Entanglement Entropy in Quantum Monte Carlo

Roger Melko

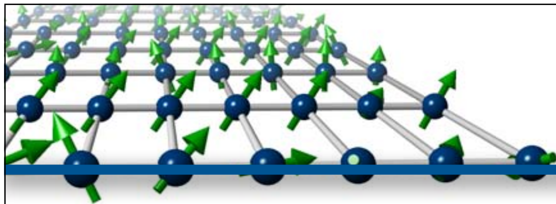
University of Waterloo

NSERC CRSNG

SHARCNET™

Ontario

MINISTRY OF RESEARCH AND INNOVATION



COLLABORATORS

Ann B Kallin

Ivan Gonzalez

CESGA

Matt Hastings

Valence Bond and von Neumann Entanglement Entropy in Heisenberg Ladders
Phys. Rev. Lett., 103, 117203 (2009)

Measuring Renyi Entanglement Entropy with Quantum Monte Carlo
Phys. Rev. Lett. 104, 157201 (2010)

Finite-size scaling of mutual information in Monte Carlo simulations: Application to the spin-1/2 XXZ model
Phys. Rev. B, 82, 180504 (2010)

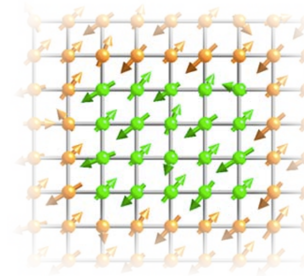
Topological Entanglement Entropy in a Kagome BH Spin Liquid
WORK IN PROGRESS

Sergei Isakov

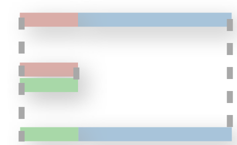
ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Outline

- Renyi Entanglement Entropy as a resource in Condensed Matter Physics

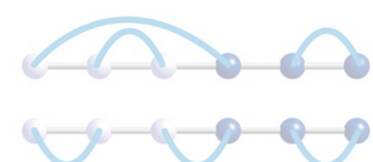


- Finite-Temperature QMC and Mutual Information



- Topological entanglement entropy in a quantum Spin Liquid

- T=0 projector QMC in the Valence Bond Basis



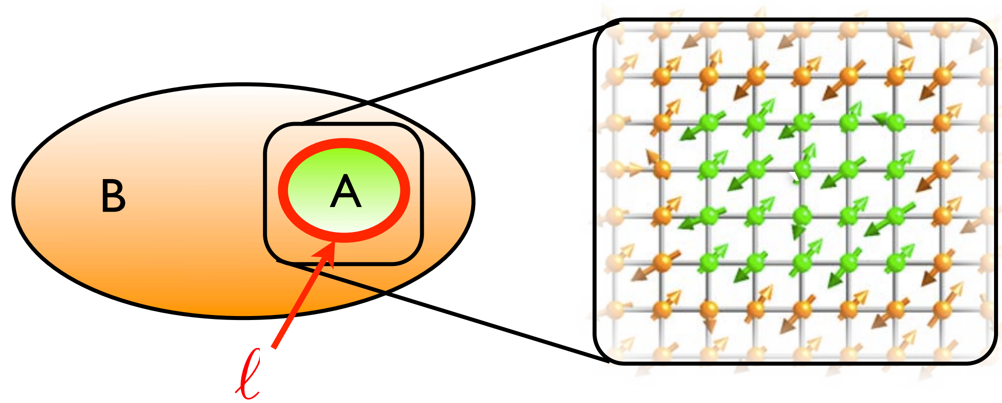
GOAL

Develop an unbiased, scalable numerical simulation procedure (QMC) that is able to measure entanglement entropy in a variety of D≥2 lattice models

von Neumann

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

$$\rho_A = \mathrm{Tr}_B |\psi\rangle\langle\psi|$$



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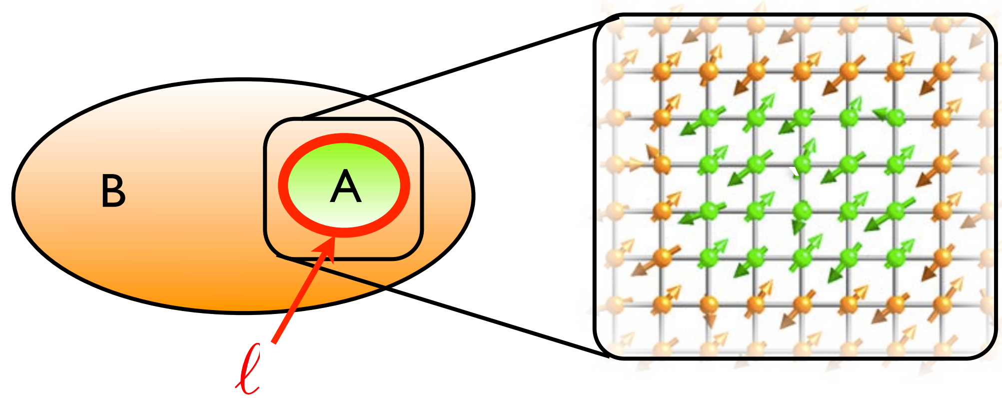
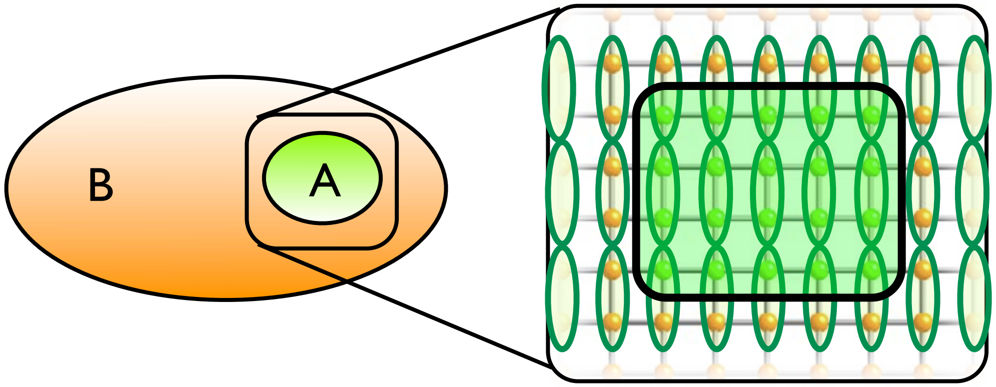
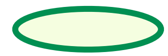


Punchline: you can calculate a variant, called Renyi EE, in both finite-T (SSE) and T=0 (VB basis) quantum Monte Carlo:

- Simulations do not have access to the wavefunction
- The “sign problem” inhibits the simulation of frustrated spins or fermions

Area Law and Corrections



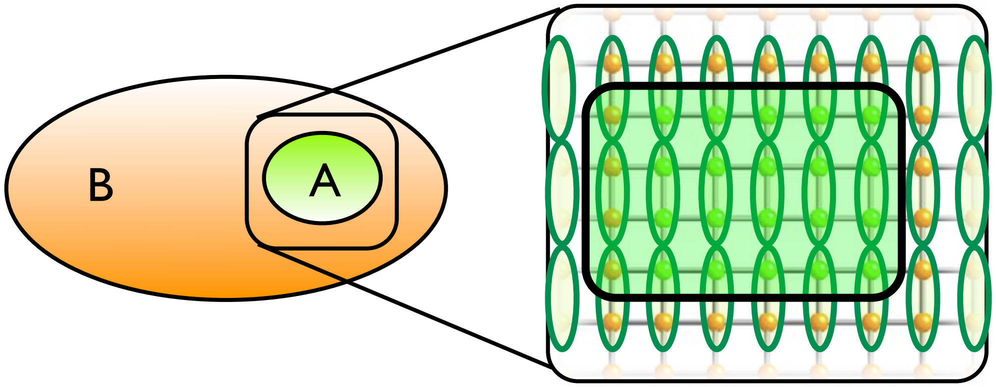
 $= \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$

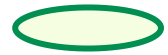
gapped phases

$S_1 = a\ell$ "area" or boundary law

M. Srednicki, Phys. Rev. Lett. 71, 666 (1993)
Eisert, Cramer, Plenio, Rev. Mod. Phys. 82, 277 (2010)

Area Law and Corrections



 $= \frac{1}{\sqrt{2}}$ (|↑↓⟩ - |↓↑⟩)

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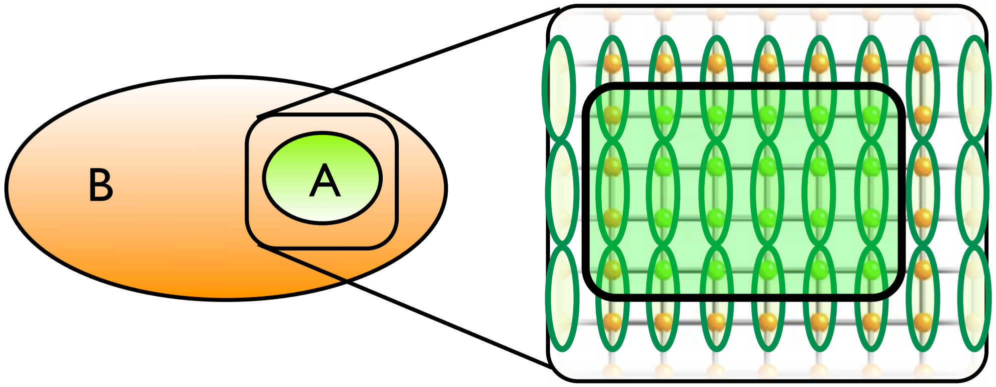
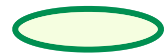
Area Law and Corrections



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

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M. Srednicki, Phys. Rev. Lett. 71, 666 (1993)
Eisert, Cramer, Plenio, Rev. Mod. Phys. 82, 277 (2010)

- Universal quantities at quantum critical points

$$S_1 = a\ell + c\log(\ell)$$

Calabrese and Cardy, J. Stat. Mech. 0406, P002 (2004).
Fradkin and Moore, PRL 97 050404 (2006)
Casini and Huerta, Nuclear Physics B, 764, 183 (2007)

$$S_1 = a\ell + \text{const.}$$

- Identification of topological spin liquids

$$S_1 = a\ell + \gamma^{\text{topo}}$$

Levin and Wen, Phys. Rev. Lett. 96, 110405 (2006)
Kitaev and Preskill Phys. Rev. Lett. 96, 110404 (2006)

Renyi Entropies

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

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

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

Properties

- **Lower bound** $S_n \geq S_m \text{ when } n < m$
- **Expected to possess the same universal properties as vN entropy**

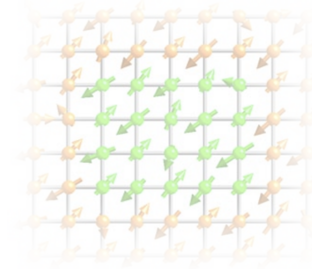
$$S_n = a\ell + c_n \log(\ell) \qquad\qquad S_n = a'\ell + \gamma^{\mathrm{topo}}$$

H. Casini and M. Huerta, Nucl. Phys. B 764, 183 (2007)
M. A. Metlitski, et.al, Phys.Rev. B 80, 115122 (2009)

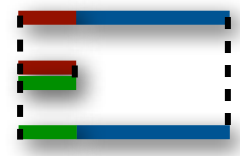
Flammia, Hamma, Huges, Wen, Phys. Rev. Lett. 103, 261601 (2009)

Outline

- Renyi Entanglement Entropy as a resource in Condensed Matter Physics

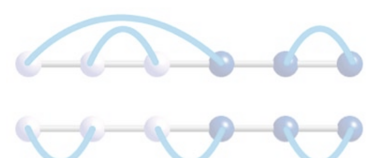


- **Finite-Temperature QMC and Mutual Information**



- Topological entanglement entropy in a quantum Spin Liquid

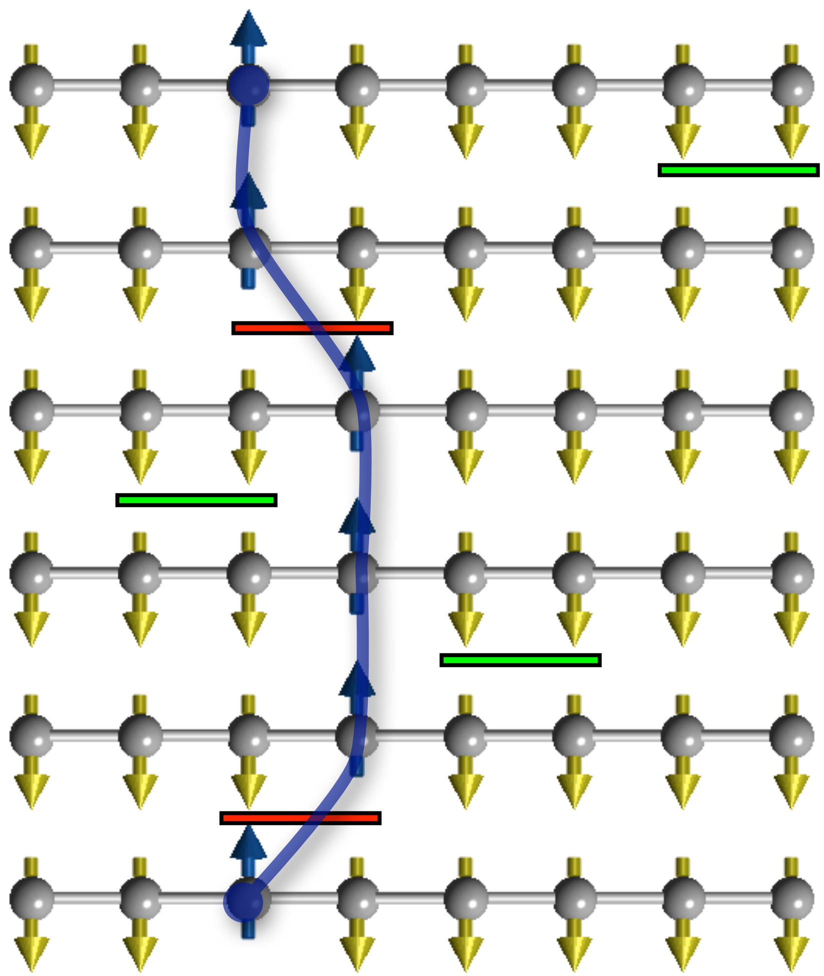
- T=0 projector QMC in the Valence Bond Basis



Stochastic Series Expansion

Sandvik

$$Z = \sum_{\alpha} \langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle \;= \sum_{\alpha} \sum_{n} \frac{(-\beta)^n}{n!} \langle \alpha | H^n | \alpha \rangle \;= \sum_{\alpha} \sum_{n} \sum_{S_n} \frac{(-\beta)^n}{n!} \langle \alpha | \prod_{i=1}^{n} H_{b_i} | \alpha \rangle$$



H_{b_i}

(green bar) $= S_i^z S_j^z$

(red bar) $= (S_i^+ S_j^- + S_i^- S_j^+)$

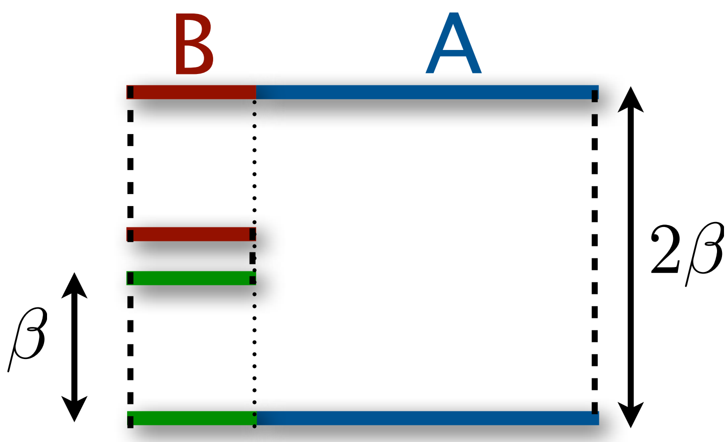
- Spin and Boson models
- Scales as N and β

Replica Trick

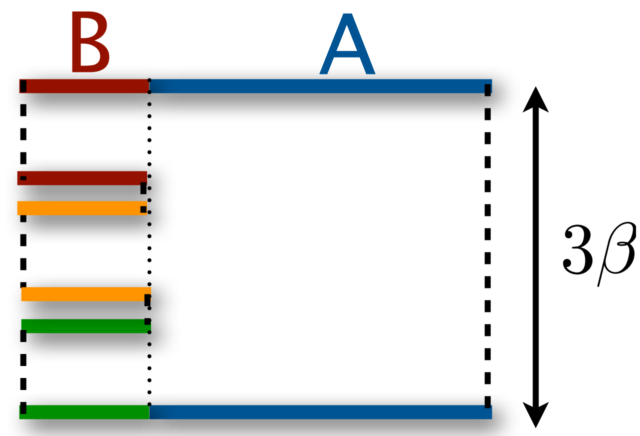
Calabrese and Cardy, J. Stat. Mech. 0406, P002 (2004).
Nakagawa, Nakamura, Motoki, and Zaharov, arXiv:0911.2596
Buividovich and Polikarpov, Nucl. Phys. B, 802, 458 (2008)
M. A. Metlitski, et.al, Phys.Rev. B 80, 115122 (2009).

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

where $Z[A,n,T]$ is the partition function of the systems having special topology - the n-sheeted Riemann surface.

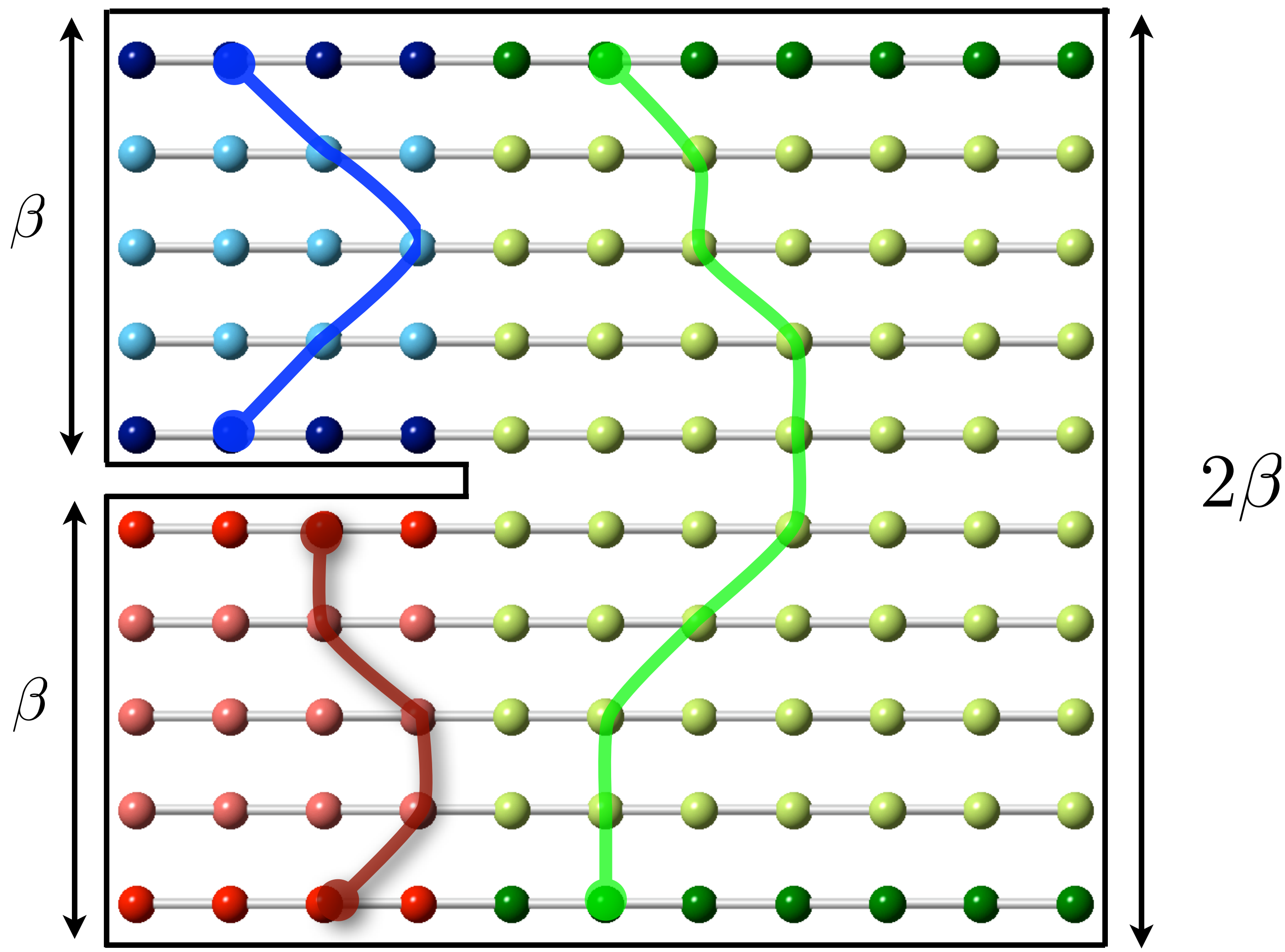


$Z[A,2,T]$



$Z[A,3,T]$

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



Thermodynamic Integration

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

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

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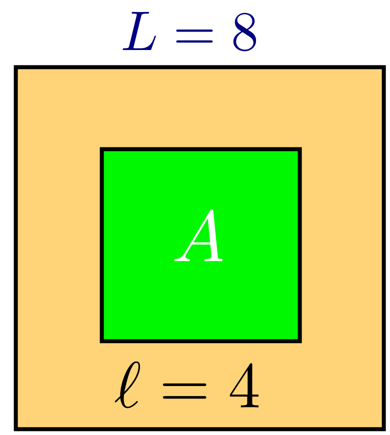
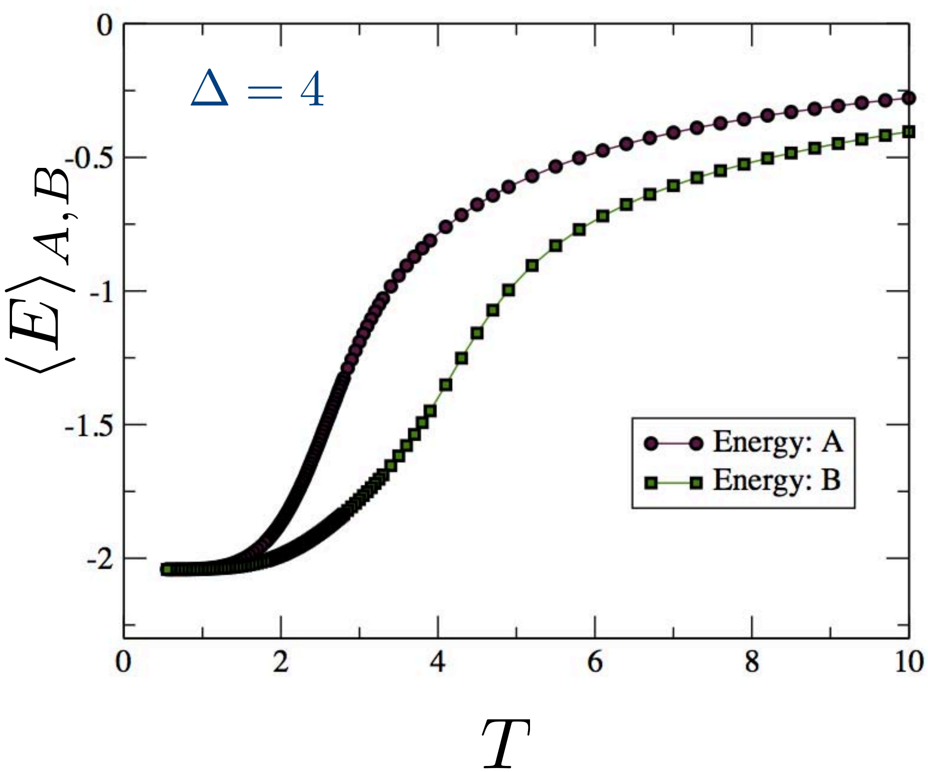
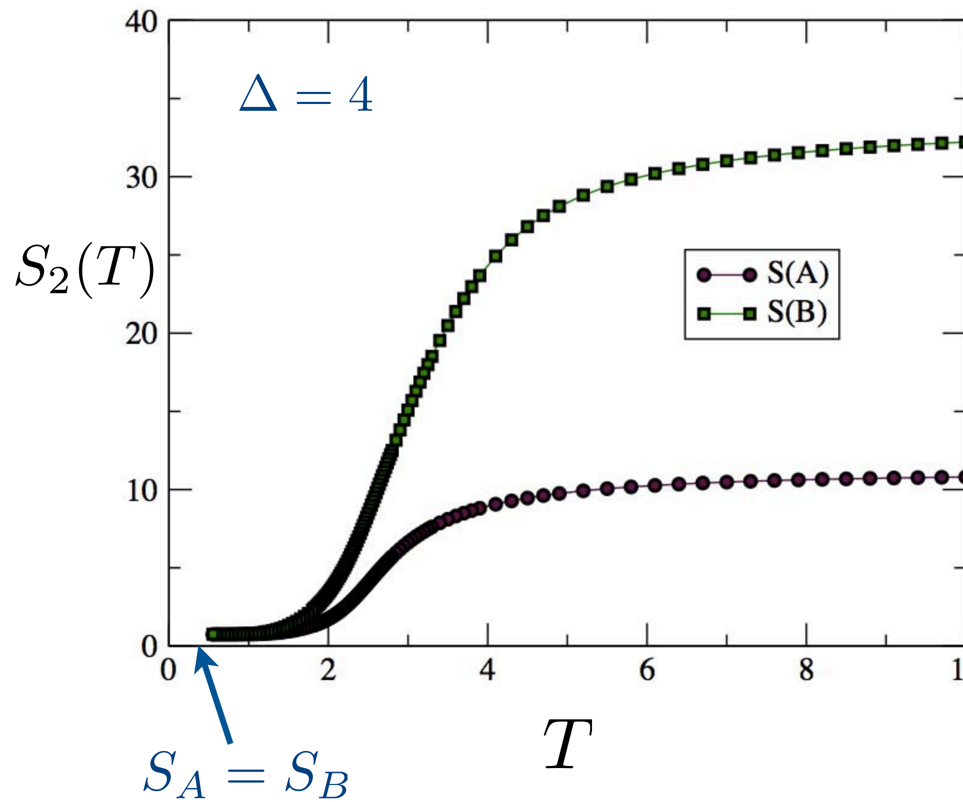


XXZ model $H = \sum_{\langle ij \rangle} \left(\Delta S_i^z S_j^z + S_i^x S_j^x + S_i^y S_j^y \right)$



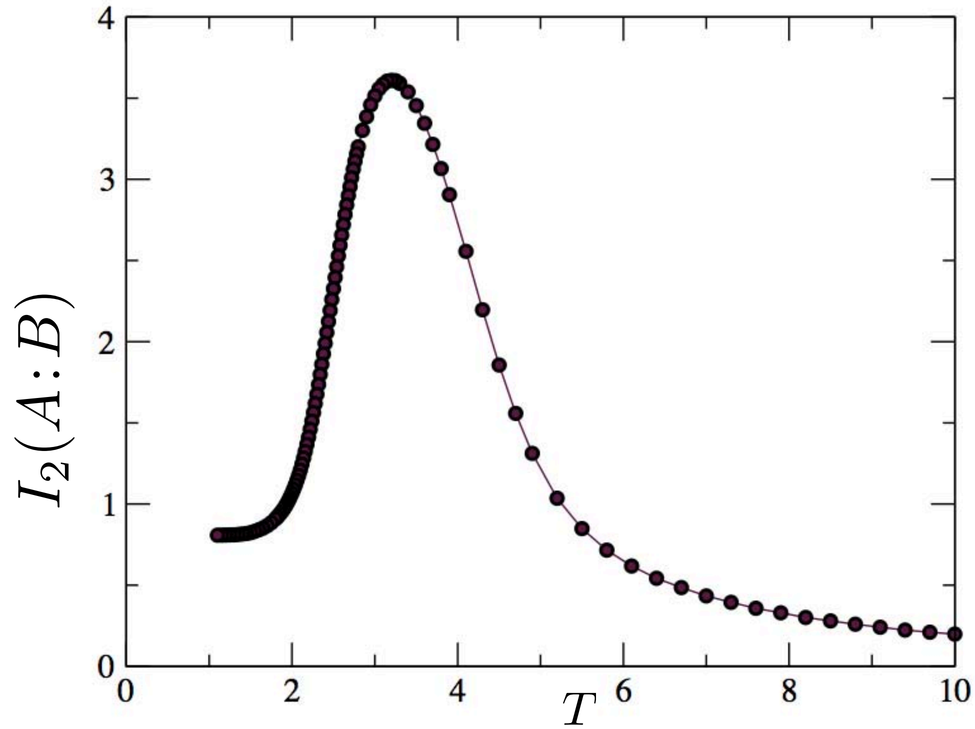


Mutual Information

Swingle, arXiv:1010.4038
Wolf et al. PRL 100, 070502 (2008)

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

$$\frac{1}{1-n} \ln \frac{Z(n\beta)}{Z(\beta)^n}$$



- Coincides with the entanglement entropy at zero temperature

$$T = 0 \qquad I_n(A:B) = 2S_n(A) = 2S_n(B)$$

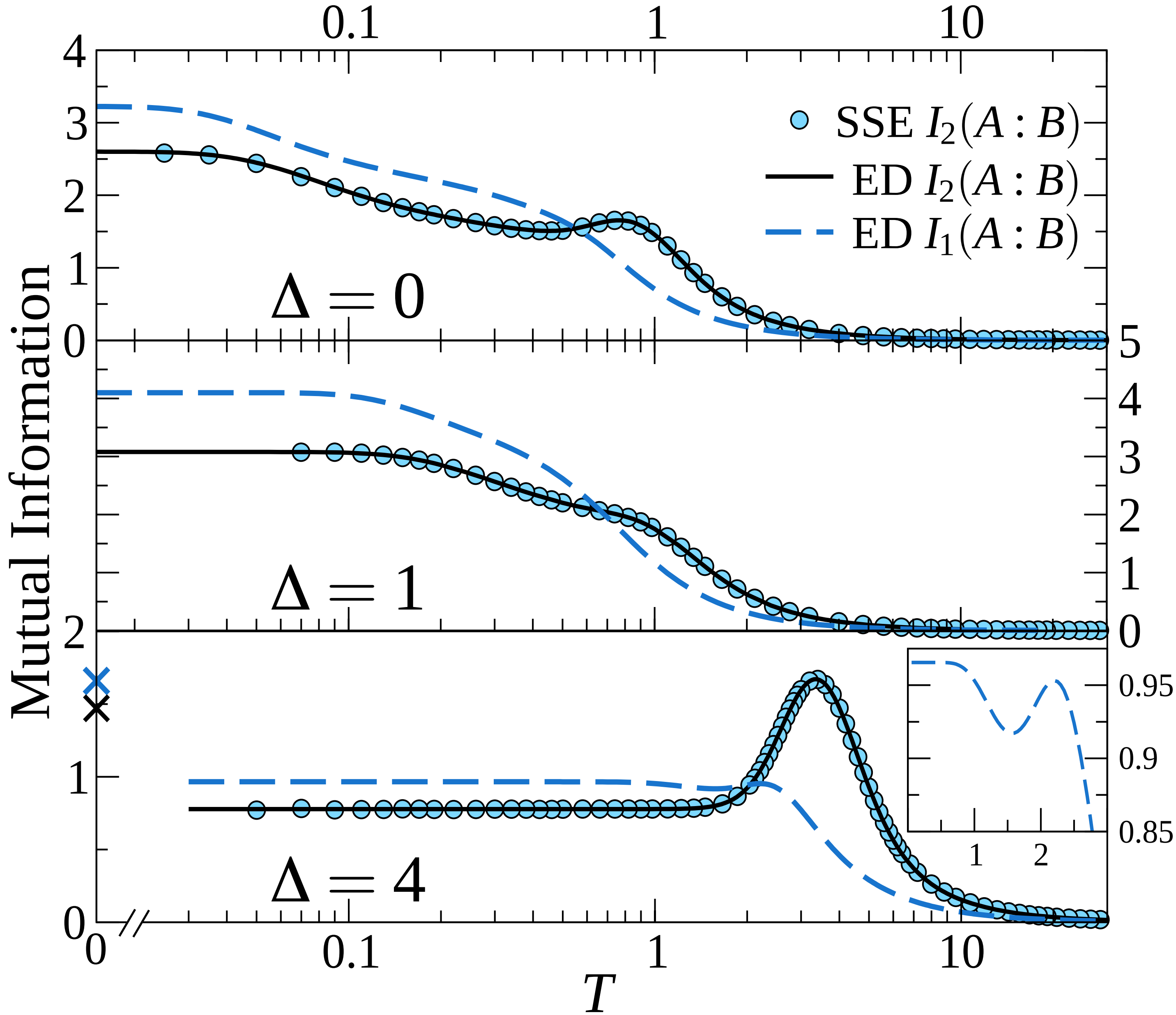
- Will give area-law scaling at finite-temperature
- Measures the total amount of correlation between two systems

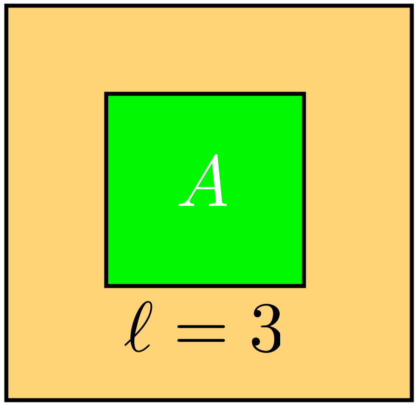
2D XXZ model: 4x4 lattice

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

$L = 4$

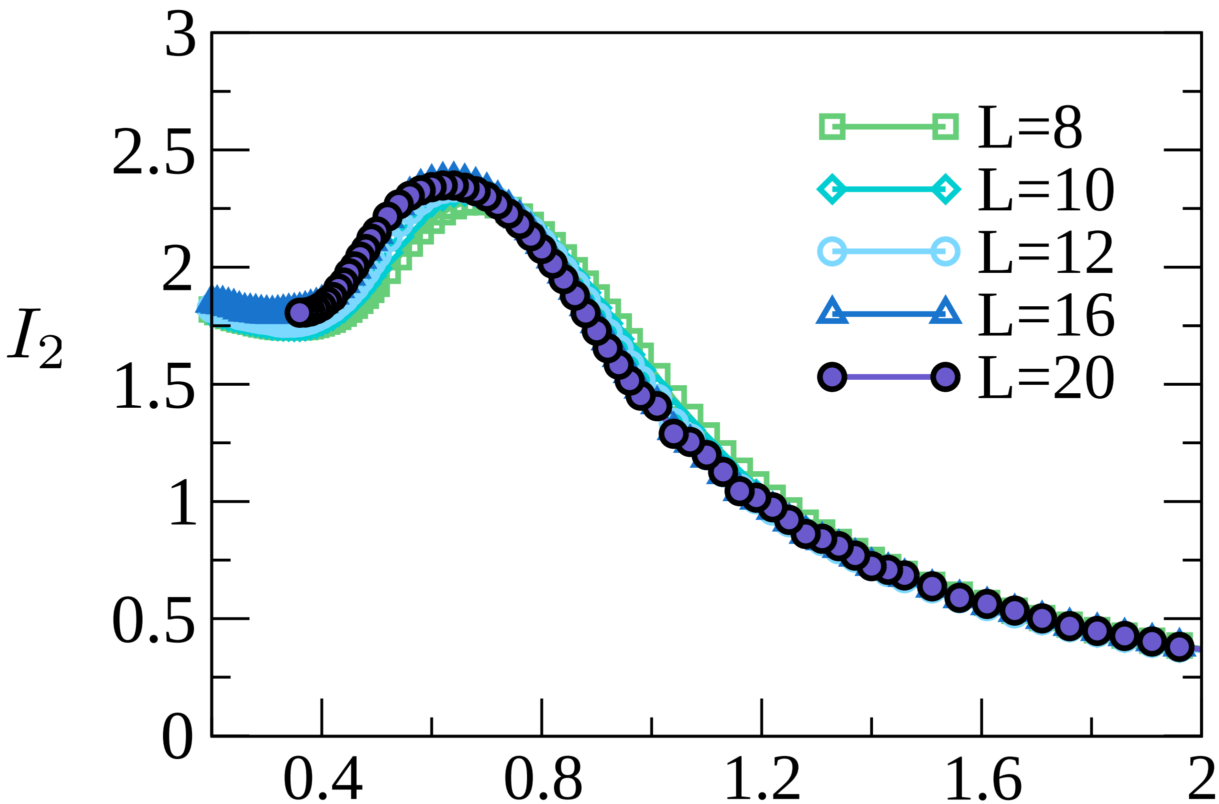
$\ell = 3$



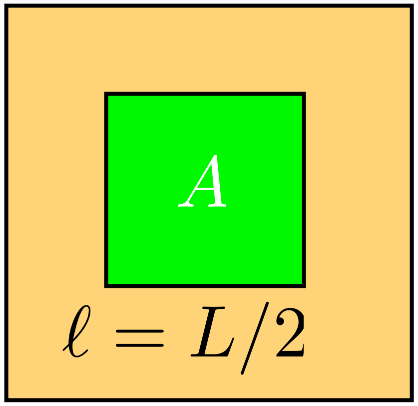


XY model

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



Finite-Size Scaling 2



XXZ model

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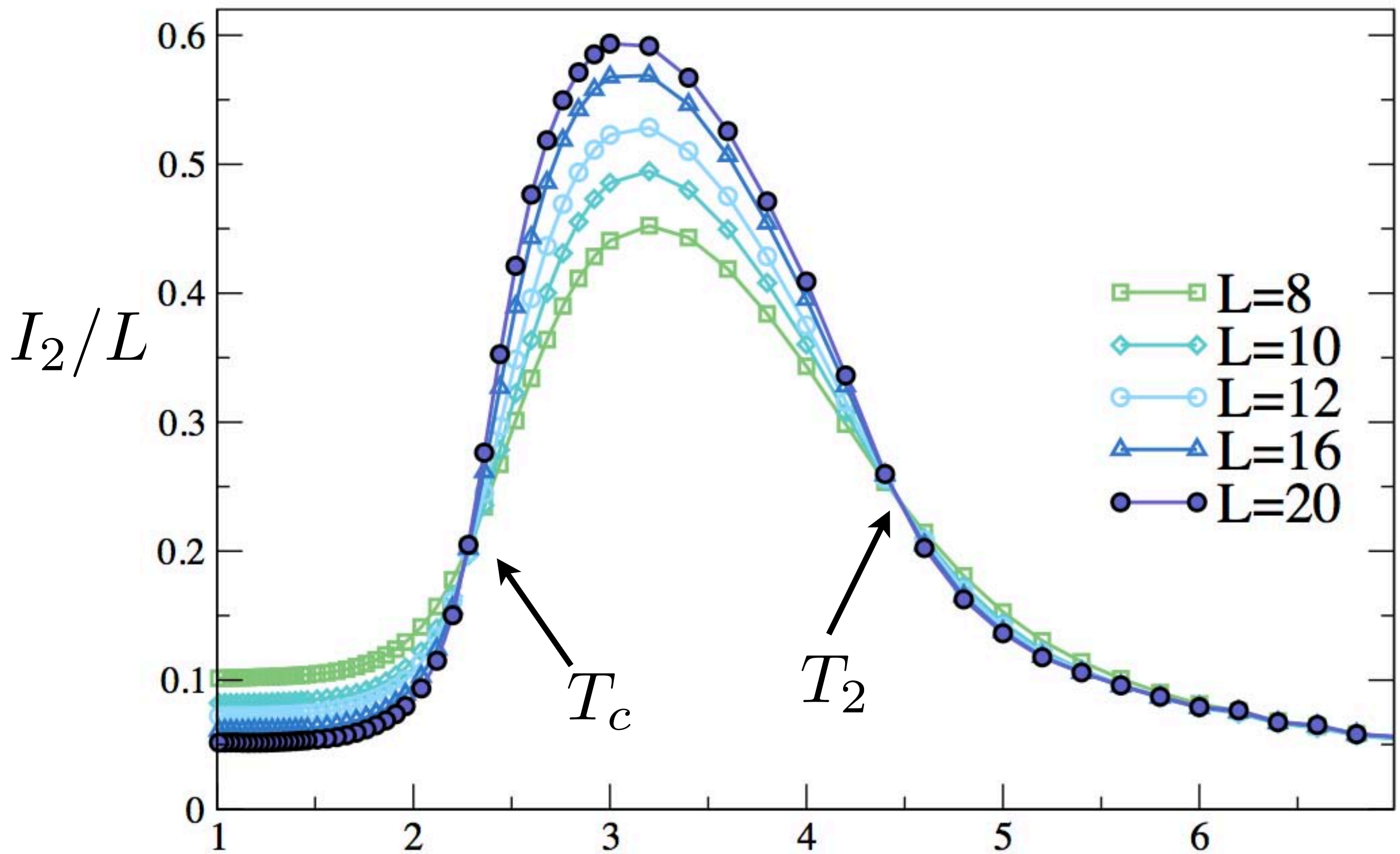


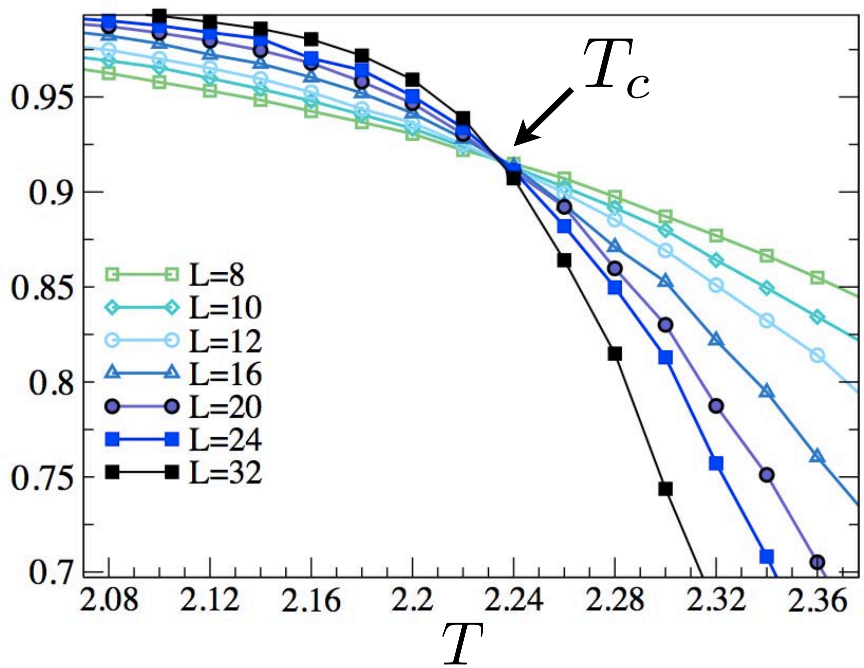
$\Delta = 4$

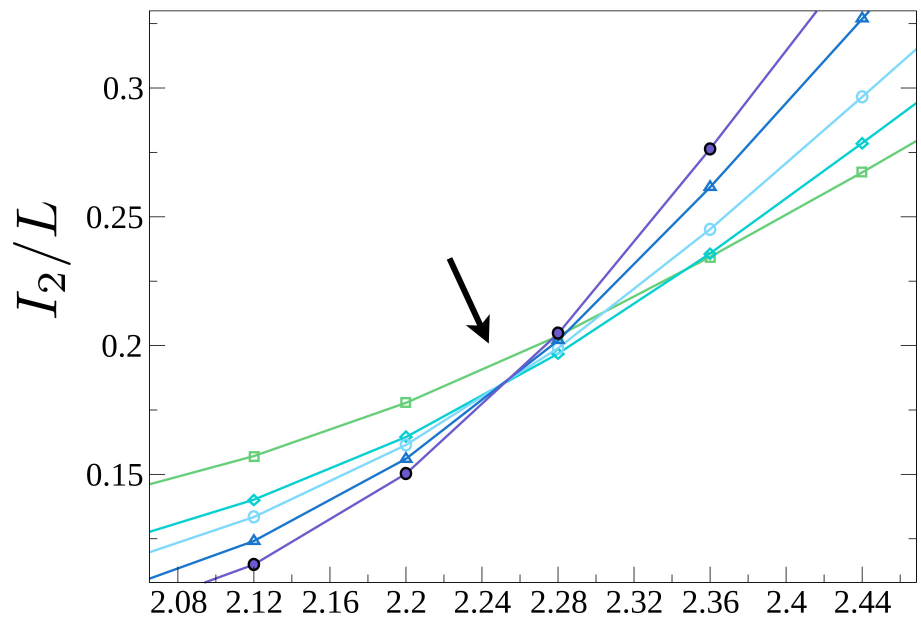
Correlating MI and Tc

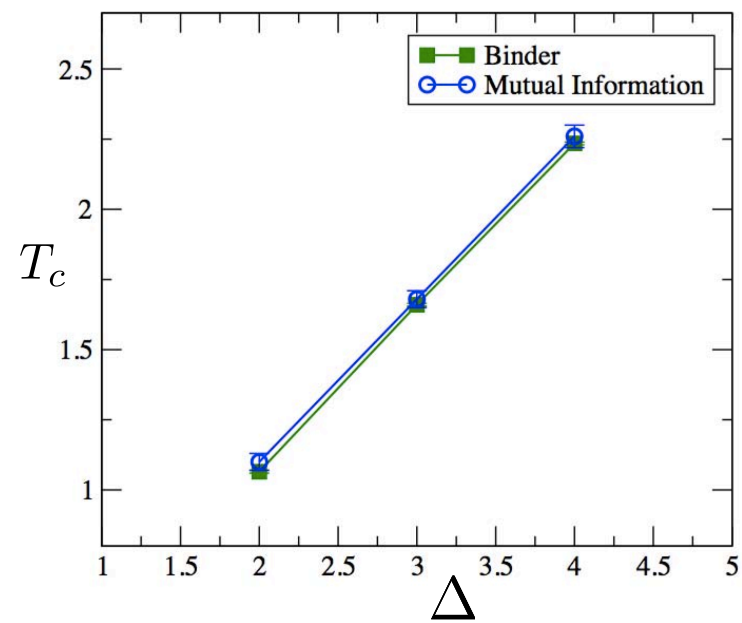
$$\Delta = 4$$

Binder Cumulant

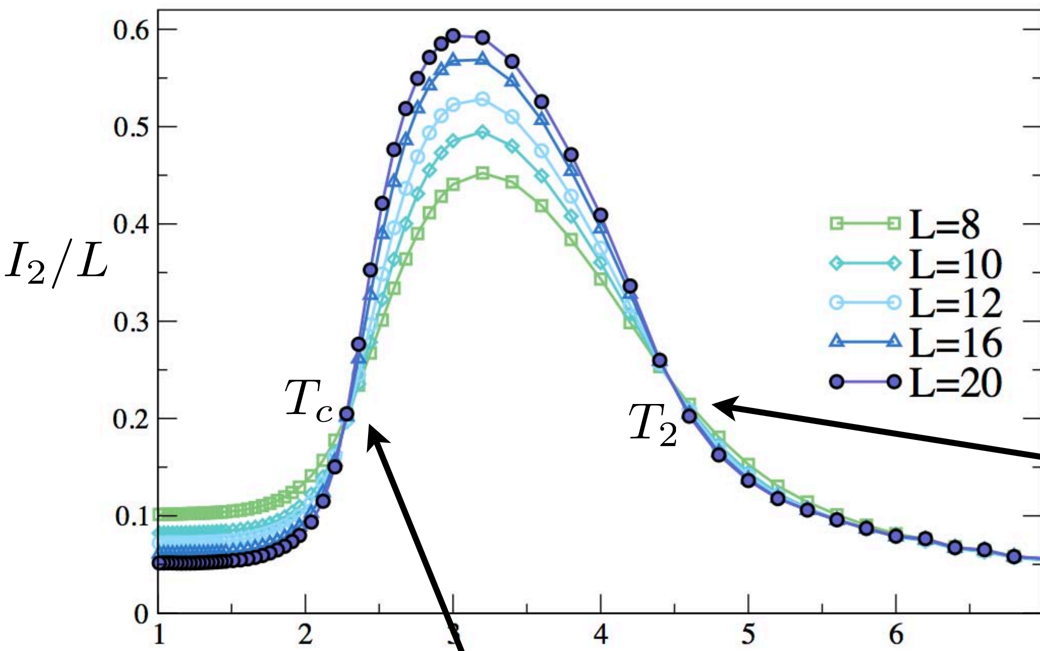
$$U_4 = \frac{3}{2}\left(1 - \frac{1}{3}\frac{\langle m_s^4\rangle}{\langle m_s^2\rangle^2}\right)$$







Source of Crossing?



$$I_2(A{:}B) = Lf(T) + g(T) + \ldots$$

$$I_2(A{:}B) = Lf(T) + L^{\kappa} k((T - T_c)^{\nu} L) + g(T) + \ldots$$

$0 < \kappa < 1$

L^{κ} dominates $g(T)$

crossing determined by some unknown
universal properties?

Outline

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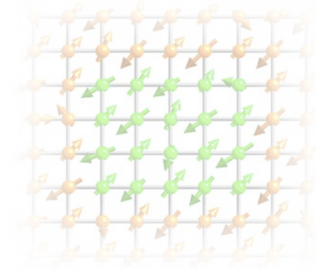

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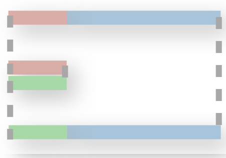
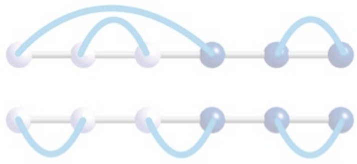


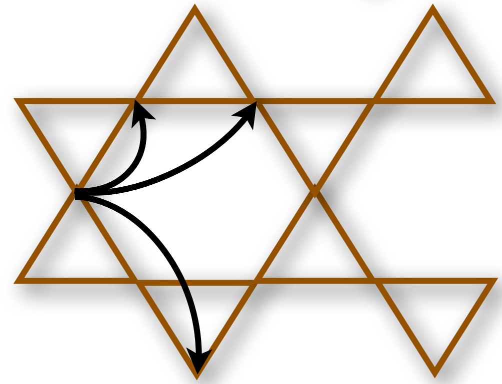
- **Topological entanglement entropy in a quantum Spin Liquid**

- T=0 projector QMC in the Valence Bond Basis



Kagome Bose-Hubbard Spin Liquid

L. Balents, M. P. A. Fisher, and S. M. Girvin,
Phys. Rev. B **65**, 224412 (2002).



Spin-Liquid Phase in a Spin-1/2 Quantum Magnet on the Kagome Lattice

Phys. Rev. Lett. 97, 207204 (2006)
S. V. Isakov, Yong Baek Kim, and A. Paramekanti

$$H_b = -t \sum_{(i,j)} (b_i^\dagger b_j + \mathrm{H.c.}) + V \sum_{\hexagon} (n_{\hexagon})^2 - \mu \sum_i n_i$$

Kagome Bose-Hubbard Spin Liquid

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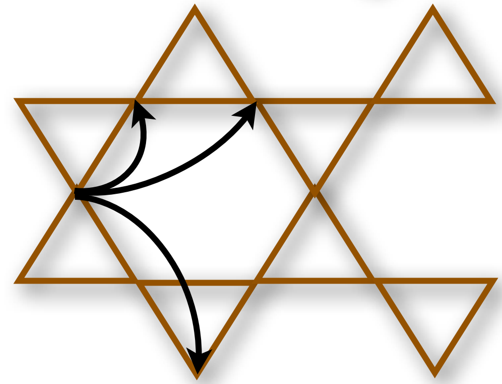

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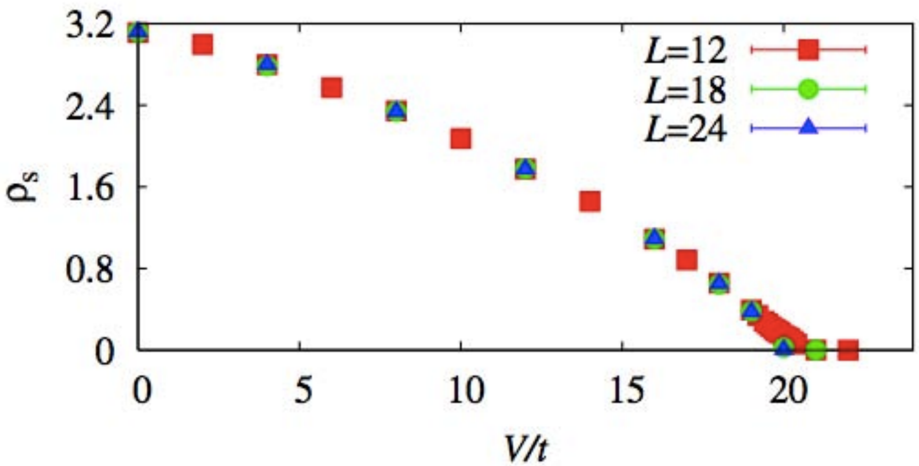
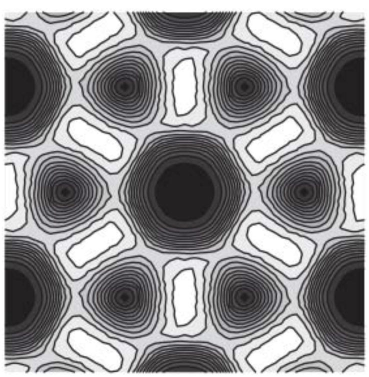
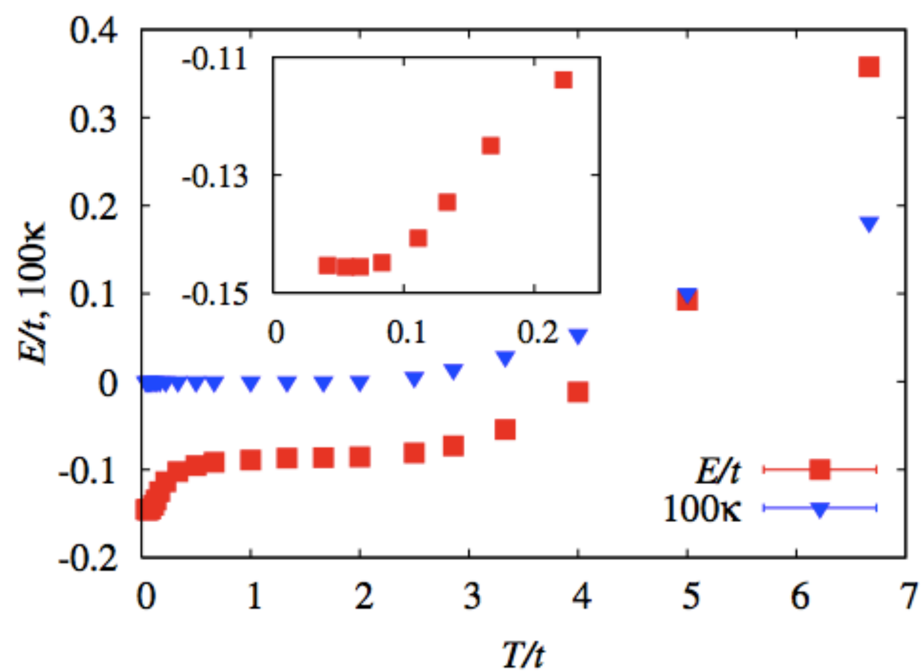
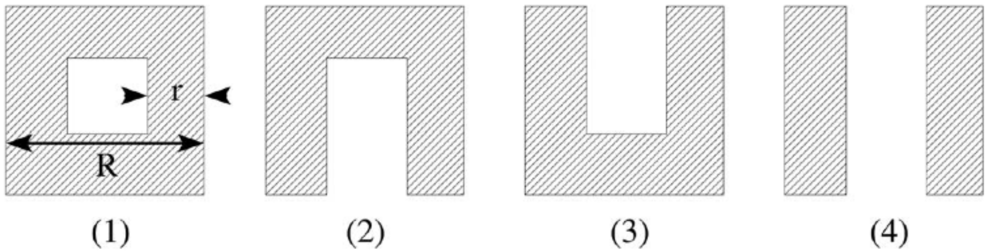




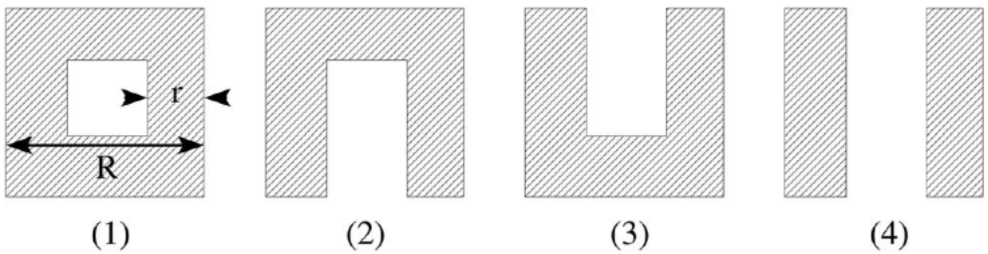


Topological Entanglement Entropy



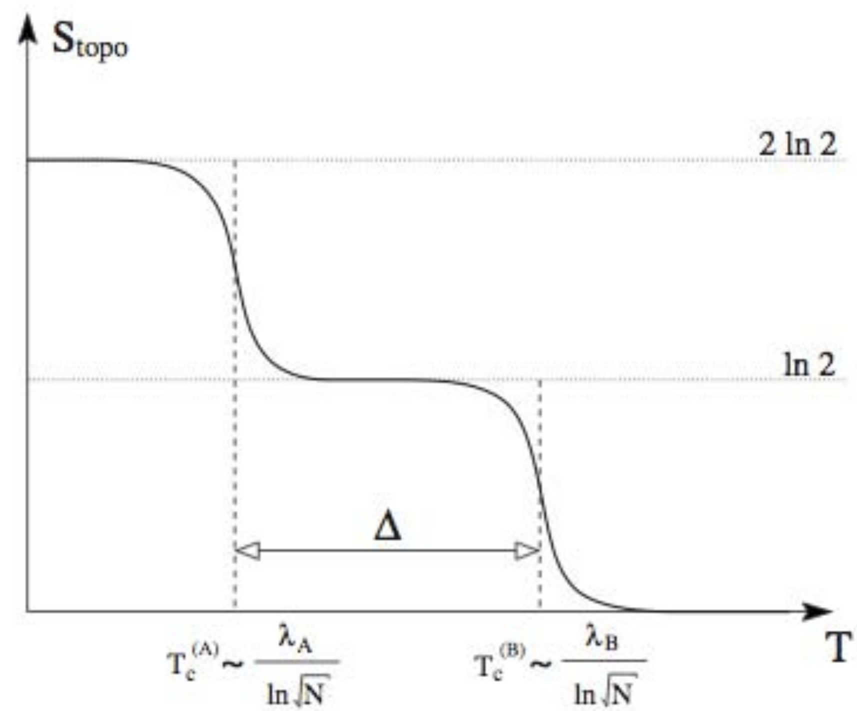
$$S_{\text{topo}} = \lim_{r,R\to\infty} [- S_{\text{VN}}^{1\mathcal{A}} + S_{\text{VN}}^{2\mathcal{A}} + S_{\text{VN}}^{3\mathcal{A}} - S_{\text{VN}}^{4\mathcal{A}}]$$

Topological Entanglement Entropy



finite-size systems retain a statistical contribution to the topological EE

$$S_{\text{topo}} = \lim_{r,R\to\infty} [-S_{\text{VN}}^{1\mathcal{A}} + S_{\text{VN}}^{2\mathcal{A}} + S_{\text{VN}}^{3\mathcal{A}} - S_{\text{VN}}^{4\mathcal{A}}]$$

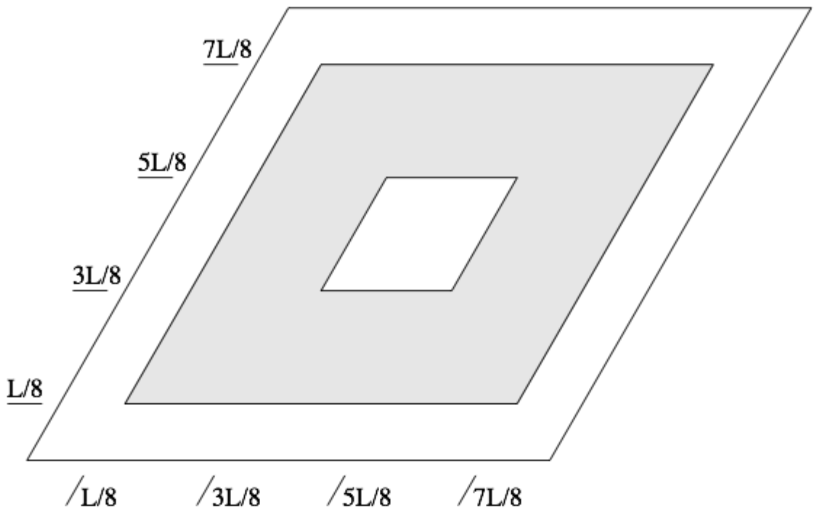


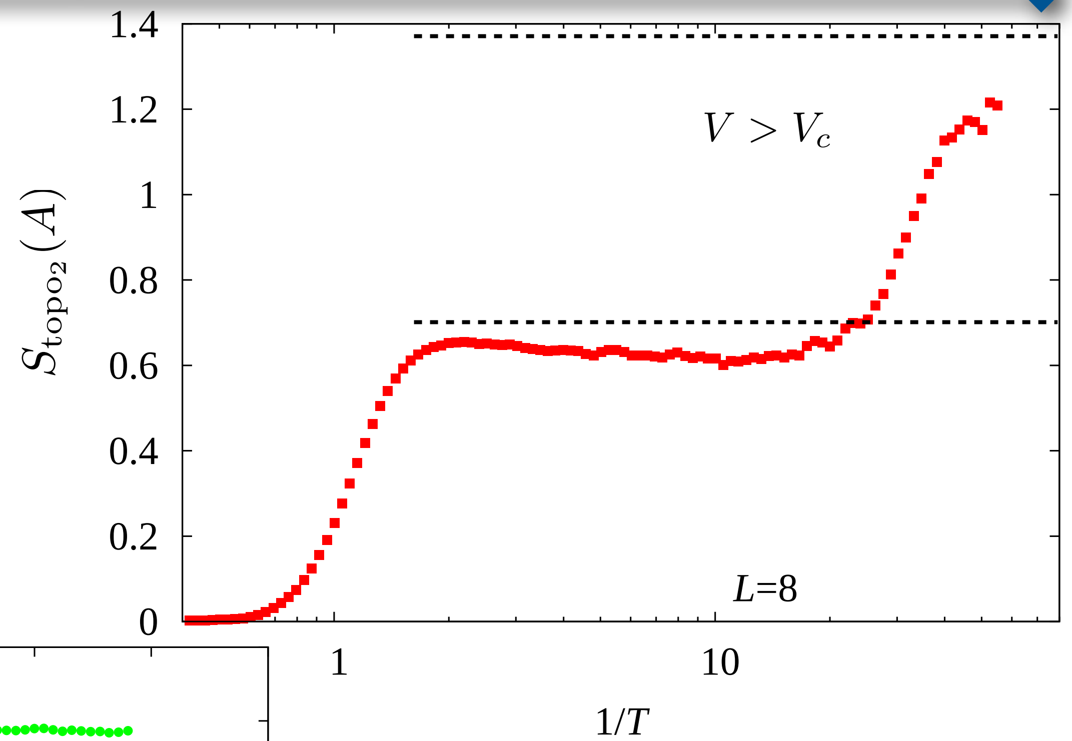
$$H = -\lambda_B \sum_{\text{plaquettes } p} B_p - \lambda_A \sum_{\text{stars } s} A_s$$

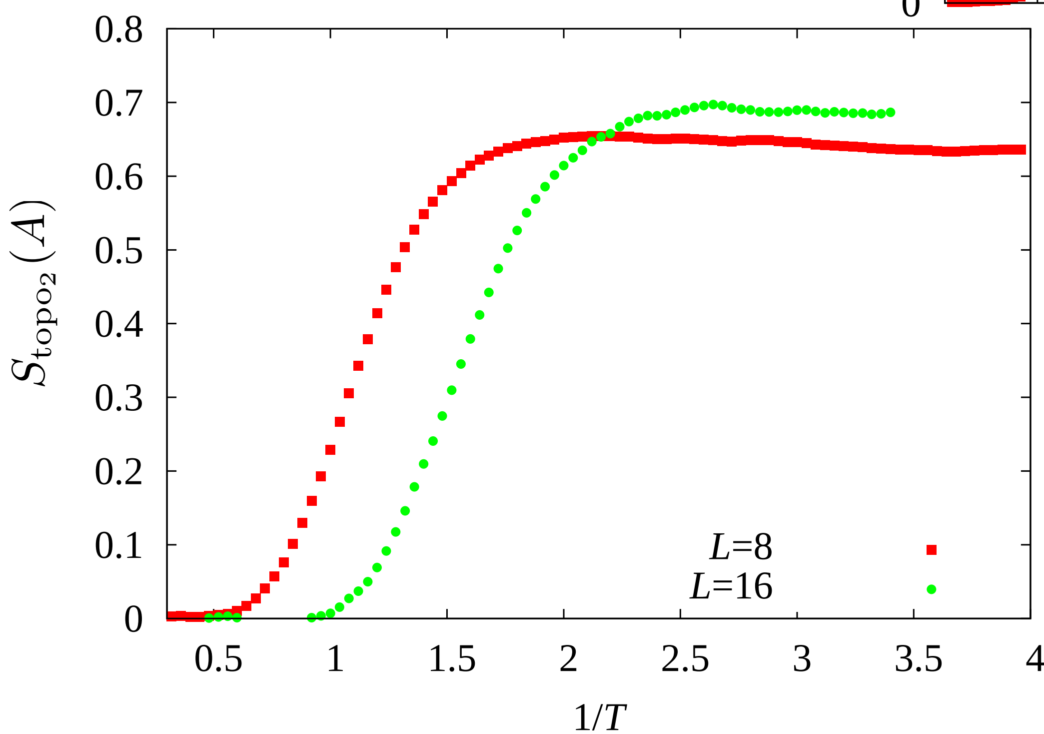
$$B_p = \prod_{i\in p} \sigma_i^z \qquad A_s = \prod_{j\in s} \sigma_j^x$$

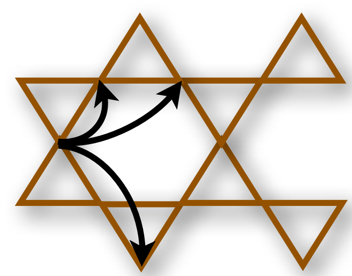
Entanglement and topological entropy of the toric code at finite temperature
Claudio Castelnovo and Claudio Chamon, PRB 76, 184442 2007

Topological Entanglement Entropy





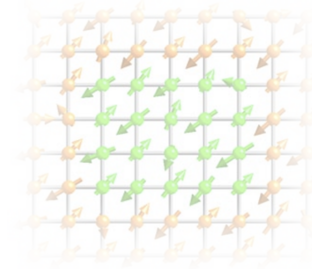




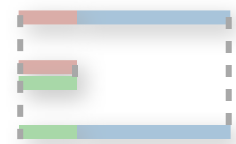
$$H_b = -t\sum_{(i,j)}(b_i^\dagger b_j + \mathrm{H.c.}) + V\sum_{\bigcirc}(n_\bigcirc)^2 - \mu\sum_i n_i$$

Outline

- Renyi Entanglement Entropy as a resource in Condensed Matter Physics

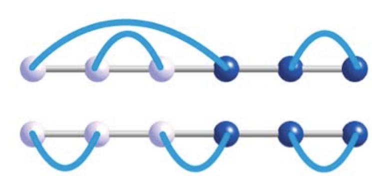


- Finite-Temperature QMC and Mutual Information



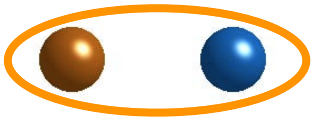
- Topological entanglement entropy in a quantum Spin Liquid

- **T=0 projector QMC in the Valence Bond Basis**

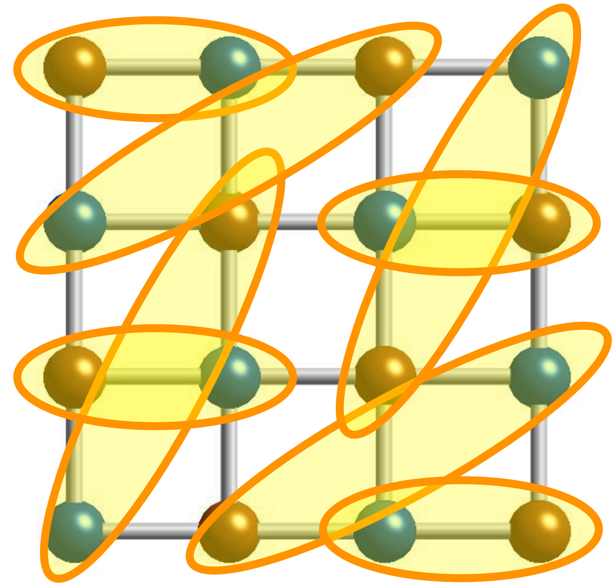


Valence Bond Basis

Pauling, Anderson, Liang, Sandvik, Beach
Sandvik, Phys. Rev. Lett. 95, 207203 (2005)



$$(i,j) = \frac{1}{\sqrt{2}}(|\uparrow_i\downarrow_j\rangle - |\downarrow_i\uparrow_j\rangle)$$



$$|V_r\rangle = |(i_{r,1},j_{r,1})(i_{r,2},j_{r,2})\cdots(i_{r,N/2},j_{r,N/2})\rangle$$

Projector QMC

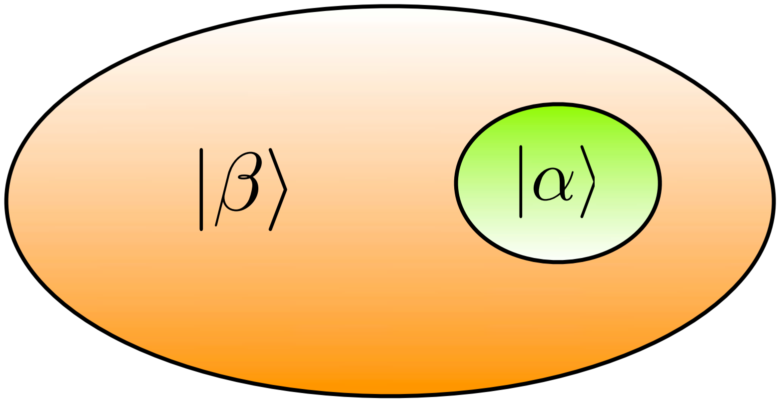
$$|\Psi_0\rangle \propto H^m|V_{\rm trial}\rangle$$

$$P_r = H_{b_1^r}H_{b_2^r}H_{b_3^r}\cdots$$

$$H^m = \left(\sum_b H_b\right)^m = \sum_r P_r$$

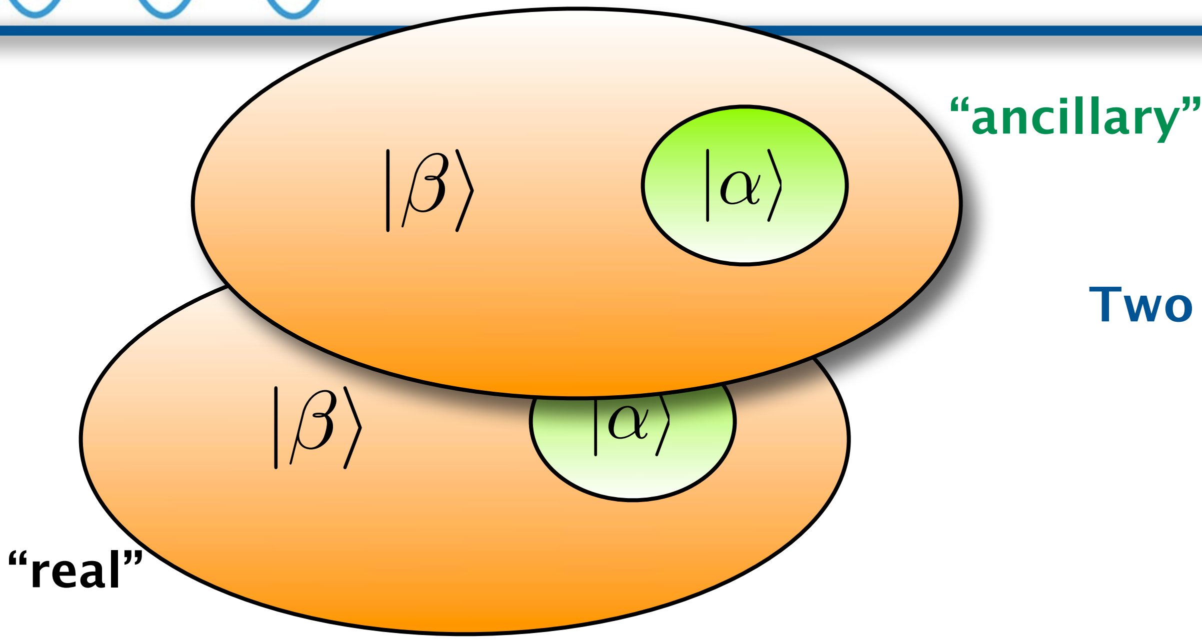
$$P_r|V_{\rm trial}\rangle = W_r|V_r\rangle$$

SWAP operator



$$|\Psi_0\rangle = \sum_{\alpha,\beta} C_{\alpha,\beta}|\alpha\rangle|\beta\rangle$$

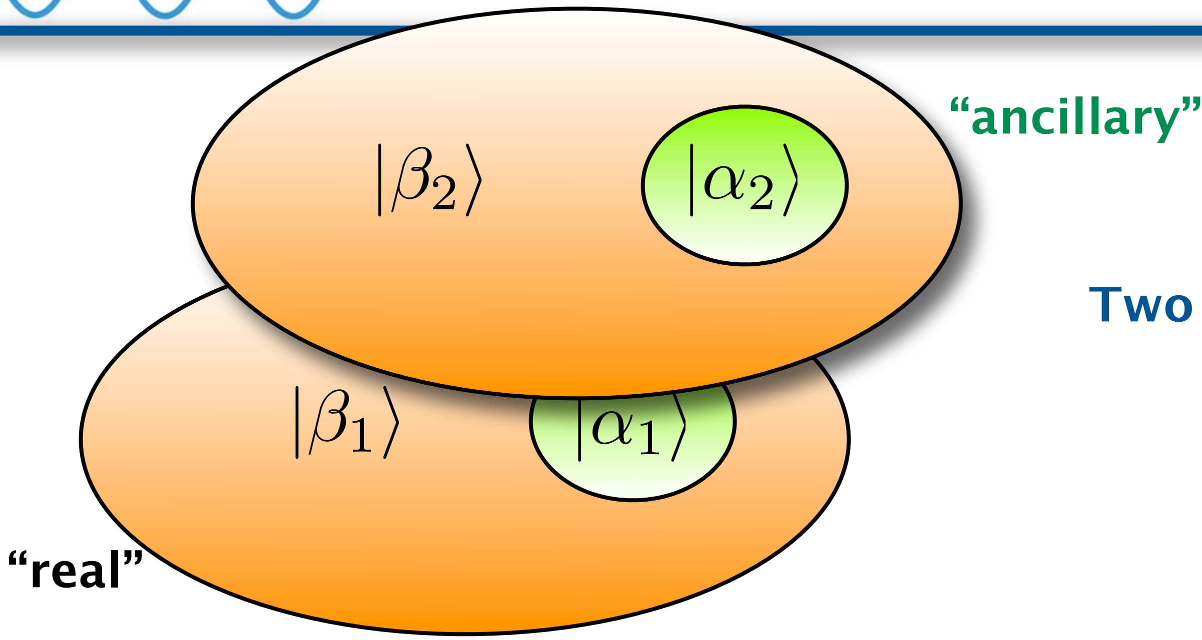
SWAP OPERATOR



Two non-interacting copies

$$|\Psi_0 \otimes \Psi_0\rangle$$

SWAP OPERATOR



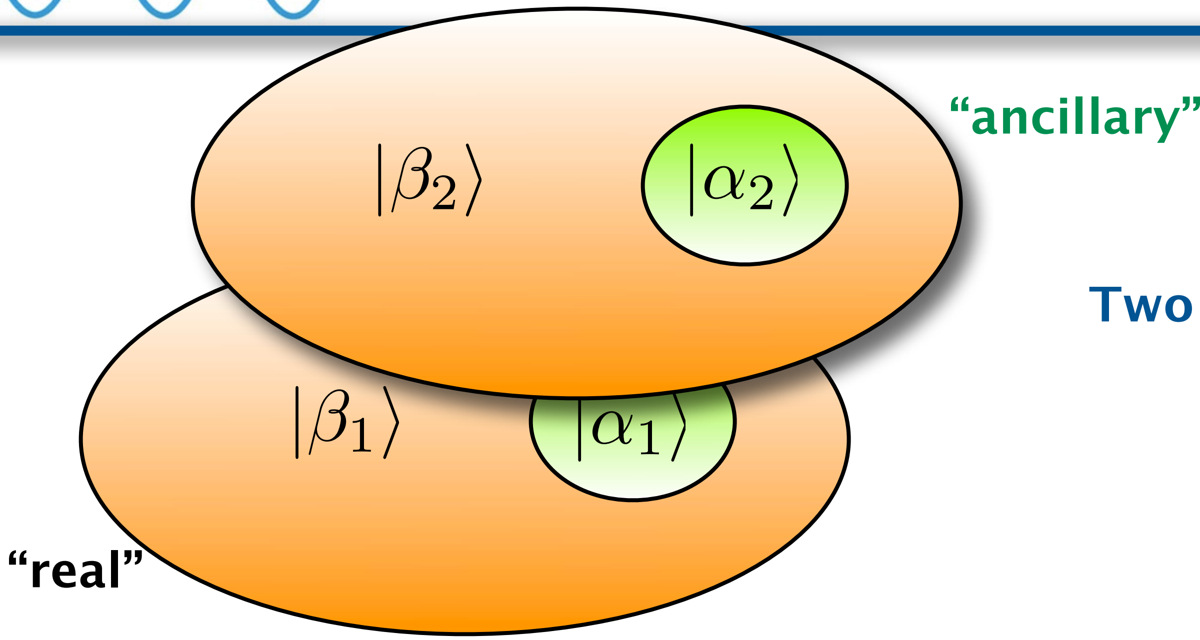
Two non-interacting copies

$$|\Psi_0 \otimes \Psi_0\rangle$$

$$Swap_A\Big(\sum_{\alpha_1,\beta_1} C_{\alpha_1,\beta_1}|\alpha_1\rangle|\beta_1\rangle\Big) \otimes \Big(\sum_{\alpha_2,\beta_2} D_{\alpha_2,\beta_2}|\alpha_2\rangle|\beta_2\rangle\Big)$$

$$= \sum_{\alpha_1,\beta_1} C_{\alpha_1,\beta_1} \sum_{\alpha_2,\beta_2} D_{\alpha_2,\beta_2}\Big(|\alpha_2\rangle|\beta_1\rangle\Big) \otimes \Big(|\alpha_1\rangle|\beta_2\rangle\Big)$$

SWAP OPERATOR



Two non-interacting copies

$$|\Psi_0 \otimes \Psi_0\rangle$$

$$\langle \Psi_0 \otimes \Psi_0 | Swap_A | \Psi_0 \otimes \Psi_0 \rangle = \sum_{\alpha_1,\alpha_2,\beta_1,\beta_2} C_{\alpha_1,\beta_1} \overline{C}_{\alpha_2,\beta_1} C_{\alpha_2,\beta_2} \overline{C}_{\alpha_1,\beta_2}$$

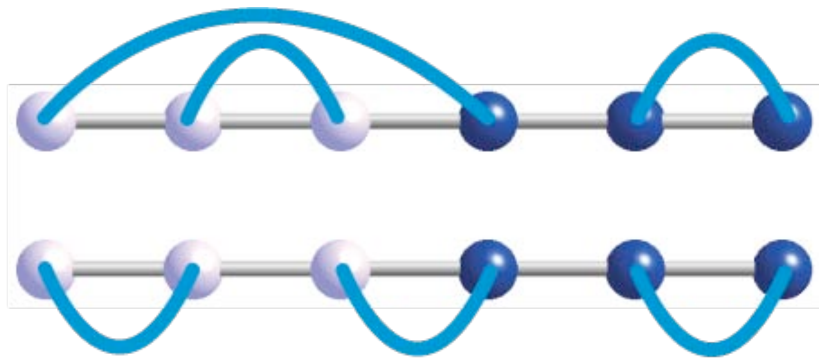
$$= \sum_{\alpha_1,\alpha_2} \langle \alpha_1 | \rho_A | \alpha_2 \rangle \langle \alpha_2 | \rho_A | \alpha_1 \rangle = \mathrm{Tr}(\rho_A^2)$$

$$S_2(\rho_A) = -\ln(\mathrm{Tr}(\rho_A^2)) = -\ln(\langle Swap_A \rangle)$$

VB Basis QMC

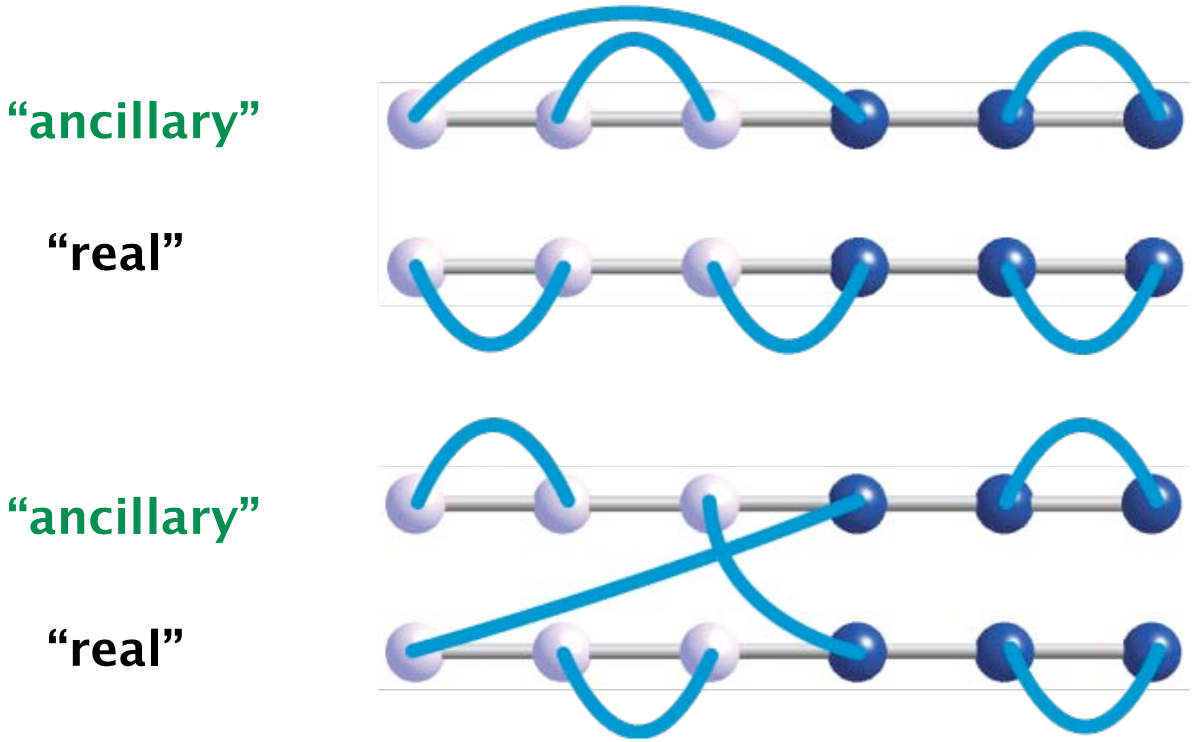
“ancillary”

“real”



$$|V_r\rangle$$

VB Basis QMC



$|V_r\rangle$

$Swap_A|V_r\rangle$

$$\langle \Psi_0 \otimes \Psi_0 | Swap_A | \Psi_0 \otimes \Psi_0 \rangle = \mathrm{Tr}(\rho_A^2)$$

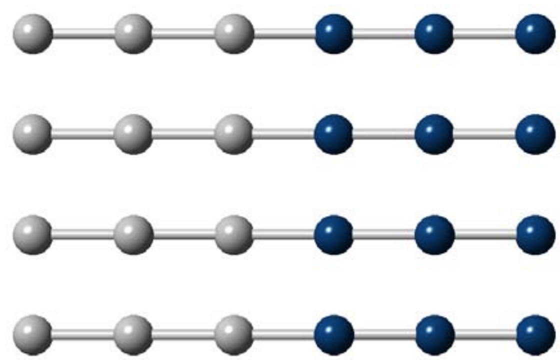
$$-\ln\langle Swap_A \rangle = S_2(\rho_A)$$

Notes:

- Best suited for calculating EE scaling in groundstate wavefunctions

- More work needed on improving statistics/scalability:
  - combining Renyi with VB QMC loop moves
  - using multicanonical histogram sampling

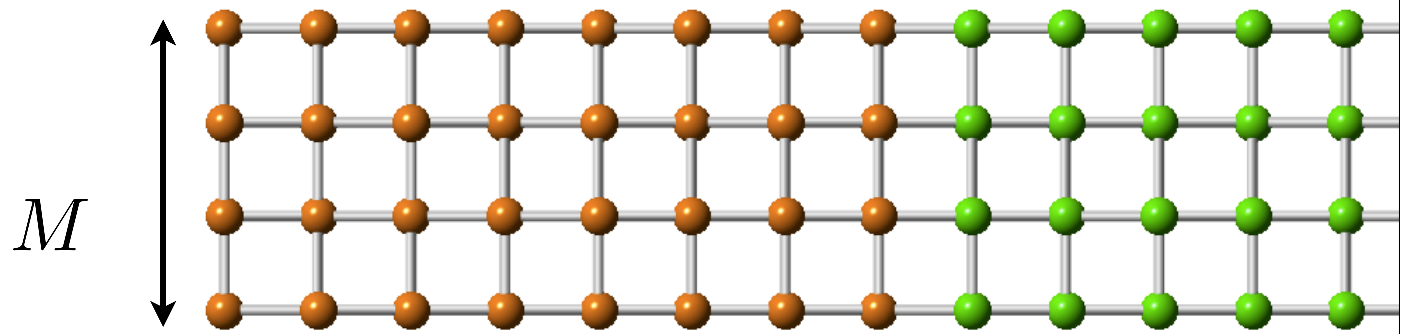
- More replicas enable the calculation of higher-n Renyi entropies

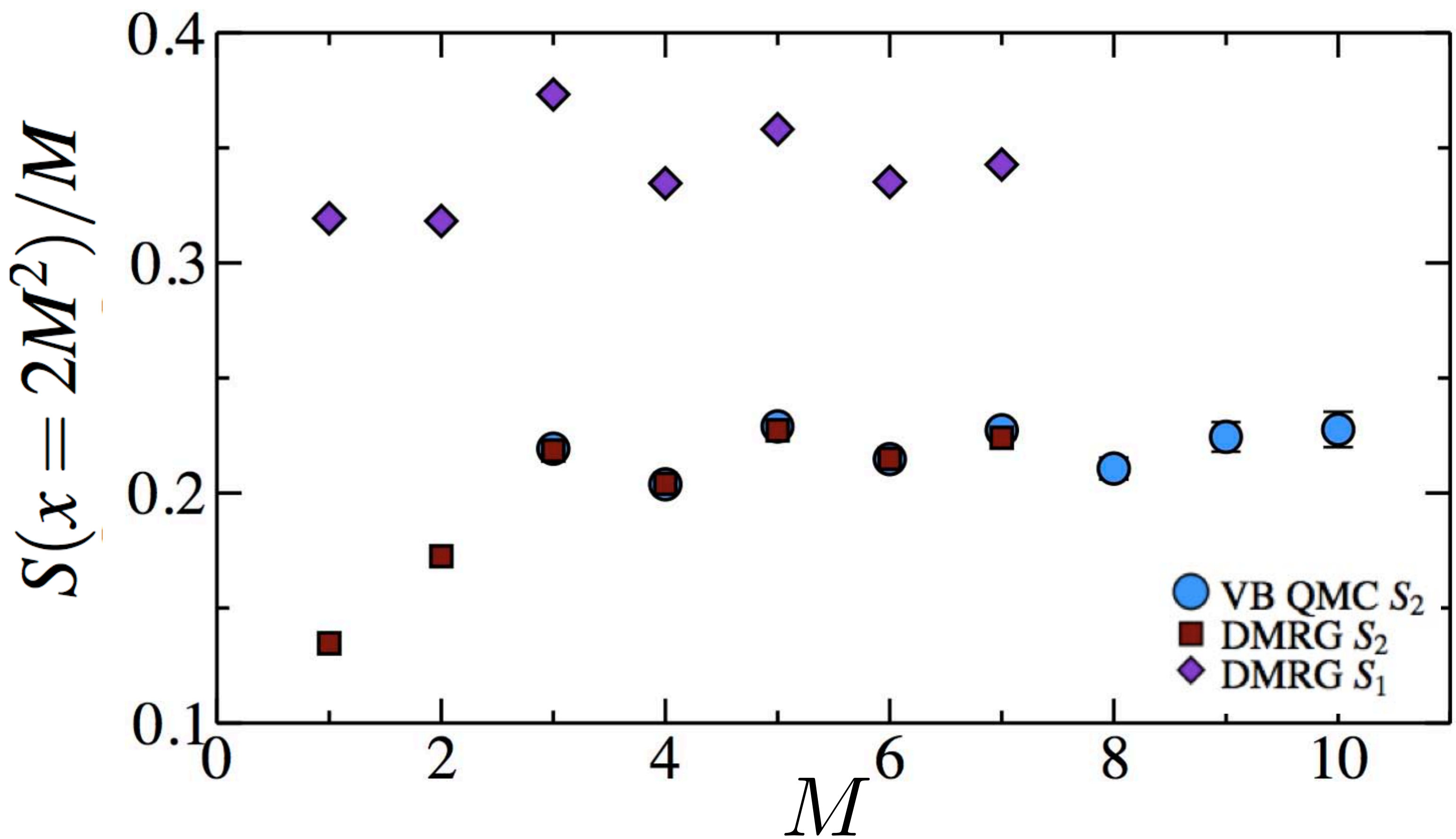


- SU(2) or SU(N) models only

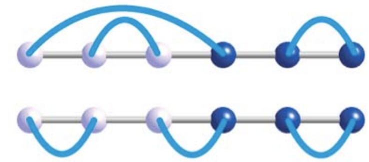
Néel State: Area Law

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

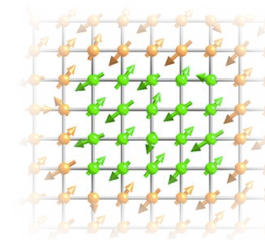




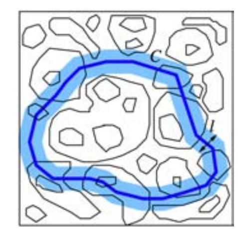
CONCLUSIONS



● Quantum Monte Carlo simulations can calculate Renyi entanglement entropy in general many-body Hamiltonians (spins, bosons, T=0 and T>0)



● QMC simulations have confirmed leading-order area law behaviour in the Néel state.



● We can access topological entanglement entropy in spin liquid phases

● Next: universal subleading corrections at T=0 QCP

$$S_n = a\ell + c_n \log(\ell)$$

● This effort is only 1 year old: expect rapid advances in scaling and efficiency.