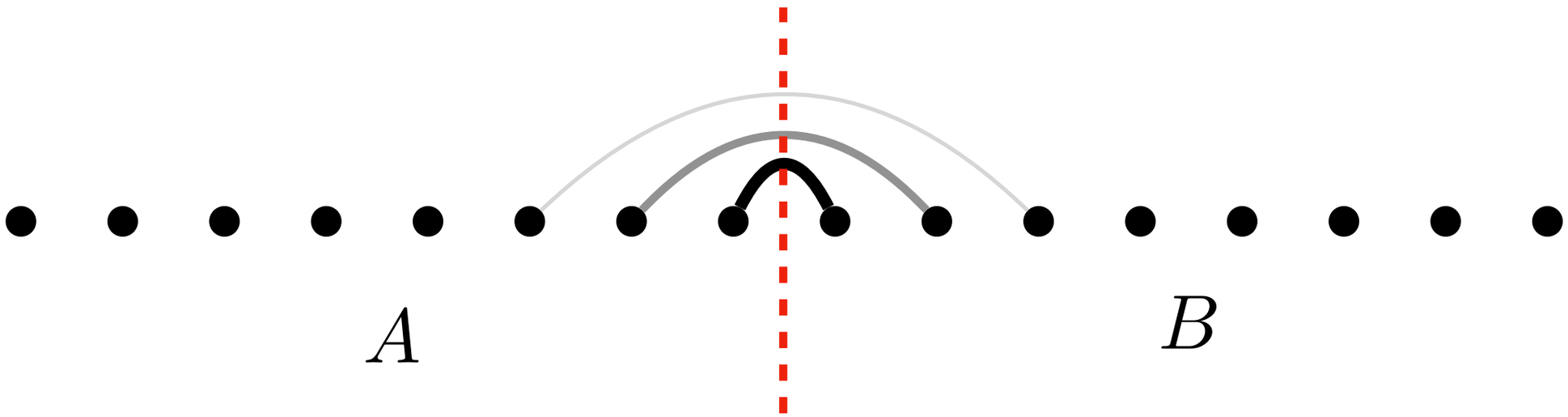
Tensor Networks and Applications



E.M. Stoudenmire

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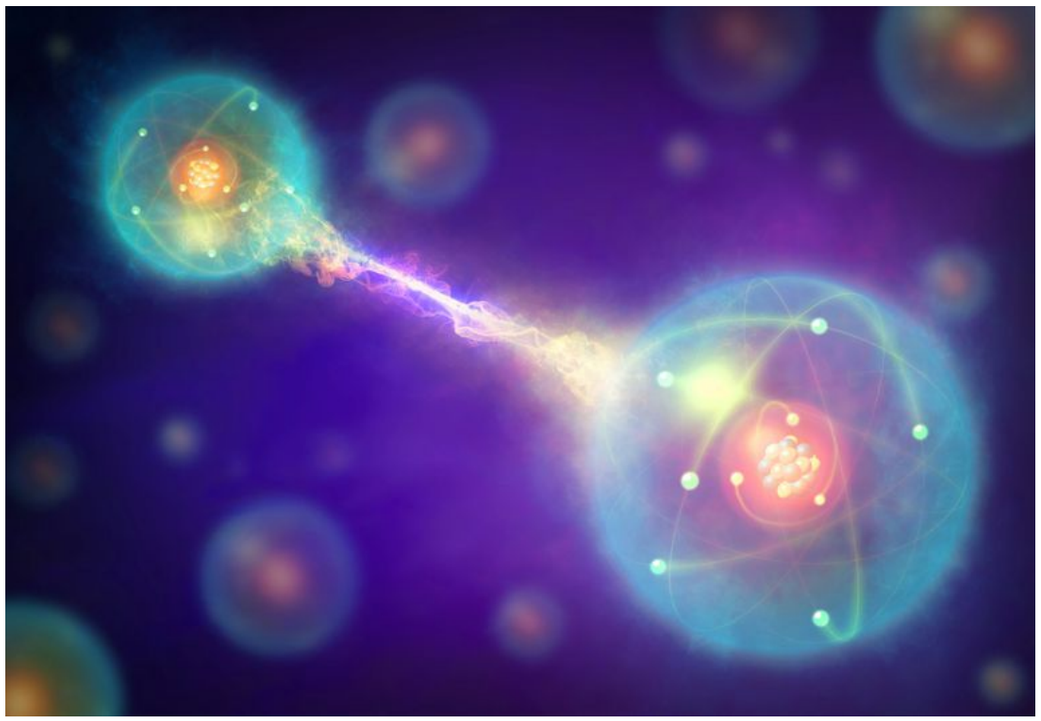
The Quantum Many-Body Problem

Quantum many-body problem is solving behavior of electrons in matter

- continuum problem
- three dimensional
- strong interaction (repulsion) between electrons



Credit: MARK GARLICK/SCIENCE PHOTO LIBRARY/Getty Images

Interestingly, we know exactly what to do

Just solve $i\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle$

With H given by

$$\hat{H} = \frac{1}{2}\int_{\mathbf{r}} \hat{\psi}^\dagger_{\mathbf{r}} \left[-\partial_x^2 + v(\mathbf{r})\right] \hat{\psi}_{\mathbf{r}} + \frac{1}{2}\int_{\mathbf{r}\mathbf{r}'} u(\mathbf{r},\mathbf{r}')\hat{\psi}^\dagger_{\mathbf{r}}\hat{\psi}^\dagger_{\mathbf{r}'}\hat{\psi}_{\mathbf{r}'}\hat{\psi}_{\mathbf{r}}$$

$$u(\mathbf{r},\mathbf{r}') = \frac{1}{|\mathbf{r}-\mathbf{r}'|} \qquad v(\mathbf{r}) = -\sum_a \frac{Z_a}{|\mathbf{r}-\mathbf{r}_a|}$$

The *"electronic structure problem"*

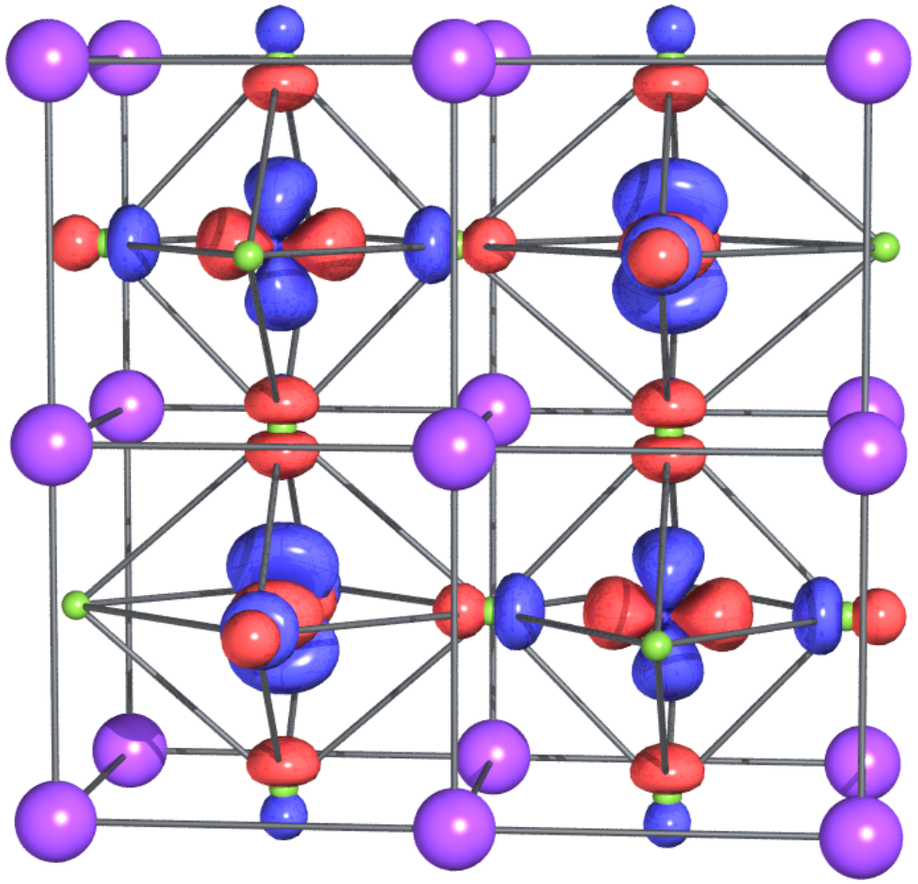
Paul Dirac remarked in 1929

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that ***approximate practical methods*** *of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems* ***without too much computation****.*

Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, Vol. 123, No. 792 (6 April 1929)

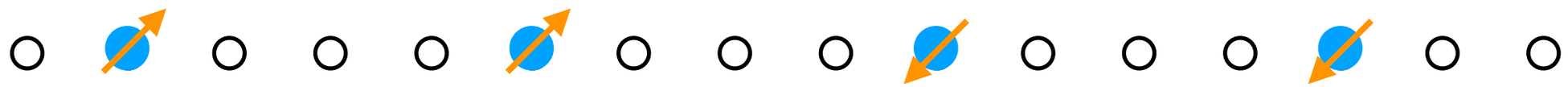
Can simplify various ways:

- Born-Oppenheimer approximation (classical nuclei)
- project electron motion to certain orbitals
- treat high & low energy states with approximations such as LDA density functional



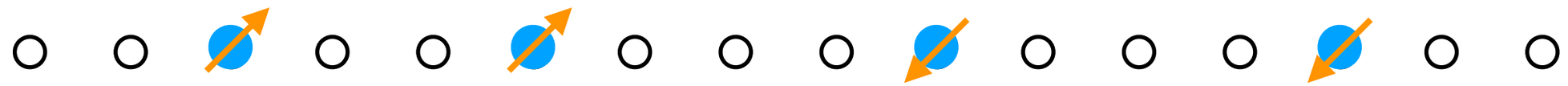
Credit: EVA PAVARINI

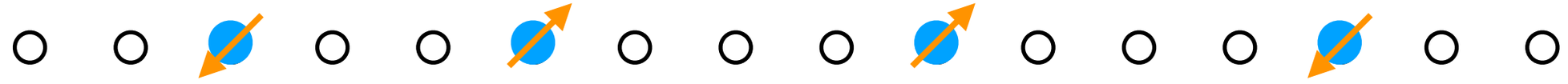
Can even reduce to model systems, fewer dimensions:



But size of problem grows **exponentially** with number of electrons

Quantum wavefunction assigns an amplitude to each classical state:

1: 

2: 

3: 

Four states per site $\{0, \uparrow, \downarrow, \uparrow\downarrow\}$

So 4^N states given N sites

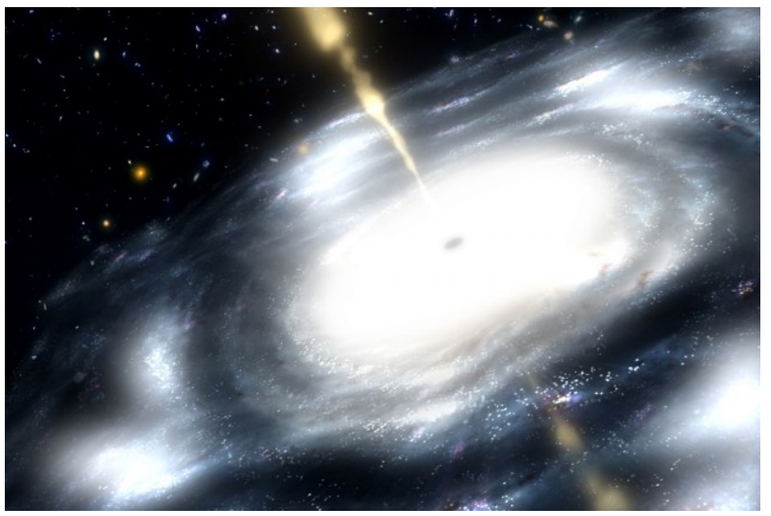
Could try to store all the amplitudes, but

$N = 10, 4^{10} \sim 10^{6}$

$N = 20, 4^{20} \sim 10^{12}$

$N = 30, 4^{30} \sim 10^{18}$

For N > 130, number of amplitudes greater than **number of atoms in the known universe**



But can "nature's computer" really work this way?

Are the amplitudes of a realistic wavefunction all different?

Or is there some relationship between them?

Many-body wavefunction is a weighted sum (superposition) of basis states

$$|\Psi\rangle = \Psi^{\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow} |\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$$

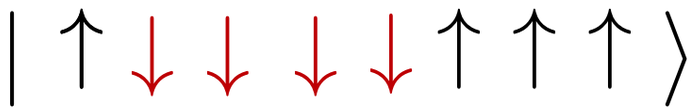
$$+ \Psi^{\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow} |\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\rangle$$

$$+ \Psi^{\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow} |\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\rangle$$

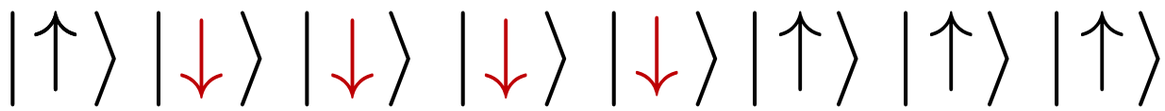
$$+ \Psi^{\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow} |\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle$$

$$+ \ldots$$

Recall that the following



is shorthand for



(tensor product of basis states)

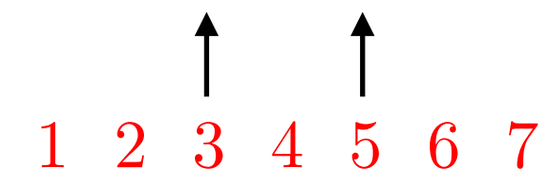
General discussion applies to any basis, for example fermions in "orbital basis"

$$|\Psi\rangle = \Psi^{1\,1\,0\,0\,0\,0\,0}\,|\,1\;1\;0\;0\;0\;0\;0\;\rangle$$

$$+\,\Psi^{1\,0\,1\,0\,0\,0\,0}\,|\,1\;0\;1\;0\;0\;0\;0\;\rangle$$

$$+\,\Psi^{0\,0\,1\,0\,0\,1\,0}\,|\,0\;0\;1\;0\;0\;1\;0\;\rangle \;+\; \ldots$$

$$\langle x_1 x_2 | 0\;0\;1\;0\;1\;0\;0\rangle = \phi_3(x_1)\phi_5(x_2) - \phi_3(x_2)\phi_5(x_1)$$



Let's write the wavefunction

$$|\Psi\rangle = \Psi^{\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow} |\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$$

$$+ \Psi^{\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow} |\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\rangle$$

$$+ \Psi^{\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow} |\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\rangle$$

$$+ \Psi^{\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow} |\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle$$

$$+ \ldots$$

in a more compact form ...

Many-body wavefunction in compact form

$$|\Psi\rangle = \sum_{\mathbf{s}} \Psi^{s_1 s_2 s_3 \cdots s_N} |s_1 s_2 s_3 \cdots s_N\rangle$$

amplitudes

basis

$\Psi^{s_1 s_2 s_3 \cdots s_N}$ amplitude tensor

Examples

Simplest state

$$|\Psi\rangle = |\uparrow\uparrow\rangle = |\uparrow\rangle|\uparrow\rangle$$

$$\Psi^{\uparrow\uparrow} = 1\,,\ \text{all other amplitudes zero}$$

Example of a product state
Has zero entanglement (factorized)

More interesting state

$$|\Psi\rangle = |\uparrow\rangle|\rightarrow\rangle$$

$$= |\uparrow\rangle(\frac{1}{\sqrt{2}}|\uparrow\rangle + \frac{1}{\sqrt{2}}|\downarrow\rangle)$$

$$= \frac{1}{\sqrt{2}}|\uparrow\rangle|\uparrow\rangle + \frac{1}{\sqrt{2}}|\uparrow\rangle|\downarrow\rangle$$

Also a product state (no entanglement)

Not obvious in z basis though!

Maximally entangled state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle|\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\rangle|\uparrow\rangle$$

"Singlet" state of two spin 1/2's

Cannot be written as a product state in any basis transformation of individual sites

Entangled because spins (anti-)correlated

Entanglement

Can evaluate entanglement of simple states "by inspection"

But what about more complicated states?

How to be sure whether state is entangled?
How to quantify amount of entanglement?

Intuition:

- limited information in two spins
- more information shared *between* spins, less information about *each* separately

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Low entanglement intuition:

Intuition:

- limited information in two spins
- more information shared *between* spins, less information about *each* separately

Low entanglement intuition:

↑ ↓

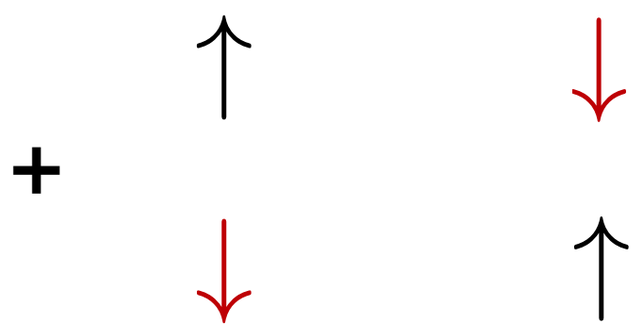
Observe state of first spin only: ↑

Remains *pure*

Intuition:

- limited information in two spins
- more information shared *between* spins, less information about *each* separately

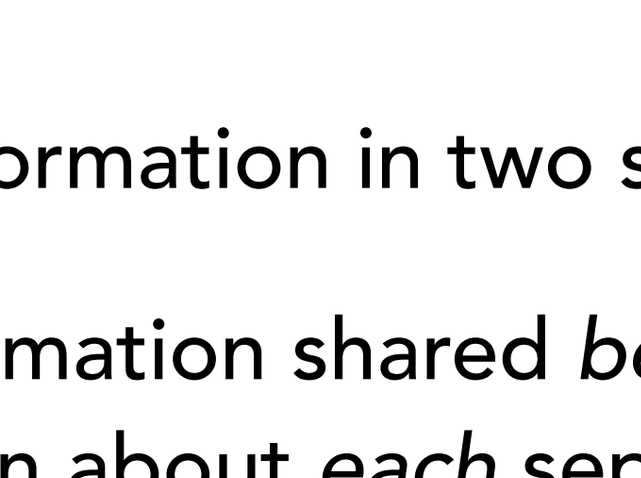
High entanglement intuition:



Intuition:

- limited information in two spins
- more information shared *between* spins, less information about *each* separately

High entanglement intuition:

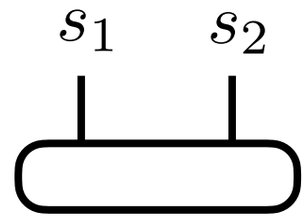


Observe state of first spin only: $\frac{1}{2}\uparrow, \frac{1}{2}\downarrow$

Highly *mixed*

Quantify by using *reduced density matrix*

$$|\Psi\rangle = \Psi^{s_1 s_2} |s_1 s_2\rangle$$



Quantify by using *reduced density matrix*

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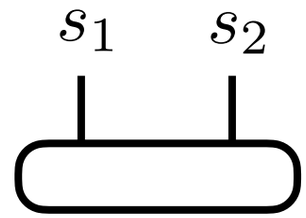
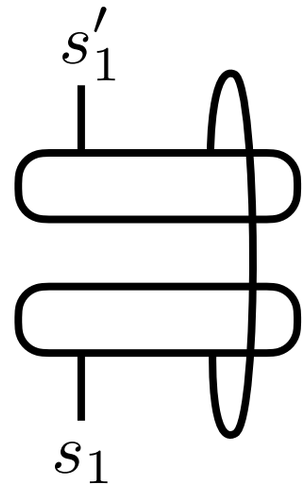


$$\rho_{s_1}^{s_1'} = \sum_{s_2} \Psi^{s_1' s_2} \Psi_{s_1 s_2}$$

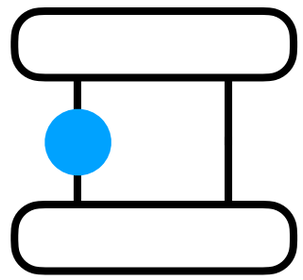


$$= \mathrm{Tr}_2[|\Psi\rangle\langle\Psi|]$$

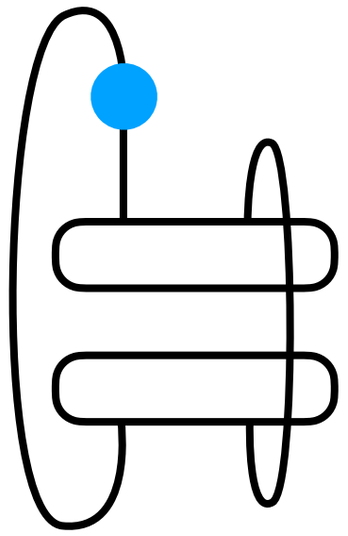
Why reduced density matrix?

Characterizes all observables of spin #1:

$$\langle \Psi | \hat{\mathcal{O}}_1 | \Psi \rangle$$



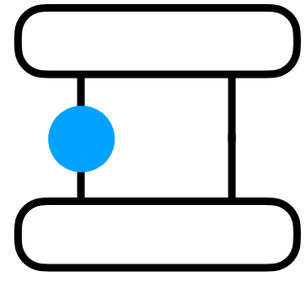
$$= \mathrm{Tr}[\rho_1 \hat{\mathcal{O}}_1]$$



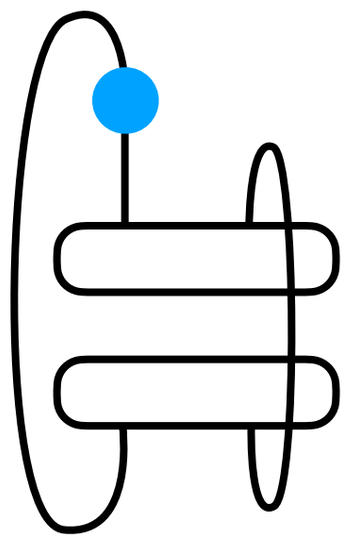
Why reduced density matrix?

Characterizes all observables of spin #1:

$$\langle\Psi|\hat{\mathcal{O}}_1|\Psi\rangle = \sum_{s_1 s_1' s_2} \Psi^*_{s_1 s_2} \hat{\mathcal{O}}^{s_1}_{s_1'} \Psi^{s_1' s_2}$$



$$= \mathrm{Tr}[\rho_1 \hat{\mathcal{O}}_1] = \sum_{s_1 s_1'} \rho^{s_1'}_{s_1} \hat{\mathcal{O}}^{s_1}_{s_1'}$$



Reduced density matrix in extreme cases

Case #1: trivial product state

$$\Psi^{s_1 s_2} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad |\Psi\rangle = |\uparrow\uparrow\rangle$$

$$\rho_{s_1}^{s_1'} = \sum_{s_2} \Psi^{s_1' s_2} \Psi^*_{s_1 s_2} = \Psi\Psi^\dagger$$

$$= \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

Case #2: singlet state $|\Psi\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle|\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\rangle|\uparrow\rangle$

$$\Psi^{s_1 s_2} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$\rho_{s_1}^{s_1'} = \sum_{s_2} \Psi^{s_1' s_2} \Psi^*_{s_1 s_2} = \Psi \Psi^\dagger$$

$$= \frac{1}{2} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Summary of cases:

Case #1: product state $|\Psi\rangle = |\uparrow\uparrow\rangle$

$$\rho_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

one non-zero eigenvalue

Case #2: singlet state $|\Psi\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle|\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\rangle|\uparrow\rangle$

$$\rho_1 = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$$

two non-zero eigenvalues

Entanglement Entropy

Convenient to summarize eigenvalues as an "entropy"

Let eigenvalues of ρ be $\{p_n\}$

Define "von Neumann entanglement entropy" as

$$S_{\mathrm{vN}} = -\sum_n p_n \ln(p_n)$$

$$= -\mathrm{Tr}\left[\rho \ln(\rho)\right]$$

Quantifies sharing of information between spins

Entanglement Entropy

Case #1: product state $|\Psi\rangle = |\uparrow\uparrow\rangle$

$$\rho_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$$S_{\mathrm{vN}} = -\sum_n p_n \ln(p_n)$$

$$= -1 \cdot \ln(1) - 0 \cdot \ln(0) = 0 + 0$$

$$= 0$$

Entanglement Entropy

Case #2: singlet state $|\Psi\rangle = \frac{1}{\sqrt{2}}|\uparrow\rangle|\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\rangle|\uparrow\rangle$

$$\rho_1 = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/2 \end{bmatrix}$$

$$S_{\mathrm{vN}} = -\sum_n p_n \ln(p_n)$$

$$= -\frac{1}{2}\ln\left(\frac{1}{2}\right) - \frac{1}{2}\ln\left(\frac{1}{2}\right) = -\ln\left(\frac{1}{2}\right)$$

$$= \ln(2)$$ maximum possible!

Entanglement Entropy

Important note: if reduced density matrix not diagonal, must diagonalize to get eigenvalues

For example,

$$\rho_1 = \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \frac{1}{\sqrt{2}}$$

Test Your Knowledge! 🤔

Compute the entanglement entropy of the following state:

$$|\Psi\rangle = \frac{1}{2}|\uparrow\uparrow\rangle + \frac{1}{2}|\uparrow\downarrow\rangle + \frac{1}{2}|\downarrow\uparrow\rangle + \frac{1}{2}|\downarrow\downarrow\rangle$$

$$\Psi^{s_1 s_2} = \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}$$

Recall: $\rho_{s_1}^{s_1'} = \sum_{s_2} \Psi^{s_1' s_2} \Psi^*_{s_1 s_2} = \Psi\Psi^\dagger$

Rényi Entropy

von Neumann entropy just one way to summarize density matrix eigenvalues

Alternative is *Rényi entropy* with *Rényi index* α

$$S_\alpha = \frac{1}{1-\alpha} \ln \mathrm{Tr}[\rho^\alpha] = \frac{1}{1-\alpha} \ln \left[\sum_n (p_n)^\alpha \right]$$

Defined to reproduce von Neumann entropy as $\alpha \to 1$

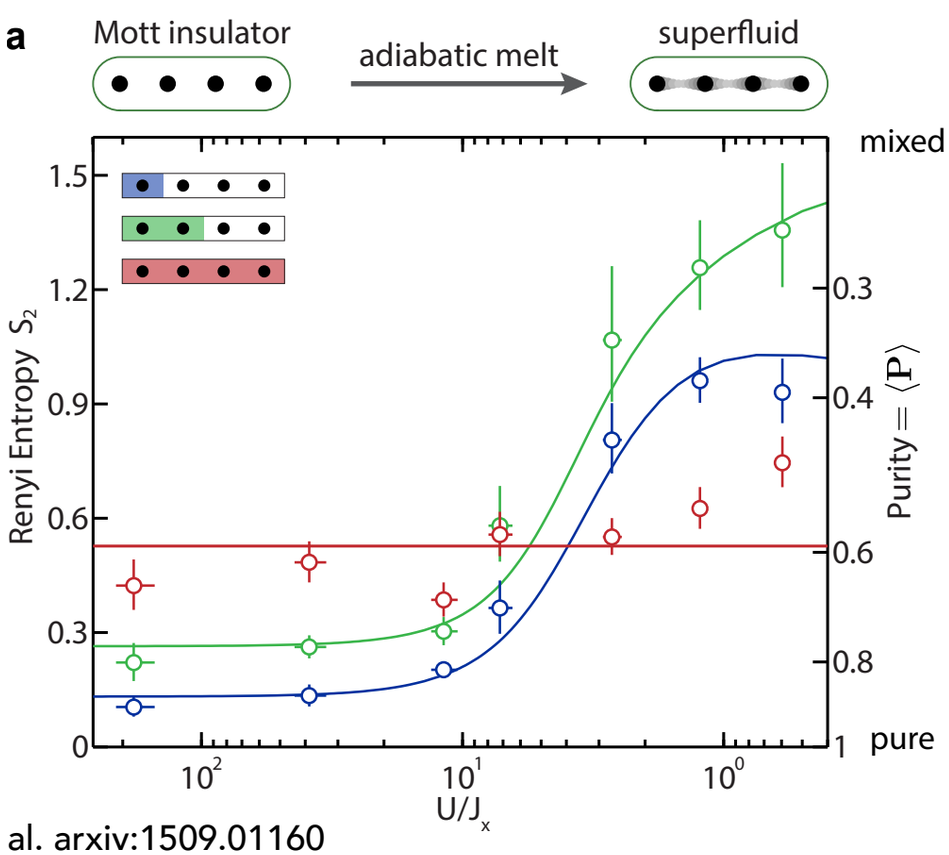
$$\lim_{\alpha \to 1} S_\alpha = S_{\mathrm{vN}}$$

Second Rényi Entropy

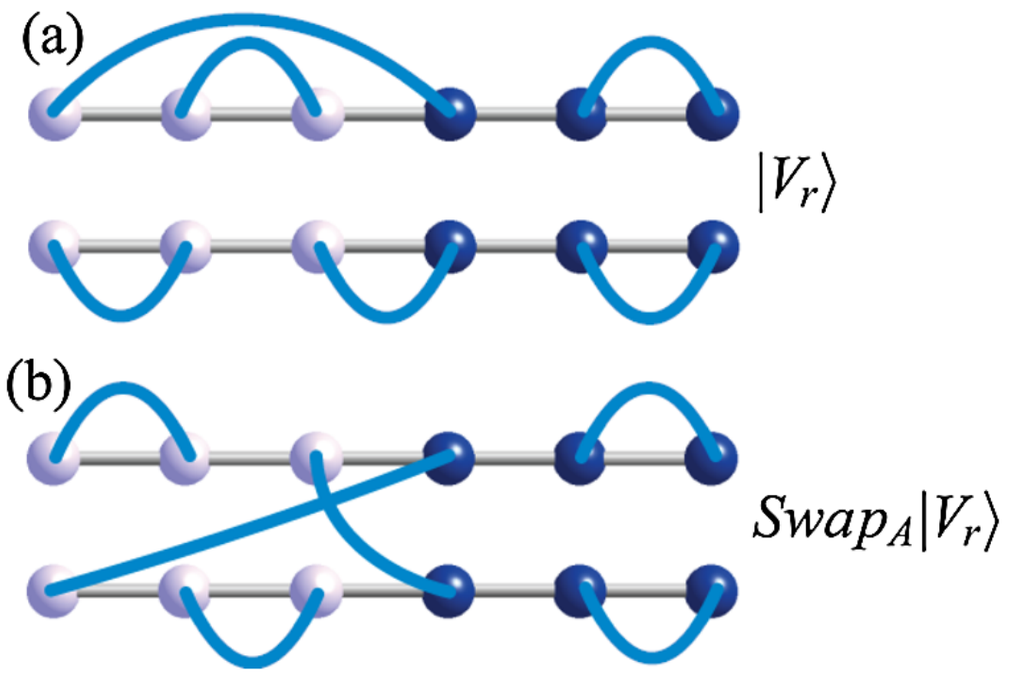
The second Rényi entropy with $\alpha = 2$
is especially interesting

$$S_2 = -\ln \mathrm{Tr}[\rho^2]$$

Can be measured in experiment and by quantum Monte Carlo



Islam, et al. arxiv:1509.01160



Hastings, Gonzalez, Kallin, Melko, PRL **104**, 157201 (2010)

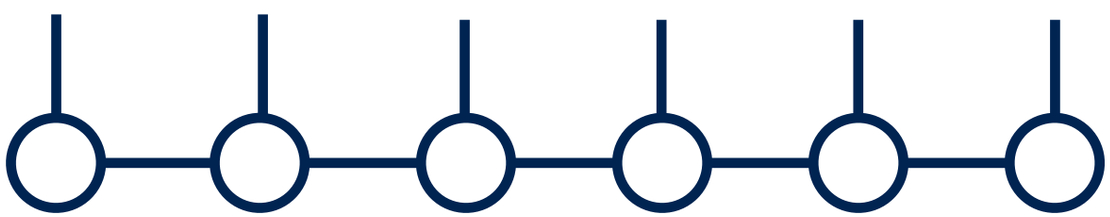
Many-Body Entanglement

To discuss many-body wavefunctions, very helpful to introduce **tensor diagrams**

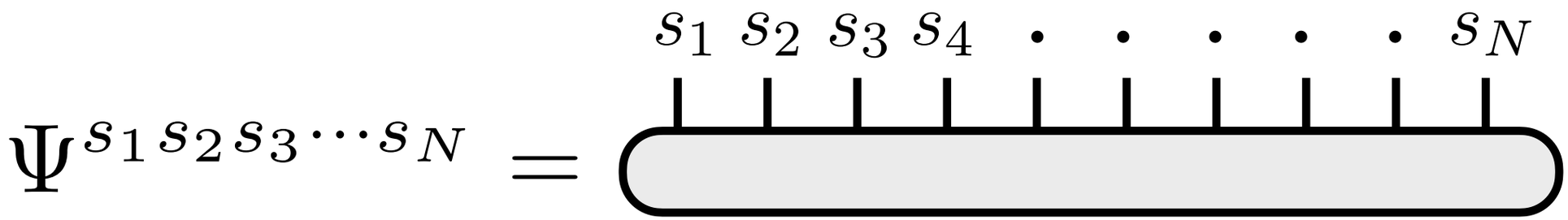
Simple way to notate large tensors & sums

$$\sum_{\alpha} M^{s_1}_{\alpha_1} M^{s_2}_{\alpha_1\alpha_2} M^{s_3}_{\alpha_2\alpha_3} M^{s_4}_{\alpha_3\alpha_4} M^{s_5}_{\alpha_4\alpha_5} M^{s_6}_{\alpha_5}$$

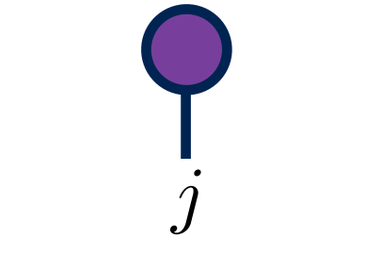
$=$



N-index tensor represented as "blob" with N lines

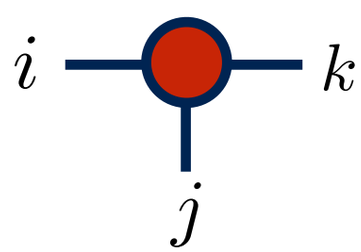


Diagrams for simple tensors



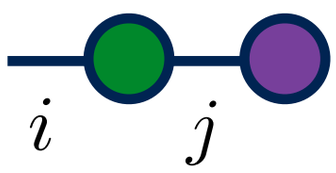
v_j

M_{ij}



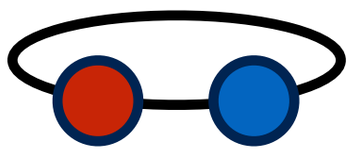
T_{ijk}

Joining lines implies contraction, can omit names



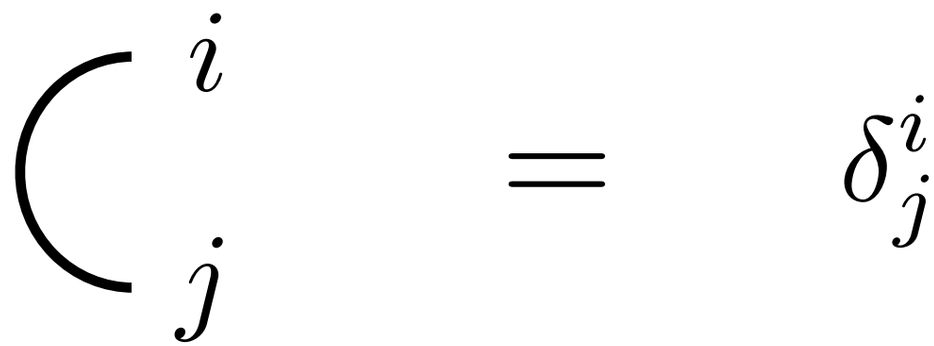
$$\longleftrightarrow \quad \sum_j M_{ij} v_j$$

$$\longleftrightarrow \quad A_{ij} B_{jk} = AB$$



$$\longleftrightarrow \quad A_{ij} B_{ji} = \mathrm{Tr}[AB]$$

Undecorated line means identity tensor
(Kronecker delta tensor)



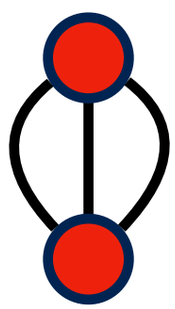
Test Your Knowledge! 🤔

Write a "classical" (index) expression for the following diagrams:

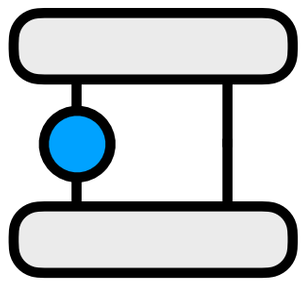
(1)

(2)

(3)



(4)

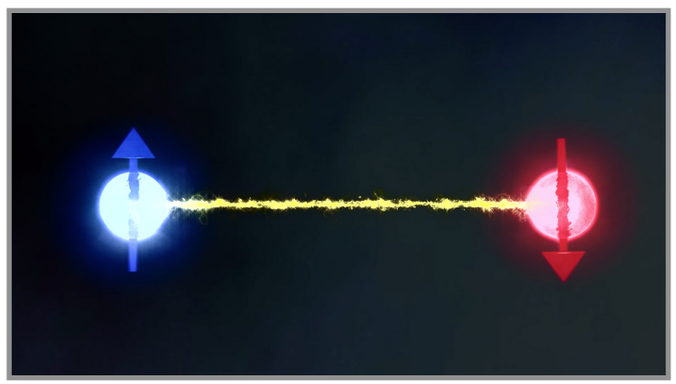


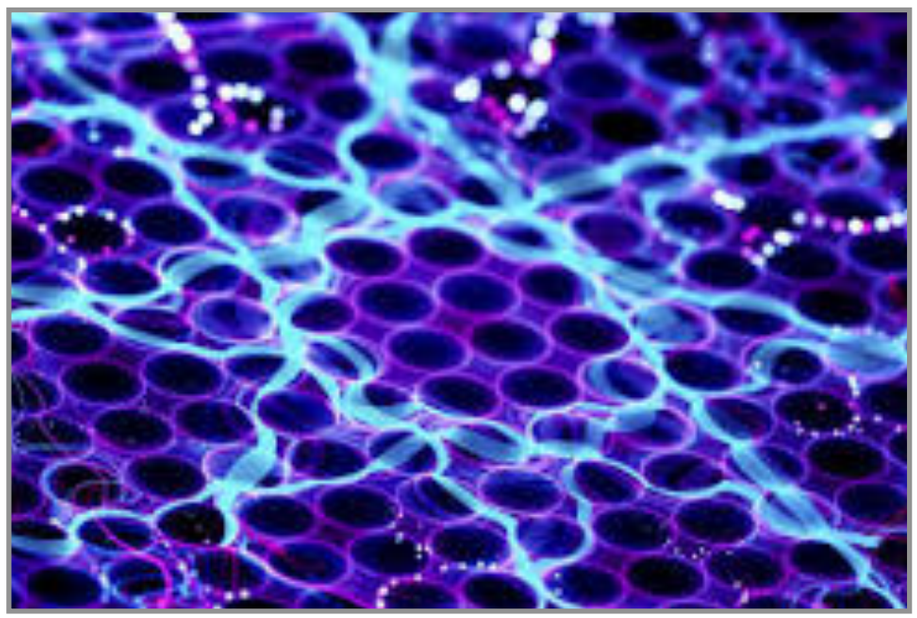
Which ones give a scalar result?

How is entanglement defined for many-body wavefunctions?

What does entanglement reveal about wavefunctions?

Which wavefunctions?

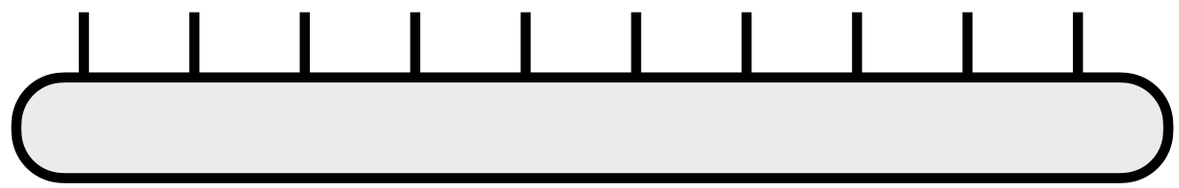




Many-Body Entanglement

Define entanglement by dividing sites into region "A" and "B"

$|\Psi\rangle =$



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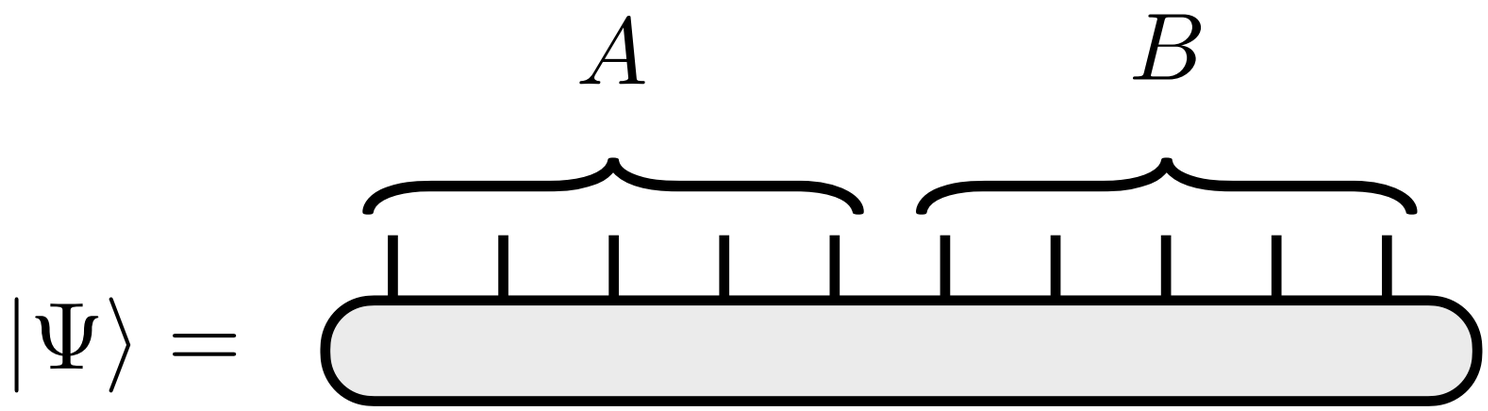
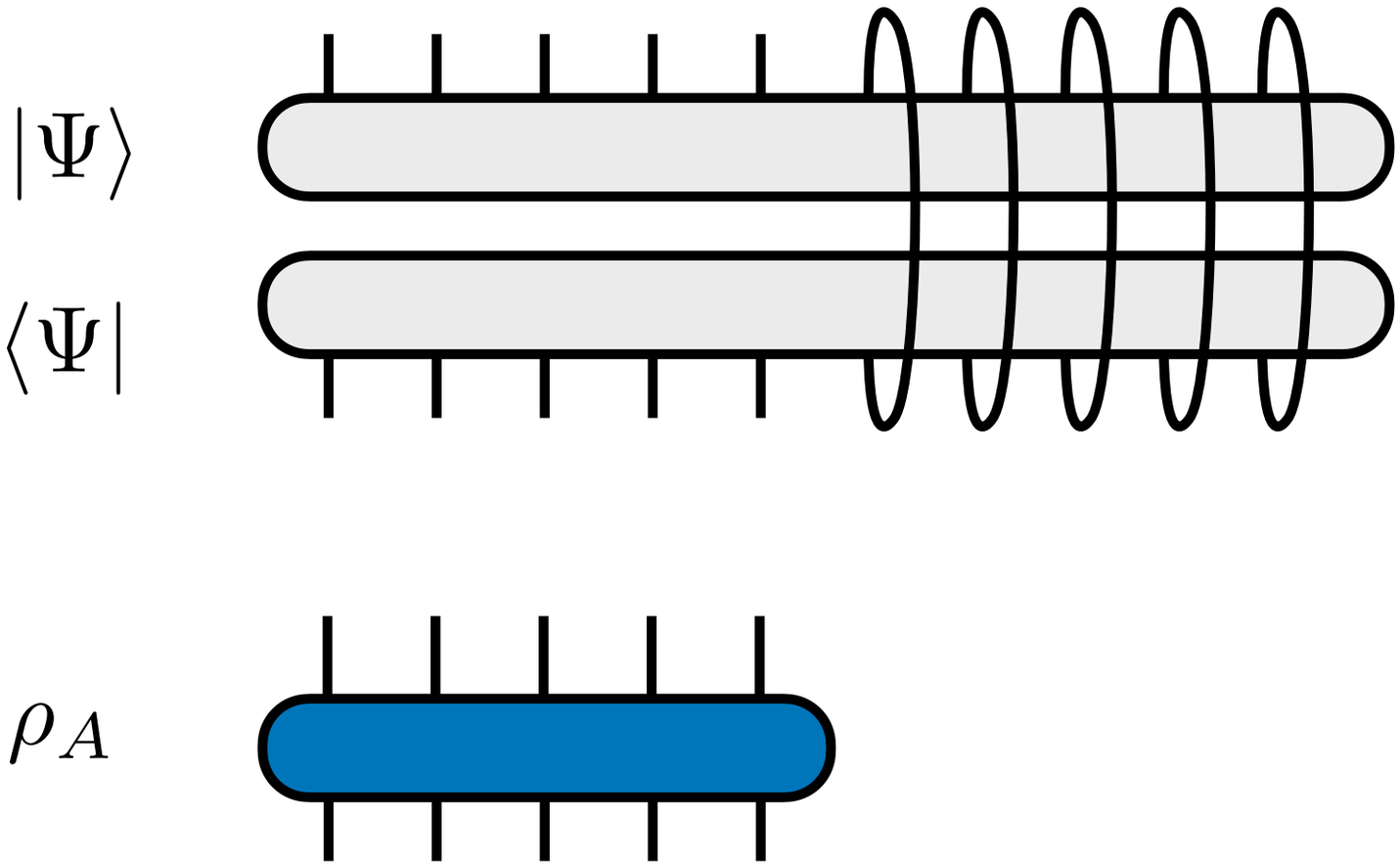


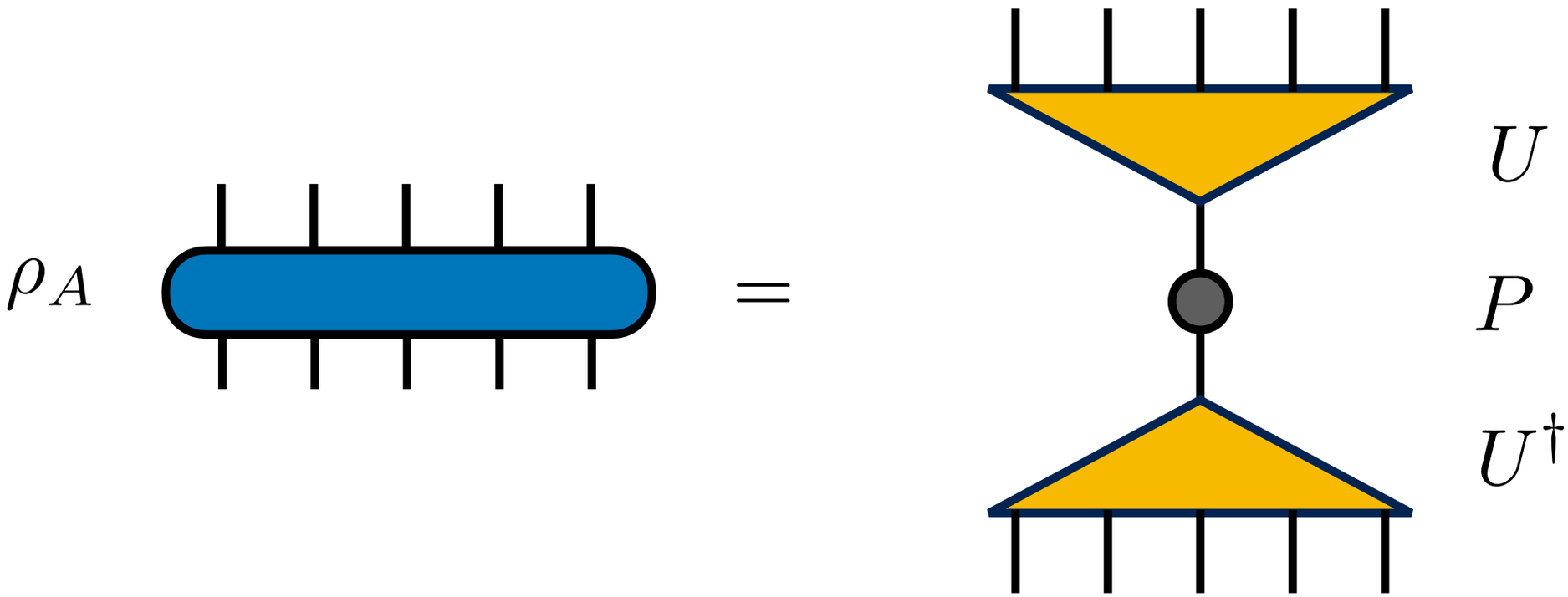
Many-Body Entanglement

Trace over region B to get reduced density matrix of A



Many-Body Entanglement

Diagonalize ρ_A to get eigenvalues



$$P = \begin{bmatrix} p_1 & & & & & \\ & p_2 & & & & \\ & & p_3 & & & \\ & & & p_4 & & \\ & & & & p_5 & \\ & & & & & \ddots \end{bmatrix}$$

Many-Body Entanglement

Use eigenvalues of ρ_A to compute S_{vN}

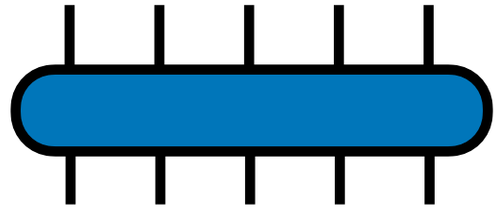
$$P = \begin{bmatrix} p_1 & & & & & \\ & p_2 & & & & \\ & & p_3 & & & \\ & & & p_4 & & \\ & & & & p_5 & \\ & & & & & \ddots \end{bmatrix}$$

$$S_{\mathrm{vN}} = -\sum_n p_n \ln(p_n)$$

Many-Body Entanglement

What is the maximum amount of entanglement?

ρ_A is a $2^{N/2} \times 2^{N/2}$ matrix



$2^{N/2}$ eigenvalues, trace has to be 1

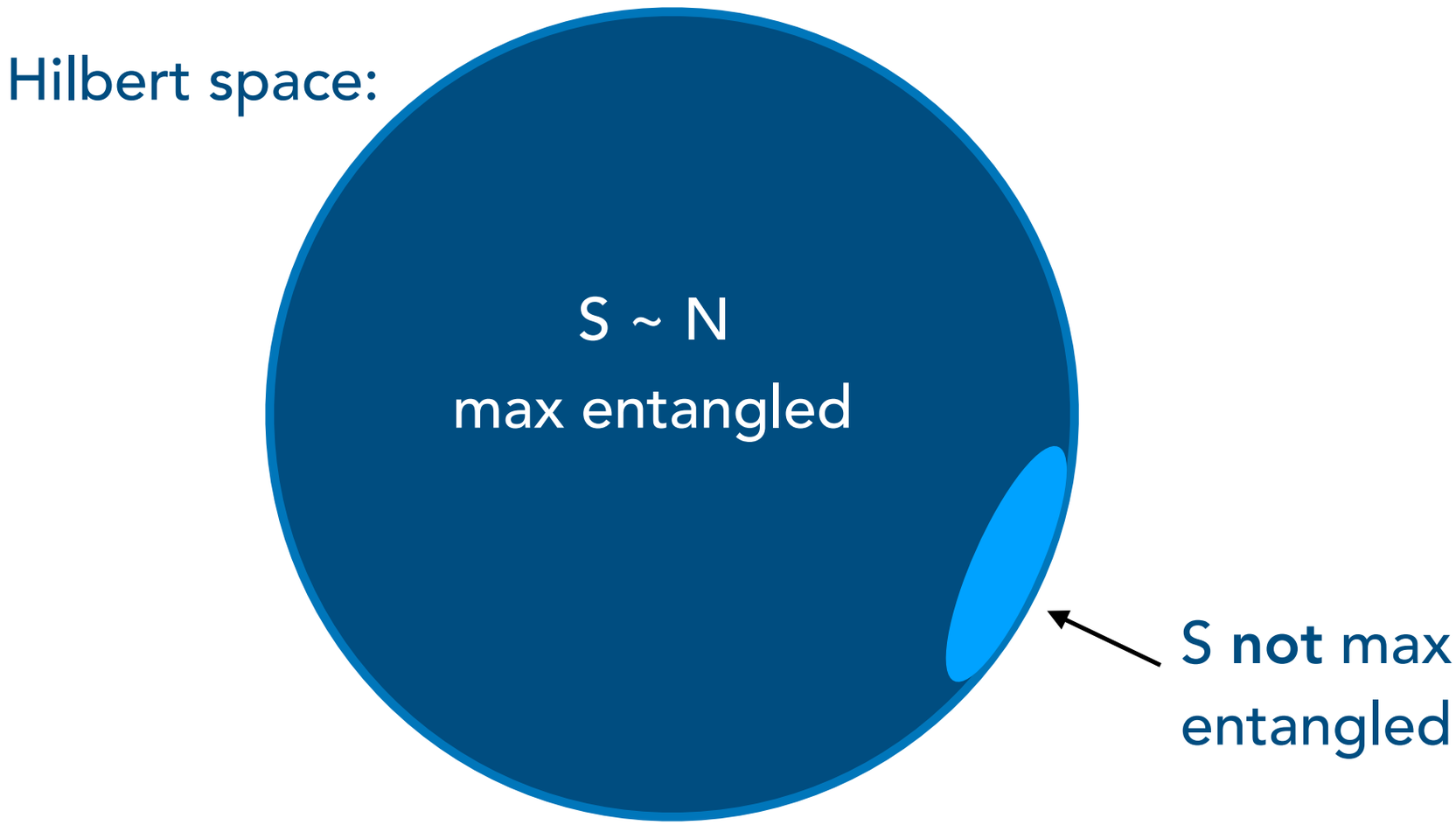
maximum entropy if all eigenvalues same, $p_n \equiv 2^{-N/2}$

$$S_{\mathrm{vN}} = -\sum_{n=1}^{2^{N/2}} p_n \ln(p_n) = -2^{N/2} \frac{1}{2^{N/2}} \ln(2^{-N/2})$$

$$= \frac{N}{2} \ln(2) \sim N$$ "volume law"

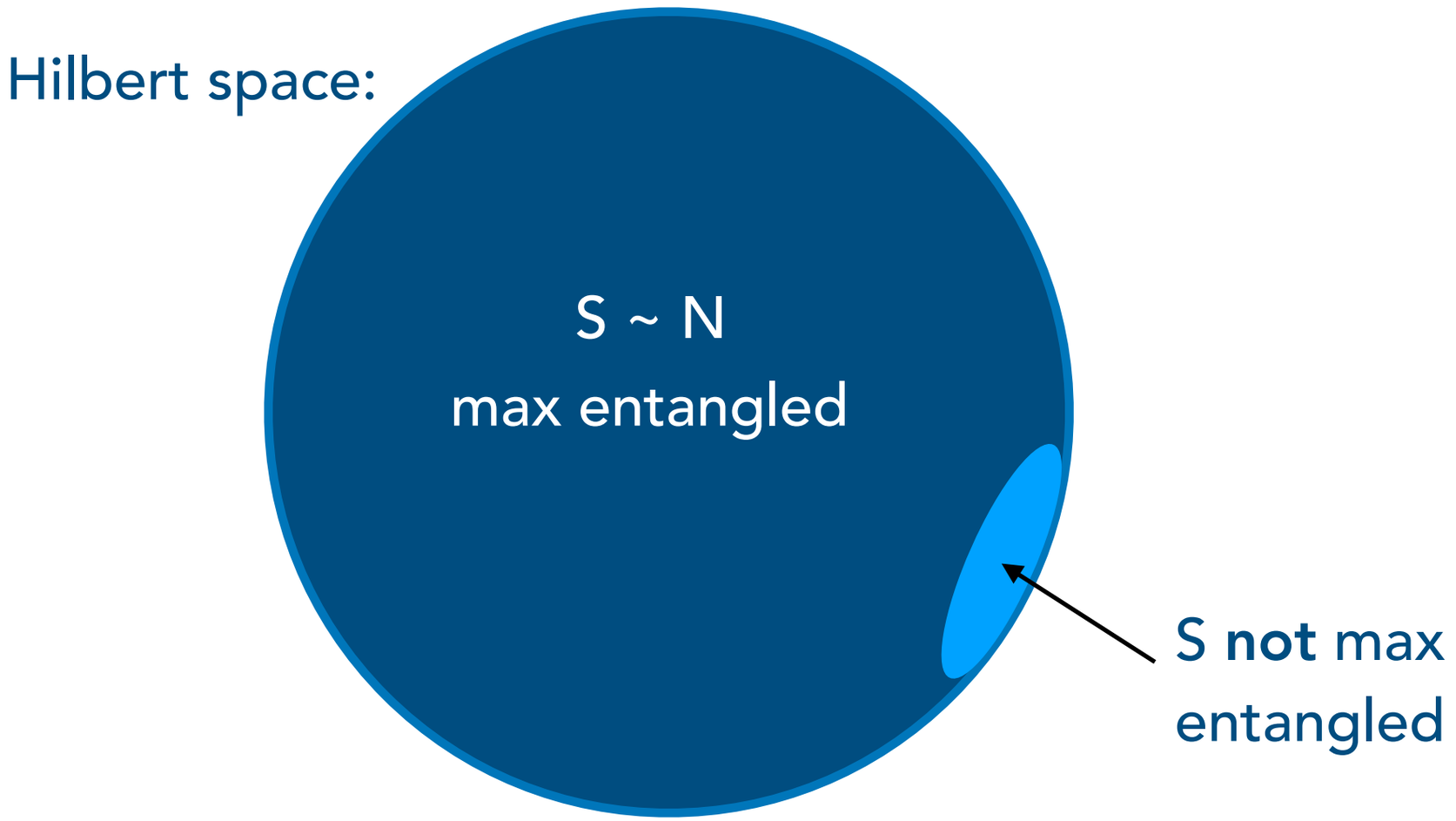
Many-Body Entanglement

Fact: randomly chosen wavefunctions have maximum entropy with probability 1.0



Many-Body Entanglement

Which wavefunctions live in the special region that is not maximally entangled?



Consider ***ground states*** of 1D Hamiltonians

Heisenberg spin chain:

$$H = \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$

Hubbard chain:

$$H = -t \sum_{j,\sigma} (c^\dagger_{j,\sigma} c_{j+1,\sigma} + c^\dagger_{j+1,\sigma} c_{j,\sigma}) + \sum_j U n_{j\uparrow} n_{j\downarrow}$$

1D "electronic structure" Hamiltonian:

$$H = \int_x \psi^\dagger(x) \Big[-\frac{1}{2}\partial_x^2 + v(x) \Big] \psi(x) + \int_{x,x'} u(x-x') n(x) n(x')$$

By ***ground state*** we mean

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle \qquad\qquad E_0 \leq E_1 \leq E_2 \leq \ldots$$

Then the ground state is $|\Psi_0\rangle$

(May be degenerate, meaning $|E_1 - E_0| \sim e^{-aN}$)

Special cases of ground states

Case #1: Heisenberg ferromagnet

$$H = -\sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$

$$|\Psi_0\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle = |\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle$$

Special cases of ground states

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zero entanglement

Special cases of ground states

Case #2: "Majumdar-Ghosh chain"

$$H = \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1} + \frac{1}{2} \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+2}$$

Ground state a product of singlets:

$|\Psi_0\rangle =$ 

Special cases of ground states

Case #2: "Majumdar-Ghosh chain"

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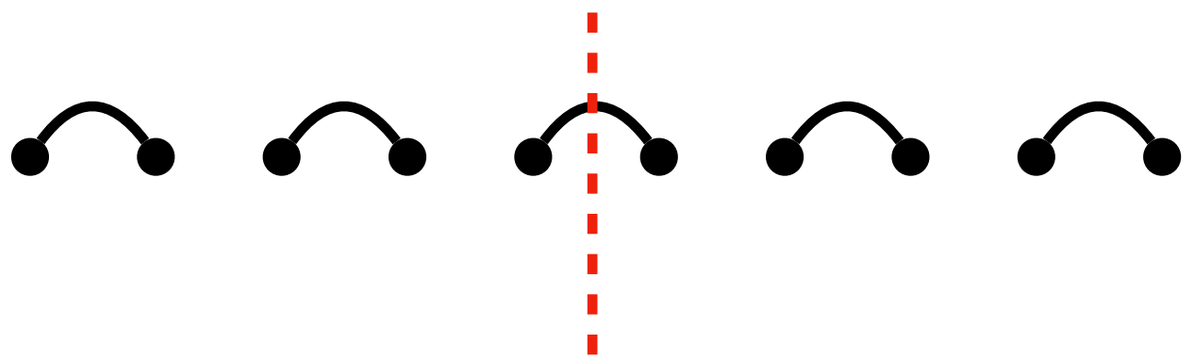
$|\Psi_0\rangle =$ 

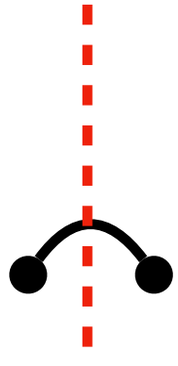
entanglement S=ln(2)

Non-extensive entanglement (not volume law)

How typical are these cases?

As system size N increases, is following possible?

$|\Psi_0\rangle =$



$$S = \ln(2)$$

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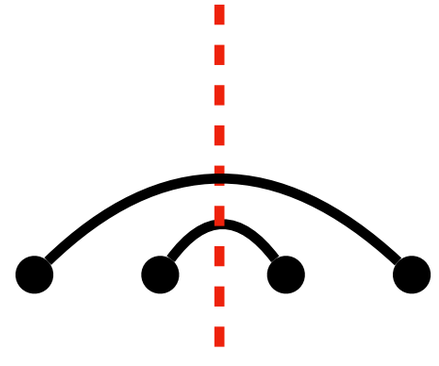

$$S = 2\ln(2)$$

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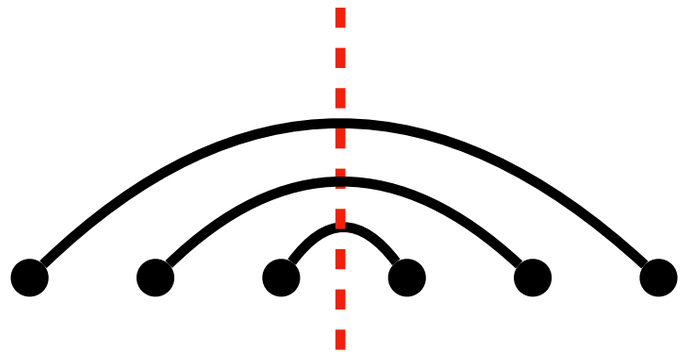
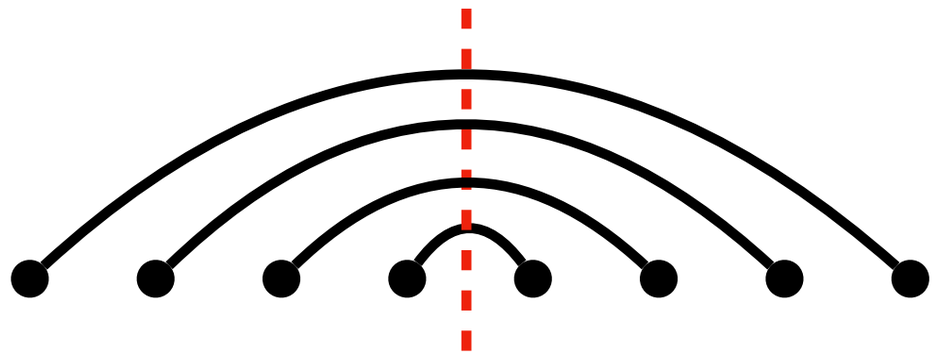


$$S = 3\ln(2)$$

How typical are these cases?

As system size N increases, is following possible?

$|\Psi_0\rangle =$



$$S = 4\ln(2)$$

Would give a "**volume law**" of entanglement: $S \sim N$

But Hamiltonian would be non-local:

$$H = \mathbf{S}_1 \cdot \mathbf{S}_8 + \mathbf{S}_2 \cdot \mathbf{S}_7 + \mathbf{S}_3 \cdot \mathbf{S}_6 + \ldots$$

What is the case for *local* Hamiltonians?

Around 2000-2005 many researchers observed for 1D systems, that $S_{\mathrm{vN}} \sim \mathrm{const.} \sim N^0$ for the ground state

But logarithmic violations also observed (Vidal, 2003)

What is the case for *local* Hamiltonians?

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But logarithmic violations also observed (Vidal, 2003)

Then in 2007, M. Hastings proved:

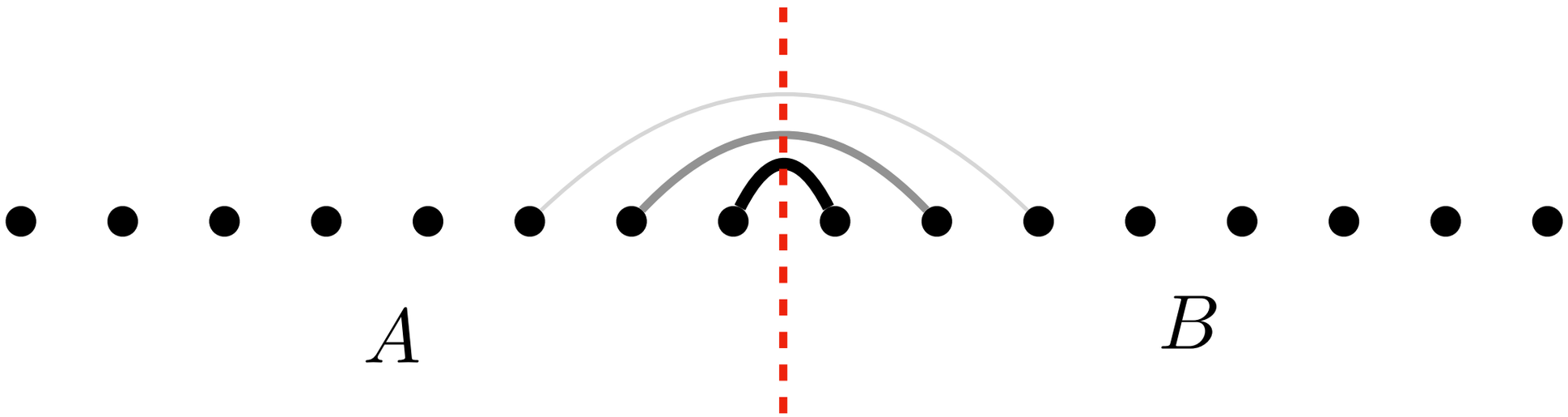
For 1D, **local** Hamiltonians with a **gap** between ground and excited states, the entanglement entropy of a bipartition is independent of system size as $N \to \infty$

this is the "**area law**" or "**boundary law**"

Hastings, J. Stat. Mech. P08024 (2007)

Intuition of **boundary law**

All entanglement between A and B due to entangled spins near their boundary



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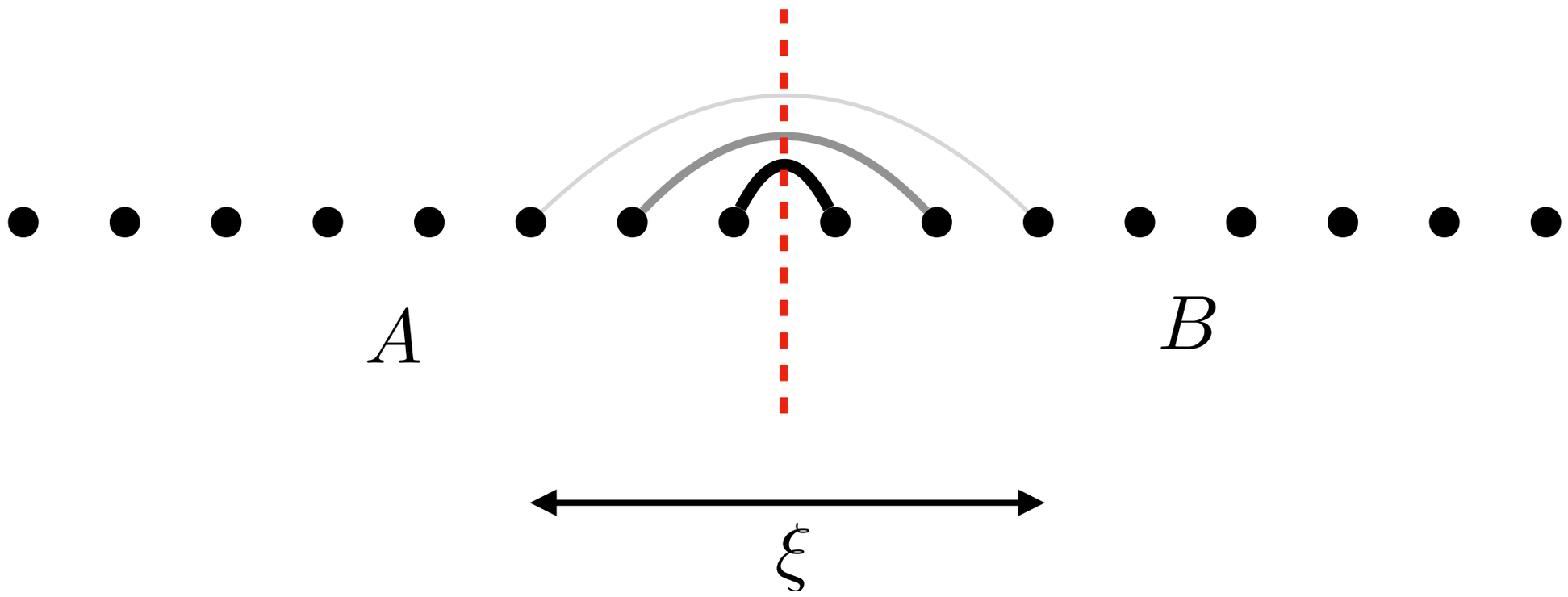

Local H and **gap** required implies a correlation length ξ