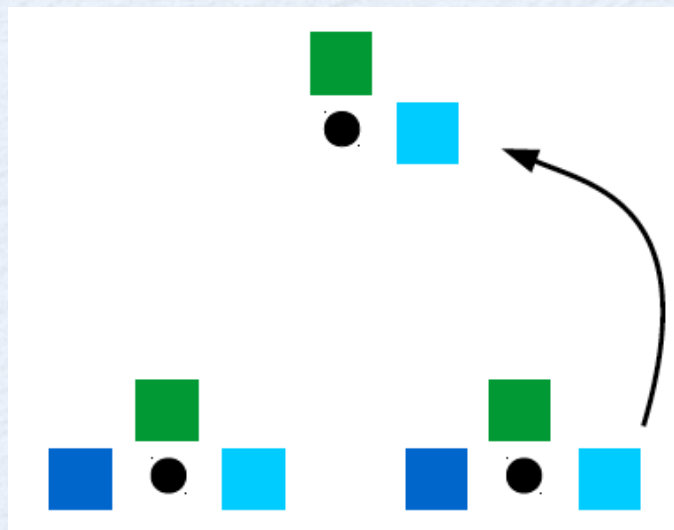
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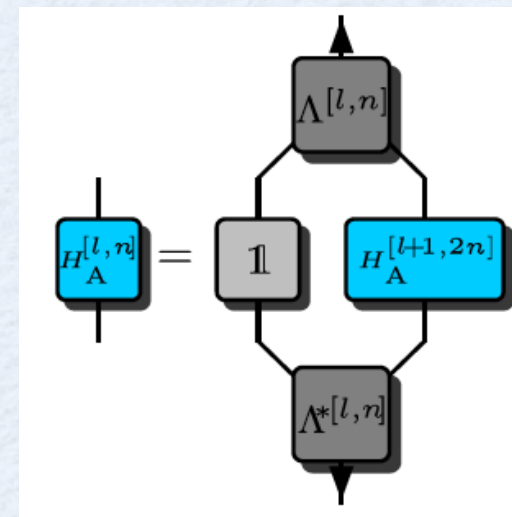
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$\equiv$



Effective Hamiltonian Construction

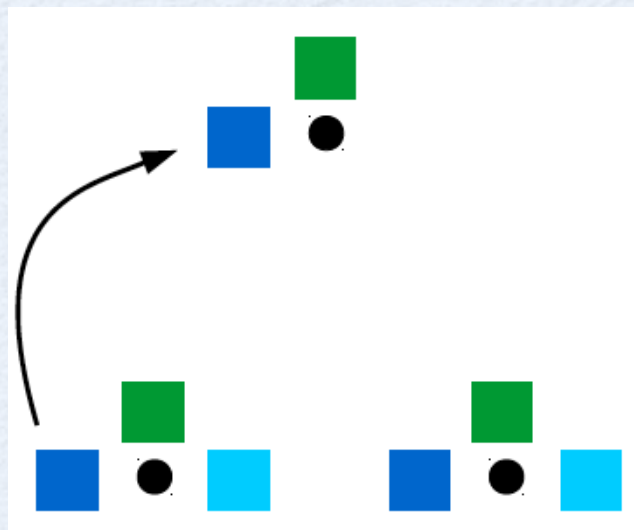
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$$H = \sum_i \underbrace{H_{\text{loc}}^i}_{\text{green}} + \sum_i \underbrace{H_A^i}_{\text{cyan}} \underbrace{H_B^{i+1}}_{\text{blue}}$$

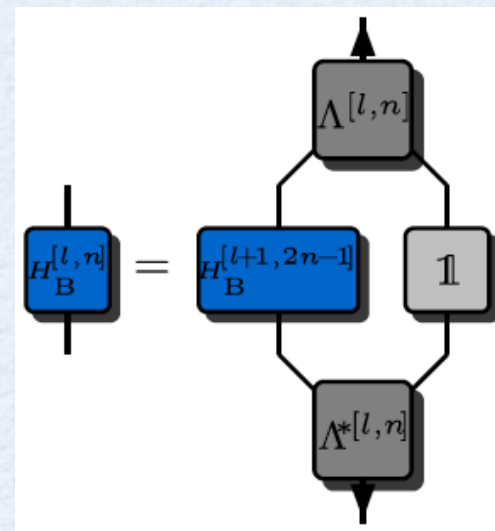
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l

 $l + 1$

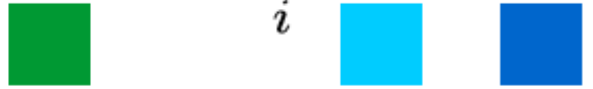


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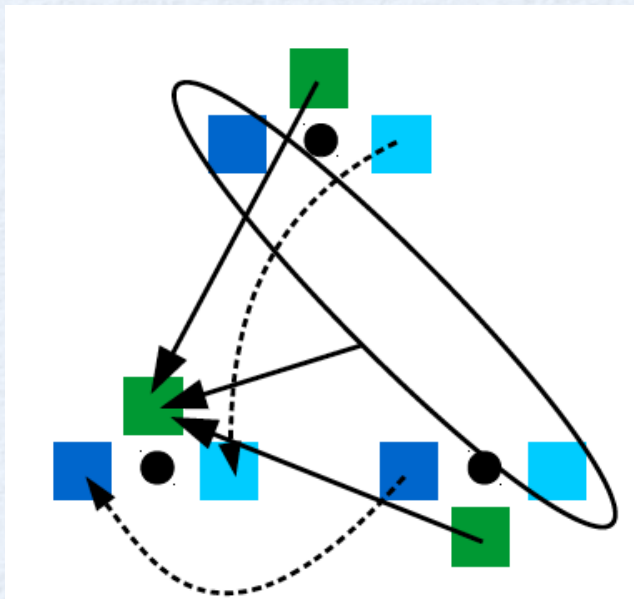
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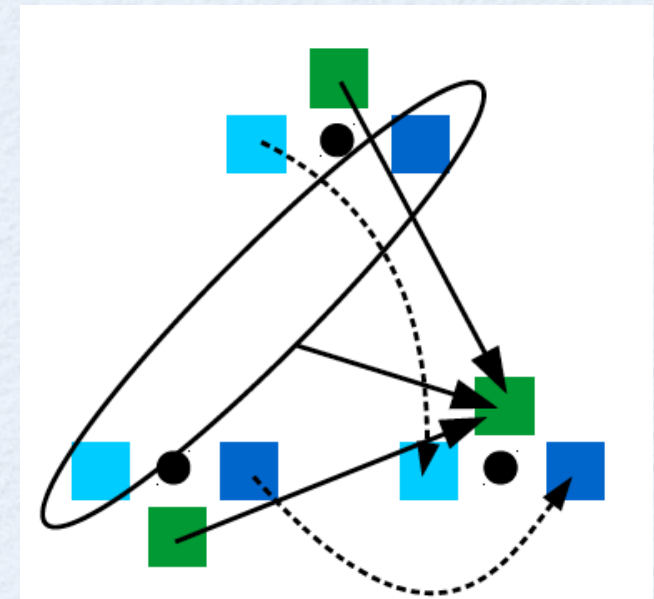
$$H = \sum_i H_{\text{loc}}^i + \sum_i H_A^i H_B^{i+1}$$


- Mapping works identically in all directions !

RG



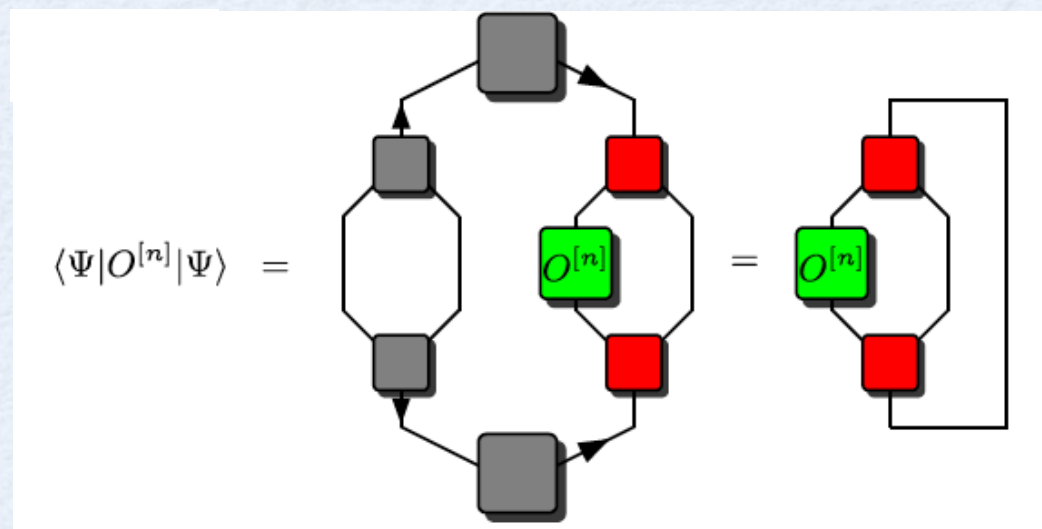
RG



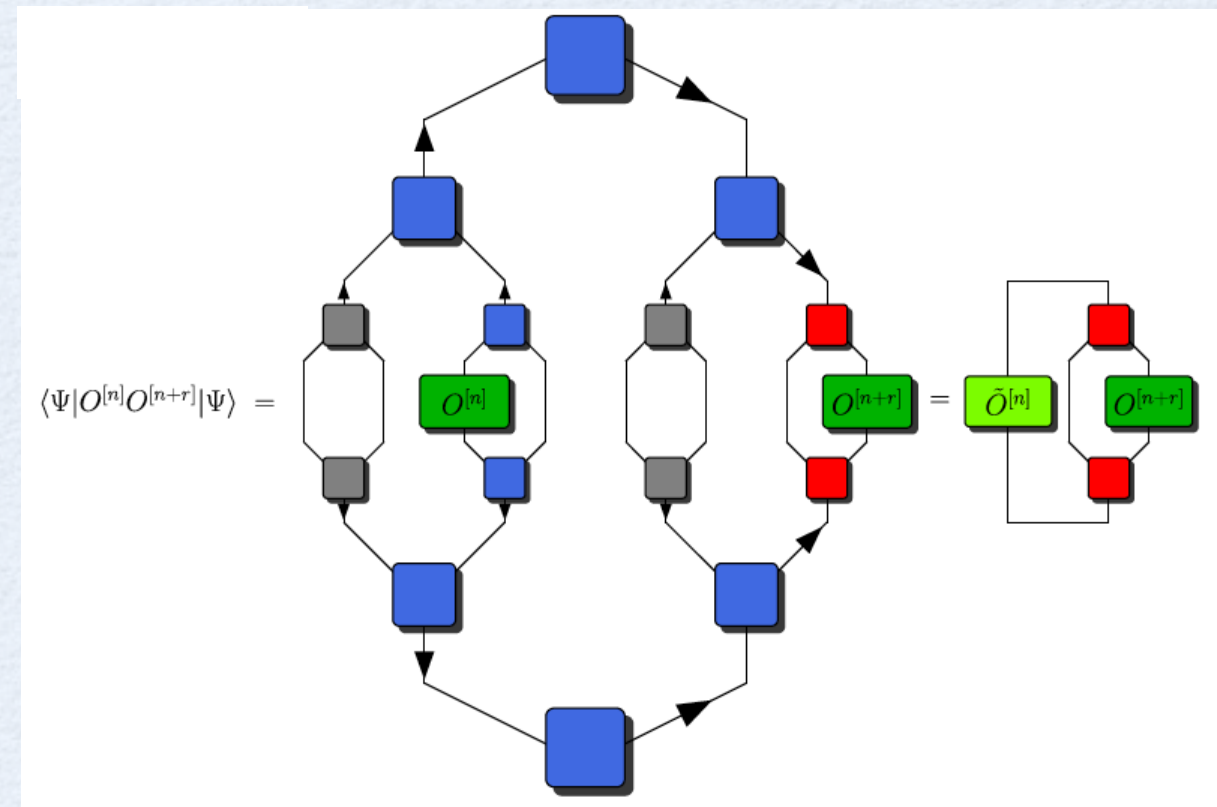
- Mapping should be performed in the same order as isometrization
(i.e., from furthest to closest tensors to the “nucleus”)

Measurement of observables

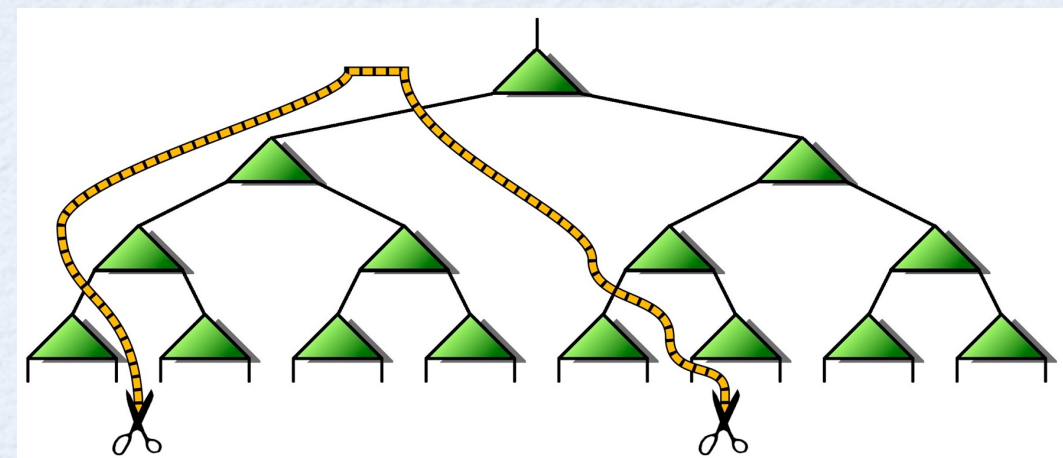
- local observables:
only 3 contractions



- correlation functions:
only $O(\log N)$ contractions



- hierarchical structure could encompass critical properties
- log divergence of entang. entropy captured “on average”



OUTLINE

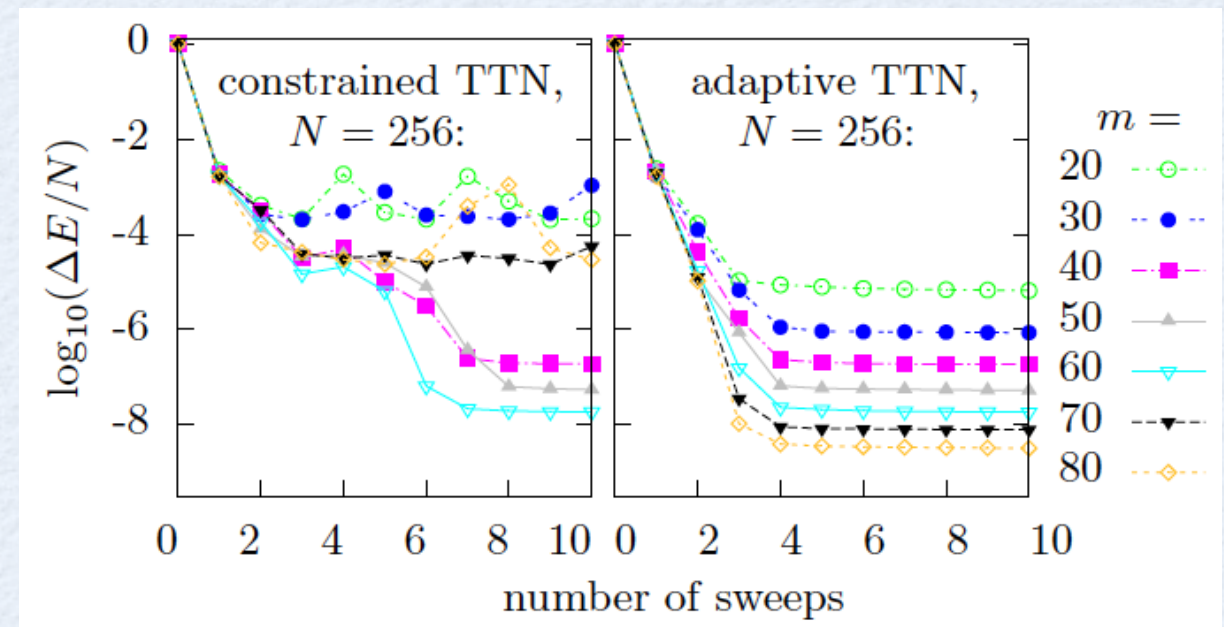
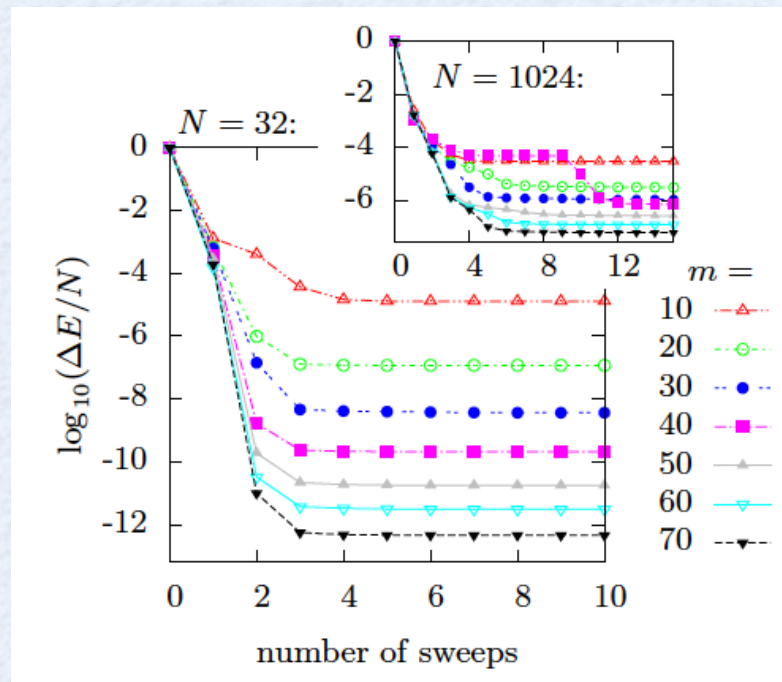
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Ising in transverse field: energy

- Convergence in few sweeps -- more stable than *standard* isometric TTN

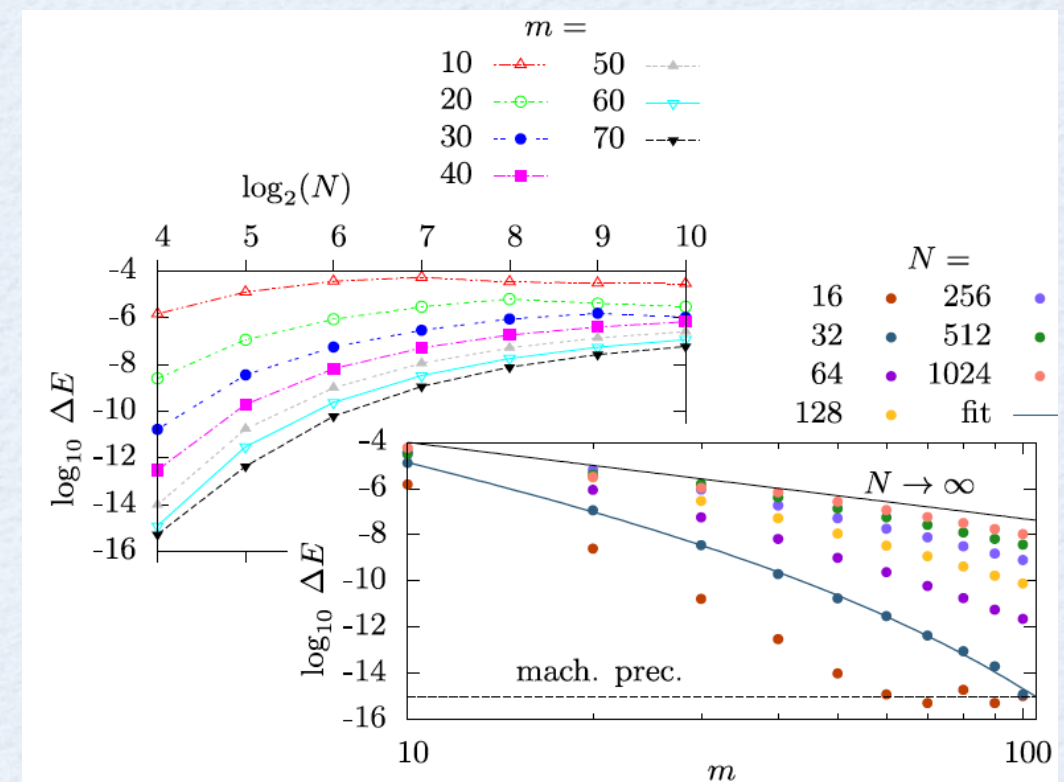


- Power-law convergence in the bond-dimension

$$\Delta E(m) \propto m^{-a} e^{-b m}$$

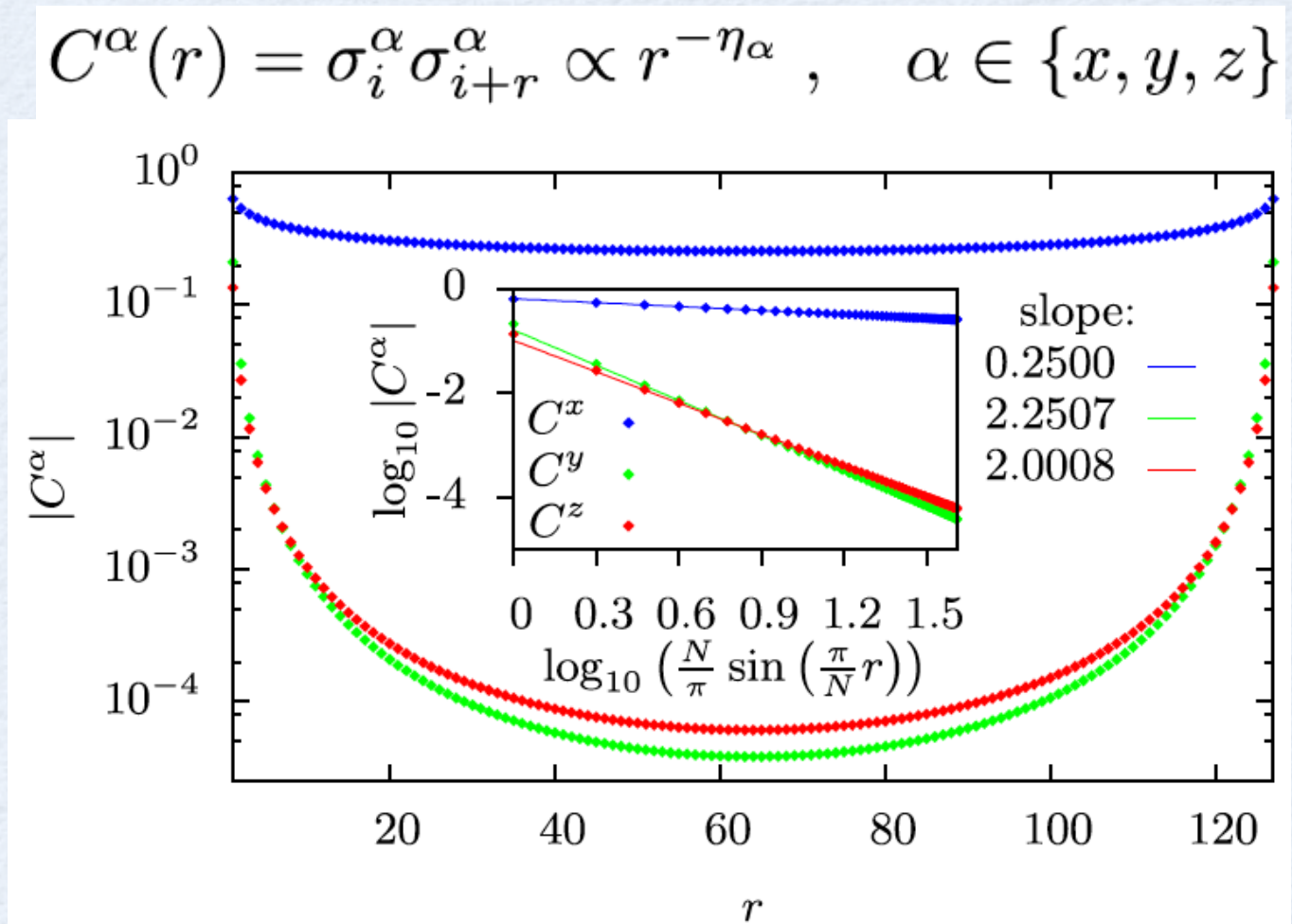
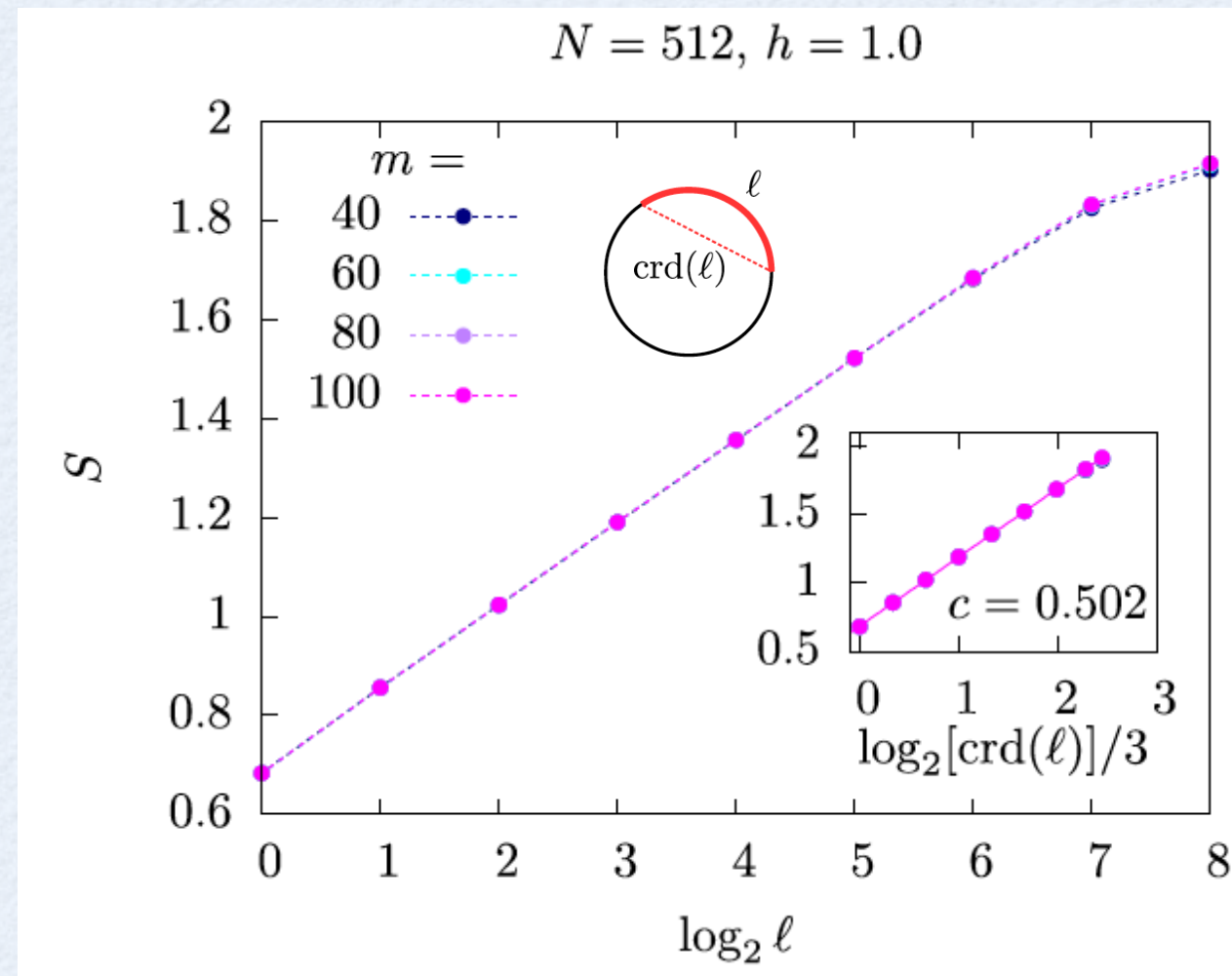
b vanishing at TL

$a \sim 3$ at TL



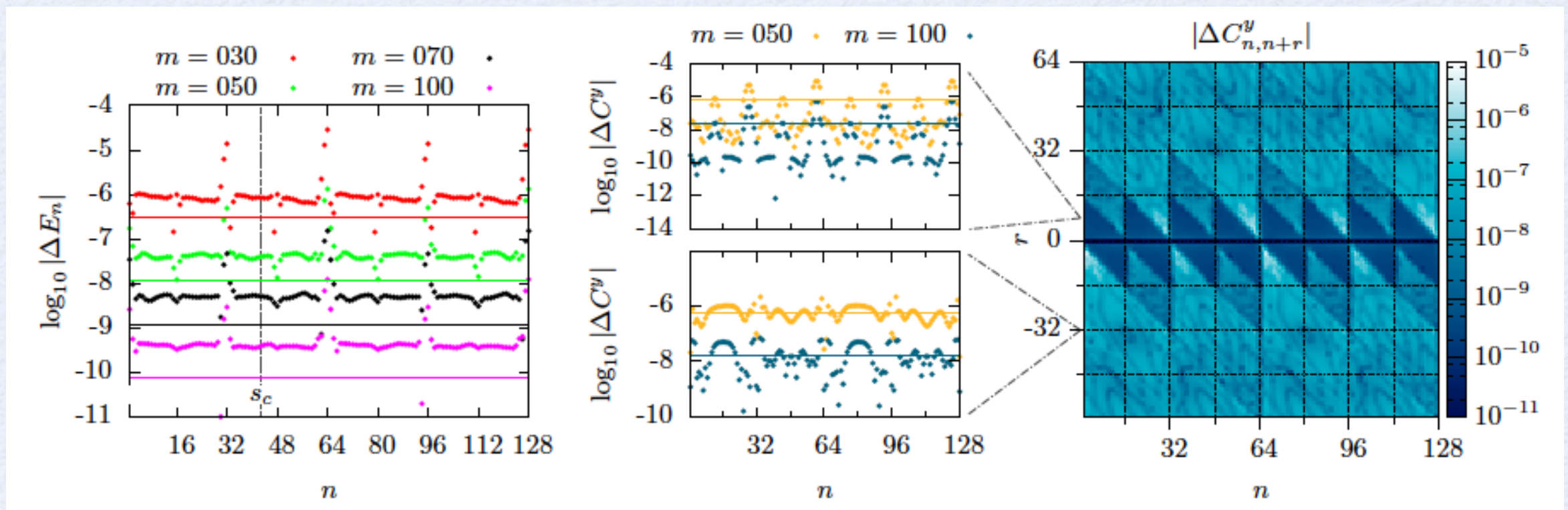
Ising in transverse field: correlations

- Critical behaviour captured with high accuracy

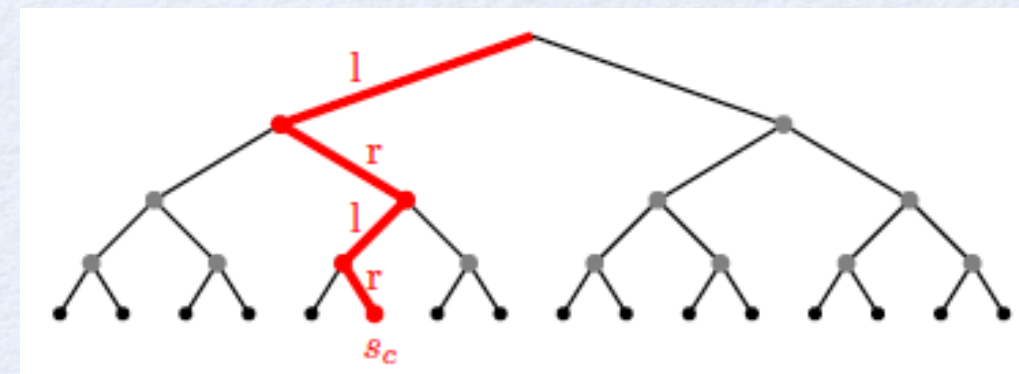


Ising in transverse field: translations

- breaking of translational invariance compensated by large bond dims.

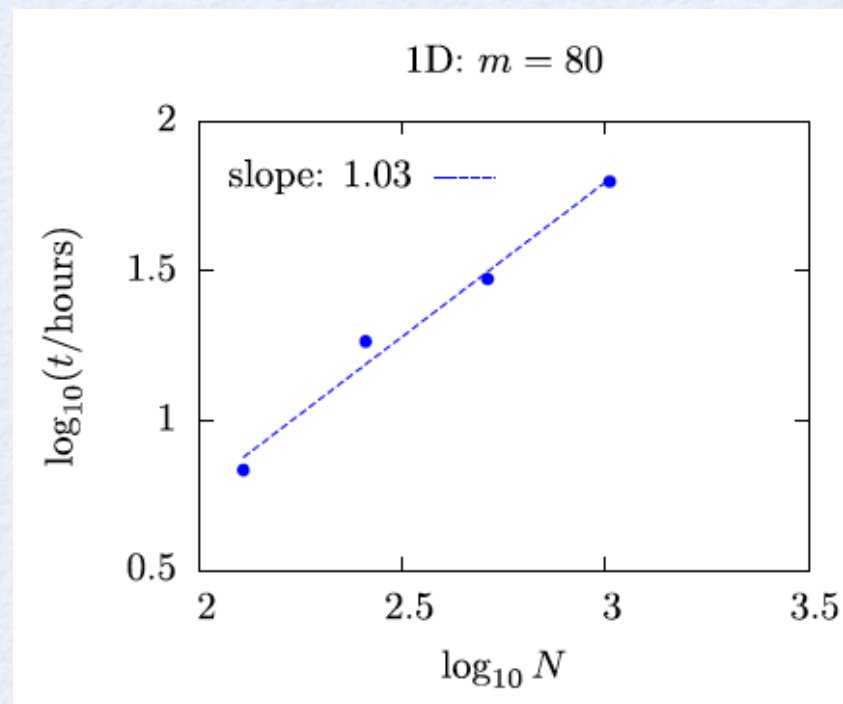


- no strict need to introduce a “central” site...

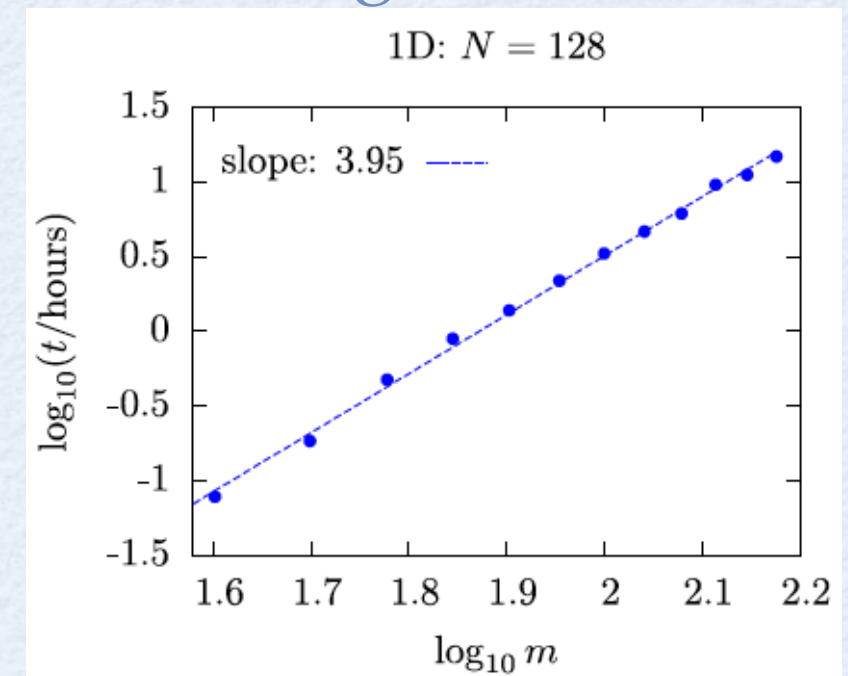


CPU running time

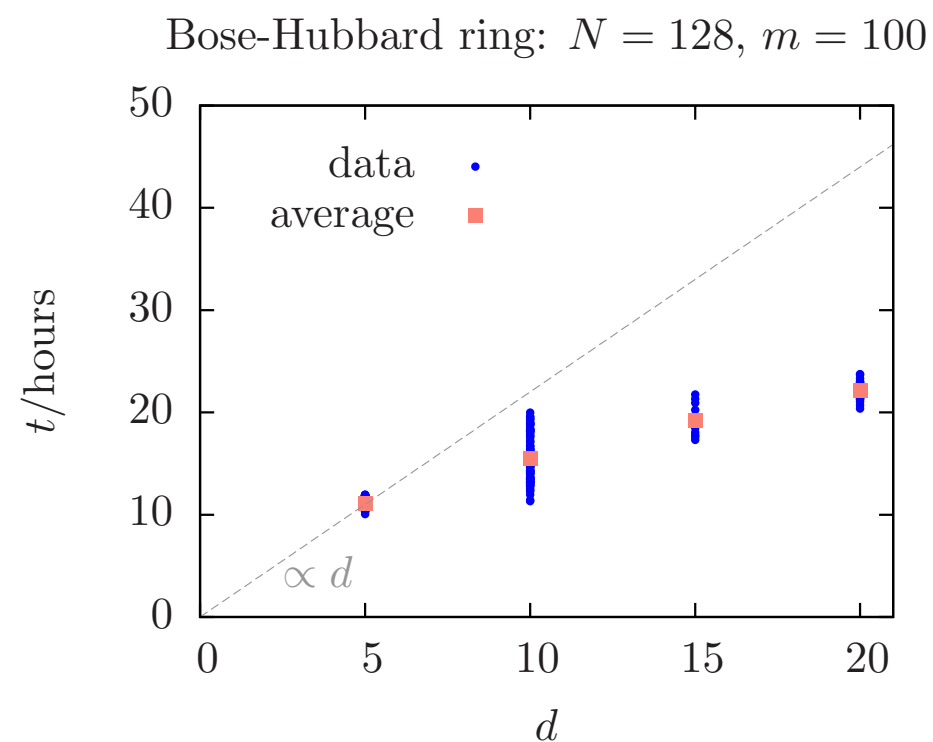
- linear scaling with system size



- $O(m^4)$ scaling with bond dim.



- sub-linear scaling
with local dimension !
[OBC is $O(d^n m^3)$]



OUTLINE

- Motivation: why periodic boundaries?
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The Hamiltonian

$$\mathcal{H} = -t \sum_j \left(b_j^\dagger b_{j+1} + \text{h.c.} \right) + \frac{U}{2} \sum_j n_j (n_j - 1) - \sum_j V_j n_j$$

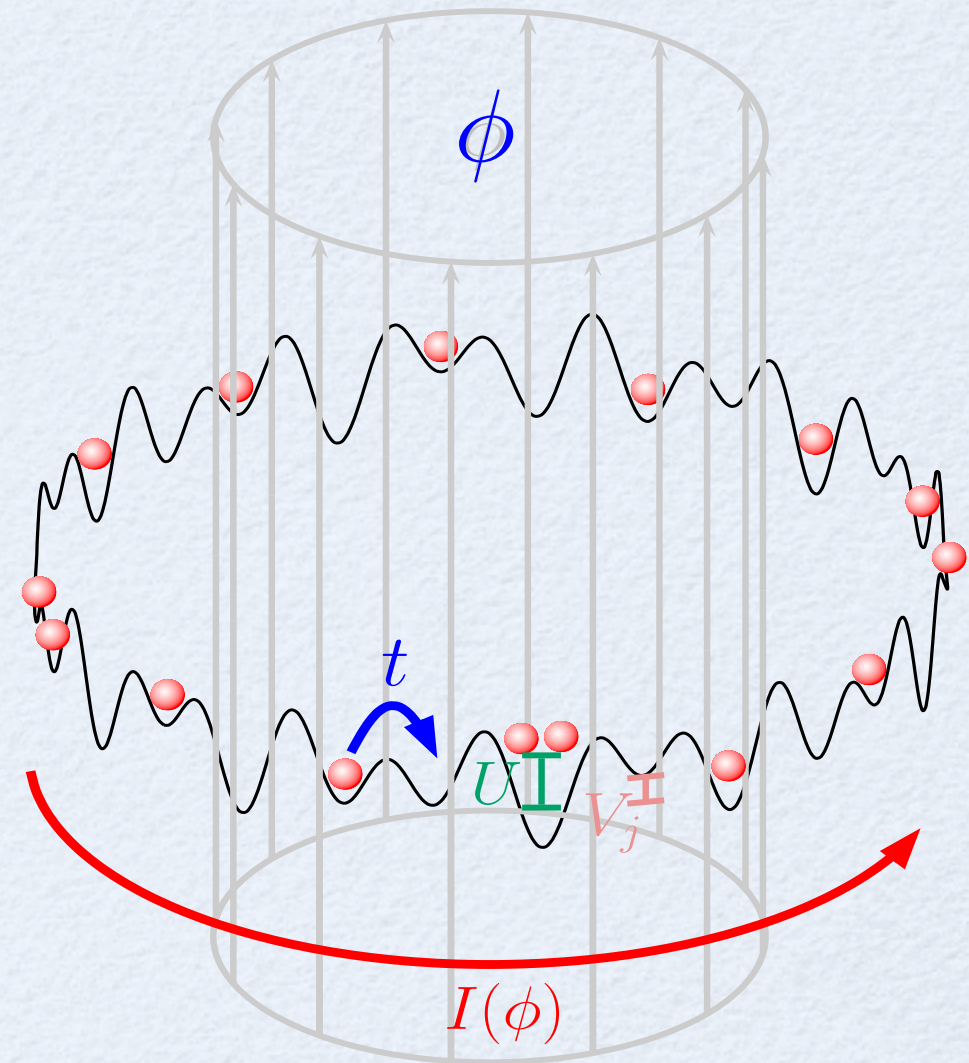
Commensurate particle density $n = N/L = 1$

Uniform disorder distribution $V_j \in [-\Delta, +\Delta]$

On-site interactions

Peierls substitution $t \longrightarrow t e^{-2\pi i \phi / N_s}$

Superfluid stiffness $\rho_s = \frac{N_s}{8\pi^2} \frac{\partial^2 E_0}{\partial \phi^2} \Big|_{\phi=0}$



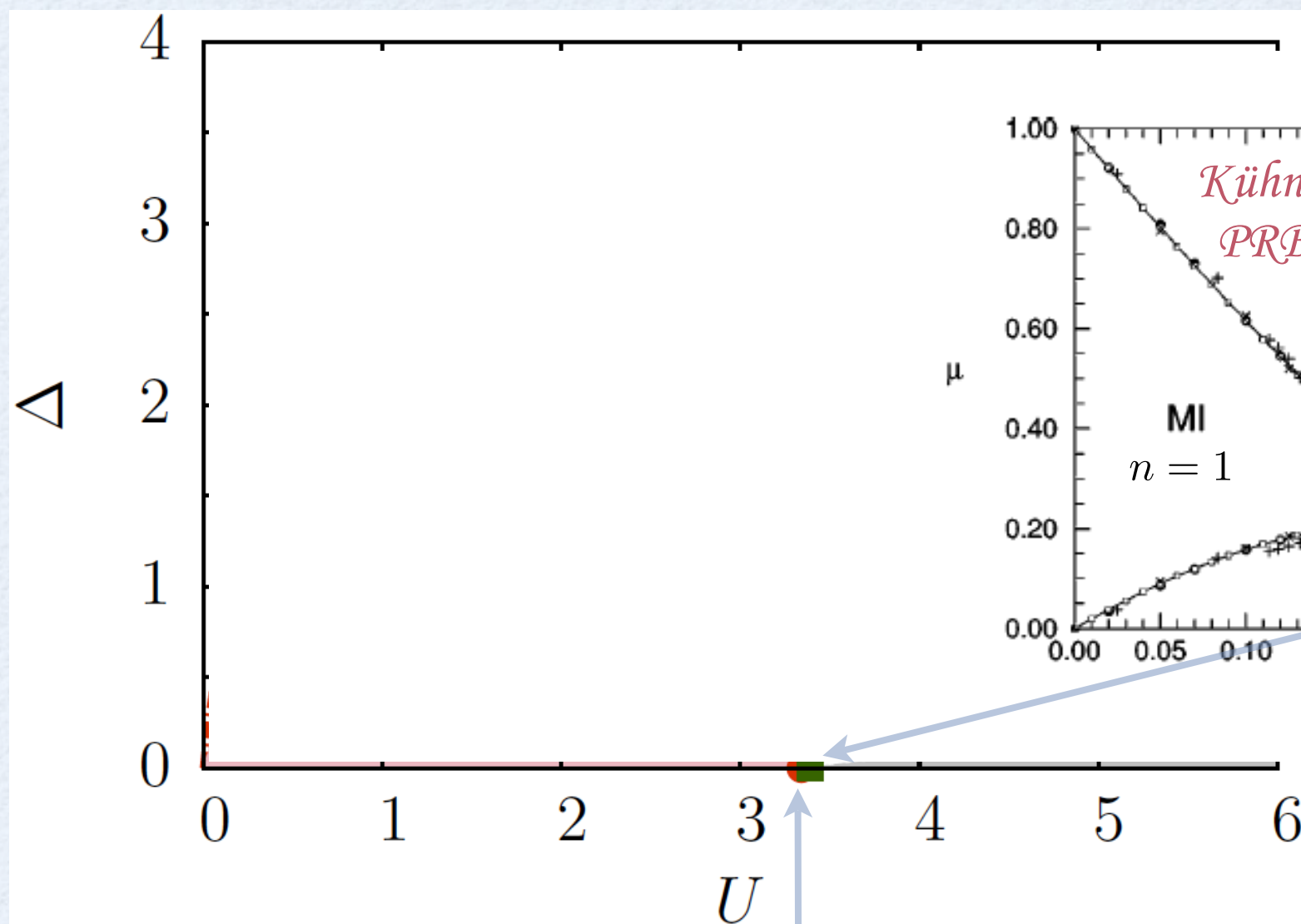
The phase diagram

$$U = 0$$



Anderson
Localization

$$\Delta \neq 0$$



$$\Delta = 0$$



Superfluid

Mott Insulator

BKT transition

$$U_c \simeq 3.3 t$$

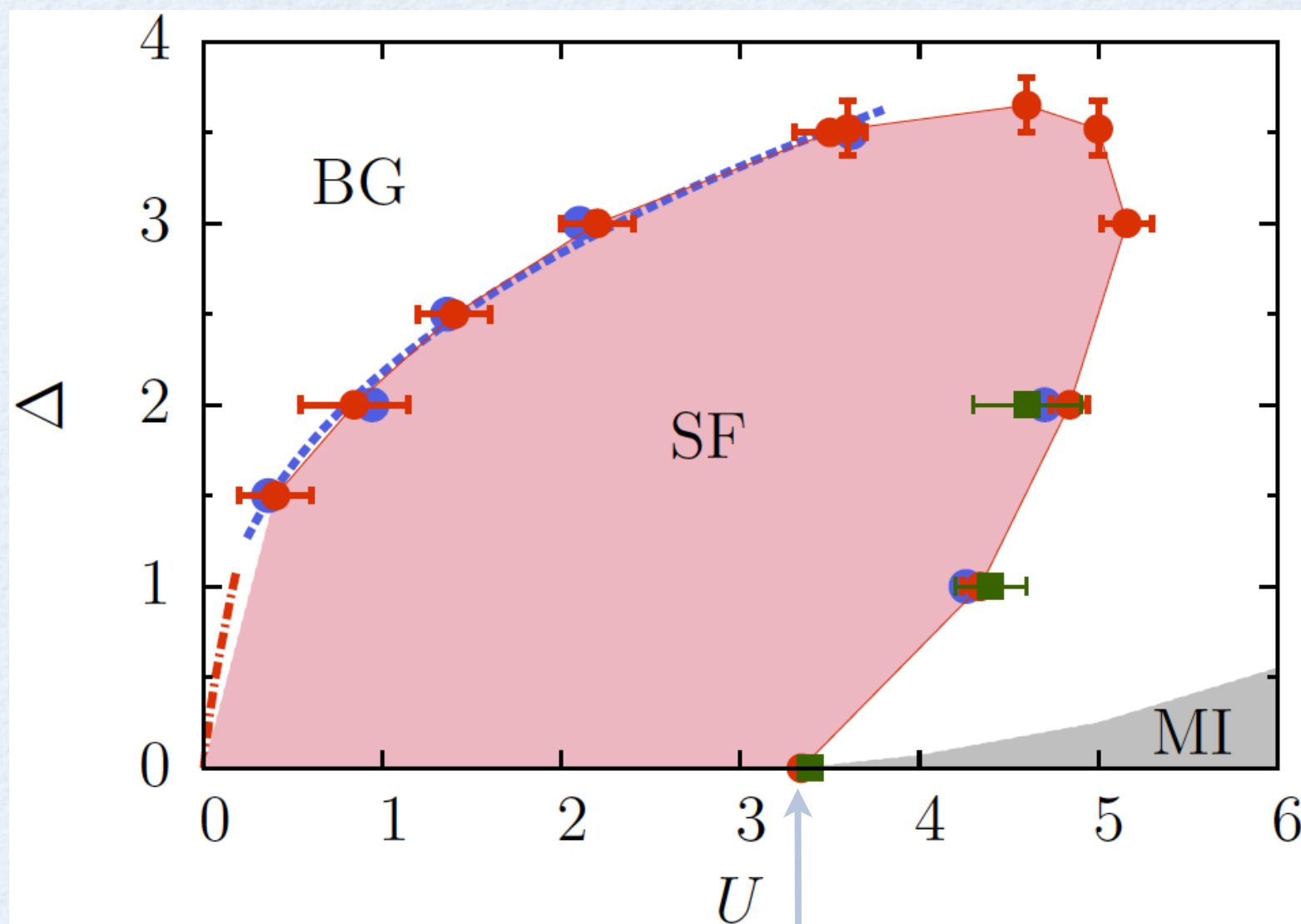
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Bose Glass

- compressible
- not coherent !

*Fisher, et al. ('89)
Giamarchi, Schulz,
Altman, Zwerver,
Prokof'ev, Svistunov,
Pollet, & many others*

$$\Delta = 0$$



Superfluid

Mott Insulator

BKT transition

$$U_c \simeq 3.3t$$

The phase diagram cold atoms experiments !?

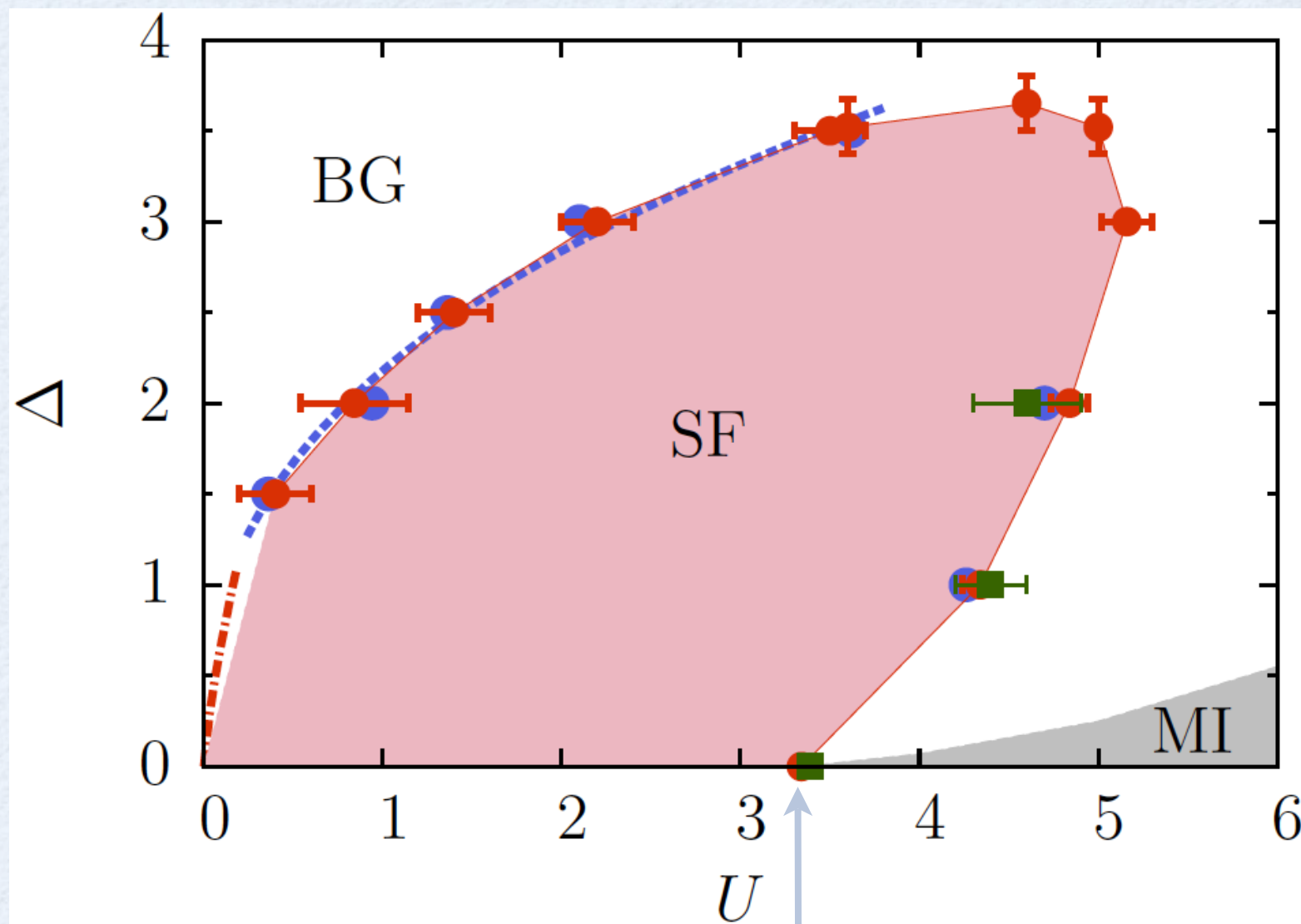
$$U = 0$$



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Localization

$$\Delta \neq 0$$

*J. Billy, et al.,
Nature 453, 891 (2008);
G. Roati, et al.,
Nature 453, 895 (2008).*



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Prokof'ev, Svistunov,
Pollet, & many others*

*C. D'Errico, et al.,
PRL 113, 095301 (2014)*

$$\Delta = 0$$



Superfluid

Mott Insulator

*M. Greiner, et al.,
Nature 415, 39 (2002).*

BKT transition

$$U_c \simeq 3.3 t$$

M. Gerster, MR, et al. NJP 18 015015 (2016)

N.V. Prokof'ev, B.V. Svistunov, PRL 80, 4355 (1998)

Indicator 1: superfluid stiffness

$$\rho_s = \frac{N_s}{8\pi^2} \frac{\partial^2 E_0}{\partial \phi^2} \bigg|_{\phi=0} \quad \longrightarrow \quad \text{universal jump} \quad (\sim \text{classical 2D XY})$$

$$\rho_s^c = \left(2/\pi^2\right) U_c$$

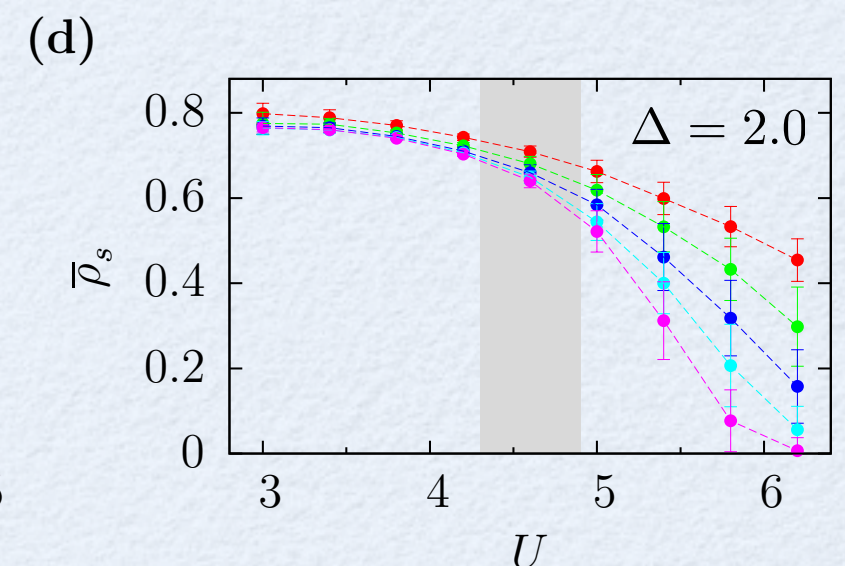
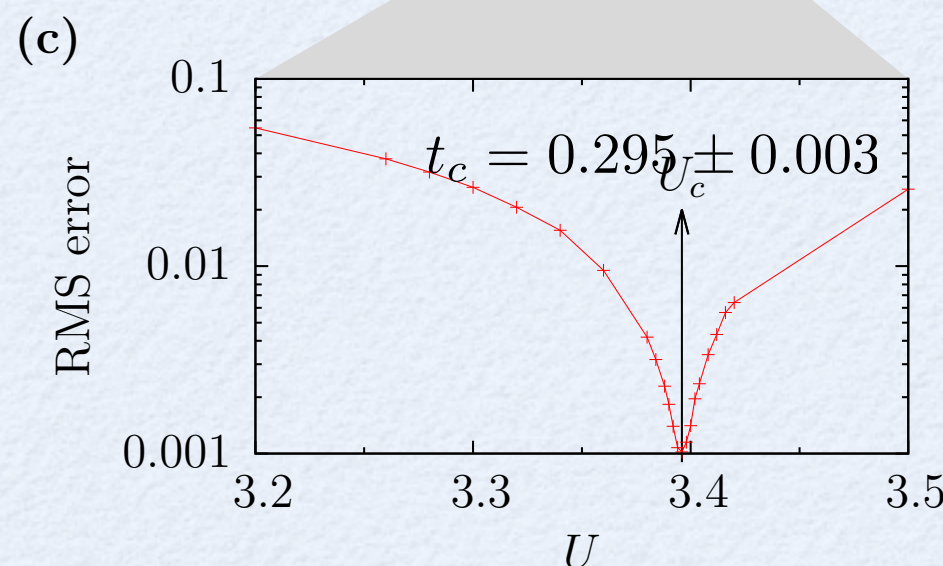
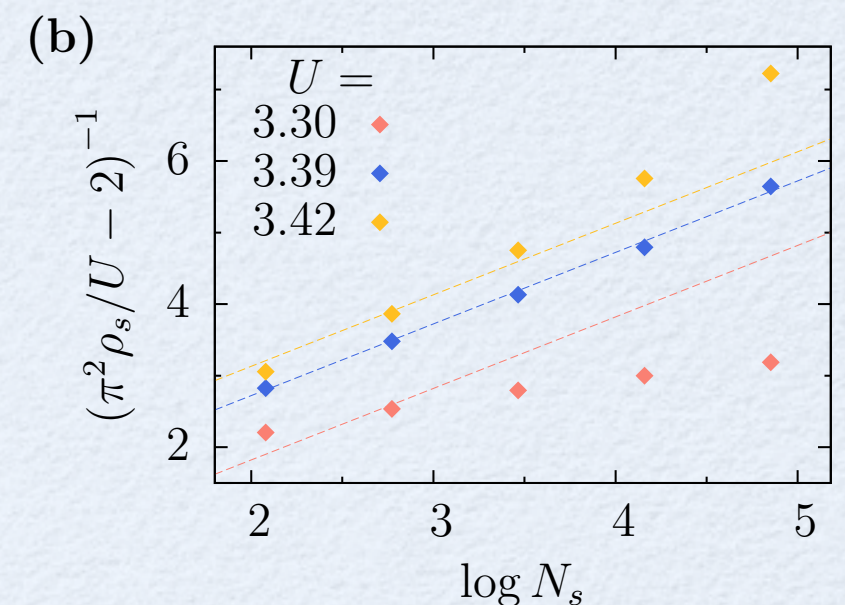
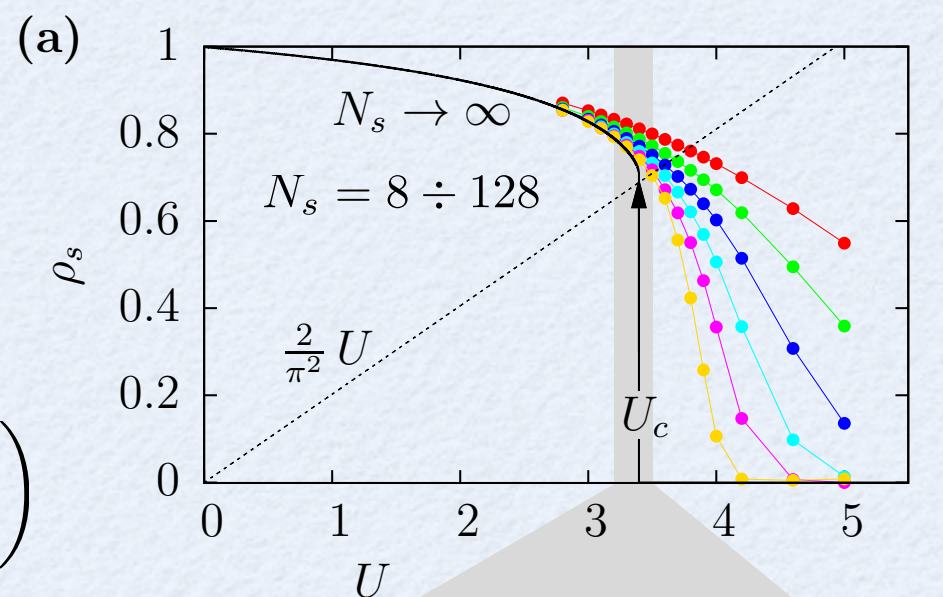
Nelson & Kosterlitz, PRL.39, 1201 (1977)

M. Fisher, et al., PRB 40, 546 (1989)

Finite size scaling

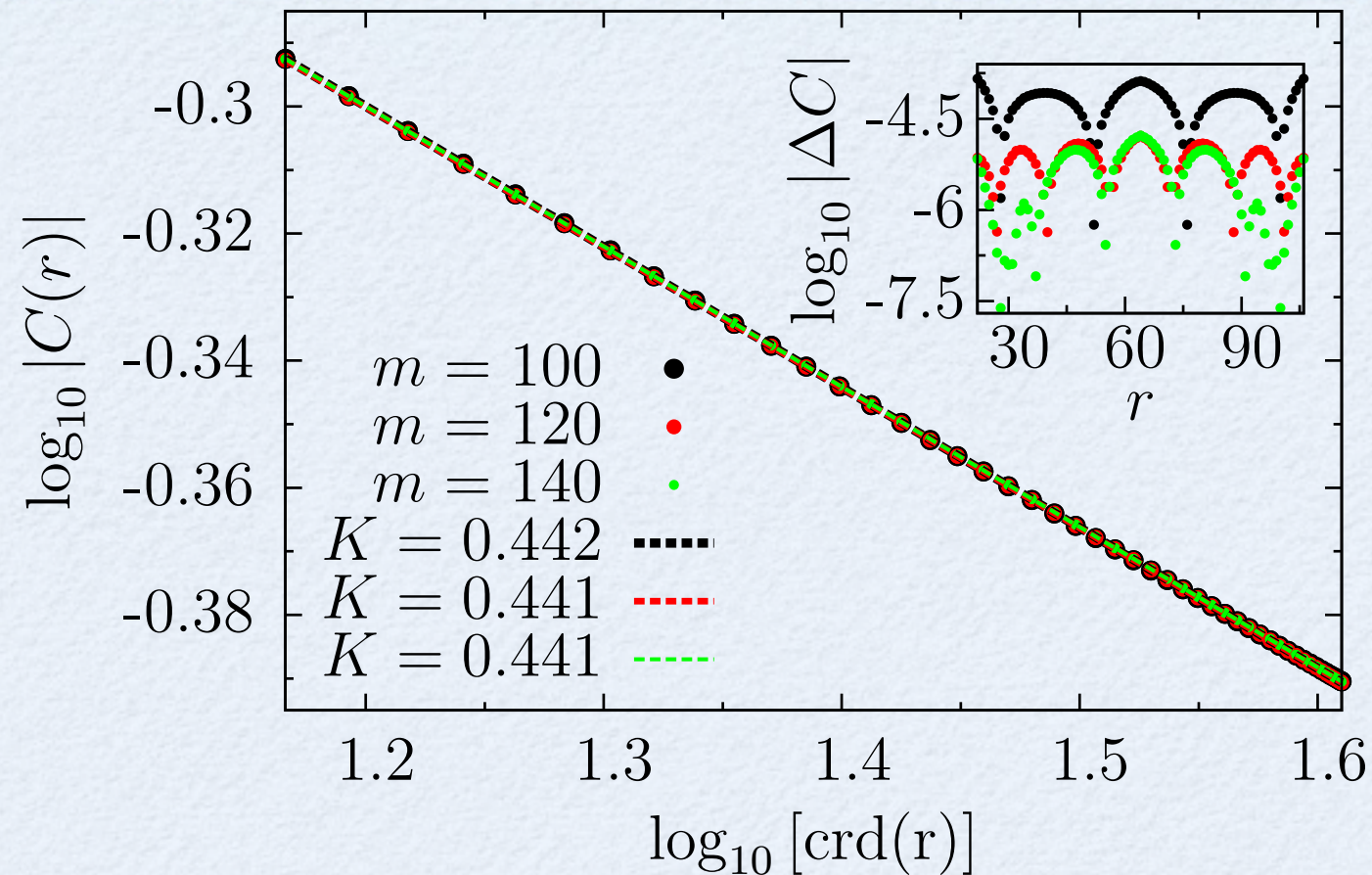
$$\rho_s^c(N) = \frac{2U}{\pi^2} \left(1 + \frac{1}{2 \log N + b}\right)$$

H. Weber, P. Minnhagen, PRB 37, 5986 (1988).



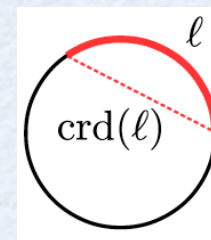
M. Gerster, MR, et al. NJP 18 015015 (2016)

Indicator 2: hopping correlation decay (K)



Luttinger liquid theory

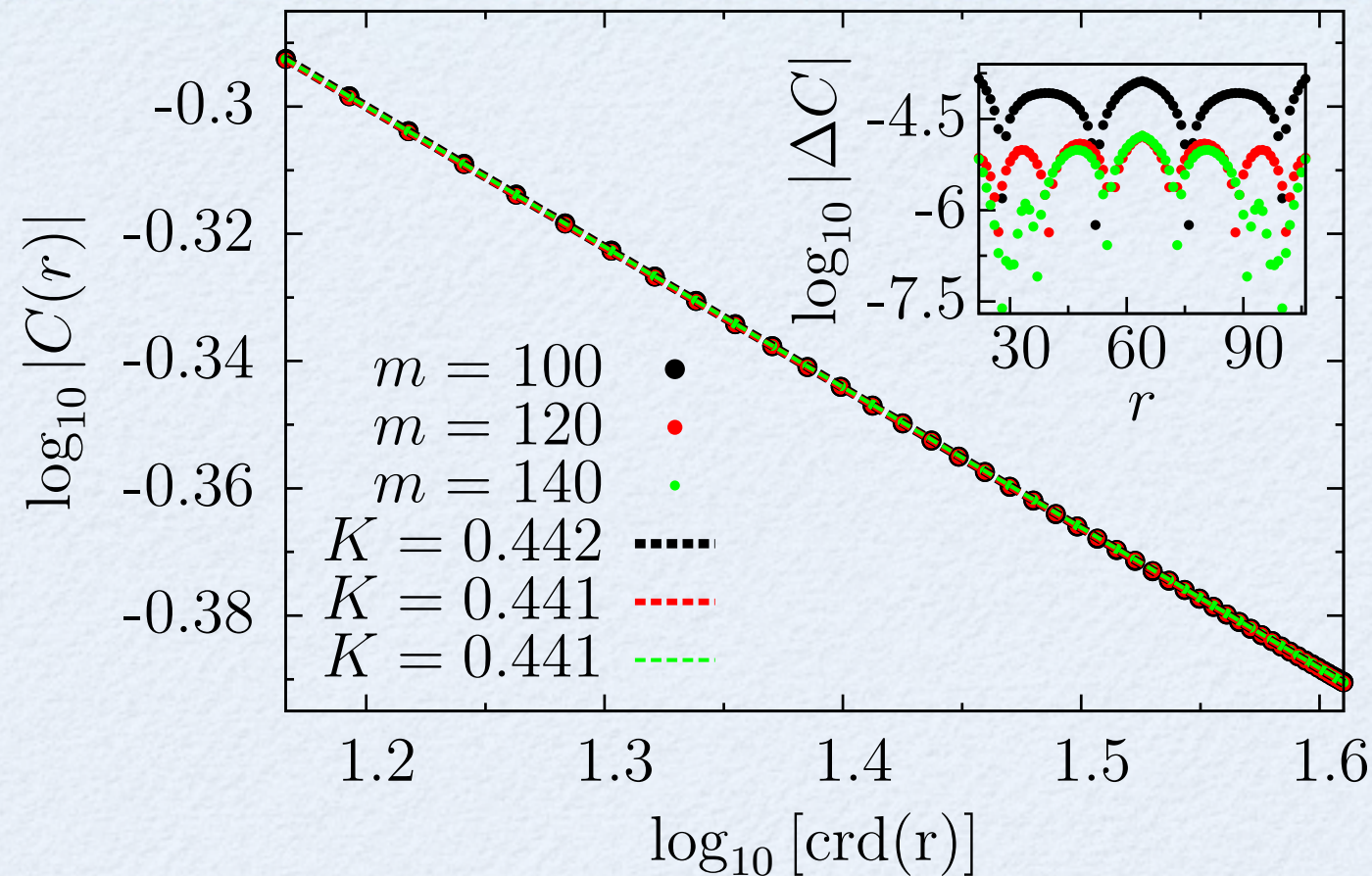
$$C(r) = \langle b_j^\dagger b_{j+r} \rangle \propto \text{crd}(r)^{-K/2}$$



PBC $\Rightarrow$ chord distance

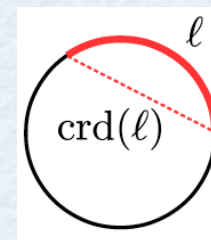
$$\text{crd}(r) = N_s / \pi \sin(\pi r / N_s)$$

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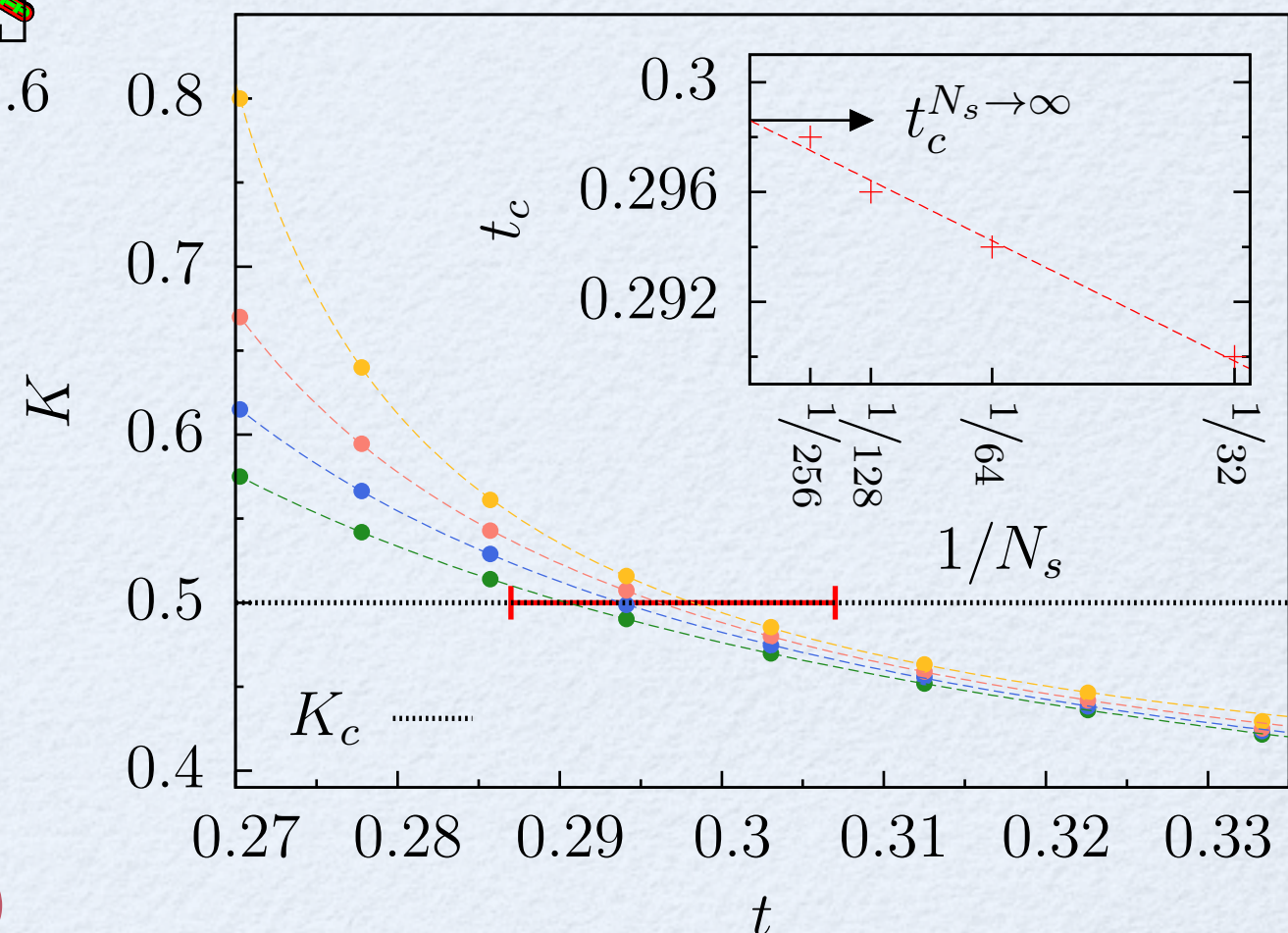
PBC $\rightarrow$ chord distance

$$\text{crd}(r) = N_s / \pi \sin(\pi r / N_s)$$

“Clean” Mott - Superfluid trans.

$$K_c = 1/2$$

$$t_c = 0.299 \pm 0.002$$

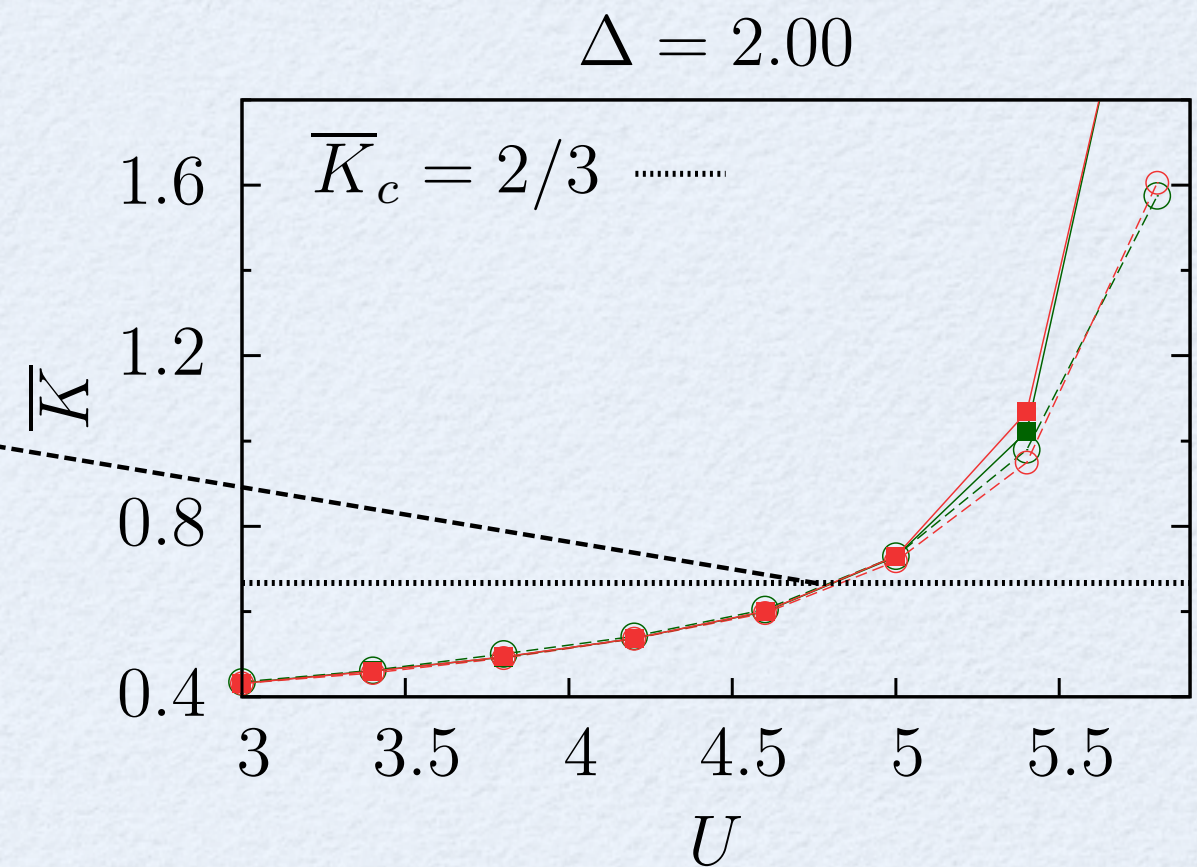
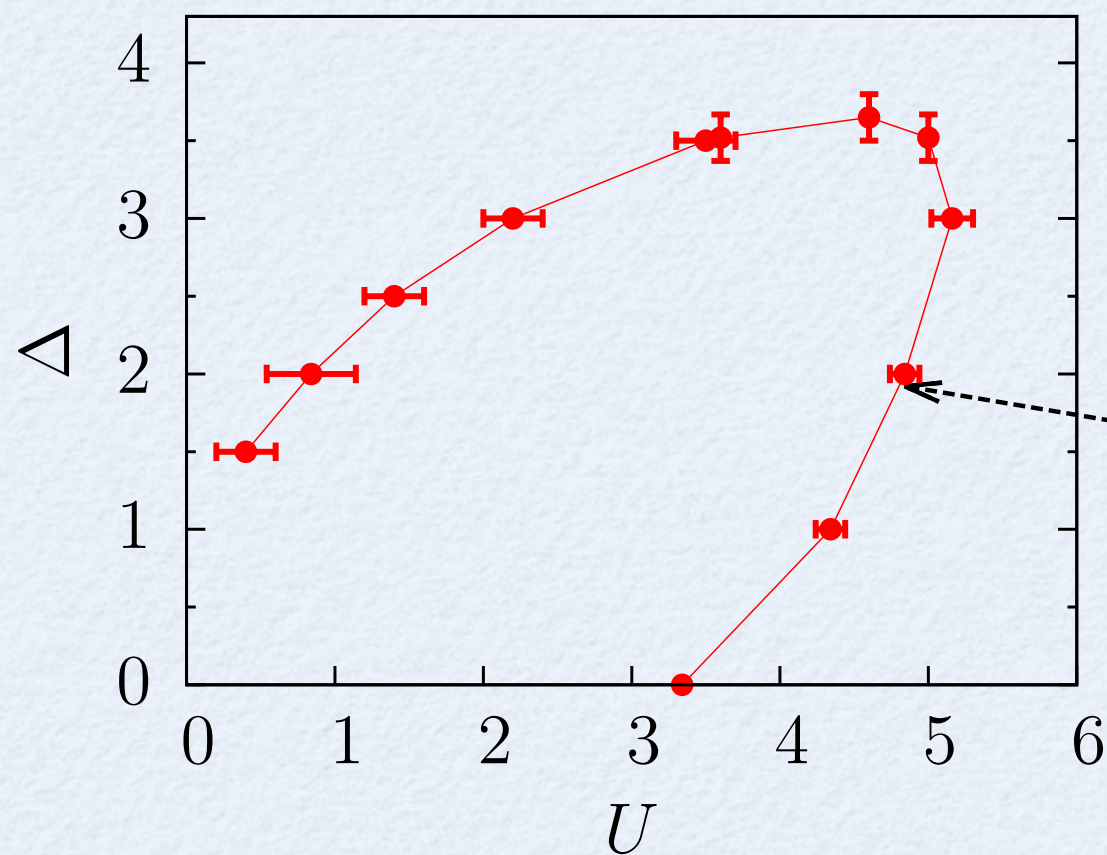


Indicator 2: hopping correlation decay (K)

Disorder-averages $\overline{A}_s \equiv \frac{1}{n_r} \sum_{\gamma=1}^{n_r} \langle A \rangle_{\gamma}$ over “reasonable” $n_r = 10^2 \div 10^3$

Giamarchi-Schulz SF criterion $\overline{K}_c = 2/3$

T. Giamarchi, H.J. Schulz, PRB 37, 325 (1988).



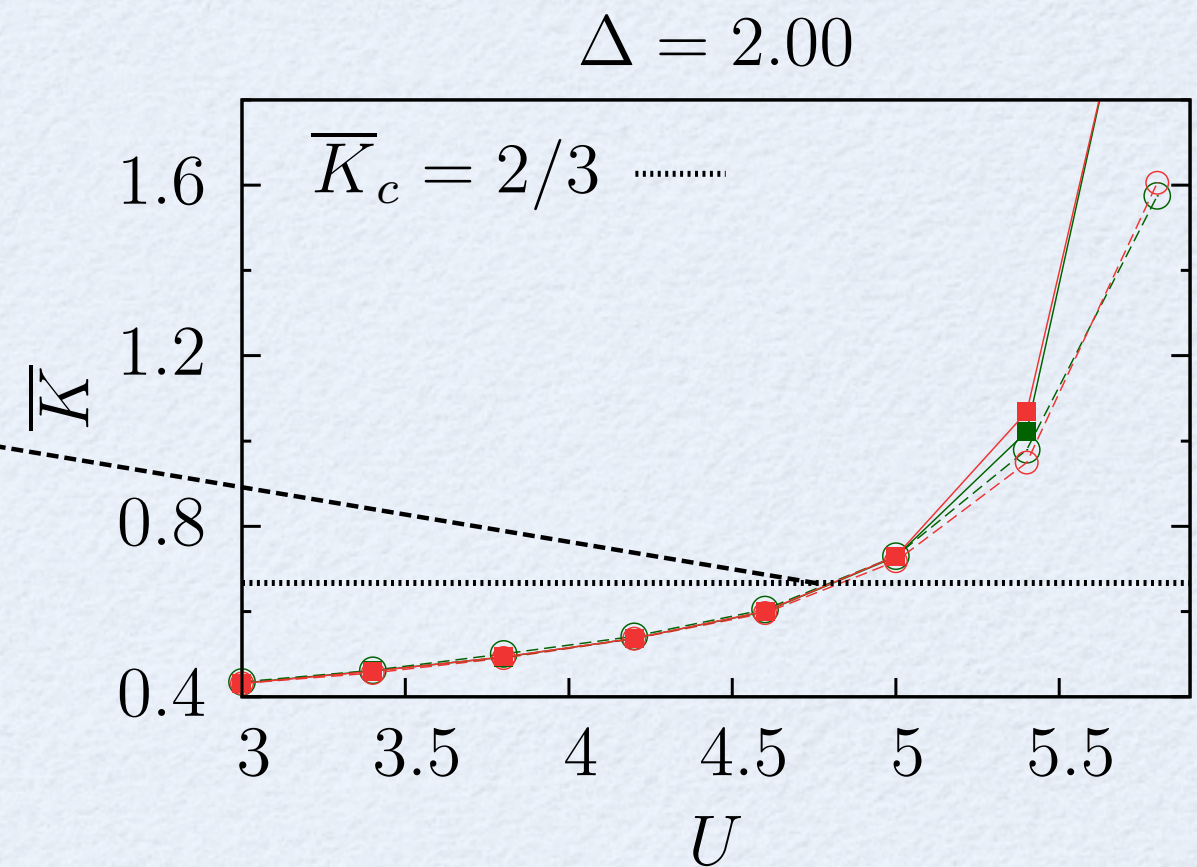
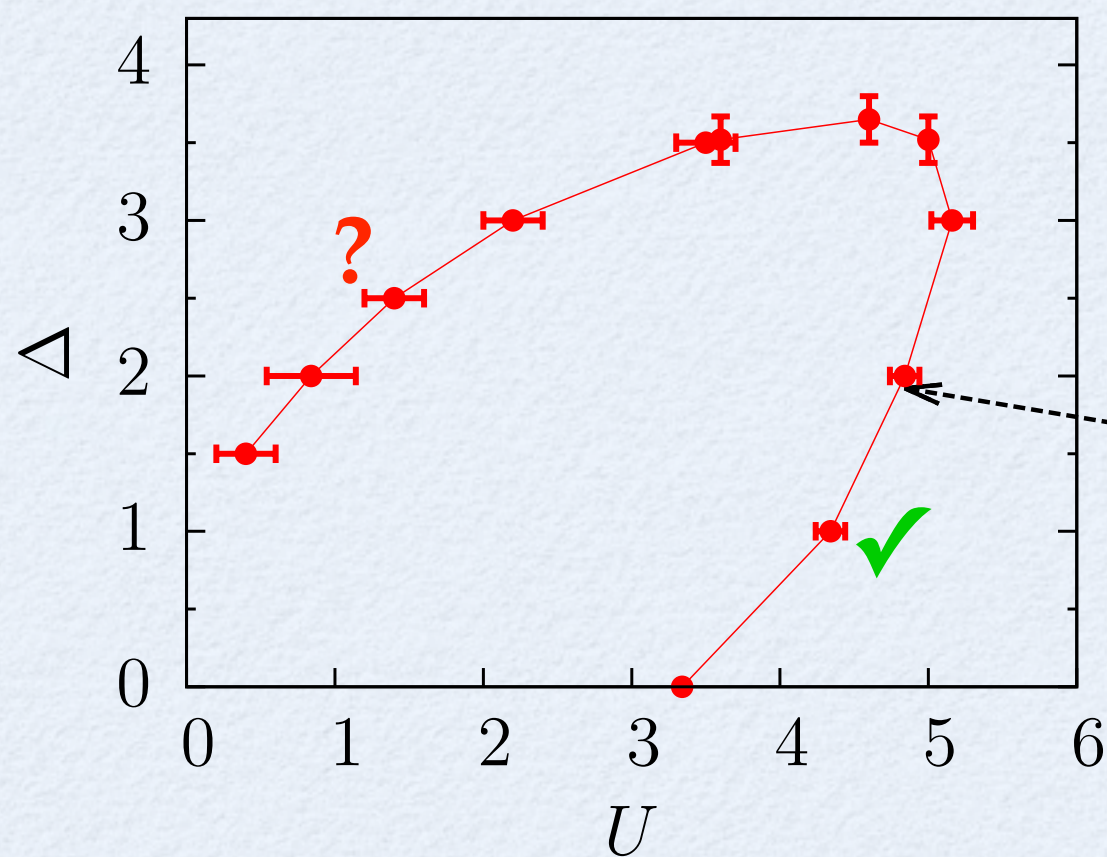
M. Gerster, MR, et al. NJP 18 015015 (2016)

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Giamarchi-Schulz SF criterion $\bar{K}_c = 2/3$ ☒ appropriate $\Delta/U \ll 1$
☐ (highly) debated $\Delta/U \gg 1$
T. Giamarchi, H.J. Schulz, PRB 37, 325 (1988).

L. Pollet, Comptes Rendus Physique 14, 712 (2013)



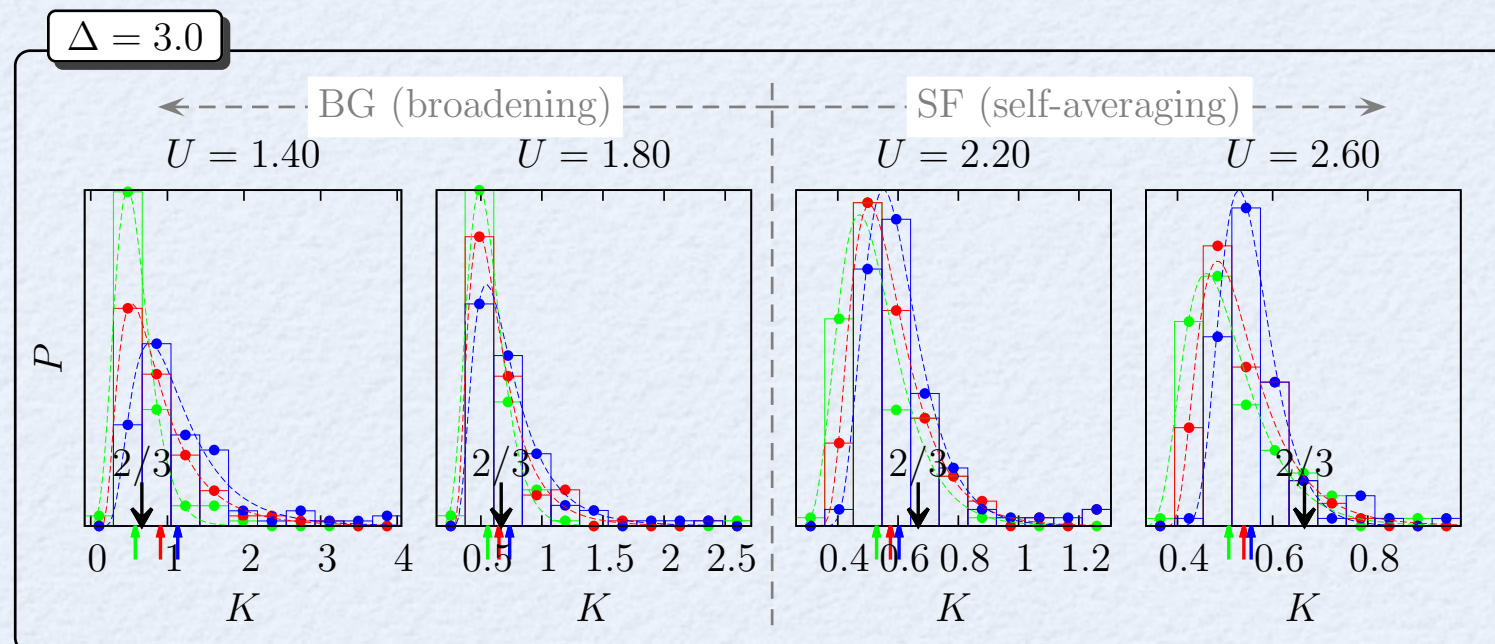
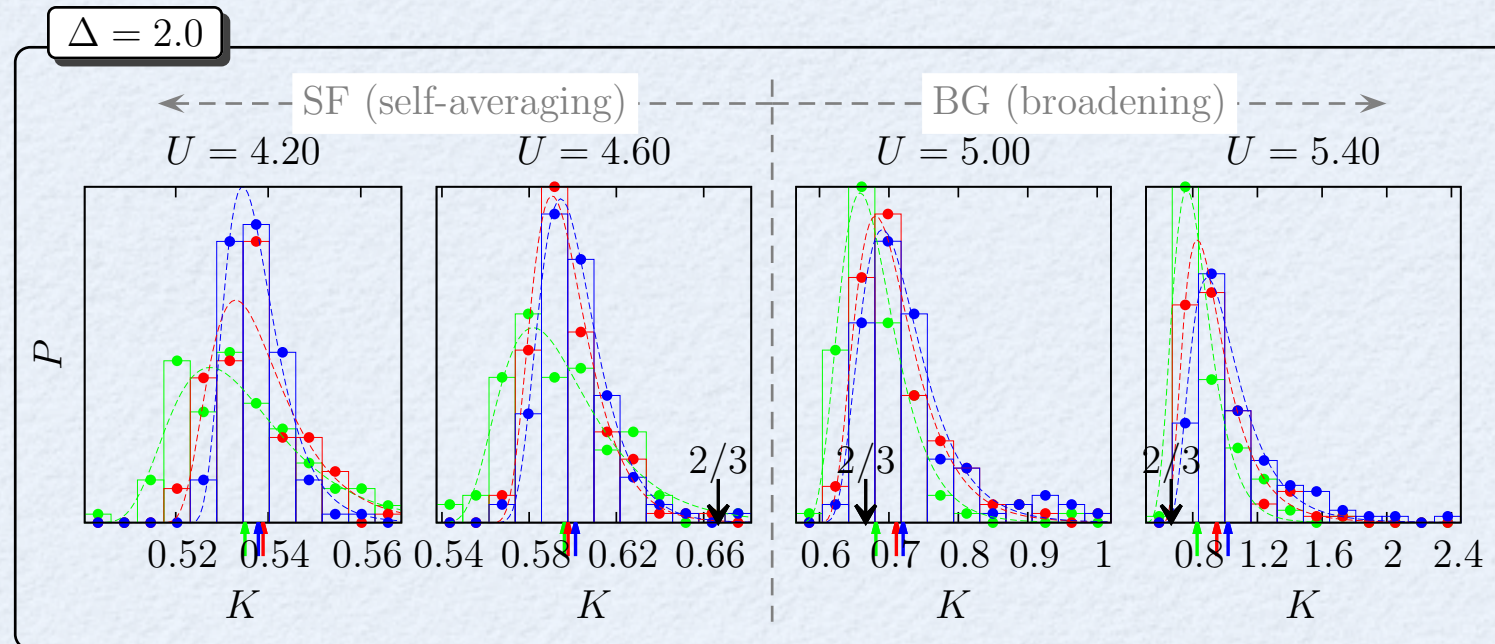
Indicator 3: $\mathcal{K}$ -distribution properties

New universality class: XY-scratched !? $\rightarrow$ Lobe shrinking due to rare events $\rightarrow$ Broadening vs. averaging with system size

*Pollet, Prokof'ev, Svistunov,
PRB 87, 144203 (2013)*

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} \frac{1}{x} \exp\left(-\frac{1}{2} \left(\frac{\log x - \mu}{\sigma}\right)^2\right)$$

$$x = K - K_{\min}$$



M. Gerster, MR, et al. NJP 18 015015 (2016)

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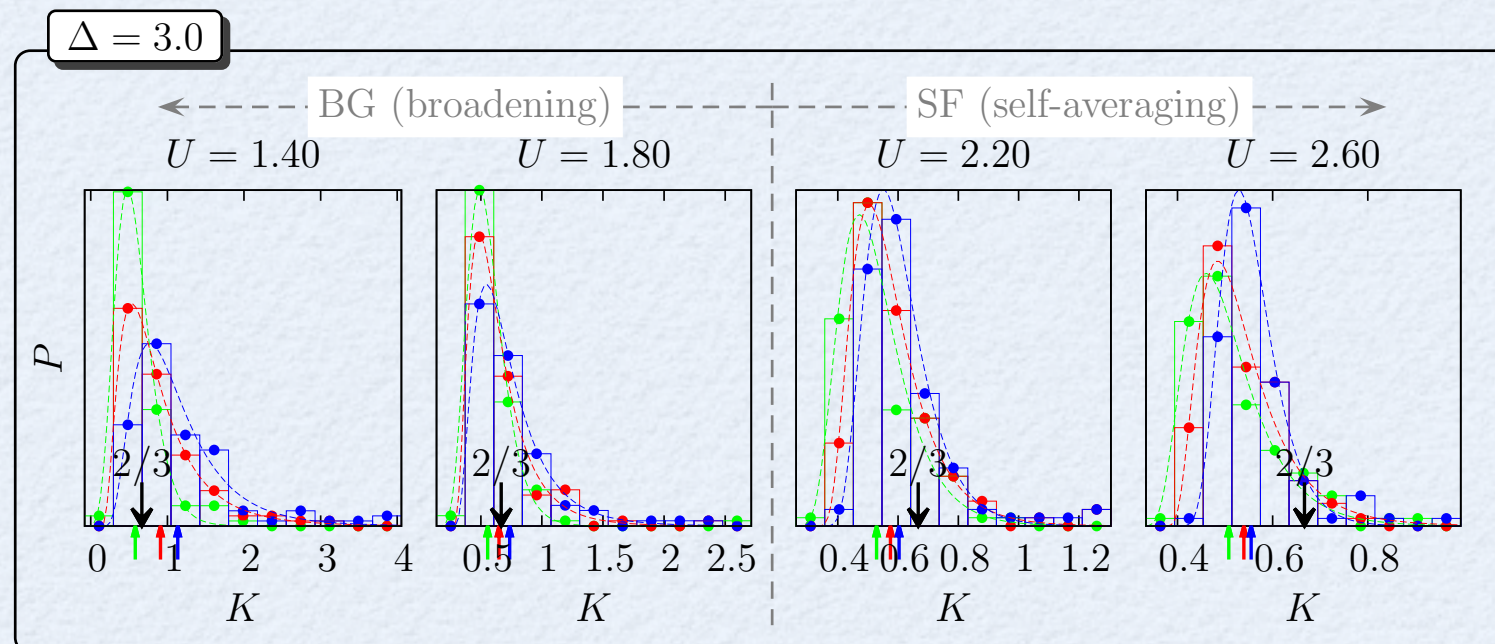
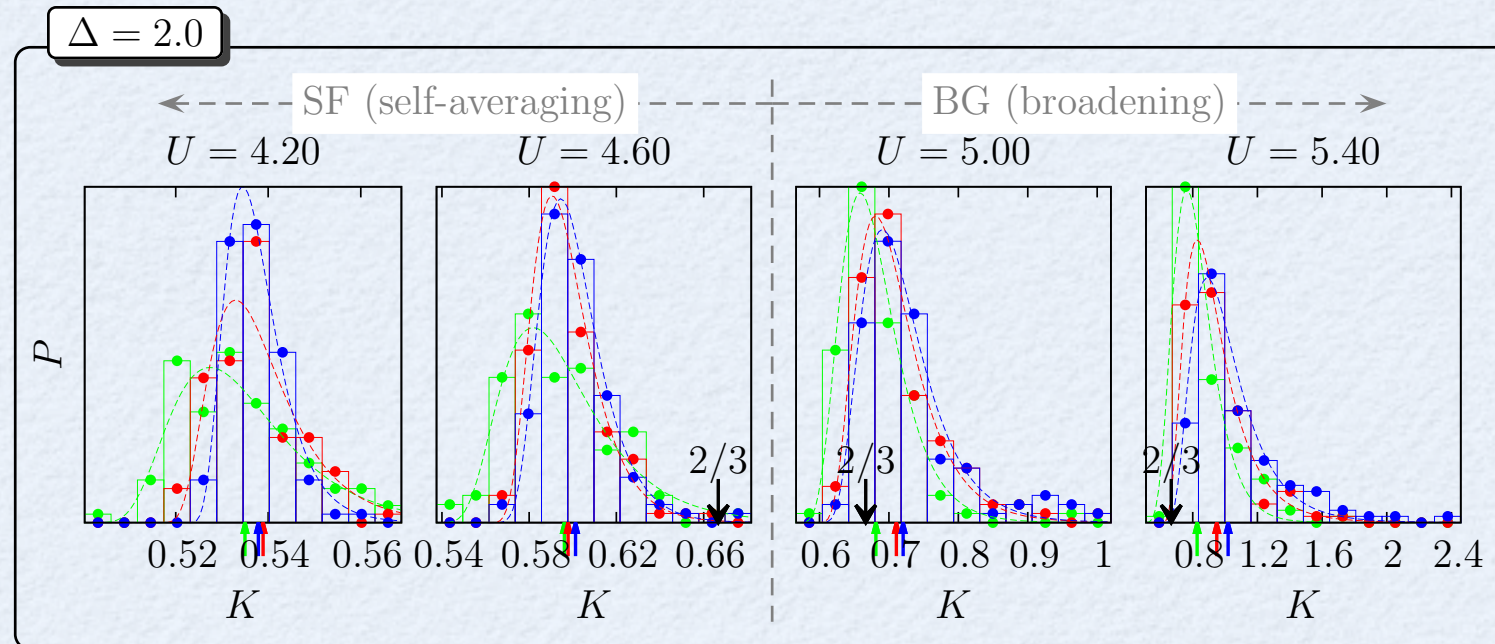
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$$x = K - K_{\min}$$



For "reasonable" sampling

$$\sigma(N_s) \simeq \sigma(N_s/2) \quad \bar{K} \simeq \bar{K}_c = 2/3$$

$$n_r \gg N_s$$

$$n_r \simeq 10^5$$

to see deviations !

Out of experimental reach !?

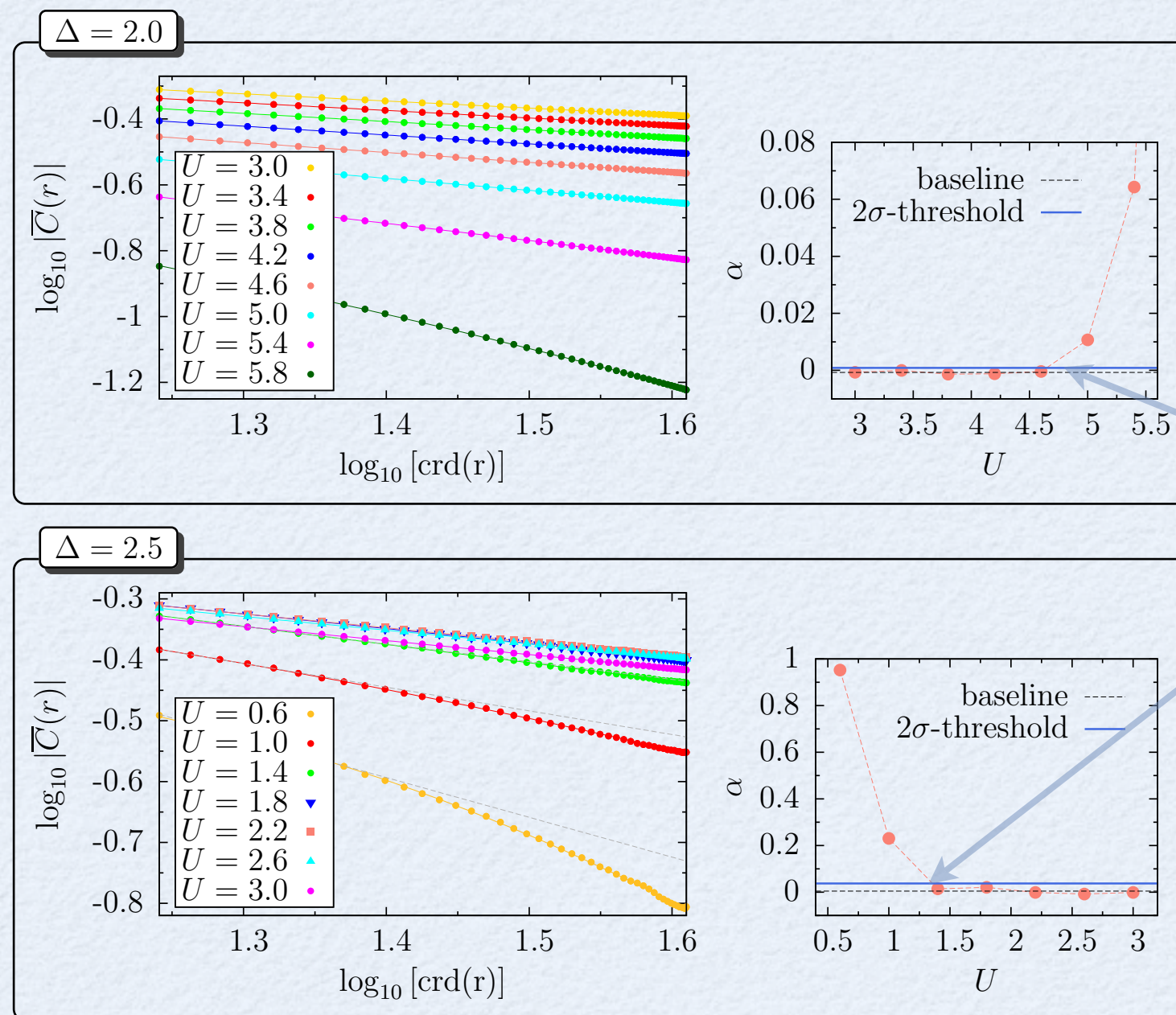
M. Gerster, MR, et al. NJP 18 015015 (2016)

Indicator 4: averaged hopping correlations

No assumption on transition class $\log [\overline{C}(r)] = -\alpha \tilde{r}^2 - \frac{K}{2} \tilde{r} + \text{const.}$
 $\tilde{r} = \text{crd}(r)$

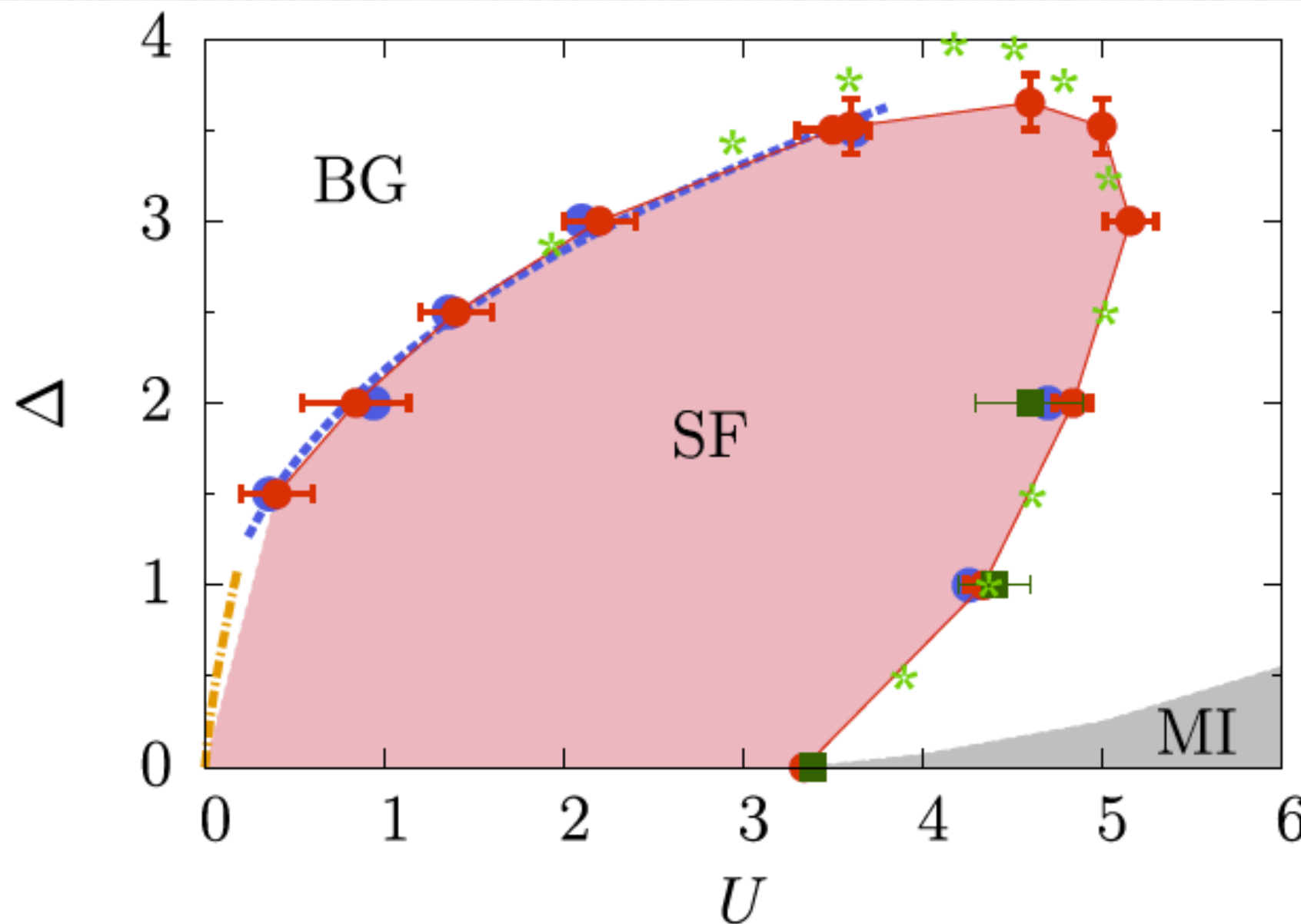
$\alpha = 0$ Superfluid

$\alpha \neq 0$ Insulator (BG)



guessed U_c

The phase diagram



jump in $\overline{\rho}_s$ ■
 $\overline{K} = 2/3$ ●
 $\overline{C}(r)$ crossover ●
 fit ---
 $\Delta_c \sim U^{3/4}$ -.-.-

Quantum MonteCarlo

*N.V. Prokof'ev, B.V. Svistunov,
PRL 80, 4355 (1998)*

“scratched XY” conjecture

$$\Delta_c \propto U^{3/4}$$

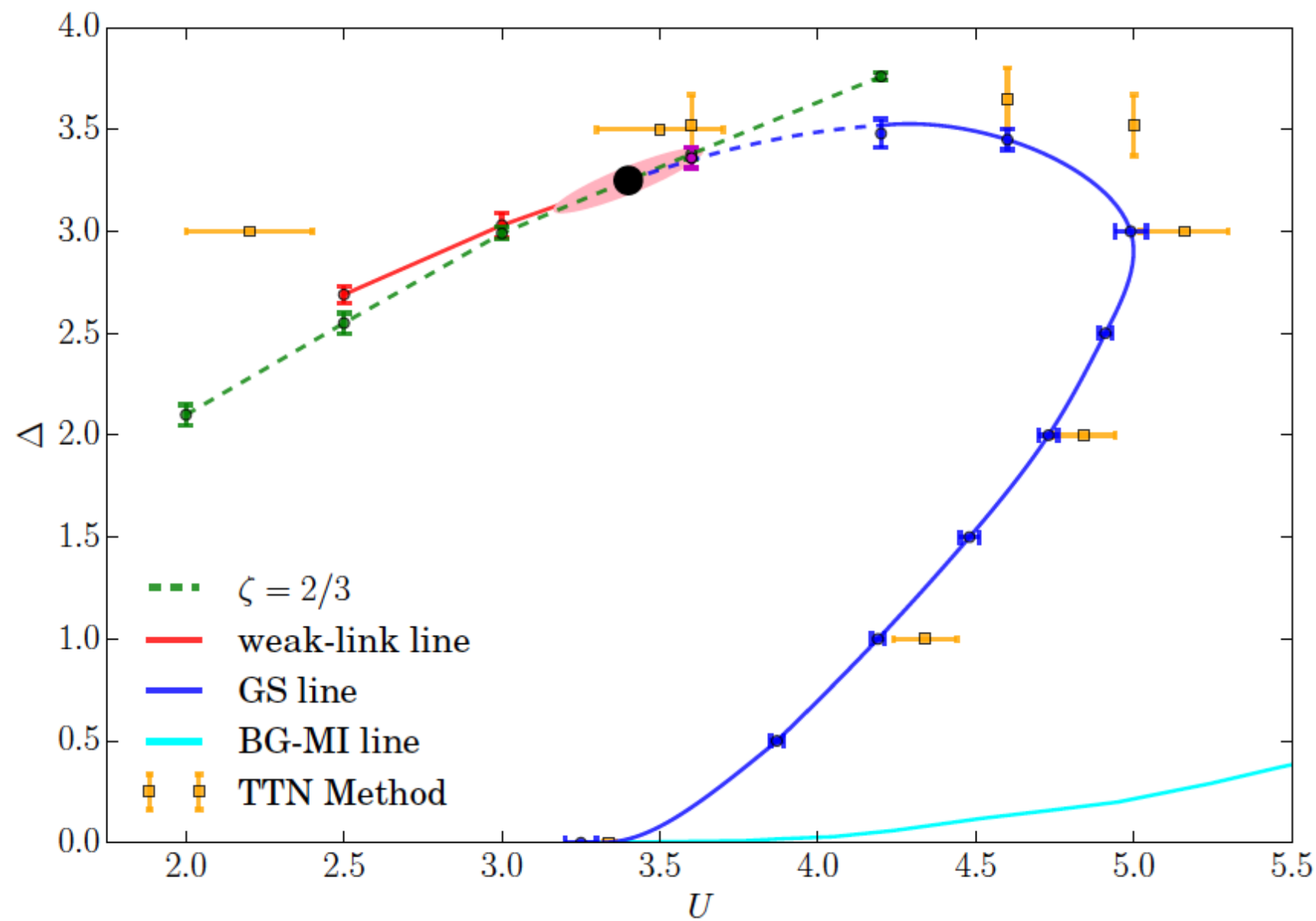
L. Pollet, Comptes Rendus Physique 14, 712 (2013)

M. Gerster, MR, et al. NJP 18 015015 (2016)

The phase diagram

Most recent QMC results - averages over 50.000 realizations

Z. Yao, et al., arXiv:1601.06185



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Persistent currents in Dirac rings



orbital magnetic susceptibility of 1D cold Dirac fermions

➔ orbital paramagnets of pure many-body origin !?

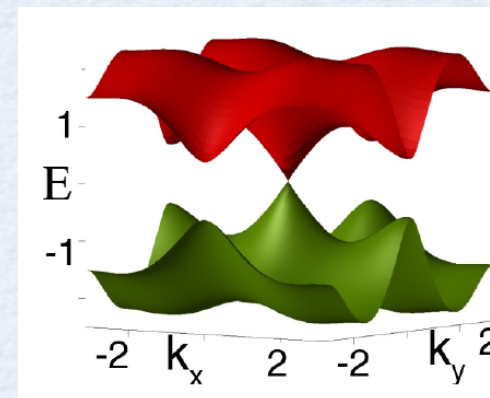
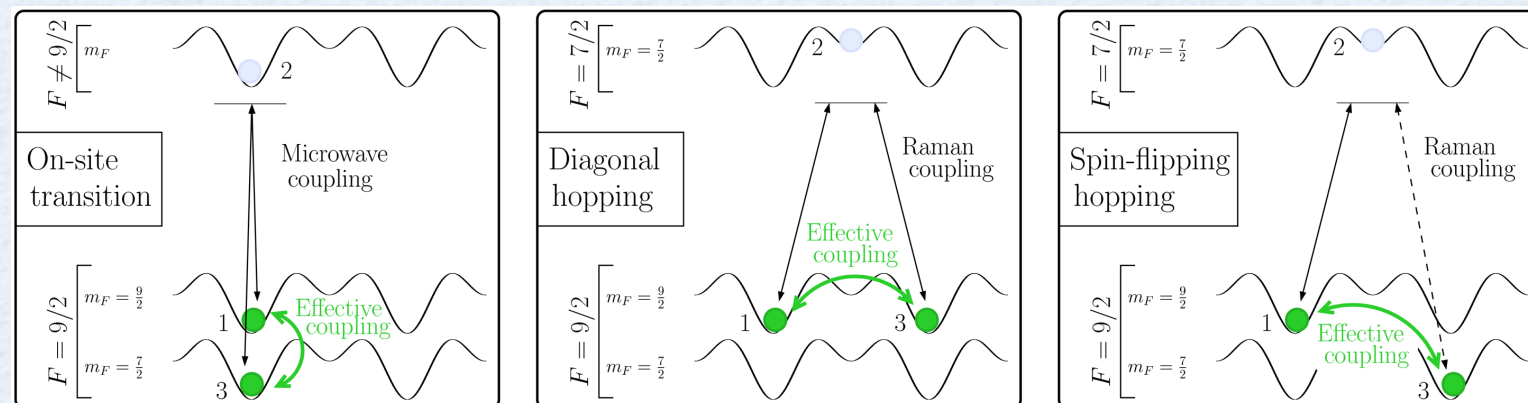
tunable gauge potentials with cold atoms



J. Jünemann



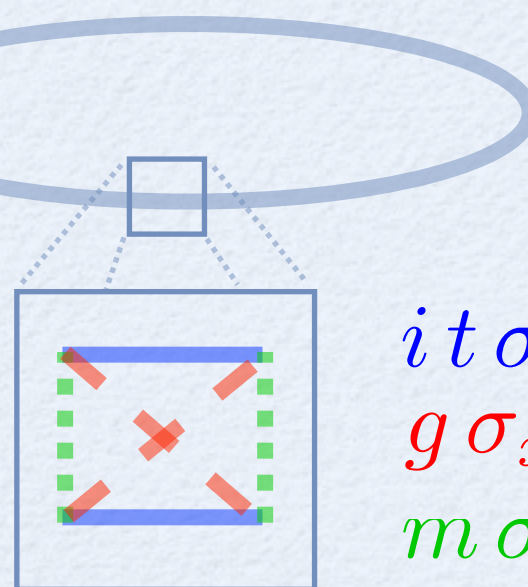
M. Bischoff



M. Rizzi, POS (SISSA) 193 (QCD-TNT-III), 036 (2013)

all that on rings!?

M. Łącki, et al. arXiv:1507.00030



$it\sigma_z$
 $g\sigma_x$
 $m\sigma_x$

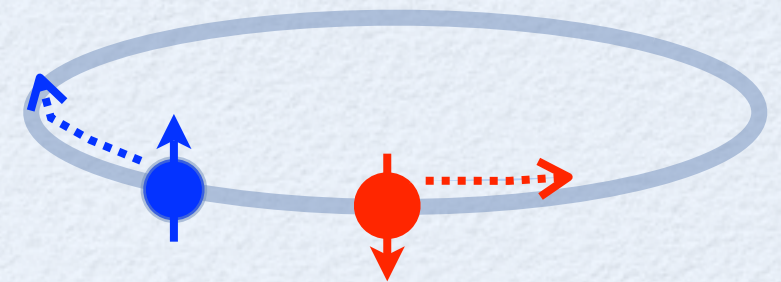
Creutz ladder at $m=g=t$

isolated cone at $k=0$

consider interactions

Future: time-dependent problems

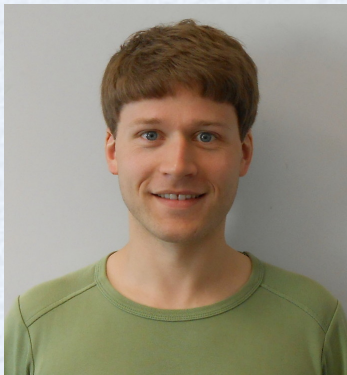
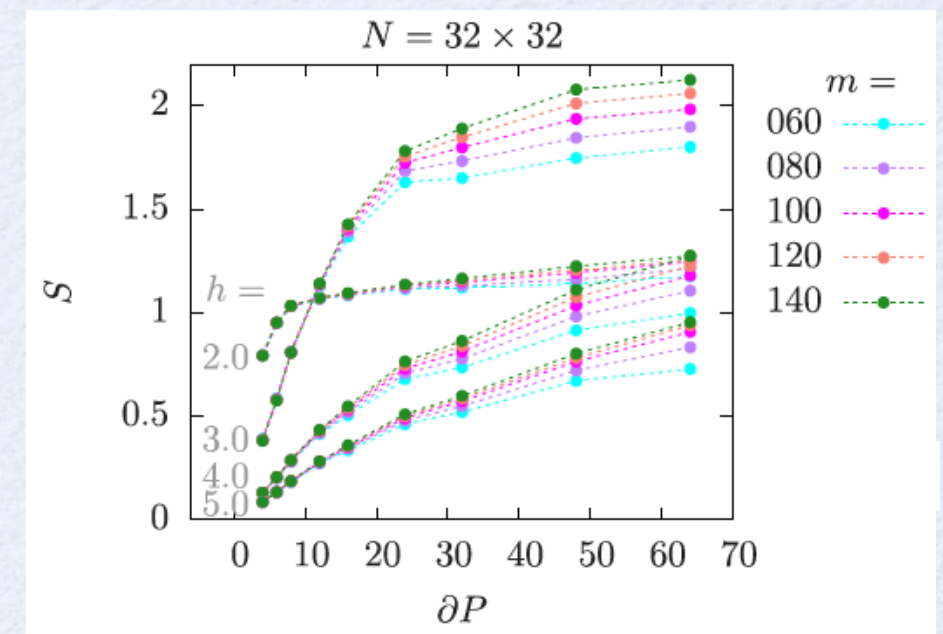
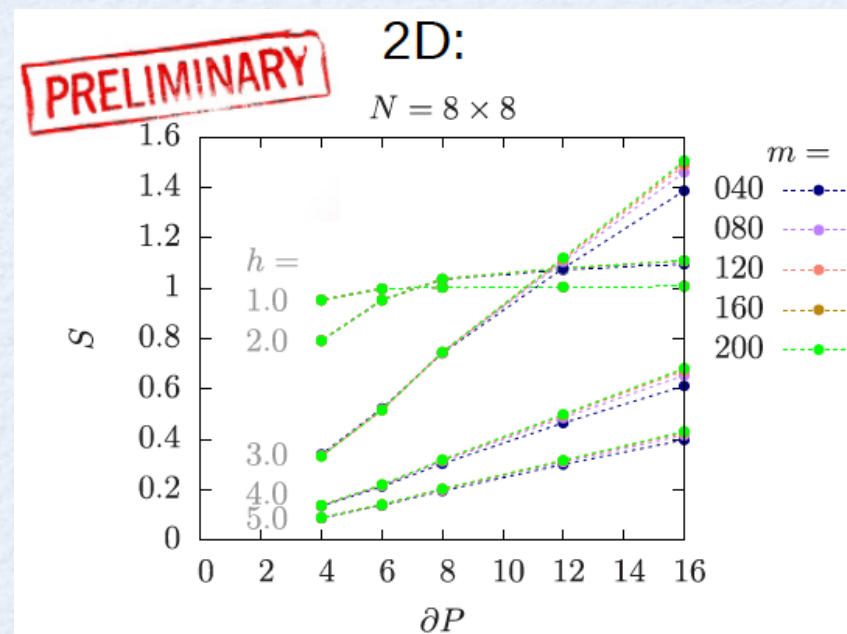
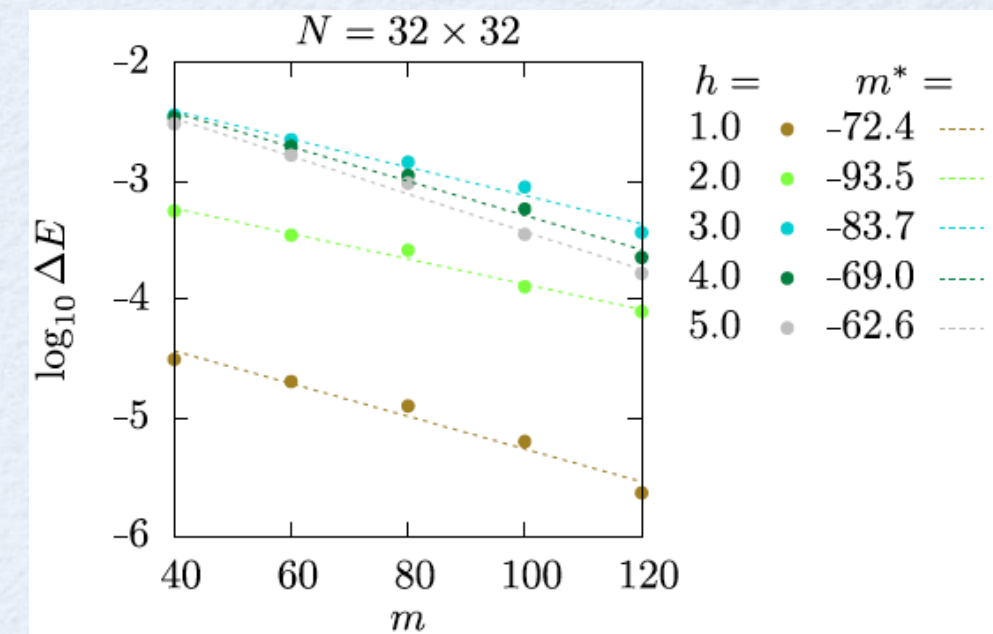
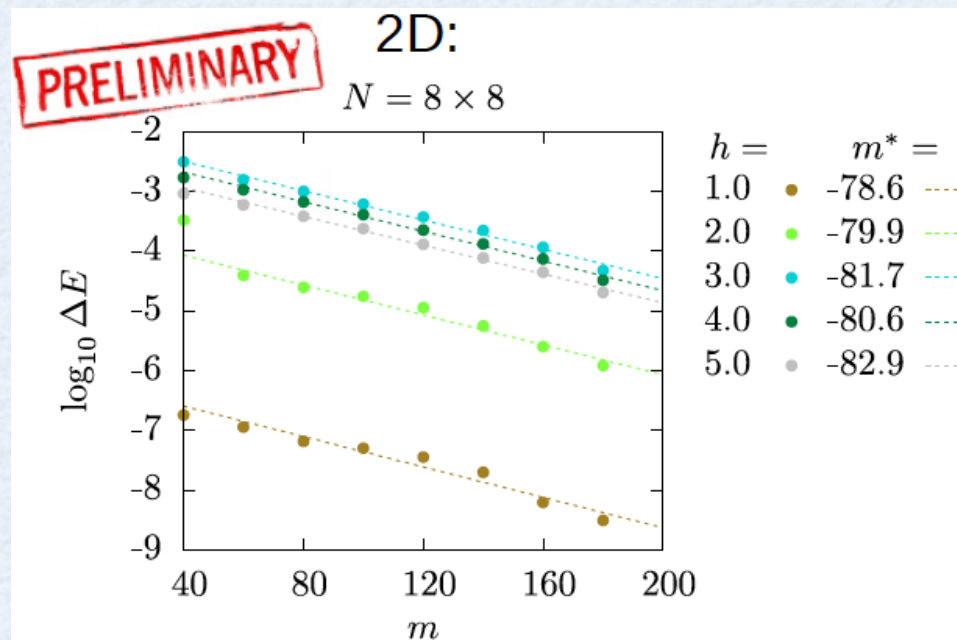
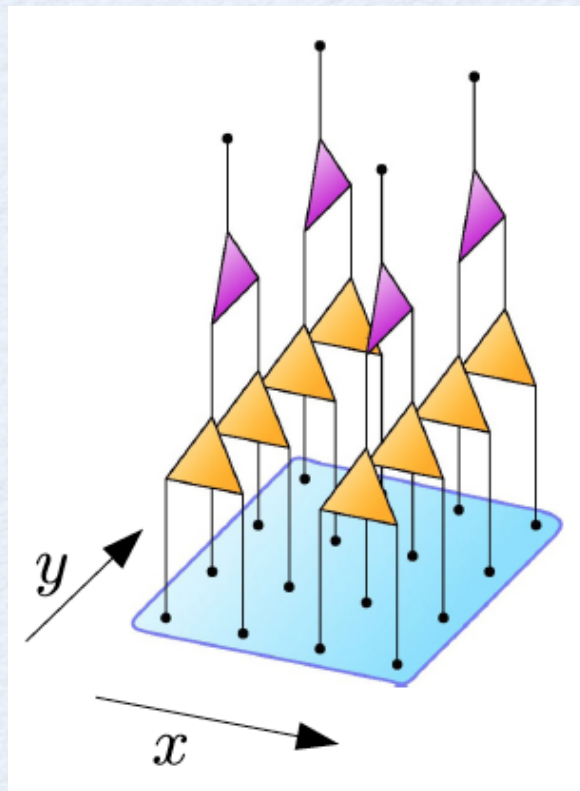
- implement time-dependence in TTN's (e.g., TEBD or TDVP like)
- study generation and decay of orbital and spin currents: spin-drag, dynamical instabilities, pairing effects, ...
- study quenches and relaxation with disorder (MBL!?)



Future: what about 2D?



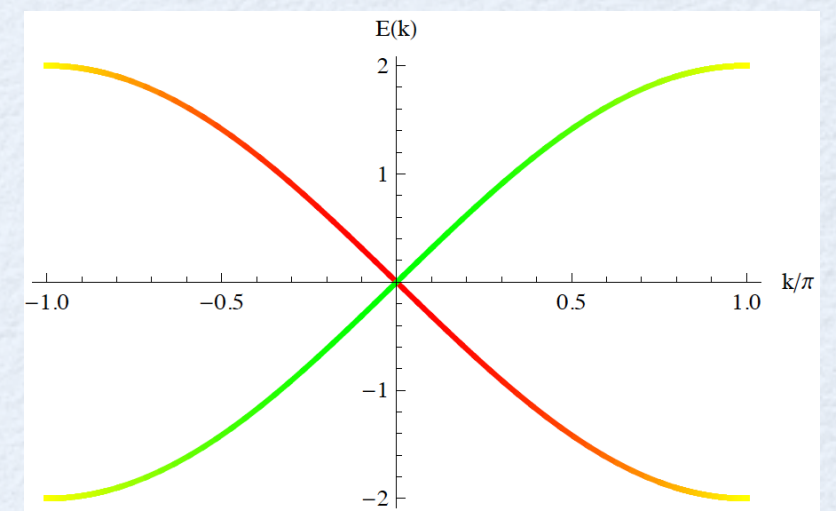
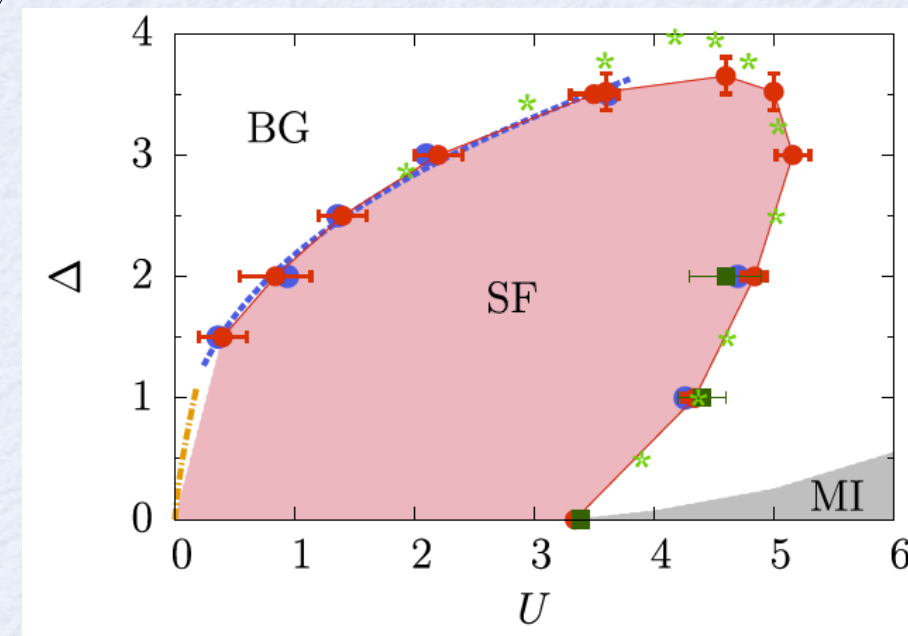
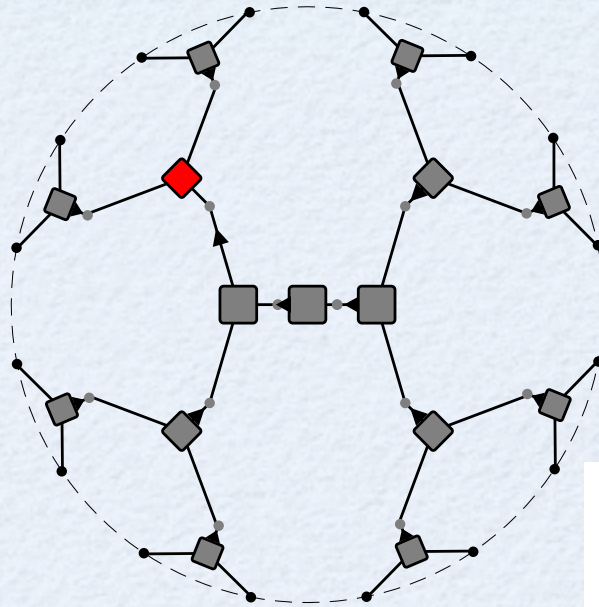
- it should **not** work, but what if brute force helps ?
- on-going tests on Ising in transverse field ($h_c \sim 3.04$)



M. Gerster (Ulm)

Summary

- Adaptive gauge strategy for Tree Tensor Networks: *pb*c enhanced performance!
PRB 90, 125154 (2015)
- 1D disordered Bose-Hubbard model: a TTN study on Bose-Glass transition
NJP 18 015015 (2016)
- Future studies on persistent currents in Dirac rings & other systems
POSTER by J. Jünemann (arriving tomorrow)



Thanks to ...

F. Hekking (Grenoble)
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D. Draxler (Wien)

P. van Dongen, R. Orus, and all KOMET337
My group: J. Jünemann, A. Haller, M. Bishoff

\$\$\$:



JOHANNES GUTENBERG
UNIVERSITÄT MAINZ



... and all of you for your attention !