

Title: Computing Entanglement in Simulations of Quantum Condensed Matter

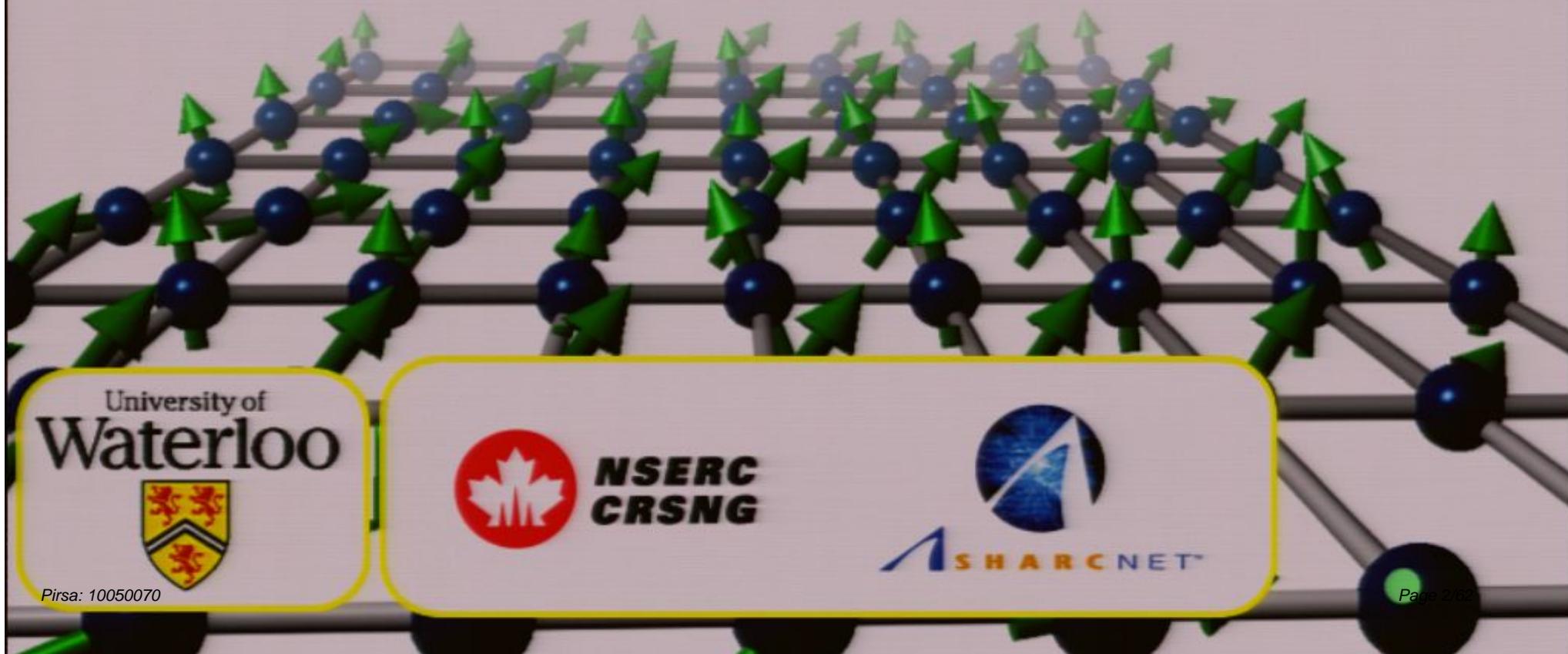
Date: May 26, 2010 10:30 AM

URL: <http://pirsa.org/10050070>

Abstract: Condensed matter theorists have recently begun exploiting the properties of entanglement as a resource for studying quantum materials. At the forefront of current efforts is the question of how the entanglement of two subregions in a quantum many-body groundstate scales with the subregion size. The general belief is that typical groundstates obey the so-called "area law", with entanglement entropy scaling as the boundary between regions. This has lead theorists to propose that sub-leading corrections to the area law provide new universal quantities at quantum critical points and in exotic quantum phases (i.e. topological Mott insulators). However, away from one dimension, entanglement entropy is difficult or impossible to calculate exactly, leaving the community in the dark about scaling in all but the simplest non-interacting systems. In this talk, I will discuss recent breakthroughs in calculating entanglement entropy in two dimensions and higher using advanced quantum Monte Carlo simulation techniques. We show, for the first time, evidence of leading-order area law scaling in a prototypical model of strongly-interacting quantum spins. This paves the way for future work in calculating new universal quantities derived from entanglement, in the plethora of real condensed matter systems amenable to numerical simulation.

COMPUTING ENTANGLEMENT IN SIMULATIONS OF QUANTUM CONDENSED MATTER

Roger Melko



University of
Waterloo



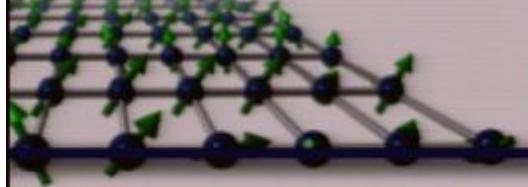
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NSERC
CRSNG



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COLLABORATORS



Ann Kallin



Ivan Gonzalez



Matt Hastings

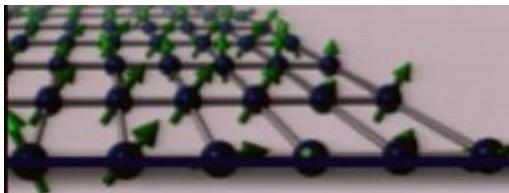
Station Q



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

Measuring Renyi Entanglement Entropy with
Quantum Monte Carlo

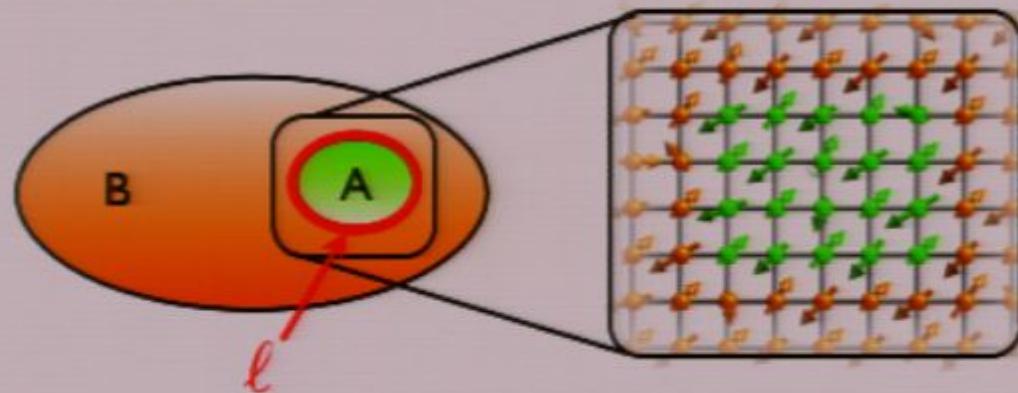
Phys. Rev. Lett., 104, 157201 (2010)

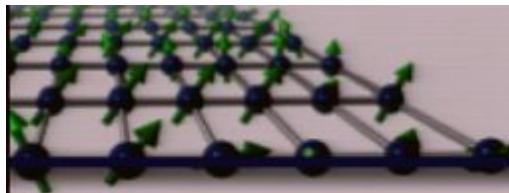


GOAL

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

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

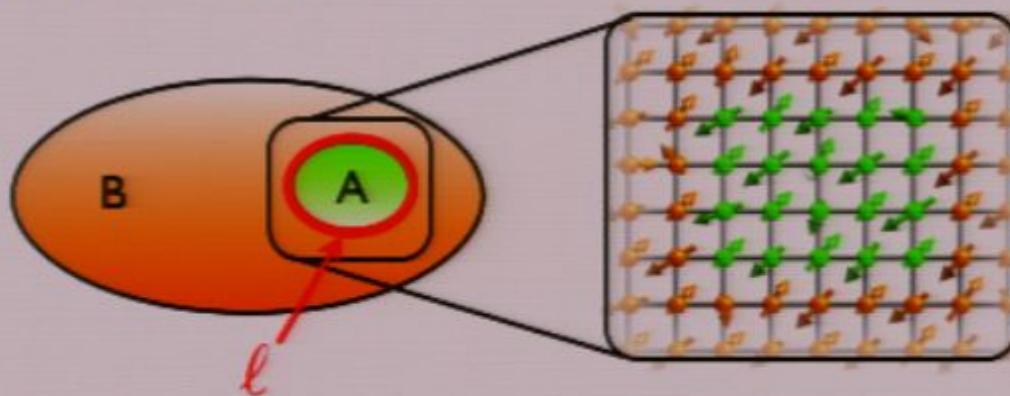




GOAL

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



- Universal quantities at quantum critical points

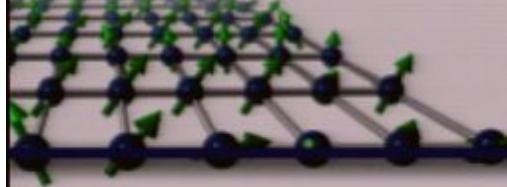
$$S_1 = a\ell + \gamma^{\text{critical}}$$

- 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)

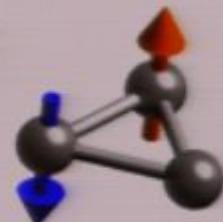


QUANTUM MONTE CARLO

- A scalable simulation method in any dimension
 N or N^2
- Finite and zero-temperature methods available

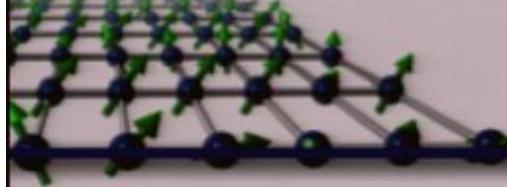
$$|\psi\rangle \approx (-\hat{H})^m |\psi_{\text{trial}}\rangle \quad Z = \sum_{\alpha} \langle \alpha | e^{-\beta \hat{H}} | \alpha \rangle$$

- The “sign problem” inhibits the simulation of frustrated spins or fermions



- Simulations do not have access to the wavefunction

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



RENYI ENTROPIES

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

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

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

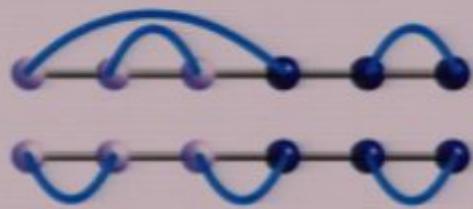
Properties

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

$$S_n = a'\ell + \gamma_n^{\text{critical}}$$

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

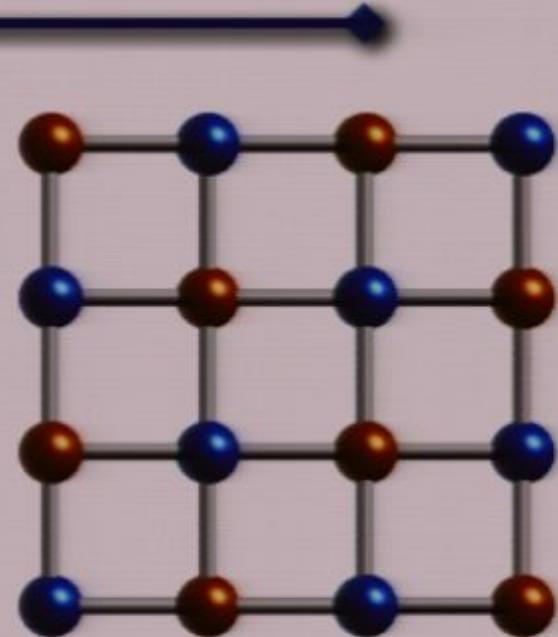
Calculating Renyi Entropy in Valence Bond Basis QMC





VALENCE BOND BASIS

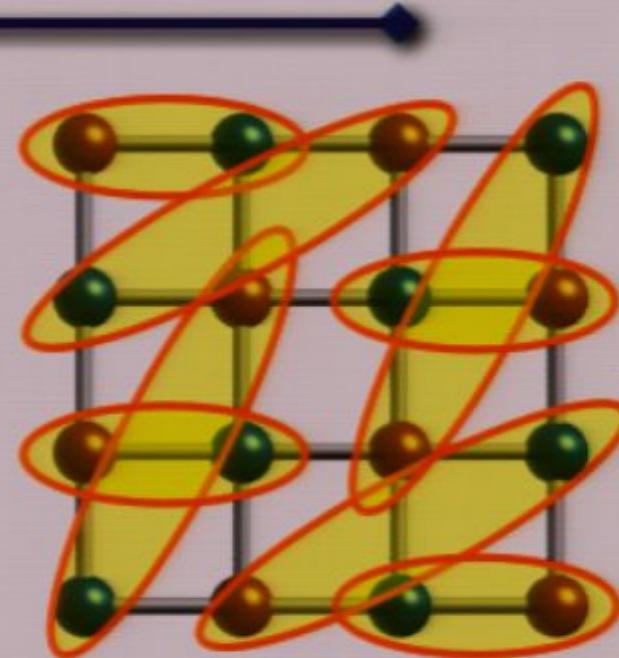

$$(i, j) = \frac{1}{\sqrt{2}}(|\uparrow_i \downarrow_j\rangle - |\downarrow_i \uparrow_j\rangle)$$





VALENCE BOND BASIS

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



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

Pauling, Anderson, Liang

Sandvik, Phys. Rev. Lett. 95, 207203 (2005)

Number of possible states in the VB basis, if we restrict valence bonds to exist between A and B sublattice: $(N/2)!$



PROJECTOR METHODS

$$(C - H)^m |\Psi\rangle \rightarrow c_o (C - E_0)^m \left[|0\rangle + \frac{c_1}{c_0} \left(\frac{C - E_1}{C - E_0} \right)^m |1\rangle + \dots \right]$$



PROJECTOR METHODS

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Consider the S=1/2 Heisenberg model

$$H = -J \sum_{\langle i,j \rangle} H_{i,j} \quad H_{i,j} = - \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} \right)$$



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$$H_{a,b} | \textcolor{cyan}{a} \textcolor{red}{\curvearrowright} \textcolor{yellow}{b} \textcolor{cyan}{c} \textcolor{red}{\curvearrowright} \textcolor{yellow}{d} \rangle = | \textcolor{cyan}{a} \textcolor{red}{\curvearrowright} \textcolor{yellow}{b} \textcolor{cyan}{c} \textcolor{red}{\curvearrowright} \textcolor{yellow}{d} \rangle$$

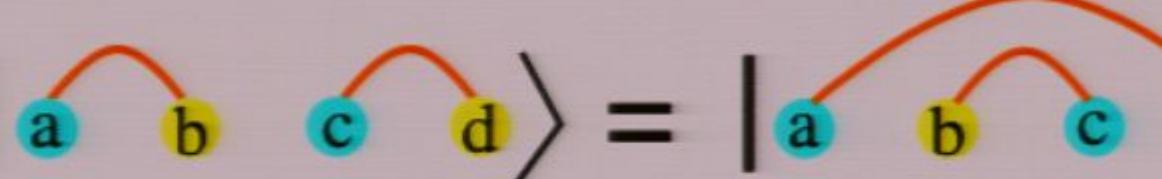


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$$H_{b,c} |a b c d\rangle = |a b c d\rangle \times \frac{1}{2}$$


PROJECTOR QMC

$$(C - H)^m = \left(\sum_b H_b \right)^m = \sum_r P_r \quad P_r = H_{b_1^r} H_{b_2^r} H_{b_3^r} \cdots$$

the sum is done through importance sampling

- a fixed (large) m is chosen
- a sequence of m bond operators propagates an initial state
- some number of operators are swapped each Monte Carlo step through a Metropolis algorithm

$$H_{b_i} \left| \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \right\rangle \rightarrow \left| \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \right\rangle$$

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$$P_r |\Psi\rangle = W_r |V_r\rangle$$

$$W_r = \left(\frac{1}{2} \right)^{m_{\text{od}}}$$

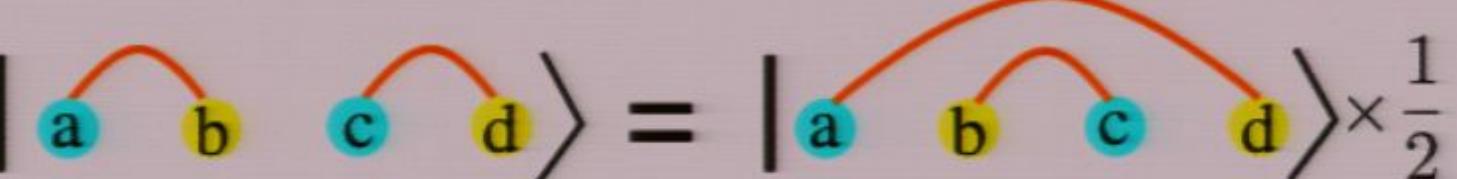


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$$H_{b_l} \left| \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right\rangle \rightarrow \left| \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right\rangle$$

$$P_s |\Psi\rangle = W_s |V_s\rangle$$

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$$H_{b_i} \left| \begin{array}{c} \text{O} \\ \text{O} \\ \text{O} \end{array} \right\rangle \rightarrow \left| \begin{array}{c} \text{O} \\ \text{O} \\ \text{O} \end{array} \right\rangle$$

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TYPICAL OBSERVABLES

Energy

$$\langle H \rangle = \frac{\sum_r W_r \langle \Psi | H | V_r \rangle}{\sum_r W_r \langle \Psi | V_r \rangle}$$

Expectation values

$$\langle A \rangle = \frac{\sum_{rl} W_r W_l \langle V_l | A | V_r \rangle}{\sum_{rl} W_r W_l \langle V_l | V_r \rangle}$$

Singlet-triplet gap

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



FEATURES

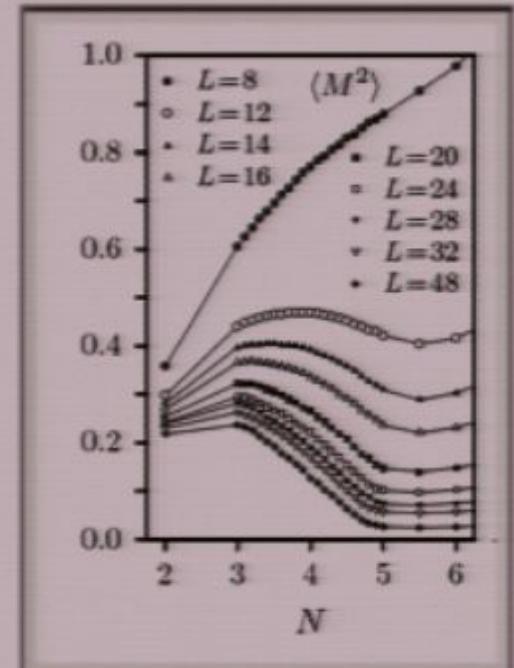
- Loop algorithm allows VB QMC to reach systems sizes comparable to SSE QMC (10^7)

Sandvik, Evertz, arXiv:0807.0682

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

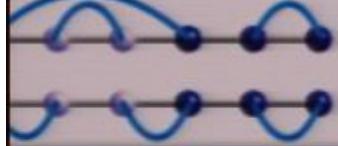
Beach, Alet, Mambrini, Capponi, Phys. Rev. B 80, 184401 (2009)

$$N_c = 4.57(5)$$

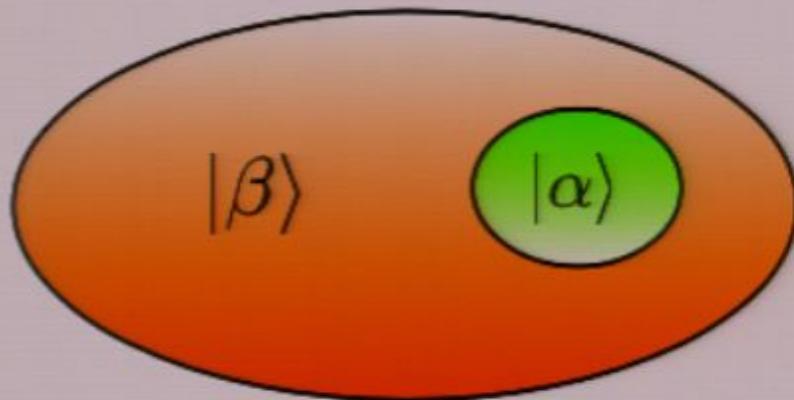
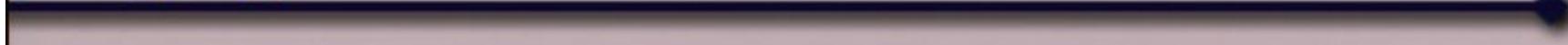


- sign problem comparable to SSE (some improvements may be possible)

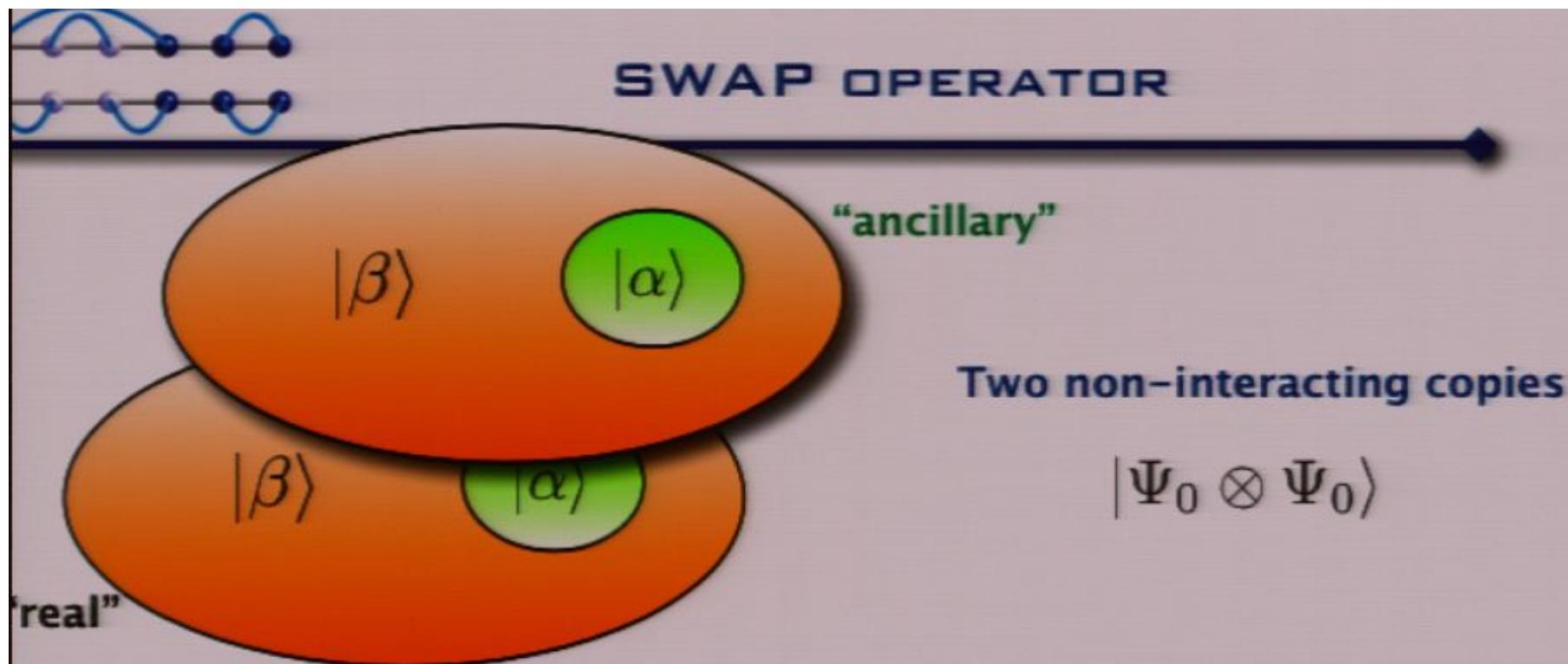
Kevin Beach

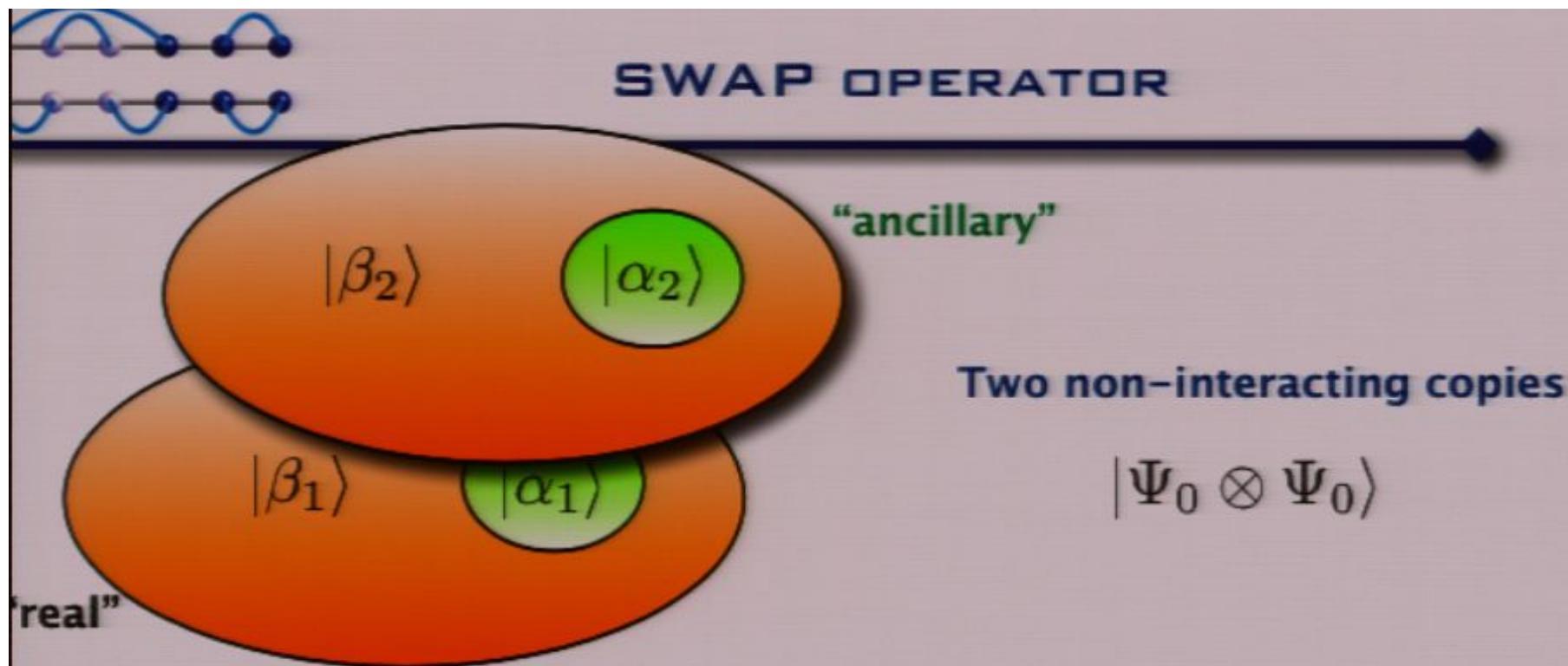


SWAP OPERATOR



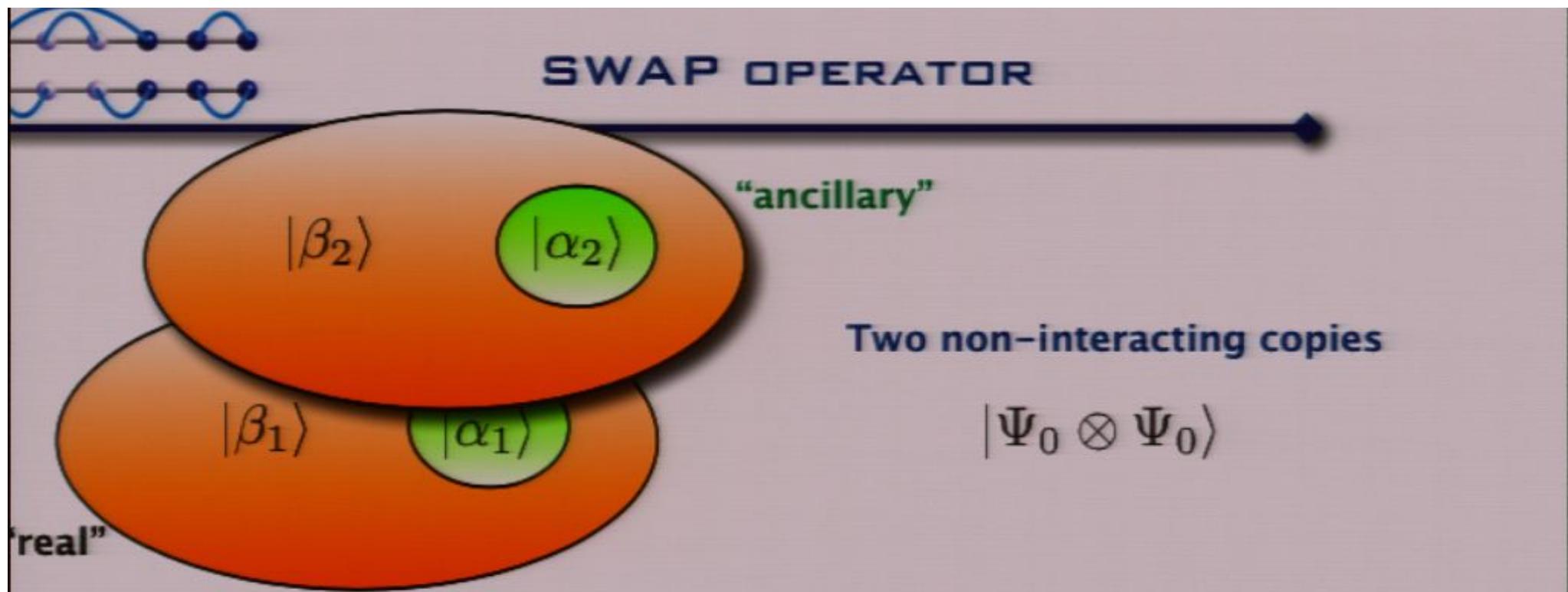
$$|\Psi_0\rangle = \sum_{\alpha,\beta} C_{\alpha,\beta} |\alpha\rangle |\beta\rangle$$



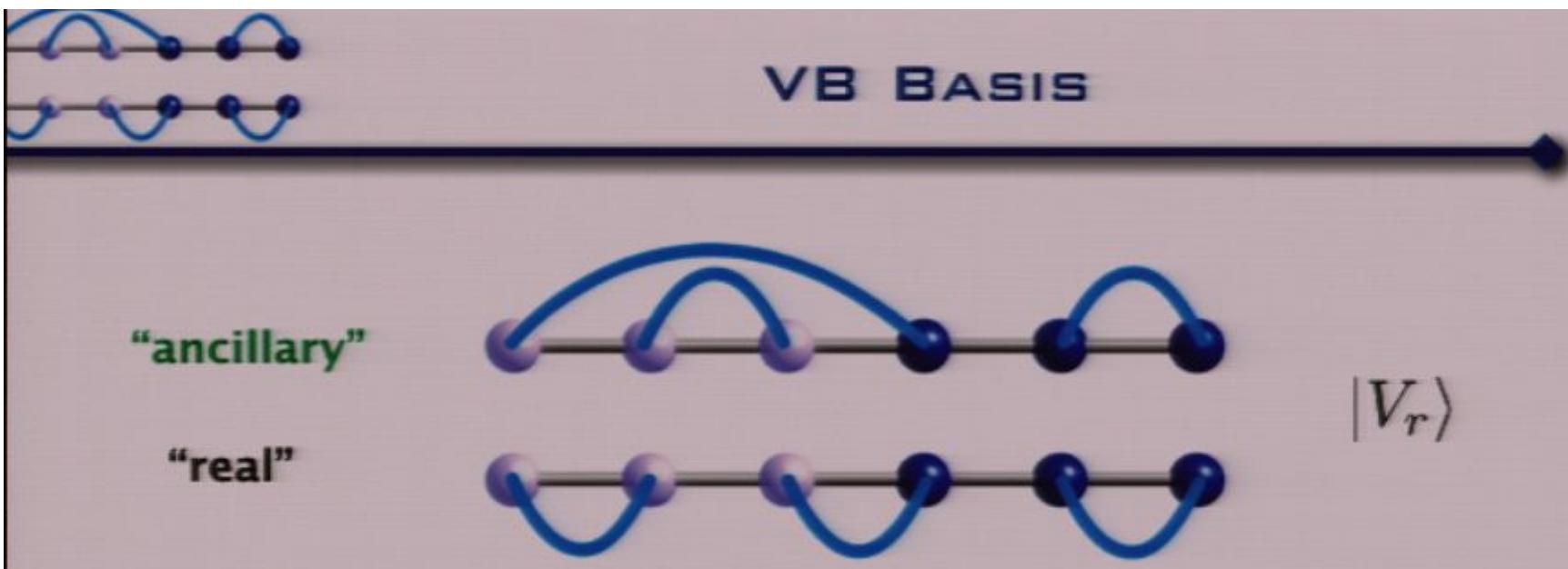


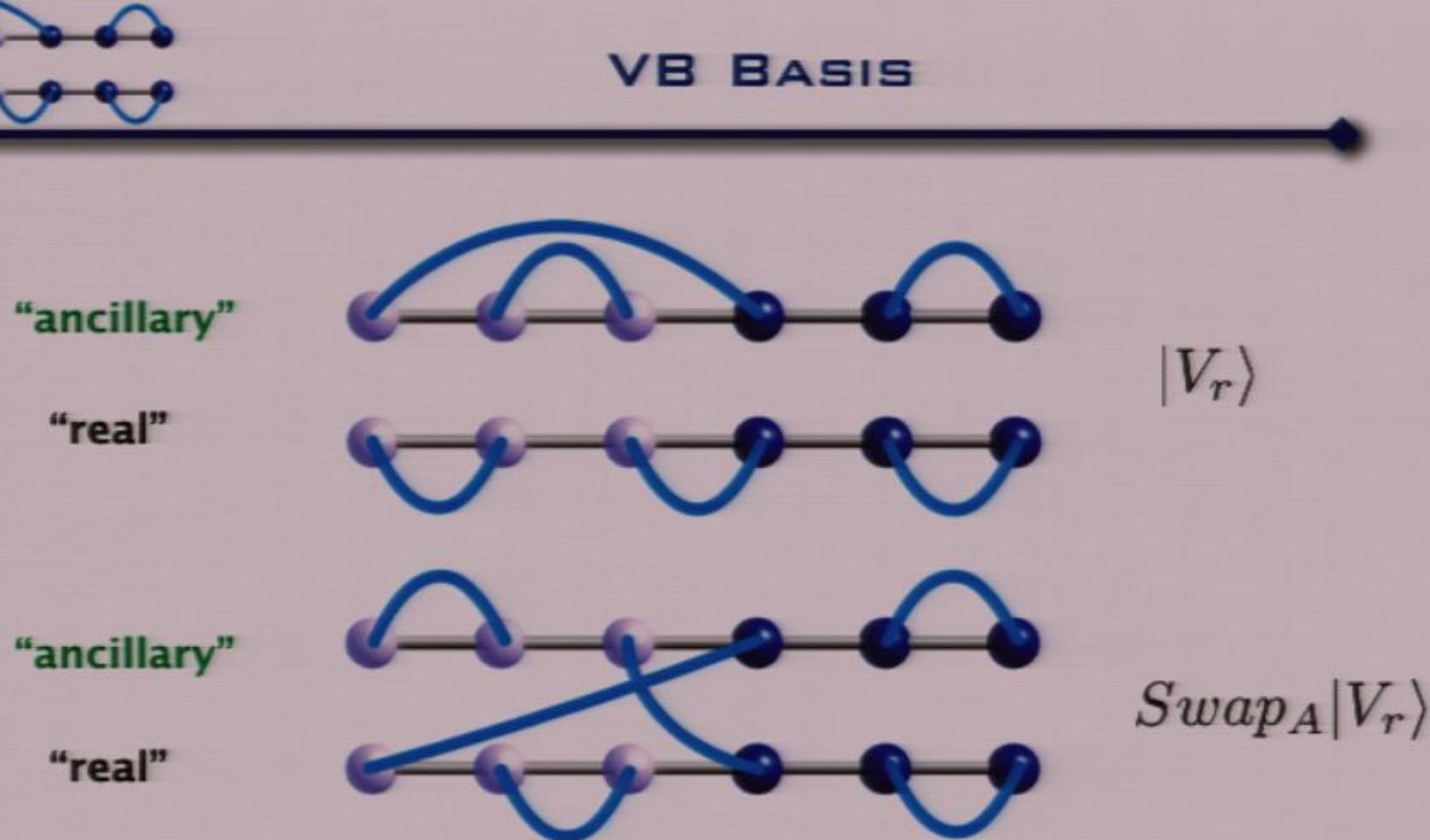
$$Swap_A \left(\sum_{\alpha_1, \beta_1} C_{\alpha_1, \beta_1} |\alpha_1\rangle |\beta_1\rangle \right) \otimes \left(\sum_{\alpha_2, \beta_2} D_{\alpha_2, \beta_2} |\alpha_2\rangle |\beta_2\rangle \right)$$

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

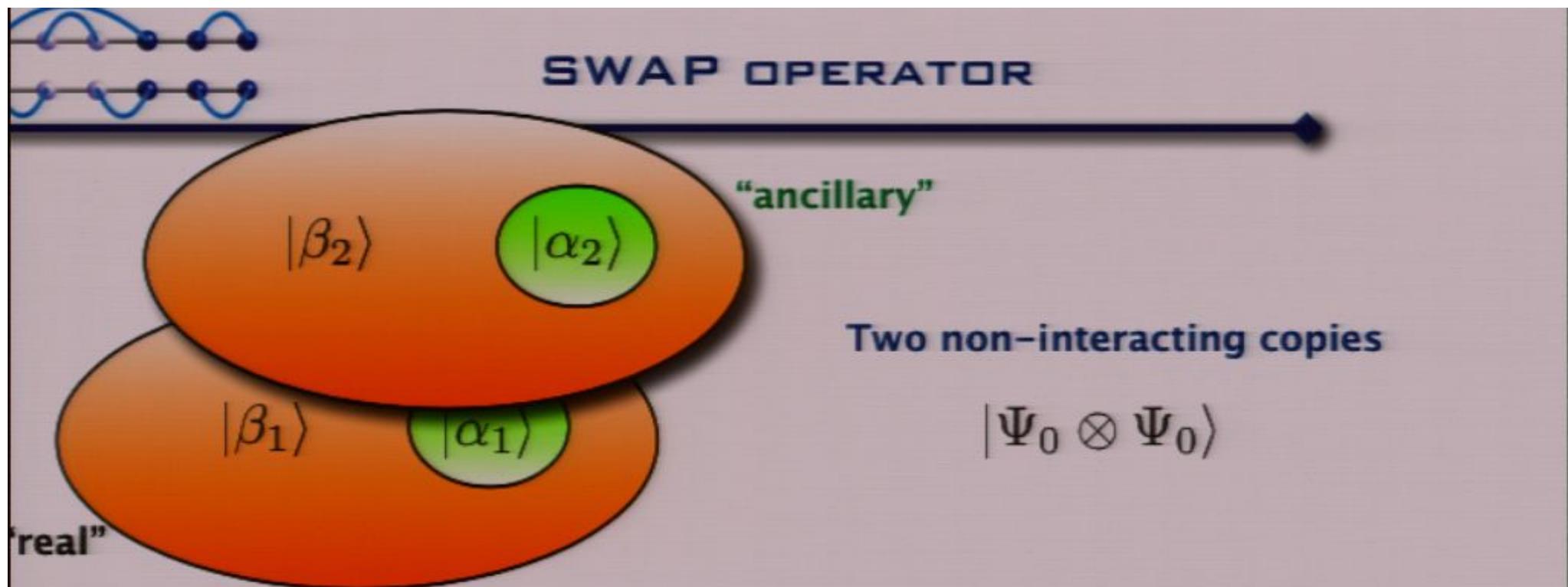


$$\begin{aligned}
 \Psi_0 \otimes \Psi_0 |Swap_A| \Psi_0 \otimes \Psi_0 \rangle &= \sum_{\alpha_1, \alpha_2, \beta_1, \beta_2} C_{\alpha_1, \beta_1} \overline{C}_{\alpha_2, \beta_1} C_{\alpha_2, \beta_2} \overline{C}_{\alpha_1, \beta_2} \\
 &= \sum_{\alpha_1, \alpha_2} (\rho_A)_{\alpha_1, \alpha_2} (\rho_A)_{\alpha_2, \alpha_1} = \text{Tr}(\rho_A^2)
 \end{aligned}$$





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



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VB BASIS

“ancillary”



$|V_r\rangle$

“real”



“ancillary”



$Swap_A |V_r\rangle$

“real”



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

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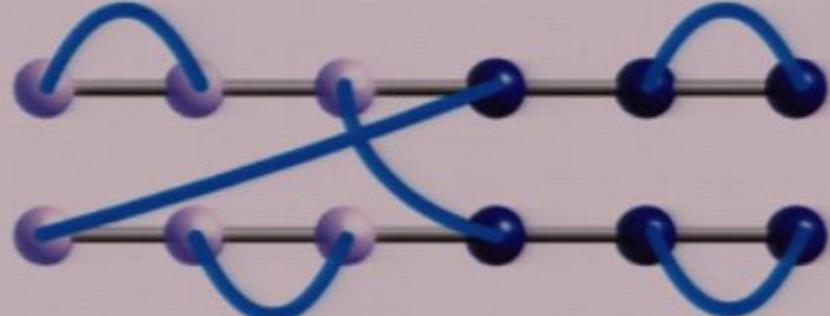


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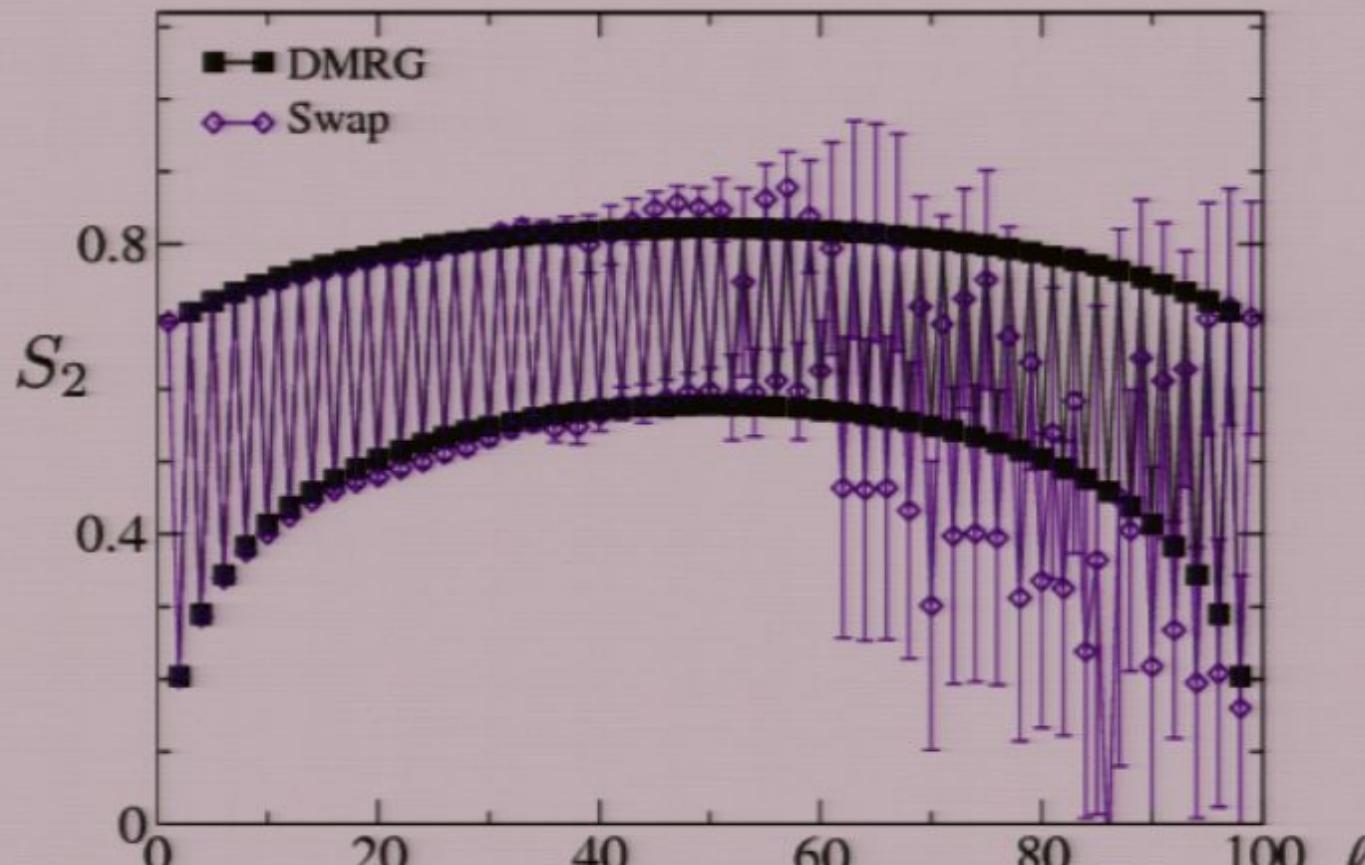
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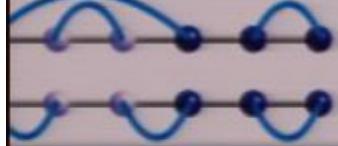
VB QUANTUM MONTE CARLO

$$\langle Swap_A \rangle = \left\langle \frac{\langle V(l) | Swap_A | V(r) \rangle}{\langle V(l) | V(r) \rangle} \right\rangle$$

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

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

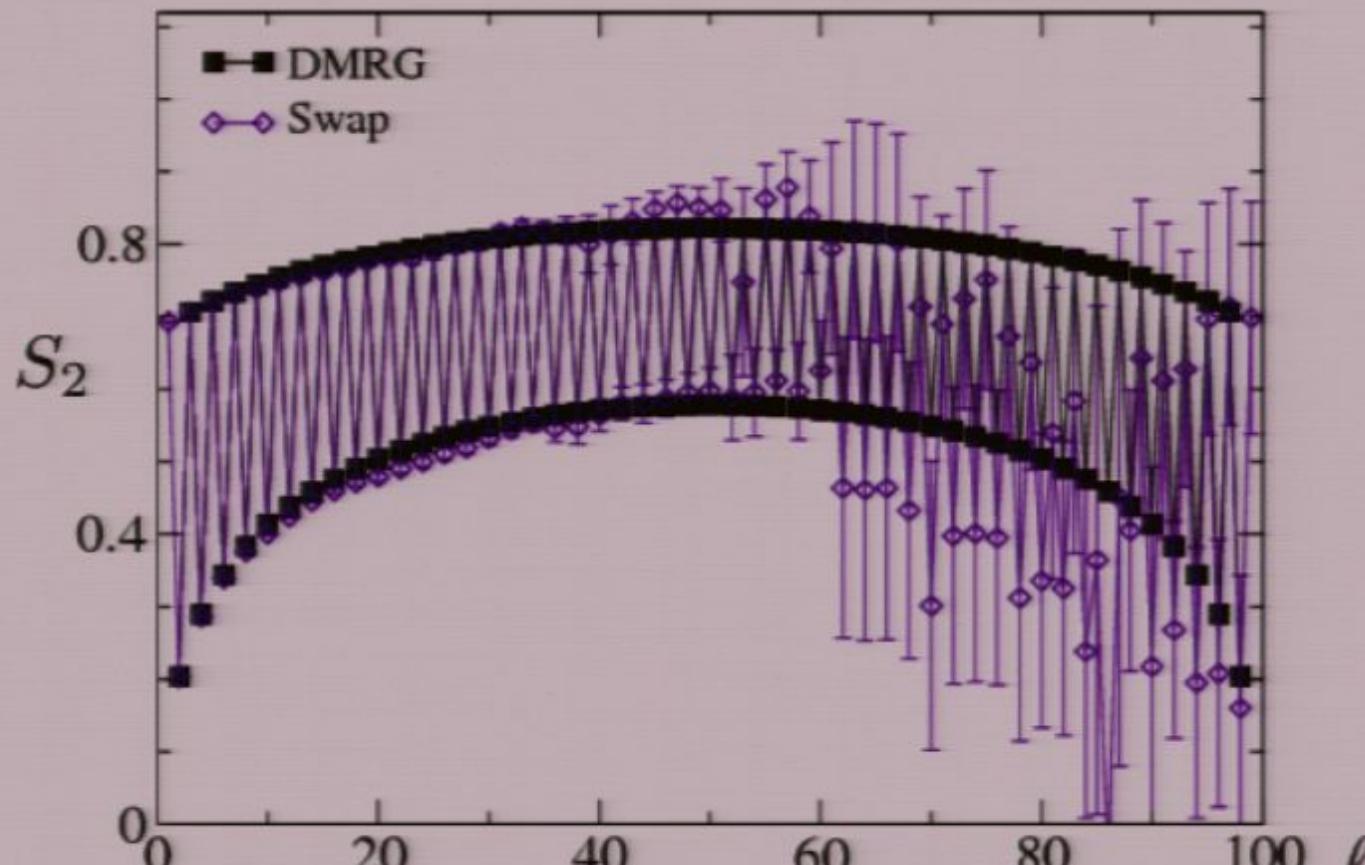


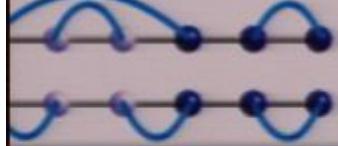


VB QUANTUM MONTE CARLO

poor sampling: we expect

$$-\ln \langle Swap_A \rangle = S_2(\rho_A) \sim a \ln \ell \quad \langle Swap_A \rangle \sim \ell^{-a}$$

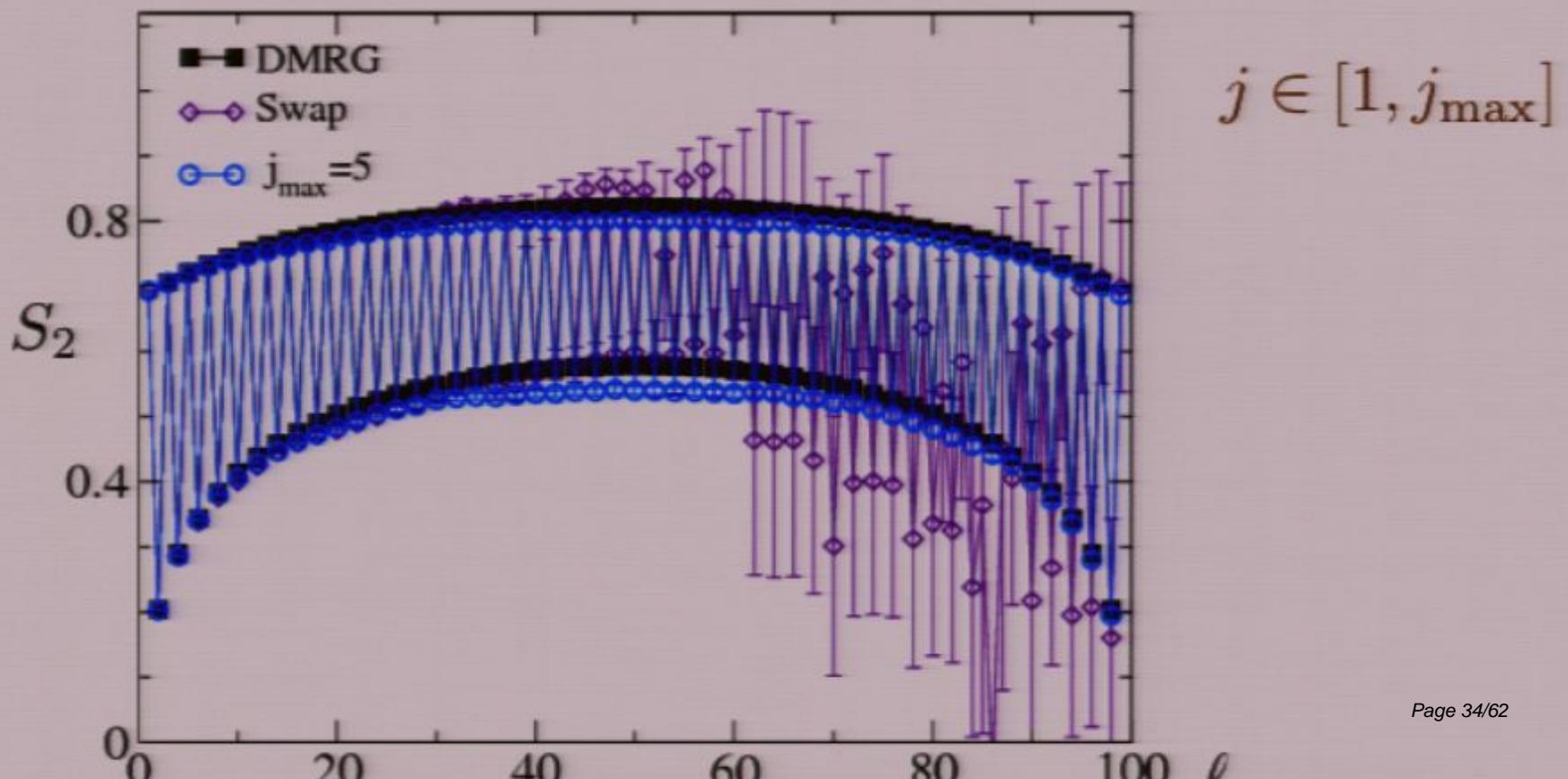


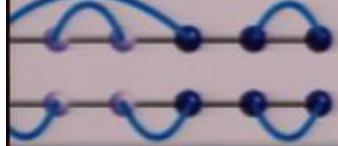


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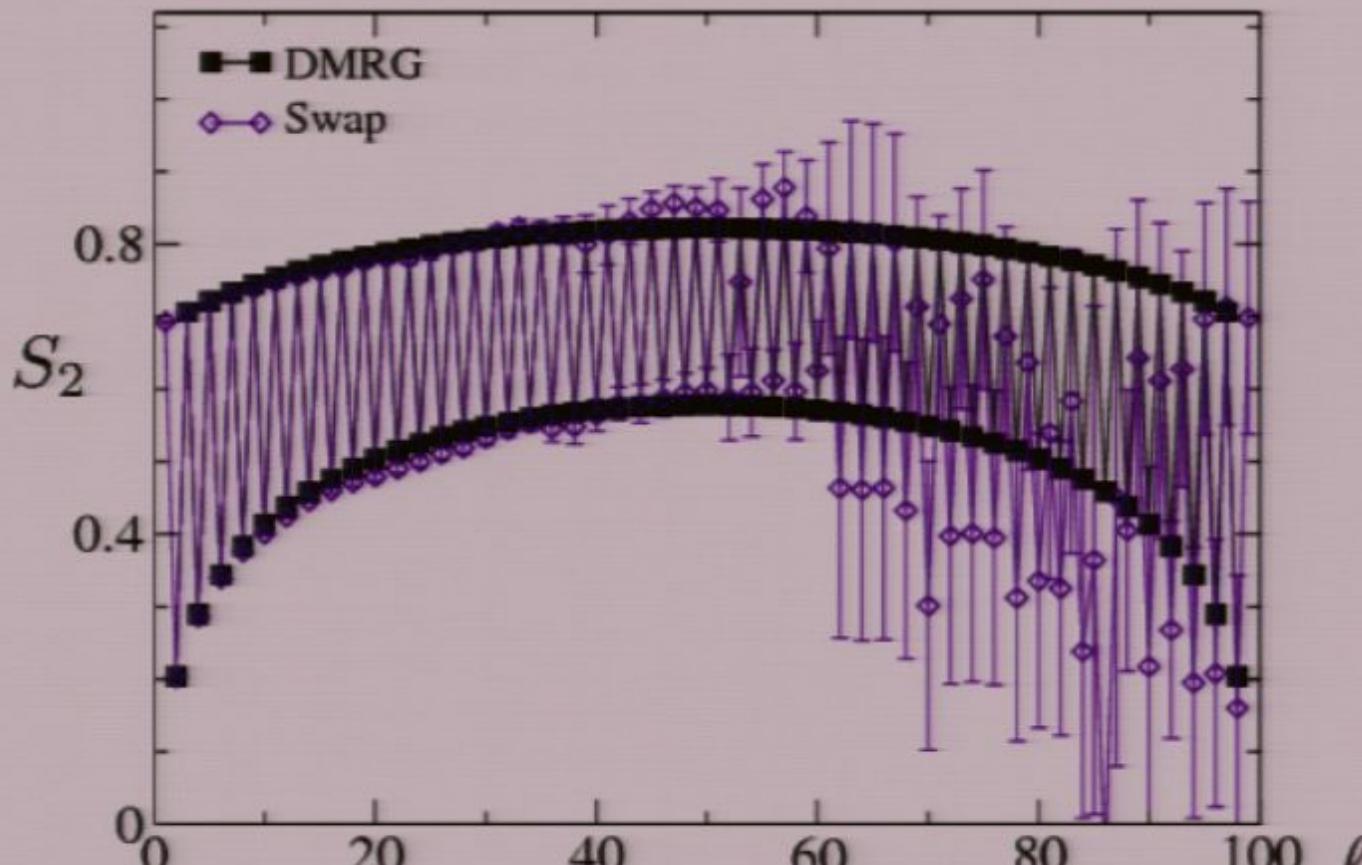




VB QUANTUM MONTE CARLO

poor sampling: we expect

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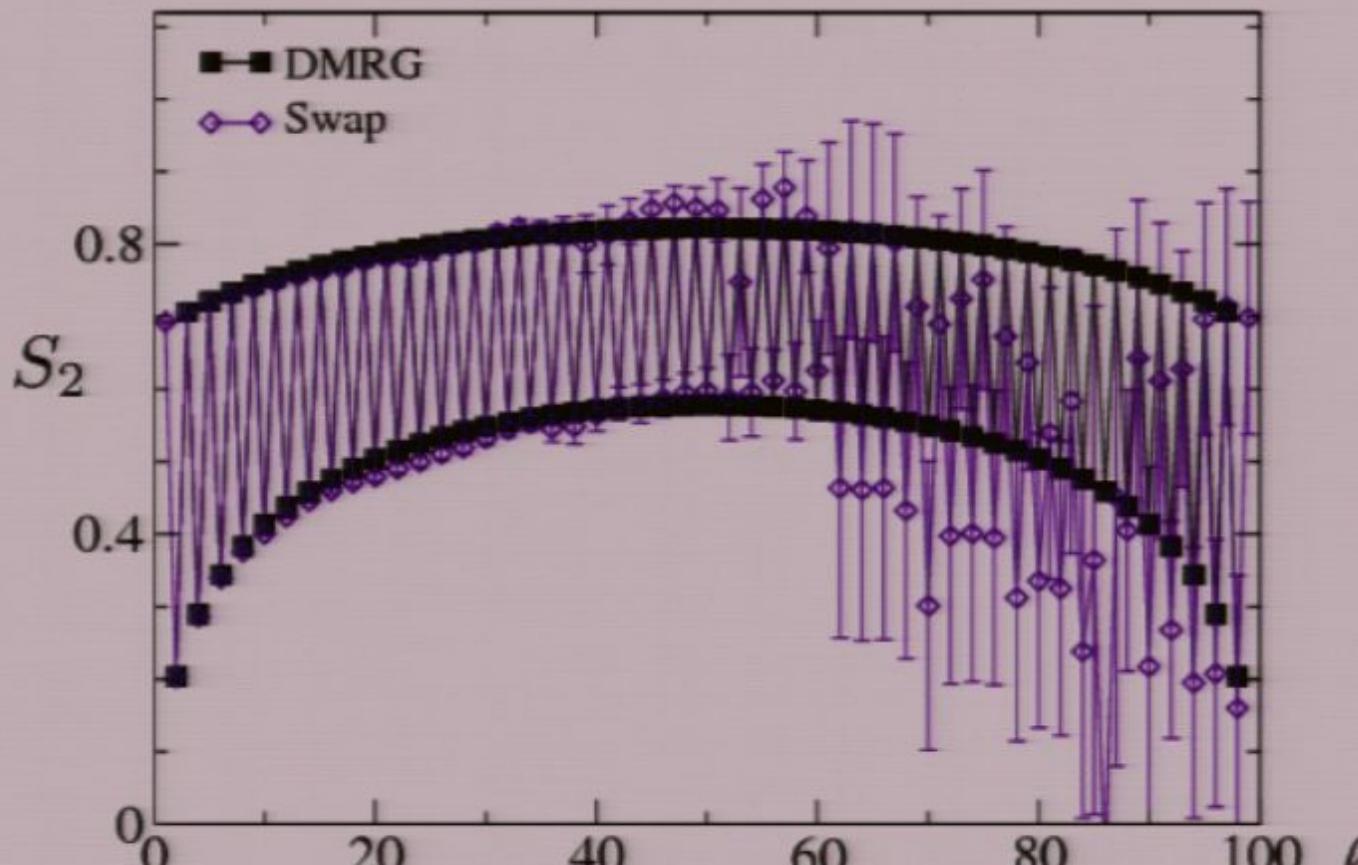
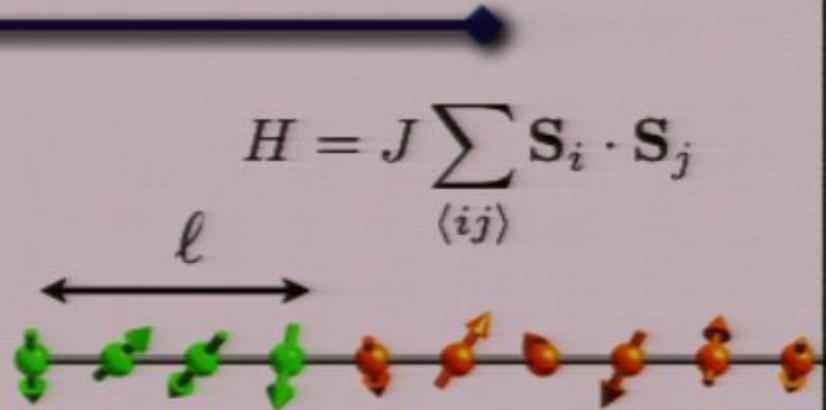


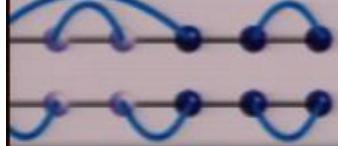
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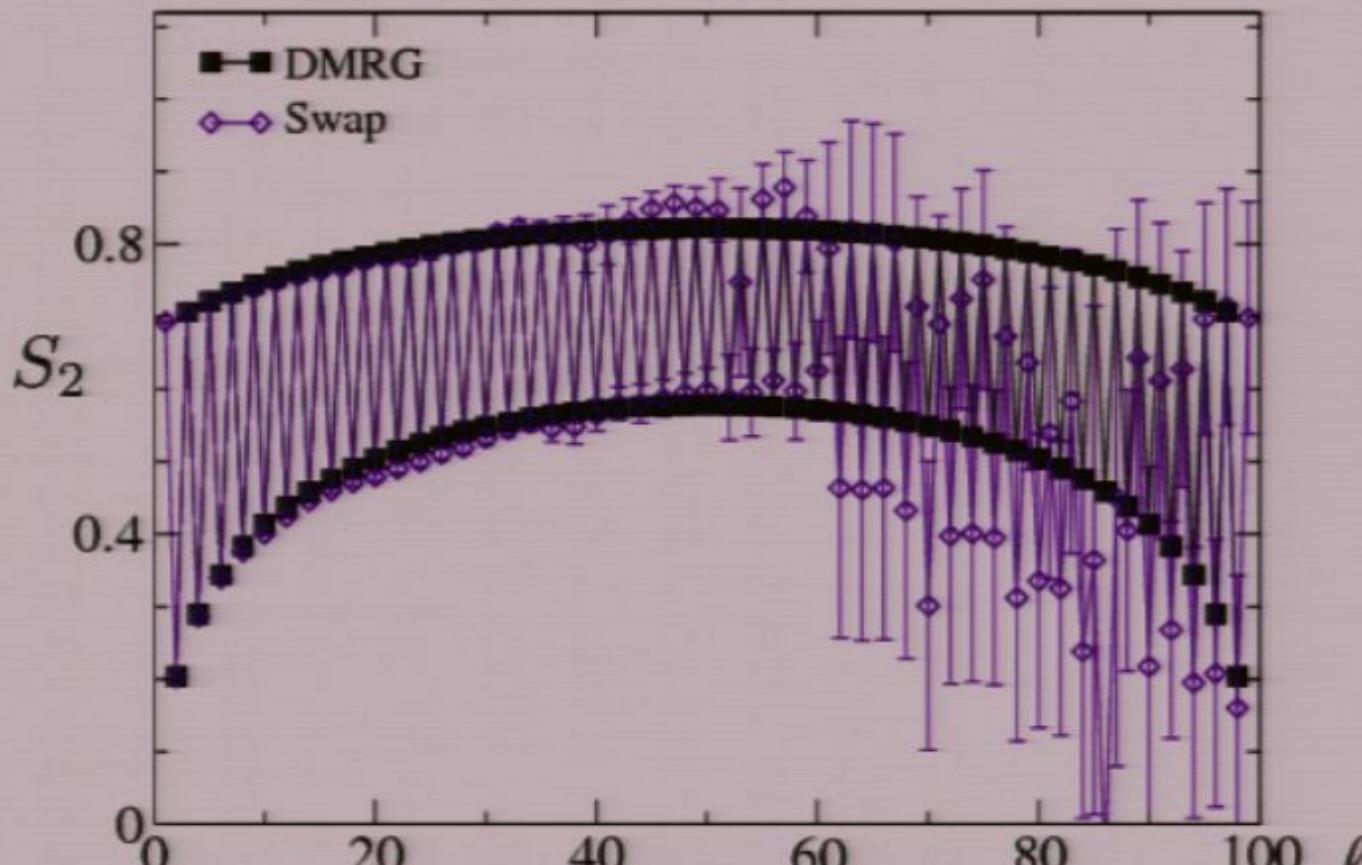


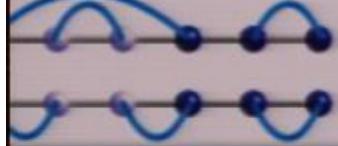


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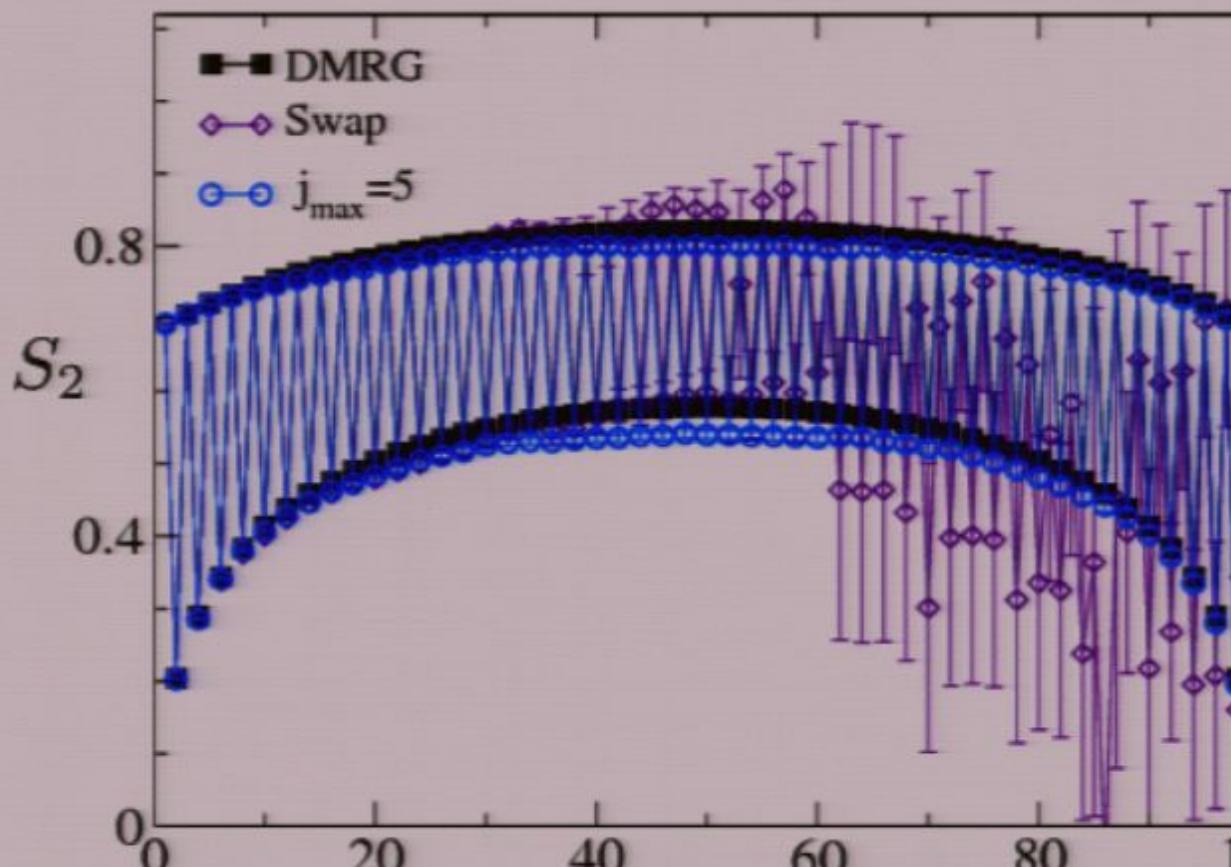
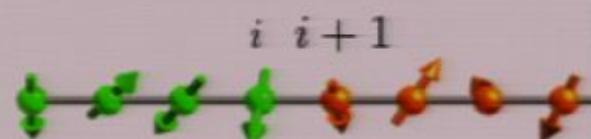




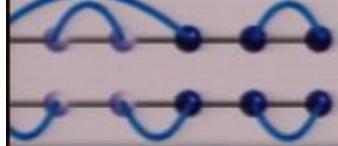
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$j \in [1, j_{\max}]$

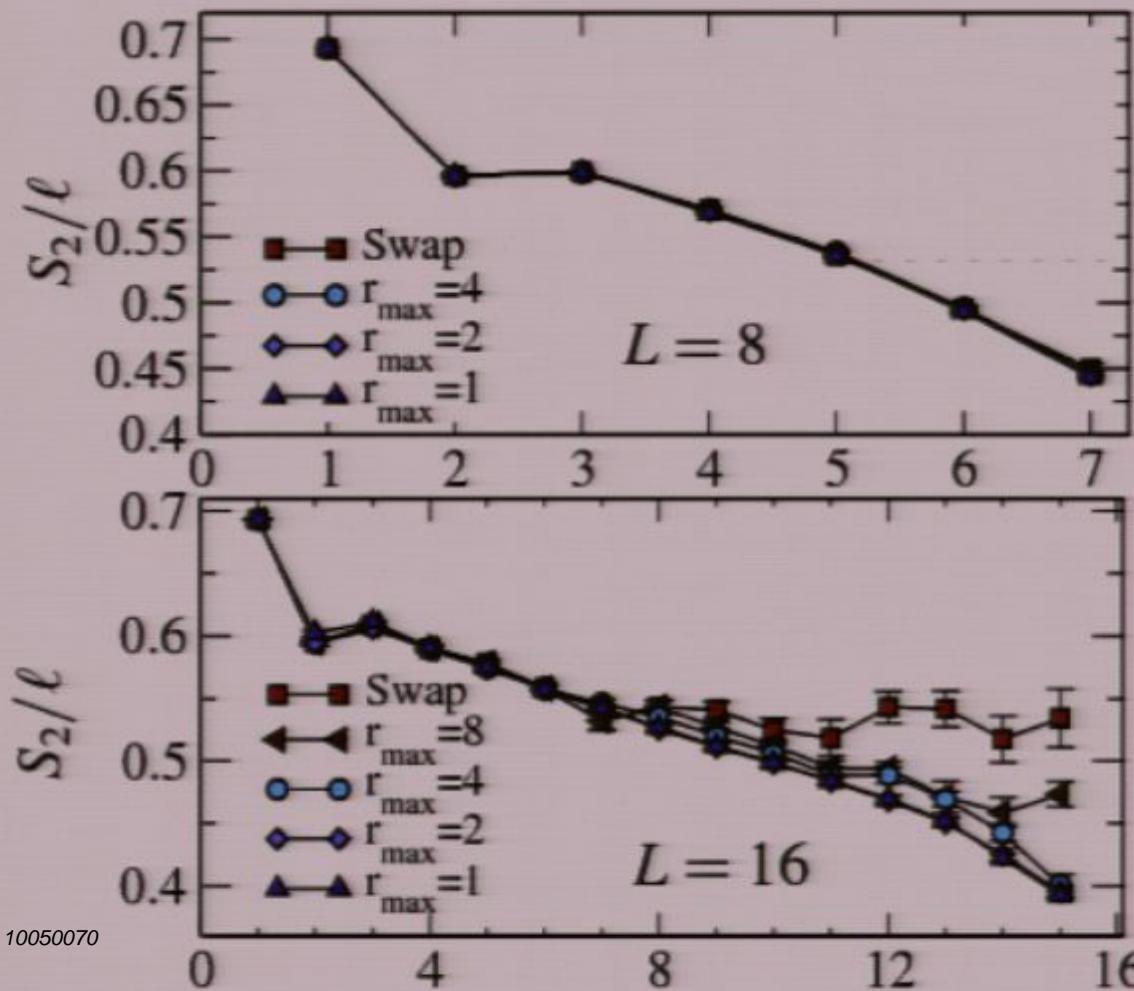


TWO-DIMENSIONAL RESULTS

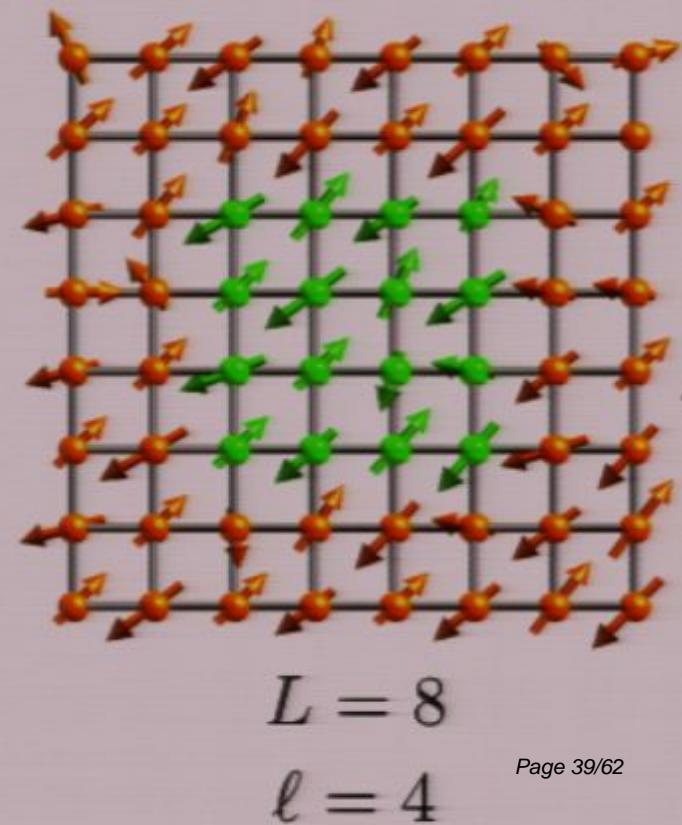


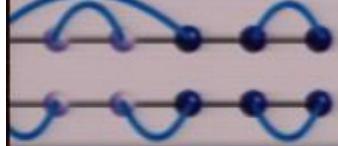
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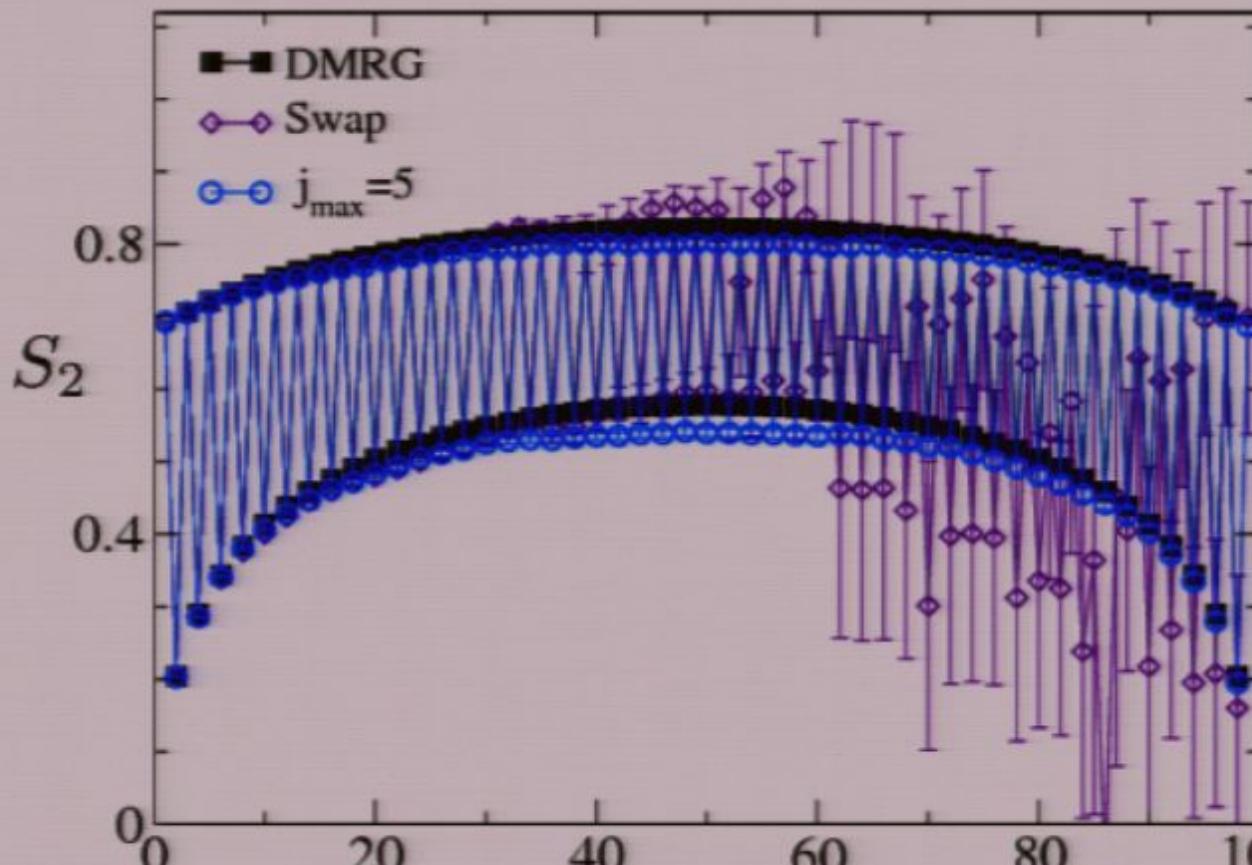
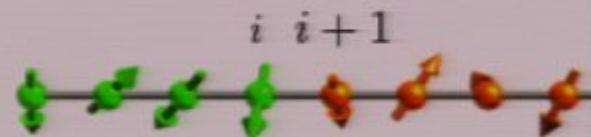




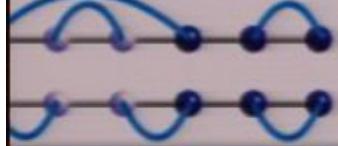
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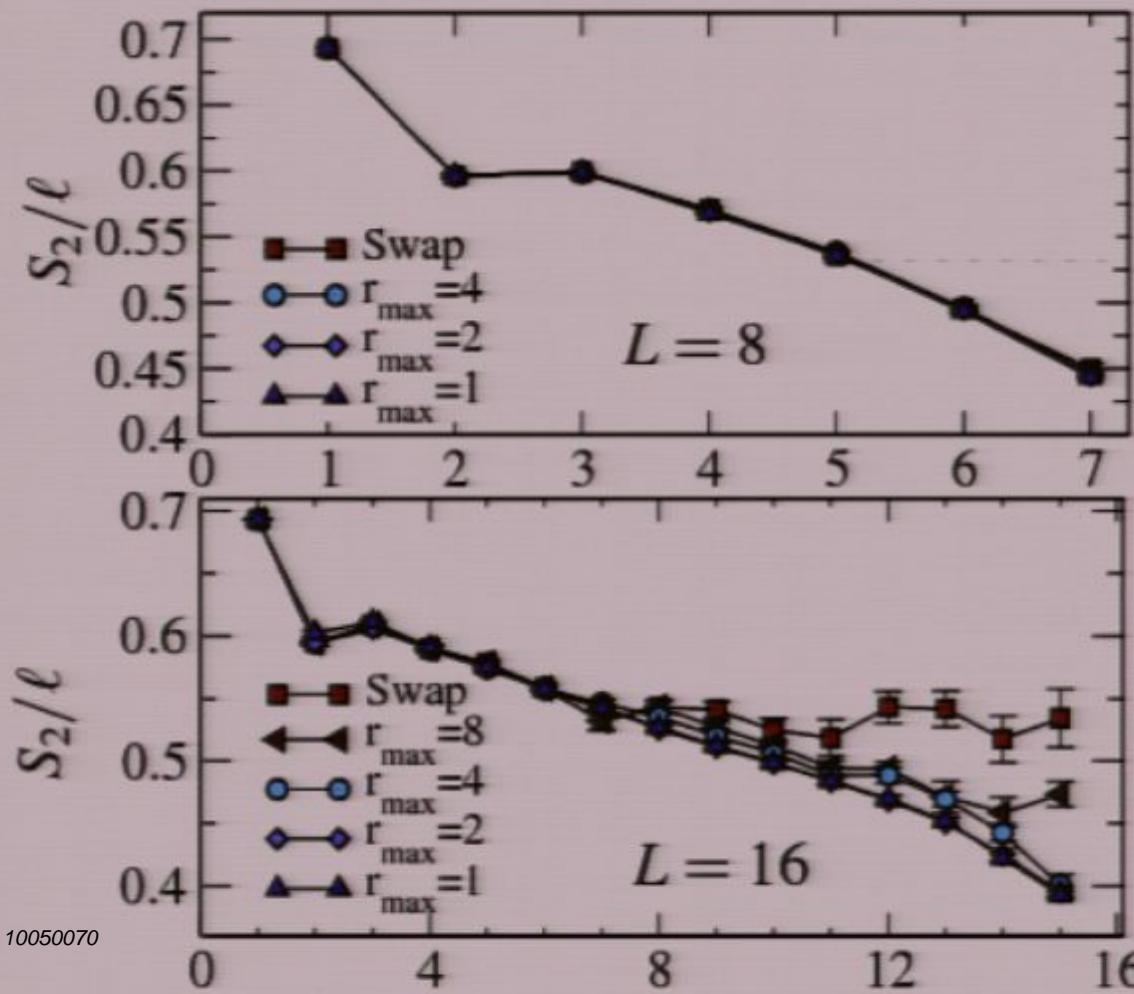
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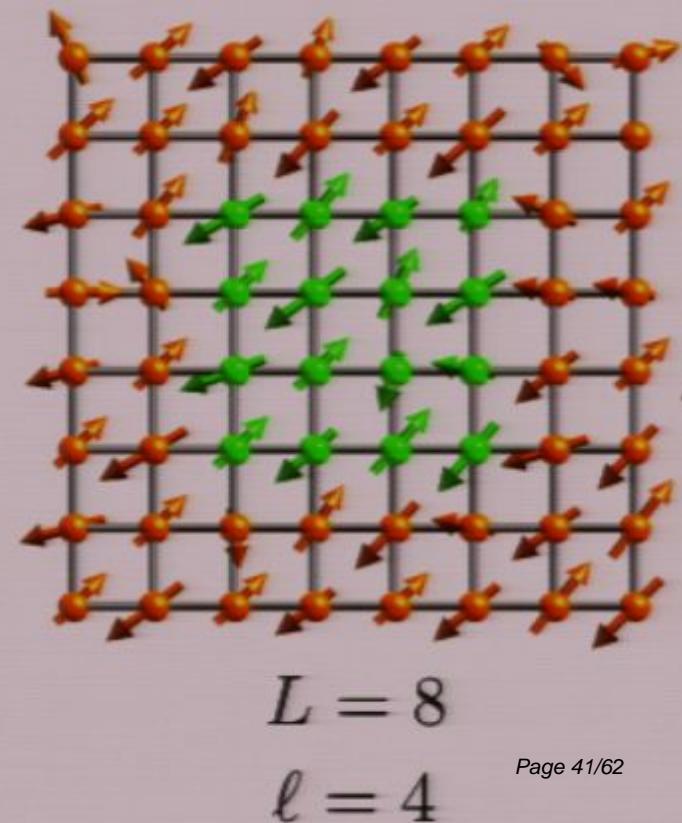
TWO-DIMENSIONAL RESULTS

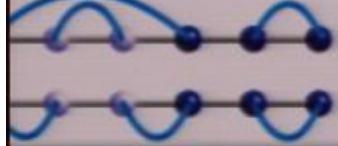
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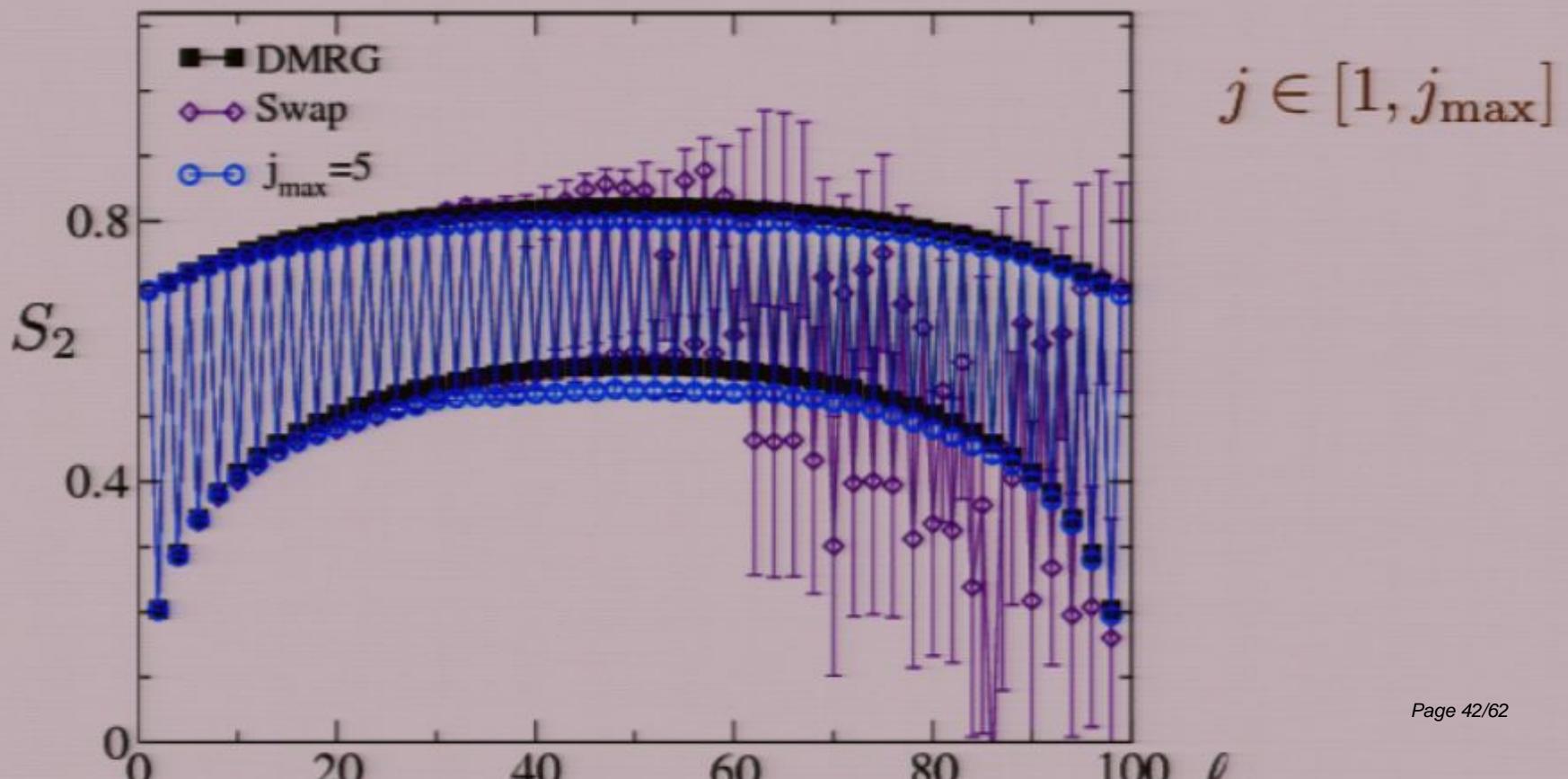
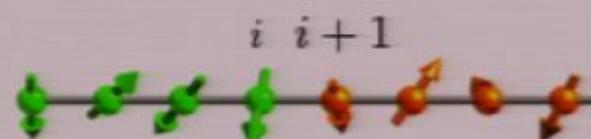


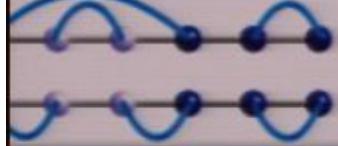


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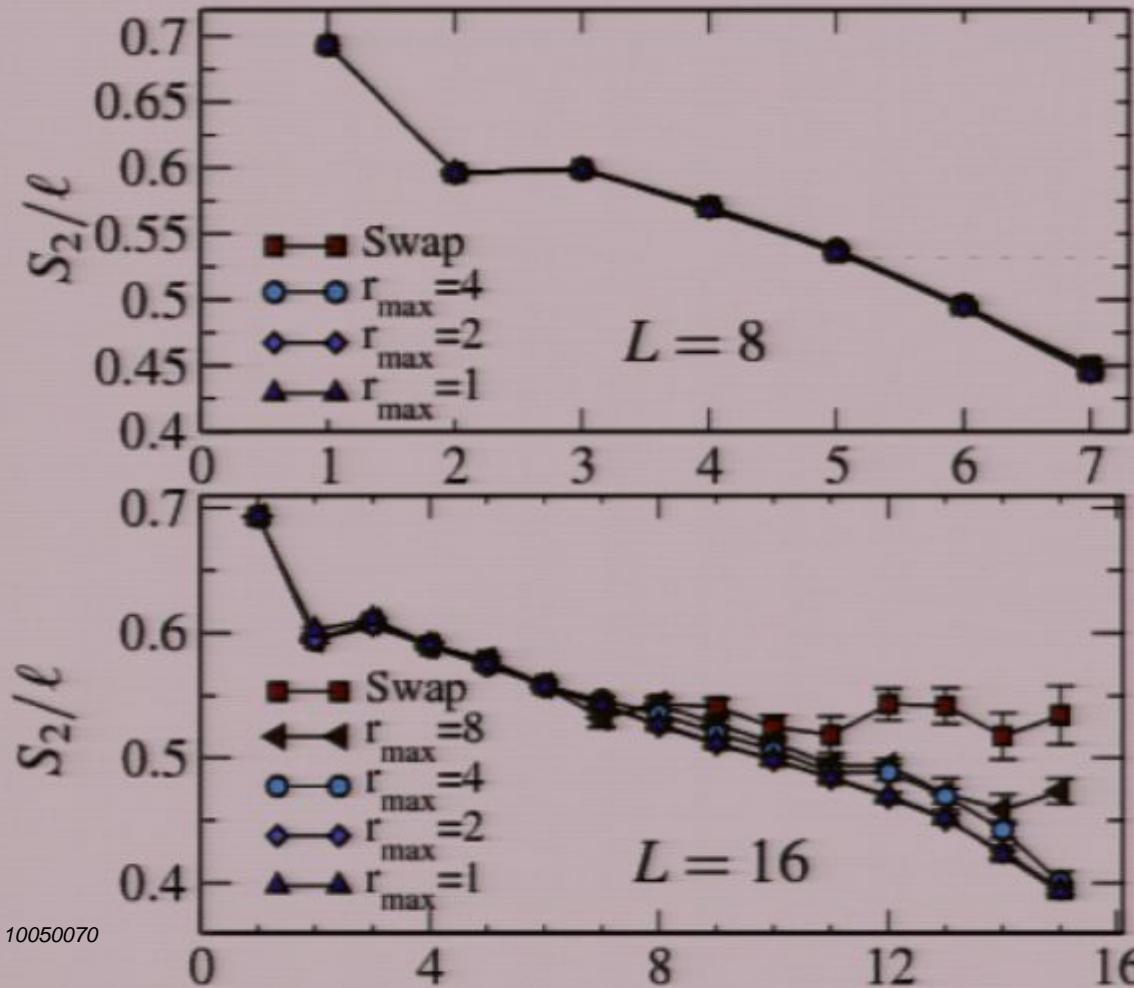


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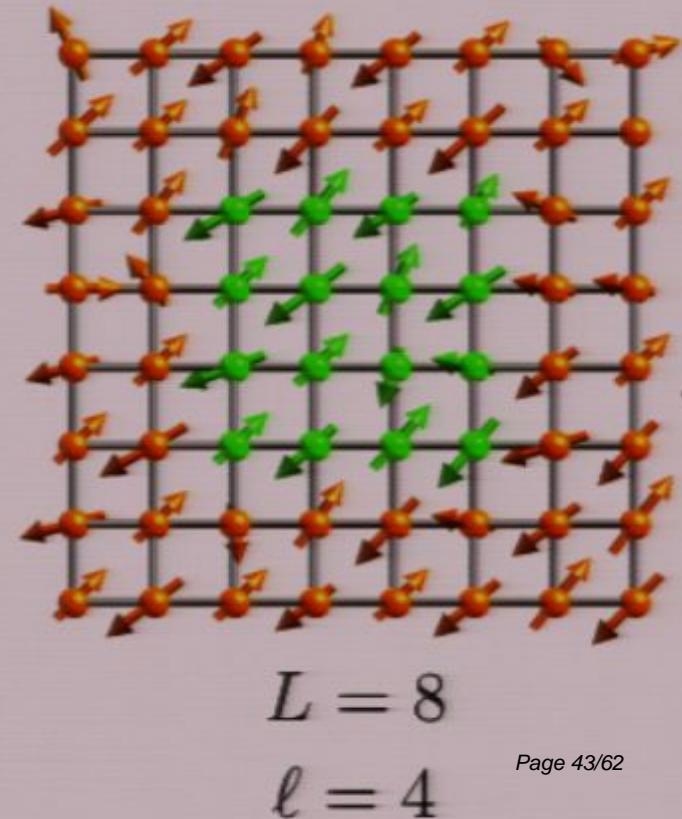


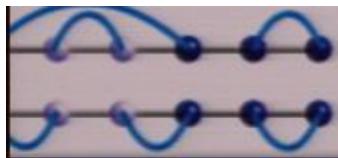
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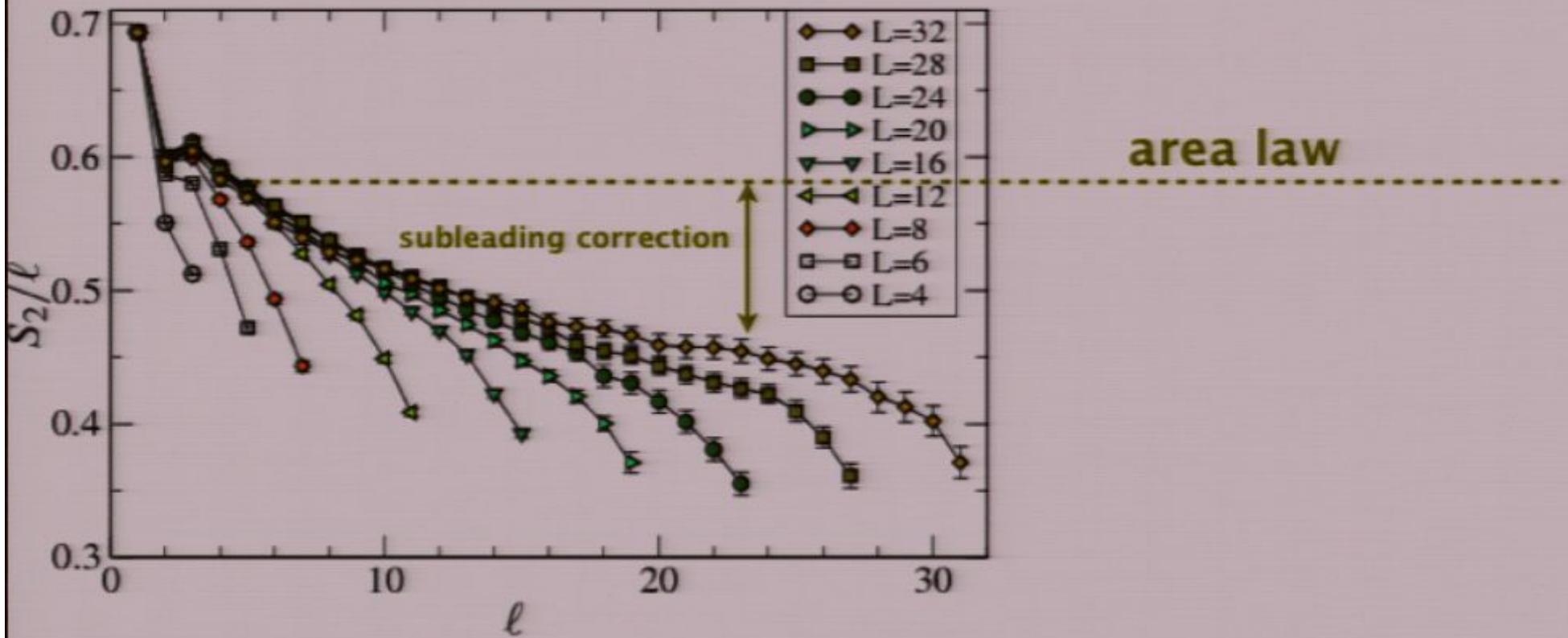
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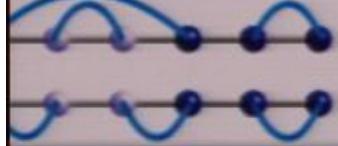




CHECK OF AREA LAW

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

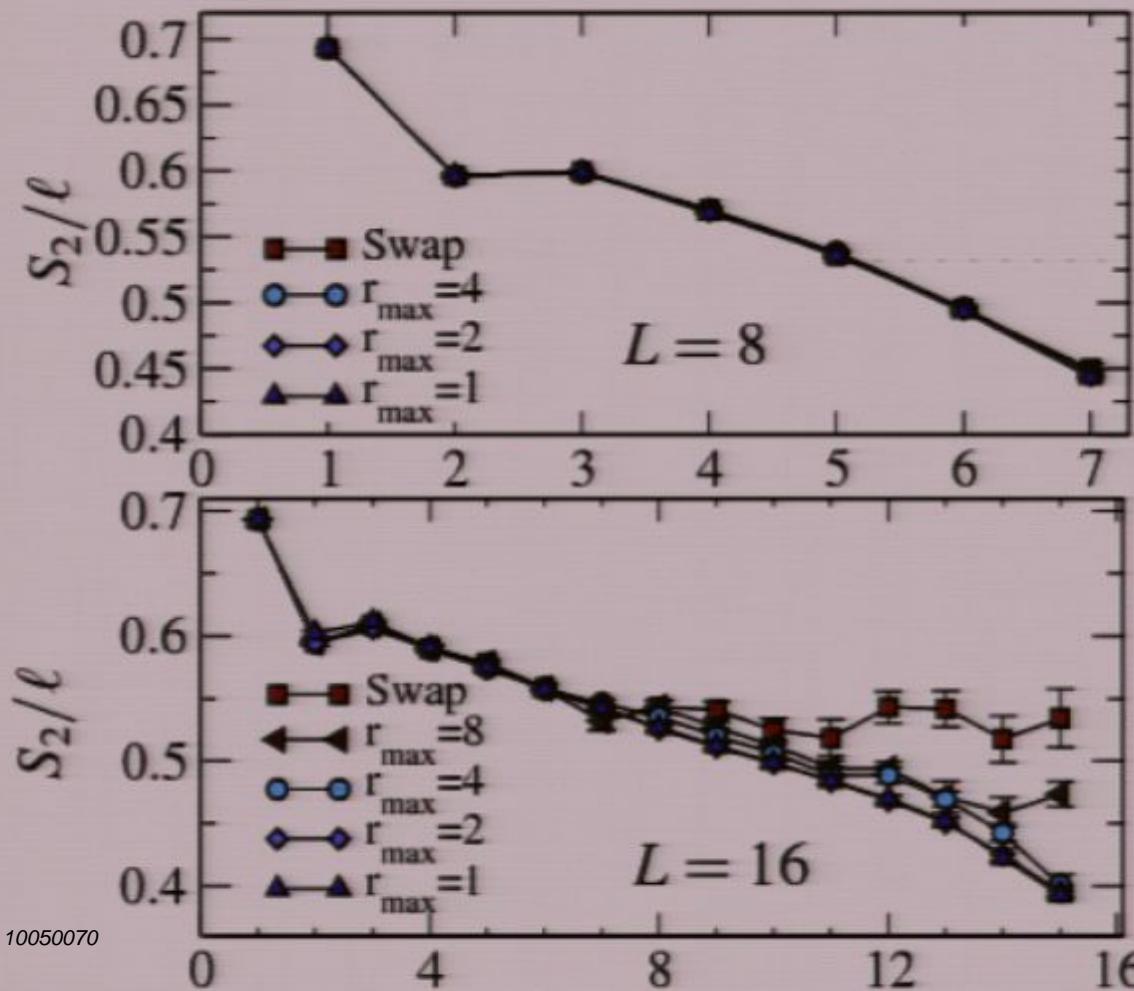




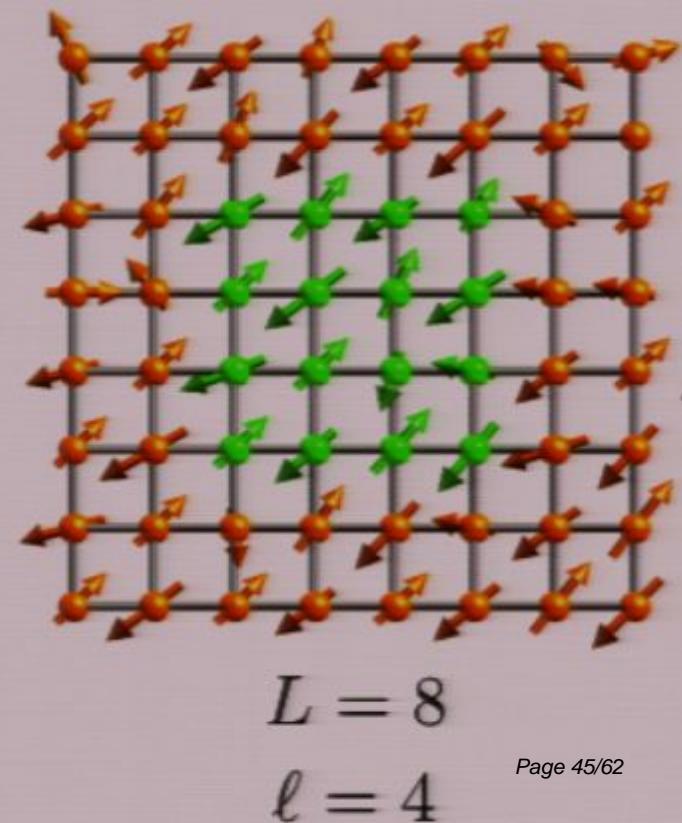
TWO-DIMENSIONAL RESULTS

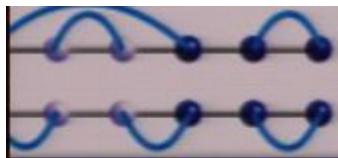
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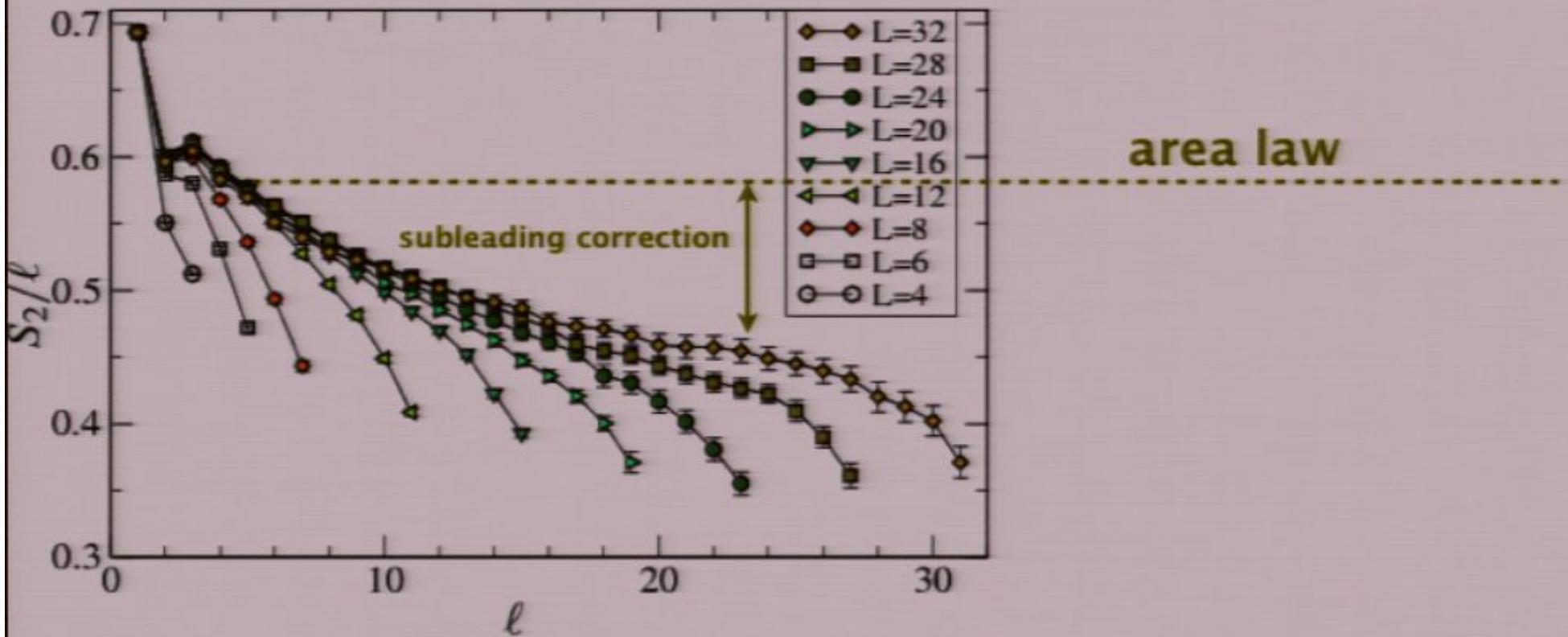
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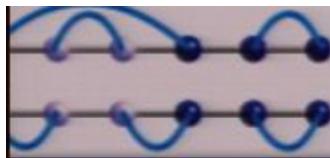




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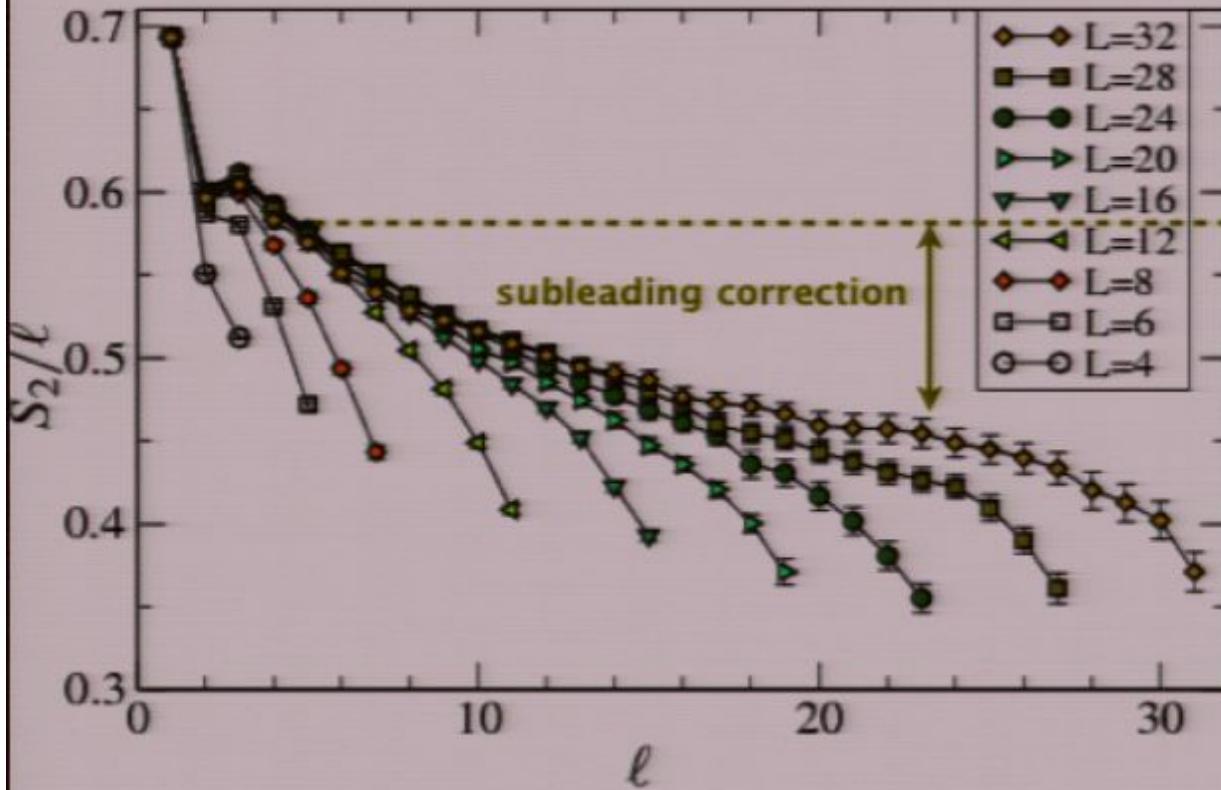
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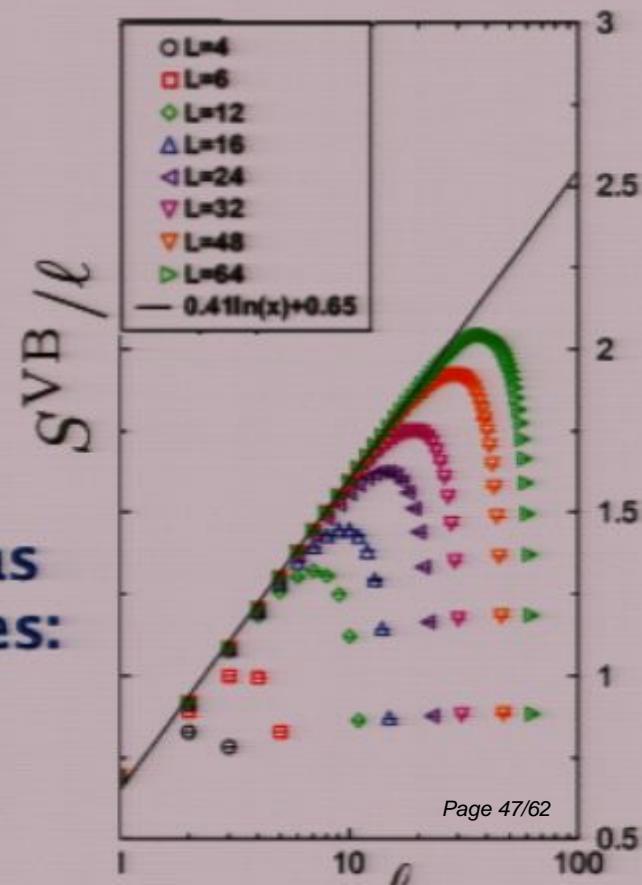


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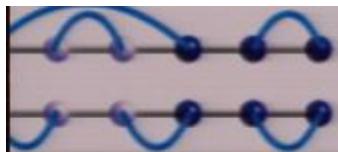
area law



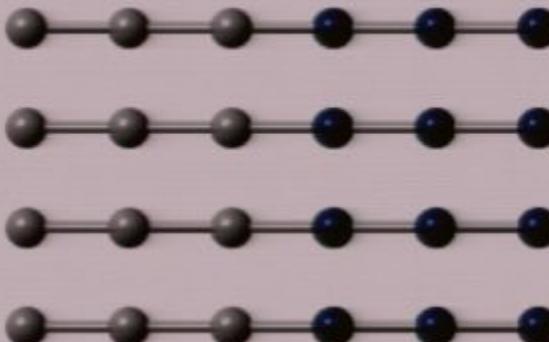
NOT a multiplicative log correction as suggested by other entropy measures:

$$S^{VB} = \ln(2)\langle N_A \rangle$$

$$S^{VB} \propto \ell \ln(\ell)$$



NOTES:

- More work needed on improving statistics/scalability:
 - combining ratio 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
- Strictly T=0 only

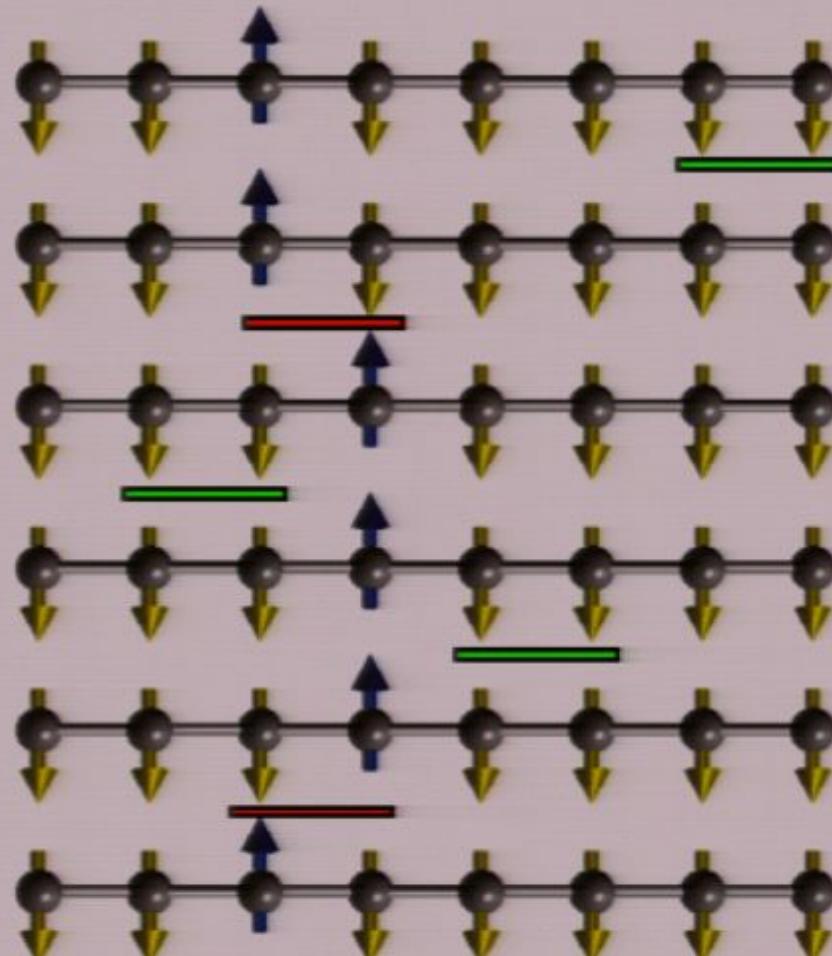
Calculating Renyi Entropy in finite-T QMC



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}

— = $S_i^z S_j^z$

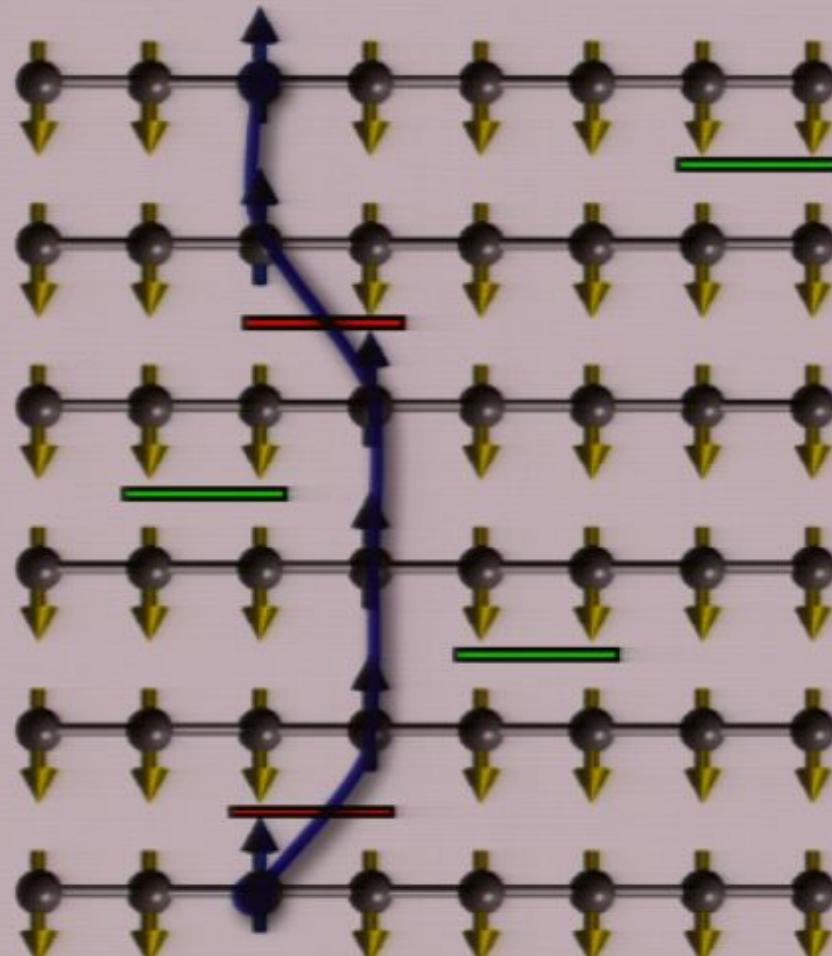
— = $(S_i^+ S_j^- + S_i^- S_j^+)$

state of the art method for
spin/boson models without the
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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).

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

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



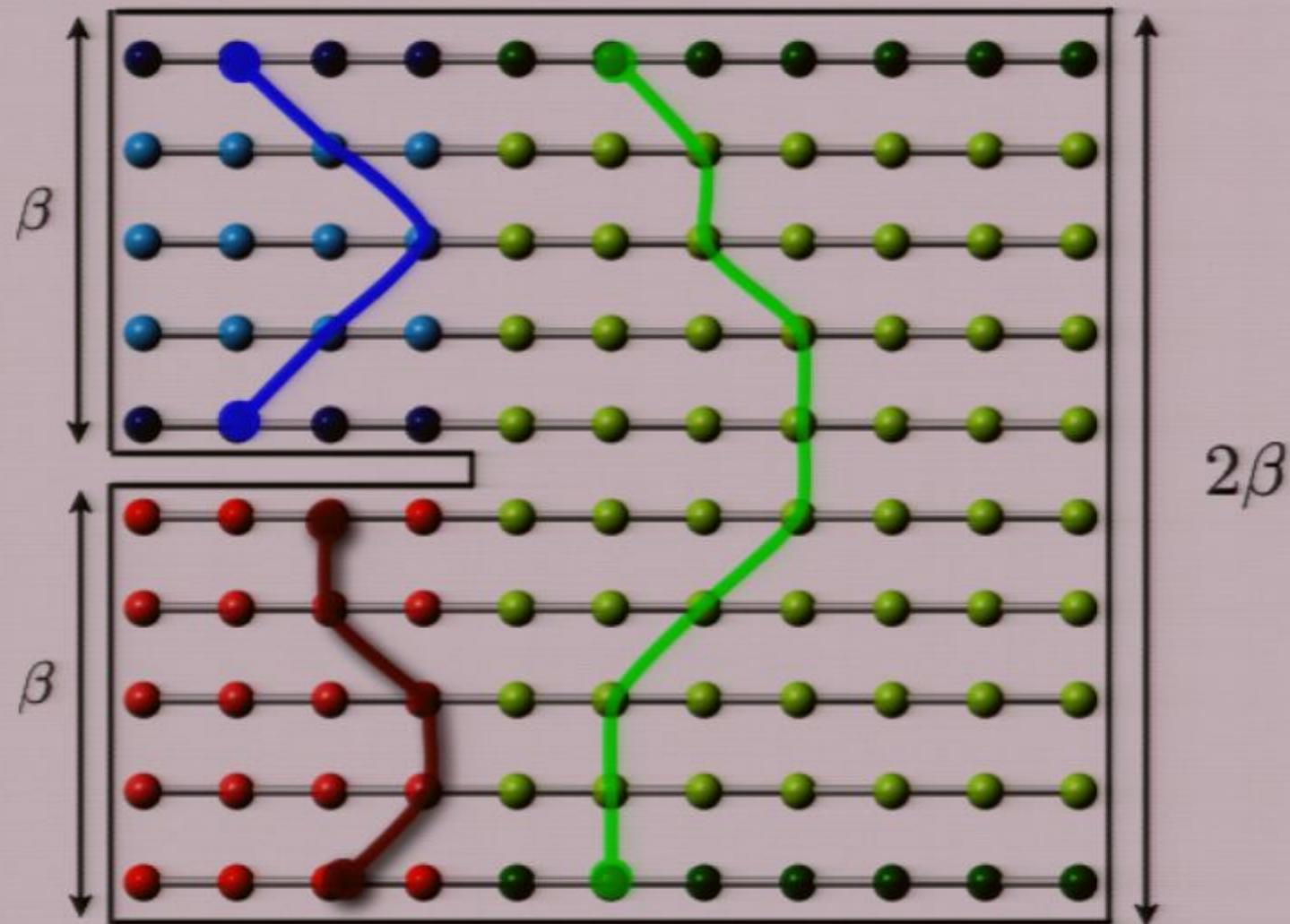
$$Z[A, 2, T]$$



$$Z[A, 3, T]$$

SSE SIMULATION CELL

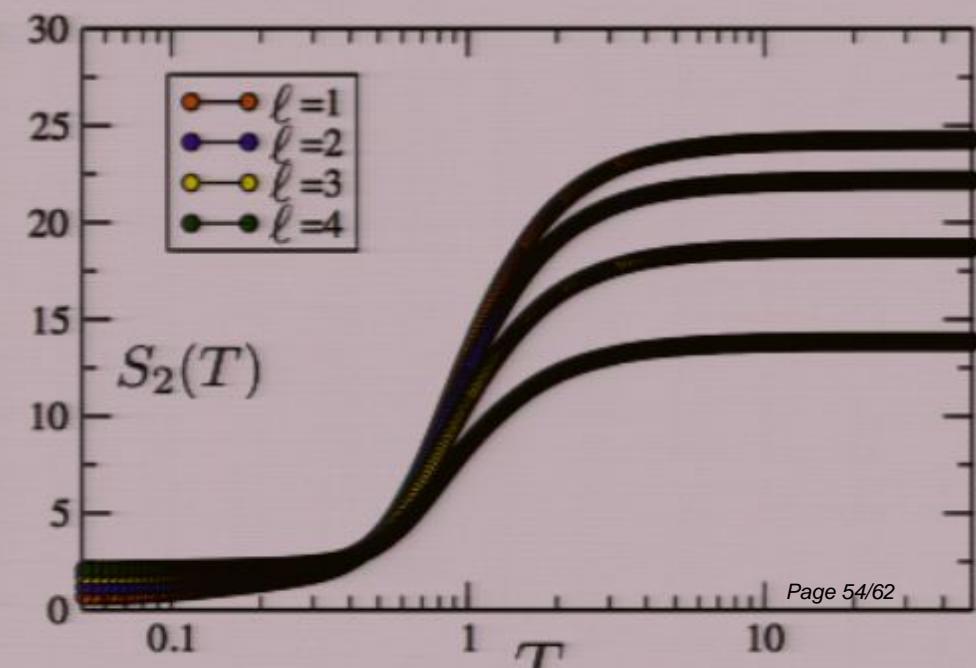
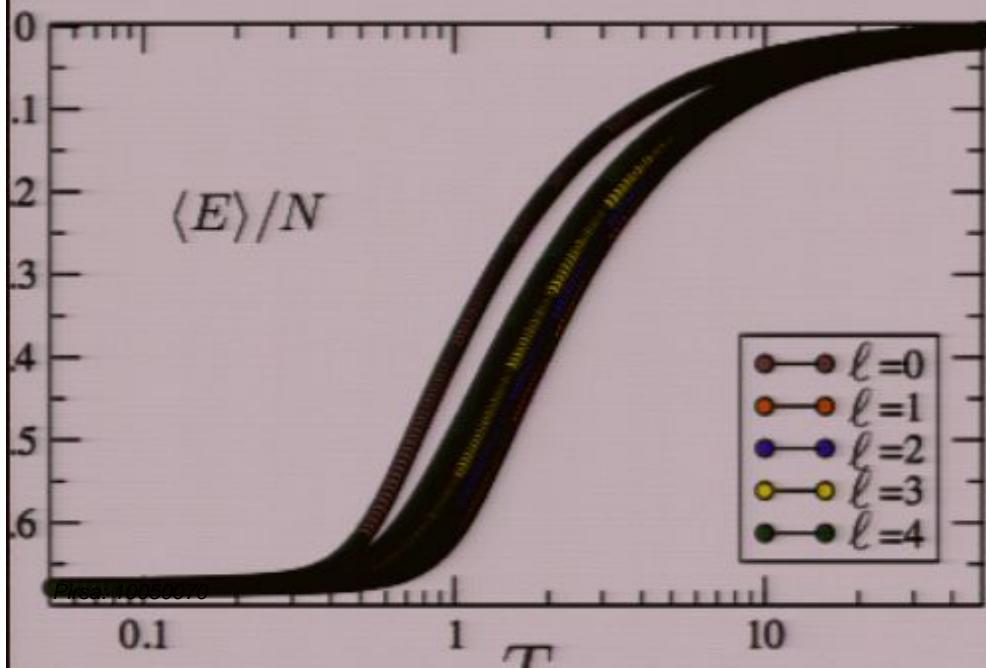
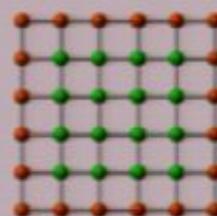
$Z[A, 2, T]$



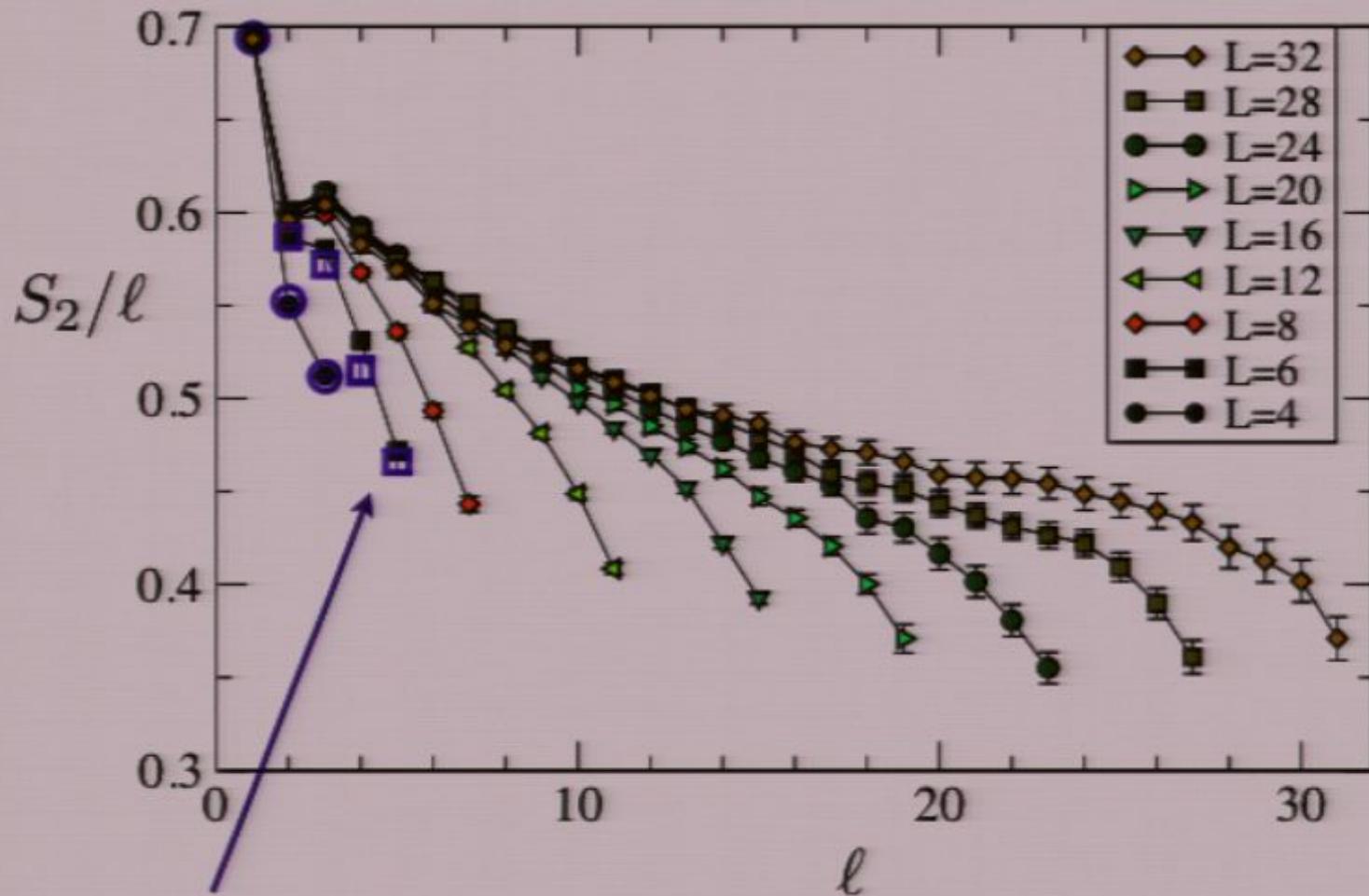
THERMODYNAMIC INTEGRATION

$$\begin{aligned}
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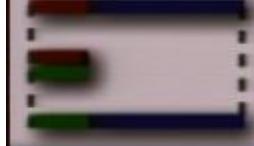
$L = 6$ Heisenberg model



THERMODYNAMIC INTEGRATION



SSE QMC with finite-T
integration

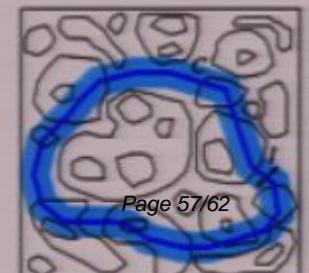
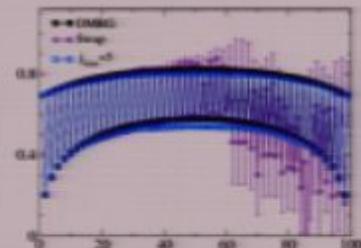
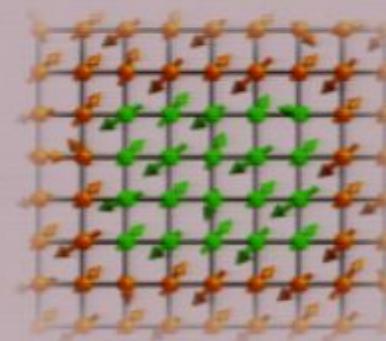
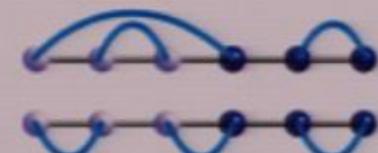


NOTES:

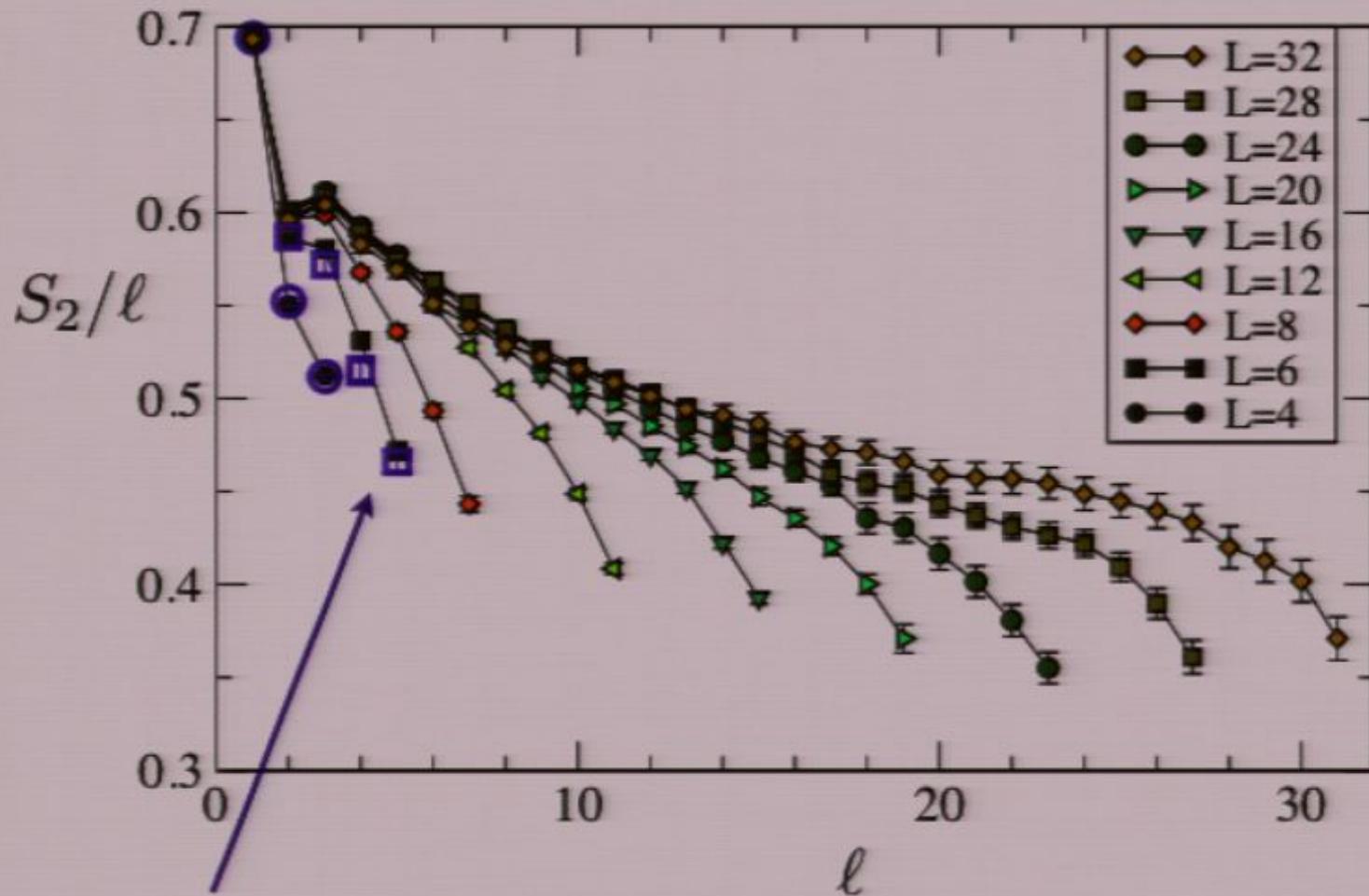
- Improvements can be made on thermodynamic integration (quantum version of umbrella sampling?)
- Easyish to code into any current SSE QMC code (realistic CM Hamiltonians, QCPs, cold atoms, etc...)
- Always scales as N and β

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.
- This effort less than 1 year old: expect rapid advances in scaling and efficiency.
- We are about to begin exploring subleading corrections at quantum critical points (and topological phases?).



THERMODYNAMIC INTEGRATION

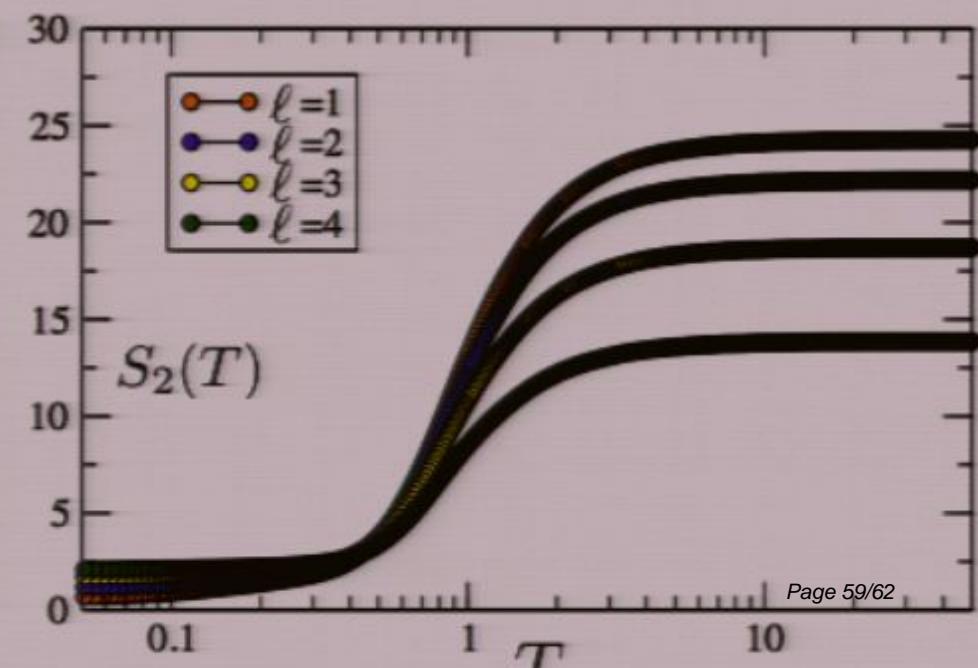
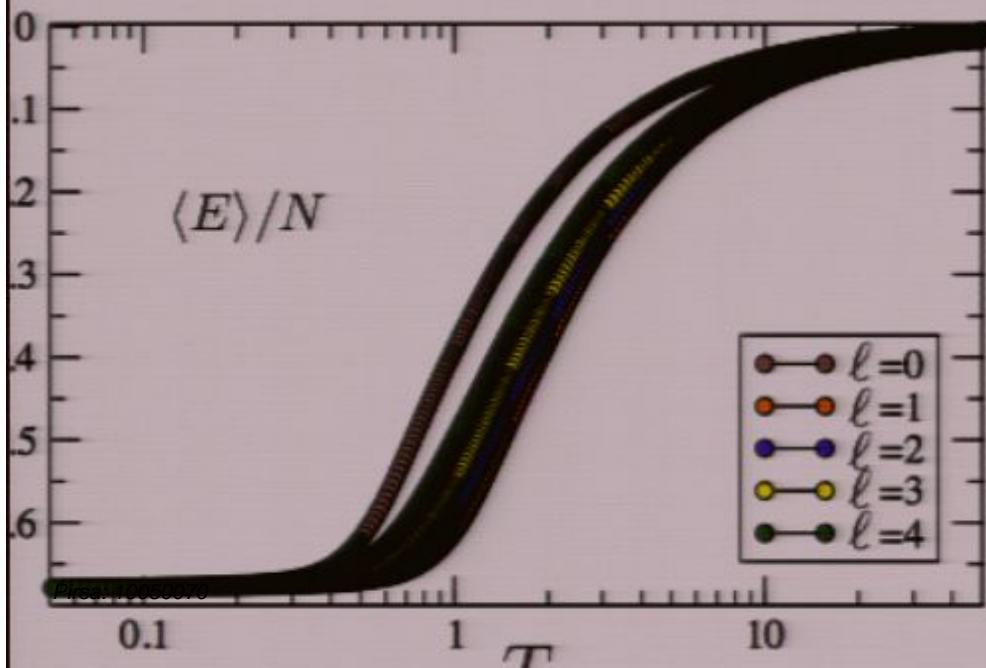
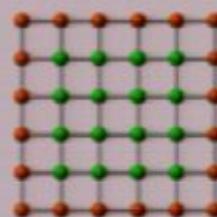


SSE QMC with finite-T
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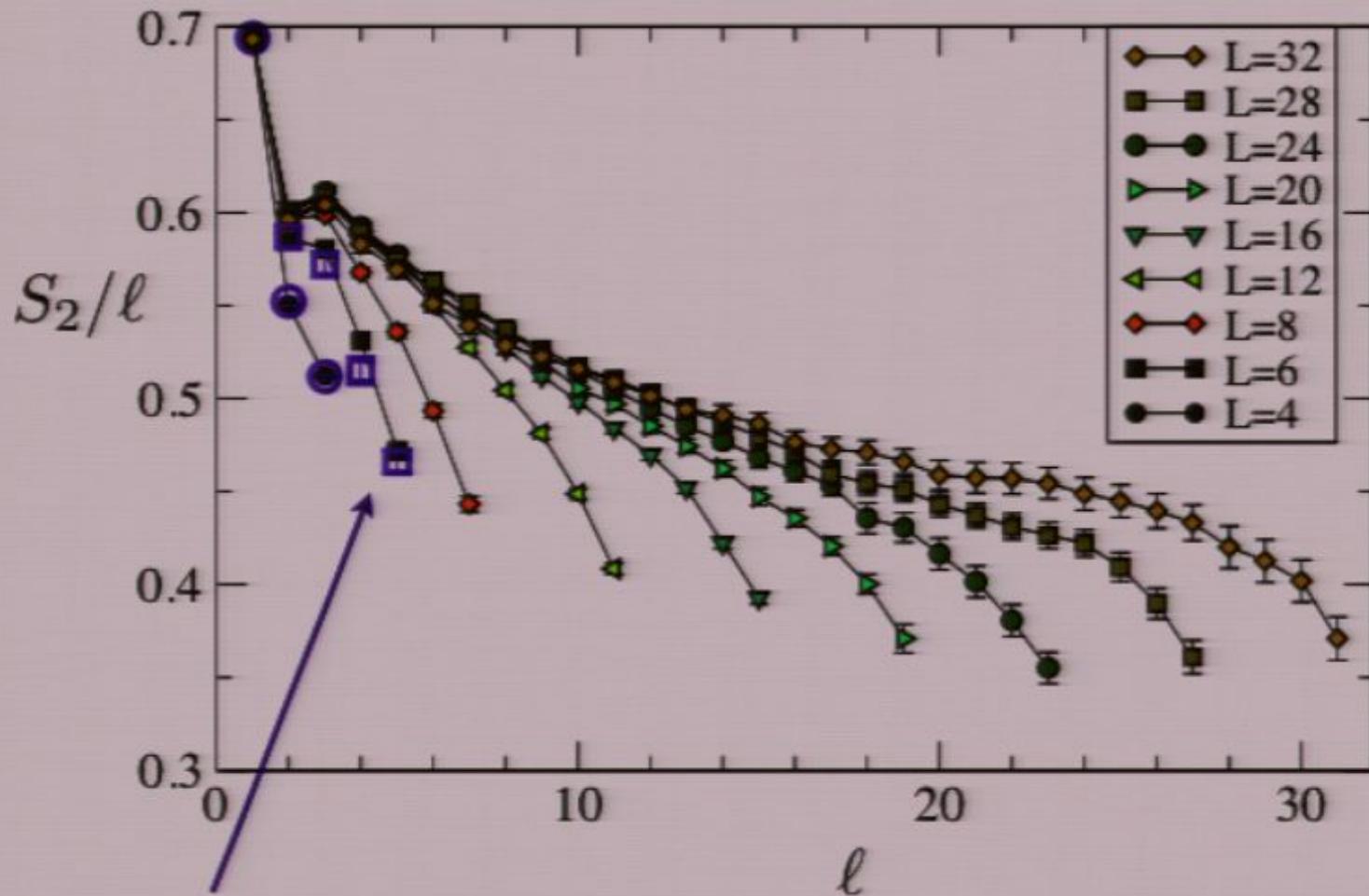
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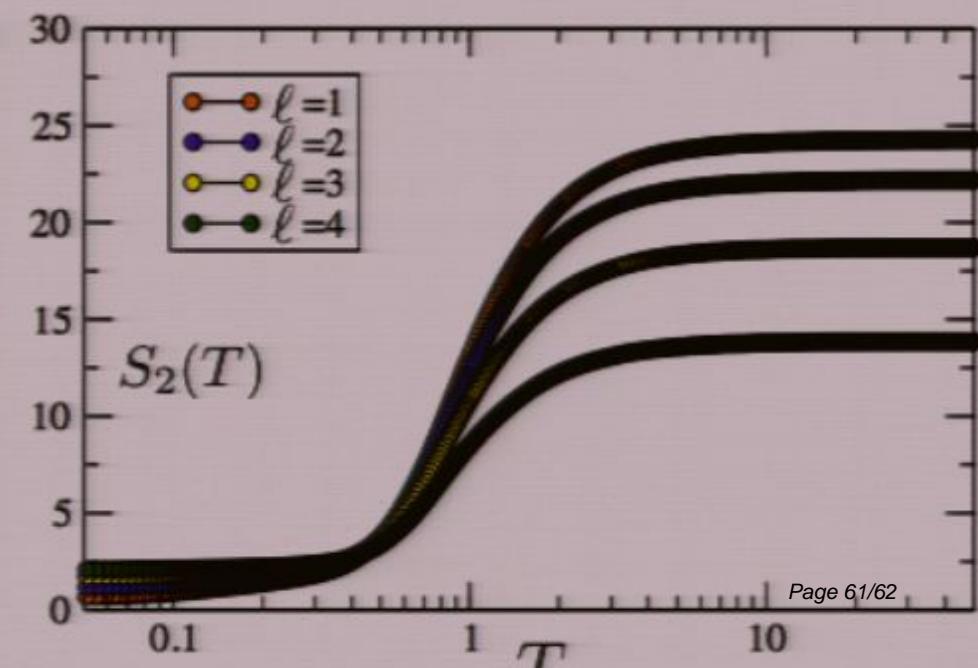
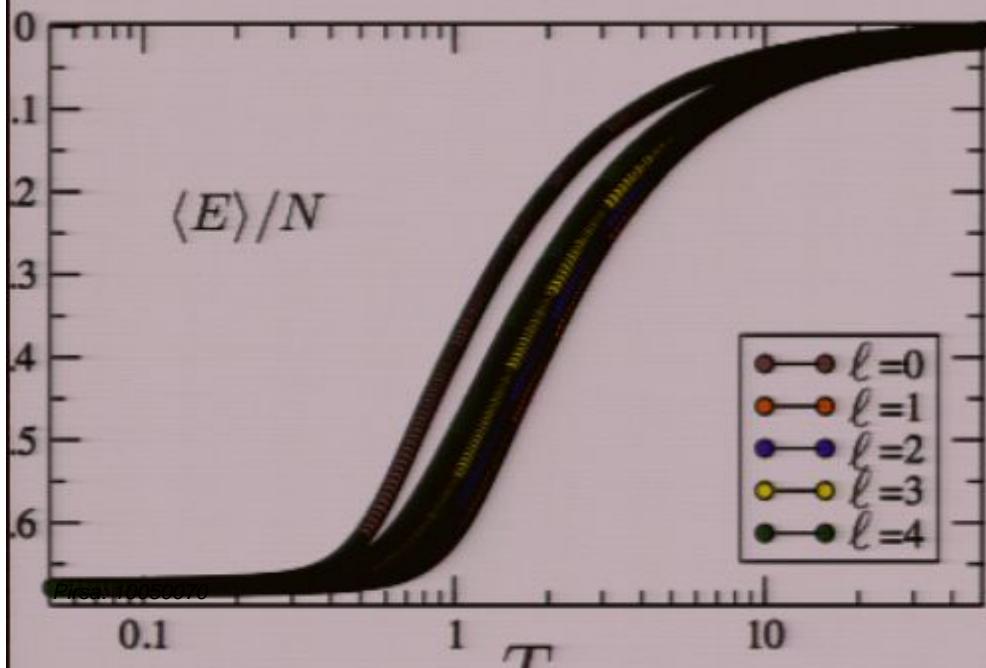
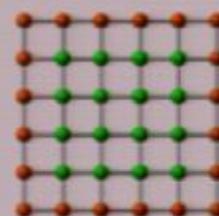


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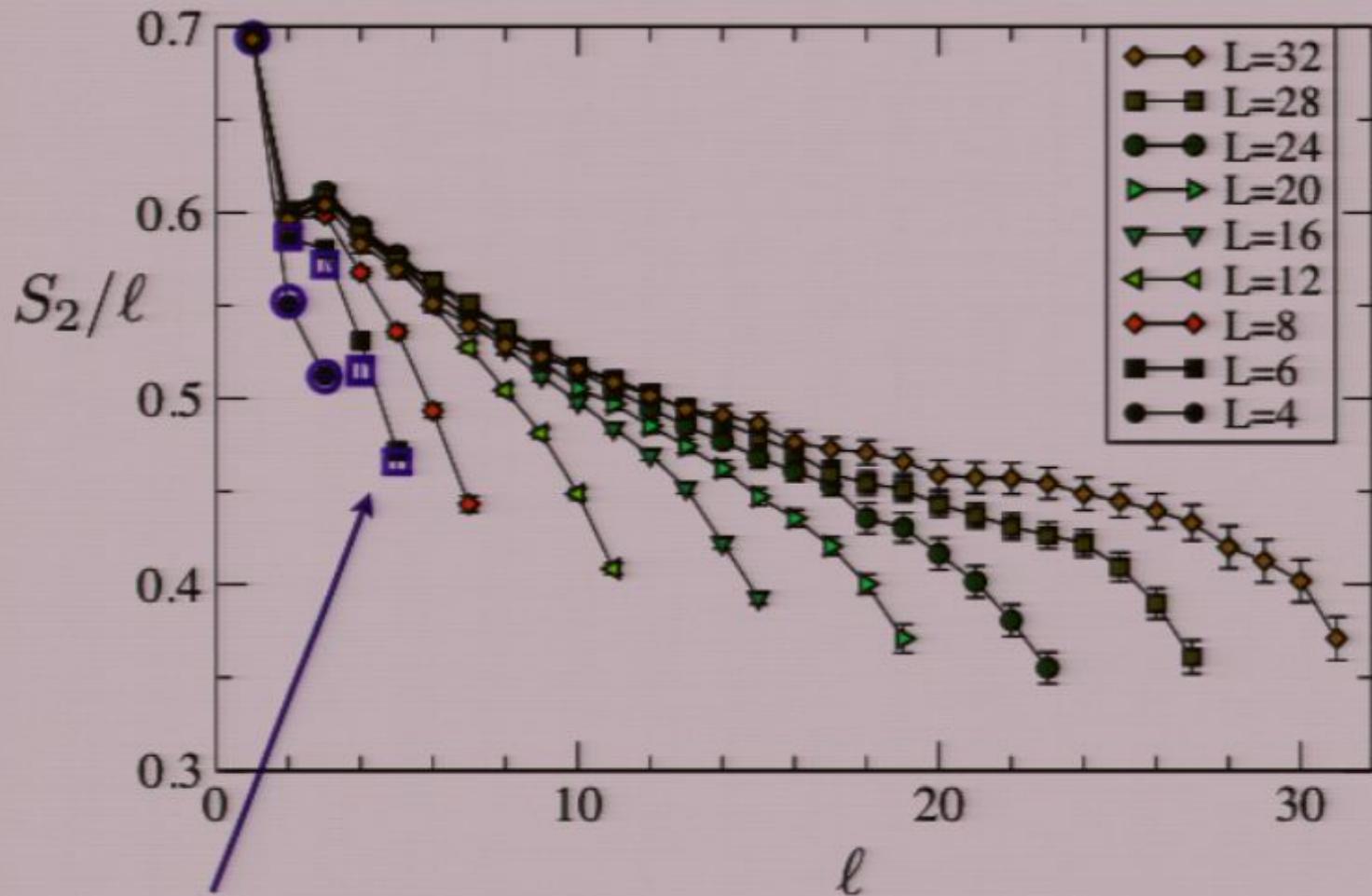
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