Tensor Networks & Entanglement

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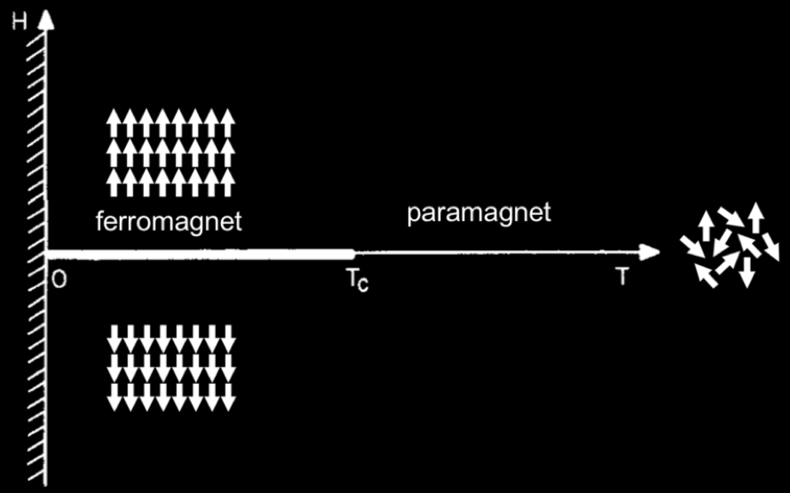
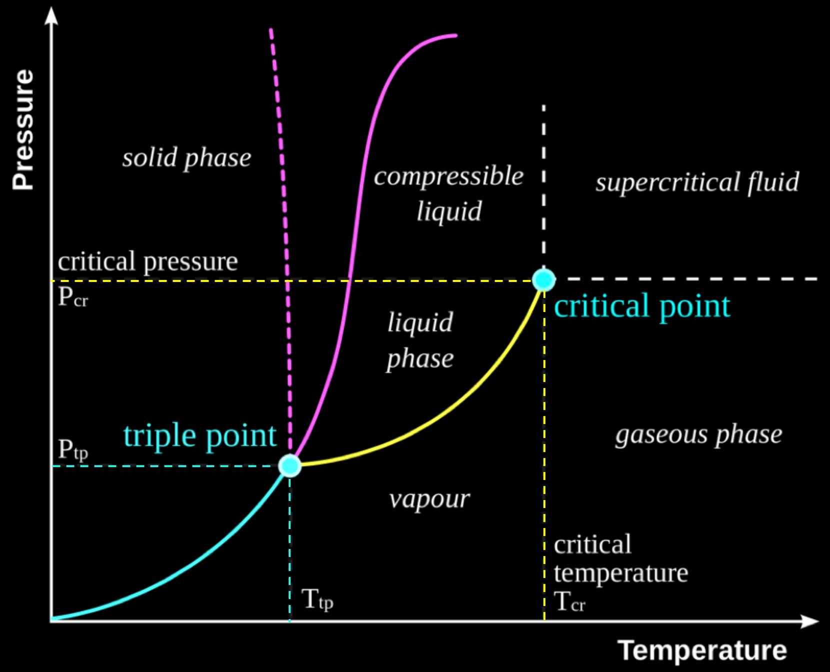
Motivation remarks

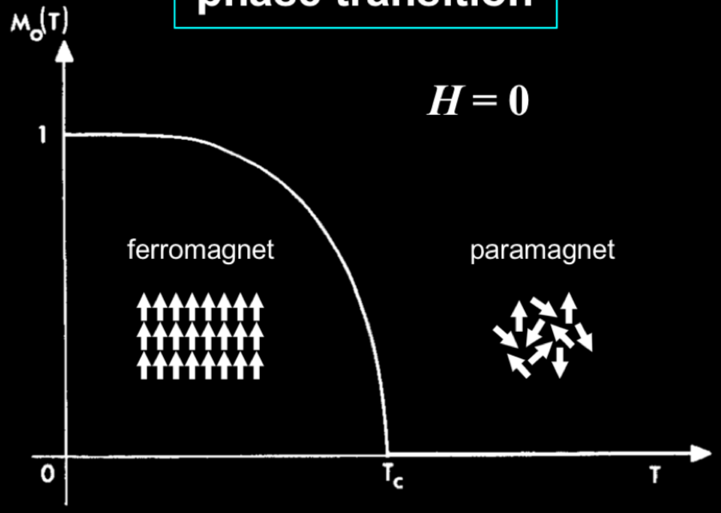
Part 1

Phase transitions

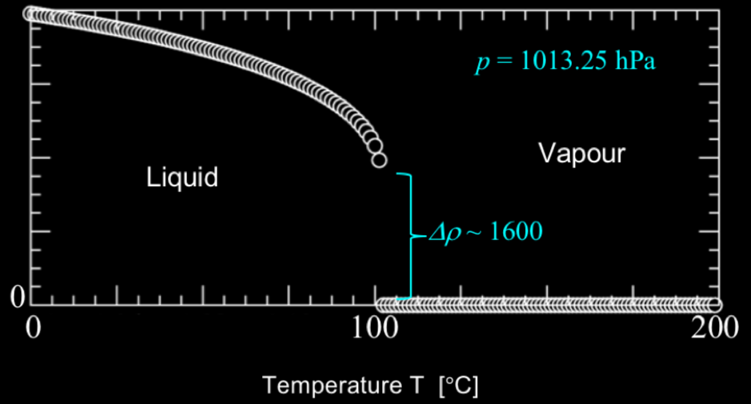


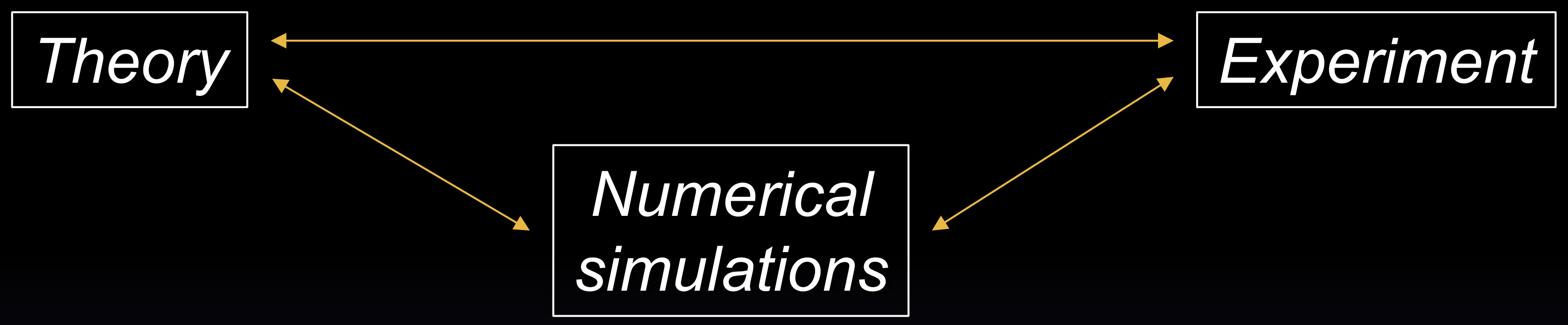


The 2nd order phase transition



The 1st order phase transition





Numerical methods *(in terms of Tensor Networks)*

- *DMRG* — *Density Matrix Renormalization Group*
- *CTMRG* — *Corner Transfer Matrix Renormalization Group*
- *MPS* — *Matrix Product States*
- *TEBD* — *Time Evolving Block Decimation*
- *HOTRG* — *Higher-Order Tensor Renormalization Group*
- *TPVF* — *Tensor Product Variational Formulation*
- *MERA* — *Multi-scale Entanglement Renormalization Ansatz*

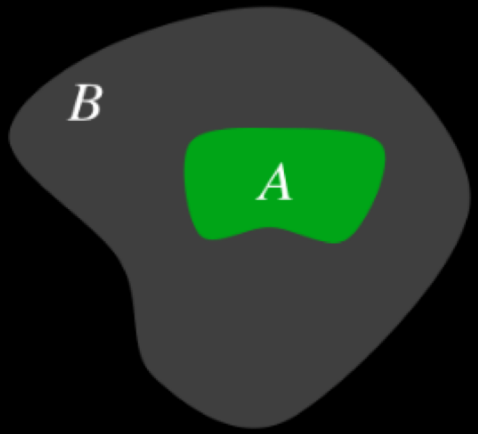
Entanglement Entropy

(What else is it good for?)

$$H|\psi_n\rangle = E_n|\psi_n\rangle, \qquad n = 0, 1, 2, \ldots$$

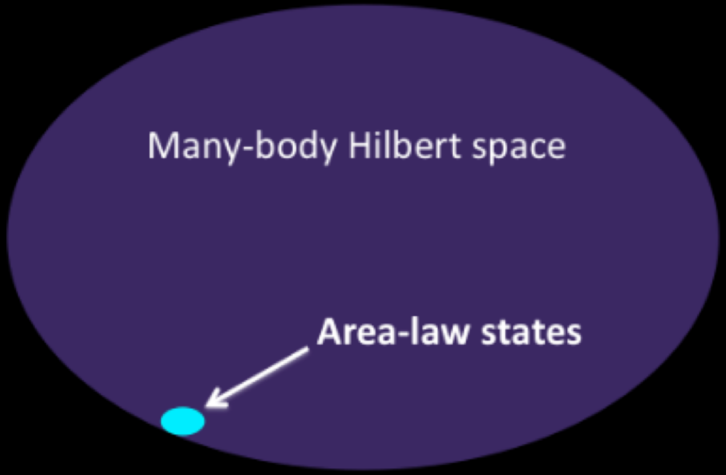
$$\rho'_A = Tr_B\{|\psi_0(A,B)\rangle\langle\psi_0(A,B)|\}$$

$$S = -Tr\left(\rho'_A \log_2(\rho'_A)\right) \geq 0$$



Area law

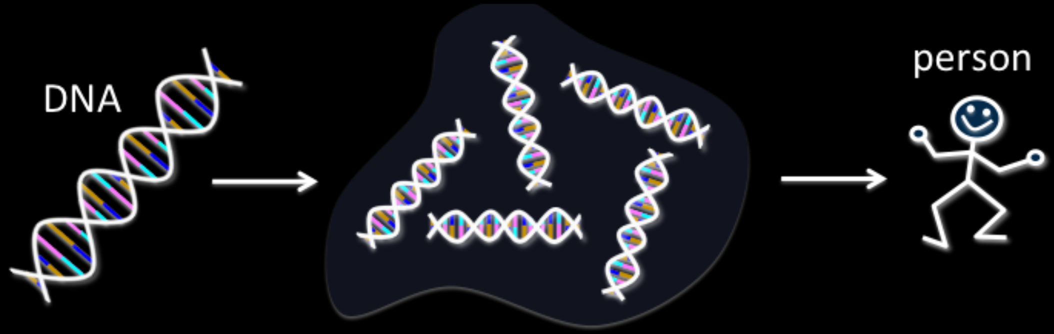
$S \sim \partial A$

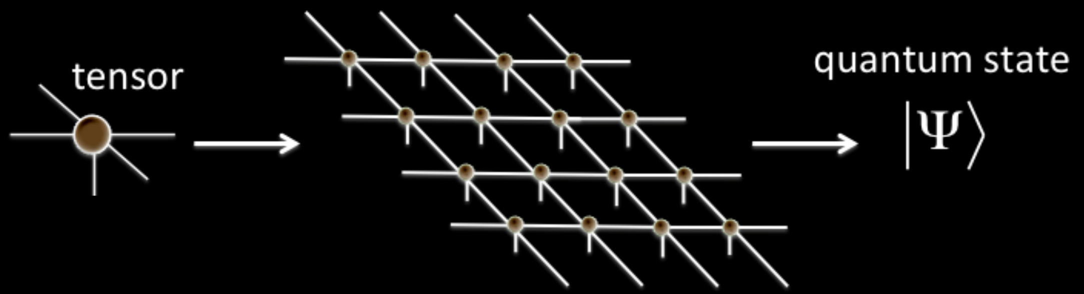


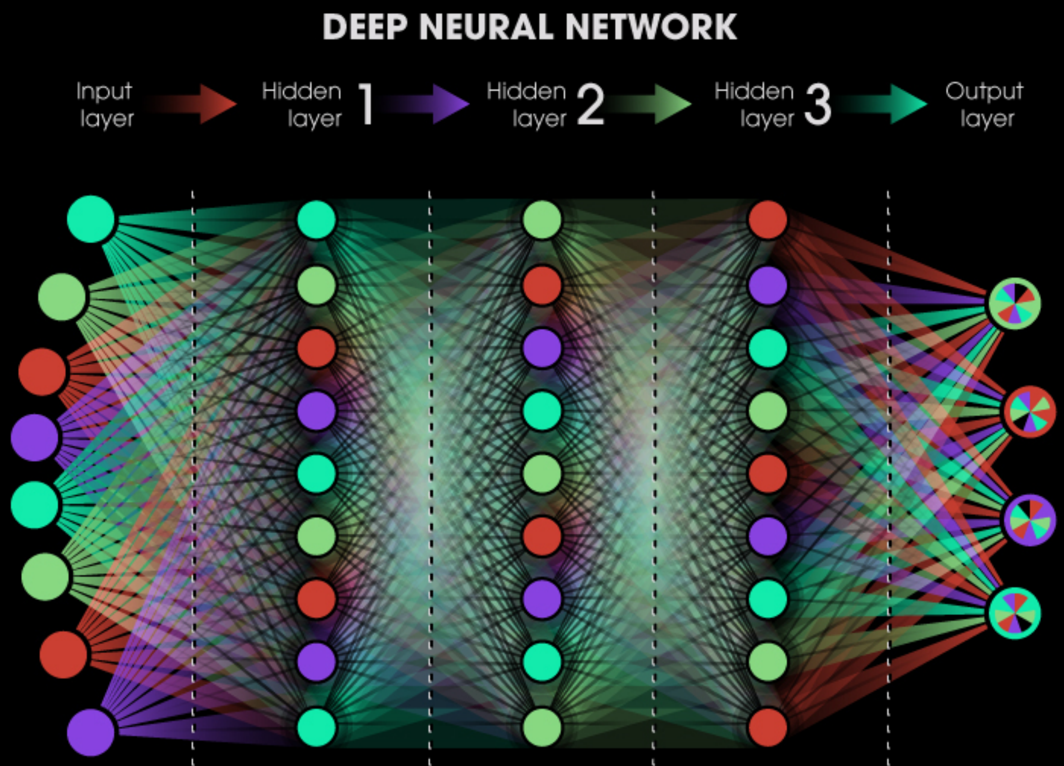
Motivation remarks

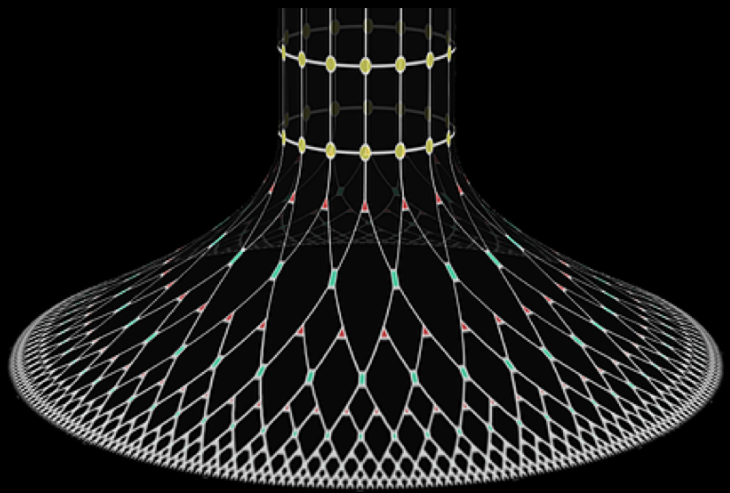
Part 2

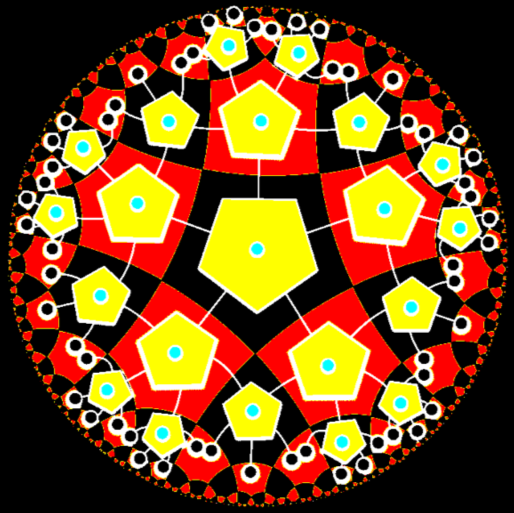
A quantum state of Hamiltonian
is like
"a state of mind in brain"

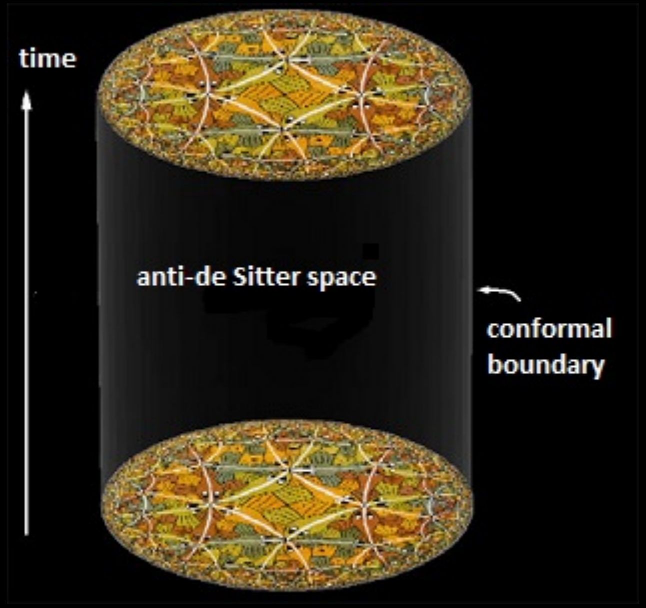

DNA
person

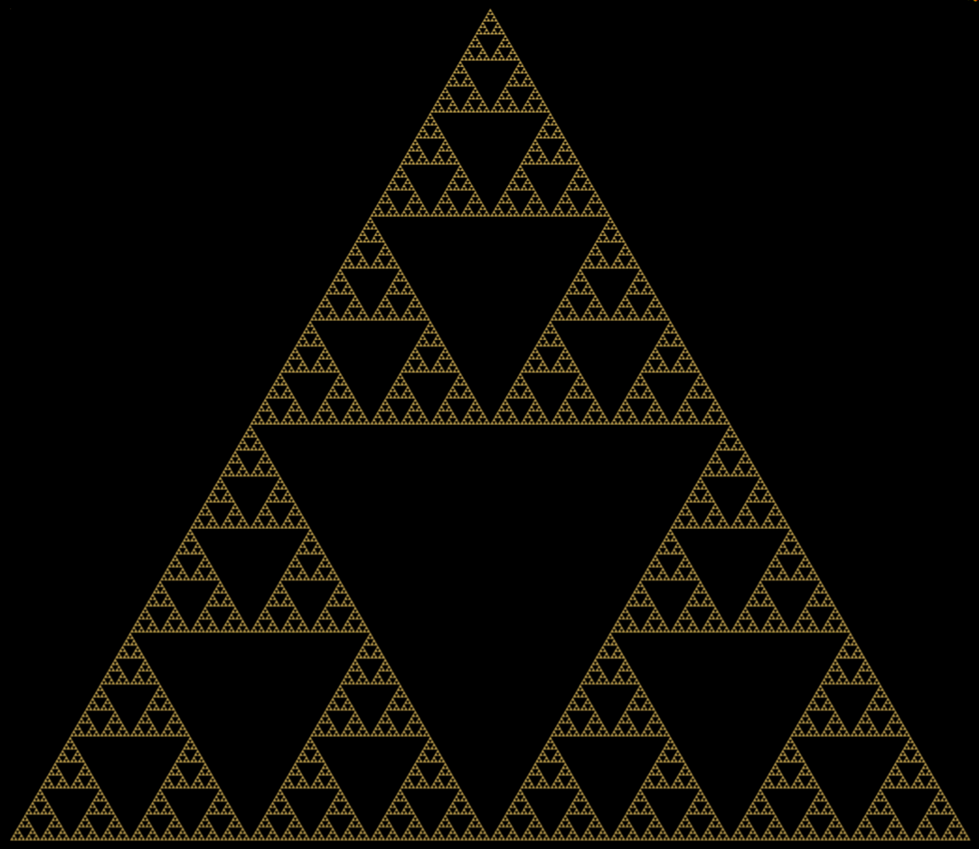

tensor
quantum state
$|\Psi\rangle$


DEEP NEURAL NETWORK
Input layer
Hidden layer 1
Hidden layer 2
Hidden layer 3
Output layer

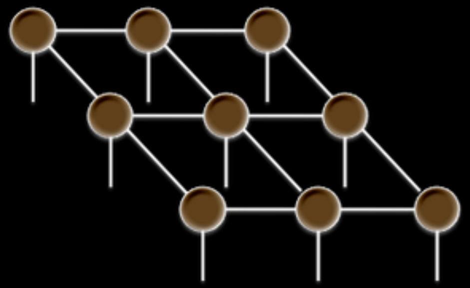








Matrix Product State → Tensor Product State



Quantum mechanics

Introduction to numerics

Introduction to solving quantum-mechanical problems

- Only <u>a few</u> simple systems are exactly (analytically) solvable!

- The aim is to find out <u>efficient approximations</u>
  - either analytically (by pen and heaps of paper and time)
  - or numerically (by computers and much shorter time)

- If exact solutions exist, they may serve as <u>benchmarks</u>

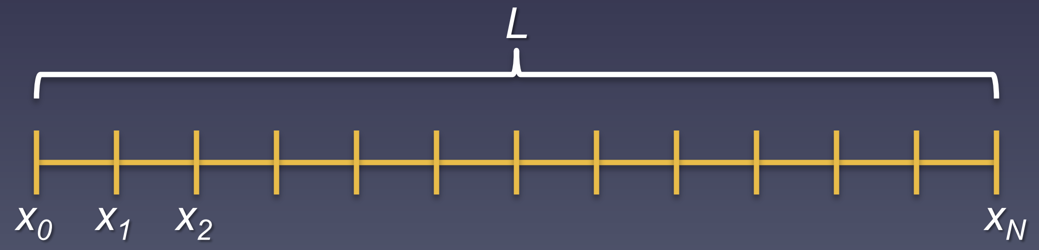
- Two examples: Let us study **<u>two simplest</u>** quantum systems numerically
  At first, continuous variables has to be discretized.

Discretization:

$$0 \le x \le L \rightarrow x_i = \frac{iL}{N} \quad \text{and} \quad i = 0,1,2,\ldots,N$$

$$x \rightarrow x_i \rightarrow i$$

$$f(x) \rightarrow f(x_i) \rightarrow f_i$$

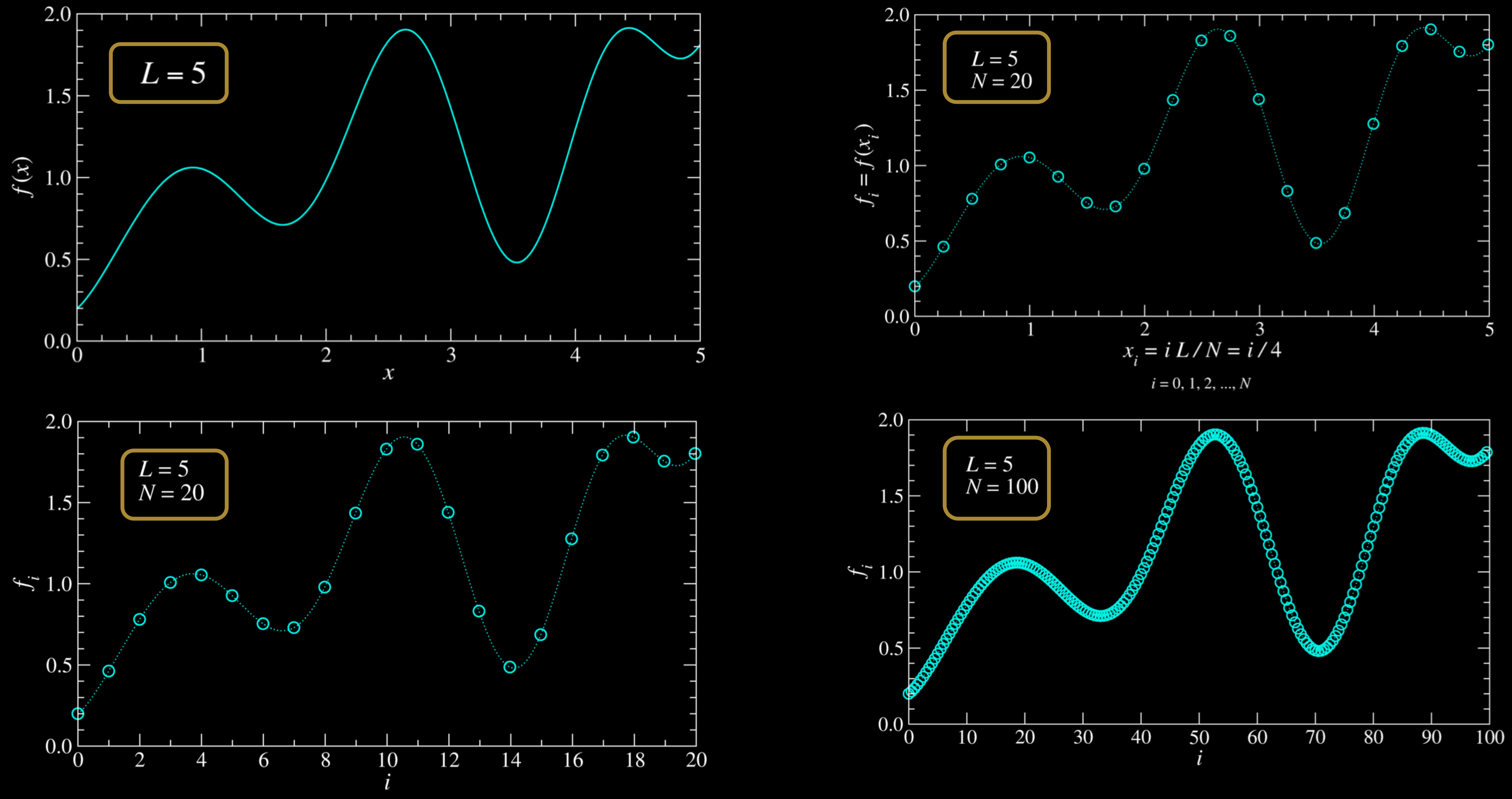


Discretization:

$$x \to x_i \to i$$

$$f(x) \to f(x_i) \to f_i$$

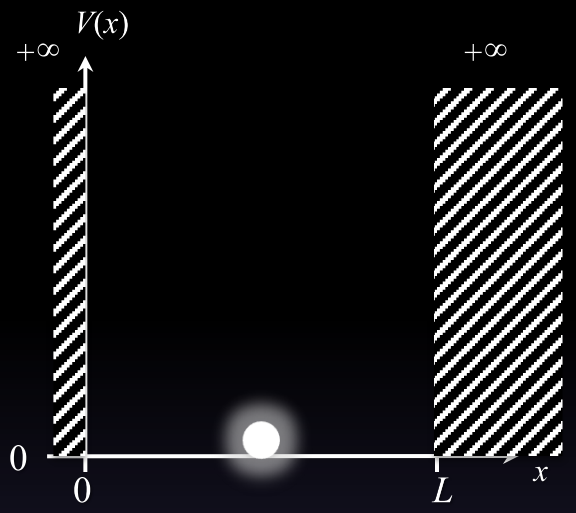
$$0 \le x \le L \to x_i = \frac{iL}{N} \quad \text{and} \quad i = 0,1,2,\dots,N$$



A simple example: 1D particle in a box (infinite potential well)

$$\left[-\frac{\hbar^2}{2m}\Delta + V(x)\right]\Psi(x) = E\ \Psi(x), \qquad V(x) = \begin{cases} 0, & 0 \le x \le L \\ \infty, & \text{otherwise} \end{cases}$$

$$-\Delta\Psi(x) = \frac{2m}{\hbar^2} E\ \Psi(x) \qquad \text{let} \qquad \hbar^2 / 2m = 1$$



discretized

$$-\Delta\Psi(x_i) = E'\ \Psi(x_i), \qquad x_i = \frac{iL}{N} \ \text{and} \ i = 0,1,2,\dots,N$$

$$-\frac{\Psi\left(\frac{(i-1)L}{N}\right) - 2\Psi\left(\frac{iL}{N}\right) + \Psi\left(\frac{(i+1)L}{N}\right)}{\left(\frac{L}{N}\right)^2} = E'\ \Psi\left(\frac{iL}{N}\right)$$

$$-\Psi_{i-1} + 2\Psi_i - \Psi_{i+1} = \tilde{E}\ \Psi_i$$

Matrix to be diagonalized to get E_0:

fixed boundary conditions:

$\Psi_{-1} = \Psi_{N+1} = 0$

periodic boundary conditions:

$\Psi_{-1} = \Psi_{N+1} = -1$

$$\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & & 0 \\ -1 & 2 & -1 & 0 & 0 & & 0 \\ 0 & -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & 0 & -1 & 2 & -1 & & 0 \\ 0 & 0 & 0 & -1 & 2 & & 0 \\ & & \vdots & & & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 2 \end{pmatrix} \begin{pmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \\ \\ \Psi_N \end{pmatrix} = \tilde{E}_0 \begin{pmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \\ \\ \Psi_N \end{pmatrix}$$

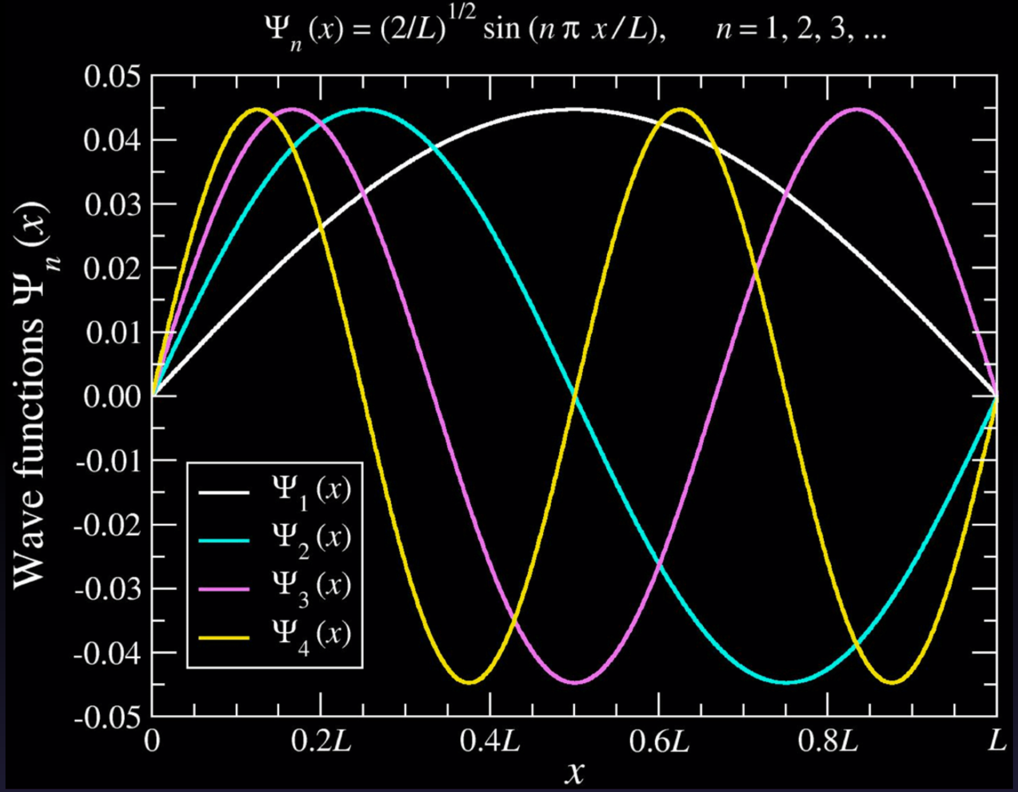
$$\hat{H} = -\frac{\partial^2}{\partial x^2} \approx -\sum_{j=1}^{N=1} \left(\hat{c}_j^+ \hat{c}_{j+1} + \hat{c}_{j+1}^+ \hat{c}_j\right) + 2\sum_{j=1}^{N=1} \hat{c}_j^+ \hat{c}_j$$

Exact solution exists!

For the 1D particle in the box we get:

$$E_n = \frac{\pi^2}{L^2} n^2, \qquad n = 1,2,\ldots$$

$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi n}{L} x\right)$$



	Relative error $\varepsilon = (E_n^{num} - E_n^{exact}) / E_n^{exact} \times 100\%$			
N	ε_0 [%]	ε_1 [%]	ε_2 [%]	ε_3 [%]
100	1.978	2.002	2.042	2.098
500	0.399	0.400	0.402	0.404
1 000	0.200	0.200	0.200	0.201
5 000	0.040	0.040	0.040	0.040
10 000	0.020	0.020	0.020	0.020
50 000	0.004	0.004	0.004	0.004

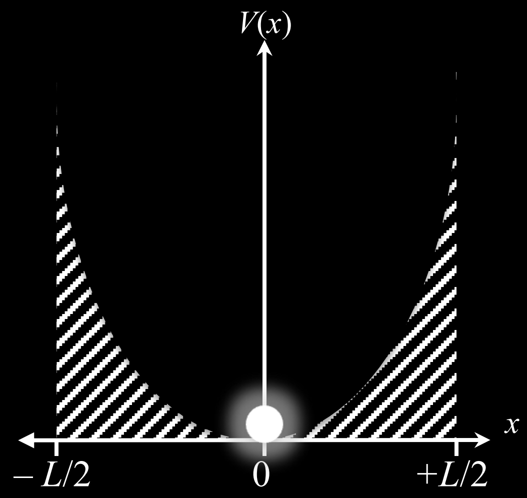
Another simple example: Linear Harmonic Oscillator in 1D

$$\left[-\frac{\hbar^2}{2m}\Delta+\frac{1}{2}m\omega^2x^2\right]\Psi(x)=E\ \Psi(x)$$

$$-\Delta\Psi(x)+x^2\Psi(x)=2E'\ \Psi(x)$$

$$-\Delta\Psi\left(x_i\right)+\left(x_i\right)^2\Psi(x_i)=2E'\ \Psi\left(x_i\right),$$

$$-\frac{\Psi\left(\frac{(i-1)L}{N}\right)-2\Psi\left(\frac{iL}{N}\right)+\Psi\left(\frac{(i+1)L}{N}\right)}{\left(\frac{L}{N}\right)^2}+\left(\frac{iL}{N}\right)^2\Psi\left(\frac{iL}{N}\right)=2E'\ \Psi\left(\frac{iL}{N}\right)$$



$$\left\{\begin{pmatrix} 2 & -1 & 0 & 0 & 0 & & 0 \\ -1 & 2 & -1 & 0 & 0 & & 0 \\ 0 & -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & 0 & -1 & 2 & -1 & & 0 \\ 0 & 0 & 0 & -1 & 2 & & 0 \\ & & \vdots & & & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 2 \end{pmatrix}+\begin{pmatrix} \ddots & & & \vdots & & & ⋰ \\ & 2^2 & 0 & 0 & 0 & 0 & \\ & 0 & 1^2 & 0 & 0 & 0 & \\ \cdots & 0 & 0 & 0 & 0 & 0 & \cdots \\ & 0 & 0 & 0 & 1^2 & 0 & \\ & 0 & 0 & 0 & 0 & 2^2 & \\ ⋰ & & & \vdots & & & \ddots \end{pmatrix}\right\}\begin{pmatrix} \Psi_{-\frac{N}{2}} \\ \vdots \\ \Psi_{-1} \\ \Psi_0 \\ \Psi_1 \\ \vdots \\ \Psi_{\frac{N}{2}} \end{pmatrix}=\tilde{E}_0\begin{pmatrix} \Psi_{-\frac{N}{2}} \\ \vdots \\ \Psi_{-1} \\ \Psi_0 \\ \Psi_1 \\ \vdots \\ \Psi_{\frac{N}{2}} \end{pmatrix}$$

$$\hat{H}=-\sum_{i=-N/2}^{N/2}\left(\hat{c}_i^+\hat{c}_{i+1}+\hat{c}_{i+1}^+\hat{c}_i\right)+\sum_{i=-N/2}^{N/2}\left[2\hat{c}_i^+\hat{c}_i+\left(i-\tfrac{L}{2}\right)^2\right]=\sum_{i=0}^{N}\left(\hat{a}_i^+\hat{a}_i+\tfrac{1}{2}\right)\approx-\frac{\partial^2}{\partial x^2}+x^2$$

Exact solution exists:

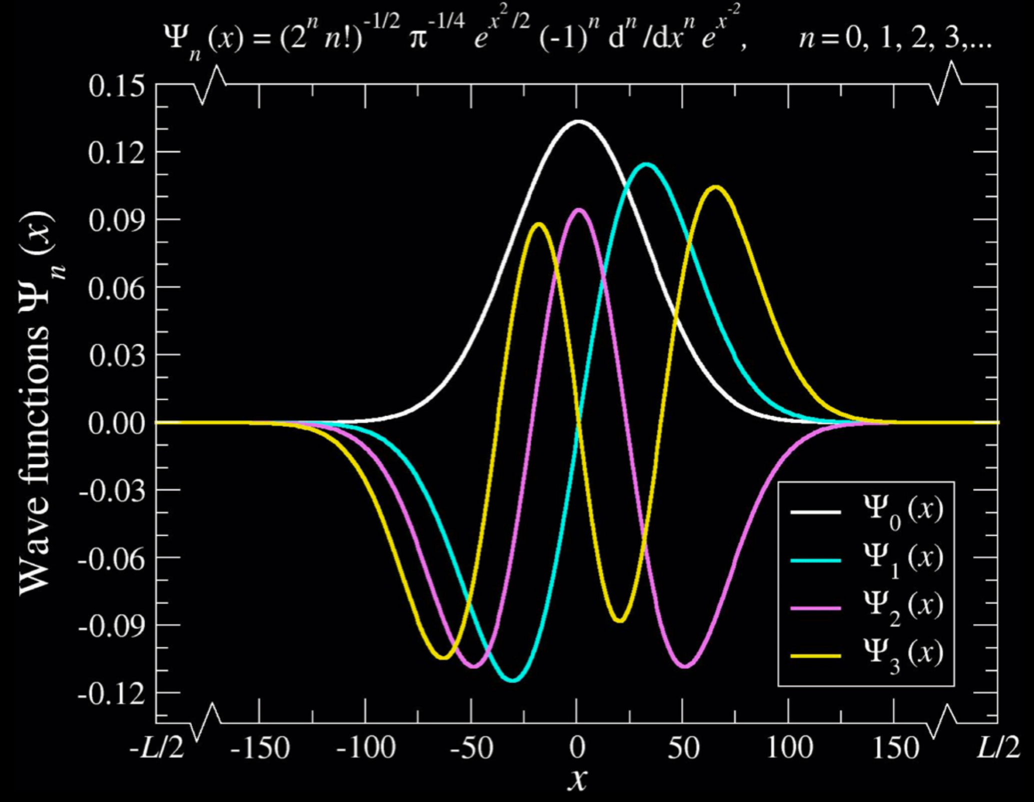
Hermite polynomials

$$E_n = \left(n + \tfrac{1}{2}\right), \qquad n = 0,1,2,\ldots$$

$$\Psi_n(x) = \frac{1}{\sqrt{2^n n!}} \sqrt{\frac{1}{\sqrt{\pi}}} \exp\left(-\frac{x^2}{2}\right) \underbrace{(-1)^n \exp\left(x^2\right) \frac{d^n}{dx^n}\left[\exp\left(-x^2\right)\right]}_{H_n(x)}$$

Recall that $\hbar = \omega = m = 1$

	Relative error $\varepsilon = (E_n^{\text{num}} - E_n^{\text{exact}})/E_n^{\text{exact}} \times 100\%$			
N	ε_0	ε_1	ε_2	ε_3
5 000	0.006	0.010	0.016	0.022



Numerical efficiency when diagonalizing matrices

DMRG: developed to reach a controlled accuracy of exact diagonalization

- Single-particle problem

Size	Matrix dimension of Hamiltonian	
N	Exact diagonalization	DMRG
10	10	4
100	100	4
1000	1000	4
10 000	10 000	4

- Many-body problem

Lattice size	Estimated memory consumption in a computer		The model
L	Exact diagonalization	DMRG	
10	1 MB	≈ 1 MB	Heisenberg model
100	10^{50} GB	≈ 100 MB	
1000	10^{600} GB	≈ 1 GB	
10	1 GB	< 8 MB	Hubbard model
100	10^{100} GB	≈ 1 GB	
1000	10^{1200} GB	≈ 10 GB	

Schrödinger equation

(for a single particle in 3D)

$$i\hbar \frac{\partial}{\partial t} |\Psi(\vec{r},t)\rangle = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right] |\Psi(\vec{r},t)\rangle$$

Time-independent Schrödinger equation

(for N particles in one-dimension)

$$\sum_{j=1}^{N}\left[-\frac{\hbar^2}{2m_j}\frac{\partial^2}{\partial x_j^2} + V(x_1, x_2, \dots, x_N)\right] |\Psi_n(x_1, x_2, \dots, x_N)\rangle = E_n |\Psi_n(x_1, x_2, \dots, x_N)\rangle$$

Time-independent Schrödinger equation in second quantization

(for N interacting particles in one-dimension)

$$\underbrace{\left[-t\sum_{j=1}^{N-1}\left(c_j^+ c_{j+1} + c_{j+1}^+ c_j\right) - \sum_{j=1}^{N} V_j c_j^+ c_j - U\sum_{j=1}^{N-1} c_j^+ c_j c_{j+1}^+ c_{j+1}\right]}_{H} |\phi_n\rangle = E_n |\phi_n\rangle$$

$$\boxed{H|\phi_n\rangle = E_n|\phi_n\rangle}$$

Solving the Schrödinger equation means to find E_n *and* $|\phi_n\rangle$ *(e.g. by diagonalizing the Hamiltonian).*

Can we prepare an entangled state(?!)

$$H = -J\left(S_1^x \otimes S_2^x + S_1^y \otimes S_2^y + S_1^z \otimes S_2^z\right) = \begin{pmatrix} -J & 0 & 0 & 0 \\ 0 & J & -2J & 0 \\ 0 & -2J & J & 0 \\ 0 & 0 & 0 & -J \end{pmatrix}$$

Diagonalize the 4 × 4 Hamiltonian matrix $H|\phi_n\rangle = E_n|\phi_n\rangle, \quad n = 0,1,2,3$

Result:

$$E = \begin{pmatrix} -J & 0 & 0 & 0 \\ 0 & -J & 0 & 0 \\ 0 & 0 & -J & 0 \\ 0 & 0 & 0 & 3J \end{pmatrix}$$

$$|\phi_0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |\phi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix},$$

$$|\phi_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad |\phi_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$$

$$|\phi_n\rangle = \sum_{i=\uparrow}^{\downarrow}\sum_{j=\uparrow}^{\downarrow} \phi_{ij}\,|ij\rangle = \phi_{\uparrow\uparrow}^{(n)}|\uparrow\uparrow\rangle + \phi_{\uparrow\downarrow}^{(n)}|\uparrow\downarrow\rangle + \phi_{\downarrow\uparrow}^{(n)}|\downarrow\uparrow\rangle + \phi_{\downarrow\downarrow}^{(n)}|\downarrow\downarrow\rangle = \phi_{\uparrow\uparrow}^{(n)}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \phi_{\uparrow\downarrow}^{(n)}\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} + \phi_{\downarrow\uparrow}^{(n)}\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} + \phi_{\downarrow\downarrow}^{(n)}\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Reduced density matrix

Let us start by finding spectrum of energies E_n and the corresponding eigenstates $|\psi_n\rangle$ of a given Hamiltonian (that is how the QM works)

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

- Reduced density matrix in a pure state $\rho' = Tr_{env}(|\psi_0\rangle\langle\psi_0|)$
- Reduced density matrix in a mixed state $\rho'' = Tr_{env}\left(\sum_j c_j|\psi_j\rangle\langle\psi_j|\right)$

- What is the reduced density matrix typically good for?
  - ✓ To obtain expectation (mean) values of operators $\langle A_s\rangle = Tr_s(A_s\rho')$
  - ✓ Quantum entanglement von Neumann entropy $S = -Tr\left(\rho' \log_2(\rho')\right)$

- Reduced density matrix (detail): $\rho'_s = Tr'_e|\psi_0(s,e)\rangle\langle\psi_0(s,e)|$
  - ✓ System interacts with environment
  - ✓ Entanglement entropy $S_s = S_e = -Tr_e\left(\rho'_e \log_2(\rho'_e)\right)$

Information inside the reduced density matrix

The reduced density matrix completely describes a subsystem (in contact with environment).

Properties of the entanglement entropy:

$$S = -Tr_s(\rho_s' \log_2 \rho_s') \geq 0$$

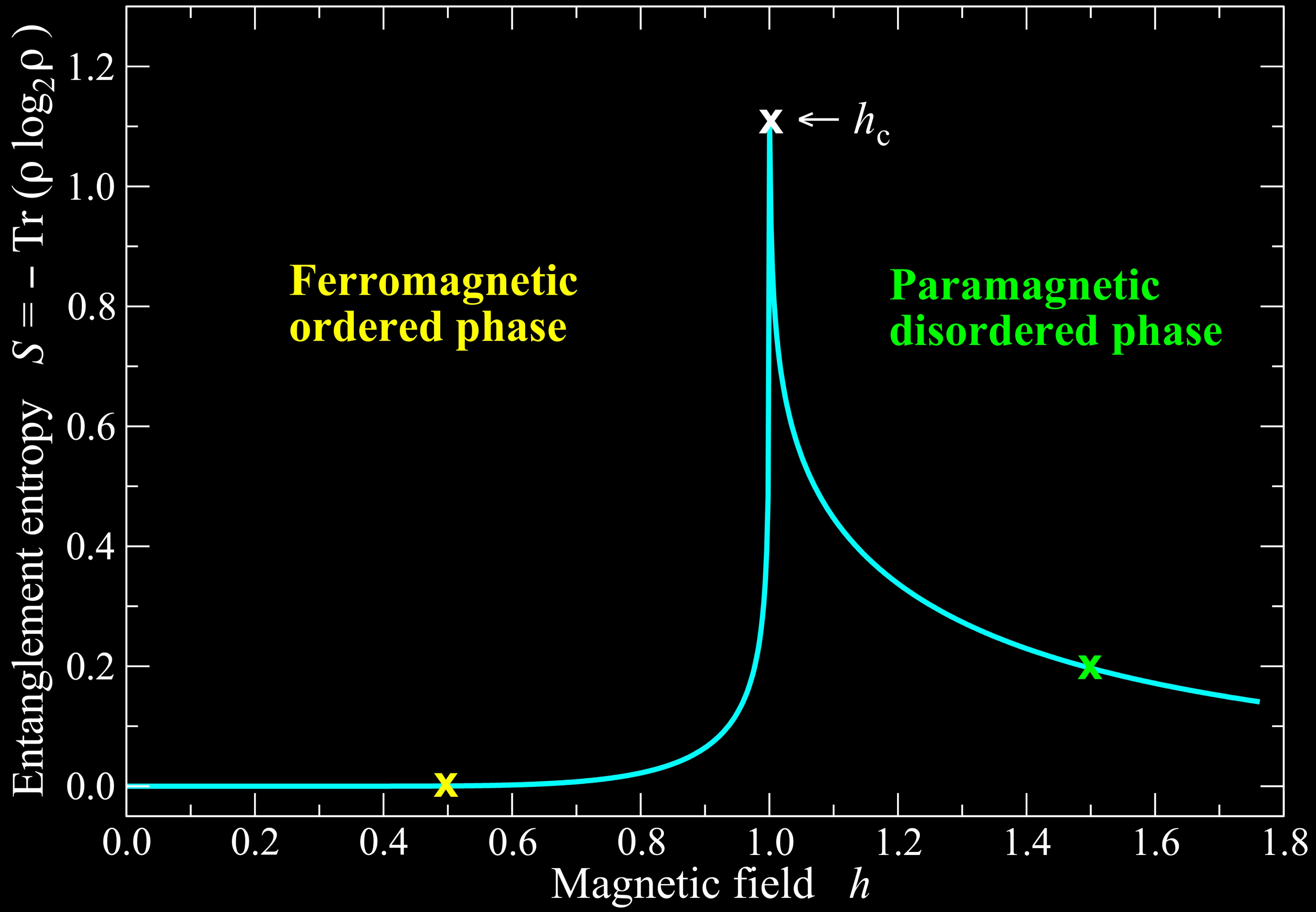
If the reduced density matrix is diagonalized $U^+ \rho_s' U = \Omega$,

the eigenvalues sorted in descending order are: $\omega_1 \geq \omega_2 \geq \omega_3 \geq \ldots \geq \omega_N$

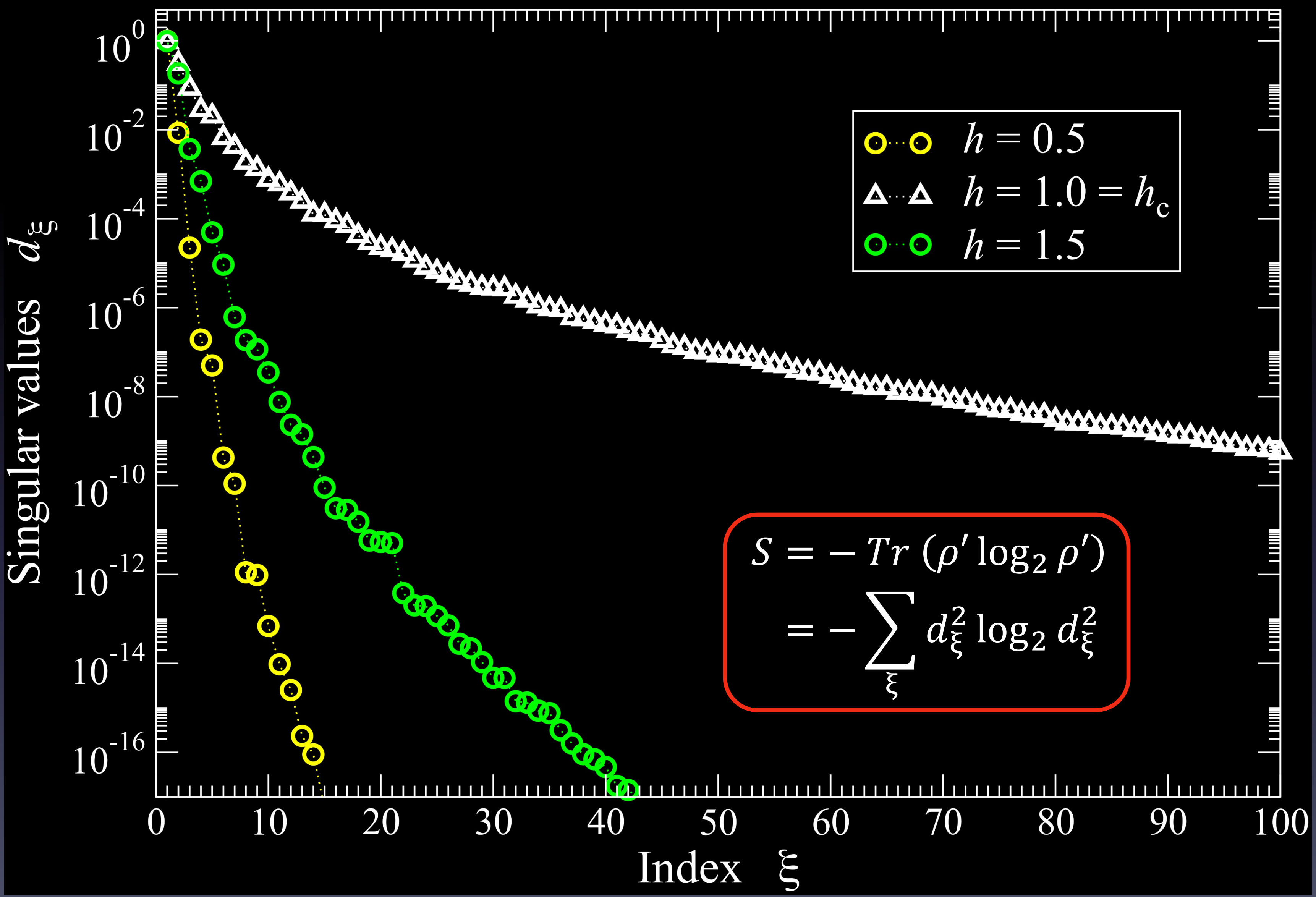
$$U^+ \rho_s' U = \Omega = \begin{pmatrix} \omega_1 & 0 & 0 & & \\ 0 & \omega_2 & 0 & \cdots & \\ 0 & 0 & \omega_3 & & \\ & \vdots & & \ddots & \\ & & & & \omega_N \end{pmatrix}$$

- ✓ No entanglement: $\omega_1 = 1, \ \omega_j = 0, \ \forall j > 1$
- ✓ Weak entanglement: $\omega_j \propto \exp(-\beta j)$
- ✓ Strong entanglement: $\omega_j \propto j^{-\alpha}$

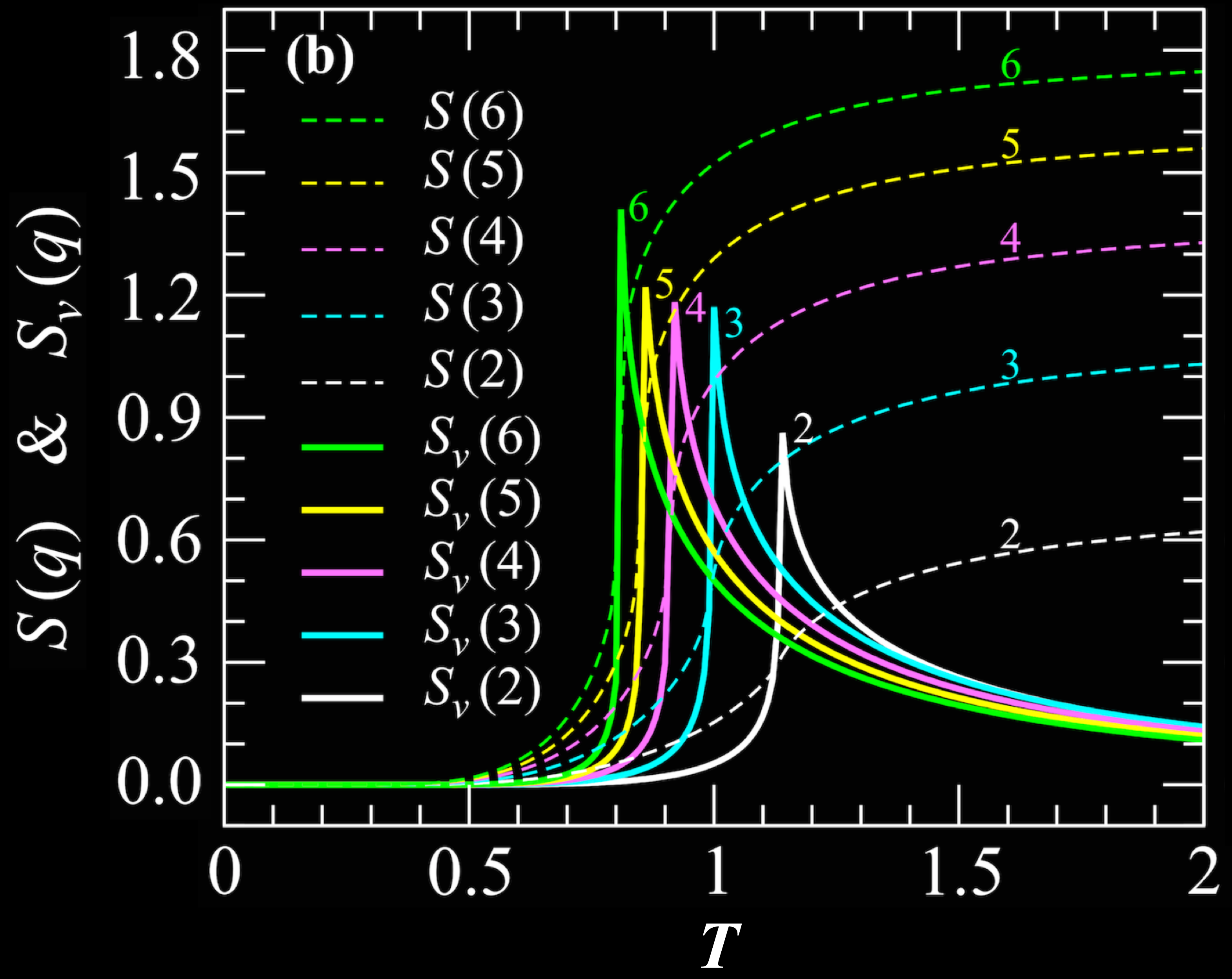
Entanglement entropy for quantum spin system $S = -\mathrm{Tr}(\rho' \log_2 \rho')$



Decay of the singular values (Schmidt coefficients) d_ξ



Comparison between the thermodynamic entropy and entanglement entropy

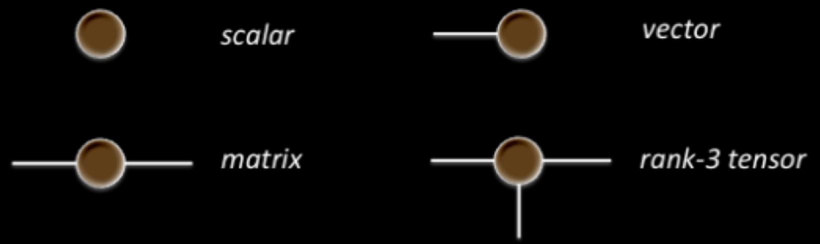


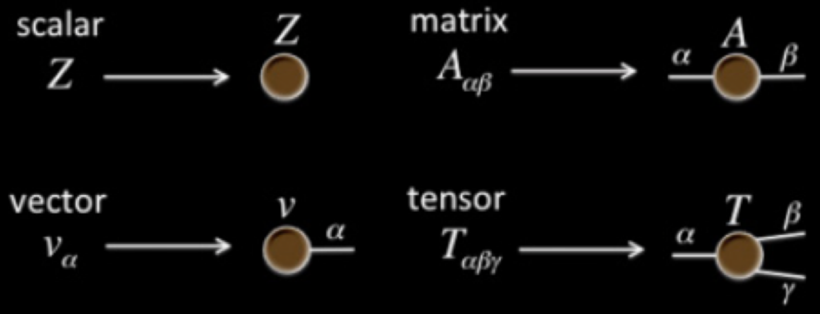
Matrix Product State

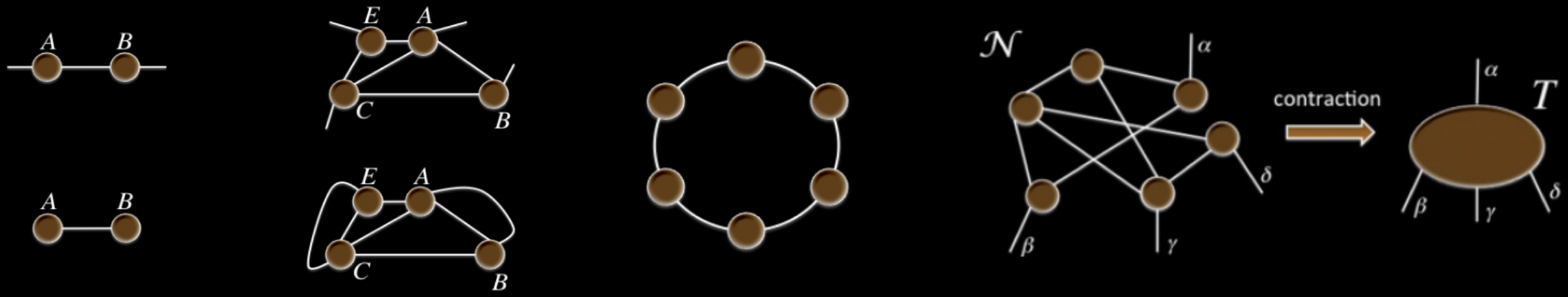
SVD and Entanglement

Tensor Network is a Tensor Product State

(and it's like playing a Tetris game...)

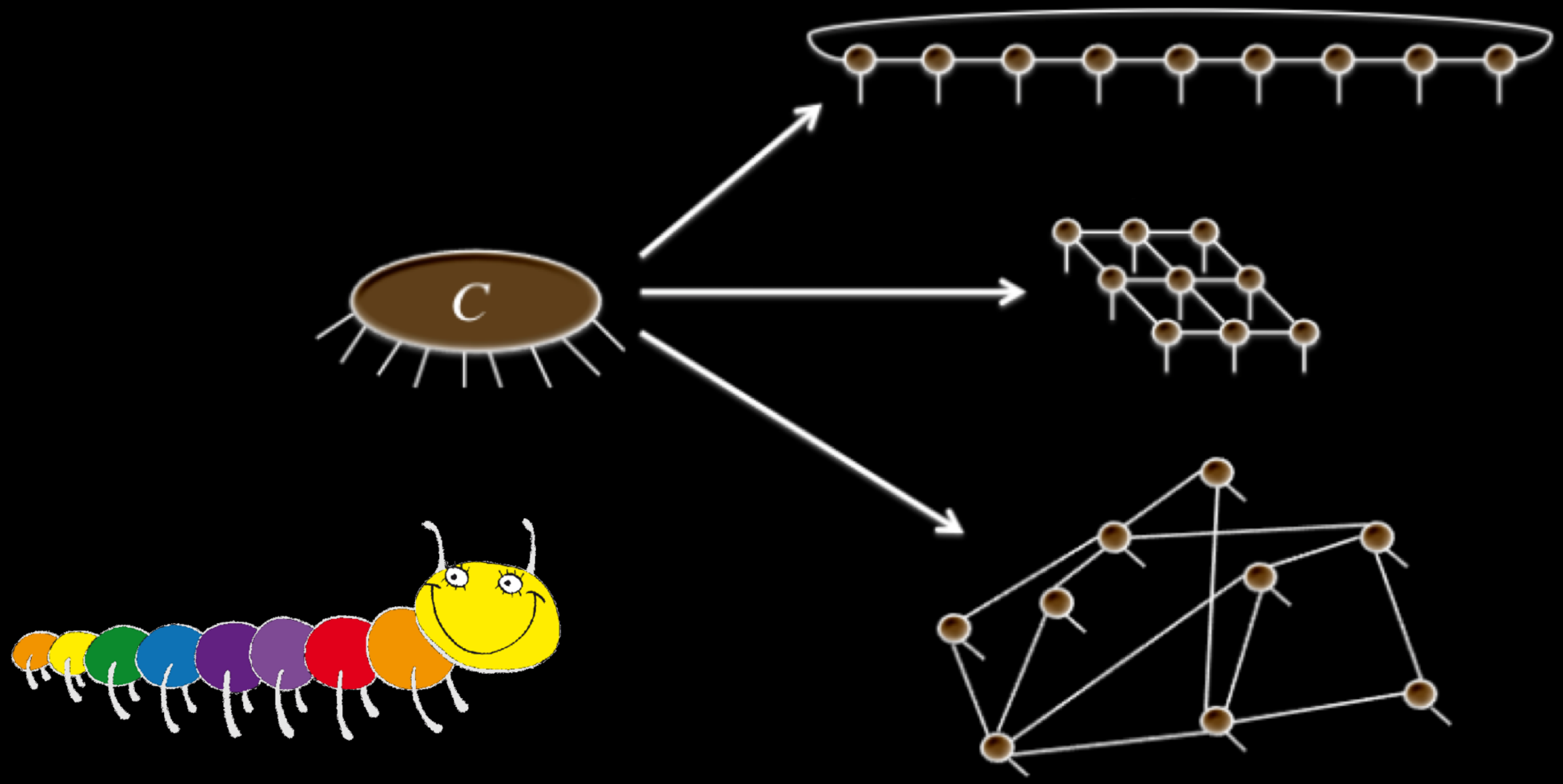






Tensor Network is a Tensor Product State

(and it‘s like playing a Tetris game...)



Tensor Network is a Tensor Product State

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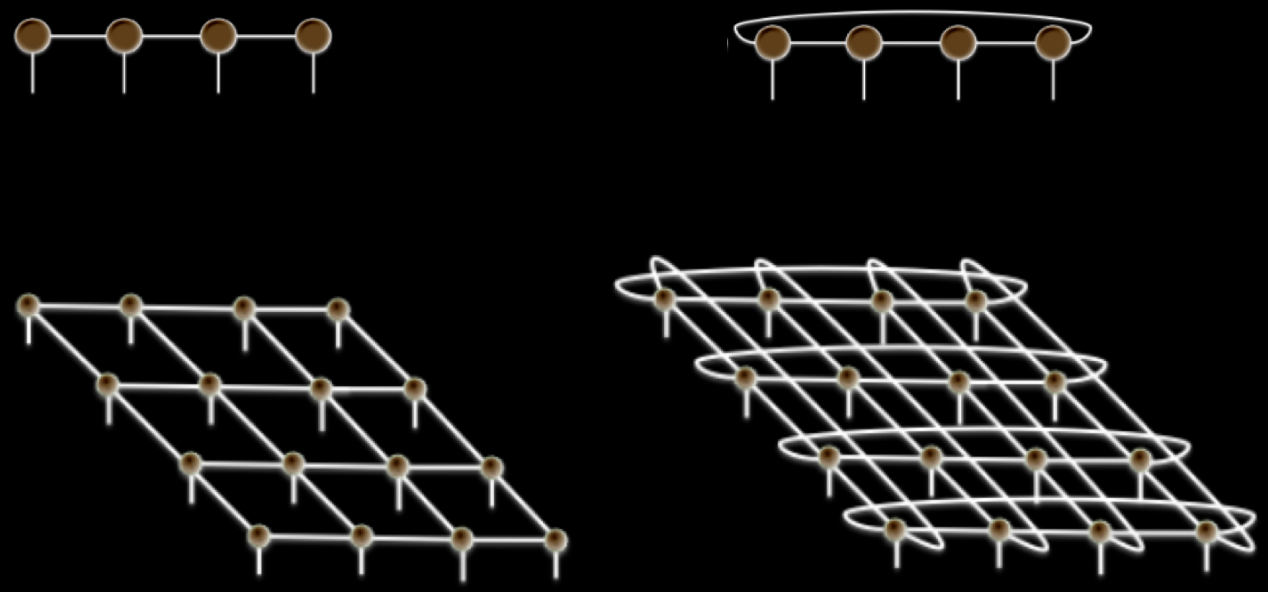


1D state $|\phi\rangle$

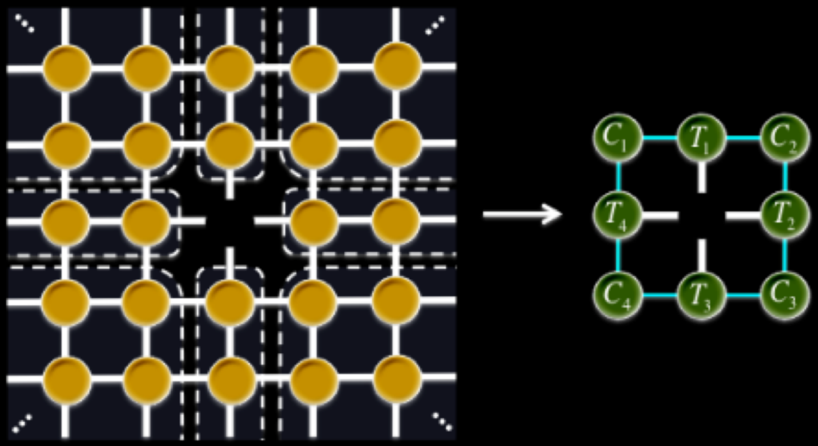
2D state $|\phi\rangle$

For open/fixed boundary conditions

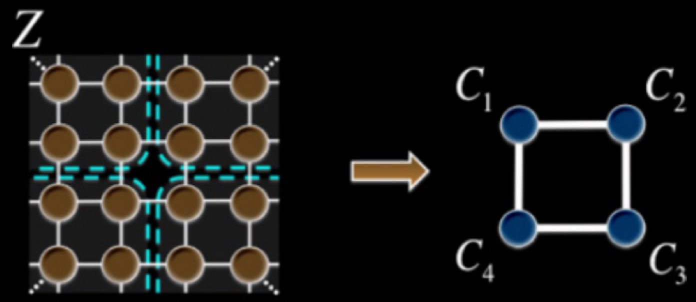
For periodic boundary conditions (it is a torus!)

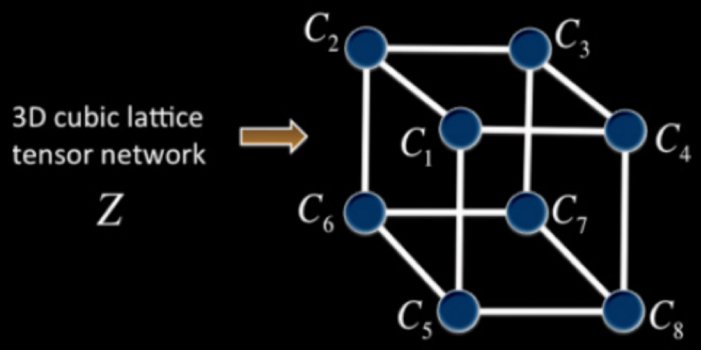
Tensor Network is a Tensor Product State

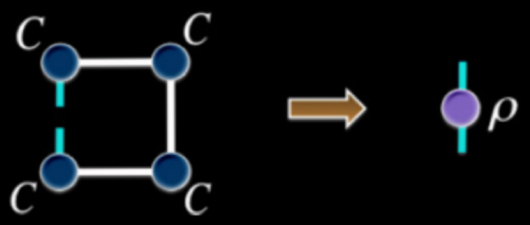
(and it's like playing a Tetris game...)



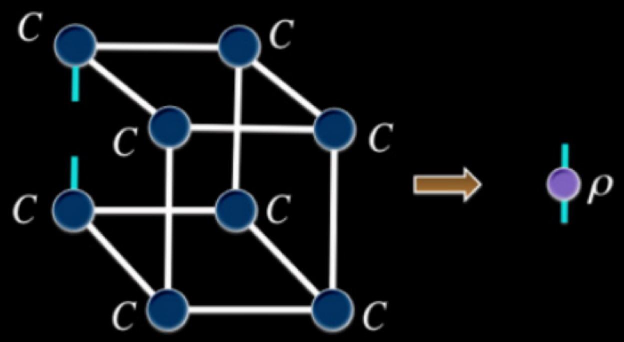
2D Tensor Network
for
Corner Transfer Matrix
Renormalization Group







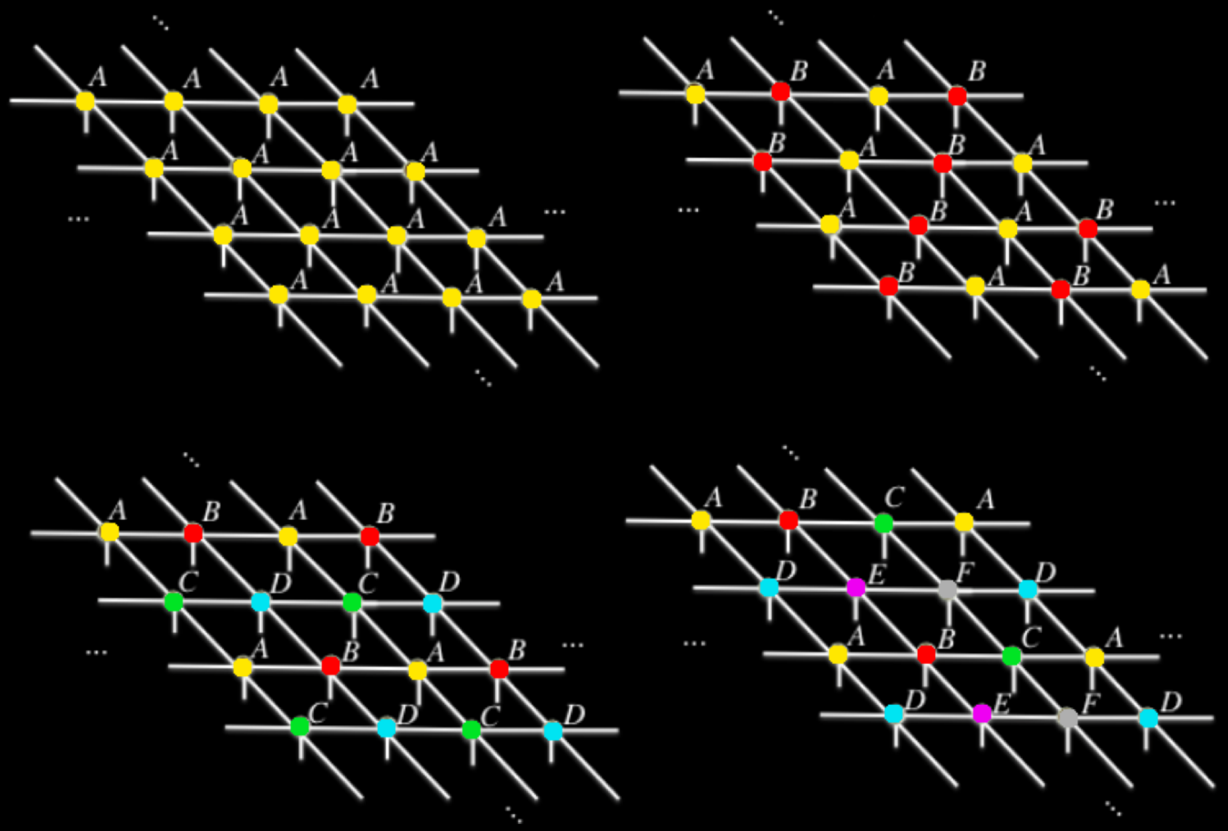
reduced density matrix



reduced density matrix

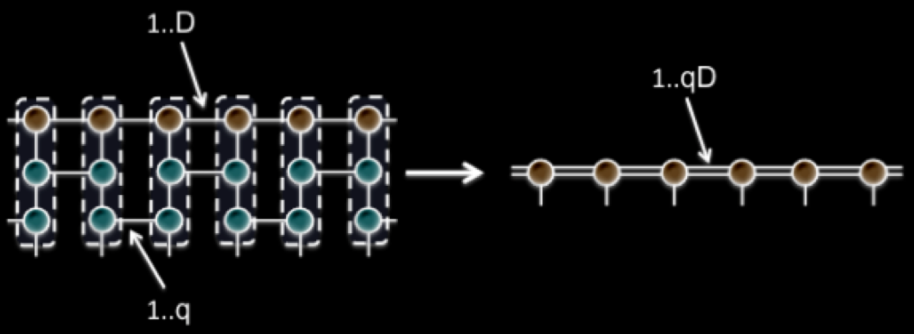
***Tensor Network** is a Tensor Product State*

(and it's like playing a Tetris game...)



If studying quantum (topological) phases

(imaginary) time evolution



For more datails, read the outstanding review by Román Orús

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A practical introduction to tensor networks: Matrix product states and projected entangled pair states

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Matrix diagonalization

M a square matrix $(n \times n)$

$$M = UDU^{-1}$$

$$M = UDU^{+} \quad \text{(if Hermitian)}$$

$$U^{+}U = \mathbb{I}$$

Singular value decomposition

(Schmidt decomposition)

M is a rectangular matrix $(n \times m)$

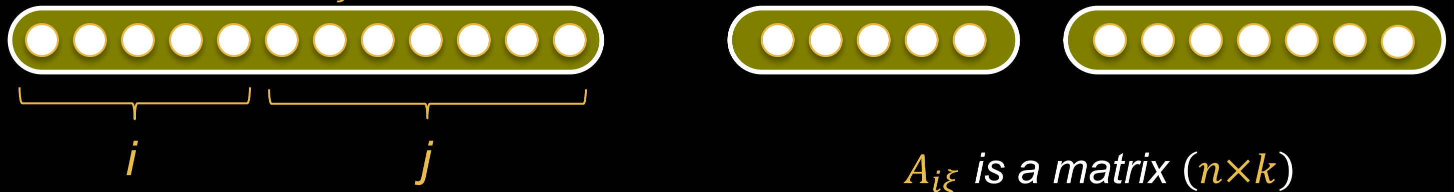
$$M = UDV^{+}$$

$$U^{+}U = V^{+}V = \mathbb{I}$$

Decomposing a vector $|\psi\rangle$ into the product of two matrices A and B

$$|\psi\rangle=\sum_{ij}\psi_{ij}|ij\rangle=\sum_{ij}\sum_{\xi}A_{i\xi}B_{\xi j}|ij\rangle \overset{SVD}{=} \sum_{ij}\sum_{\xi\xi'}U_{i\xi}D_{\xi\xi'}V^{+}_{\xi' j}|ij\rangle$$

ψ_{ij} $\quad$ $A_{i\xi}=U_{i\xi}\sqrt{D_{\xi\xi}}$ $\quad$ $B_{\xi j}=\sqrt{D_{\xi\xi}}V^{+}_{\xi' j}$



ψ_{ij} *is a matrix* $(n\times m)$

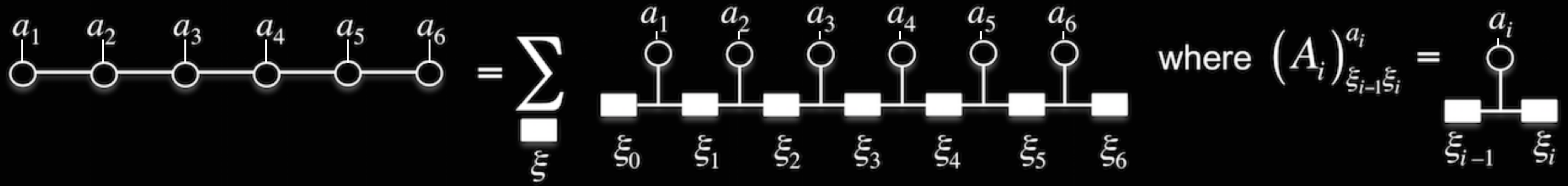
$i=0,1,2,\dots,2^n,\;\; j=0,1,2,\dots,2^m$

$A_{i\xi}$ *is a matrix* $(n\times k)$

$B_{\xi j}$ *is a matrix* $(k\times m)$

$k=\min(n,m)$

The case of L=6 $|\Psi\rangle =$



$$|\Psi\rangle=\sum_{a_1a_2\cdots a_6}\underbrace{\Psi_{a_1a_2a_3a_4a_5a_6}}|a_1a_2a_3a_4a_5a_6\rangle \overset{\substack{MPS\ (SVD)\\ decomposition}}{\equiv} \sum_{a_1a_2\cdots a_6}\sum_{\xi_0\cdots\xi_6}(A_1)^{a_1}_{\xi_0\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}(A_5)^{a_5}_{\xi_4\xi_5}(A_6)^{a_6}_{\xi_5\xi_6}|a_1a_2a_3a_4a_5a_6\rangle$$

$$\underbrace{\Psi_{a_1a_2a_3a_4a_5a_6}}_{vector\ (1\times 2^6)} \overset{reshape}{=} \underbrace{\Psi^{a_1}_{a_2a_3a_4a_5a_6}}_{matrix\ (2\times 2^5)} \overset{SVD}{=} \sum_{\xi_1=1}^{\min\left(\substack{\dim a_1,\\ \dim a_2a_3\dots a_6}\right)=2^1} \underbrace{U^{a_1}_{\xi_1}}_{(A_1)^{a_1}_{\xi_1}} \underbrace{S^{\xi_1}_{\xi_1}\left(V^T\right)^{\xi_1}_{a_2a_3a_4a_5a_6}}_{\Psi^{\xi_1}_{a_2a_3a_4a_5a_6}} = \sum_{\xi_1=1}^{2^1}(A_1)^{a_1}_{\xi_1}\underbrace{\Psi^{a_2\xi_1}_{a_3a_4a_5a_6}}_{\substack{\Psi^{\xi_1}_{a_2a_3a_4a_5a_6}\\ (reshaped)}} \overset{SVD}{=} \sum_{\xi_1=1}^{2^1}(A_1)^{a_1}_{\xi_1} \sum_{\xi_2=1}^{\min\left(\substack{\dim a_2\xi_1,\\ \dim a_3\dots a_6}\right)=2^2} \underbrace{U^{a_2\xi_1}_{\xi_2}}_{(A_2)^{a_2}_{\xi_1\xi_2}} \underbrace{S^{\xi_2}_{\xi_2}\left(V^T\right)^{\xi_2}_{a_3a_4a_5a_6}}_{\Psi^{\xi_2}_{a_3a_4a_5a_6}} =$$

Singular Value Decomposition (Schmidt decomposition)

of a $m \times n$ rectangular matrix M is the following decomposition:

$$M = USV^{+}$$

U is a unitary $m \times m$ square matrix
S is a diagonal $m \times n$ rectangular matrix (with non-negative real numbers)
V is a unitary $n \times n$ square matrix (V^{+} is conjugate transpose of V)

and $U^{+}U = V^{+}V = 1$. Let $k = min(m,n)$

The decomposition of a eigenstate Ψ_0 (Schmidt decomposition) onto the product of two matrices A_s and A_e:

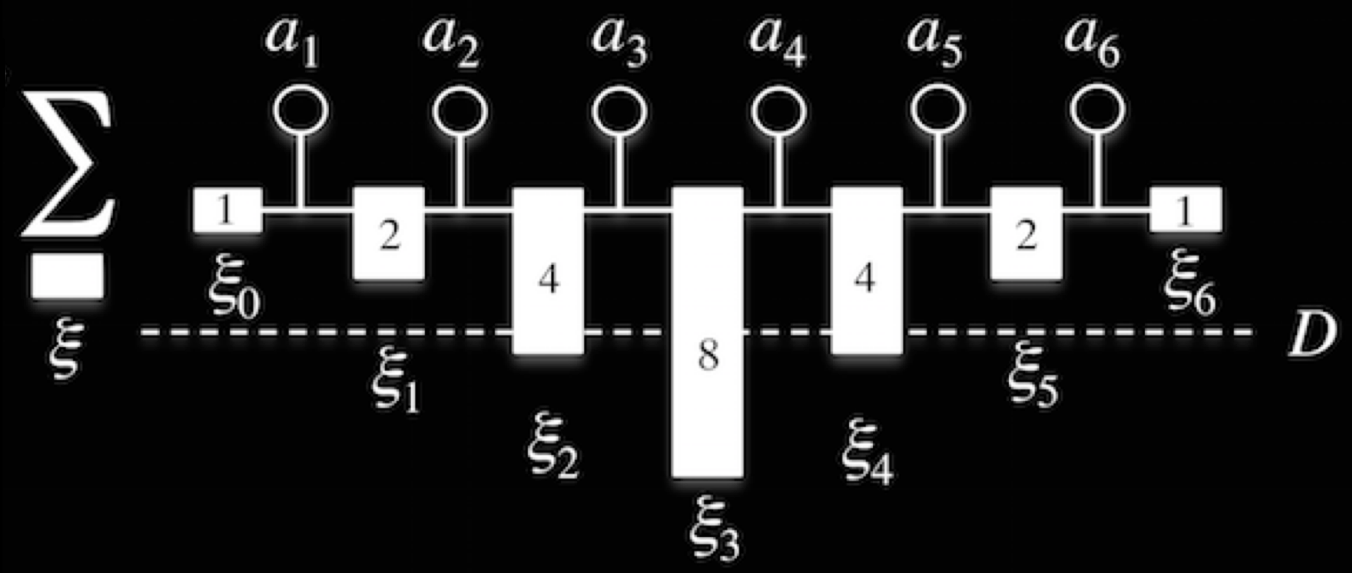
$$|\Psi_0\rangle = \Sigma_{ij}\, \Psi_{ij}\, |i\rangle_s\, |j\rangle_e$$

Analytically:

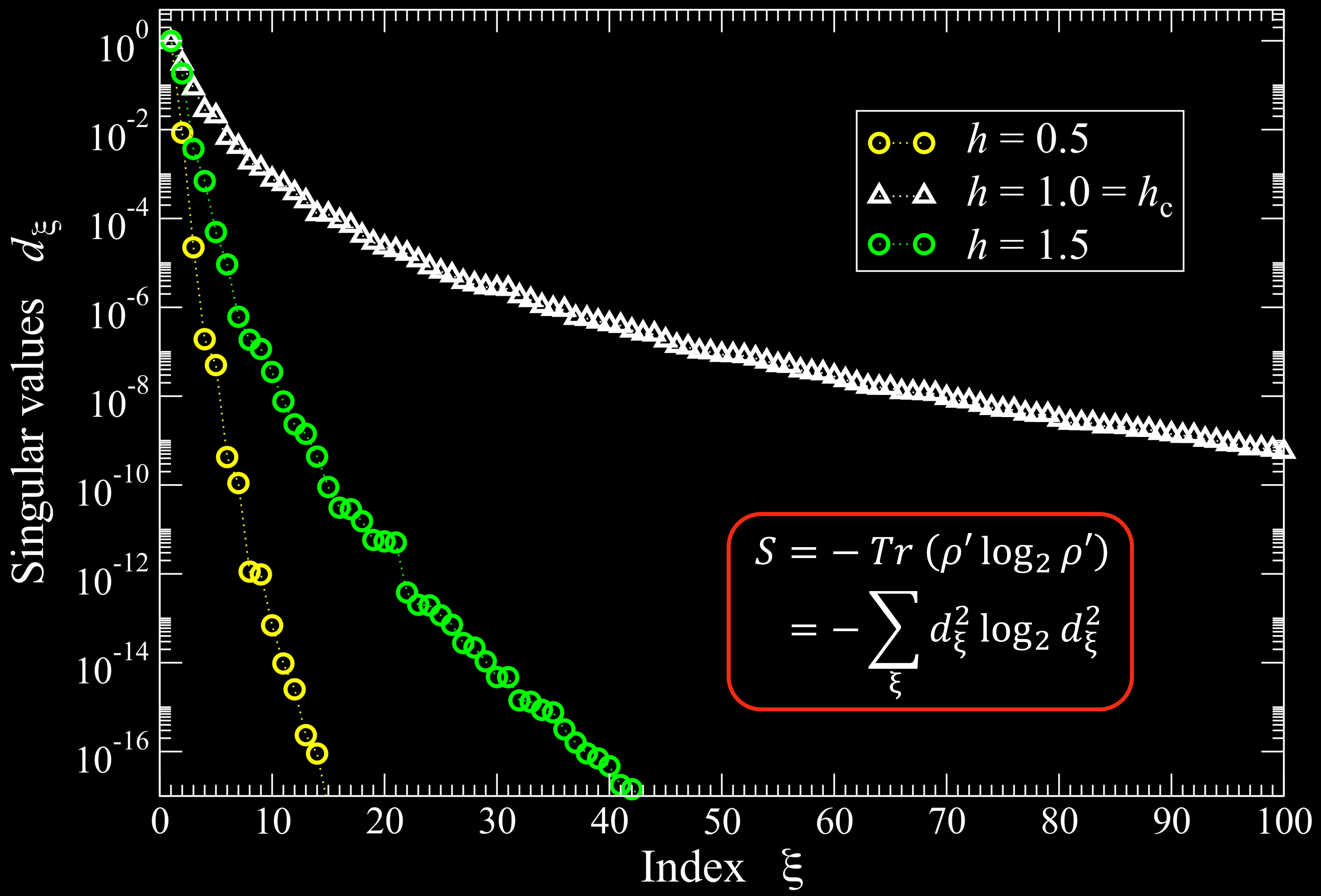
$$\Psi_0\left(a_1, a_2, \ldots, a_{L/2}, a_{L/2+1}, \ldots, a_L\right) = \Psi^{a_1, a_2, \ldots, a_{L/2}}_{a_{L/2+1}, \ldots, a_L} \underset{SVD}{=} \sum_{m}^{D} \underbrace{U^{a_1, a_2, \ldots, a_{L/2}}_{m}}_{A_s} \underbrace{D^{m}_{m} V^{+\ m}_{a_{L/2+1}, \ldots, a_L}}_{A_e}$$

$$|\Psi\rangle = \sum_{a_1a_2\cdots a_6} \underbrace{\Psi_{a_1a_2a_3a_4a_5a_6}}_{} |a_1a_2a_3a_4a_5a_6\rangle \overset{\substack{\text{MPS (SVD)} \\ \text{decomposition}}}{\equiv} \sum_{a_1a_2\cdots a_6} \sum_{\xi_0\cdots\xi_6} (A_1)^{a_1}_{\xi_0\xi_1} (A_2)^{a_2}_{\xi_1\xi_2} (A_3)^{a_3}_{\xi_2\xi_3} (A_4)^{a_4}_{\xi_3\xi_4} (A_5)^{a_5}_{\xi_4\xi_5} (A_6)^{a_6}_{\xi_5\xi_6} |a_1a_2a_3a_4a_5a_6\rangle$$

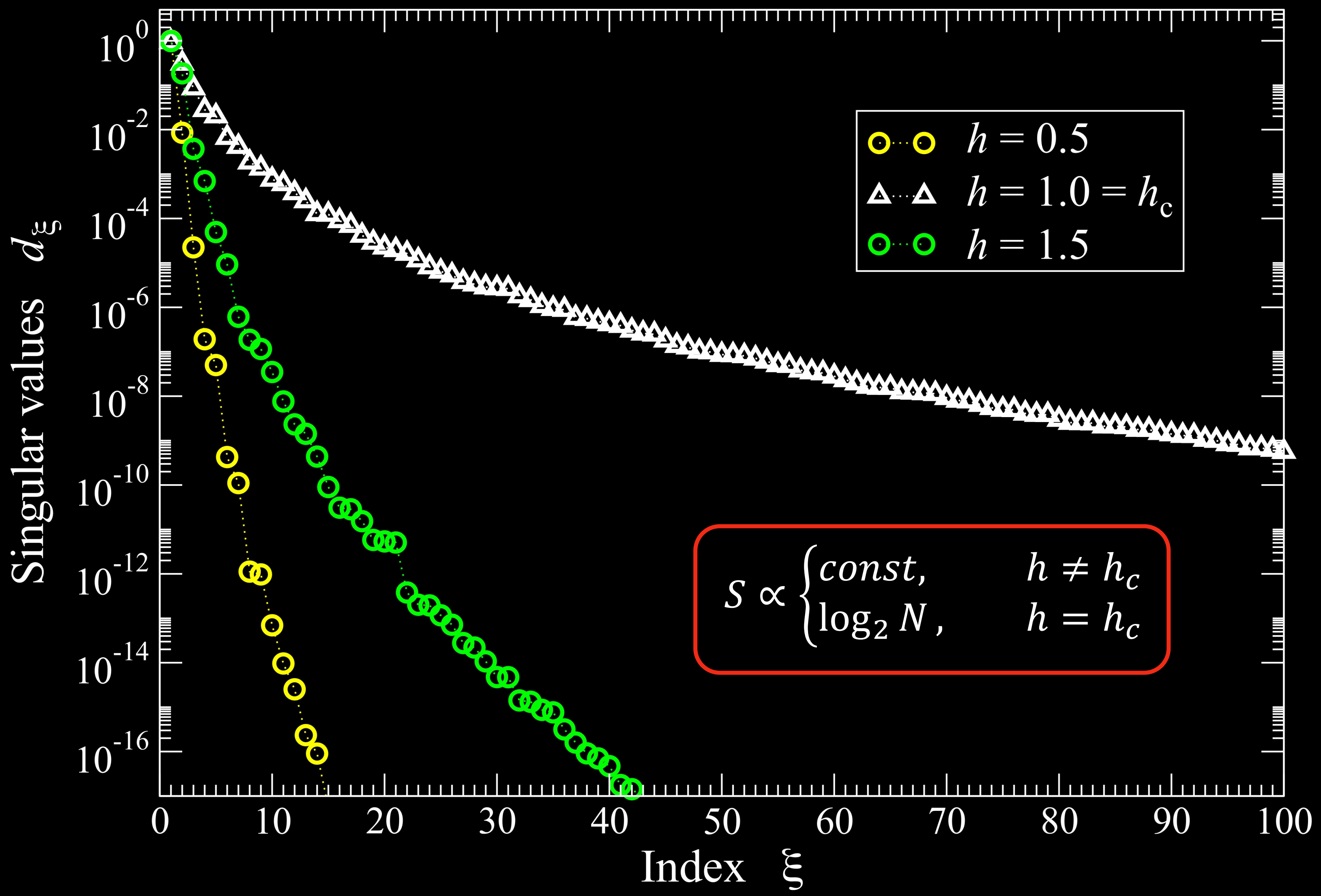
=



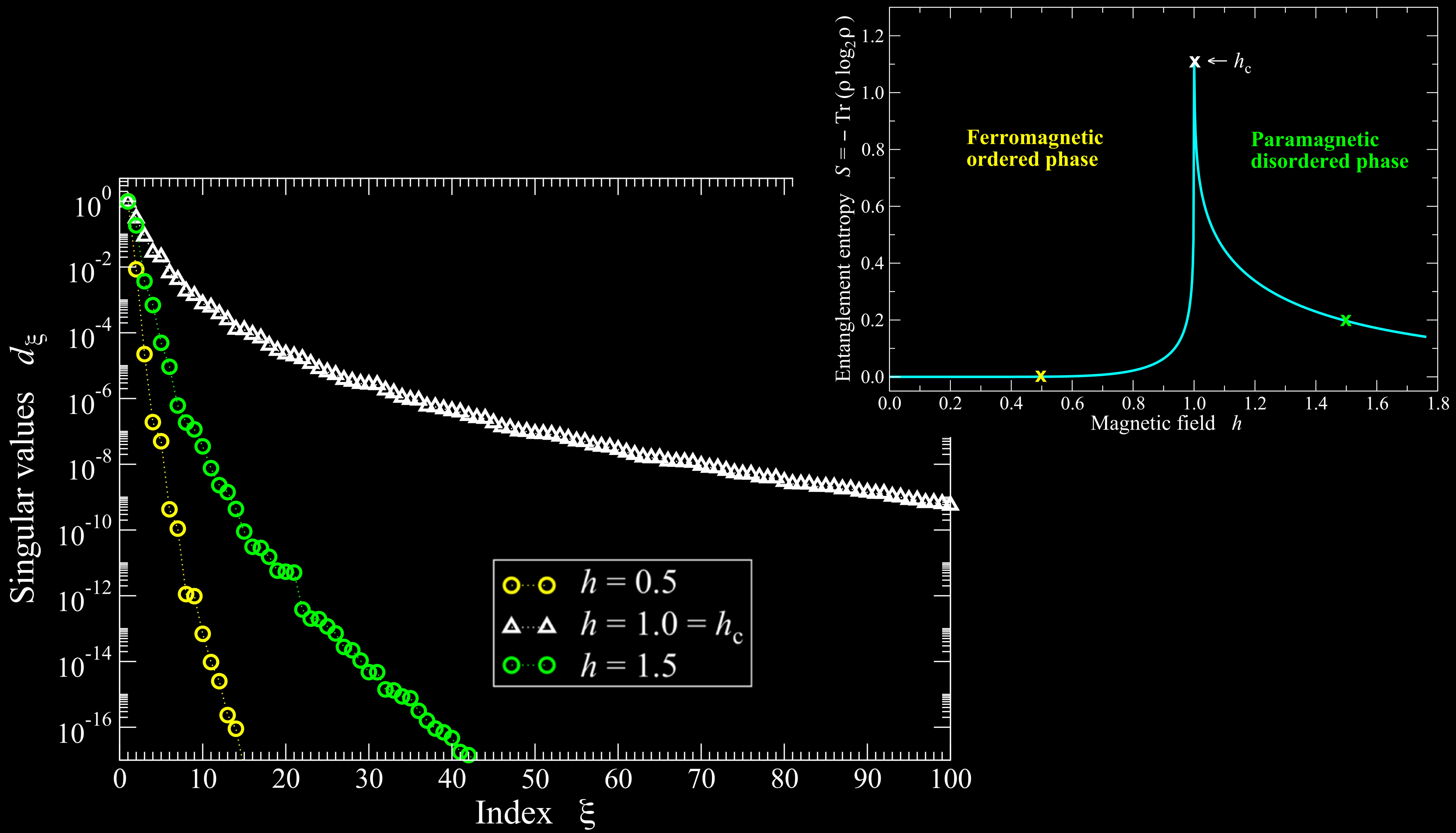
Decay of the singular values (Schmidt coefficients) d_ξ



Decay of the singular values (Schmidt coefficients) d_ξ



$$S \propto \begin{cases} const, & h \neq h_c \\ \log_2 N\,, & h = h_c \end{cases}$$



Singular values d_ξ
Index ξ
$h = 0.5$
$h = 1.0 = h_c$
$h = 1.5$
Entanglement entropy $S = -\mathrm{Tr}(\rho \log_2 \rho)$
Magnetic field h
$\leftarrow h_c$
Ferromagnetic ordered phase
Paramagnetic disordered phase

Thank you

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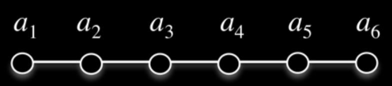
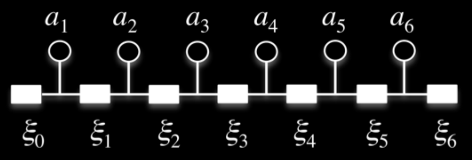
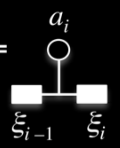
More details on singular value decomposition in 1D chain of 6 spins

The case of L=6 $|\Psi\rangle =$  $= \sum_{\xi}$  where $(A_i)^{a_i}_{\xi_{i-1}\xi_i} =$ 

$$|\Psi\rangle = \sum_{a_1 a_2 \cdots a_6} \underbrace{\Psi_{a_1a_2a_3a_4a_5a_6}} |a_1a_2a_3a_4a_5a_6\rangle \overset{\text{MPS (SVD) decomposition}}{\equiv} \sum_{a_1a_2\cdots a_6}\sum_{\xi_0\cdots\xi_6}(A_1)^{a_1}_{\xi_0\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}(A_5)^{a_5}_{\xi_4\xi_5}(A_6)^{a_6}_{\xi_5\xi_6}|a_1a_2a_3a_4a_5a_6\rangle$$

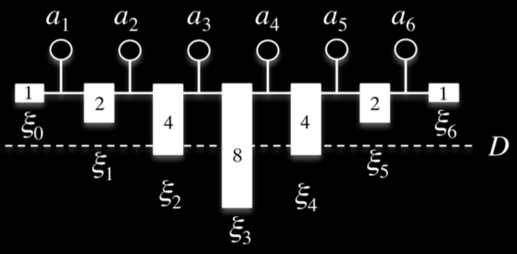
$$\underbrace{\Psi_{a_1a_2a_3a_4a_5a_6}}_{\text{vector }(1\times 2^6)} \overset{\text{reshape}}{=} \underbrace{\Psi^{a_1}_{a_2a_3a_4a_5a_6}}_{\text{matrix }(2\times 2^5)} \overset{\text{SVD}}{=} \sum_{\xi_1=1}^{\min\left(\dim a_1,\ \dim a_2a_3\ldots a_6\right)=2^1} \underbrace{U^{a_1}_{\xi_1}}_{(A_1)^{a_1}_{\xi_1}} \underbrace{S^{\xi_1}_{\xi_1}\left(V^T\right)^{\xi_1}_{a_2a_3a_4a_5a_6}}_{\Psi^{\xi_1}_{a_2a_3a_4a_5a_6}} = \sum_{\xi_1=1}^{2^1}(A_1)^{a_1}_{\xi_1}\underbrace{\Psi^{a_2\xi_1}_{a_3a_4a_5a_6}}_{\Psi^{\xi_1}_{a_2a_3a_4a_5a_6}\ (\text{reshaped})} \overset{\text{SVD}}{=} \sum_{\xi_1=1}^{2^1}(A_1)^{a_1}_{\xi_1}\sum_{\xi_2=1}^{\min\left(\dim a_2\xi_1,\ \dim a_3\ldots a_6\right)=2^2}\underbrace{U^{a_2\xi_1}_{\xi_2}}_{(A_2)^{a_2}_{\xi_1\xi_2}}\underbrace{S^{\xi_2}_{\xi_2}\left(V^T\right)^{\xi_2}_{a_3a_4a_5a_6}}_{\Psi^{\xi_2}_{a_3a_4a_5a_6}} =$$

$$= \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}\underbrace{\Psi^{a_3\xi_2}_{a_4a_5a_6}}_{\Psi^{\xi_2}_{a_3a_4a_5a_6}\ (\text{reshaped})} \overset{\text{SVD}}{=} \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}\sum_{\xi_3=1}^{\min\left(\dim a_3\xi_2,\ \dim a_4a_5a_6\right)=2^3}\underbrace{U^{a_3\xi_2}_{\xi_3}}_{(A_3)^{a_3}_{\xi_2\xi_3}}\underbrace{S^{\xi_3}_{\xi_3}\left(V^T\right)^{\xi_3}_{a_4a_5a_6}}_{\Psi^{\xi_3}_{a_4a_5a_6}} = \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}\underbrace{\Psi^{a_4\xi_3}_{a_5a_6}}_{\Psi^{\xi_3}_{a_4a_5a_6}\ (\text{reshaped})} \overset{\text{SVD}}{=}$$

$$\overset{\text{SVD}}{=} \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}\sum_{\xi_4=1}^{\min\left(\dim a_4\xi_3,\ \dim a_5a_6\right)=2^2}\underbrace{U^{a_4\xi_3}_{\xi_4}}_{(A_4)^{a_4}_{\xi_3\xi_4}}\underbrace{S^{\xi_4}_{\xi_4}\left(V^T\right)^{\xi_4}_{a_5a_6}}_{\Psi^{\xi_4}_{a_5a_6}} = \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}\sum_{\xi_4=1}^{2^2}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}\underbrace{\Psi^{a_5\xi_4}_{a_6}}_{\Psi^{\xi_4}_{a_5a_6}\ (\text{reshaped})} \overset{\text{SVD}}{=}$$

$$\overset{\text{SVD}}{=} \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}\sum_{\xi_4=1}^{2^2}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}\sum_{\xi_5=1}^{\min\left(\dim a_5\xi_4,\ \dim a_6\right)=2^1}\underbrace{U^{a_5\xi_4}_{\xi_5}}_{(A_5)^{a_5}_{\xi_4\xi_5}}\underbrace{S^{\xi_5}_{\xi_5}\left(V^T\right)^{\xi_5}_{a_6}}_{\Psi^{\xi_4}_{a_6}\equiv(A_6)^{a_6}_{\xi_5}} = \sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}\sum_{\xi_4=1}^{2^2}\sum_{\xi_5=1}^{2^1}(A_1)^{a_1}_{\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}(A_5)^{a_5}_{\xi_4\xi_5}(A_6)^{a_6}_{\xi_5}$$

$$\overset{\text{in general}}{\equiv} \sum_{\xi_0=1}^{2^0}\sum_{\xi_1=1}^{2^1}\sum_{\xi_2=1}^{2^2}\sum_{\xi_3=1}^{2^3}\sum_{\xi_4=1}^{2^2}\sum_{\xi_5=1}^{2^1}\sum_{\xi_6=1}^{2^0}(A_1)^{a_1}_{\xi_0\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}(A_5)^{a_5}_{\xi_4\xi_5}(A_6)^{a_6}_{\xi_5\xi_6} \overset{\text{graphically}}{=} \sum_{\xi}$$



$$\overset{(D<2^{L/2})}{\approx} \sum_{\xi_0=1}^{D}\sum_{\xi_1=1}^{D}\sum_{\xi_2=1}^{D}\sum_{\xi_3=1}^{D}\sum_{\xi_4=1}^{D}\sum_{\xi_5=1}^{D}\sum_{\xi_6=1}^{D}(A_1)^{a_1}_{\xi_0\xi_1}(A_2)^{a_2}_{\xi_1\xi_2}(A_3)^{a_3}_{\xi_2\xi_3}(A_4)^{a_4}_{\xi_3\xi_4}(A_5)^{a_5}_{\xi_4\xi_5}(A_6)^{a_6}_{\xi_5\xi_6}$$

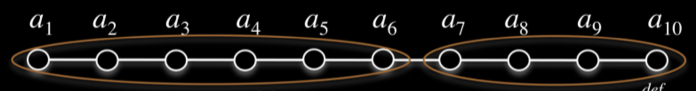
For any finite L

$$|\Psi\rangle = \sum_{a_1a_2\cdots a_L} \Psi_{a_1a_2\cdots a_L}|a_1a_2\cdots a_L\rangle \overset{\substack{MPS\ \ (SVD)\\ decomposition}}{\equiv} \sum_{a_1a_2\cdots a_L}\sum_{\xi_0\cdots\xi_L}\prod_{i=1}^{L}(A_i)^{a_i}_{\xi_{i-1}\xi_i}|a_1a_2\cdots a_L\rangle$$

$$= \sum_{a_1a_2\cdots a_L}\sum_{\xi_0=1}^{2^0}\sum_{\xi_1=1}^{2^1}\cdots\sum_{\xi_{L/2-1}=1}^{2^{L/2-1}}\sum_{\xi_{L/2}=1}^{2^{L/2}}\sum_{\xi_{L/2+1}=1}^{2^{L/2-1}}\cdots\sum_{\xi_L=1}^{2^0}\prod_{i=1}^{L}(A_i)^{a_i}_{\xi_{i-1}\xi_i}|a_1a_2\cdots a_L\rangle \overset{(D<<2^{L/2})}{\approx} \sum_{a_1a_2\cdots a_L}\sum_{\xi_0\cdots\xi_L}^{D}\prod_{i=1}^{L}(A_i)^{a_i}_{\xi_{i-1}\xi_i}|a_1a_2\cdots a_L\rangle$$

Note that $\dim\left\{(A_i)^{a_i}_{\xi_{i-1}\xi_i}\right\} = qD^2$, where , e.g., $q = \begin{cases} 2 & Heisenberg, \\ 4 & Hubbard. \end{cases}$

Consider spinless electrons on a linear chain with a finite length L divided into two parts with sizes k and $L - k$, where ($1 \leq k \leq L-1$). We show that von Neumann entanglement entropies S_{sys} and S_{env} for both of the chains are identical for a fixed k.



$|a_1a_2\cdots a_{k=6}\rangle_{system} \overset{def}{=} |i\rangle_{sys}$ $\qquad |a_{k+1}\cdots a_L\rangle_{environment} \overset{def}{=} |j\rangle_{env}$

$$S_{\substack{sys\\env}} = -Tr\left(\rho_{\substack{sys\\env}}\log_2\rho_{\substack{sys\\env}}\right)$$

$$\rho_{sys} = Tr_{env}|\Psi\rangle\langle\Psi| = \sum_j \Psi_{ij}\Psi^+_{ji}$$

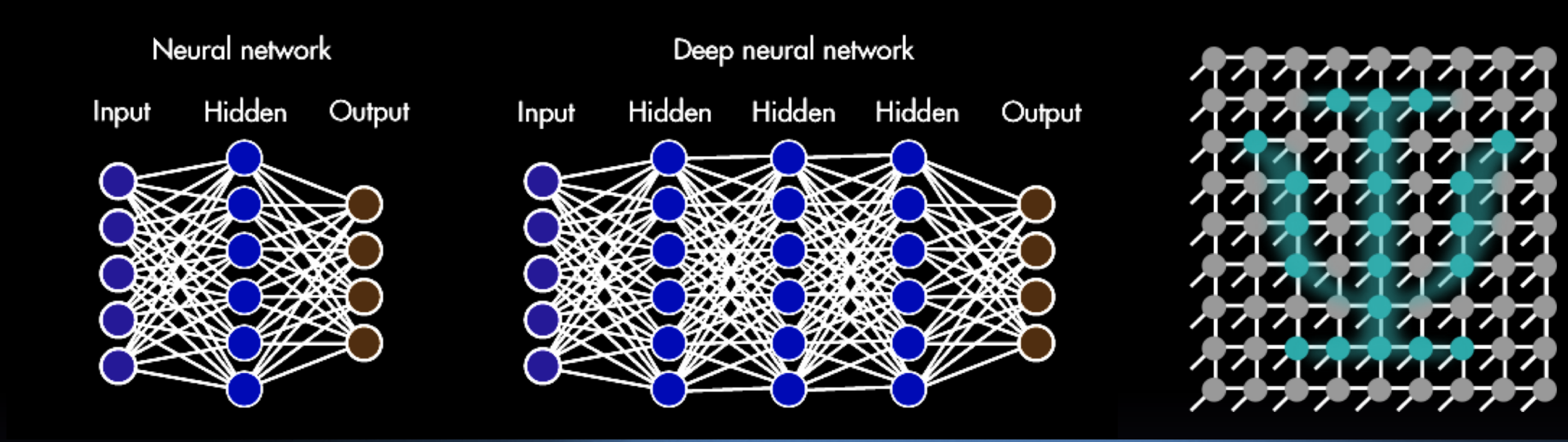
$$\rho_{env} = Tr_{sys}|\Psi\rangle\langle\Psi| = \sum_i \Psi^+_{ji}\Psi_{ij}$$

$$|\Psi\rangle = \sum_{i=1}^{2^k}\sum_{j=1}^{2^{L-k}}\Psi^i_j|i\rangle_{sys}|j\rangle_{env} \overset{SVD}{=} \sum_{i=1}^{2^k}\sum_{j=1}^{2^{L-k}}\sum_{\xi=1}^{m=\min(2^k,2^{L-k})} U^i_\xi \underbrace{S^\xi_\xi}_{\substack{\equiv s_\xi\\ diag.\\ matrix}} (V^T)^\xi_j|i\rangle_{sys}|j\rangle_{env} = \sum_{\xi=1}^{m}s_\xi\underbrace{\sum_{i=1}^{2^k}U^i_\xi|i\rangle_s}_{=|\xi\rangle_{sys}}\underbrace{\sum_{j=1}^{2^{L-k}}(V^T)^\xi_j|j\rangle_e}_{=|\xi\rangle_{env}} = \sum_{\xi=1}^{m}s_\xi|\xi\rangle_{sys}|\xi\rangle_{env}$$

$$\rho_{sys} = Tr_{env}|\Psi\rangle\langle\Psi| = \sum_{j=1}^{2^{L-k}}\sum_{\xi=1}^{m}s_\xi|\xi\rangle_{sys}|\xi\rangle_{env}\sum_{\eta=1}^{m}\left[s_\eta|\eta\rangle_{sys}|\eta\rangle_{env}\right]^+ = \sum_{\xi=1}^{m}\sum_{\eta=1}^{m}\underbrace{s_\xi s^+_\eta}_{s^+_\eta=s_\eta}|\xi\rangle_{sys}\underbrace{\sum_{j=1}^{2^{L-k}}|\xi\rangle_{env}\langle\eta|_{env}}_{=\delta_{\xi,\eta}}\langle\eta|_{sys} = \sum_{\xi=1}^{m}s_\xi^2|\xi\rangle_{sys}\langle\xi|_{sys}$$

$$\rho_{env} = Tr_{sys}|\Psi\rangle\langle\Psi| = \sum_{i=1}^{2^k}\sum_{\xi=1}^{m}\left[s_\xi|\xi\rangle_{sys}|\xi\rangle_{env}\right]^+\sum_{\eta=1}^{m}s_\eta|\eta\rangle_{sys}|\eta\rangle_{env} = \sum_{\xi=1}^{m}\sum_{\eta=1}^{m}\underbrace{s^+_\xi s_n}_{s^+_\xi=s_\xi}|\xi\rangle_{env}\underbrace{\sum_{i=1}^{2^k}|\xi\rangle_{sys}\langle\eta|_{sys}}_{=\delta_{\xi,\eta}}\langle\eta|_{env} = \sum_{\xi=1}^{m}s_\xi^2|\xi\rangle_{env}\langle\xi|_{env}$$

For any fixed k, even if $k \neq L/2$, we get $\begin{cases} S_{sys} = -Tr_{sys}\left(\rho_{sys}\log_2\rho_{sys}\right) = \sum_{\xi=1}^{m}s_\xi^2\log_2\left(s_\xi^2\right) \\ S_{env} = -Tr_{env}\left(\rho_{env}\log_2\rho_{env}\right) = \sum_{\xi=1}^{m}s_\xi^2\log_2\left(s_\xi^2\right) \end{cases} \Rightarrow \boxed{S_{sys} \equiv S_{env}.}$


Neural network
Input
Hidden
Output
Deep neural network
Input
Hidden
Hidden
Hidden
Output