Introduction to DMRG

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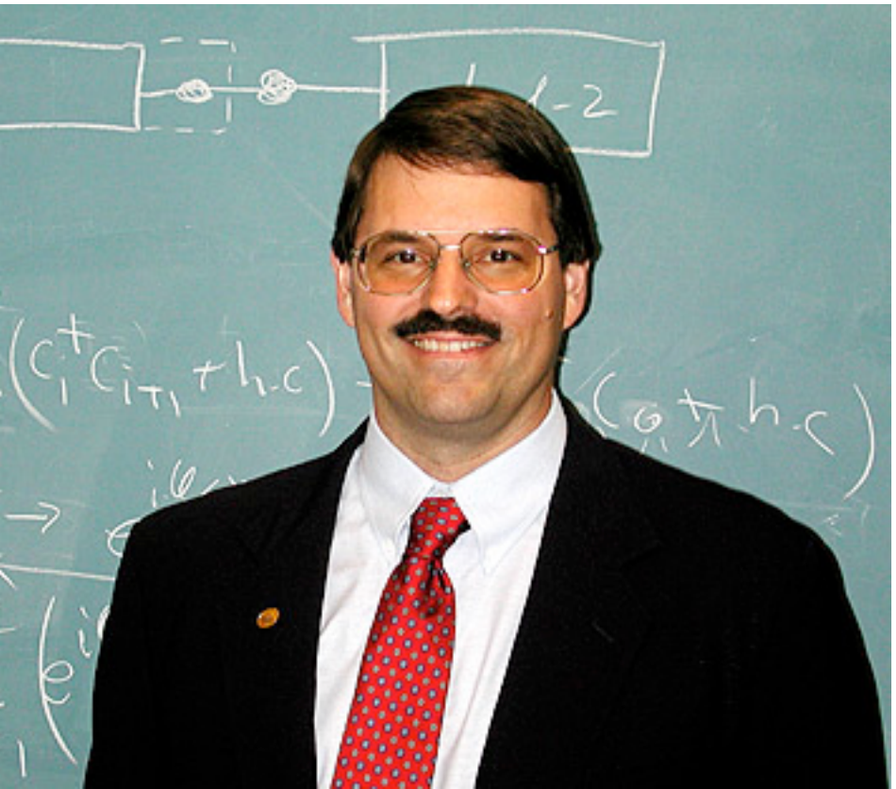
Outline

1) Density Matrix Renormalization Group - overview and basics

2) Entanglement Entropy in condensed matter systems

What is the Density Matrix Renormalization Group?

- DMRG is the established leading method for simulation of statistics and dynamics of **one-dimensional** strongly-correlated quantum lattice models.



Steve White

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

Why do we need DMRG?

- There are only a few “exact” numerical methods capable of tackling quantum many-body problems using classical computers

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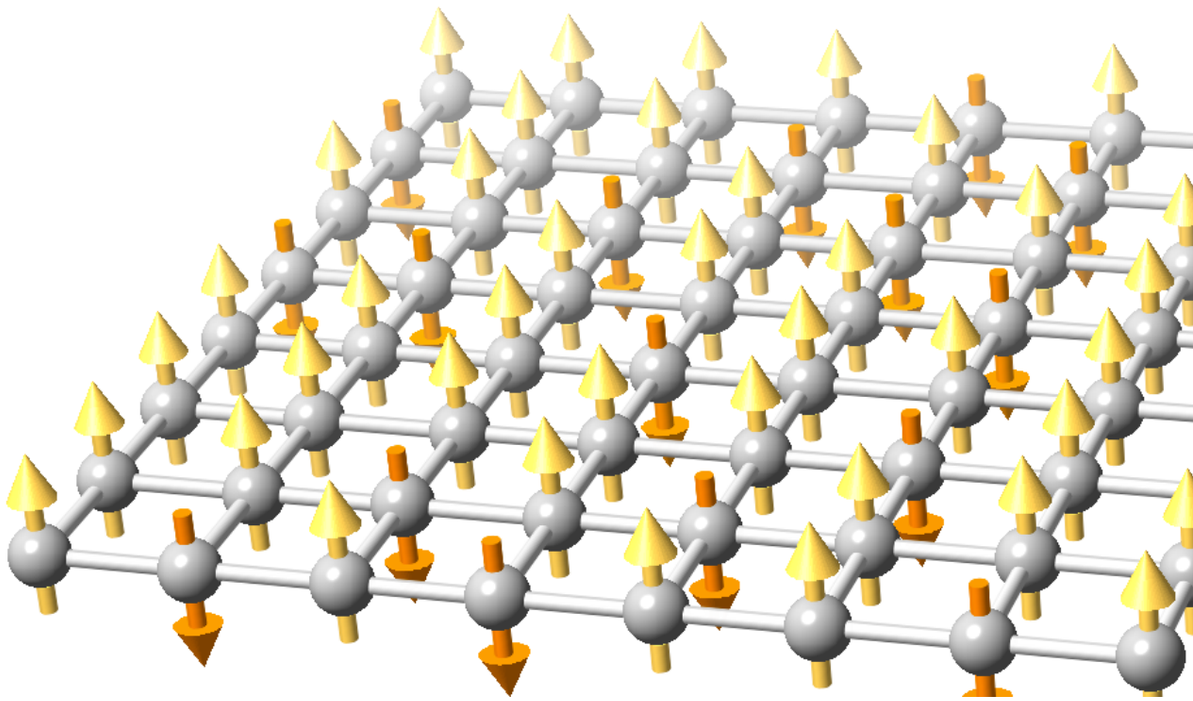
Exponential state space

$$\Omega = 2^N$$

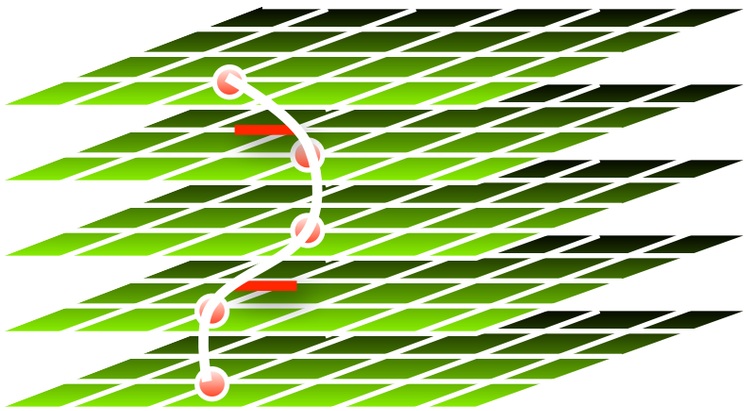


$$H = -J \sum_{\langle ij \rangle} S_i^z S_j^z$$

Why do we need DMRG?

- There are only a few “exact” numerical methods capable of tackling quantum many-body problems using classical computers

Quantum Monte Carlo simulations avoid this direct sum by statistical sampling based on random numbers.



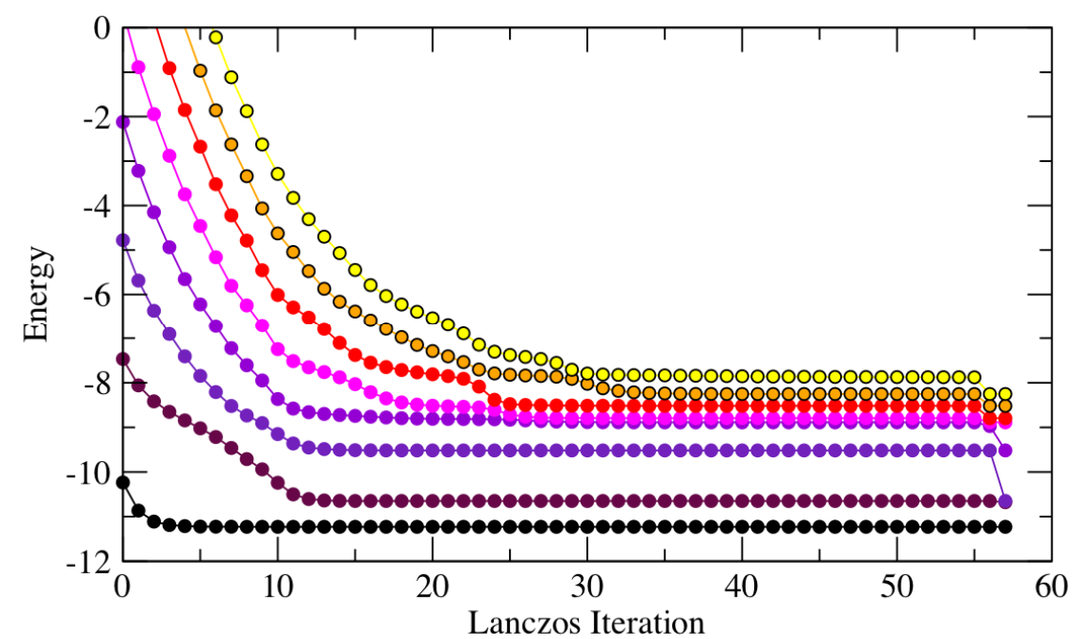
$$\langle \mathcal{O} \rangle = \frac{1}{Z} \sum_{i=1}^{\Omega} \mathcal{O}_i e^{-\beta E_i}$$

Cannot simulate fermions (or frustrated spins)

Why do we need DMRG?

- There are only a few “exact” numerical methods capable of tackling quantum many-body problems using classical computers

Exact Diagonalization

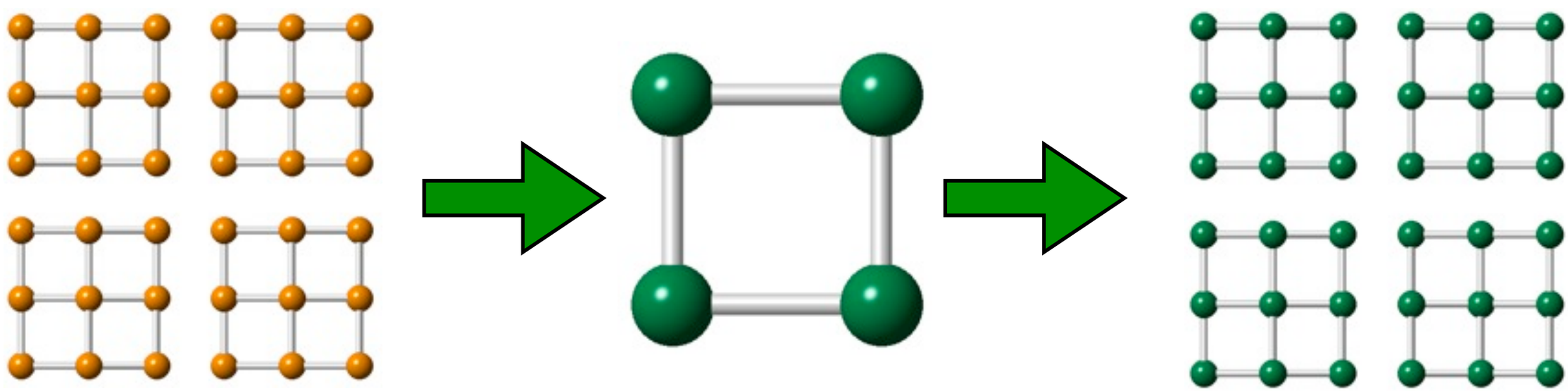


Exponential Hilbert Space: 2^N

Maximum number of S=1/2 spins: 40~44

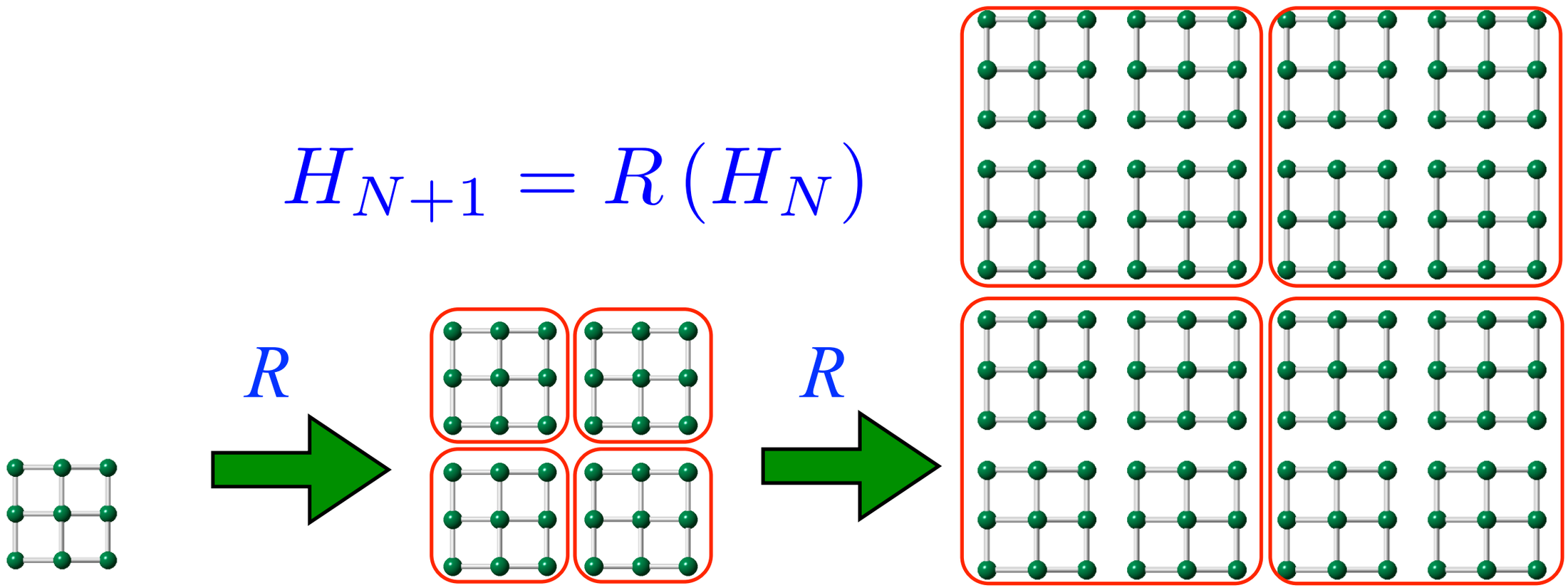
Renormalization Group

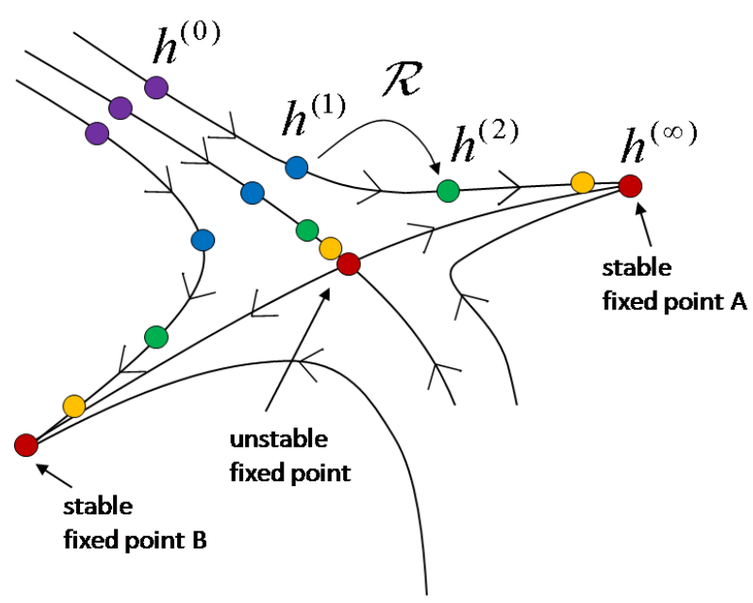
- Reduce the size of this Hilbert space through some clever decimation procedure
- Keep only the important information
- Perform an ED using the remaining Hilbert space



Renormalization Group

$$H_{N+1} = R\left(H_N\right)$$

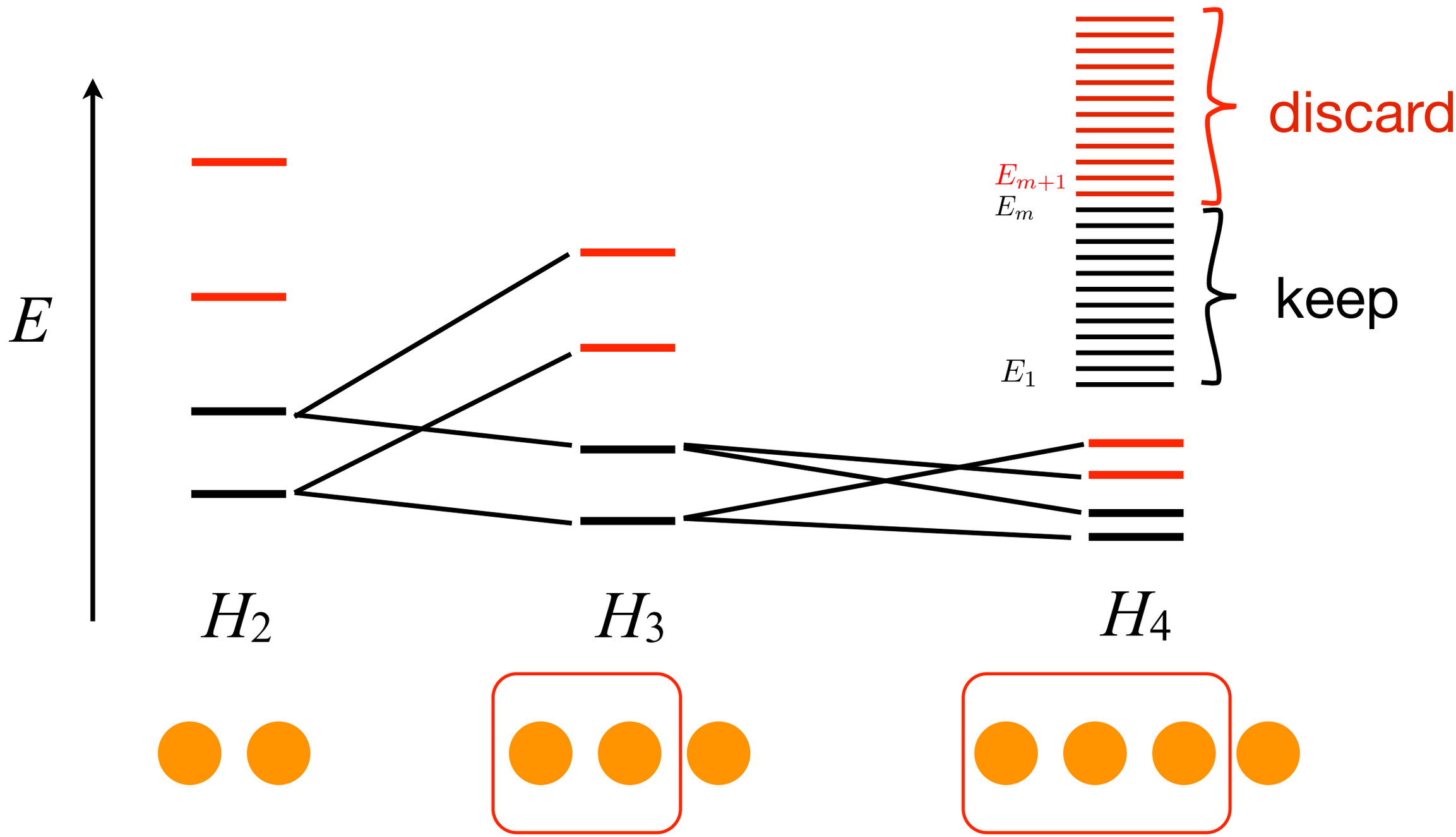




see: Tomorrow's talks

Wilson's Numerical RG

- Reduce the size of the Hilbert space by an RG-like procedure that truncates the **energy levels**

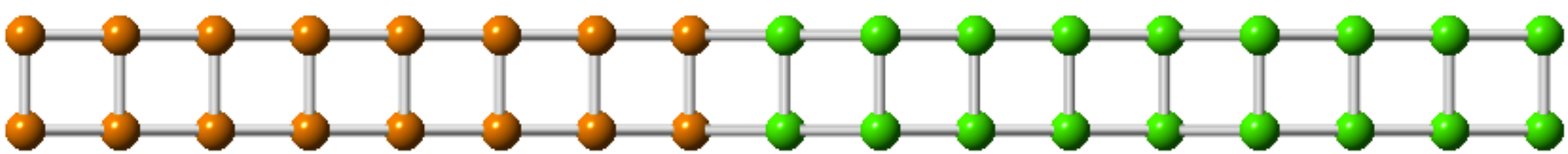


this can give very poor results

- Truncating the higher energy eigenvalues only works well for a few specific models - fails in general

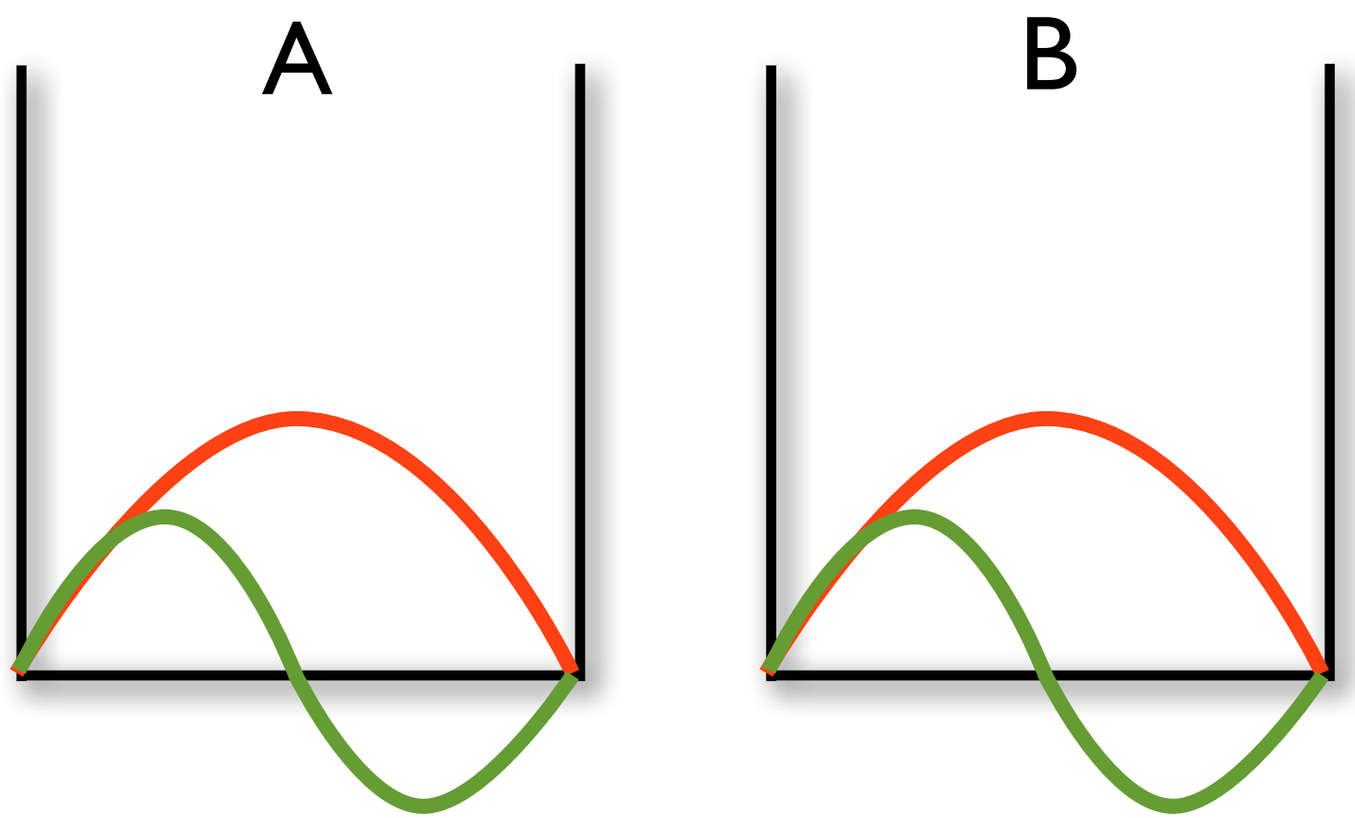
- 20 years after Wilson's original idea, Steve White fixed the method to produce DMRG

- The right quantity to truncate is the number of **entanglement** degrees of freedom represented



Particle in a box

- Consider a particle in a box



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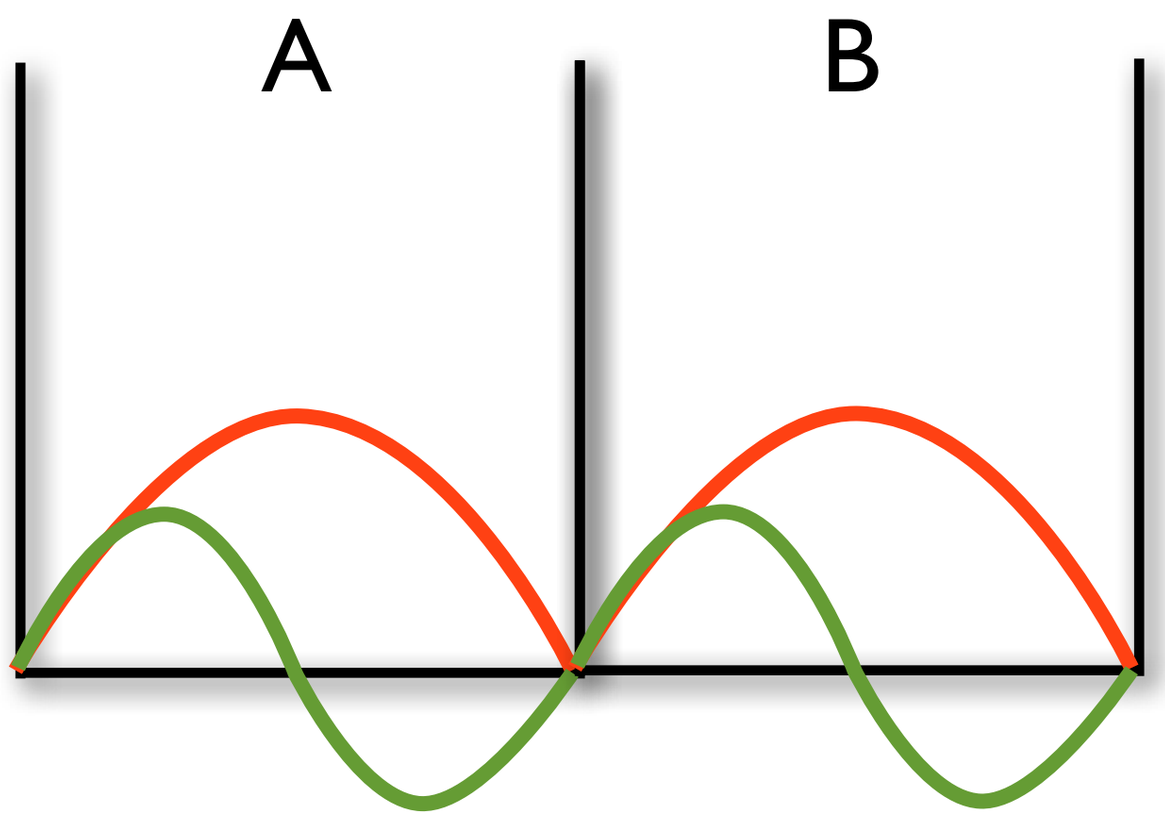
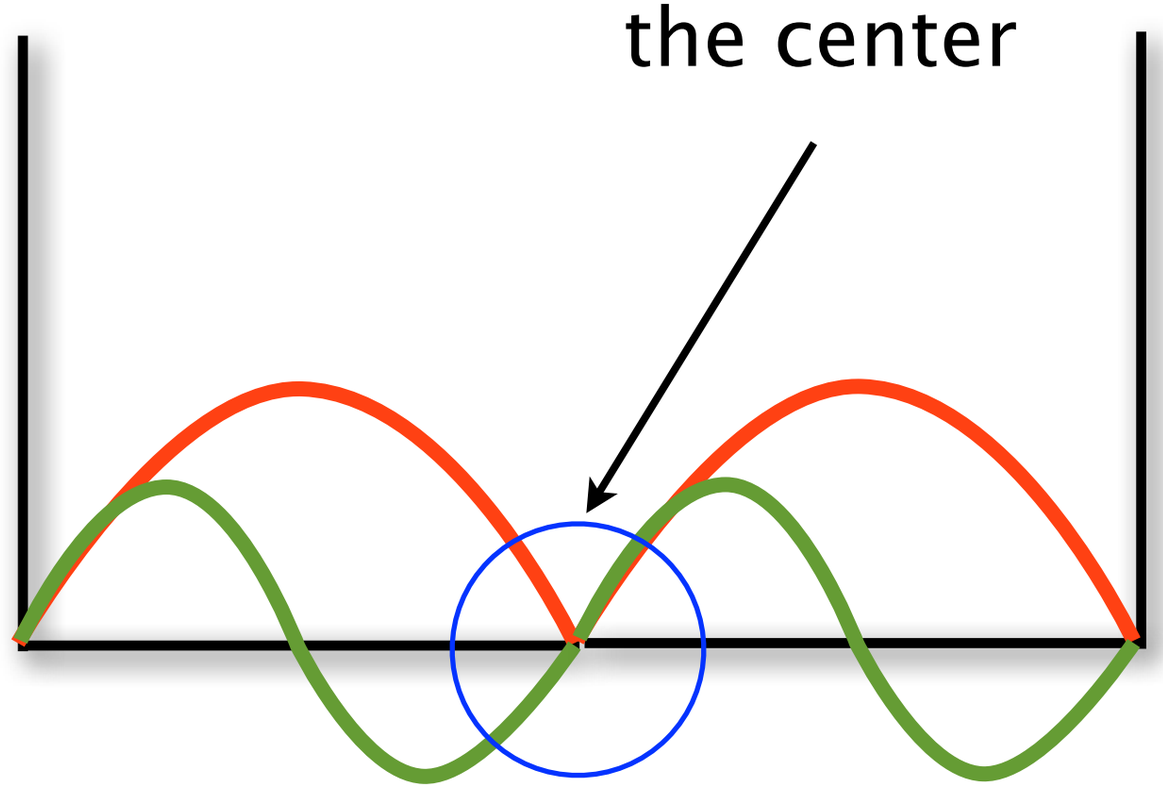


Particle in a box

- Consider a particle in a box

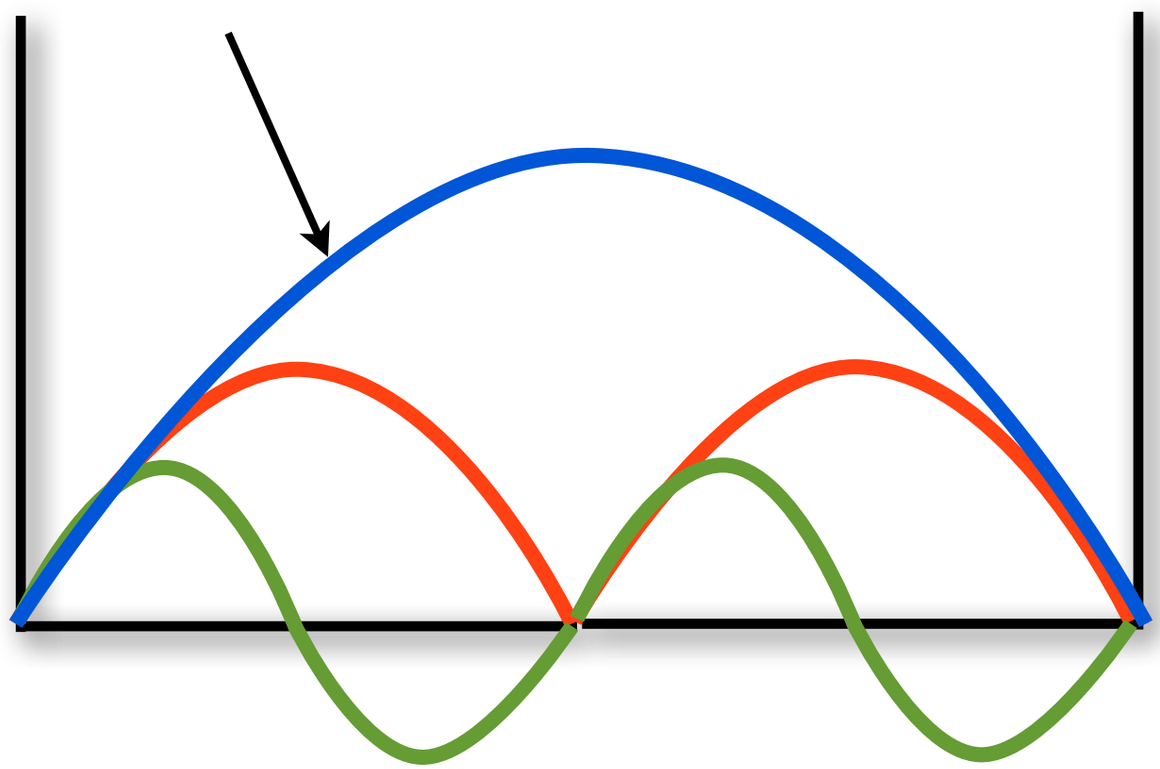
Solutions built from the smaller blocks have a node at the center



Particle in a box

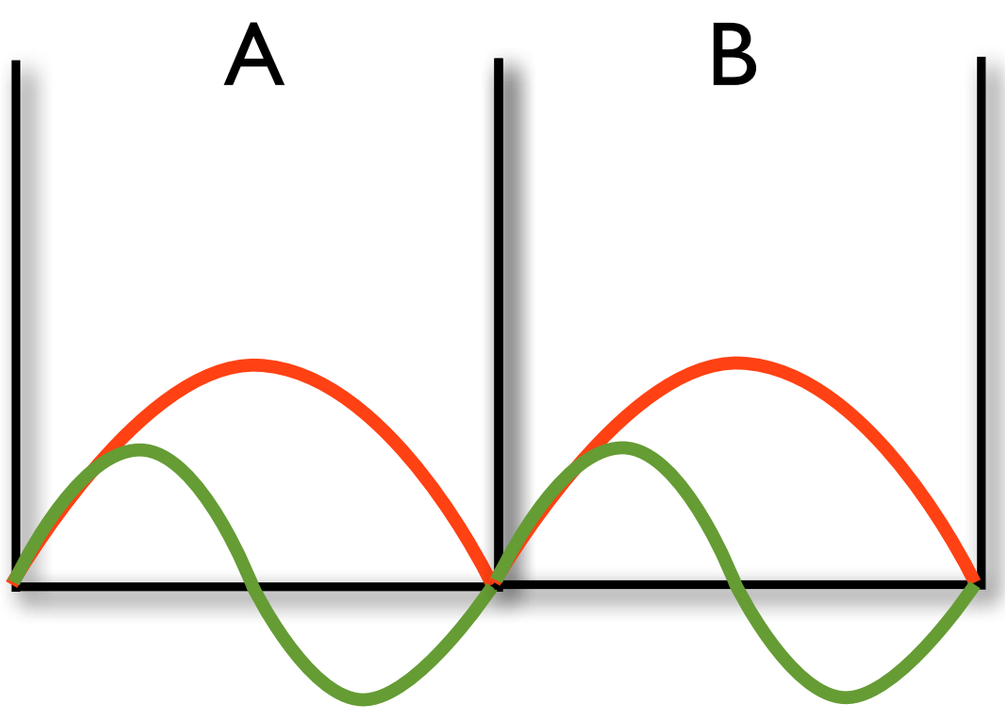
- Consider a particle in a box

System ground state ≠ product of subsystem low energy states



Numerical RG results

- 10 blocks (2048 sites), 8 states kept
- Very poor results
- Treatment of boundary condition is critical

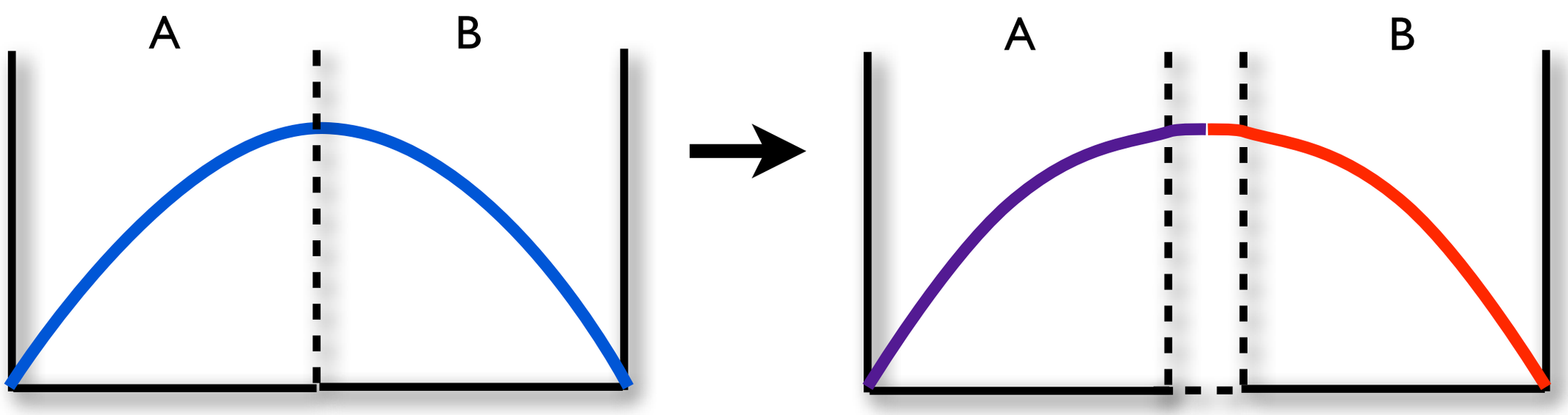


State	Exact	NRG
E_0	2.351×10^{-6}	1.9207×10^{-2}
E_1	9.403×10^{-6}	1.9209×10^{-2}
E_2	2.116×10^{-5}	1.9714×10^{-2}

S.R. White and R.M. Noack, PRL 68, 3487 (1992)

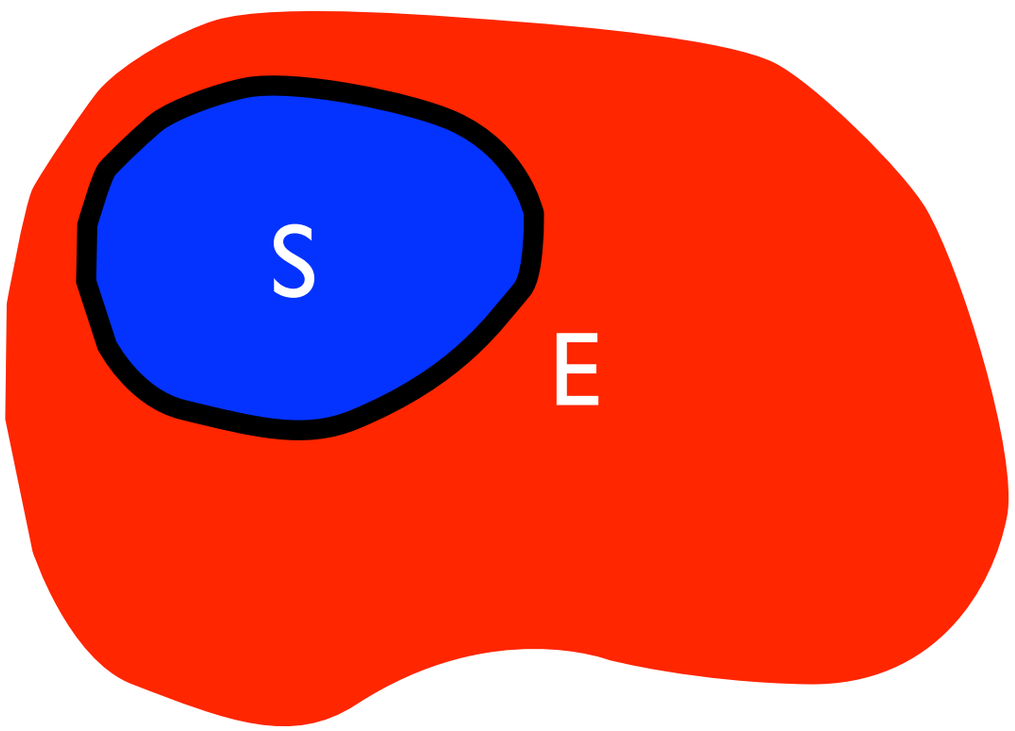
Particle in a box: Better Solution

- Embed A in an environment
- Diagonalize the system+ environment, then increase size



Subsystem States

- What are the most important subsystem states ?



Hamiltonian

$$H = H_S + H_E + H_{SE}$$

Wavefunction

$$|\psi\rangle = \sum_{i,\alpha} \psi_{i,\alpha} \, |i\rangle_S \, |\alpha\rangle_E$$

Best approximation with m subsystem states:

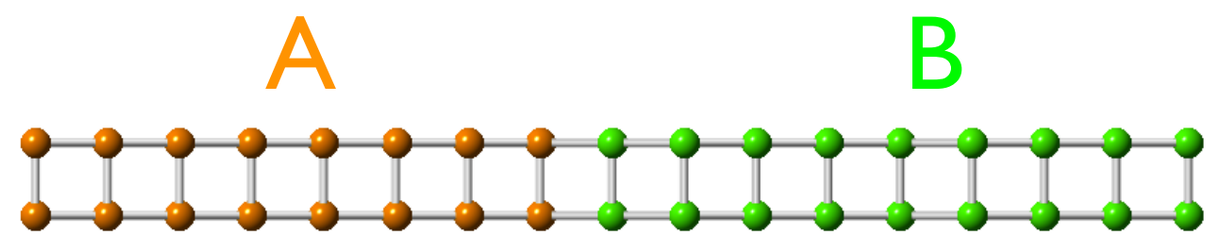
$$|\tilde{\psi}\rangle = \sum_{n=1}^{m} \sum_{\alpha} \tilde{\psi}_{n,\alpha} \, |\phi_n\rangle_S \, |\alpha\rangle_E$$

Minimize the distance between states: $S = \left| |\tilde{\psi}\rangle - |\psi\rangle \right|^2$

Reduced density matrix

- Instead of energy levels, truncate the eigenvalues of the reduced density matrix

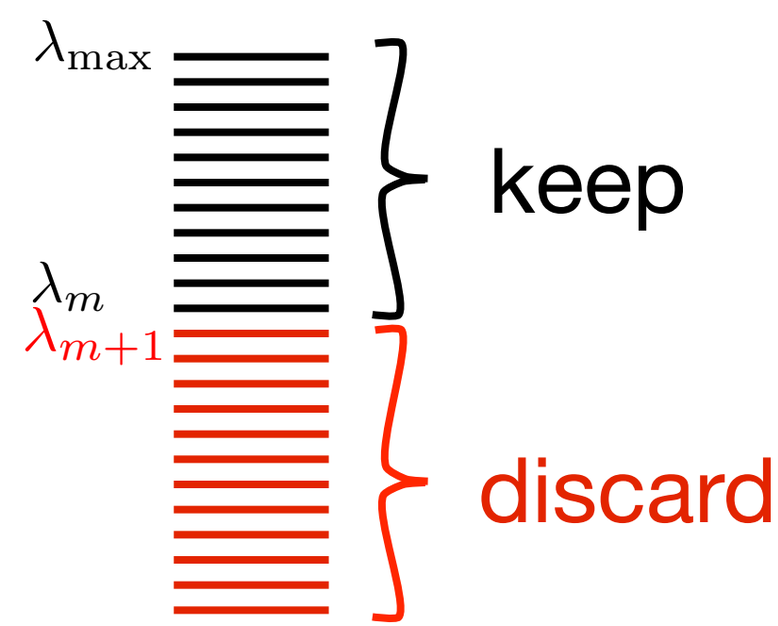
$$|\psi\rangle = \sum_i \lambda_i |i_A\rangle |i_B\rangle$$



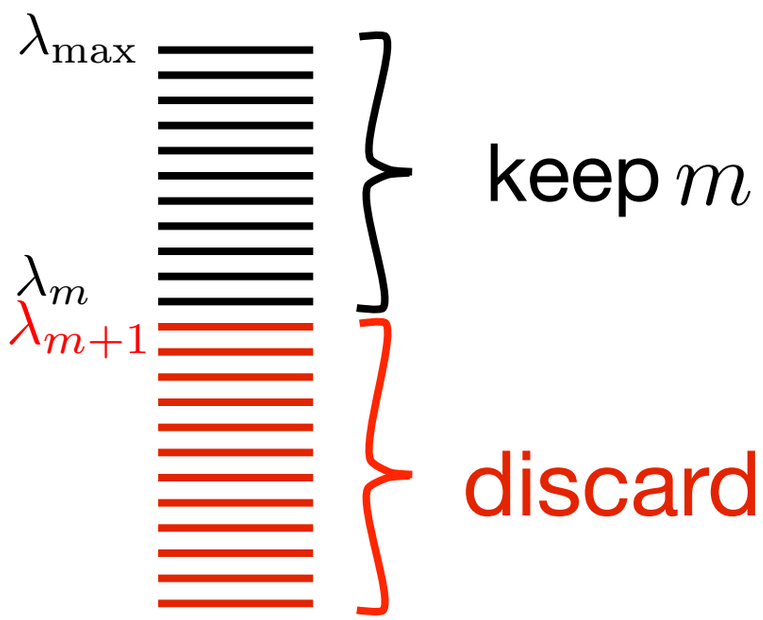
$$\rho_A = \sum_i \lambda_i^2 |i_A\rangle\langle i_A|$$

- The eigenvalues are probabilities

$$\sum_i \lambda_i^2 = 1$$



number of “states”



eigenvalues of the reduced density matrix

- In general, the number of DMRG states that you need to keep to faithfully represent a wavefunction is related to the **entanglement entropy** between the two blocks:

$$m = f(S) \quad ?$$

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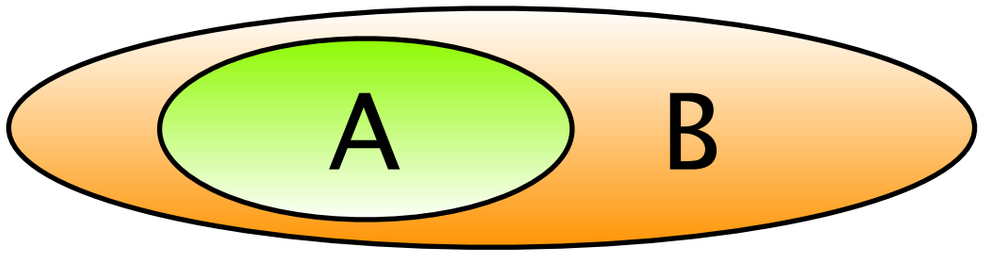
1) Density Matrix Renormalization Group - overview and basics

2) Entanglement Entropy in condensed matter systems

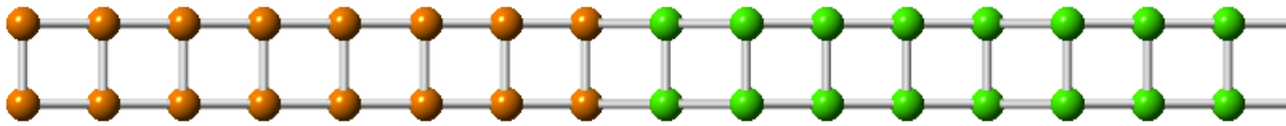
entanglement entropy

von Neumann



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

$$\rho_A = \mathrm{Tr}_B(\rho)$$



- Quantifies the entanglement between subregions A and B
- Does not depend on any choice of observable
- $S_1(\rho_A) = S_1(\rho_B)$
- $S_1(\rho_A) = 0$ if region A and B are unentangled

entanglement entropy of two spins

$$|\Psi\rangle = \cos\phi\ |\uparrow\rangle|\downarrow\rangle + \sin\phi\ |\downarrow\rangle|\uparrow\rangle$$

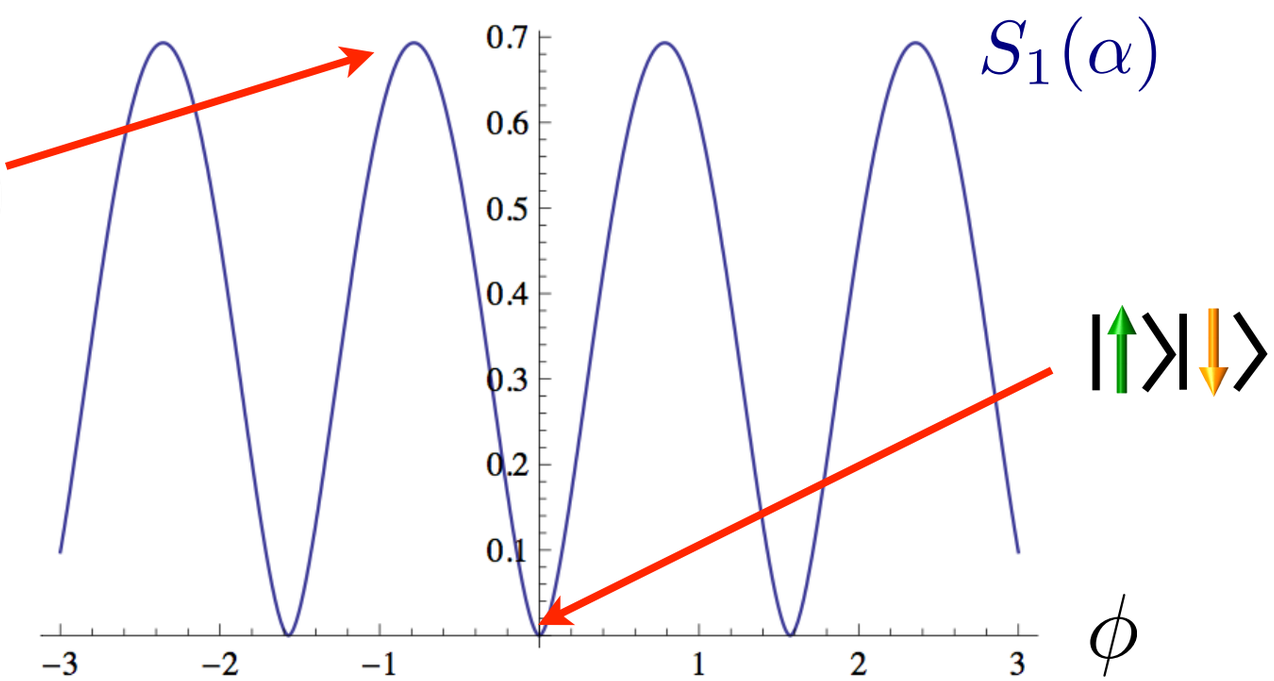
$\uparrow = A$

$\uparrow = B$

$$\rho_A = \begin{pmatrix} \cos^2\phi & 0 \\ 0 & \sin^2\phi \end{pmatrix}$$

$$S_1 = -\cos^2\phi \ln\cos^2\phi - \sin^2\phi \ln\sin^2\phi$$

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



$|\uparrow\rangle|\downarrow\rangle$

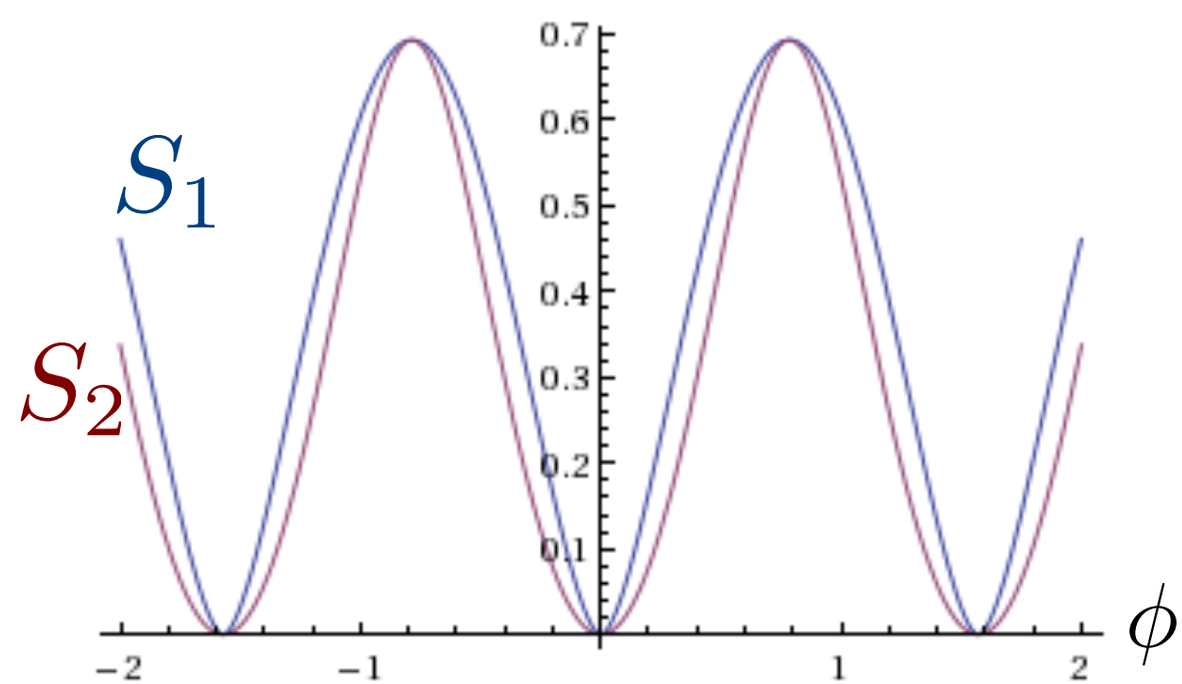
Renyi entanglement entropy

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

$$S_1(\rho_A) = -\mathrm{Tr}(\rho_A \ln \rho_A) \qquad S_2(\rho_A) = -\ln \left[\mathrm{Tr}(\rho_A^2) \right]$$

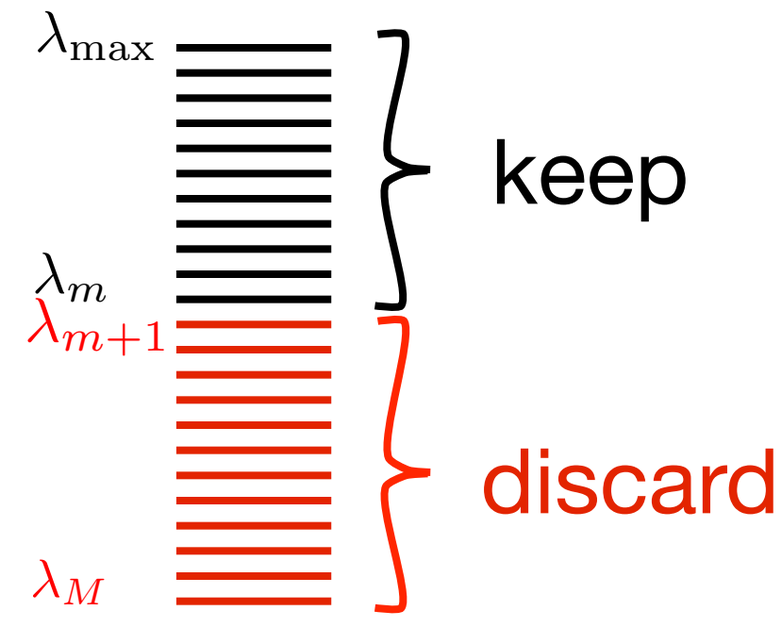
two spins:

$$|\Psi\rangle = \cos\phi \; |\uparrow\rangle|\downarrow\rangle + \sin\phi \; |\downarrow\rangle|\uparrow\rangle$$



entanglement and number of "states"

$$\rho_A = \sum_i \lambda_i^2 |i_A\rangle\langle i_A|$$



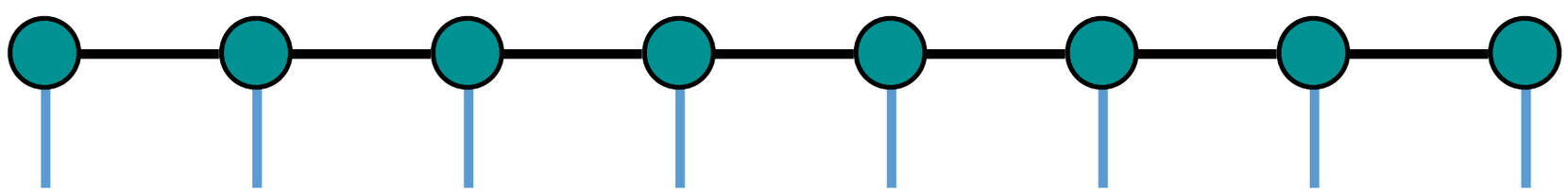
- $S_1(\rho_A) = 0$ minimally (for a product state)
- $S_1(\rho_A) = \ln(M)$ maximally (when all eigenvalues are equal)

in analogy, the effective number of states one needs in order to properly capture the entanglement between A and B is:

$$m \propto \mathrm{e}^{S_1}$$

DMRG and entanglement cutoff

- Therefore, the success of DMRG depends on the wavefunctions of interest having a “low degree” of entanglement
- This is the basis of the reformulation of DMRG in the **Matrix Product State** representation (see talks tomorrow)

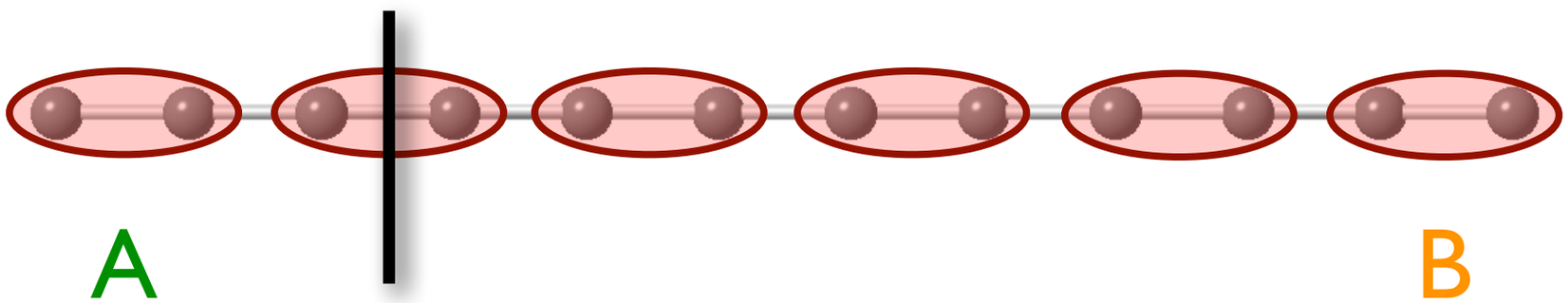


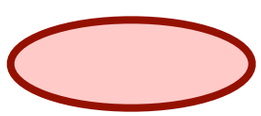
- We take a minute to examine entanglement in some prototypical models of condensed-matter physics

entanglement in one dimension

- gapped system

AKLT

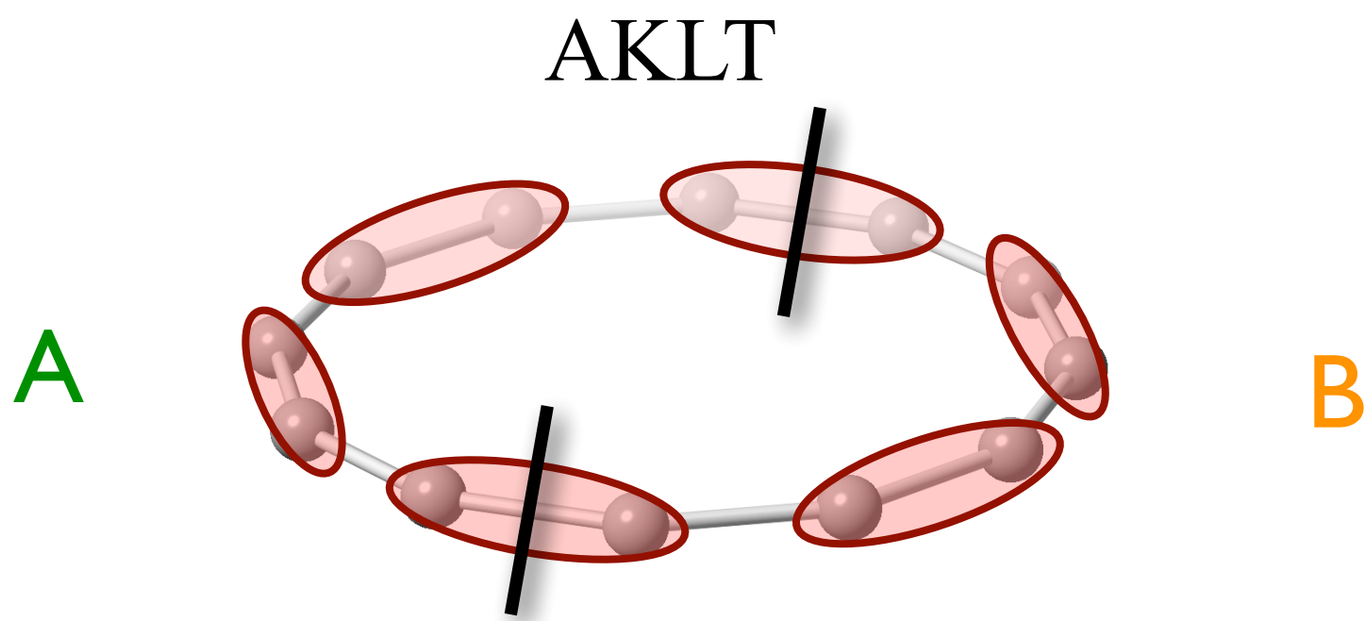




$= \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$ $\quad S_1(\rho_A) = \ln(2)$

$m \propto e^{S_1} \Rightarrow \quad m \propto 2$ (constant)

entanglement in one dimension



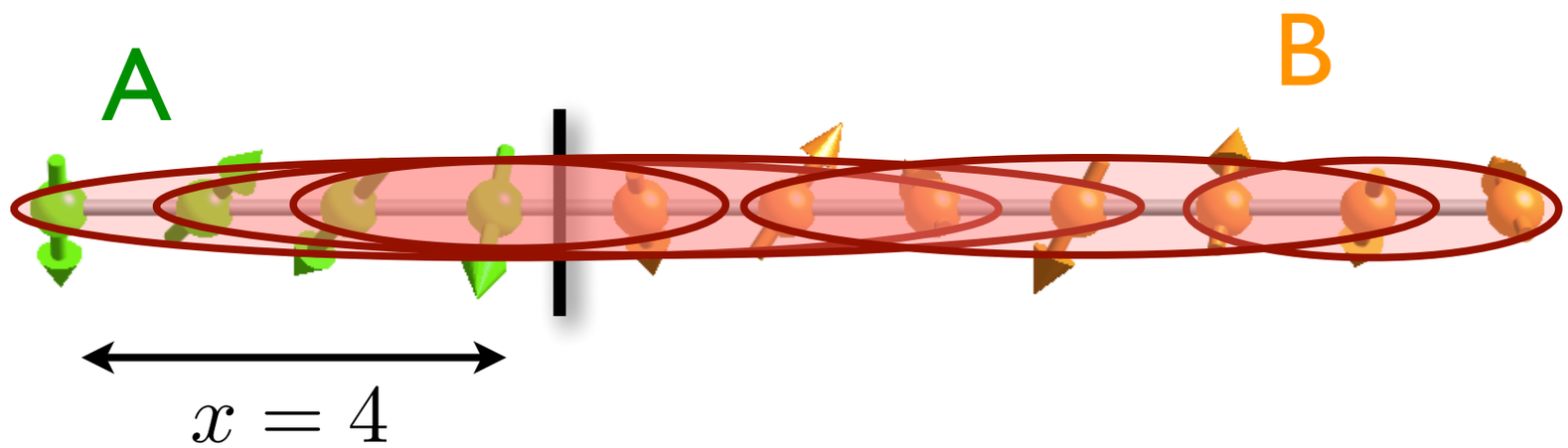
$$S_1(\rho_A) = 2\ln(2) = \ln(2^2)$$

$$m \propto \mathrm{e}^{S_1} \Rightarrow m \propto 2^2$$

- For periodic boundary conditions in 1D, you need to keep the **square** of the number of states needed for open boundary conditions

entanglement in one dimension

- gapless/critical system $$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



$$L = 11$$

$$S_1 \propto c \ln[L] \quad \Rightarrow m \propto L^{\text{const.}}$$

- computational cost grows as the size of the system
- it is still possible to simulate large systems if c is small

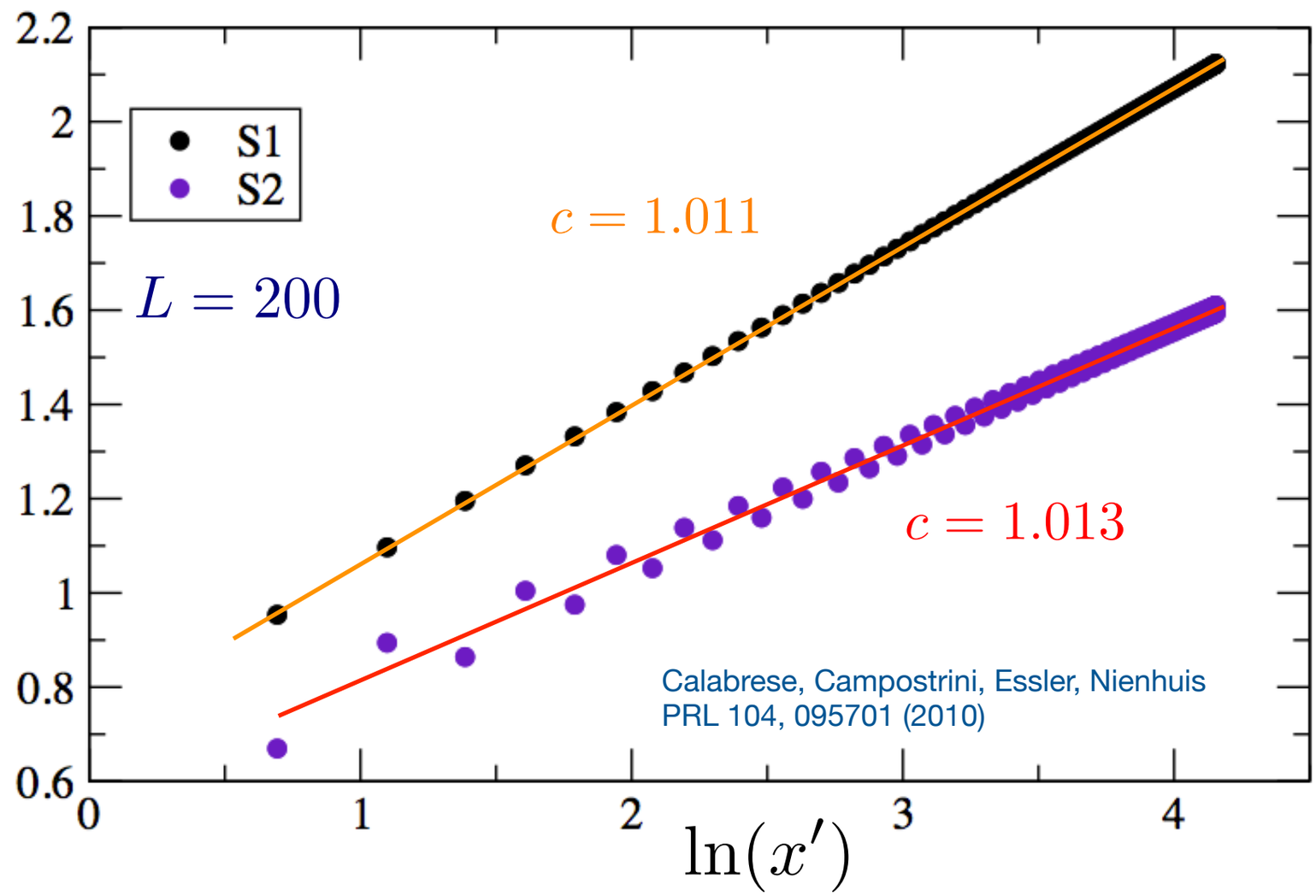
entanglement in one dimension

- gapless/critical system $$H = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

$$S_n(x) = \frac{c}{6}\left(1 + \frac{1}{n}\right) \cdot \ln\left[x'\right] + \cdots$$

$$x' = \frac{L}{\pi} \sin\left(\frac{\pi x}{L}\right)$$

c=1: central charge of a conformal field theory

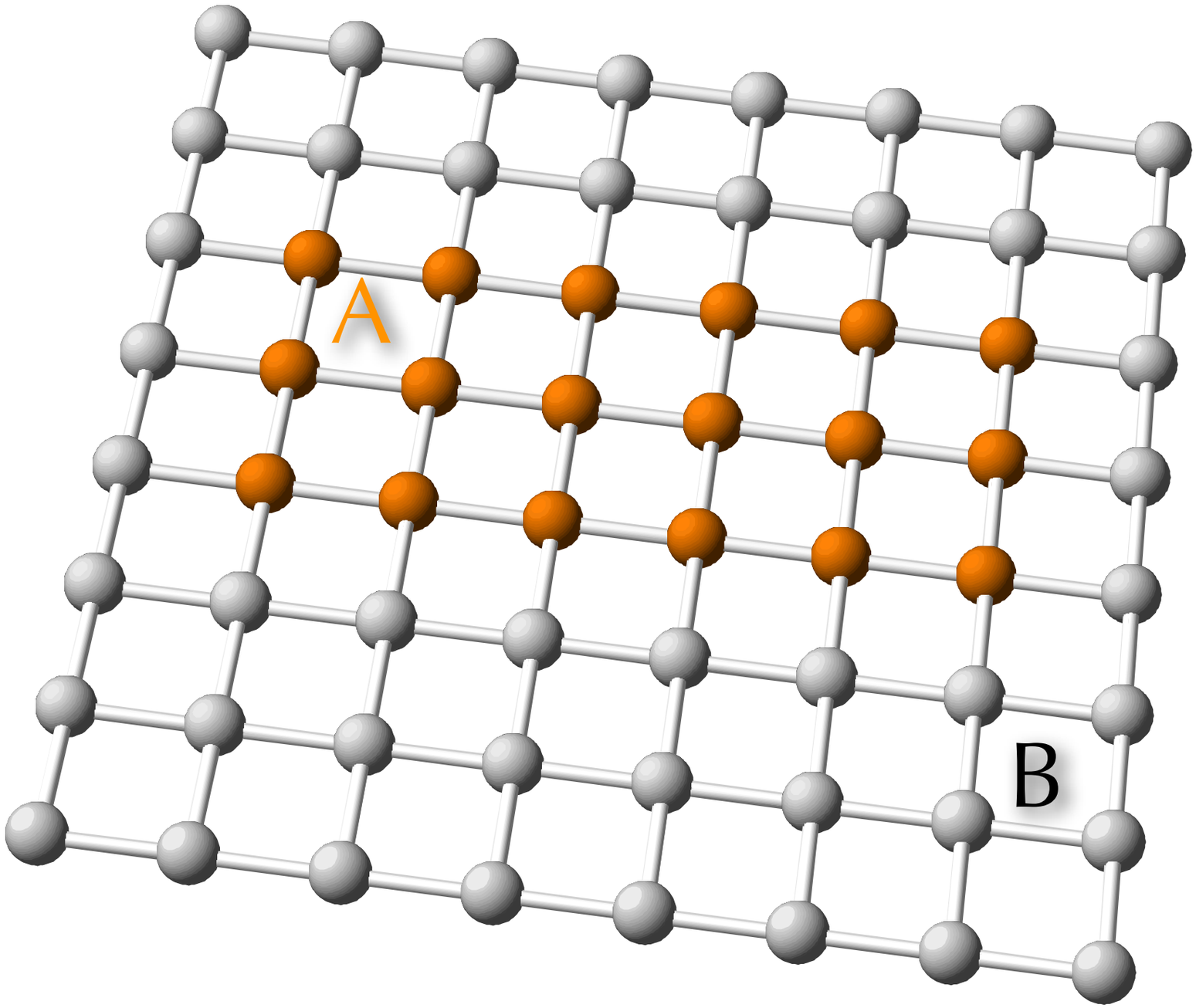


Calabrese, Campostrini, Essler, Nienhuis
PRL 104, 095701 (2010)

Holzhey, Larsen, Wilczek Nucl. Phys. B 424 443 (1994)

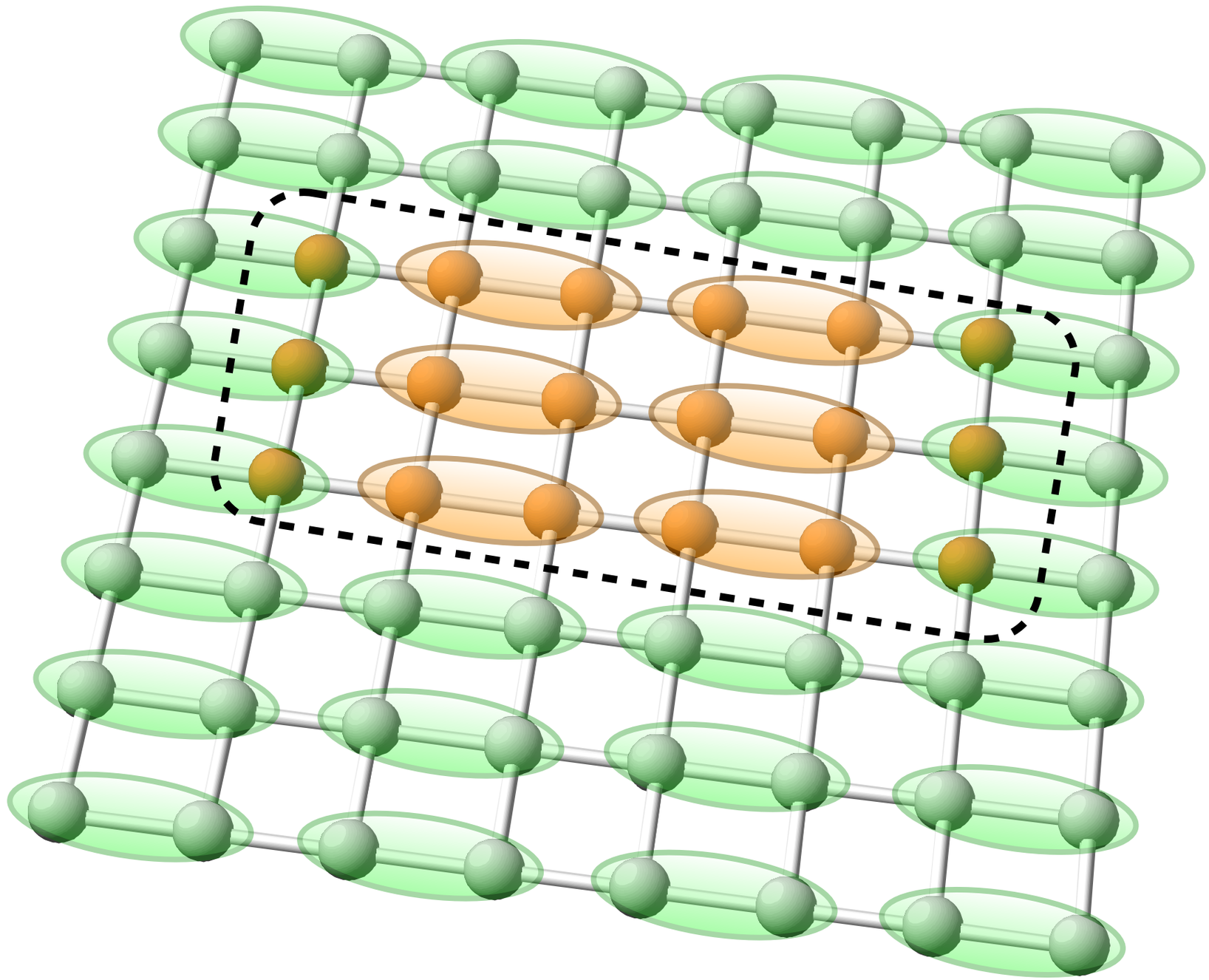
Calabrese and Cardy, J. Stat. Mech: Theory Exp. P06002 (2004)

entanglement in two dimensions



entanglement in two dimensions

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



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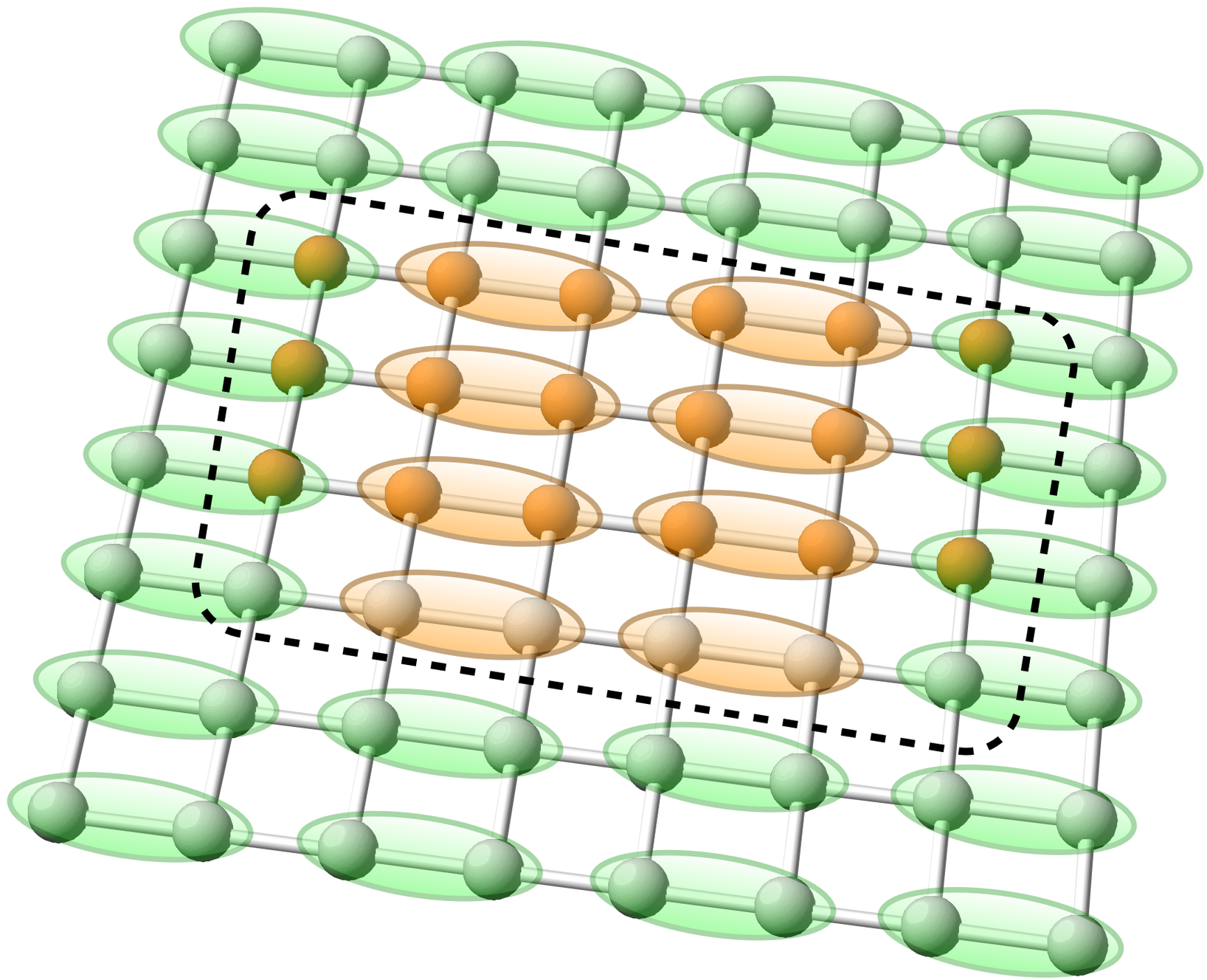

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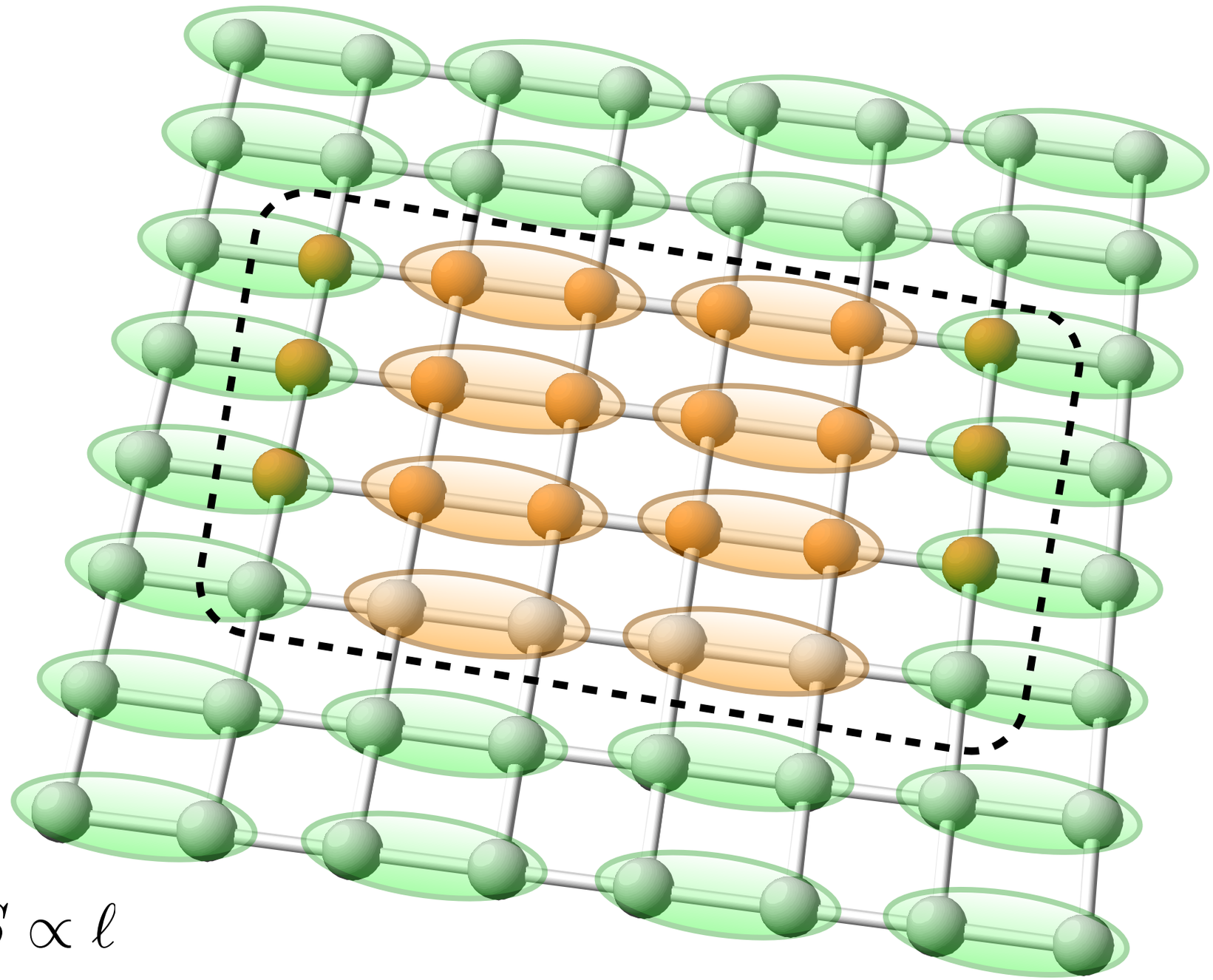


$$S \propto \ell$$

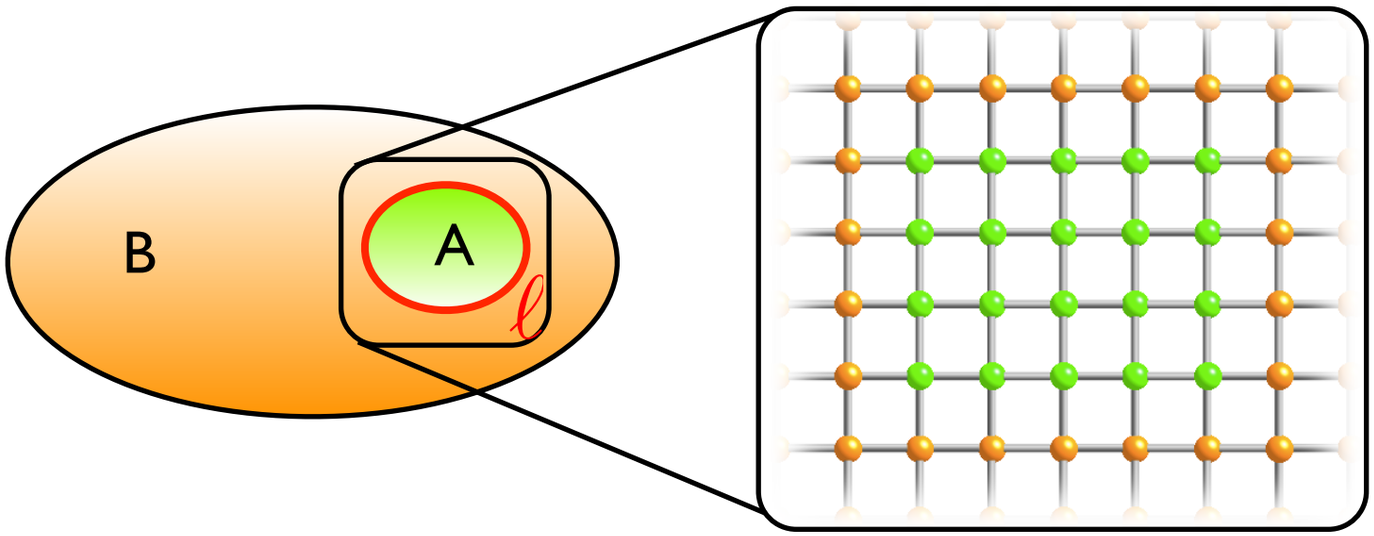
Here, the entanglement depends on the boundary: the **“Area Law”**

the **area law**: a special property of groundstates

- or the "boundary rule-of-thumb"

$$S_n = a\ell + \cdots$$

coefficient is non-universal



- **groundstate** wavefunctions of local many-body Hamiltonians

- heuristically related to short-range correlations

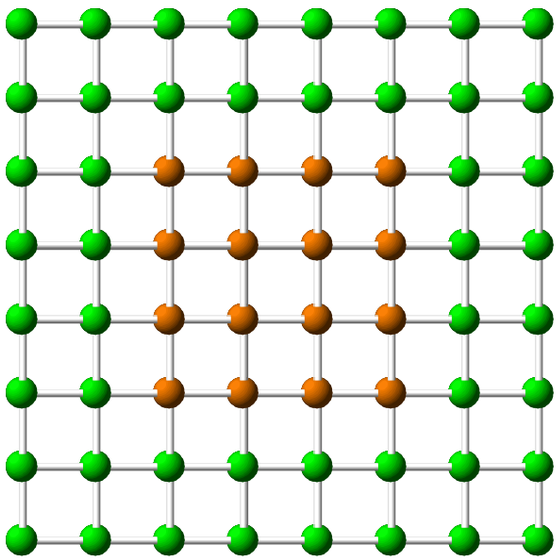
Wolf et al. Phys. Rev. Lett. 100, 070502 (2008)

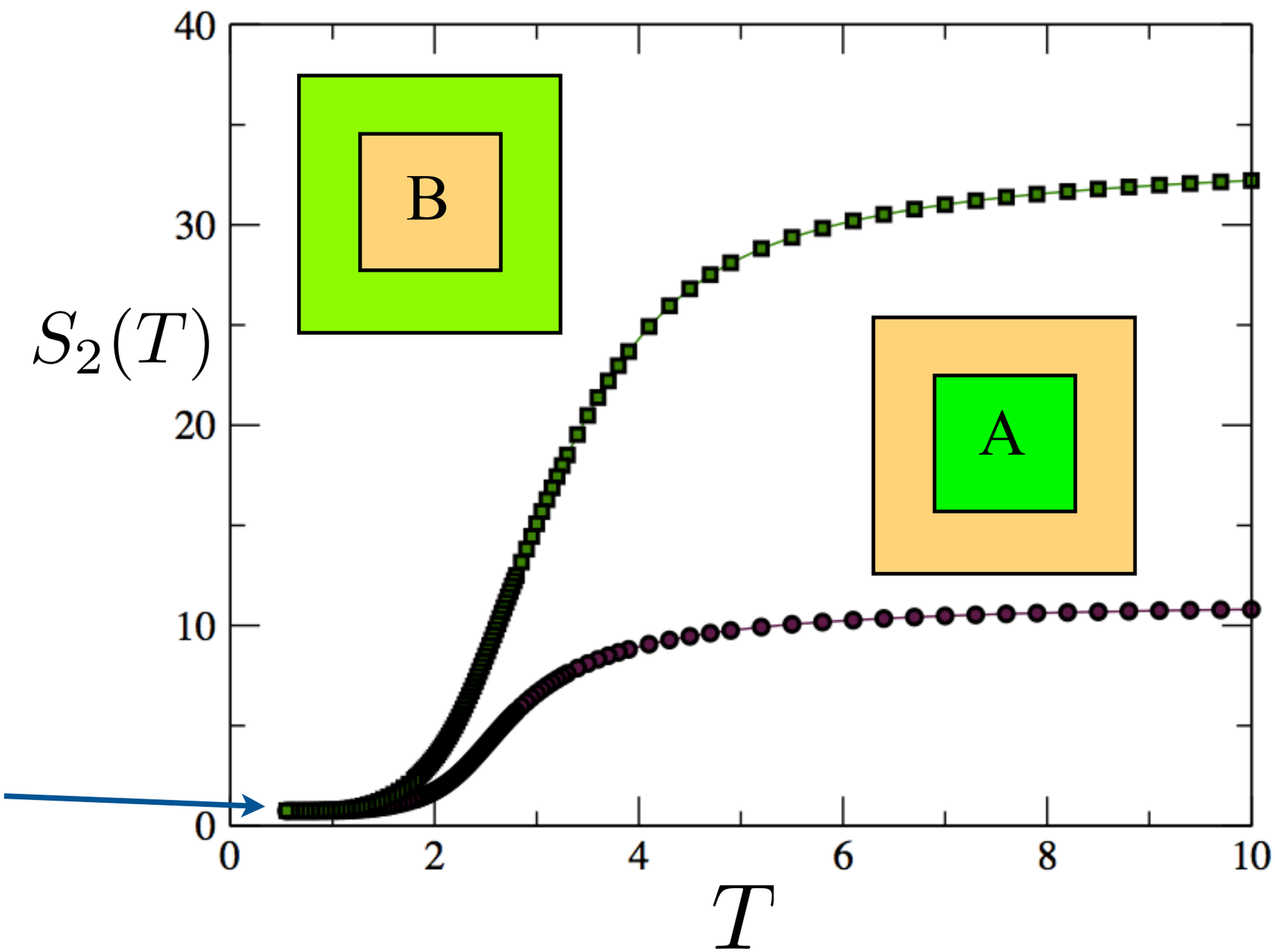
- generally speaking, excited states exhibit a **volume law**

$$S \approx a\ell^2$$

entanglement at finite-temperatures

The entanglement entropy at finite-T picks up a “volume” law due to thermal mixing





$S_A = S_B$

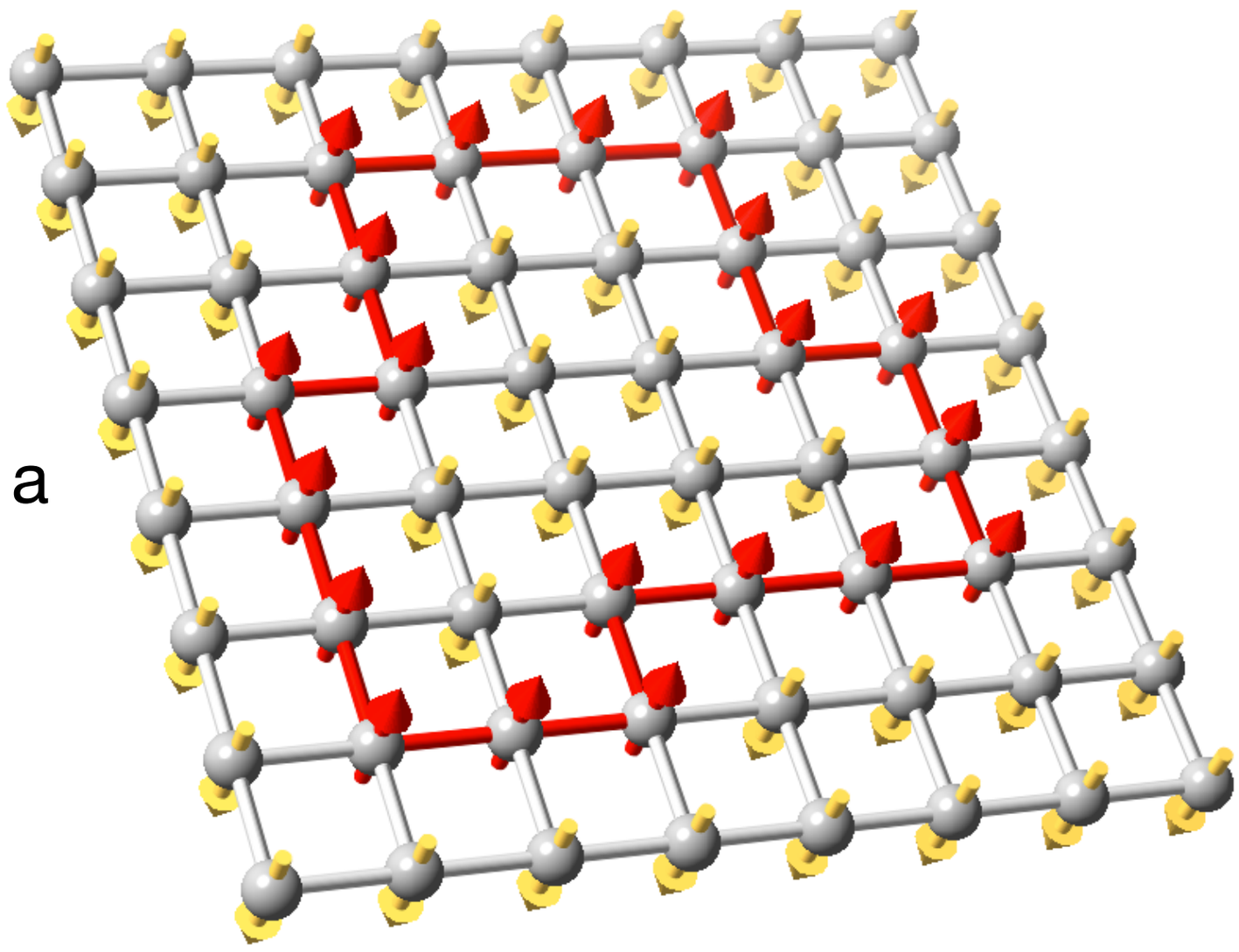
additive corrections to the area law (T=0)

gapped systems in two dimensions can have subleading terms in the entanglement entropy

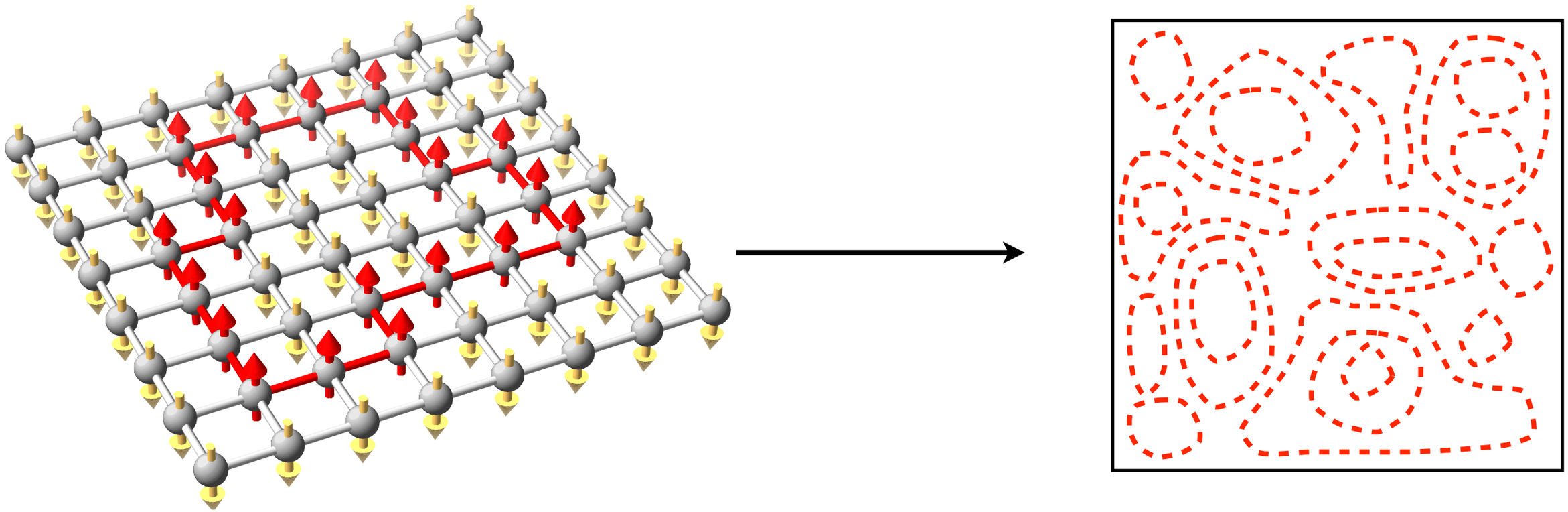
$$S_n = a\ell + \cdots$$

$$S_n = a\ell - \ln(2)$$

For example, a spin liquid (fluctuating loop gas) can have a **topological entanglement entropy**



The groundstate of a (Z_2) spin liquid can be thought of as a fluctuating “loop gas”



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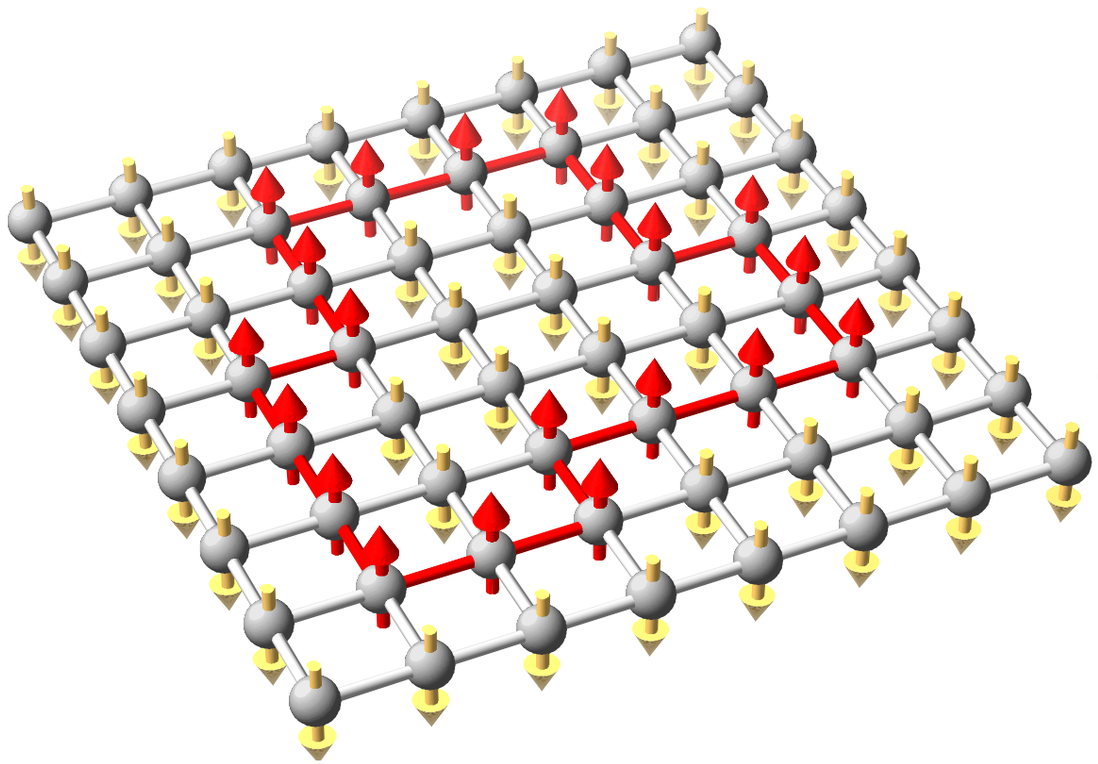
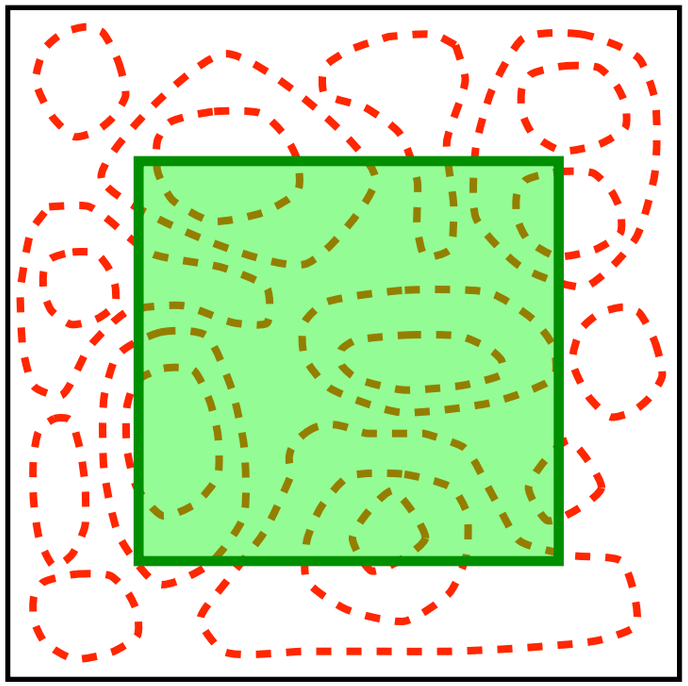




This loop structure imposes **constraints** that subtract from the entanglement entropy of a pure area law:

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

possible boundary configurations

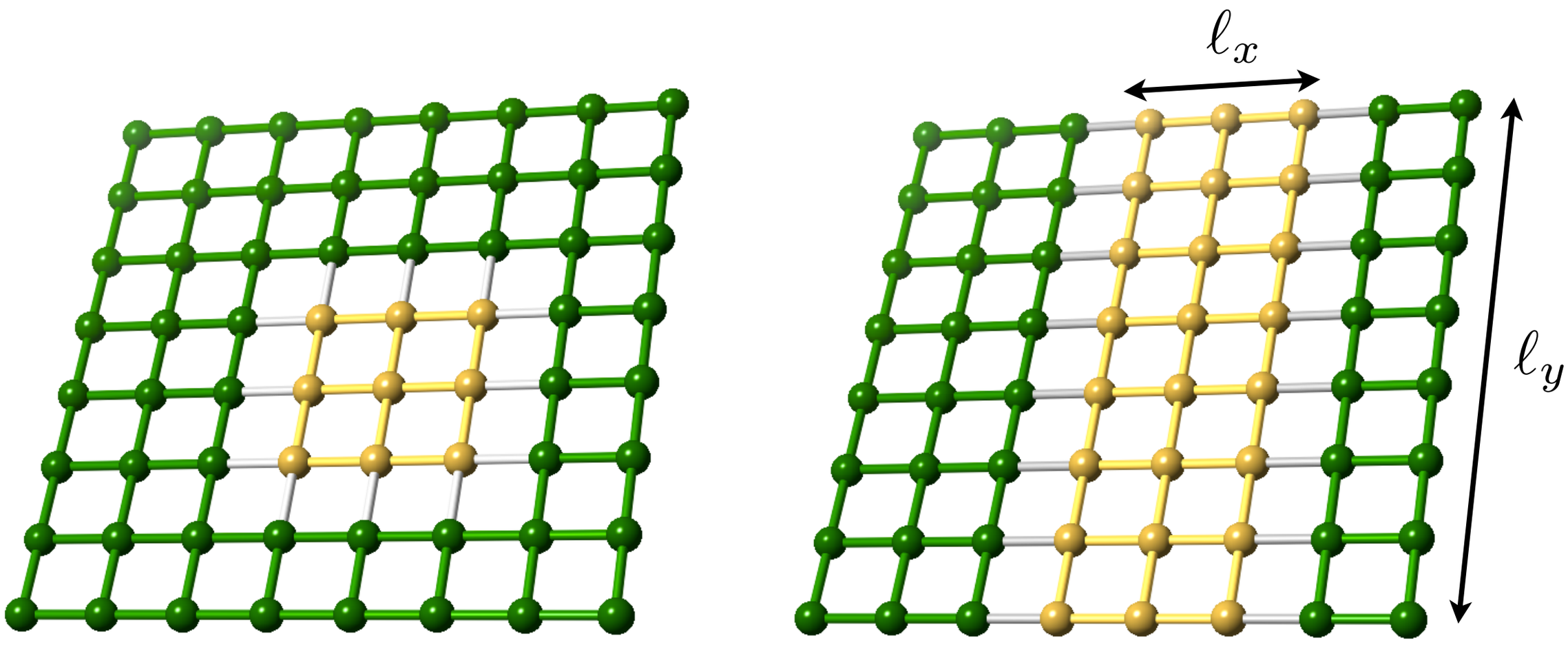
$$S_n = a\ell - \gamma$$

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

additive corrections to the area law (T=0)

gapless systems in two dimensions generally have subleading shape-dependent terms in the entanglement entropy

$$S_n = a\ell + \gamma(\ell_x, \ell_y)$$



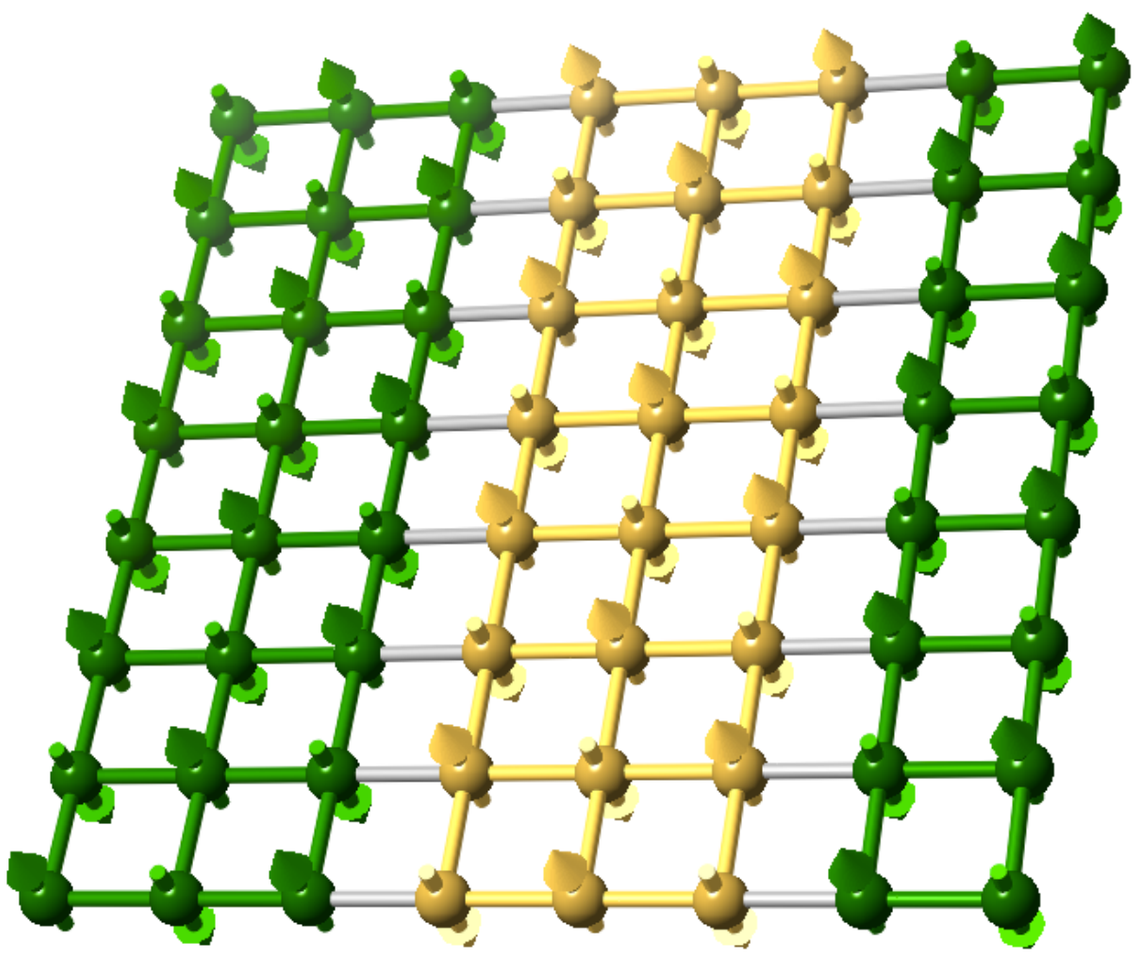
additive corrections to the area law (T=0)

Neel order, e.g. the groundstate of the 2D spin-1/2 Heisenberg model

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

$$S_n = a\ell + b\ln(\ell) + \cdots$$

The subleading term is a consequence of Goldstone modes - has a **universal** coefficient



Kallin et. al. PRB 84, 165134 (2011)
Metlitski and Grover, arXiv:1112.5166

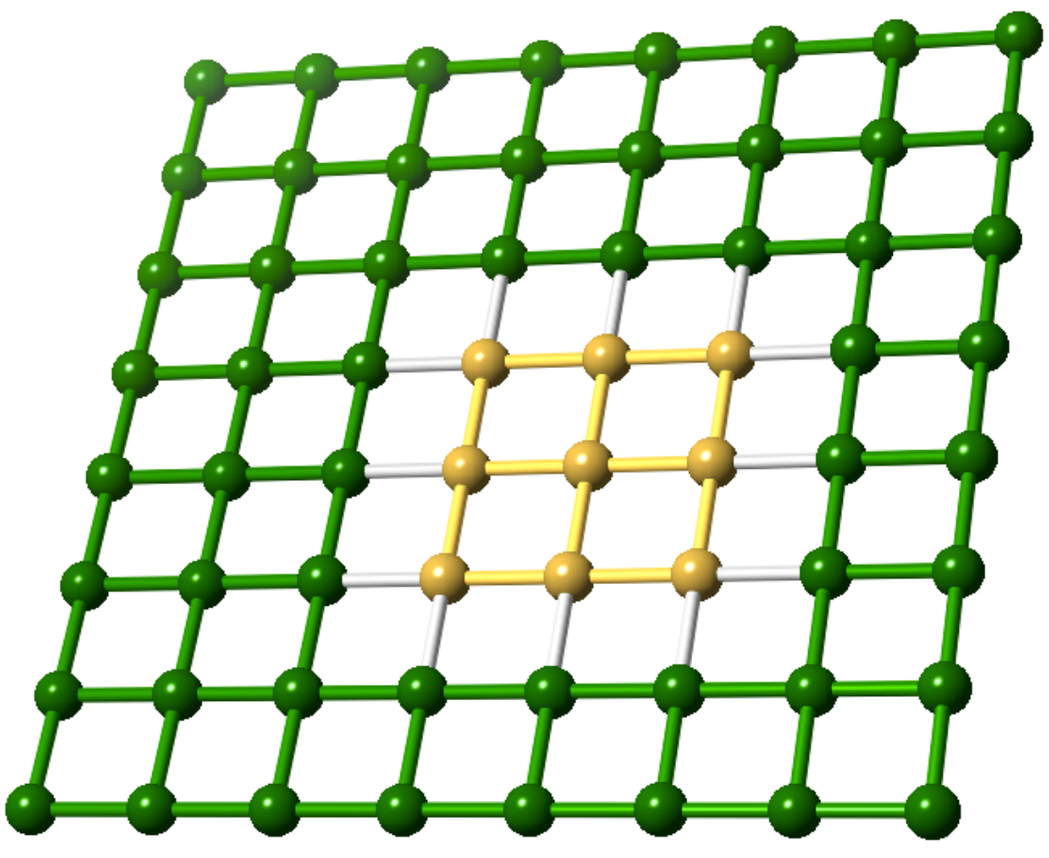
additive corrections to the area law (T=0)

Quantum critical systems, e.g. transverse-field Ising model

$$H = J \sum_{\langle ij \rangle} S_i^z S_j^z + h \sum_i S_i^x$$

$$S_n = a\ell + c_n \ln(\ell) + \cdots$$

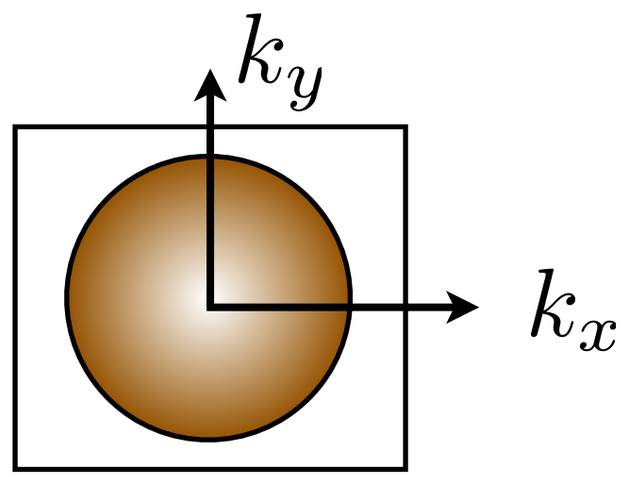
A subleading logarithm arises when one has **corners** in the region - the coefficient of this terms is universal for that particular universality class



Casini and Huerta Nucl. Phys. B 764 183 (2007)

“violations” of the area law in 2D

Multiplicative logarithmic corrections to the area law occur in cases where one has a fermi surface in 2D



$$S_n = \mathrm{c}\, \ell \ln(\ell) + \cdots$$

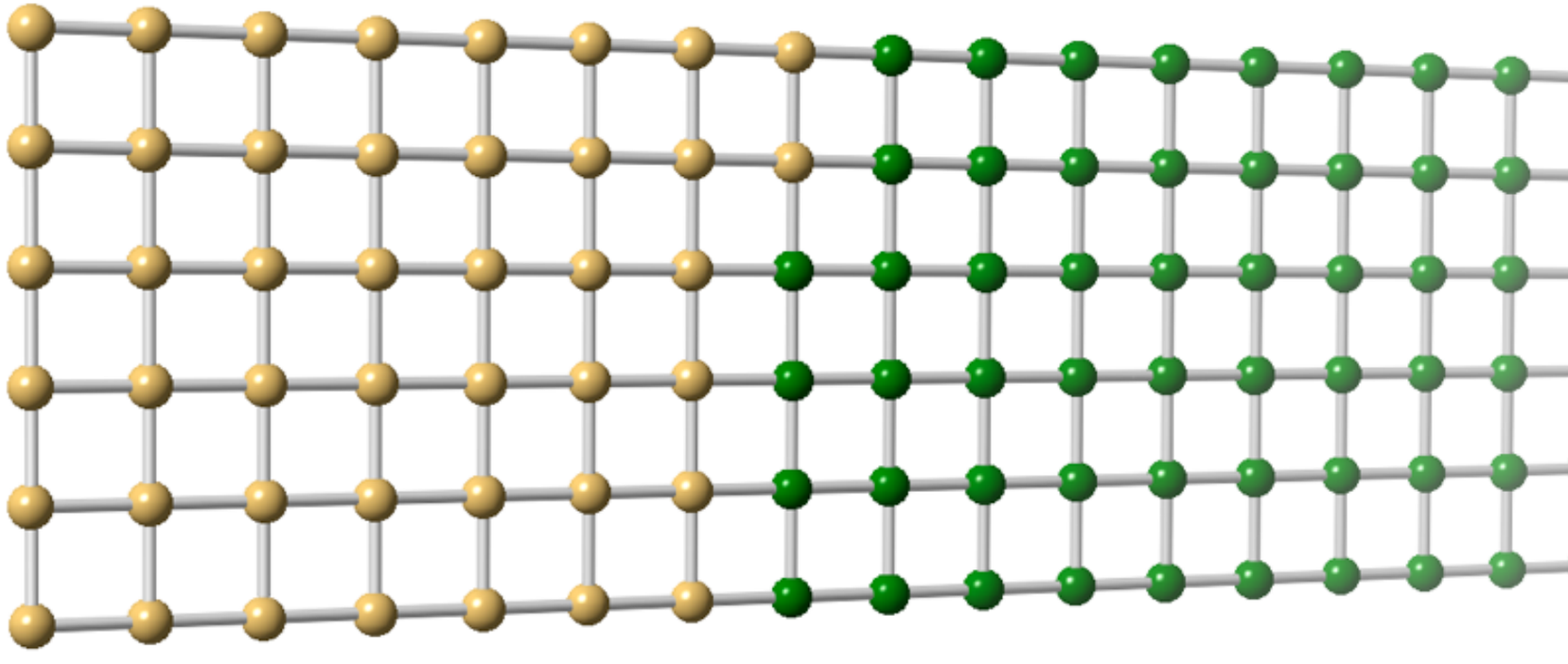
M.M. Wolf, Phys. Rev. Lett. **96**, 010404 (2006).
D. Gioev, I. Klich, Phys. Rev. Lett. **96**, 100503 (2006).

... will this be the new “sign problem” for the 21st century?

the challenge for DMRG

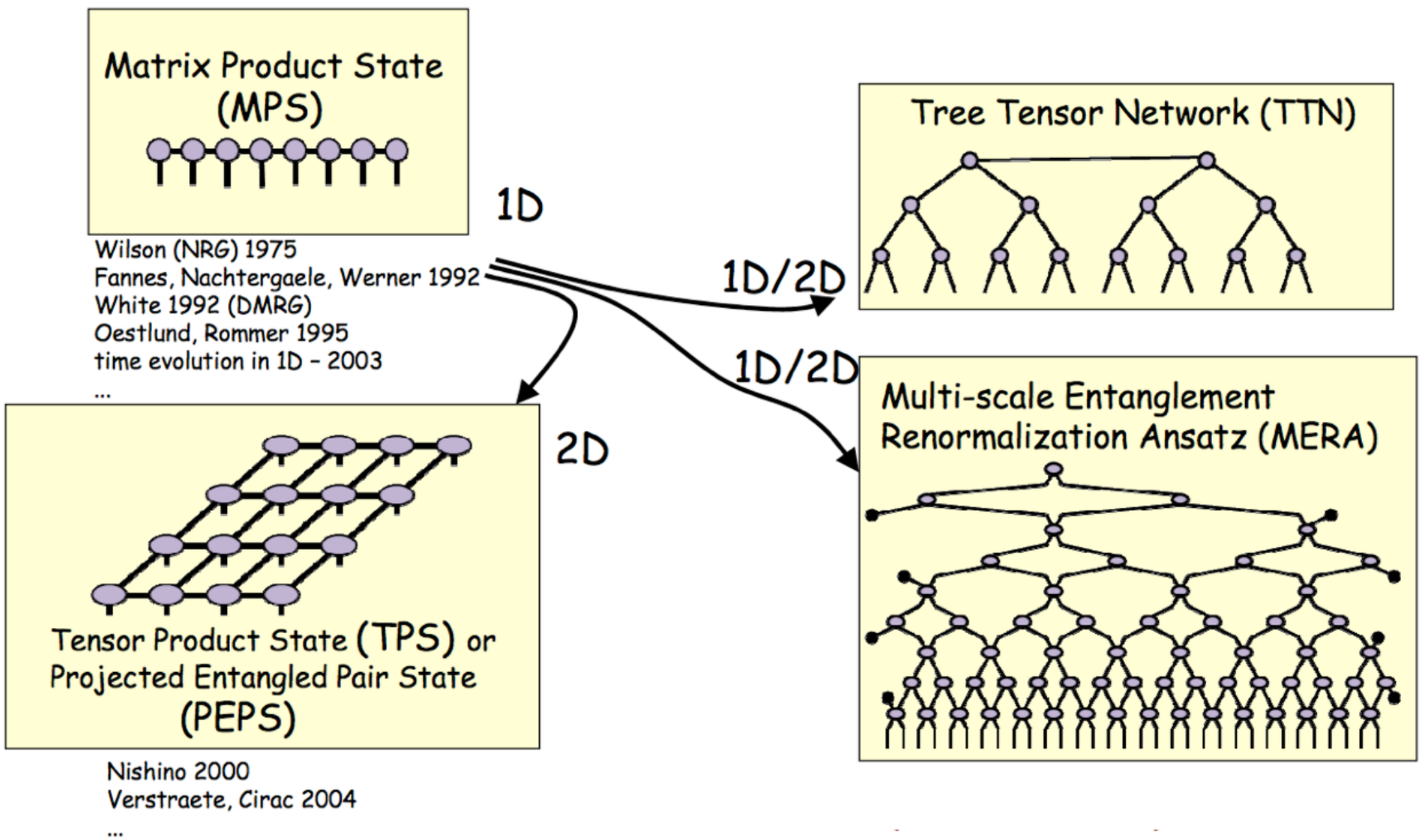
$$m \propto \mathrm{e}^{S_1} \Rightarrow \; m \propto \mathrm{e}^{\ell}$$

- in general, the number of DMRG states that you need to keep to represent a groundstate wavefunction is exponential in the width



higher dimensions? Tensor Networks

- methods based on a “low-entanglement” ansatz in the wavefunction



conclusion

DMRG is the established method for solving the ground states of strongly interacting systems in 1D

It continues to revolutionize the way we think of dealing with the strongly-interacting quantum many-body problem numerically