Renyi entropies
in
Theory, Numerics, and Experiment

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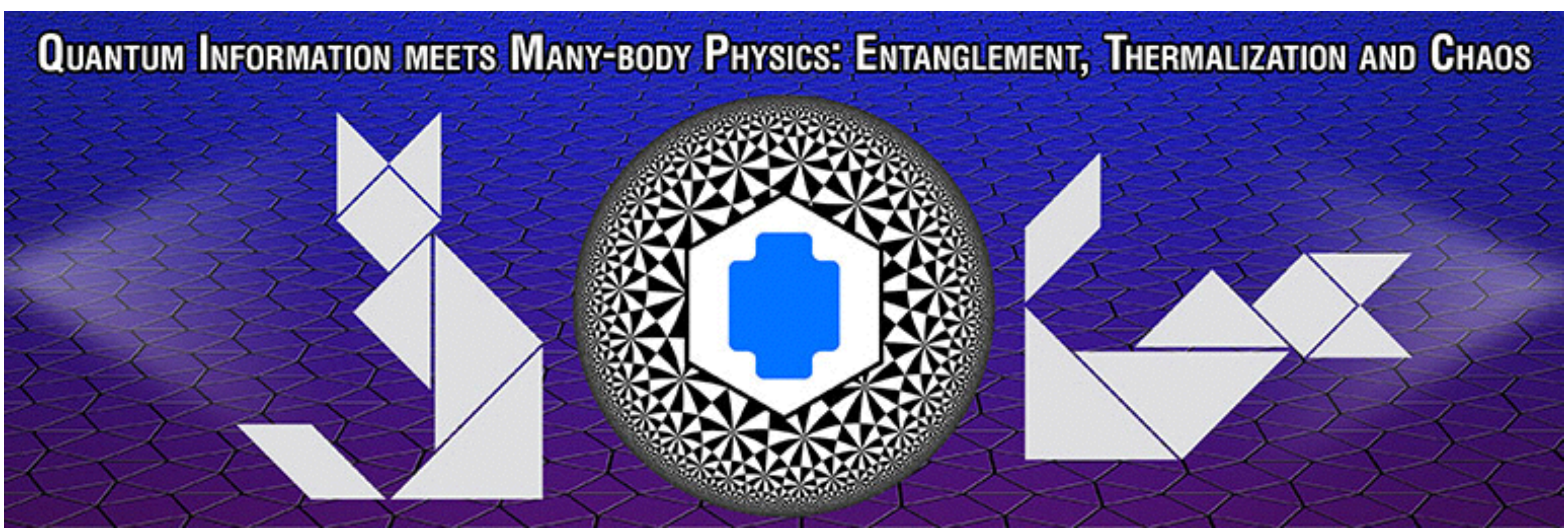
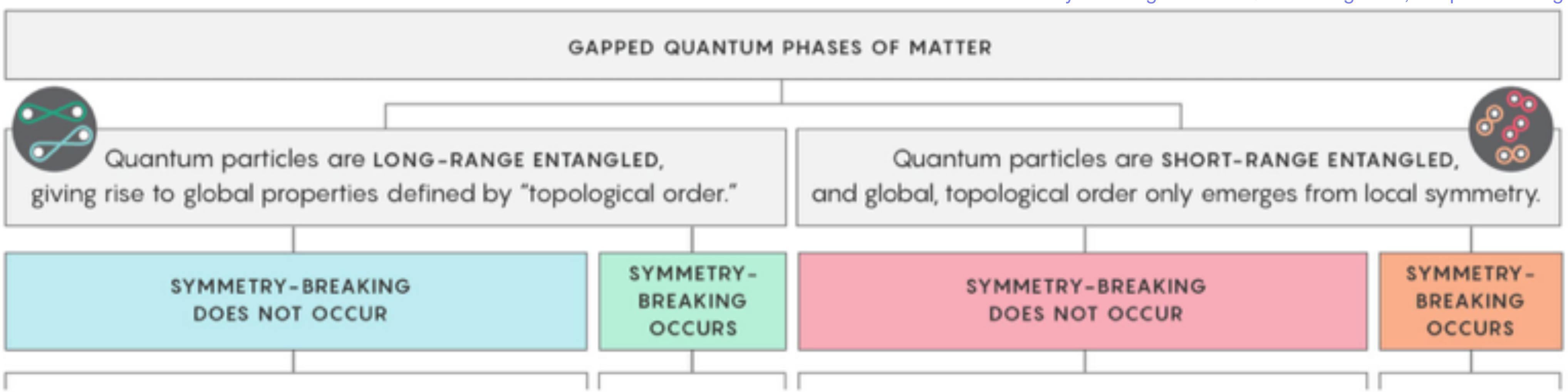


Why are we interested in entanglement?

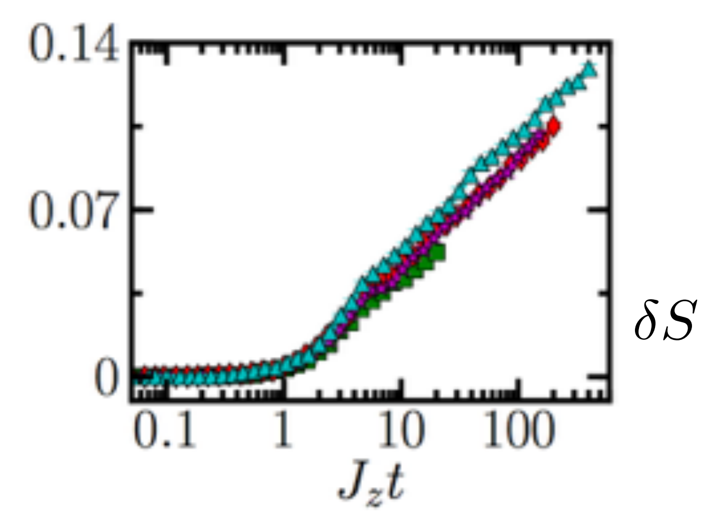
- To characterize equilibrium phases (including topological order)

Lucy Reading-Ikkanda/Quanta Magazine, adapted from figure by Xiao-Gang Wen

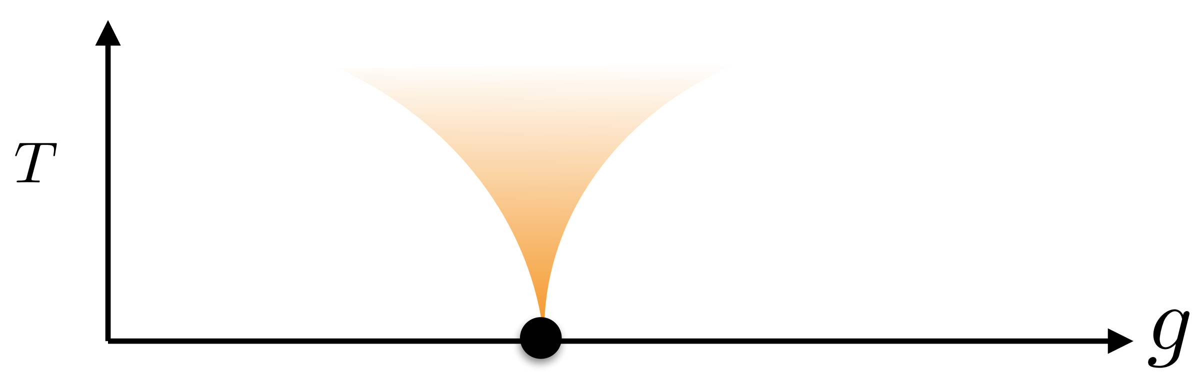


- To distinguish thermalized and localized states

Bardarson, Pollmann, Moore, Phys. Rev. Lett. 109, 017202 (2012)

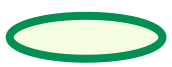


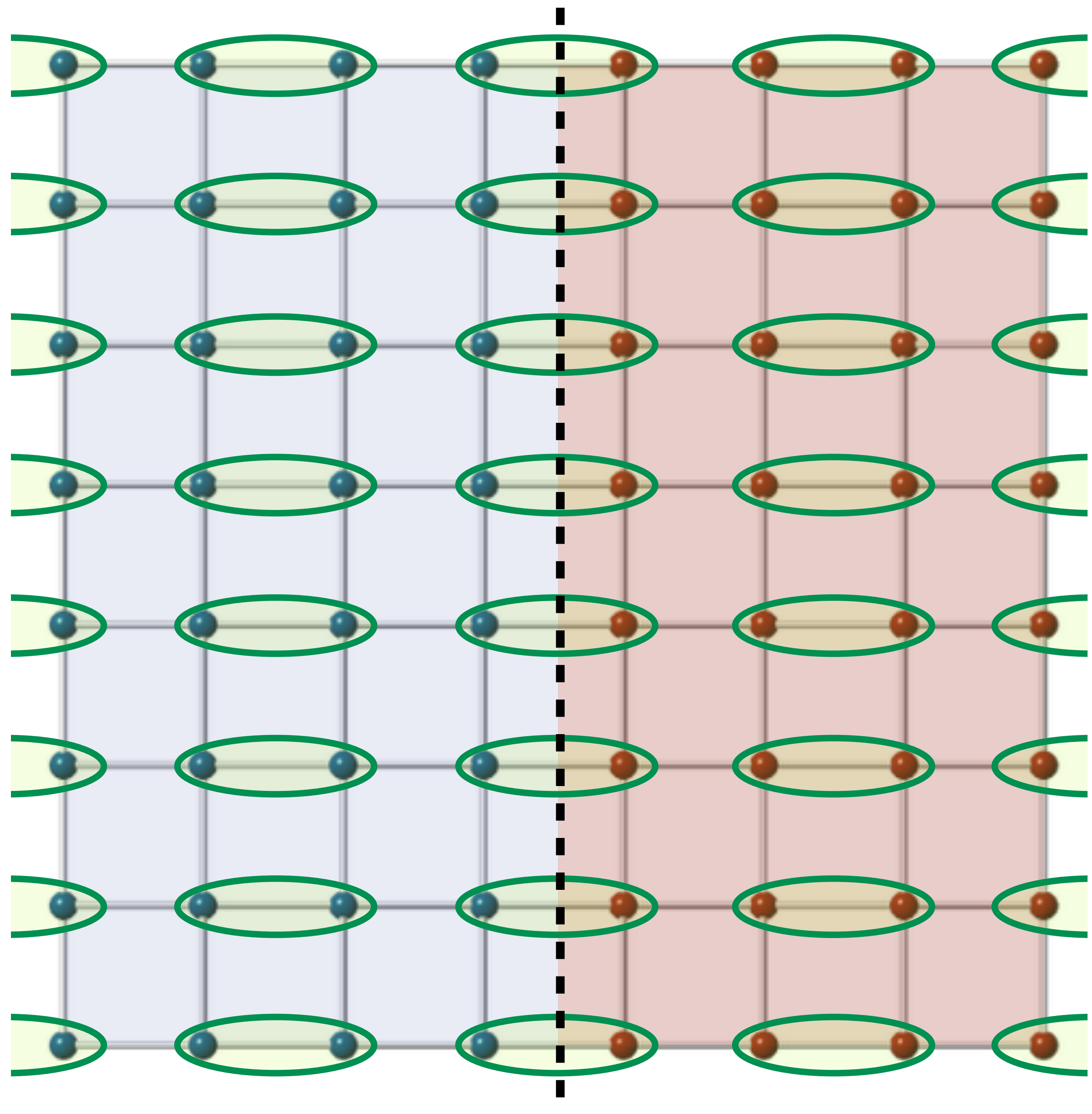
- To characterize quantum critical points and QFTs



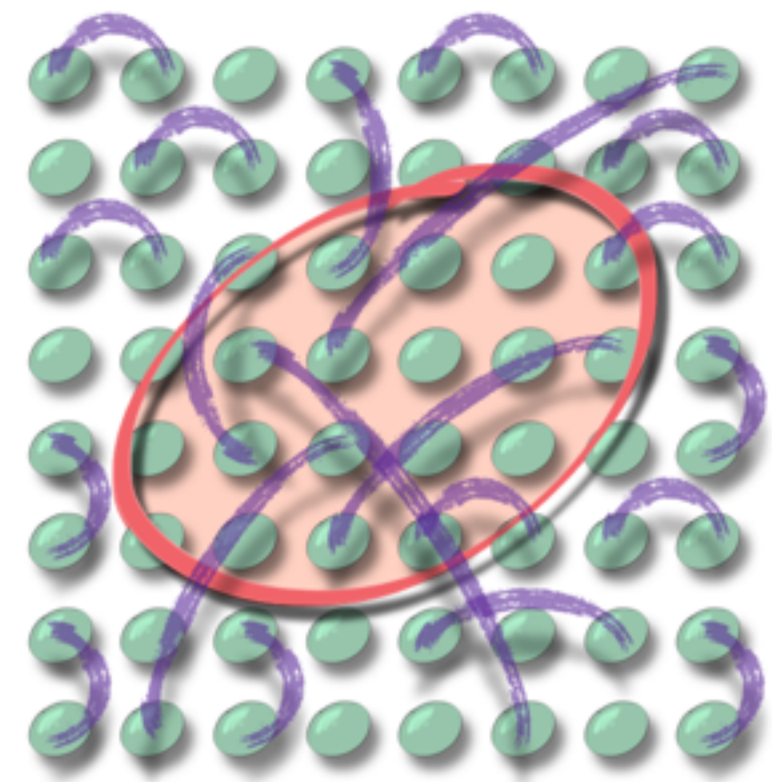
$$S[\phi] = \int d^3x \ \frac{1}{2}\left\{(\partial\phi)^2 - m^2\phi^2\right\}$$

- To determine how much entanglement exists in matter (e.g. for QIP) an **area law** is heuristically related to short-range correlations:

 $= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$



Entanglement in quantum many-body systems



- A powerful probe of many-body properties

- Entanglement entropy "**area law**" is the paradigm for groundstate wavefunctions

$$S = a\,\ell^{d-1}$$

- Violations, and subleading scaling terms may provide universal quantities useful for identifying phases and phase transitions

$$S = a\,\ell^{d-1}\log\ell$$ Fermi surface

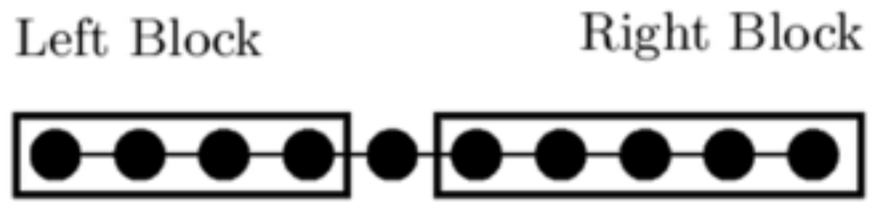
$$S = a\,\ell + \gamma$$ Topological order in two dimensions

$$S = \frac{c}{3}\log\ell$$ 1+1 conformal field theory

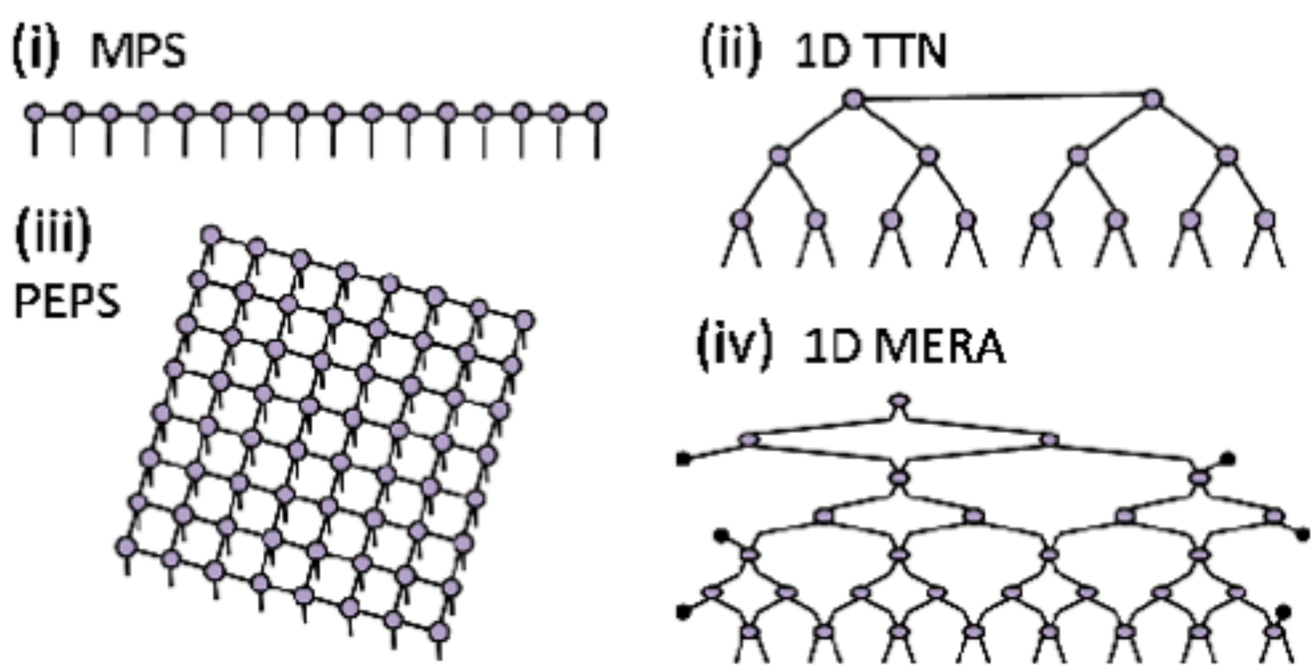
$$S = a\ell^{d-1} + \gamma(\text{geom.})$$ d+1 quantum critical point

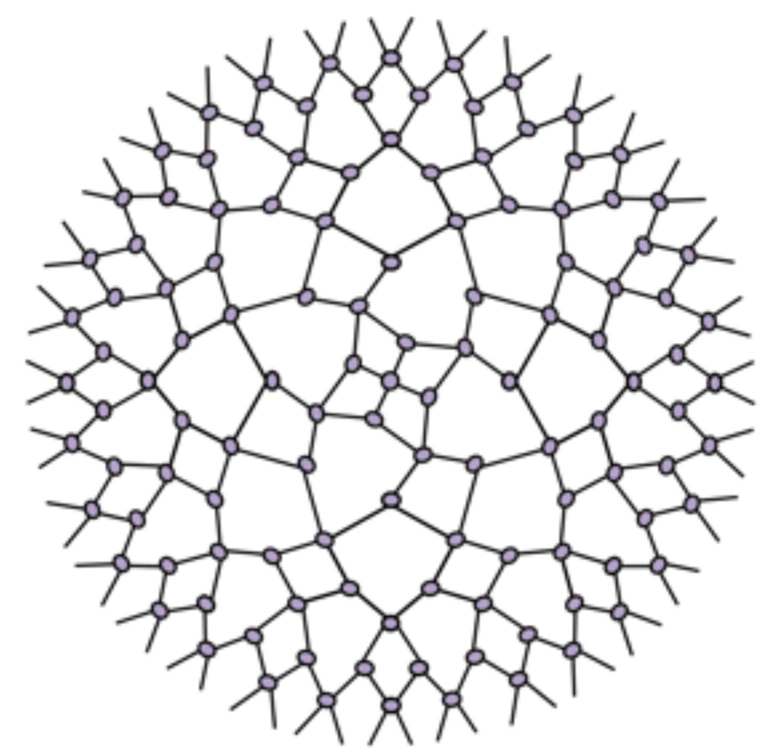
Entanglement and Algorithms

• The area law has emerged as a powerful paradigm underlying the success of DMRG in one-dimensional systems



• Higher dimensional extensions are called **tensor networks**, and hold great promise both as theoretical and numerical tools

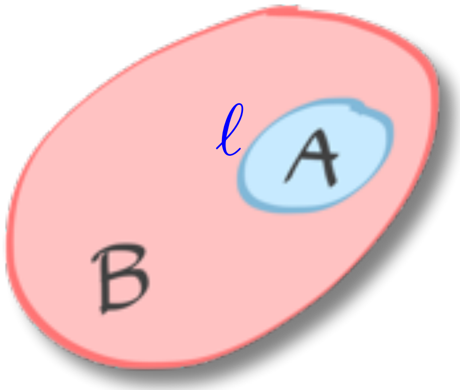




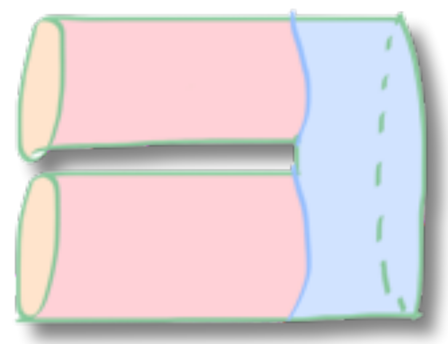
Outline

- A brief introduction to Renyi entropies in condensed matter physics

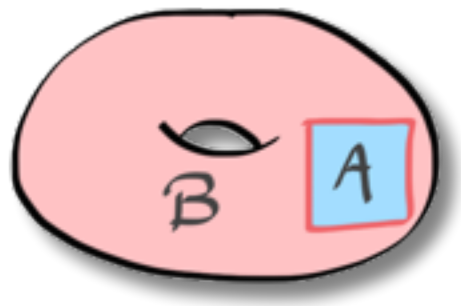
- Renyi entropies in classical Monte Carlo



- Renyi entropies in quantum Monte Carlo

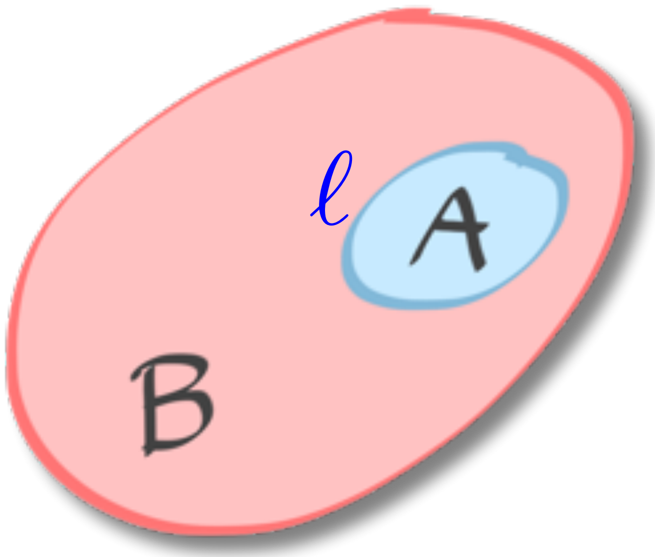


- An example of universal Renyi entropies in 2+1



von Neumann entanglement entropy

$$S_1(\rho_A) = -\mathrm{Tr}(\rho_A \ln \rho_A)$$

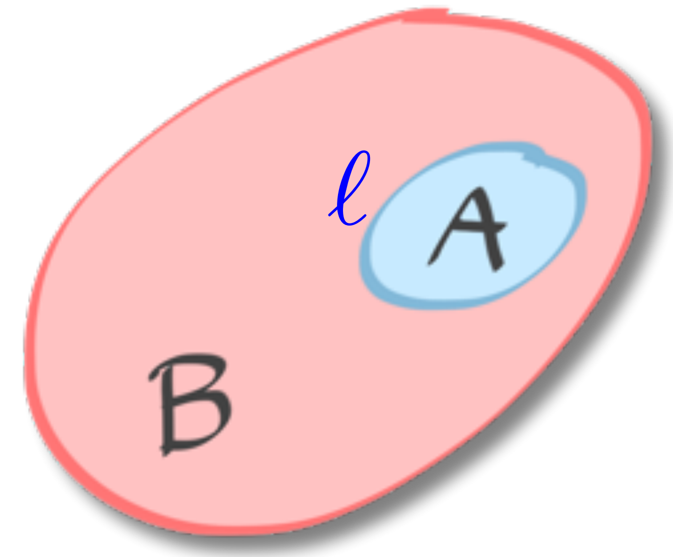


$$\rho = |\Psi\rangle\langle\Psi| \qquad \rho_A = \mathrm{Tr}_B(\rho)$$

- Quantifies the entanglement between spins A and B
- Positive $S_1(\rho_A) \geq 0$
- $S_1(\rho_A) = 0$ if A and B are unentangled
- $S_1(\rho_A) = S_1(\rho_B)$ (if the full density matrix describes a pure state)
- Basis independent
- Strongly subadditive $S_1(\rho_{ABC}) + S_1(\rho_B) \leq S_1(\rho_{AB}) + S_1(\rho_{BC})$

Renyi entanglement entropies

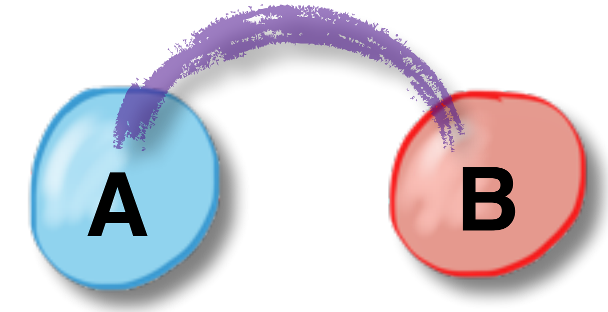
$$S_n(\rho_A) = \frac{1}{1-n} \ln\left[\mathrm{Tr}\left(\rho_A^n\right)\right]$$



$$S_2(\rho_A) = -\ln\left[\mathrm{Tr}(\rho_A^2)\right]$$

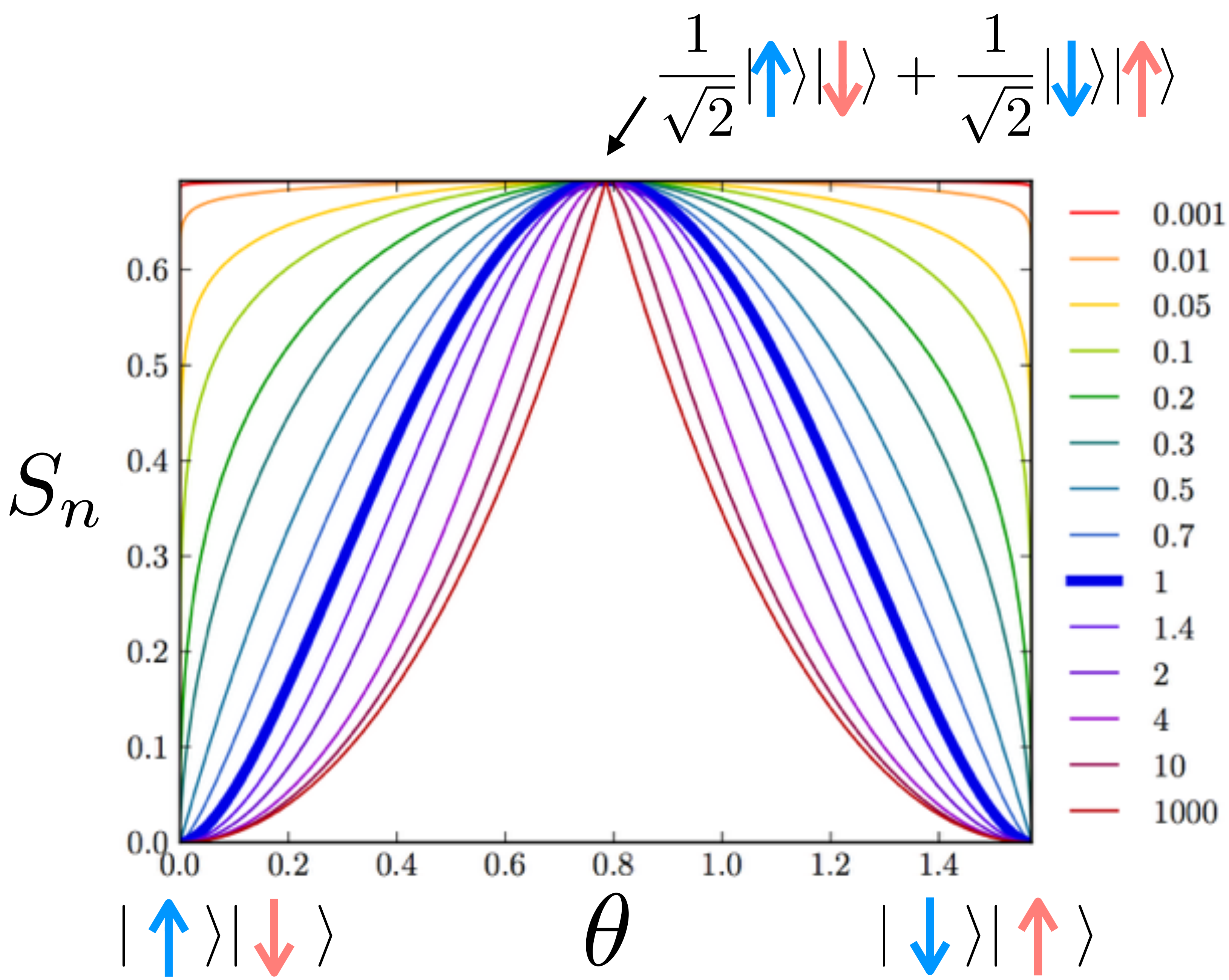
- Quantifies the entanglement between spins A and B
- Positive $S_n(\rho_A) \geq 0$
- $S_n(\rho_A) = 0$ if A and B are unentangled
- $S_n(\rho_A) = S_n(\rho_B)$ (if the full density matrix describes a pure state)
- Basis independent
- Strongly subadditive $S_1(\rho_{ABC}) + S_1(\rho_B) \leq S_1(\rho_{AB}) + S_1(\rho_{BC})$

$$|\Psi\rangle = \cos(\theta)|\uparrow\rangle|\downarrow\rangle + \sin(\theta)|\downarrow\rangle|\uparrow\rangle$$



$$\rho_A = \begin{pmatrix} \cos^2(\theta) & 0 \\ 0 & \sin^2(\theta) \end{pmatrix}$$

$$S_1 = -\cos^2(\theta)\ln\cos^2(\theta) - \sin^2(\theta)\ln\sin^2(\theta)$$



- Renyi entropies satisfy the inequalities $S_m \geq S_n \qquad m < n$

- They are all equal in the minimal and **maximal** entangled case

$$\sum_{i=1}^{d} \lambda_i = 1$$

max. entanglement

$$\lambda_i = \frac{1}{d}$$

$$S_n = \frac{1}{1-n} \ln \sum_{i=1}^{d} \lambda_i^n = \frac{1}{1-n} \ln \sum_{i=1}^{d} \frac{1}{d^n}$$

$$= \frac{1}{1-n} \ln \frac{d}{d^n} = \frac{1}{1-n} \ln \frac{1}{d^{n-1}}$$

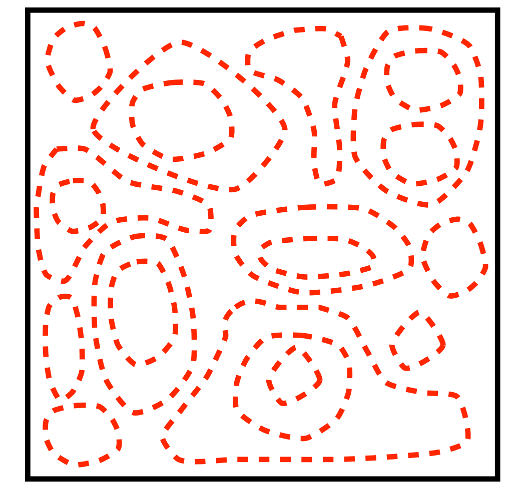
$$= \ln(d)$$

- No Renyi entropies are generally considered to be “observables” due to their non-linear dependence on the reduced density matrix… (but let’s take a closer look at n>1 integers Renyis)

$$S_2, \quad S_3, \quad S_4, \quad \text{etc.}$$

Are Renyis “as good” as vN?

- Topological entanglement entropy is Renyi-index independent



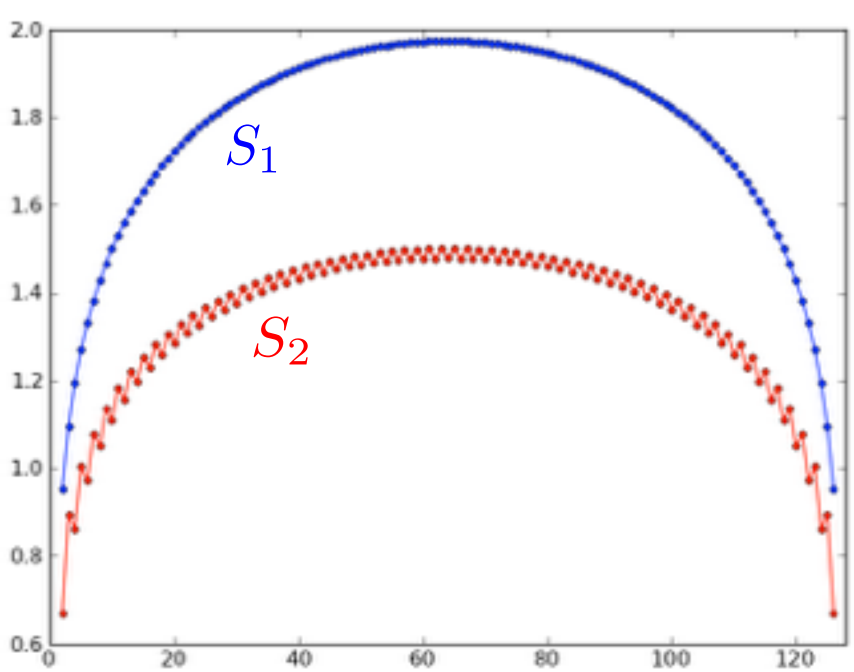
$$S_n = A\ell + \gamma_n \qquad \gamma_n = -\ln(2)$$

Kitaev and Preskill - Phys. Rev. Lett. 96, 110404 (2006)

Levin and Wen, - Phys. Rev. Lett. 96, 110405 (2006)

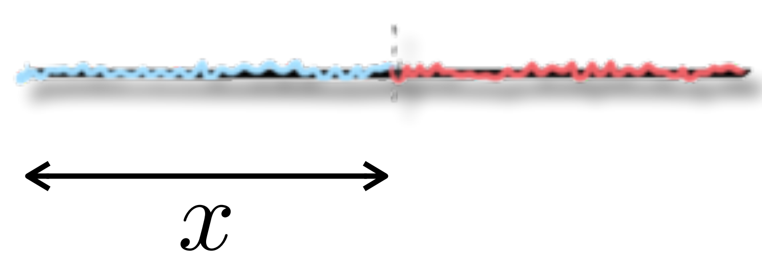
Flammia, Hamma, Hughes, Wen Phys. Rev. Lett. 103, 261601 (2009)

- In critical systems, universal quantities may depend on n



Calabrese and Cardy. J. Phys. A: Math. Theor., 42:504005, 2009

$$S_n = \frac{c}{6}\left(1 + \frac{1}{n}\right) \log\left[\frac{L}{\pi} \sin\frac{\pi x}{L}\right]$$



How do we calculate the Renyi entropies?

- Directly from the density matrix

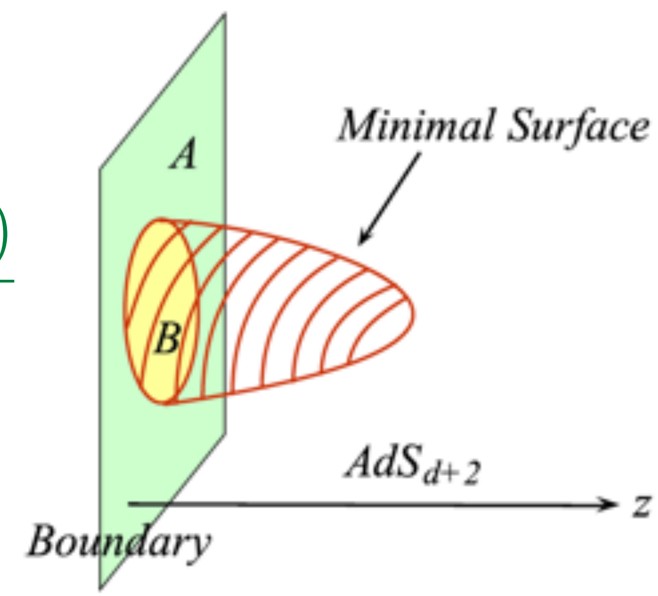
$$S_n(\rho_A) = \frac{1}{1-n} \ln \left[\mathrm{Tr}\left(\rho_A^n\right) \right]$$

– exact diagonalization
– density matrix renormalization group
– quantum state tomography

- Using holographic formulas

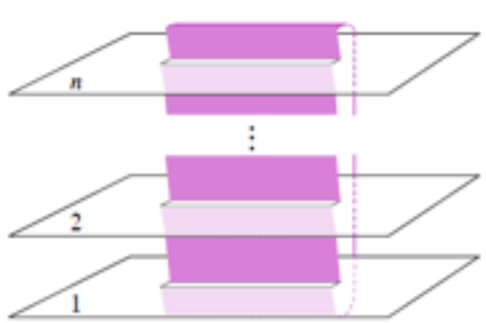
$$S_1 = \frac{\mathrm{Length}(\gamma_A)}{4G_N^{(3)}} = \frac{c}{3} \ln \frac{x}{a}$$

$$S_1 = \frac{\mathrm{Area}(\gamma_A)}{4G_N^{(d+2)}}$$



J. M. Maldacena, Adv. Theor. Math. Phys. **2**, 231 (1998)
S. Ryu and T. Takayanagi, Phys. Rev. Lett. 96, 181602 (2006)

- From a multi-sheeted Riemann surface



$$S_1 = -\lim_{n \to 1} \frac{d}{dn} \mathrm{Tr} \rho_A^n$$

J. Callan, Curtis G. and F. Wilczek, Phys. Lett. B333 , 55–61 (1994)
P. Calabrese and J. L. Cardy, J. Stat. Mech. 0406, P002 (2004)

– field theory
– Monte Carlo methods
– Cold atom experiments

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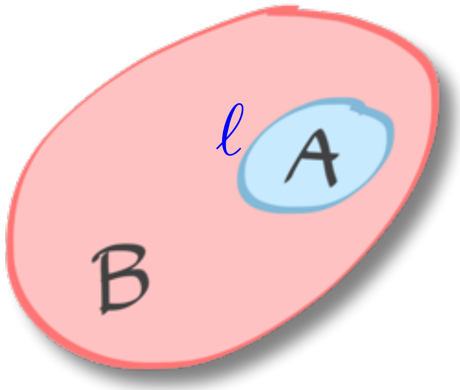
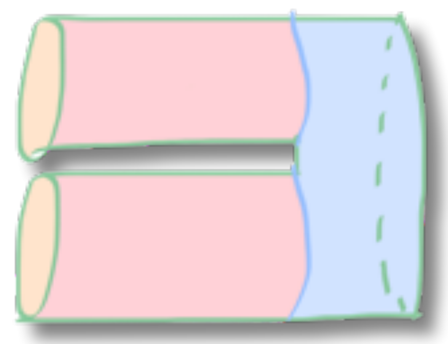
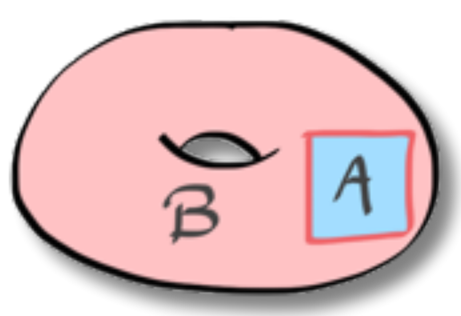


- Renyi entropies in quantum Monte Carlo

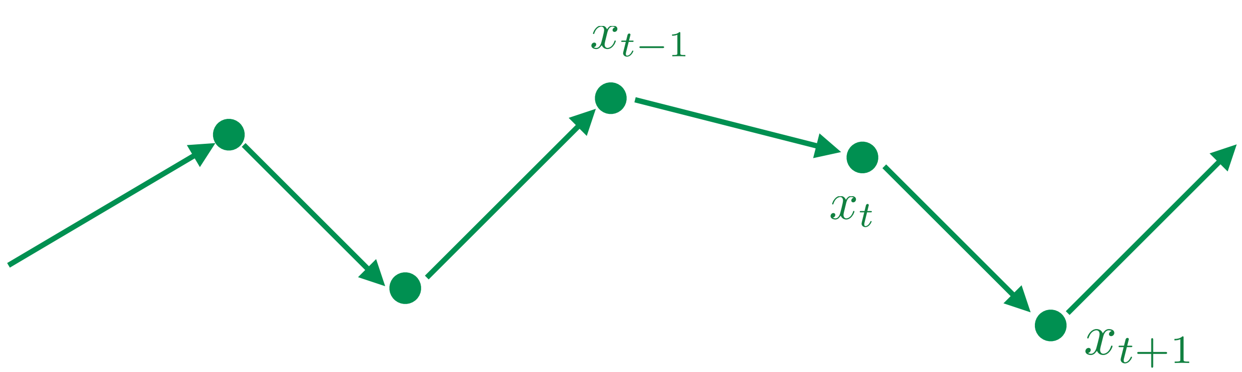


- An example of universal Renyi entropies in 2+1



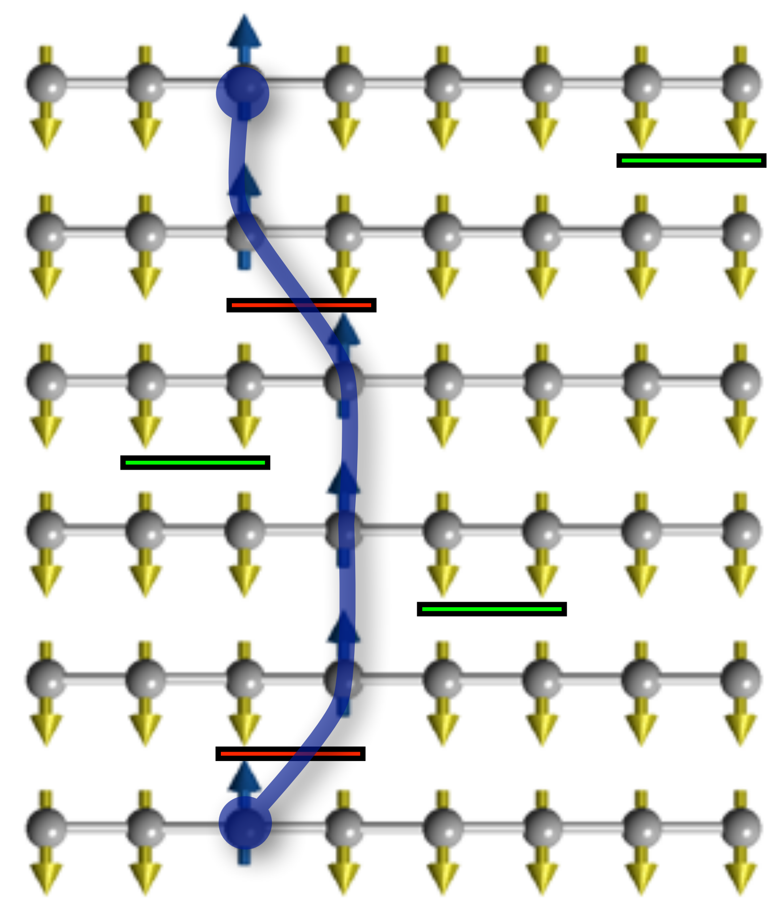
(one-slide) reminder of Monte Carlo strategies

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \mathrm{Tr}\left[e^{-\beta H} \mathcal{O} \right] = \frac{\sum_x \mathcal{O}(x) W_x}{\sum_x W_x}$$

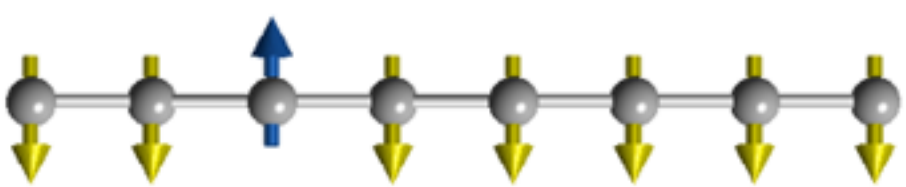


$$W_x P(x \to y) = W_y P(y \to x)$$

Quantum:

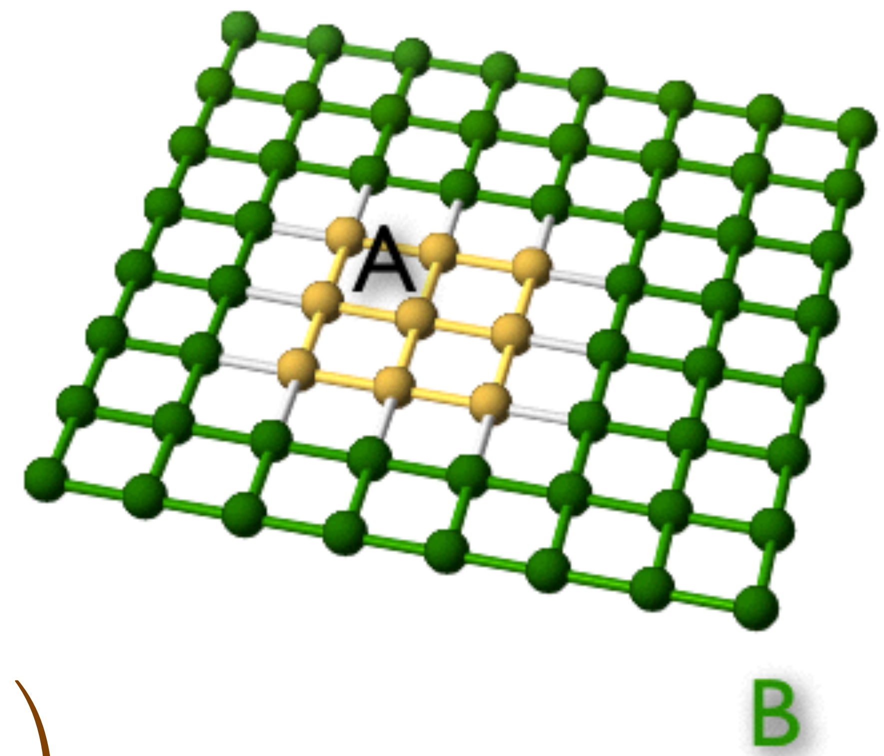


Classical:



A multi-sheeted Riemann surface can be used in Monte Carlo: a “replica trick”

V. Alba, J. Stat. Mech. P05013 (2013)
Iaconis, Inglis, Kallin, RGM: PRB 87, 195134 (2013)



- Define the entropy of a subregion A:

$$p_{i_A} = \frac{\sum_{i_B} e^{-\beta E(i_A, i_B)}}{Z}$$

$$p_{i_A}^2 = Z^{-2} \left(\sum_{i_B} e^{-\beta E(i_A, i_B)} \right) \left(\sum_{j_B} e^{-\beta E(i_A, j_B)} \right)$$

$$S_2(A) = -\ln \left(Z^{-2} \sum_{i_A} \sum_{i_B} \sum_{j_B} e^{-\beta (E(i_A, i_B) + E(i_A, j_B))} \right) = -\ln \left(\frac{Z[A, 2, T]}{Z^2} \right)$$

~ one copy of A at $T/2$

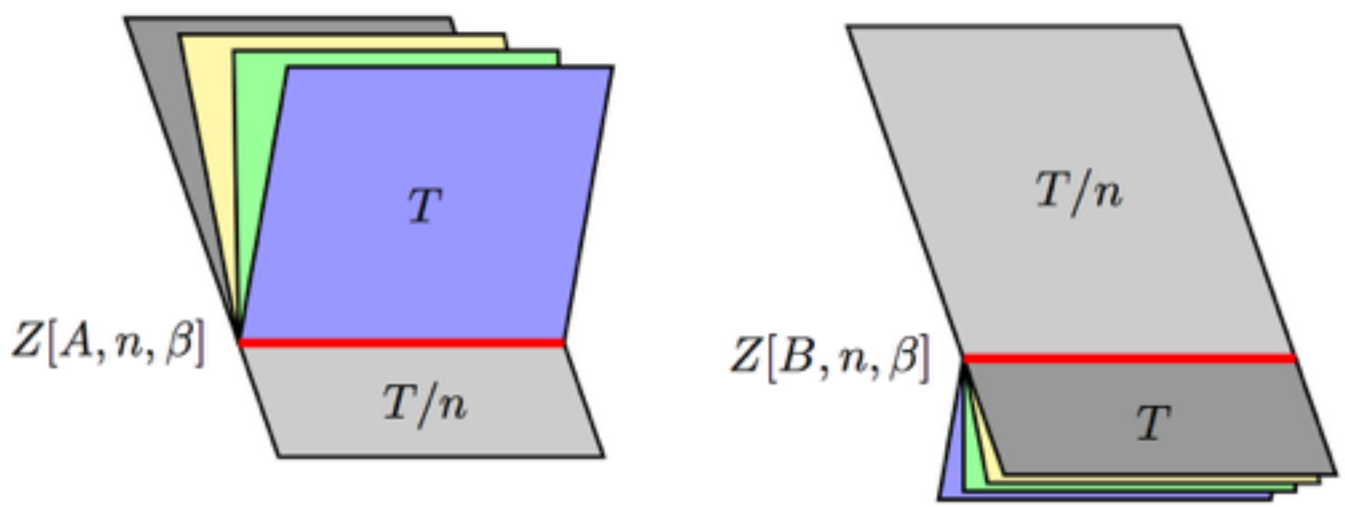
~ two copies of B at T

Classical "entanglement" entropy of a bipartition

$$S_n(A) = \frac{1}{1-n} \ln \left[\mathrm{Tr}\left(\rho_A^n\right) \right]$$

$$= \frac{1}{1-n} \ln \left[\frac{Z[A,n,\beta]}{Z^n} \right]$$

For general n, a n-sheeted "book" gives you the Renyi entropy



Stéphan, Misguich, Pasquier PRB 82, 125455 (2010)

- This general picture gives the basic idea how integer Renyi entropies are amenable to "measurement" in both Monte Carlo (and experiment)

Cardy, PRL 106, 150404 (2011)
Abanin, Demler, PRL 109, 020504 (2012)
Pichler, Bonnes, Daley, Läuchli, Zoller, NJP. 15 (2013) 063003

Measuring the Renyi entropy of a two-site Fermi-Hubbard model on a trapped ion quantum computer
Linke et. al arXiv:1712.08581

Rajibul Islam: Tomorrow 8:30am

Calculation of the entropy of a bipartition is technically equivalent to calculating the difference of two free energies:

- Thermodynamic integration

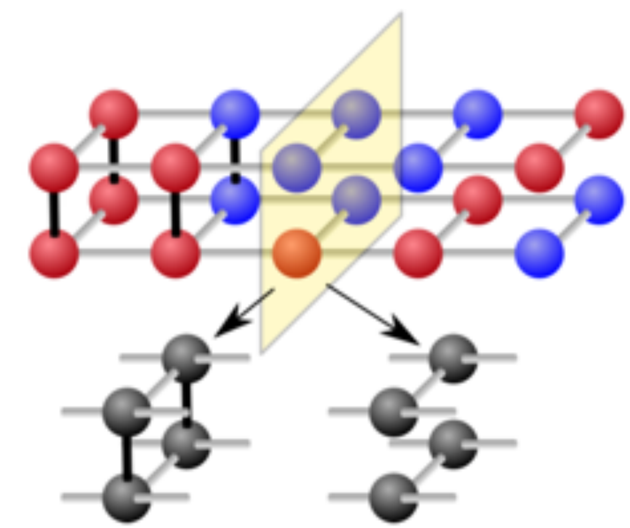
$$S_2 = -\ln \mathrm{Tr}(\rho_A^2) = -\ln\left\{\frac{Z[A,2,\beta]}{Z(\beta)^2}\right\} = -\ln Z[A,2,\beta] + 2\ln Z(\beta)$$

$$= -S_A(\beta=0) + \int_0^\beta \langle E\rangle_A d\beta + 2S_0(\beta=0) - 2\int_0^\beta \langle E\rangle_0 d\beta$$

- Extended ensemble methods

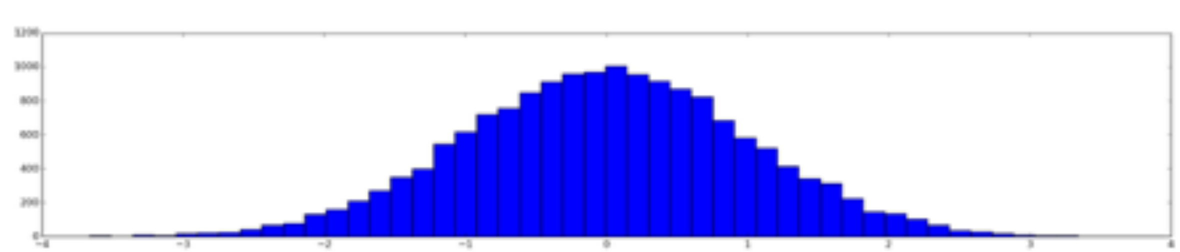
  – Ratio trick

$$\frac{Z[A_1,2,\beta]}{Z[A_2,2,\beta]} = \left\langle \frac{N_1}{N_2} \right\rangle_{\mathrm{MC}}$$



Humeniuk, Roscilde. Phys. Rev. B, 86, 235116 (2012)

  – Wang-Landau & multicanonical methods

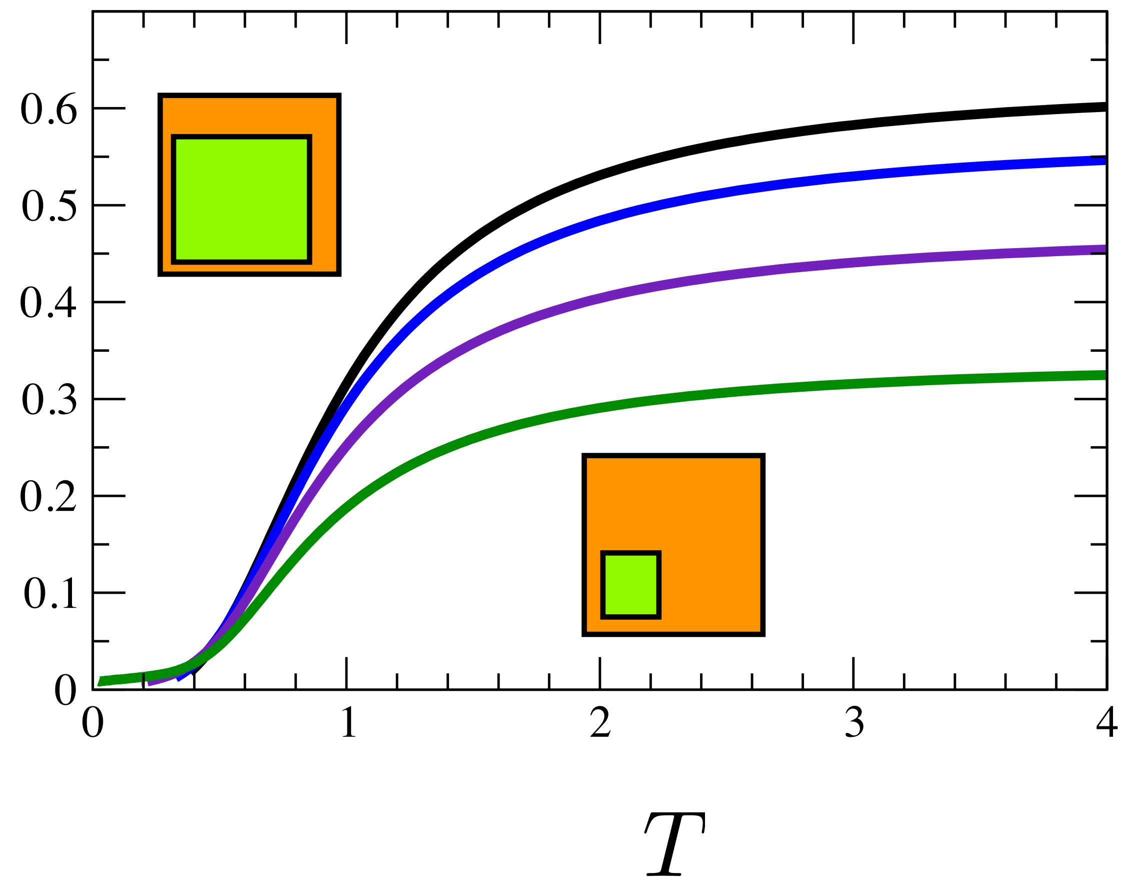


Inglis, RGM, Phys. Rev. E 87, 013306 (2013)

In general:

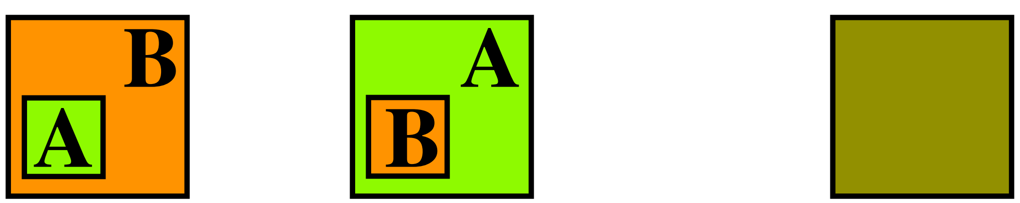
$$S_n(A) \neq S_n(B)$$

each becomes an extensive quantity
at finite temperature (volume-law)



One can consider the **Mutual Information**

$$I_n(A;B) = S_n(A) + S_n(B) - S_n(A \cup B)$$

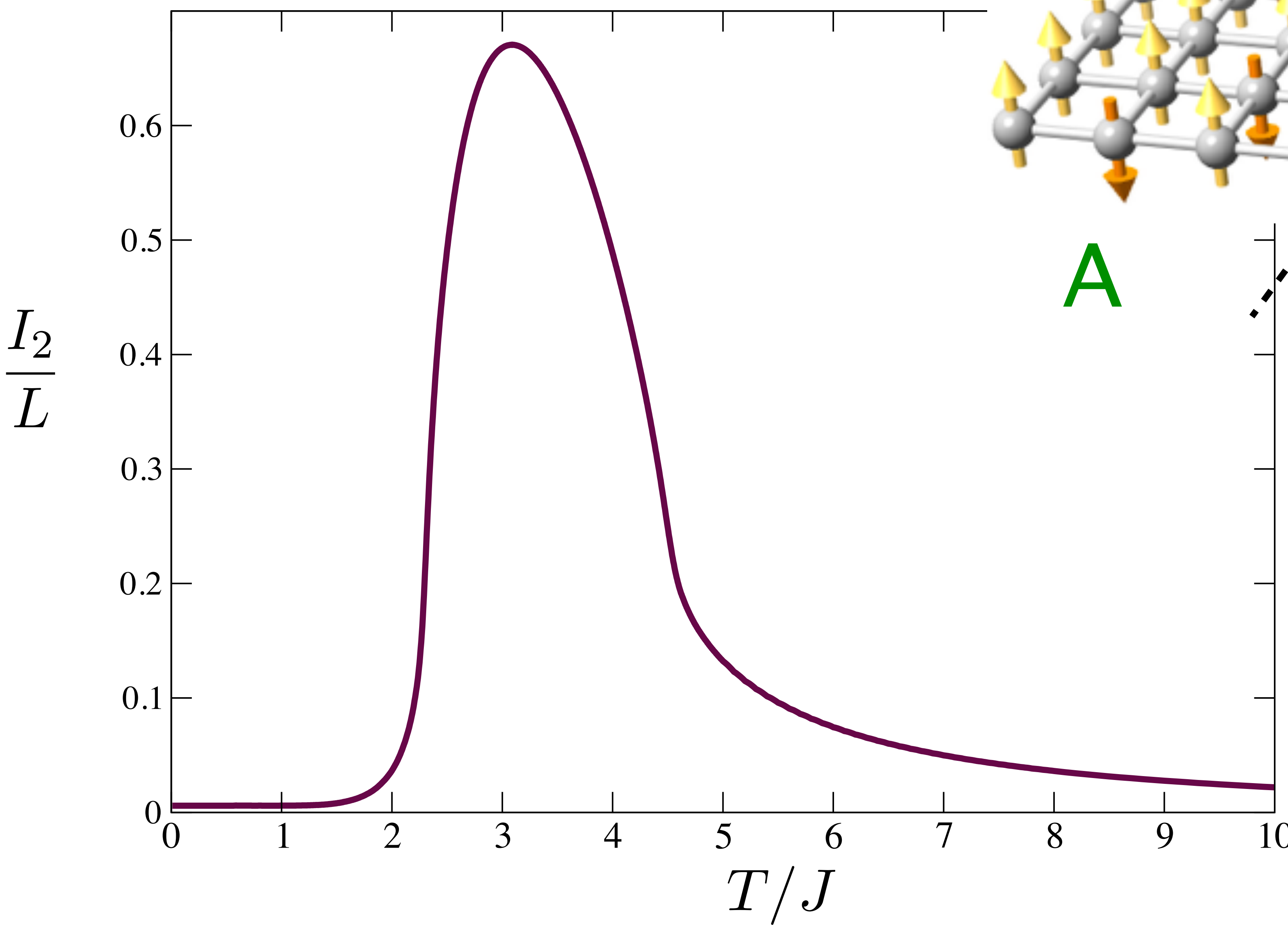


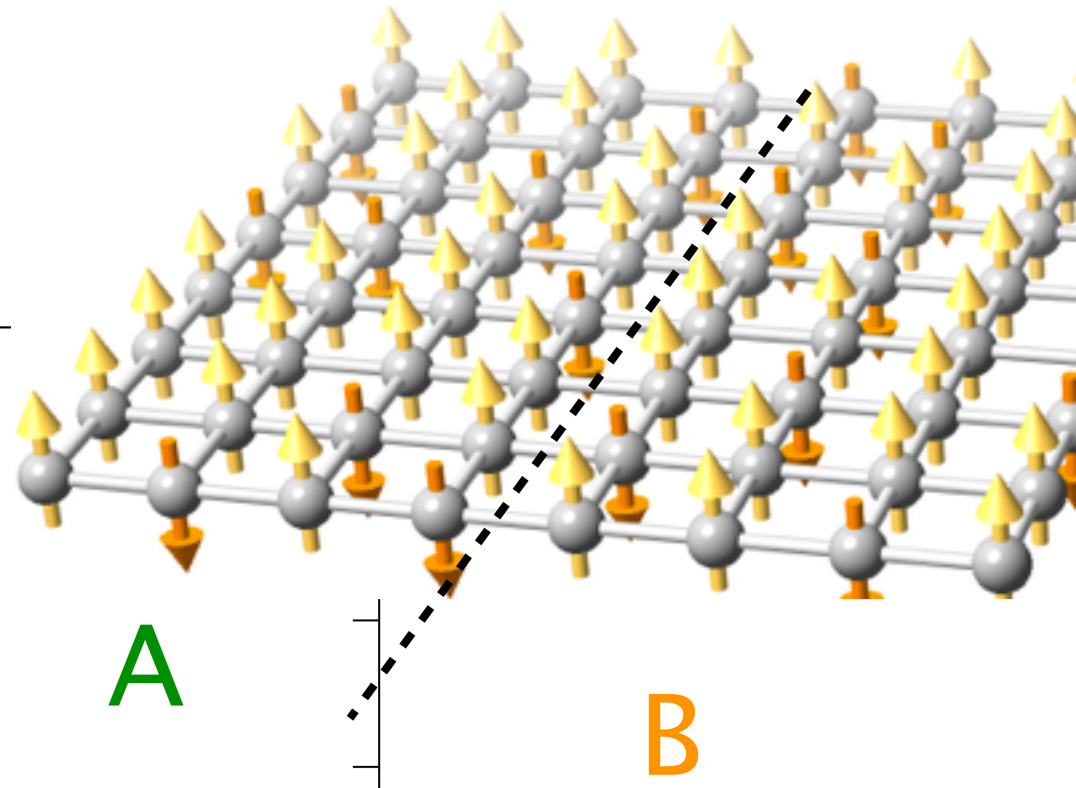
The Mutual Information is the amount of information about A contained in B: is sensitive to all correlations

Wolf, Verstraete, Hastings, Cirac, PRL **100,** 070502 (2008)

Example: Mutual Information of the 2D Ising model

$$H = -J \sum_{\langle ij \rangle} S_i^z S_j^z$$





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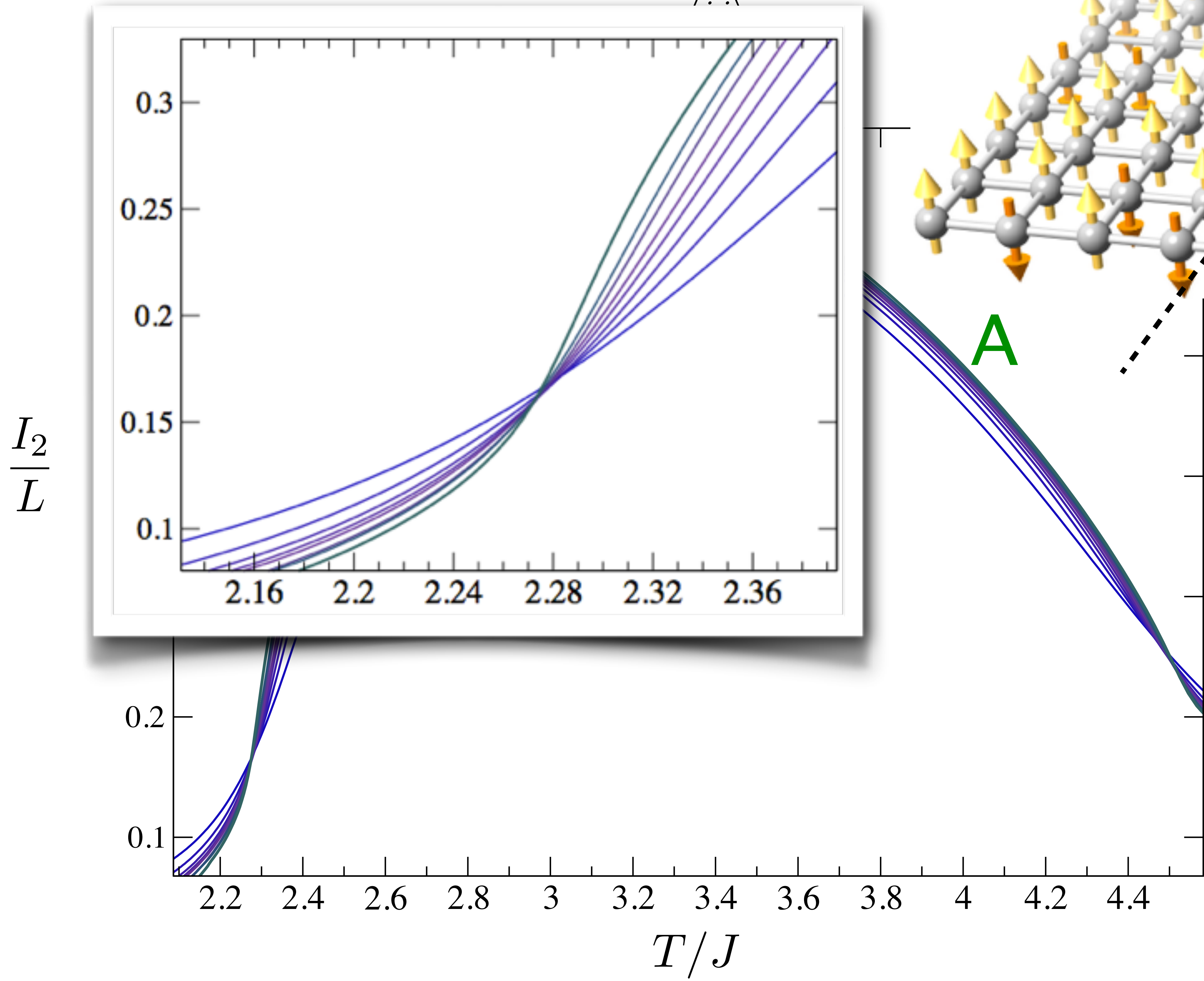
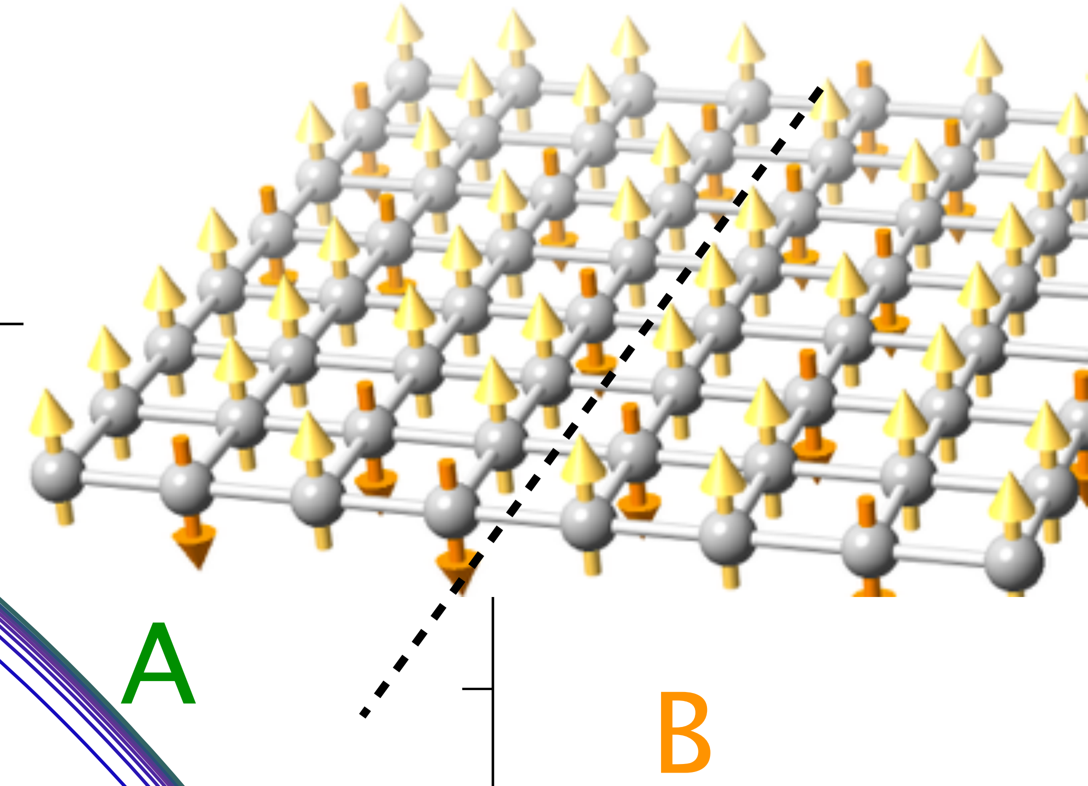
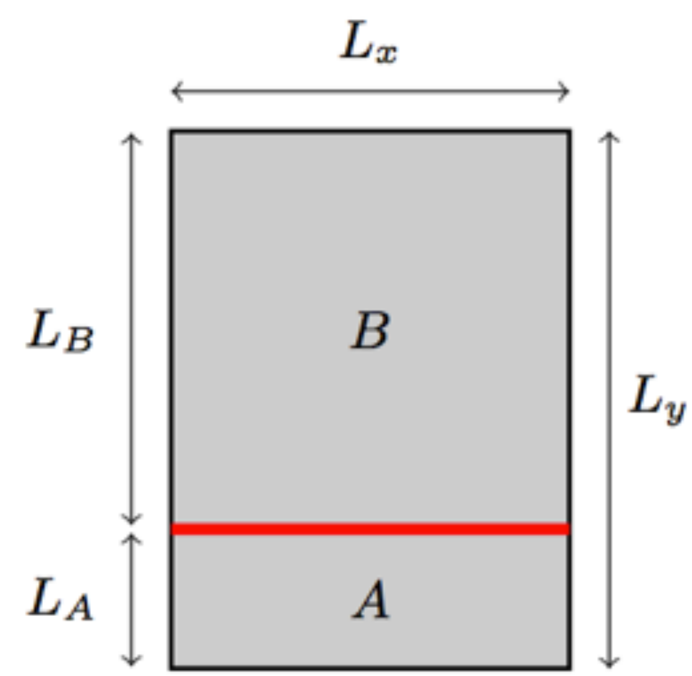




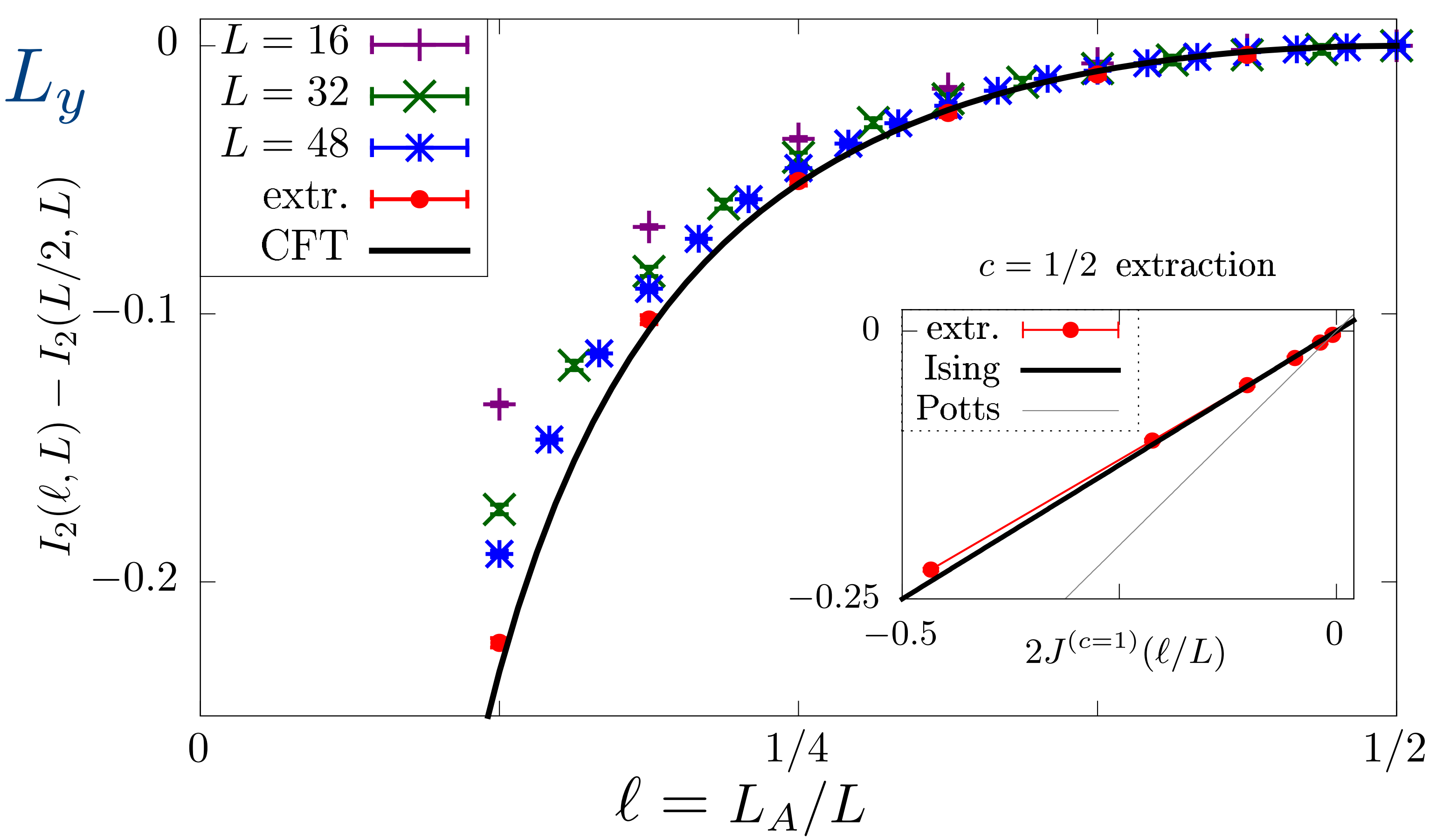
“Geometric” Mutual Information at the 2D Ising critical point

$$I_n(A;B) = a_n L + \mathcal{G}_n + \cdots$$

$$\mathcal{G}_n = \frac{c}{2}\left(\frac{n}{n-1}\right)\log\left(\frac{f(L_A/L_x)f(L_B/L_x)}{\sqrt{L_x}f(L_y/L_x)}\right)$$



$L_x = L_y$



Gives a simple way to extract the central charge c=1/2 of the CFT (with no non-universal velocities)

c.f. DMRG on the 1D quantum Ising model

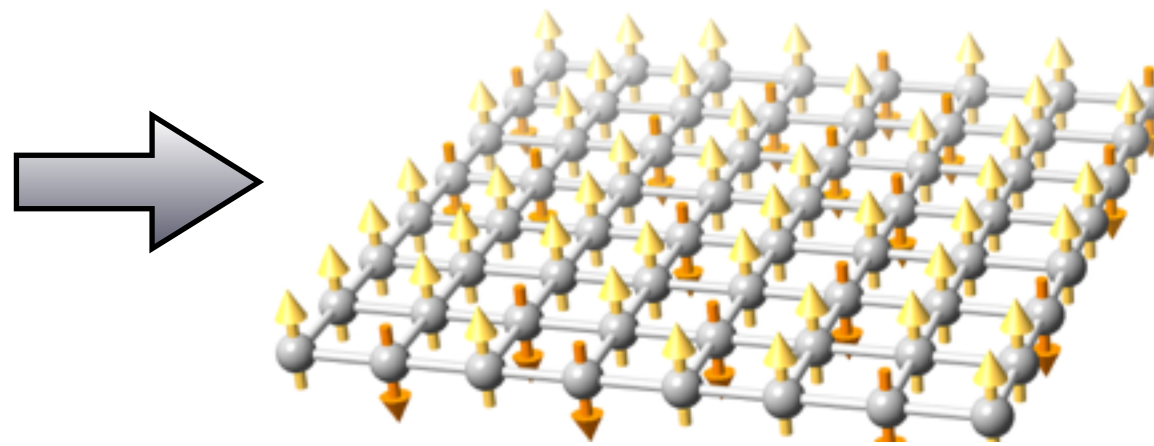
J.-M. Stephan, S. Inglis, P. Fendley, RGM, Phys. Rev. Lett. 112, 127204 (2014)

General quantum–classical correspondence

- If studying **universal** properties of entanglement entropy at a quantum critical point, can look instead at a classical (thermal) phase transition in a d+1 model

$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x$$

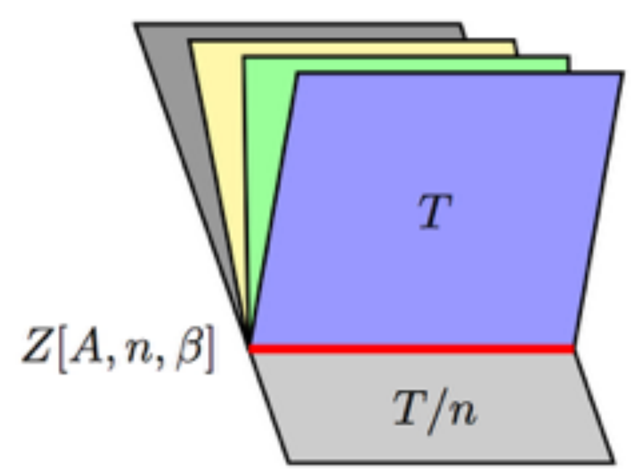
$$(h/J)_c = 1$$



$$H = -J \sum_{\langle ij \rangle} S_i^z S_j^z$$

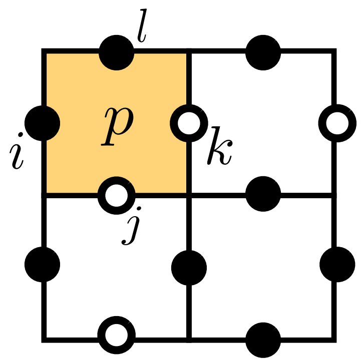
$$(T/J)_c = 2.269$$

- Since EE depends on subregion geometry, once must take care in how the d+1 classical system is defined (c.f. QMC, next)

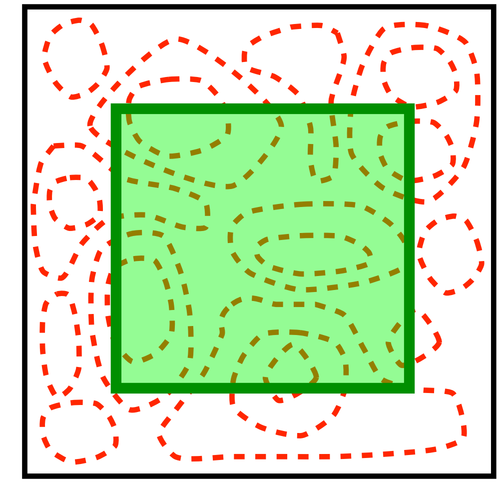


Exercise: Classical Z_2 Ising gauge theory

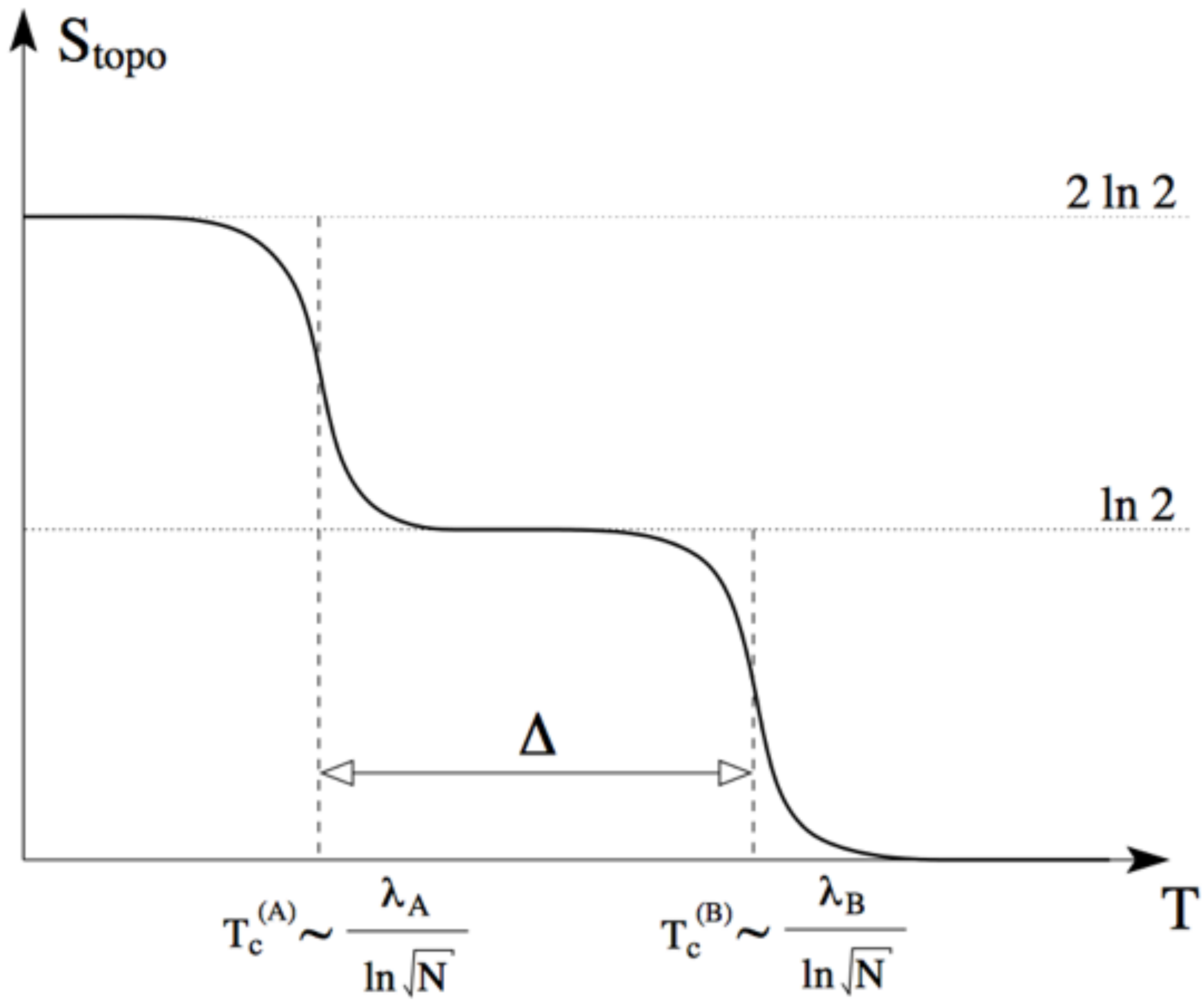
$$H = -\sum_p \sigma_i^z \sigma_j^z \sigma_k^z \sigma_l^z$$



$$\Omega \sim 2^{\ell - 1}$$



$$S_n = A\ell + \gamma$$

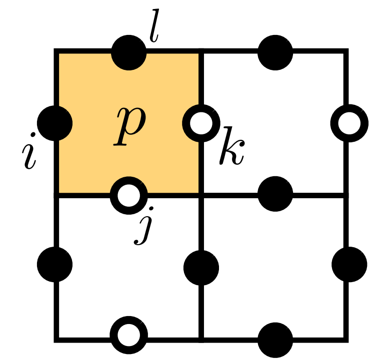


Castelnovo, Chamon Phys. Rev. B 76, 184442 (2007)

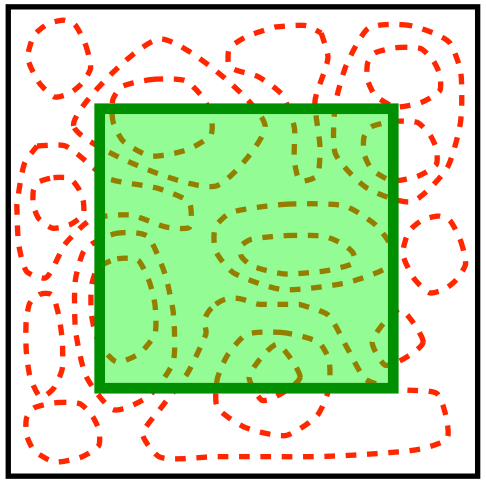
$$H = -\lambda_B \sum_{\text{plaquettes } p} B_p - \lambda_A \sum_{\text{stars } s} A_s$$

Exercise: Classical Z_2 Ising gauge theory

$$H = -\sum_p \sigma_i^z \sigma_j^z \sigma_k^z \sigma_l^z$$

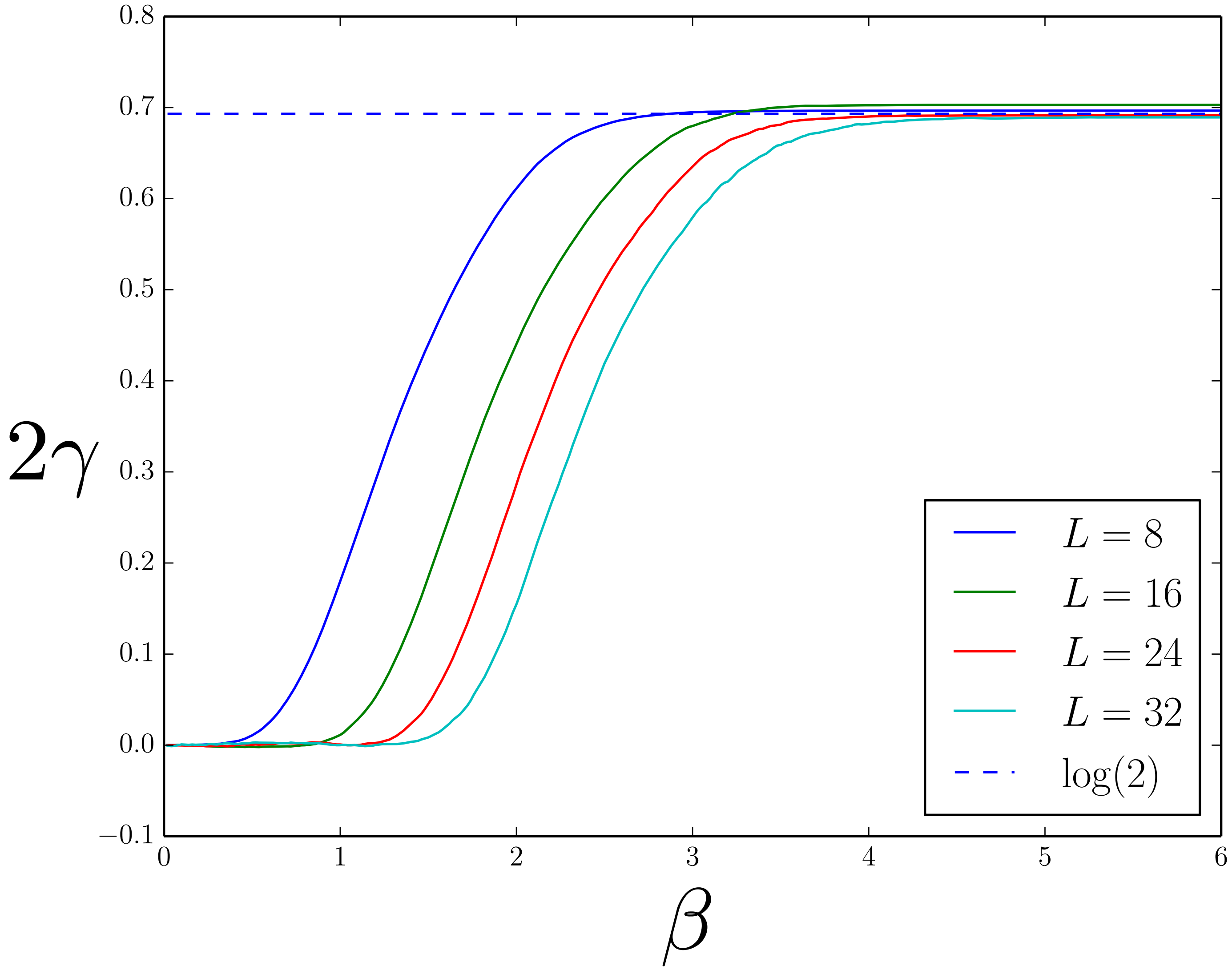


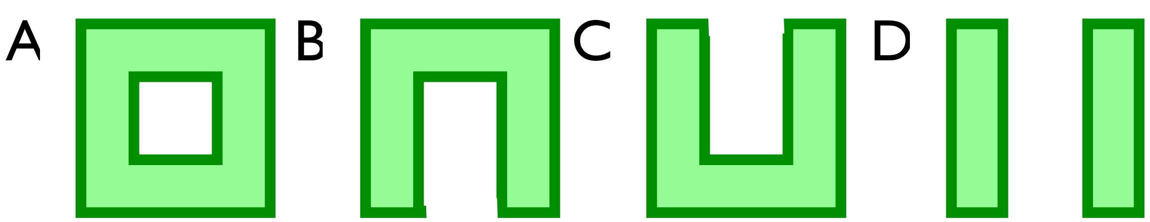
$$\Omega \sim 2^{\ell-1}$$



$$S_n = A\ell + \gamma$$

$$\gamma = -\ln(2)/2$$





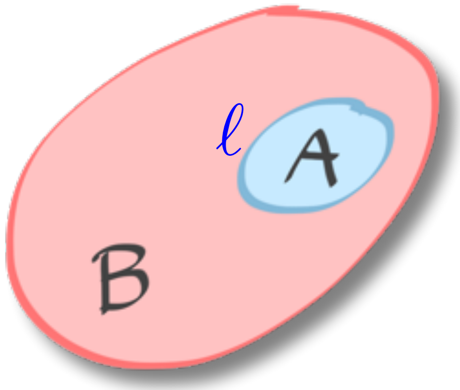
$$2\gamma = -S_n^A + S_n^B + S_n^C - S_n^D$$

Levin and Wen, Phys. Rev. Lett. 96, 110405 (2006)

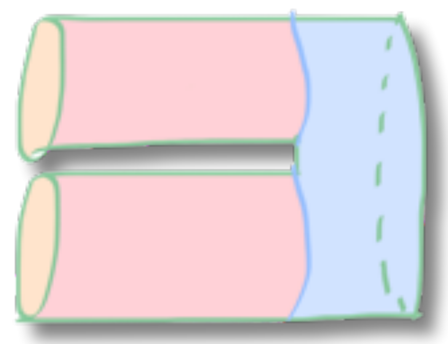
Outline

- A brief introduction to Renyi entropies in condensed matter physics

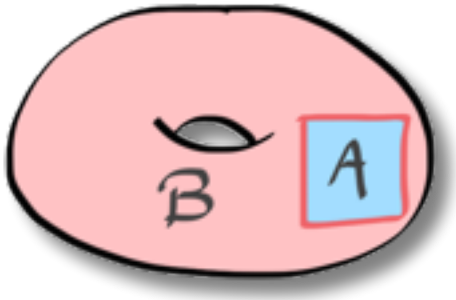
- Renyi entropies in classical Monte Carlo



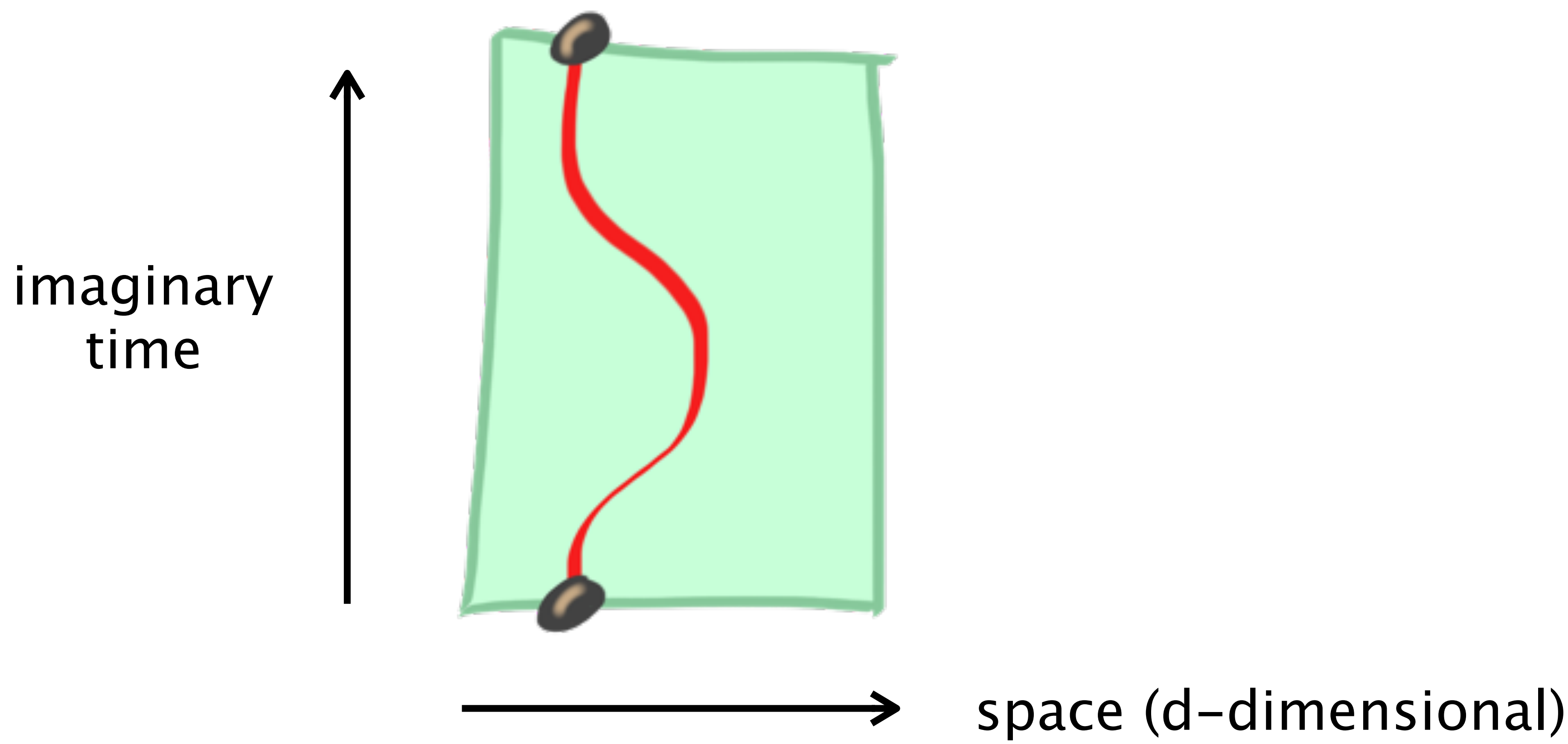
- Renyi entropies in quantum Monte Carlo



- An example of universal Renyi entropies in 2+1



Quantum Monte Carlo

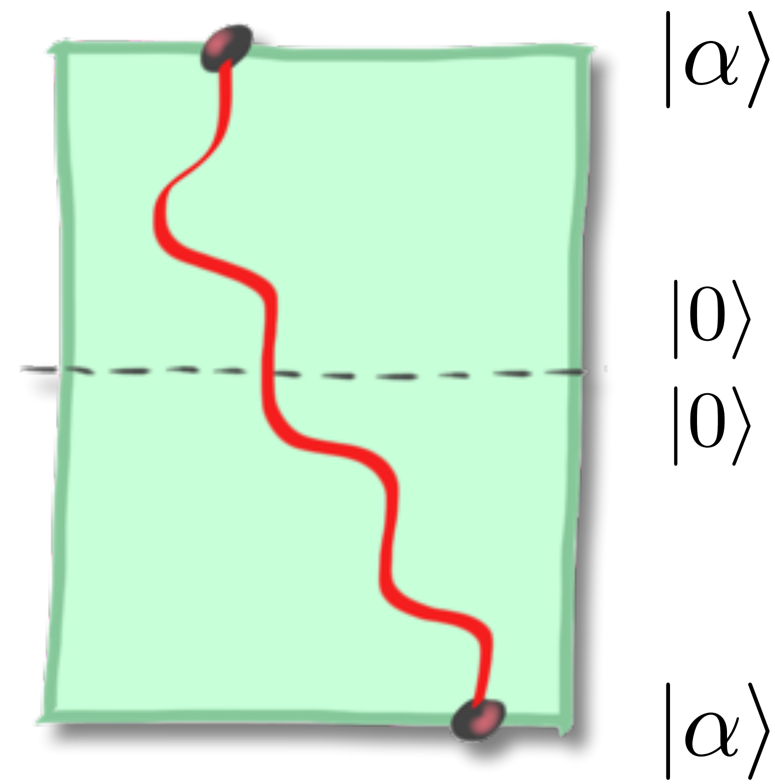


- d+1 dimensional simulation cell
- can have periodic or open boundaries in imaginary time
- sign problem may exist
- no direct access to the reduced density matrix

Ground-state projector QMC

$$Z = \langle 0 | 0 \rangle$$

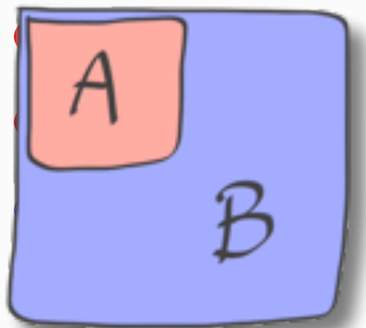
$$\langle \mathcal{O} \rangle = \frac{1}{Z} \langle 0 | \mathcal{O} | 0 \rangle$$



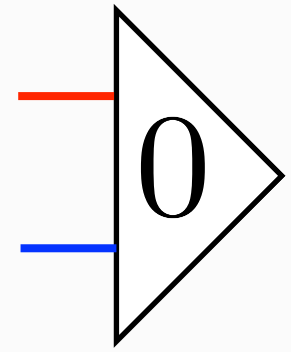
$$(-H)^m |\alpha\rangle = c_0 |E_0|^m \left[|0\rangle + \frac{c_1}{c_0} \left(\frac{E_1}{E_0} \right)^m |1\rangle \cdots \right]$$

$$= c_0 |E_0|^m |0\rangle \;\; \text{as} \;\; m \to \infty$$

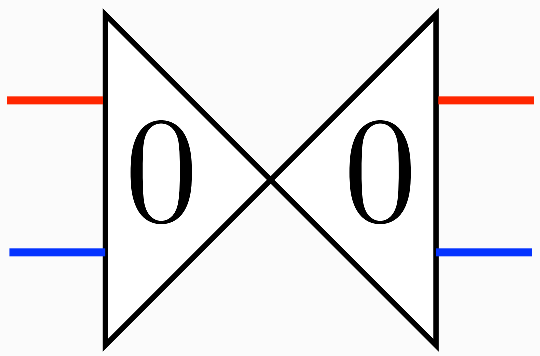
The “replica” trick



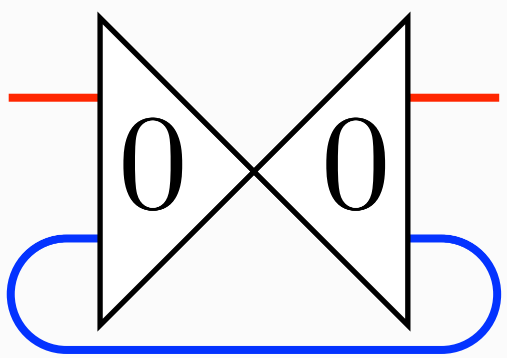
$\Leftrightarrow$



$\Leftrightarrow |0\rangle$

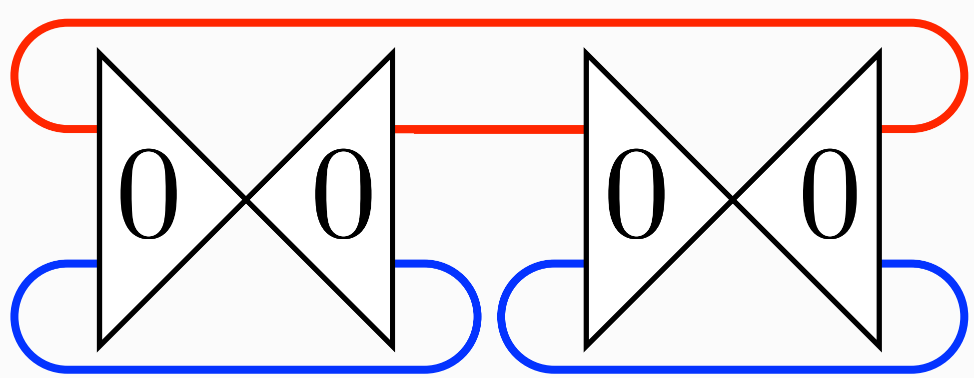


$\Leftrightarrow |0\rangle\langle 0| \quad \Leftrightarrow \quad \rho_{\mathrm{AB}}$

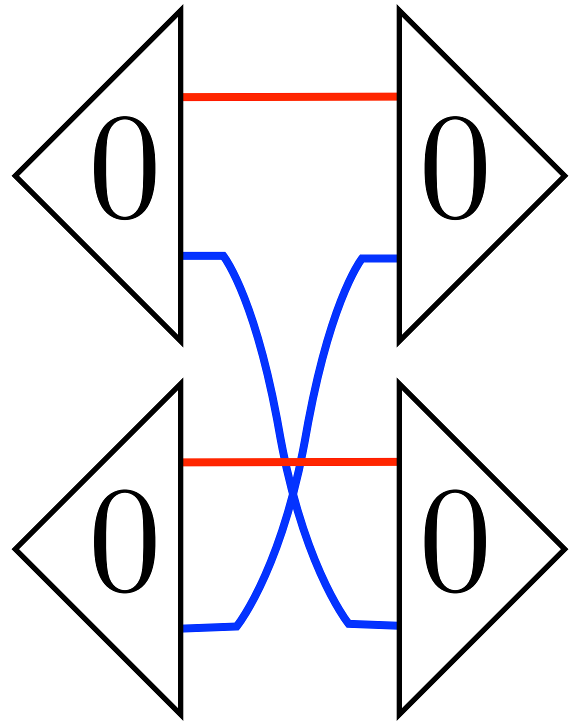


$\Leftrightarrow \mathrm{Tr}_{\mathrm{B}}(\rho_{\mathrm{AB}}) = \rho_{\mathrm{A}}$

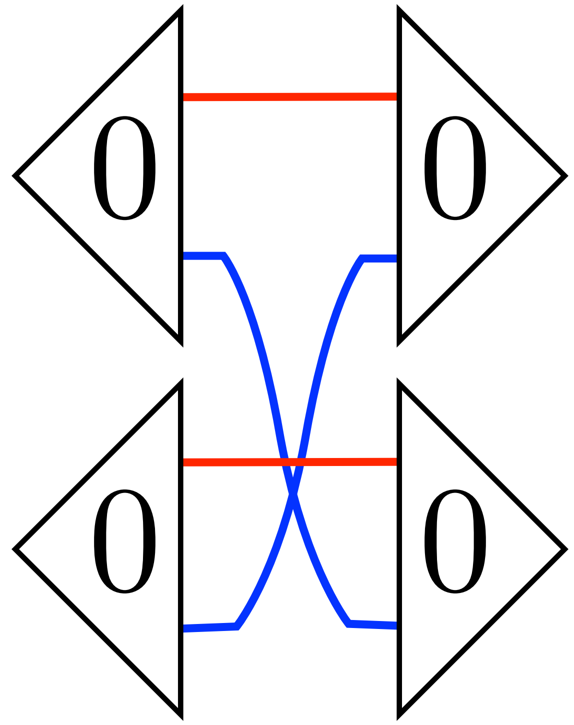
$\mathrm{Tr}(\rho_{\mathrm{A}}^2) \Leftrightarrow$



$$\mathrm{Tr}(\rho_A^2) \Leftrightarrow$$



$$\mathrm{Tr}(\rho_{\mathrm{A}}^2) \Leftrightarrow$$

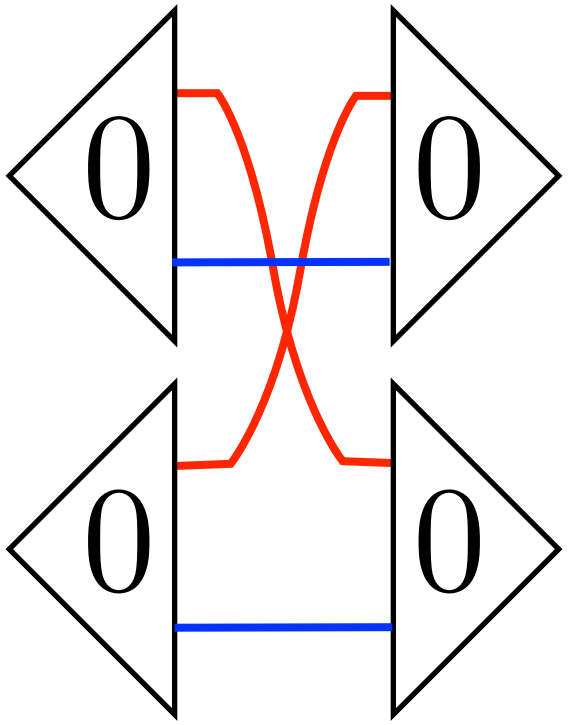


$$\Leftrightarrow \langle Swap_{\mathrm{B}} \rangle$$

$$S_2 = -\ln \mathrm{Tr}(\rho_{\mathrm{A}}^2)$$

$$\begin{aligned} \mathrm{Tr}(\rho_{\mathrm{A}}^2) &= \langle 0 \otimes 0 | Swap_{\mathrm{B}} | 0 \otimes 0 \rangle \\ &= \langle Swap_{\mathrm{B}} \rangle = \langle Swap_{\mathrm{A}} \rangle \end{aligned}$$

$$\mathrm{Tr}(\rho_{\mathrm{A}}^2) \Leftrightarrow$$

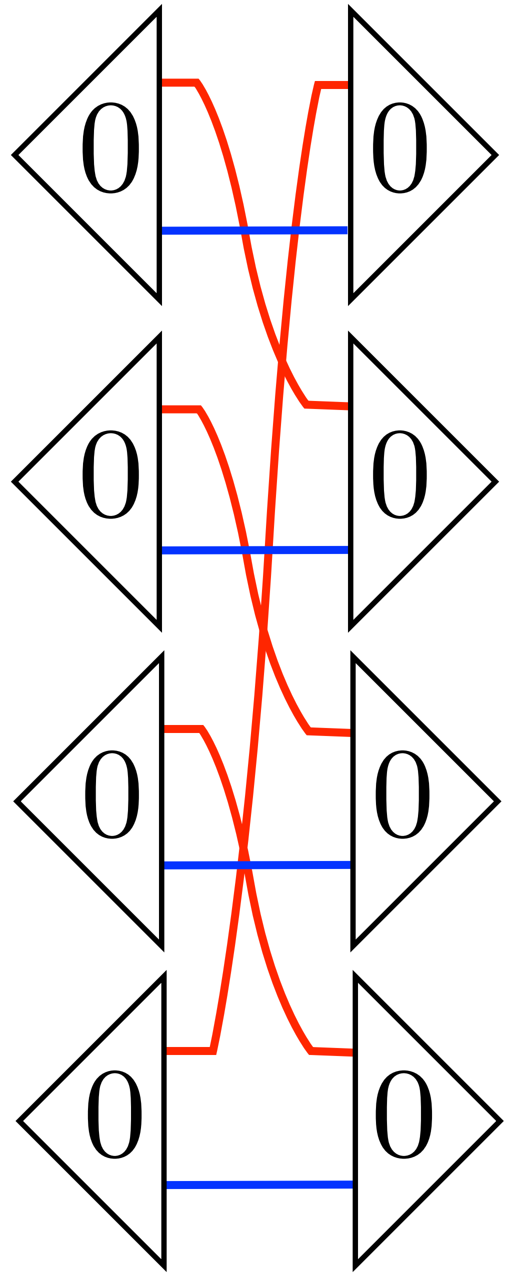


$$\Leftrightarrow \langle Swap_{\mathrm{A}} \rangle$$

$$S_2 = -\ln \mathrm{Tr}(\rho_{\mathrm{A}}^2)$$

$$\begin{aligned} \mathrm{Tr}(\rho_{\mathrm{A}}^2) &= \langle 0 \otimes 0 | Swap_{\mathrm{B}} | 0 \otimes 0 \rangle \\ &= \langle Swap_{\mathrm{B}} \rangle = \langle Swap_{\mathrm{A}} \rangle \end{aligned}$$

$$\mathrm{Tr}(\rho_{\mathrm{A}}^4) \quad \Leftrightarrow$$



$$\Leftrightarrow \quad \langle \Pi_{\mathrm{A}}^{(4)} \rangle$$

Can be used in to obtain the higher-order Renyi entropies, and hence the

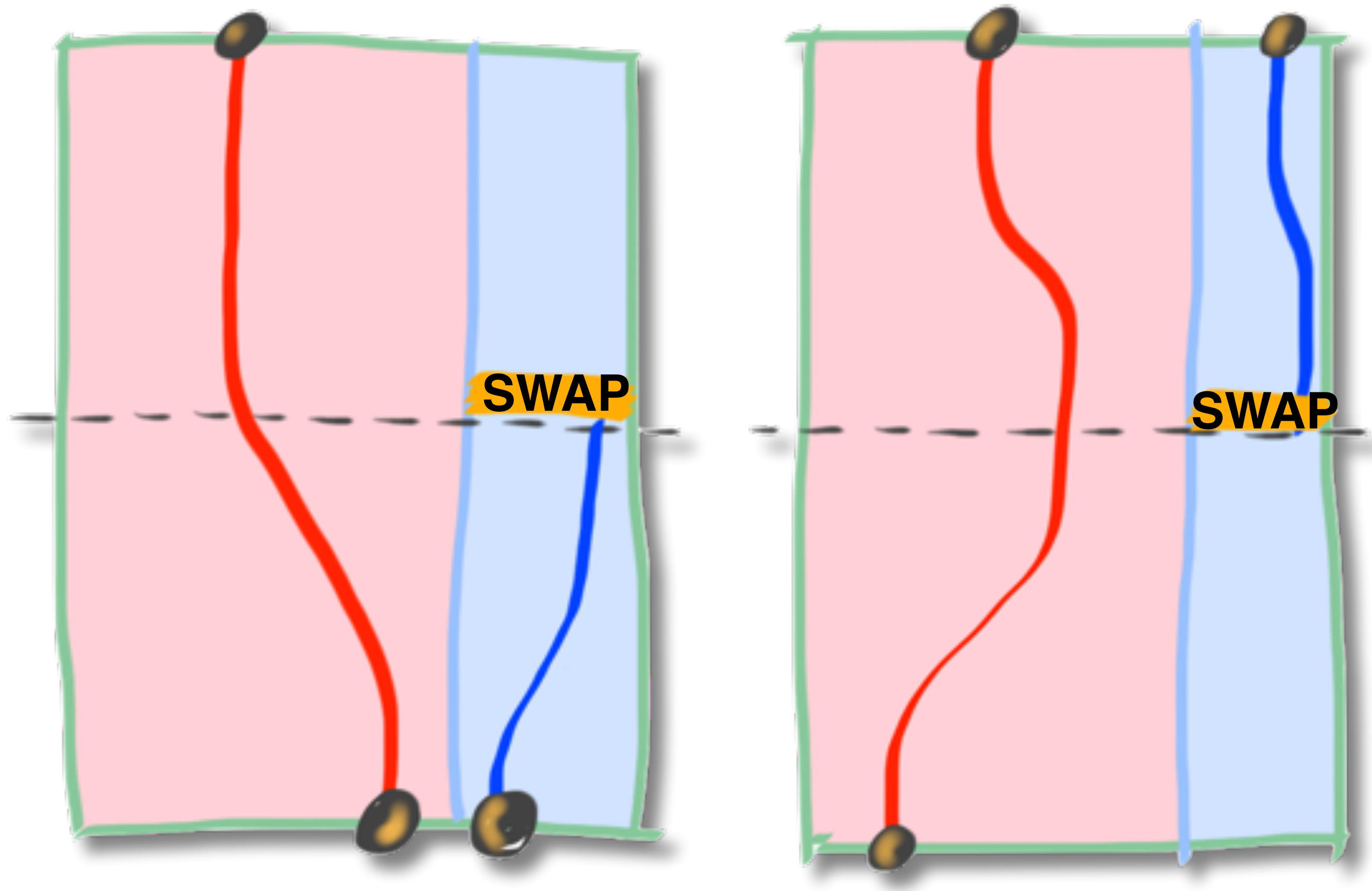
- entanglement spectrum

Chung, Bonnes, Chen, Lauchli, arXiv:1305.6536
Tubman, Yang, arXiv:1402.0503

- logarithmic negativity

Chung, Alba, Bonnes, Chen, and Lauchli, arXiv:1312.1168
V Alba, J. Stat. Mech. P05013 (2013)

Renyi entropies can be easily accessed in any flavor quantum Monte Carlo that estimates the ground-state wavefunction



– Valence-bond basis QMC

Kallin, Gonzalez, Hastings, RGM, PRL., 103, 117203 (2009)

– Variational MC

Zhang, Grover, and Vishwanath, PRB 84, 075128 (2011)

McMinis, Tubman, Phys. Rev. B 87, 081108(R) (2013)

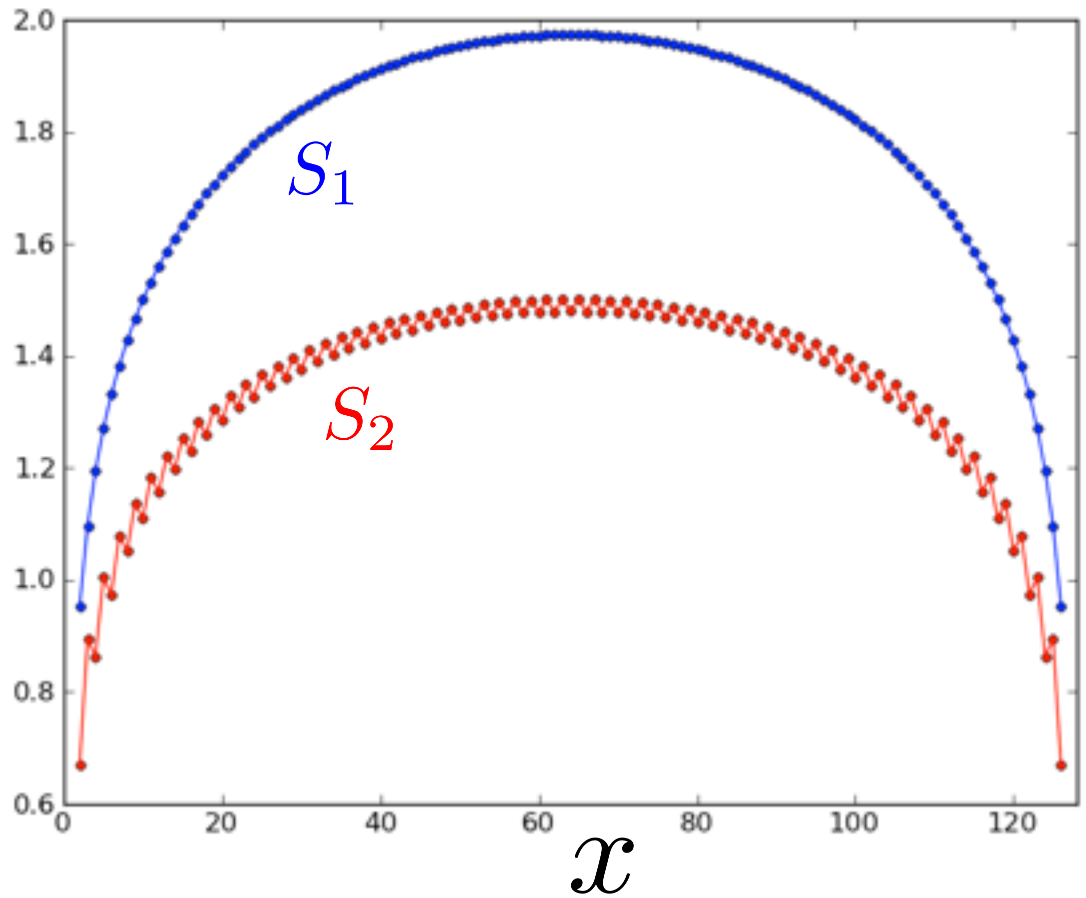
– Path Integral Ground State (PIGS)

Herdman, Roy, RGM, Del Maestro, Phys. Rev. B 89, 140501 (2014)
Phys. Rev. E 90, 013308 (2014)

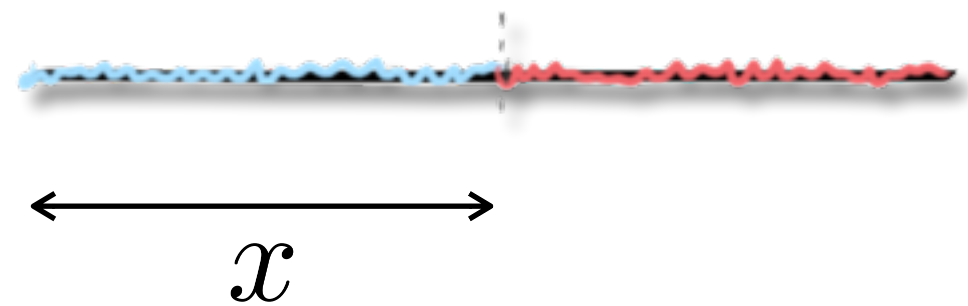
– Auxiliary Field/Determinental QMC

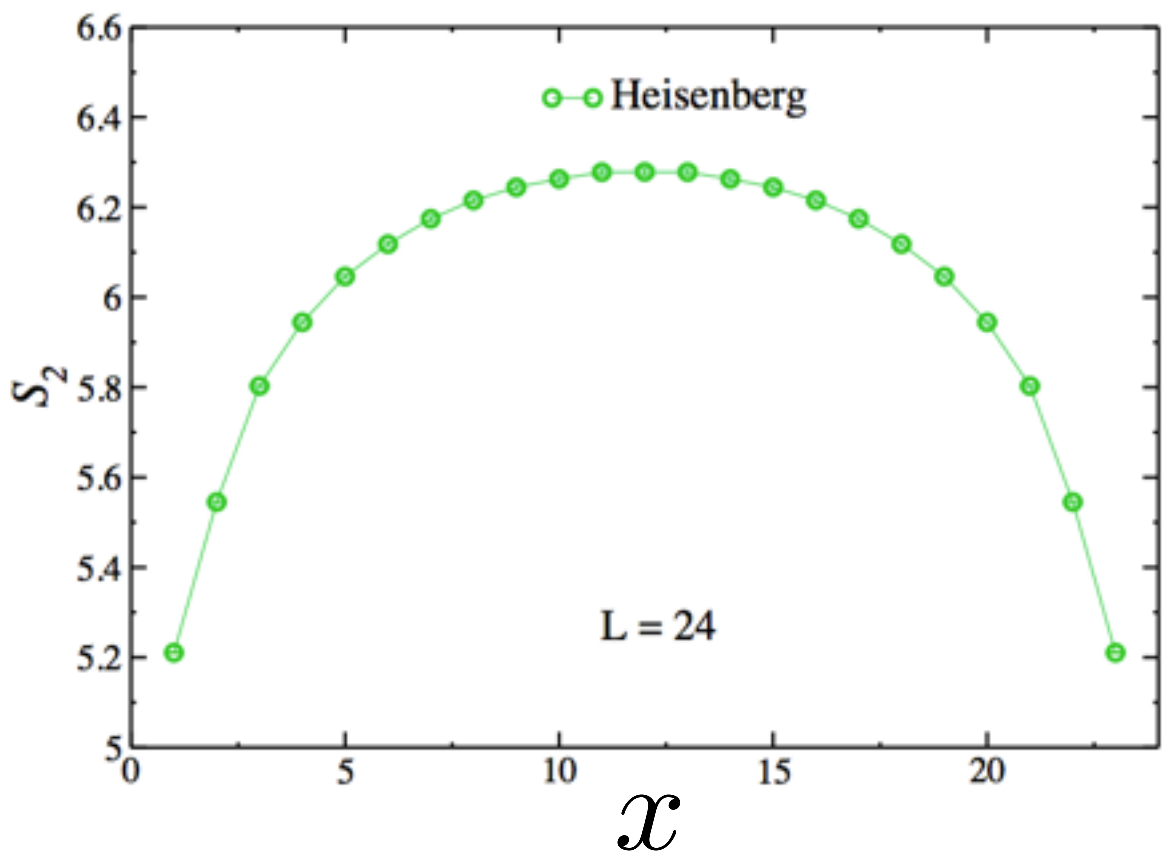
T. Grover, Phys. Rev. Lett. 111, 130402 (2013)
Assaad, Lang, Toldin, Phys. Rev. B 89, 125121 (2014)
Broecker and Trebst, J. Stat. Mech. (2014) P08015

Example:ground-state Renyi entropy QMC

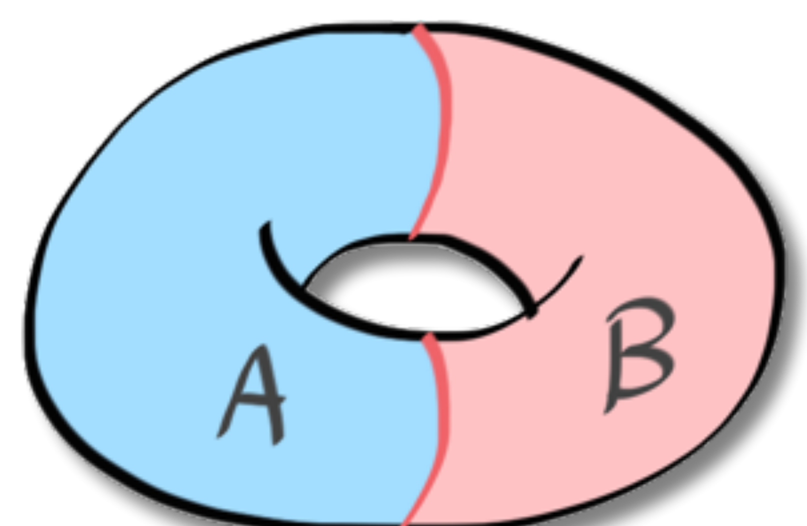


$$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

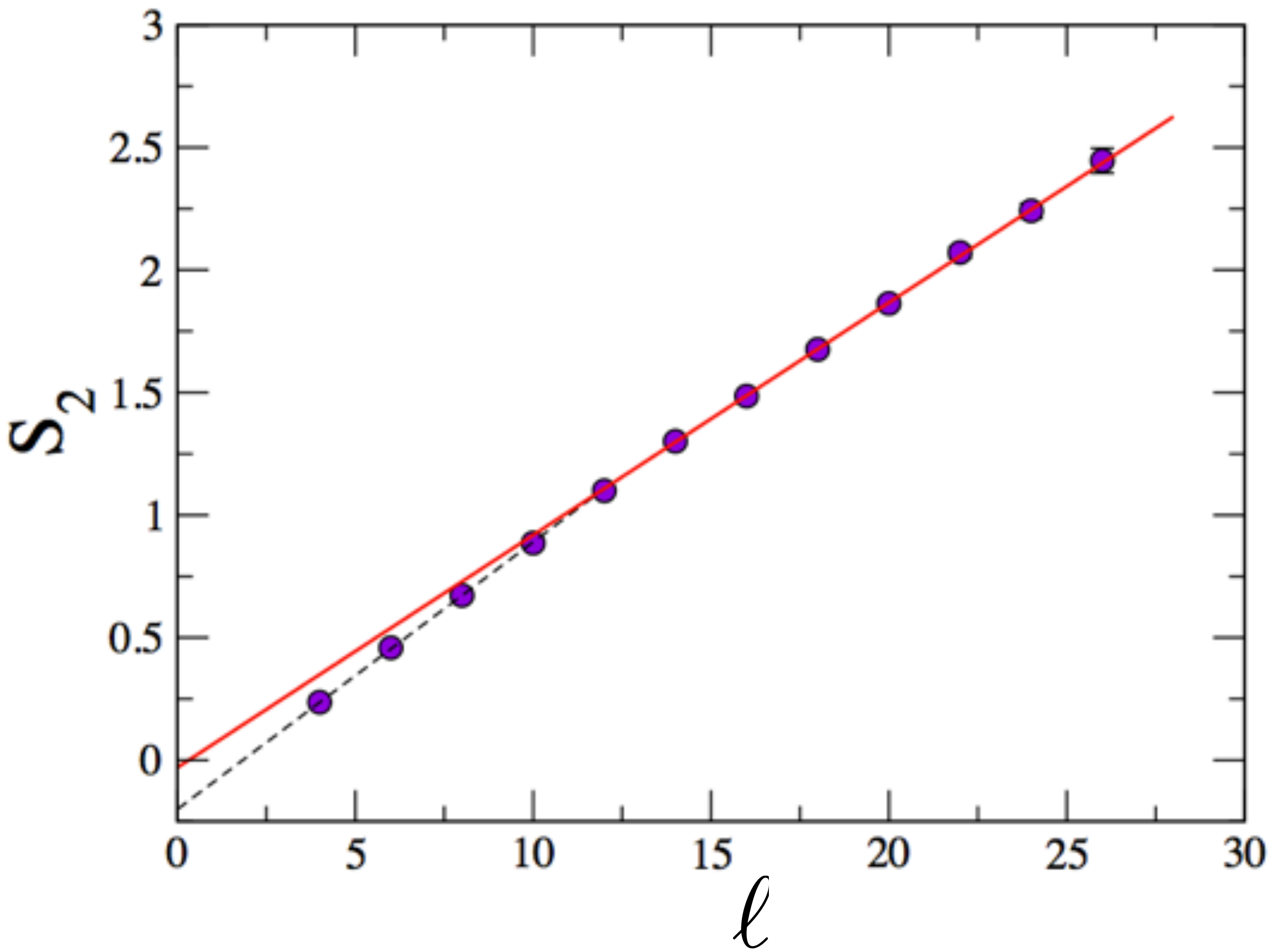


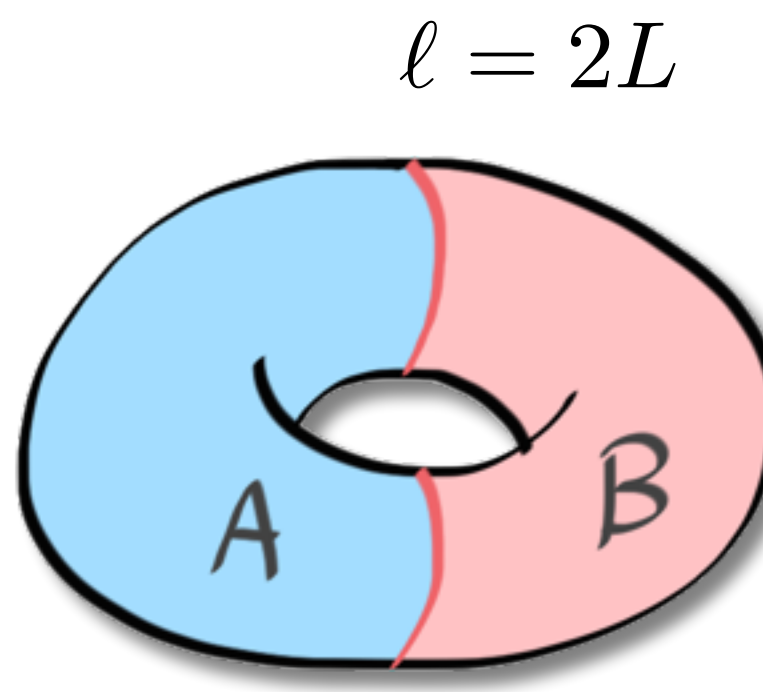


$$\ell = 2L$$



Example: Area Law at T=0

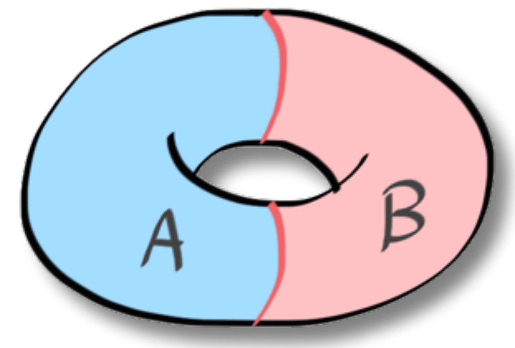


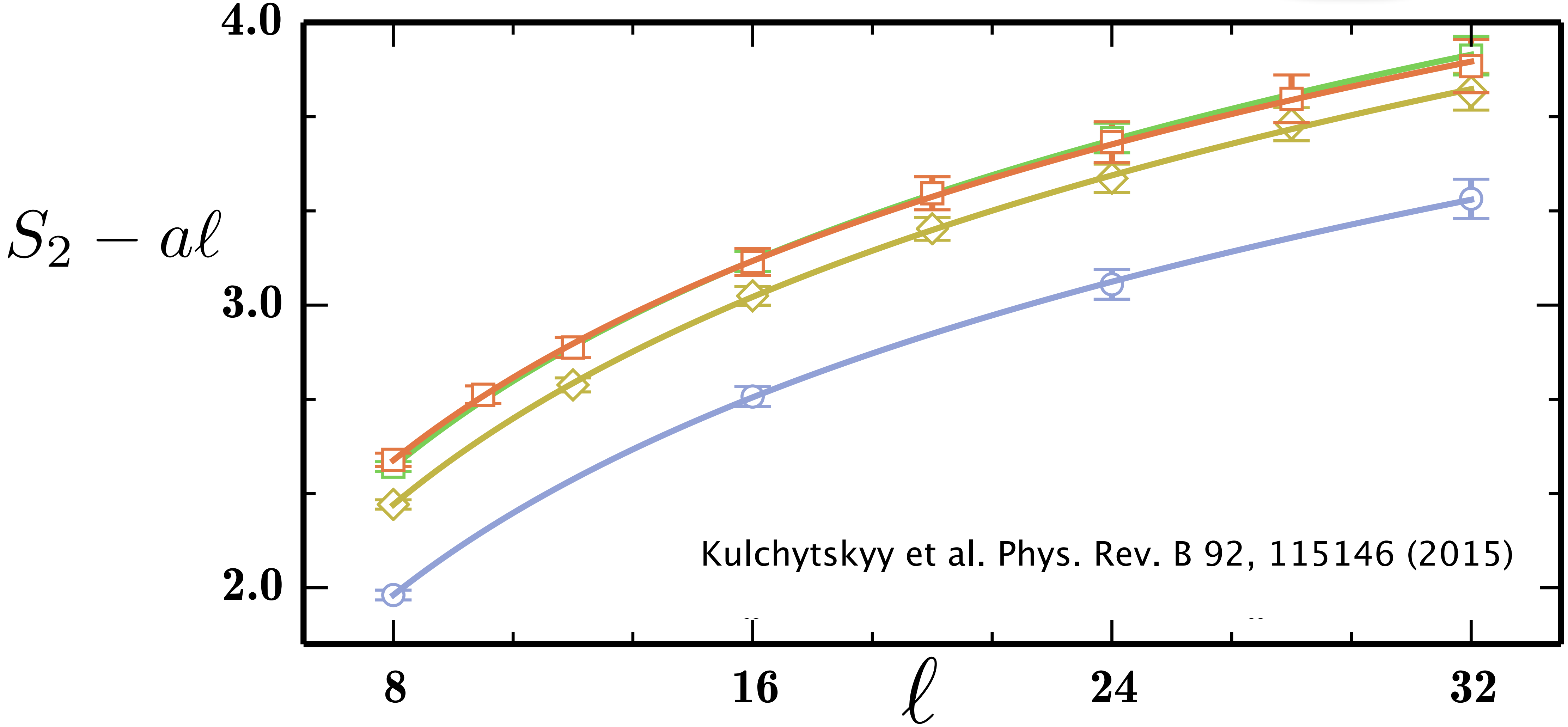


$$S_2 = a\frac{\ell}{\delta} + \mathcal{O}\left(\frac{\delta}{\ell}\right) + \cdots$$

Example: log correction from a broken continuous symmetry

$$H = \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y)$$



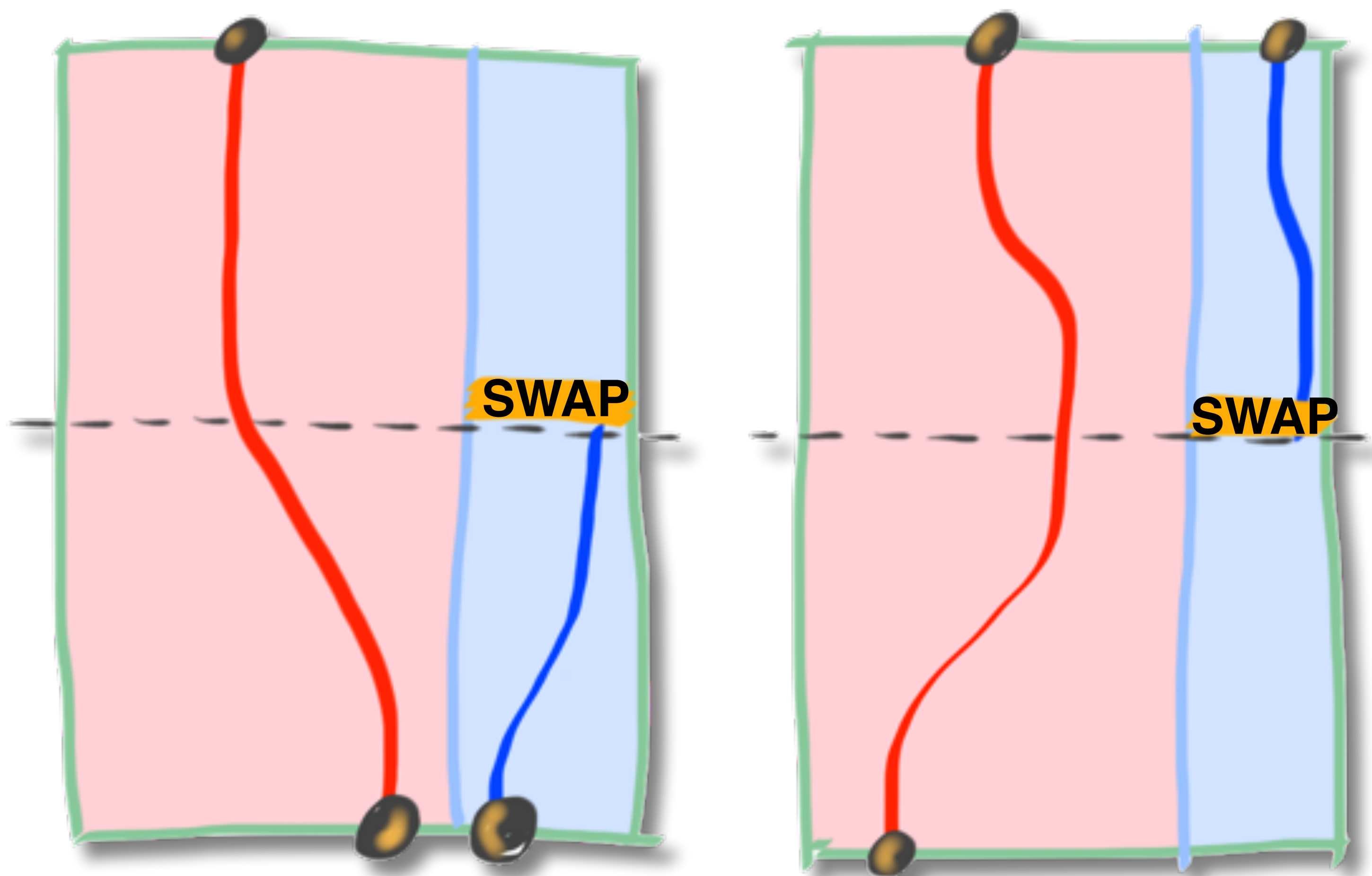


$$S_2 = a\ell + N_G \log(\ell \rho_s / c) + \gamma$$

Metlitski and Grover arXiv:1112.5166

Finite-temperature QMC

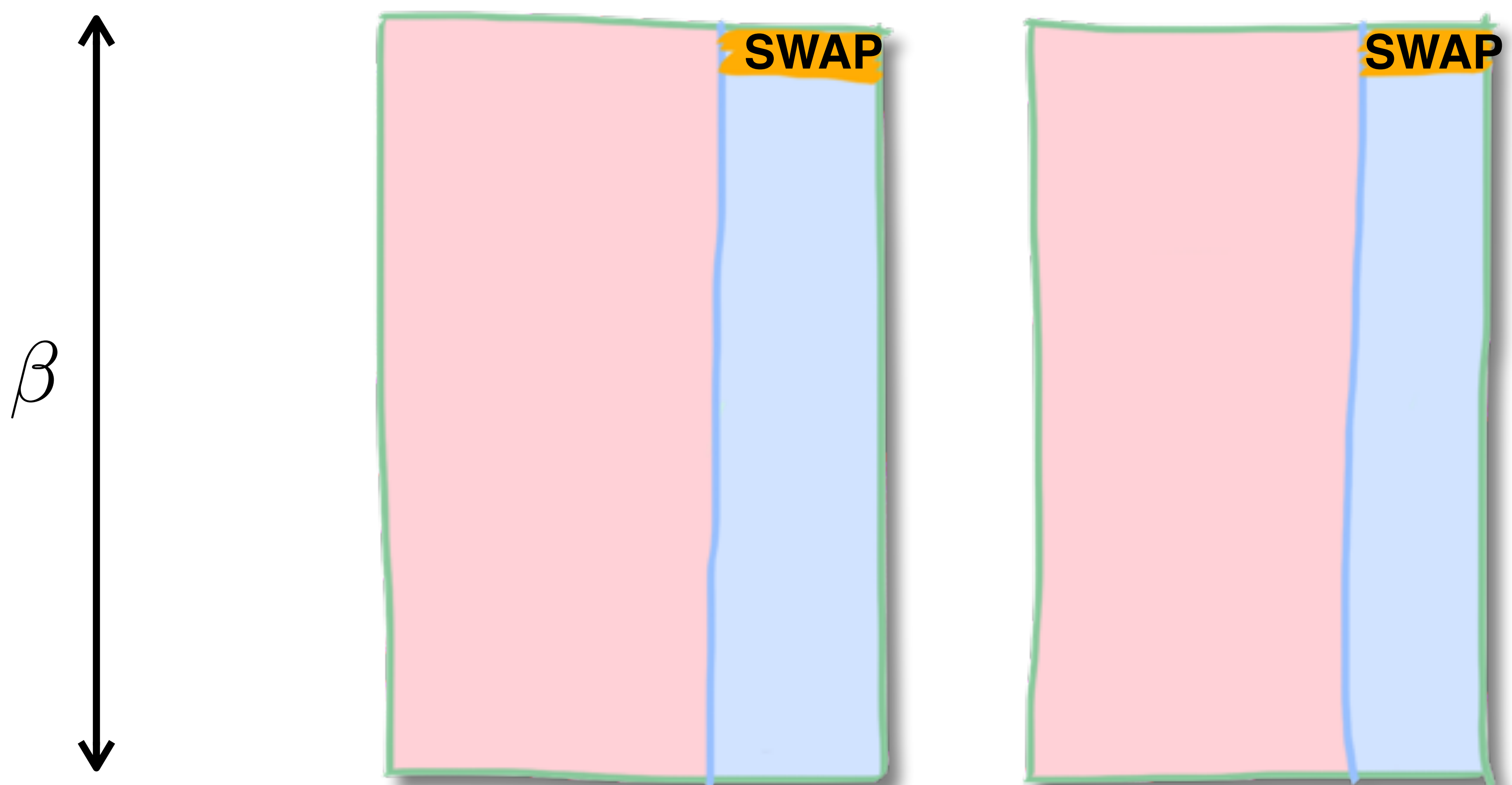
$$Z = \mathrm{Tr}\left[e^{-\beta H}\right] = \sum_{\alpha} \langle \alpha | e^{-\beta H} | \alpha \rangle$$



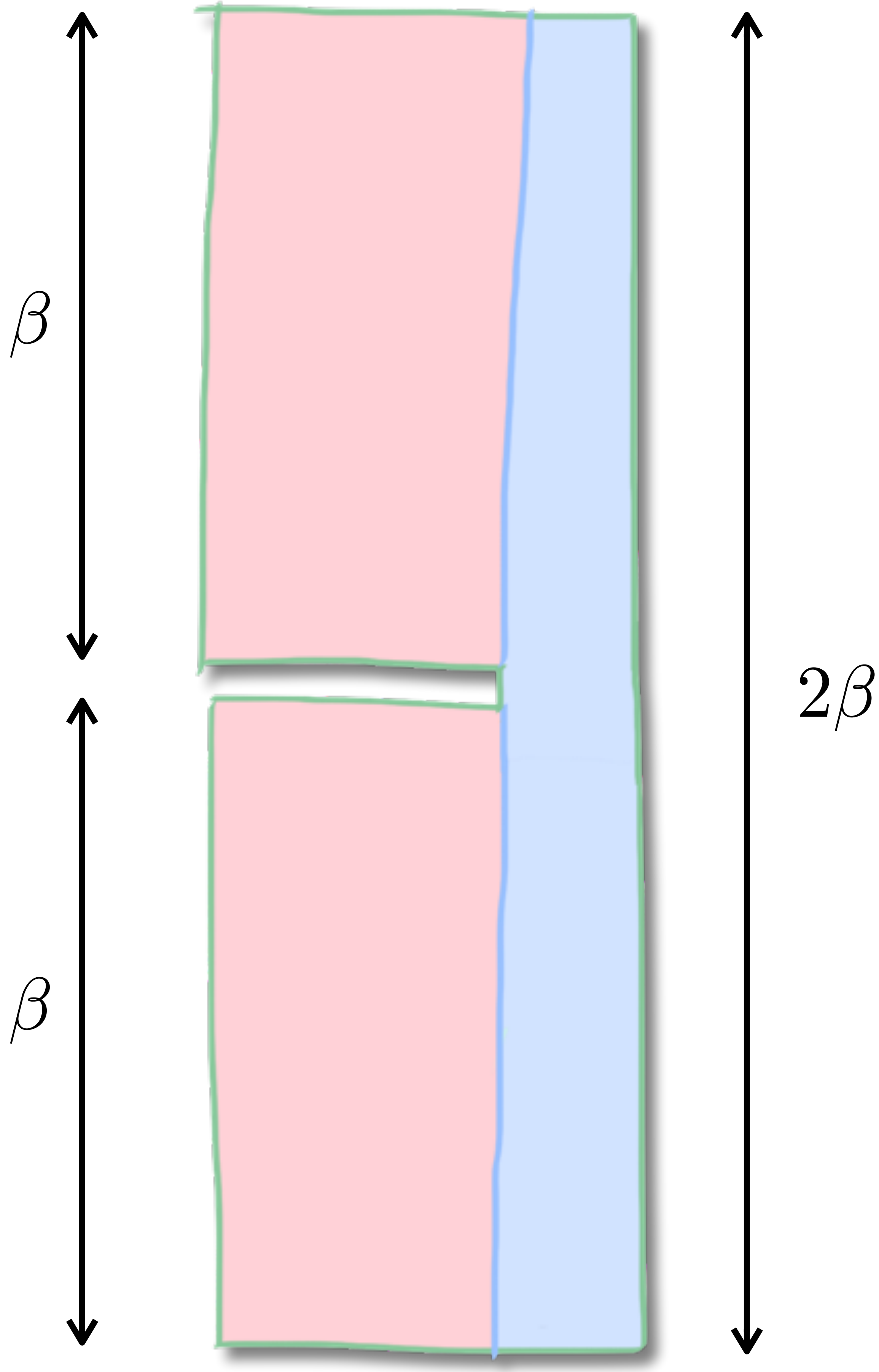
need periodic boundary conditions in imaginary time

Finite-temperature QMC

$$Z = \mathrm{Tr}\left[e^{-\beta H}\right] = \sum_{\alpha} \langle \alpha | e^{-\beta H} | \alpha \rangle$$



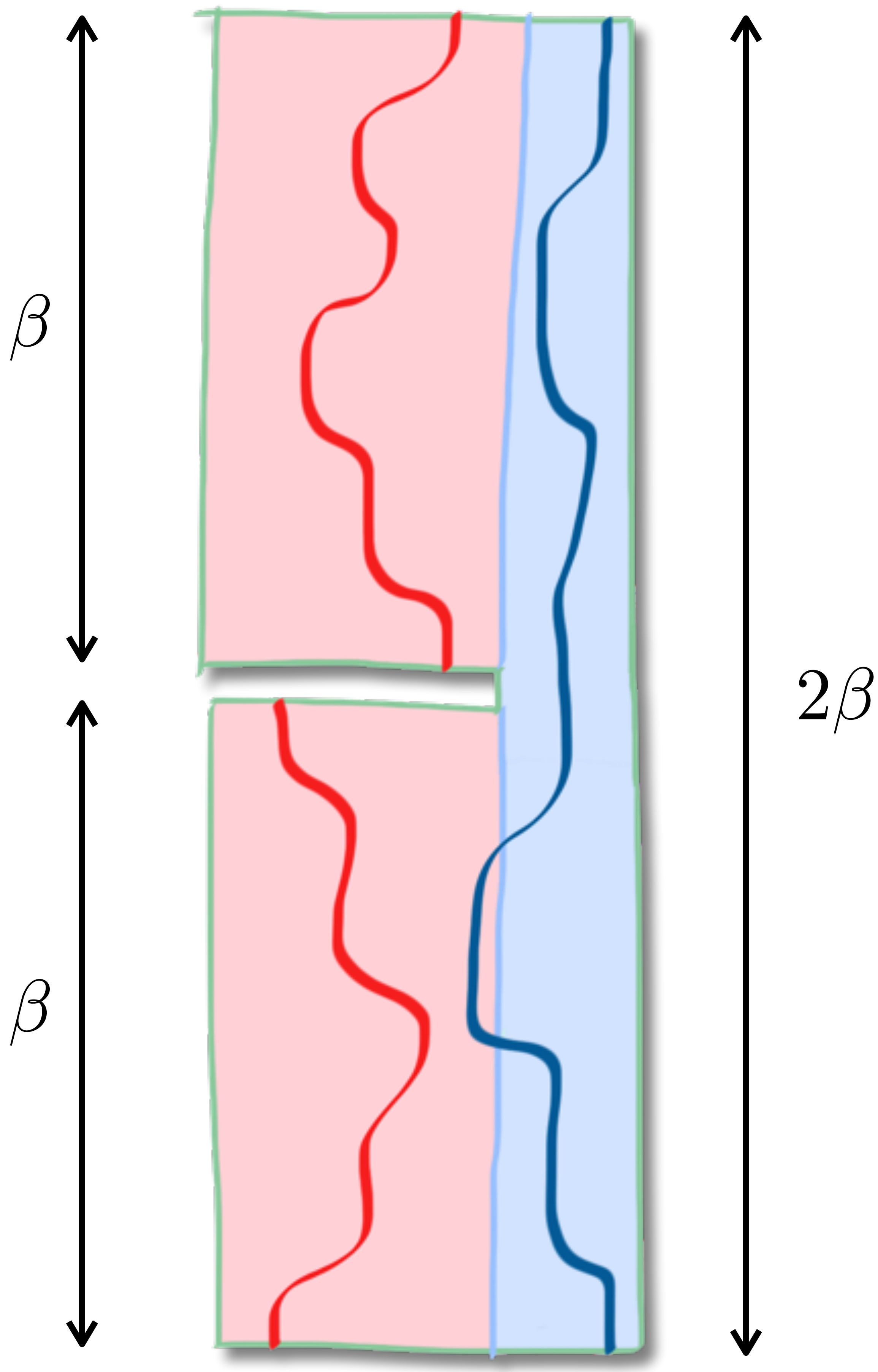
need periodic boundary conditions in imaginary time



Multi-sheeted Riemann surface

$$Z[A,2,T]$$

$$S_2 = -\log \frac{Z[A,2,T]}{Z^2}$$



Multi-sheeted Riemann surface

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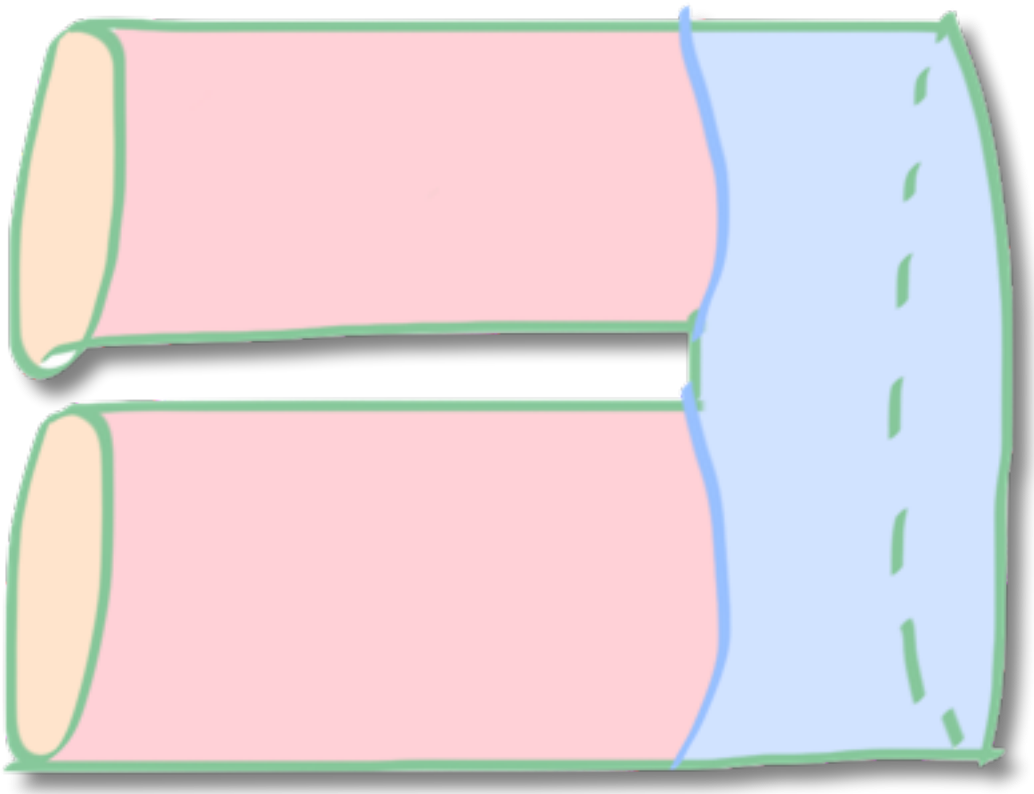


Multi-sheeted Riemann surface

$$Z[A, 2, T]$$

$$S_2 = -\log \frac{Z[A, 2, T]}{Z^2}$$

- Stochastic Series Expansion

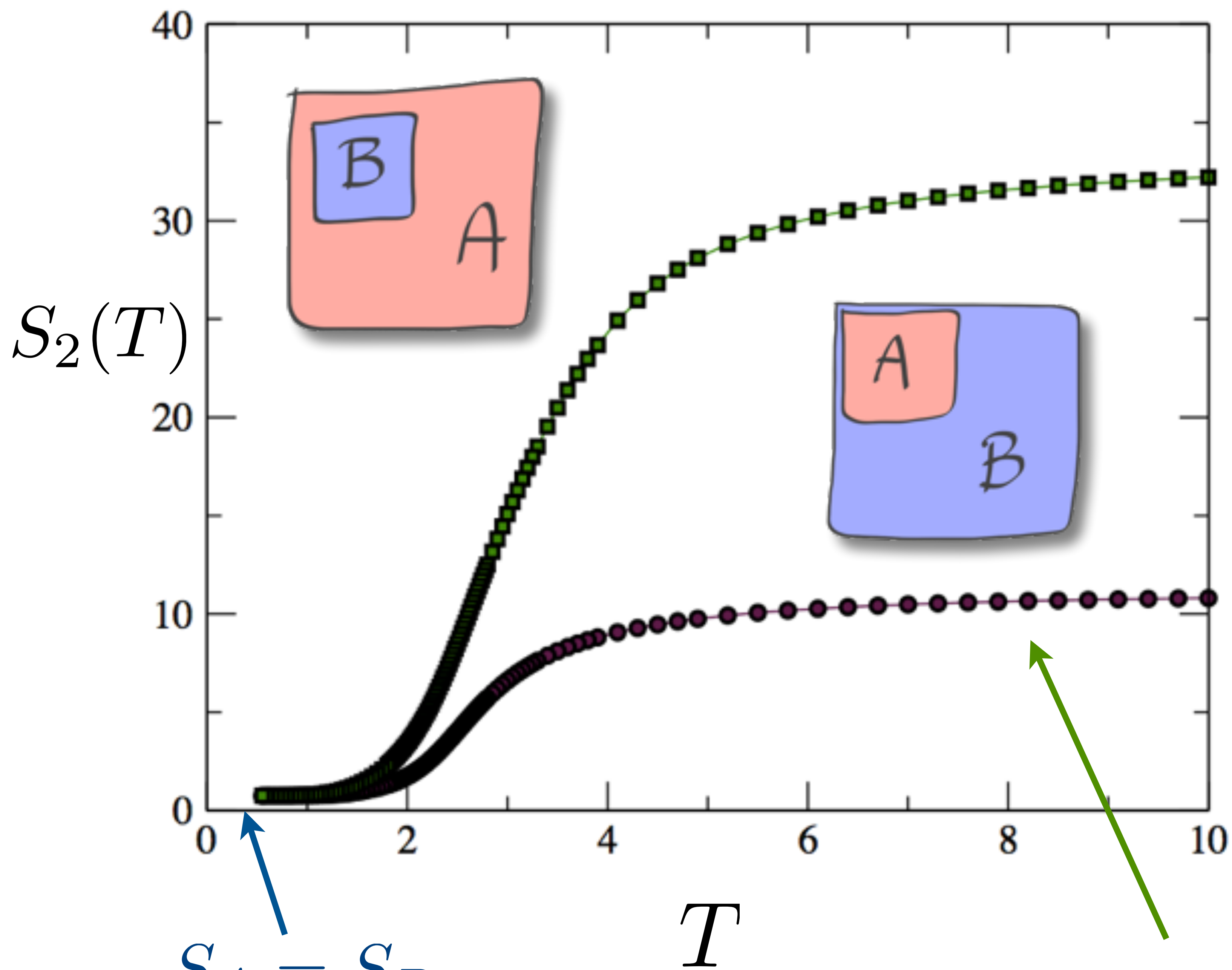
RGM, Kallin, Hastings Phys. Rev. B 82, 100409(R) (2010)

- Path Integral Monte Carlo

Del Maestro: Thursday 1:30pm

Like in the classical case:

$S_n(A) \neq S_n(B)$ in the presence of thermal mixing.



$S_A = S_B$

extensive scaling

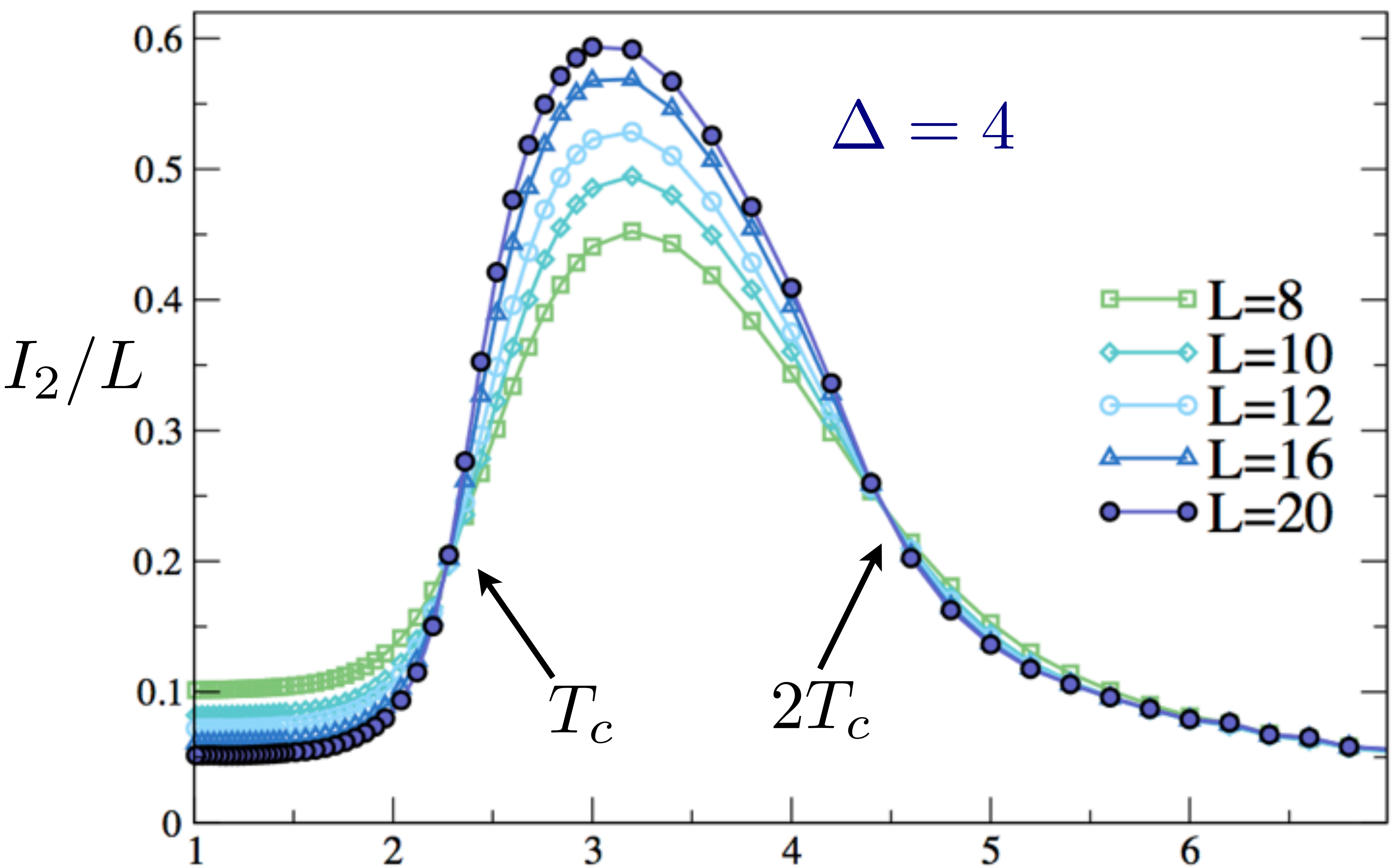
Example: Mutual information of quantum XXZ model

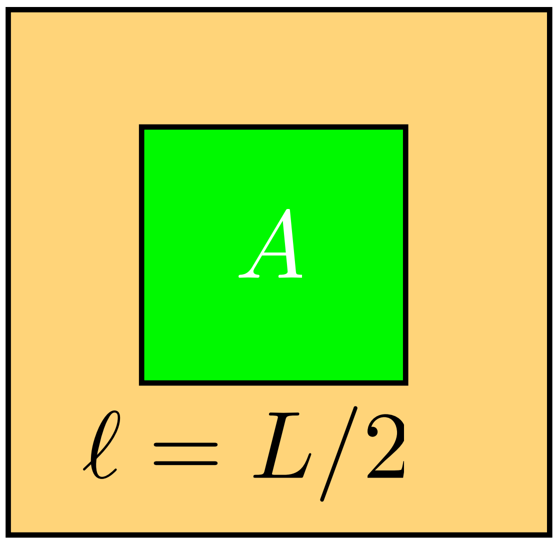
Singh, Hastings, Kallin, RGM, Phys. Rev. Lett. 106, 135701 (2011)

$$I_n(A\!:\!B) = S_n(A) + S_n(B) - S_n(A \cup B)$$

- picks up all correlations (classical and quantum)
- exhibits critical scaling at finite-T phase transitions

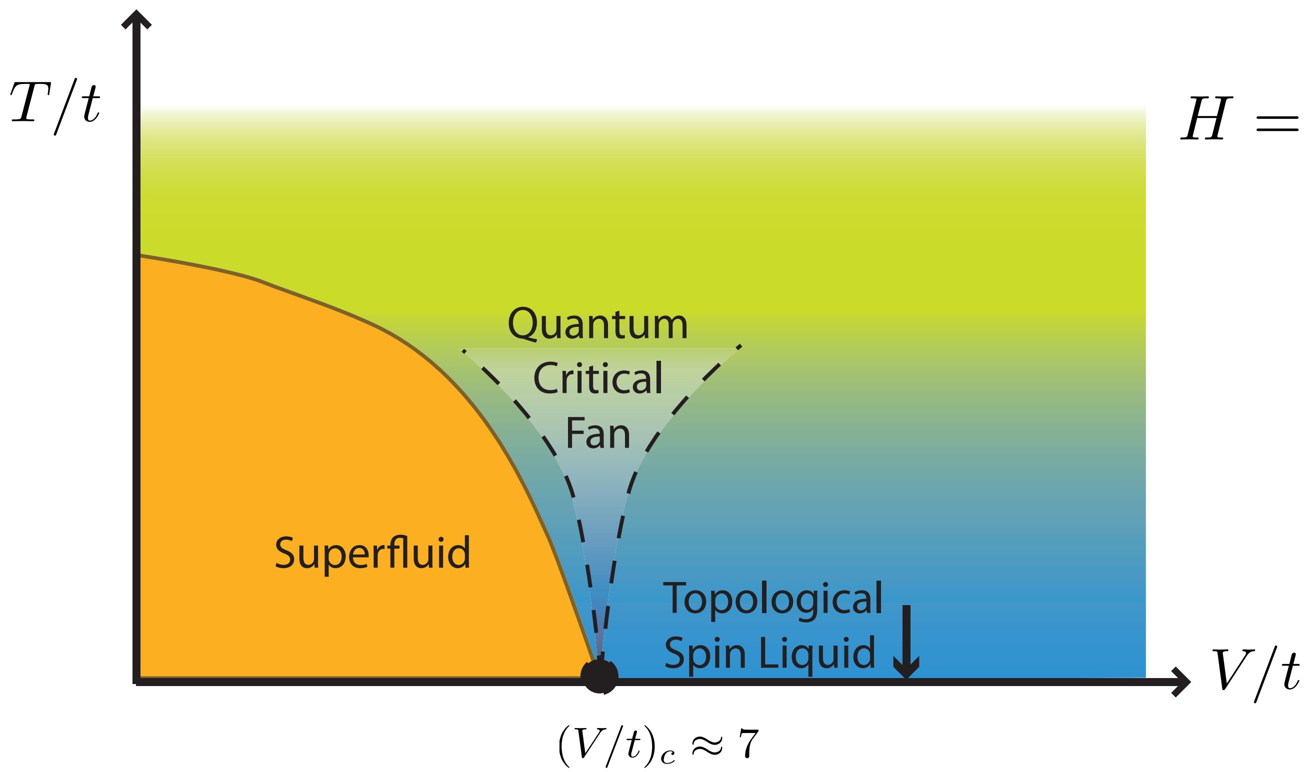
$$H = \sum_{\langle ij \rangle} \left(\Delta S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y \right)$$





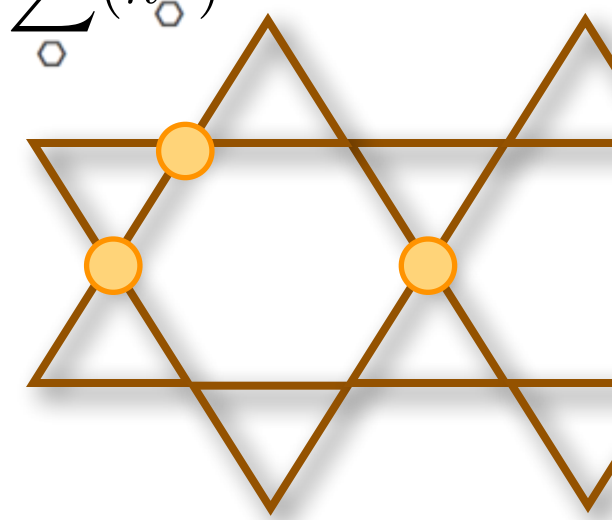
Example: Topological Entanglement Entropy of a Bose–Hubbard Spin Liquid

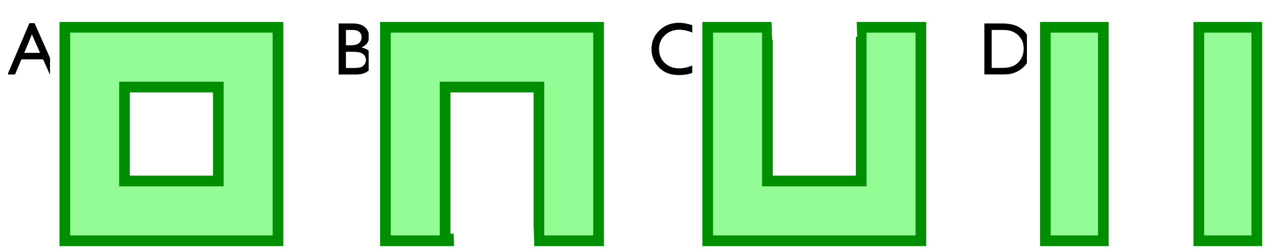
Isakov, Hastings, RGM
Nature Physics 7, 772 (2011)
Science 335, 193 (2012)



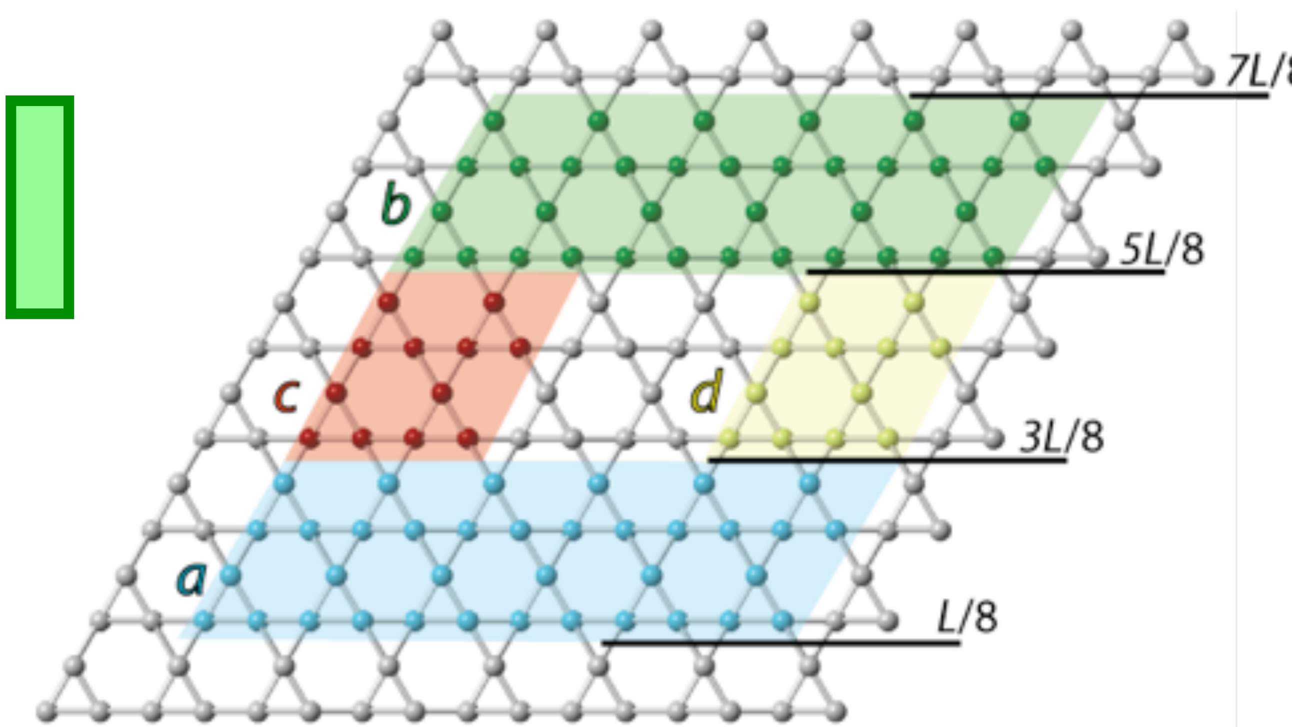
$$H = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + b_i b_j^\dagger) + V \sum_{\hexagon} (n_{\hexagon})^2$$

$$n_{\hexagon} = \sum_{i \in \hexagon} (n_i - 1/2)$$





$$2\gamma = -S_n^A + S_n^B + S_n^C - S_n^D$$



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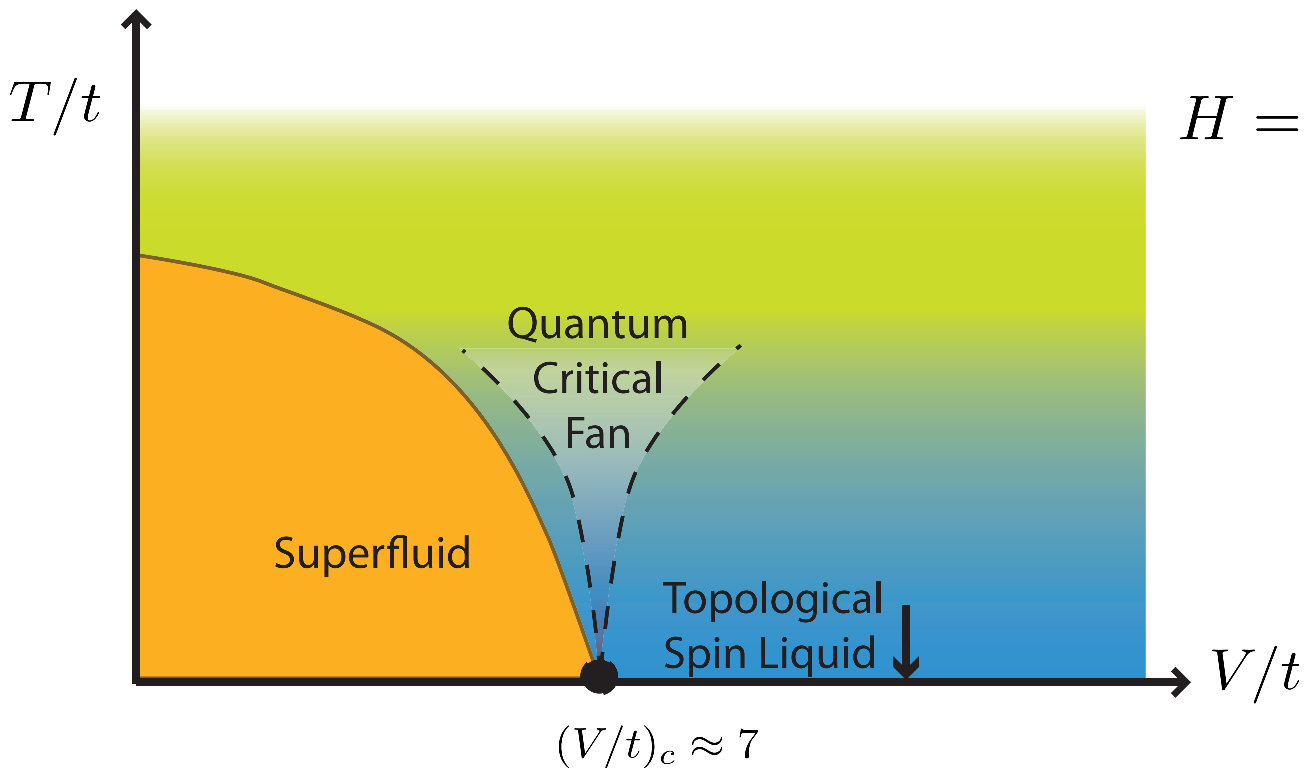

$$H = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + b_i b_j^\dagger) + V \sum_{\hexagon} (n_{\hexagon})^2$$

$$n_{\hexagon} = \sum_{i \in \hexagon} (n_i - 1/2)$$