Machine learning quantum states and entanglement

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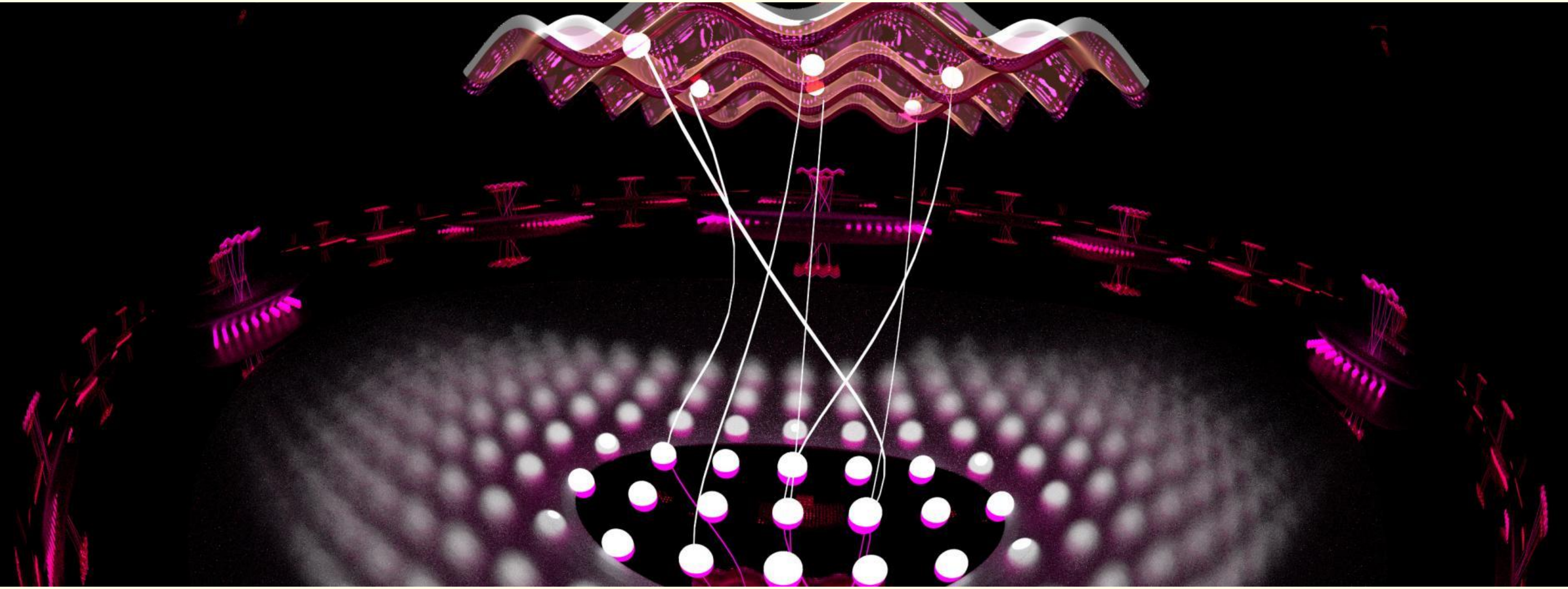


Kavli Institute for Theoretical Sciences, UCAS, Beijing, 07/06/2017

References:

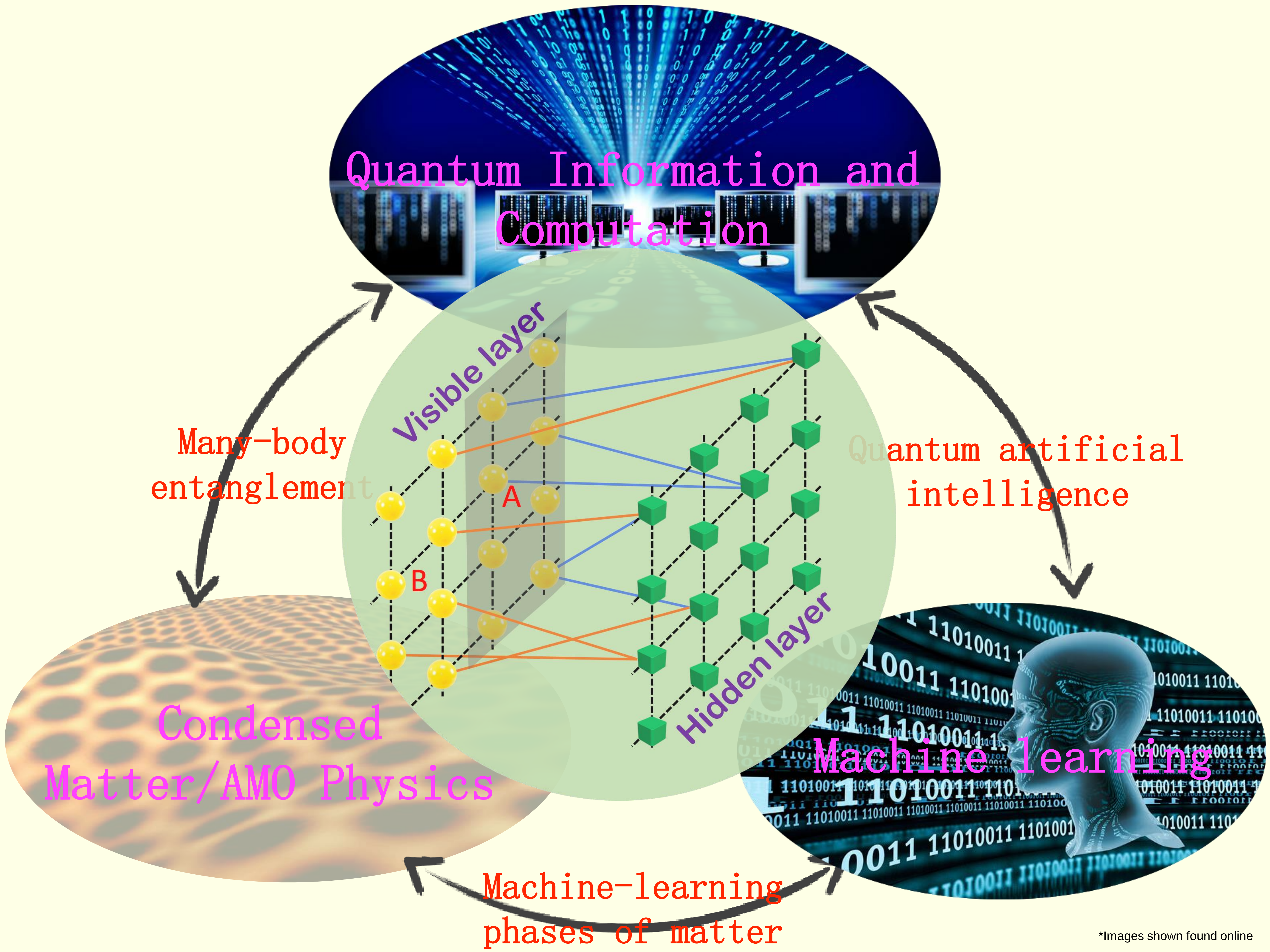
[1] **DLD**, Xiao... (2016)

[2] **DLD**, X...

Dong-Li... Xiaopeng

Outline

- Background and motivation
- Restricted Boltzmann machine (RBM)
- Exact RBM representation of topological states
- Quantum entanglement in neural network states
- Summary and outlook



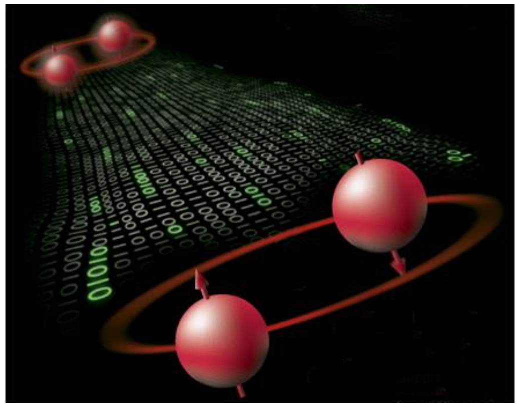
Quantum Information and Computation
Visible layer
Hidden layer
A
B
Many-body entanglement
Quantum artificial intelligence
Condensed Matter/AMO Physics
Machine learning
Machine-learning phases of matter
*Images shown found online

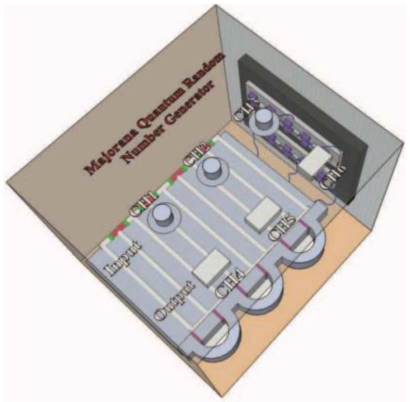
Quantum entanglement and machine-learning phases of matter

Power of machine learning →

Big data, deep learning, symmetry, locality, renormalization group …

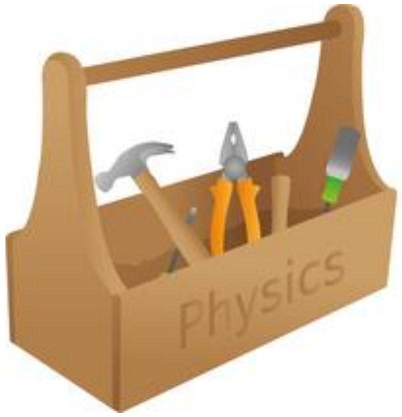
Quantum entanglement →





Quantum cryptography, supremacy, simulation, many-body localization, hamiltonian complexity, time crystals, DMRG, MERA …

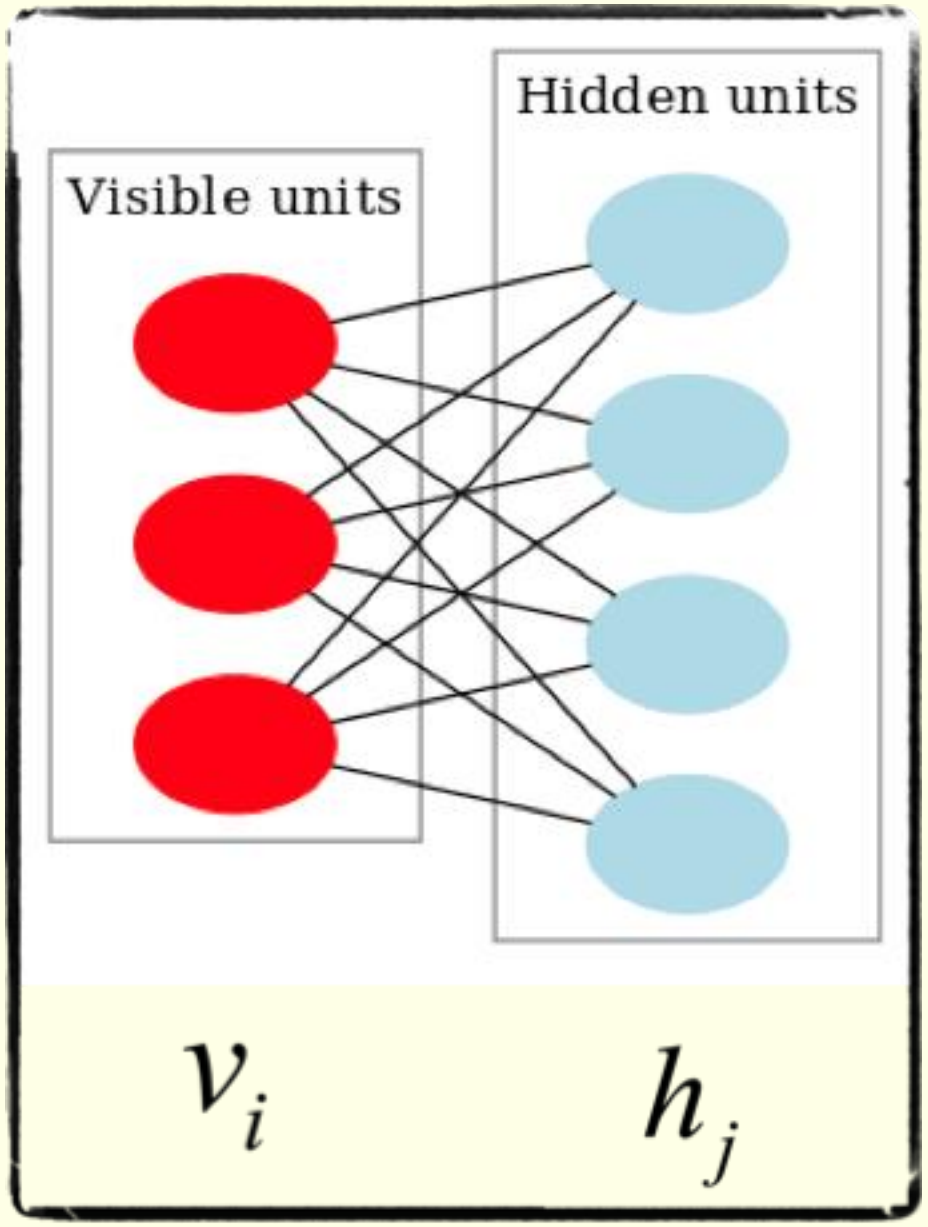
Machine-learning phases of matter →



Phase transitions, topological phases, thermalization, many-body problems …

*Images shown found online

Restricted Boltzmann machine



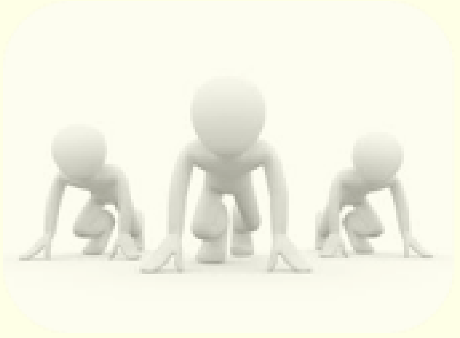
Configuration probability:

$$P(v) \propto \sum_h \exp\left[\sum_i a_i v_i + \sum_j b_j h_j + \sum_{ij} W_{ij} v_i h_j\right]$$

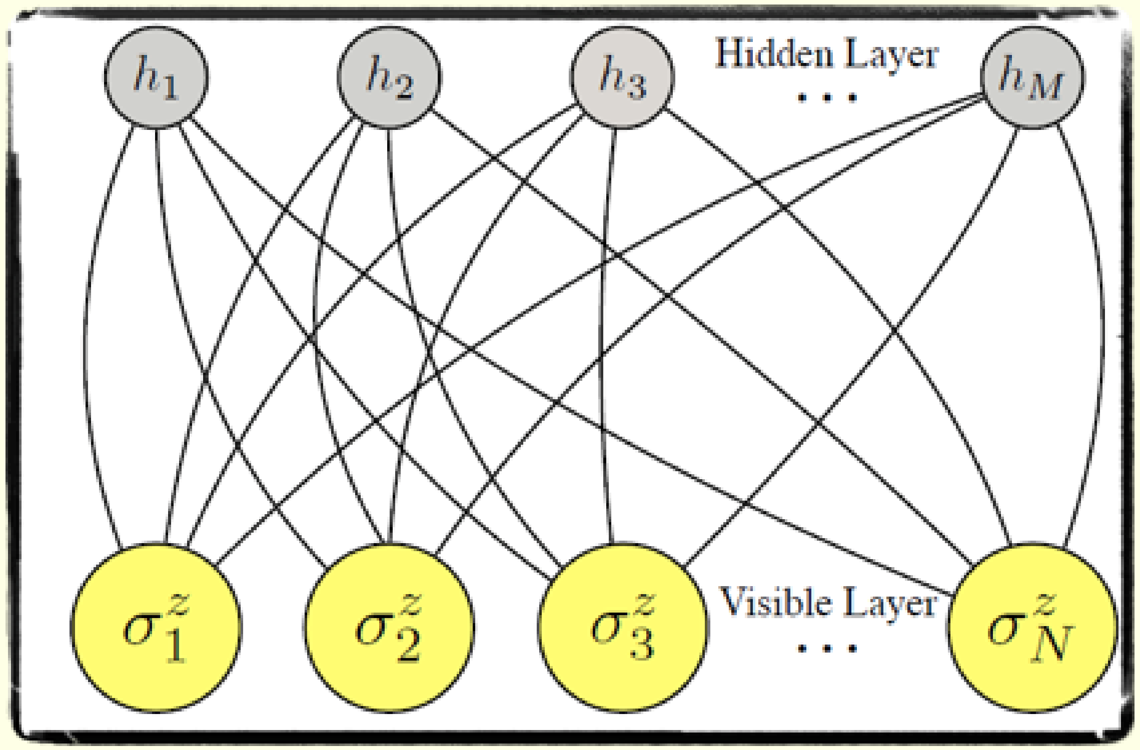
- No intra-layer coupling
- decoupled when *h* is fixed
- easy to sample

$$P(h) \propto \exp\left(\sum b_j h_j\right)$$

$$P(v|h) \propto \exp\left(\sum a_i v_i + \sum W_{ij} v_i h_j\right)$$



RBM representation of quantum states



Examples for quantum models:

Transverse field Ising:

$$\mathcal{H}_{\text{TFI}} = -h\sum_i \sigma_i^x - \sum_{\langle i,j\rangle} \sigma_i^z \sigma_j^z$$

Anti-Ferro Heisenberg:

$$\mathcal{H}_{\text{AFH}} = \sum_{\langle i,j\rangle} \sigma_i^x\sigma_j^x + \sigma_i^y\sigma_j^y + \sigma_i^z\sigma_j^z$$

Allow complex parameters and regard the probability as the coefficients for spin configurations:

$$\Psi_M(\mathcal{S};\mathcal{W}) = \sum_{\{h_k\}} e^{\sum_j a_j\sigma_j^z + \sum_k b_k h_k + \sum_{kj} W_{kj} h_k \sigma_j^z}$$

The actual quantum state:

$$|\Phi\rangle = \sum_{\mathcal{S}} \Psi_M(\mathcal{S},\mathcal{W})|\mathcal{S}\rangle$$

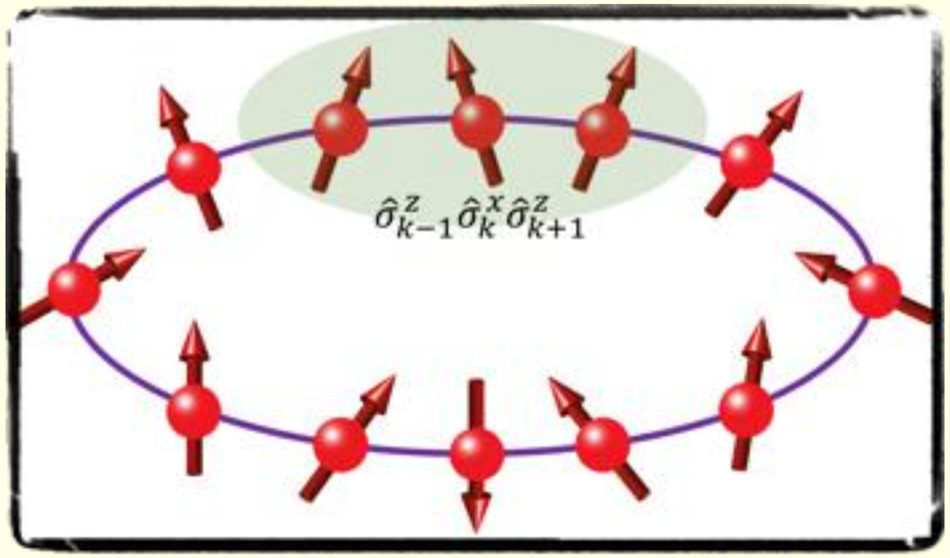
G. Carleo and M. Troyer, Science 355, 602 (2017)

Question: can RBM represents topological states?

1D symmetry protected topological (SPT) states

Hamiltonian:

$$H_{spt} = -\sum_{k=1}^{N} \hat{\sigma}^z_{k-1}\hat{\sigma}^x_k\hat{\sigma}^z_{k+1}$$



Symmetry: $Z_2 \times Z_2$

tabilizer ground state: $\hat{\sigma}^z_{k-1}\hat{\sigma}^x_k\hat{\sigma}^z_{k+1}|G\rangle = |G\rangle, \ \forall k$

Aim: an exact RBM representation

Reminder:

$$\Psi_M(\mathcal{S};\mathcal{W}) = \sum_{\{h_k\}} e^{\sum_j a_j\sigma^z_j + \sum_k b_k h_k + \sum_{kj} W_{kj} h_k \sigma^z_j}$$

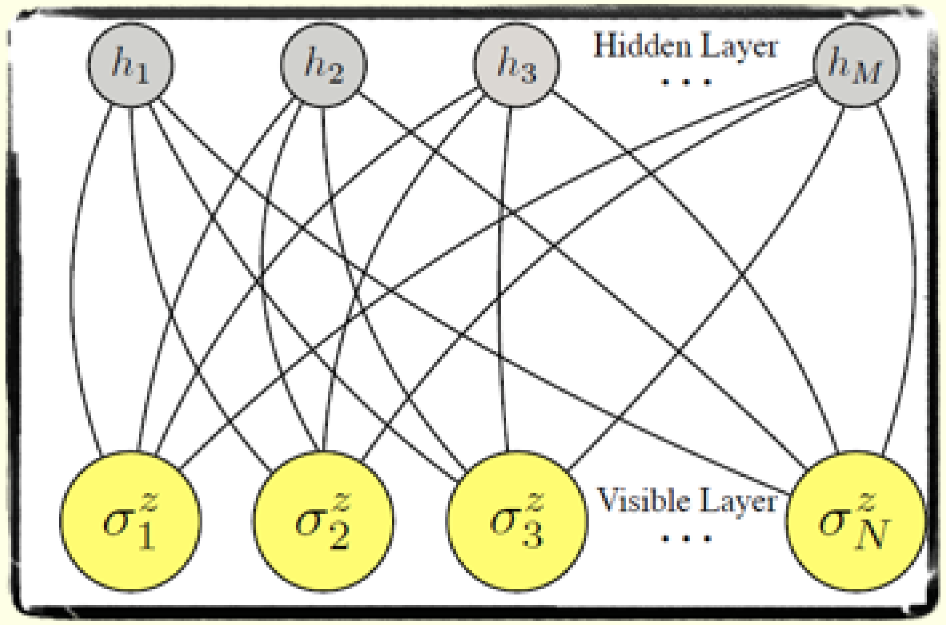
$$|\Phi\rangle = \sum_{\mathcal{S}} \Psi_M(\mathcal{S},\mathcal{W})|\mathcal{S}\rangle$$

aively, solve equations: $\hat{\sigma}^z_{k-1}\hat{\sigma}^x_k\hat{\sigma}^z_{k+1}|\Phi\rangle = |\Phi\rangle$

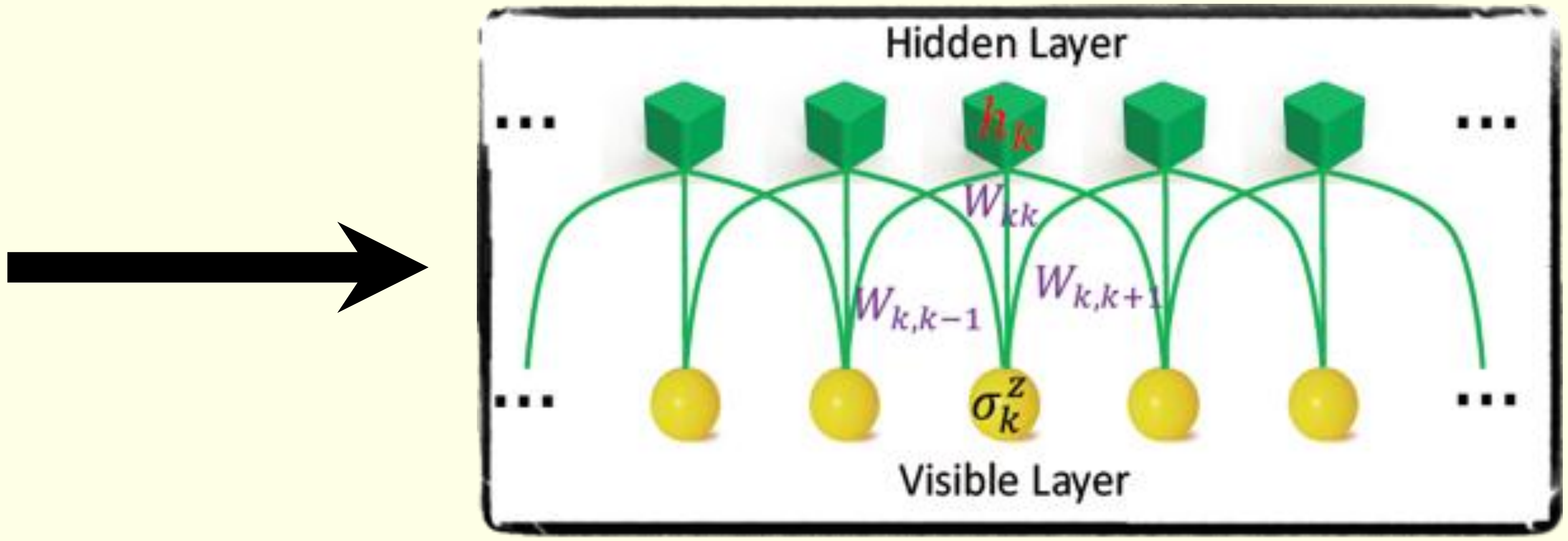
But, with exponentially many highly-nonlinear equations!

Idea: build in locality to RBM to reduce equations

A further-restricted RBM



G. Carleo and M. Troyer, **Science 355**, 602 (2017)



DLD, X.-P. Li, S. Das Sarma, arXiv: 1609.09060(2016)

Symmetry constraints: $a_k = ia, b_k = ib, W_{kk} = \omega_0, W_{kk\pm1} = \omega_{\pm1}$

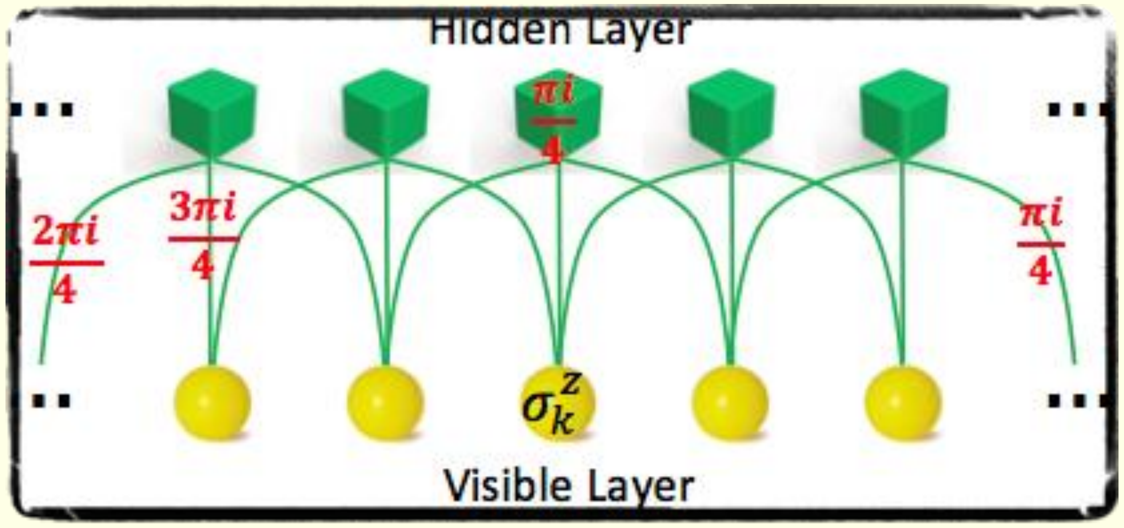
Product form: $\Psi_M = \prod e^{a_j \sigma_j^z} \prod \Gamma_k(\mathcal{S}), \Gamma_k(\mathcal{S}) = 2\cosh(b_k + \sum_j W_{kj}\sigma_j^z)$

Reduced to 32 equations with 5 variables.

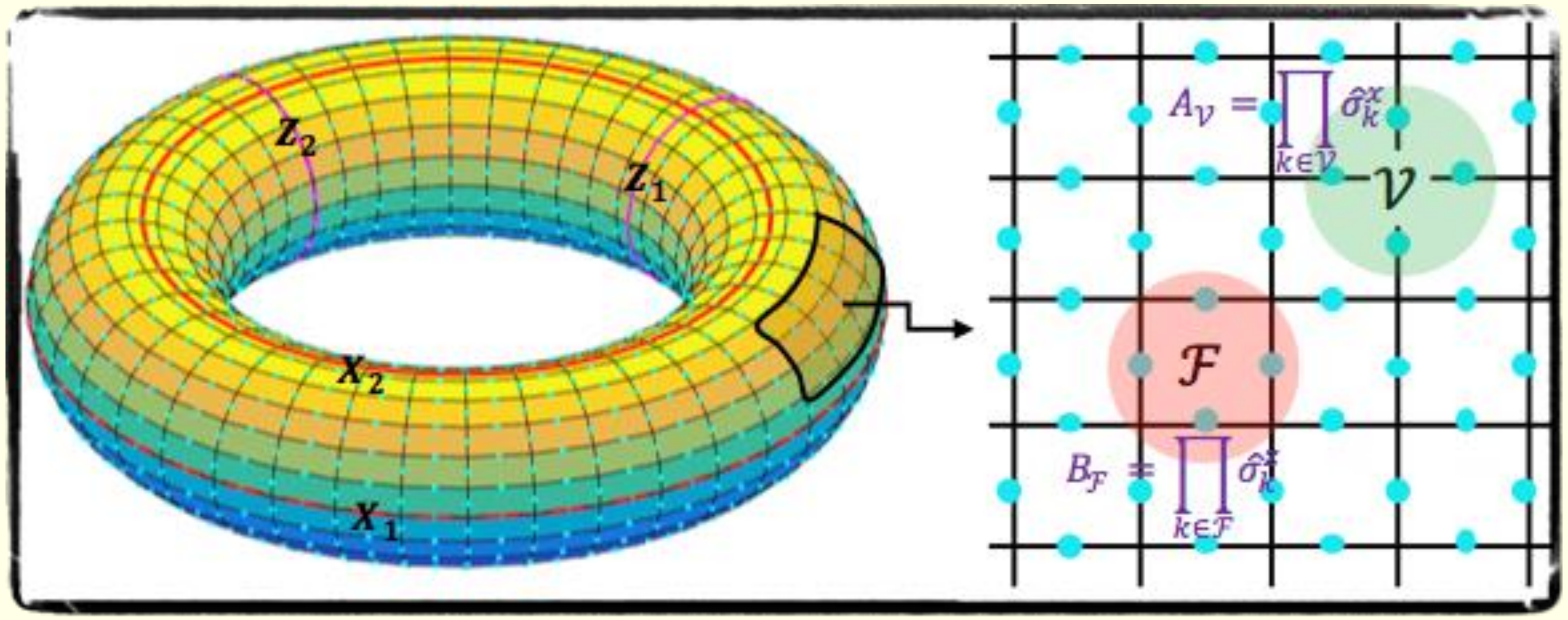
A explicit solution:

$$(a, b, \omega_{-1}, \omega_0, \omega_1) = \frac{\pi}{4}(0, 1, 2, 3, 1)$$

$$\Psi(\mathcal{S}, \mathcal{W}) = \sum_{\{h_k\}} \exp\left\{\frac{i\pi}{4}\sum_k h_k(1 + 2\sigma_{k-1}^z + 3\sigma_k^z + \sigma_{k+1}^z)\right\}$$



2D Kitaev toric code model

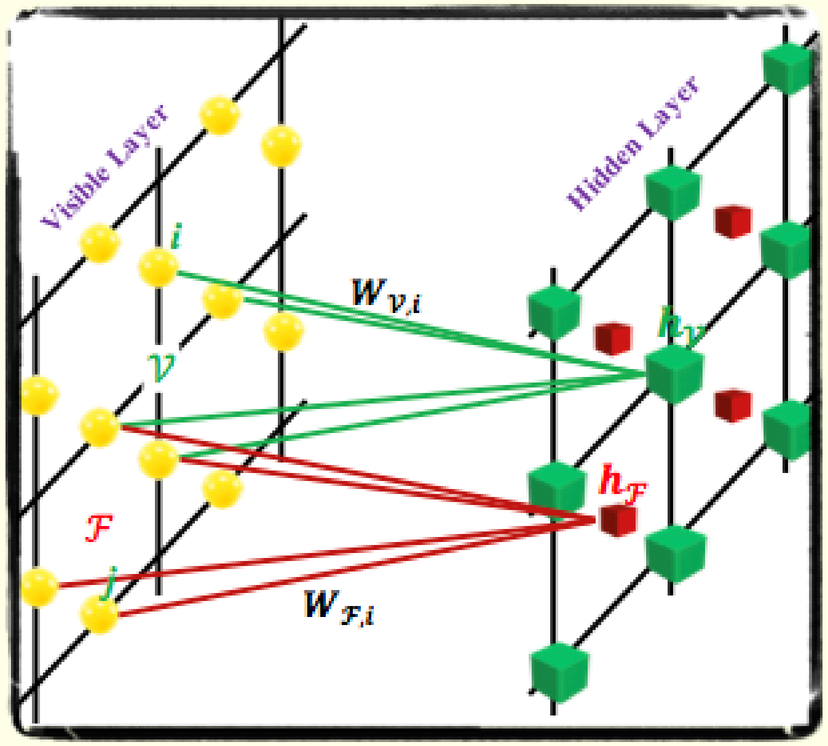


Hamiltonian: $$H_{tor} = -\sum_{\mathcal{V}\in\mathbb{T}^2} A_{\mathcal{V}} - \sum_{\mathcal{F}\in\mathbb{T}^2} B_{\mathcal{F}}$$

Ground state:

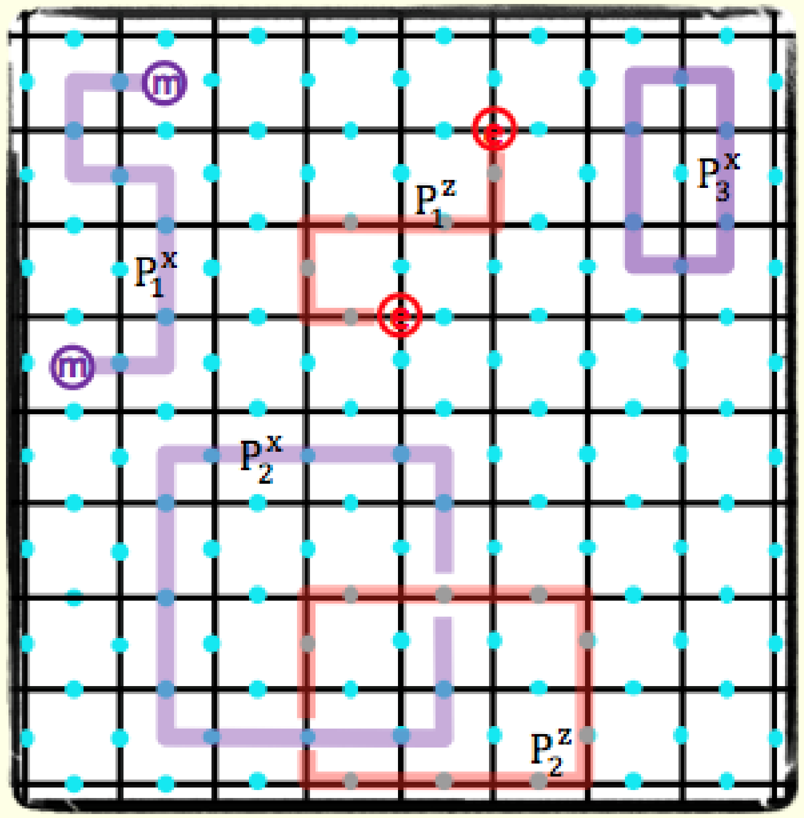
$$A_{\mathcal{V}}|G_{tor}\rangle = |G_{tor}\rangle$$
$$B_{\mathcal{F}}|G_{tor}\rangle = |G_{tor}\rangle$$

- ☆ **Intrinsic topological order with long-range entanglement**
- ☆ **Four-fold degeneracy on a torus**
- ☆ **Low-energy excitations are abelian anyons**



Solution: $$\Psi(\mathcal{S},W) = \sum_{\{h_{\mathcal{V},\mathcal{F}}\}} \exp\left\{\frac{i\pi}{2}\sum_{k,\mathcal{V}} h_{\mathcal{V}}\sigma_k^z + \frac{i\pi}{4}\sum_{k,\mathcal{F}} h_{\mathcal{F}}\sigma_k^z\right\}$$

Excited states with abelian anyons



Two types of anyons created by different string operators:

$$S^x_{P^x} = \prod_{j \in P^x} \hat{\sigma}^x_j$$ creates a pair of x-type quasiparticles (m) at the end of P^x

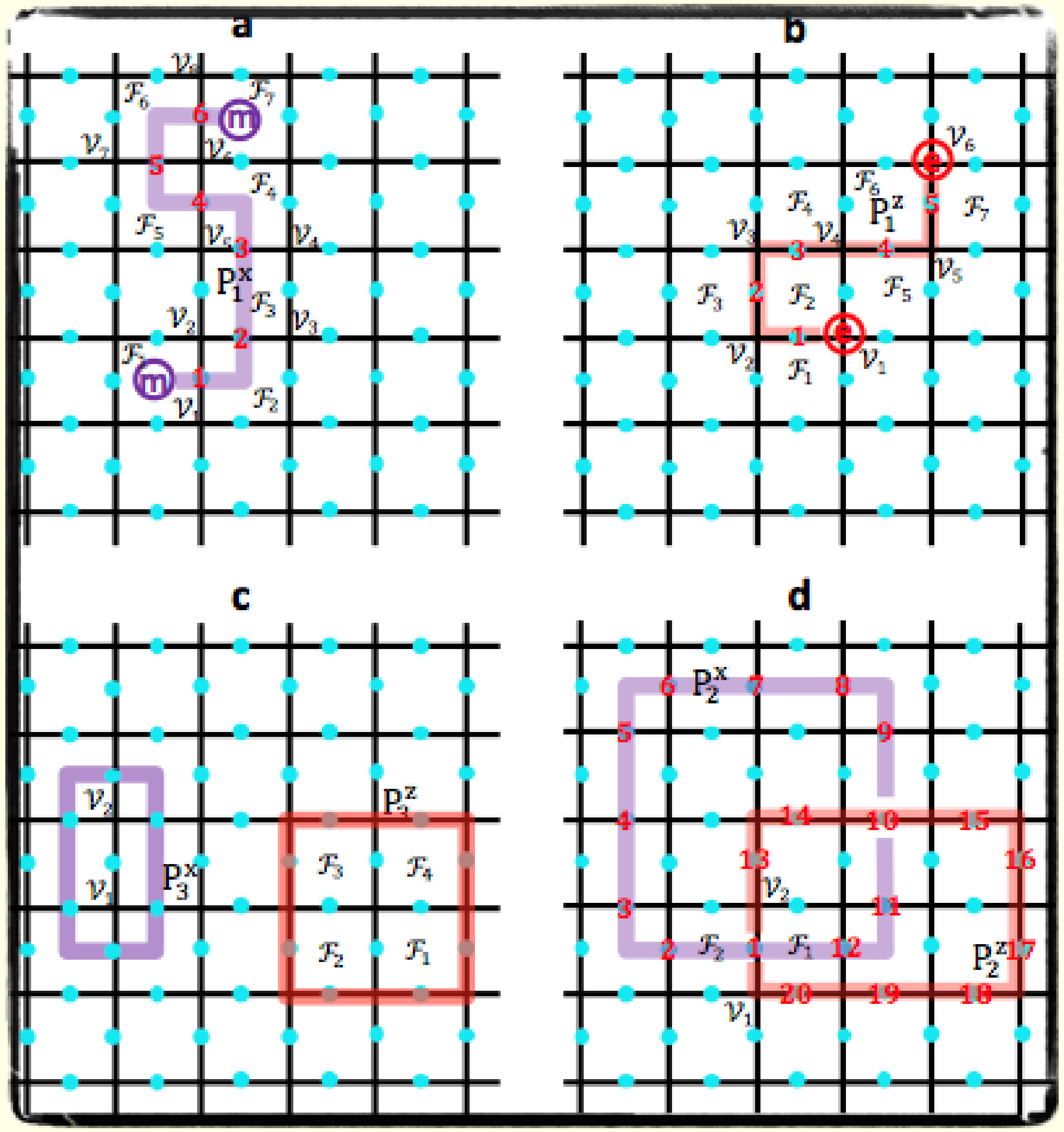
$$S^z_{P^z} = \prod_{j \in P^z} \hat{\sigma}^z_j$$ creates a pair of z-type quasiparticles (e) at the end of P^z

Fusion rule: $e \times e = 1; m \times m = 1; e \times m = \psi$

Nontrivial mutual statistics: braiding of e and m yields an overall

Kitaev, **Ann. Phys.** 321,2 (2006)

An exact neural network description



Two key observations:

1) applying $S^x_{P^x}$ is equivalent to flipping all signs of the weight parameters associated with the visible neurons living on the path P^x

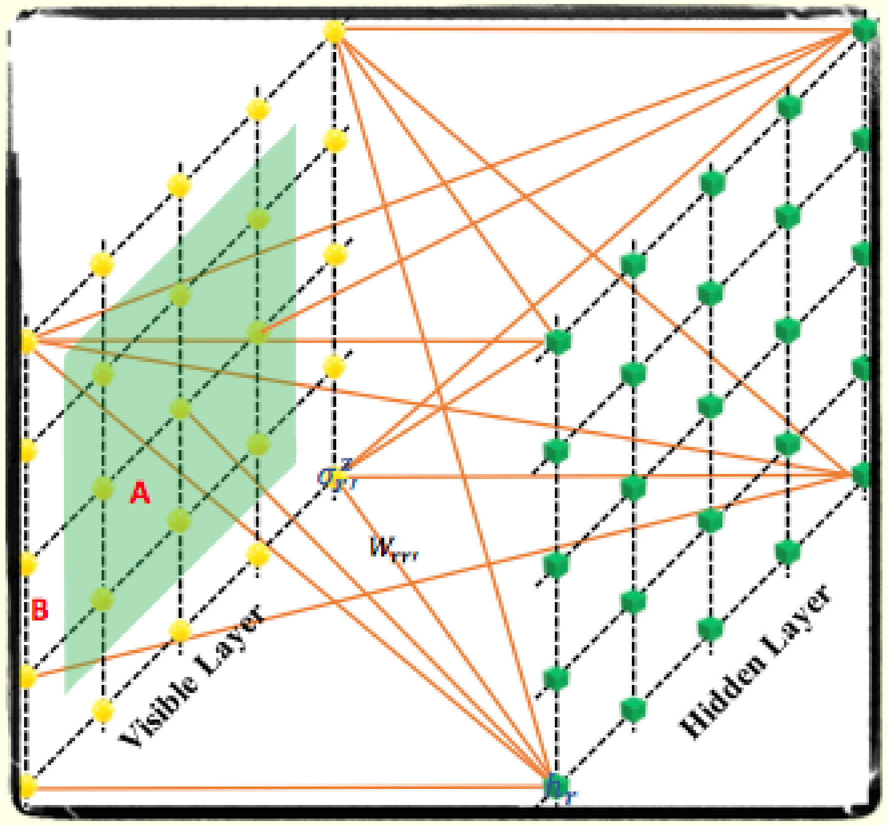
2) applying $S^z_{P^z}$ is equivalent to adding hidden neurons along P^z, with each of them connecting only to the corresponding visible neuron.

Two *m* particles at the ends of P_1^x:

$$\Psi(\mathcal{S},\mathcal{W}) = \sum_{\{h_\mathcal{V},h_\mathcal{F}\}} \exp\left\{ \frac{i\pi}{2}\sum_\mathcal{V} h_\mathcal{V}\left[\sum_{j\in\mathcal{V};j\notin P_1^x}\sigma_j^z - \sum_{j\in\mathcal{V};j\in P_1^x}\sigma_j^z\right] + \frac{i\pi}{4}\sum_\mathcal{F} h_\mathcal{F}\left[\sum_{k\in\mathcal{F};k\notin P_1^x}\sigma_k^z - \sum_{k\in\mathcal{F};k\in P_1^x}\sigma_k^z\right]\right\}$$

Quantum entanglement in neural network states

Entanglement area law for short-range RBMs



DLD, Xiaopeng Li, S. Das Sarma, PRX, 7, 021021 (2017)

The α−th order Renyi entropy:

$$S_\alpha^A \equiv \frac{1}{1-\alpha}\log[\mathrm{Tr}(\rho_A^\alpha)]$$

Theorem 1: All short-range RBM states satisfy an area law:

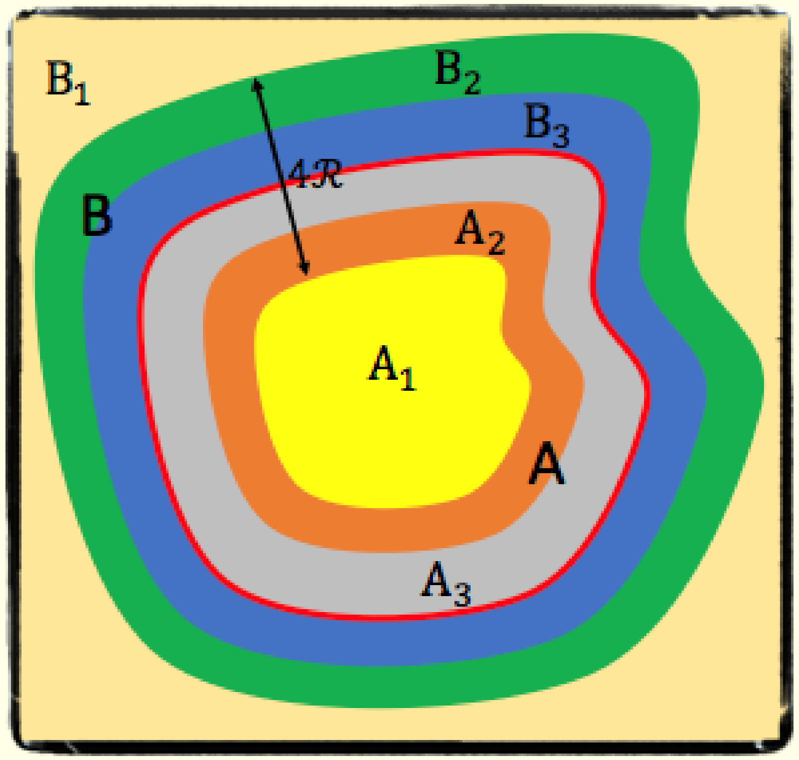
$$S_\alpha^A \leq 2\mathcal{S}(A)\mathcal{R}\log 2, \quad \forall\alpha$$

Basic idea for the proof:

- Using the product form

$$\Psi_M = \prod e^{a_j\sigma_j^z}\prod \Gamma_k(\mathcal{S})$$

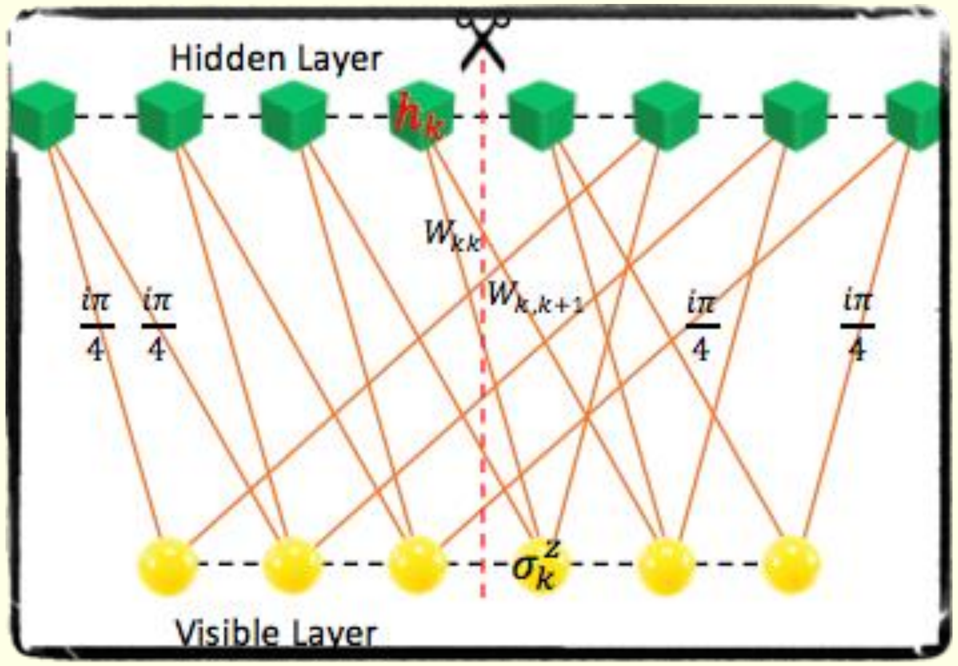
- A deliberate partitions



Remarks:

- The proof is independent of the dimensionality or the geometry of the bipartition
- The 1D SPT cluster states and the toric code states in both 2D and 3D all obey area-law entanglement
- 1D short-range RBM states can be efficiently represented by matrix product states (MPS)
- Speed up reinforcement learning
- New approach to prove entanglement area law for the ground states of local gapped Hamiltonians in higher dimensions?

Exact RBM states with volume-law entanglement



Theorem 2: the right RBM state has a volume law entanglement

$$S_\alpha^A = l \log 2, \quad \alpha$$

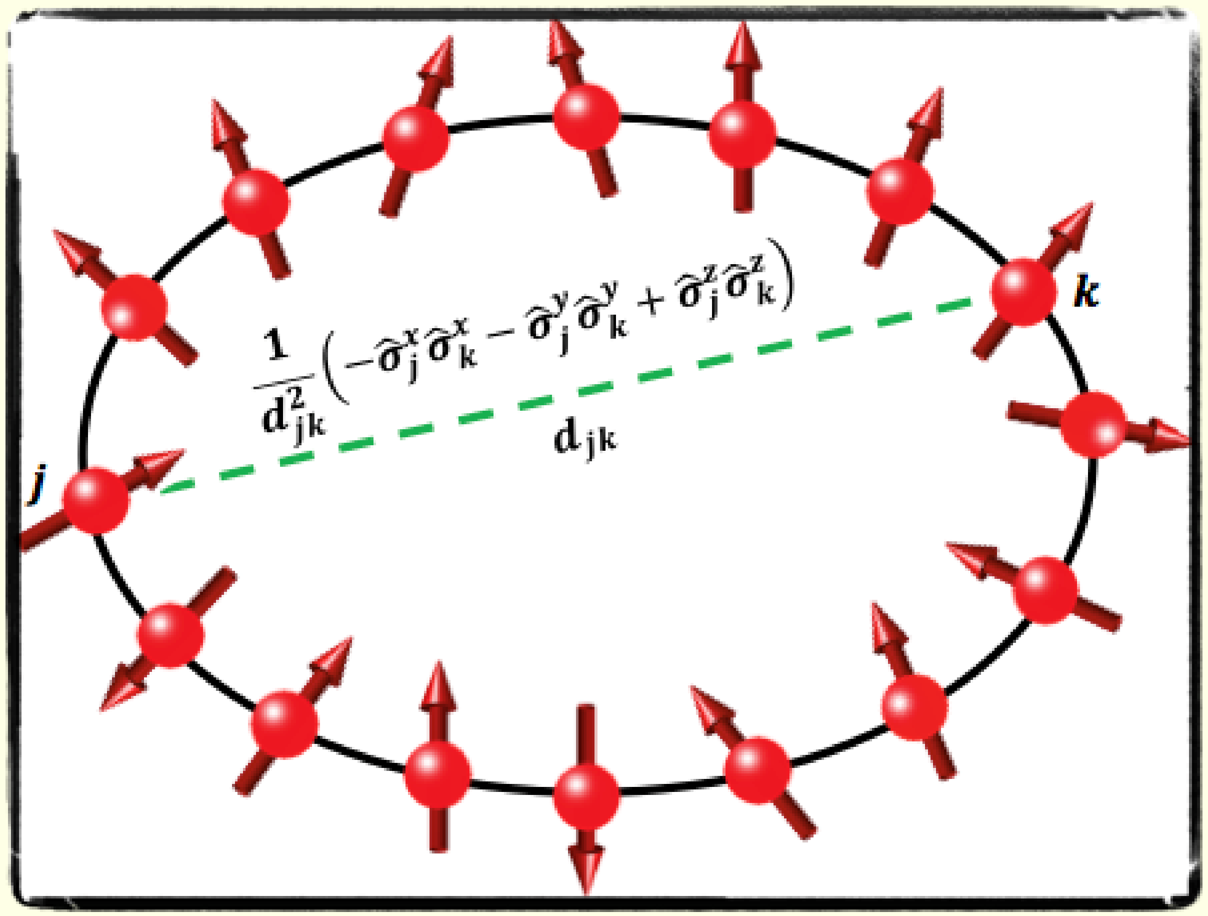
Remarks:

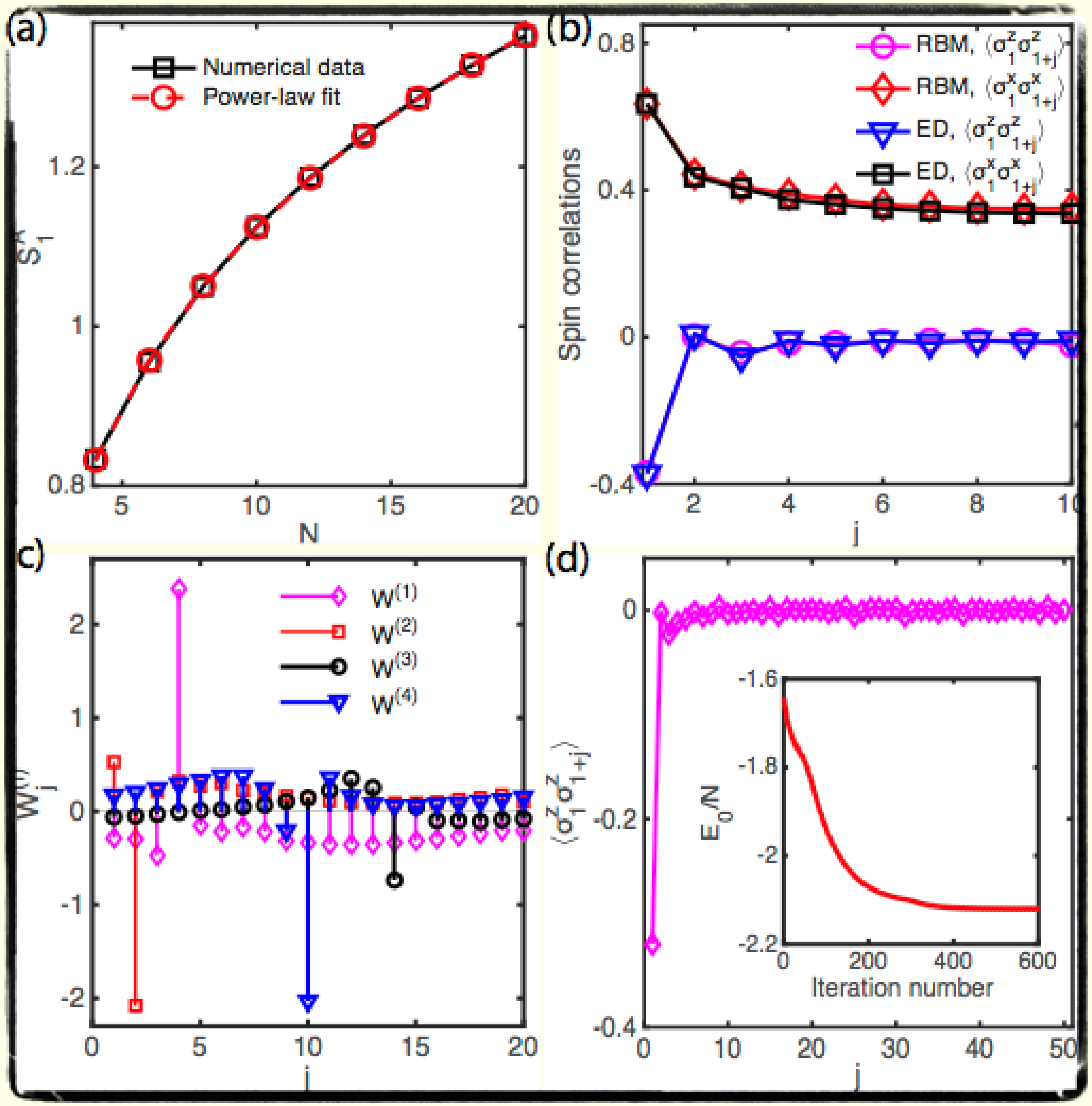
- The construction carries over to higher dimensions
- The representation is very efficient
- Unlike MPS/Tensor-network states, entanglement is not the limiting factor for RBMs

DLD, Xiaopeng Li, S. Das Sarma, **PRX**, 7, 021021 (2017)

Reinforcement learning of ground states with massive entanglement

Modified Haldane-Shastry model



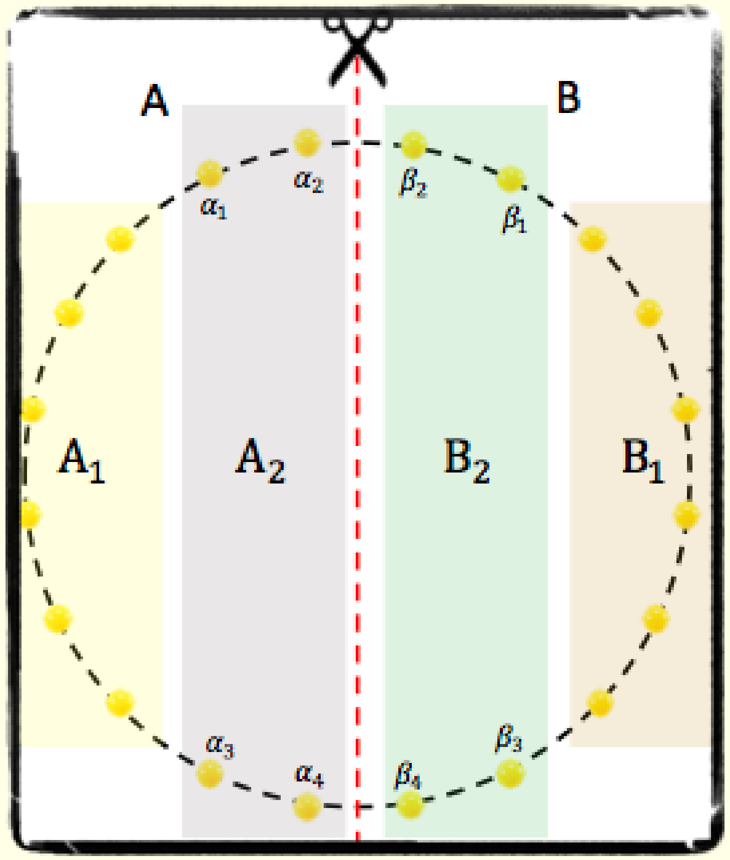


Hamiltonian:

$$H_{\mathrm{MHS}} = \sum_{j<k} \frac{1}{d_{jk}^2}(-\hat{\sigma}_j^x\hat{\sigma}_k^x - \hat{\sigma}_j^y\hat{\sigma}_k^y + \hat{\sigma}_j^z\hat{\sigma}_k^z)$$

DLD, Xiaopeng Li, S. Das Sarma, **PRX**, 7, 021021 (2017)

An analytical RBM recipe for computing entanglement



Entanglement for the 1D SPT cluster state:

Entanglement entropy:

$$S_\alpha^A = 2\log 2,\ \forall\alpha$$

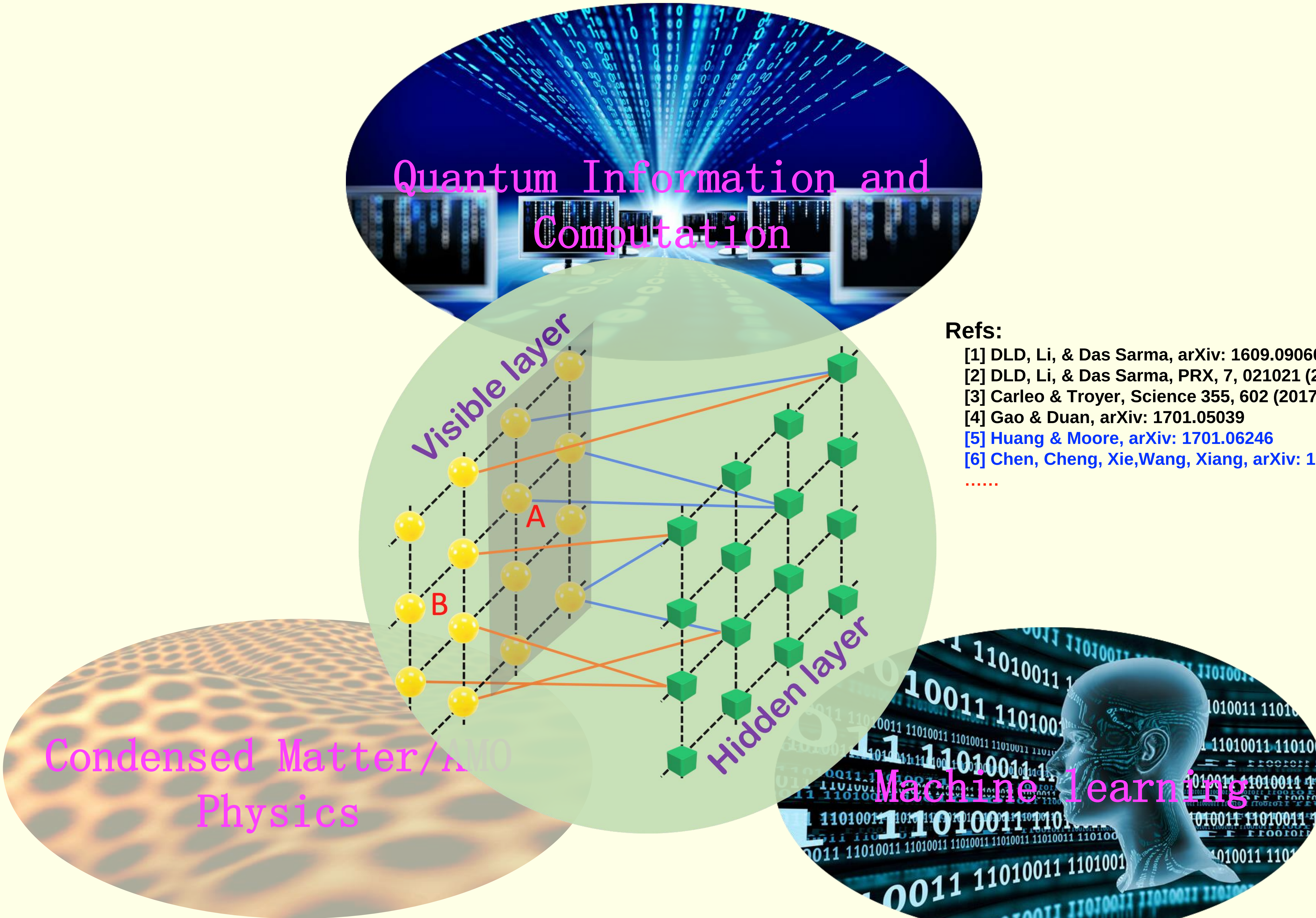
Entanglement spectrum:

$$\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = 1/4, \lambda_{k>4} = 0$$

Remarks:

- Simple, no sophisticated math
- Can deal with *finite* systems with *any* bipartition
- Entanglement spectrum has four-fold degeneracy, a signature of SPT phases
- Carry over to the toric code states straightforwardly
- Only works for certain specific cases
- No systematic way to covert a quantum many body state to RBM

Summary and outlook



Refs:

[1] DLD, Li, & Das Sarma, arXiv: 1609.09060(2016)
[2] DLD, Li, & Das Sarma, PRX, 7, 021021 (2017)
[3] Carleo & Troyer, Science 355, 602 (2017)
[4] Gao & Duan, arXiv: 1701.05039
[5] Huang & Moore, arXiv: 1701.06246
[6] Chen, Cheng, Xie,Wang, Xiang, arXiv: 1701.04831
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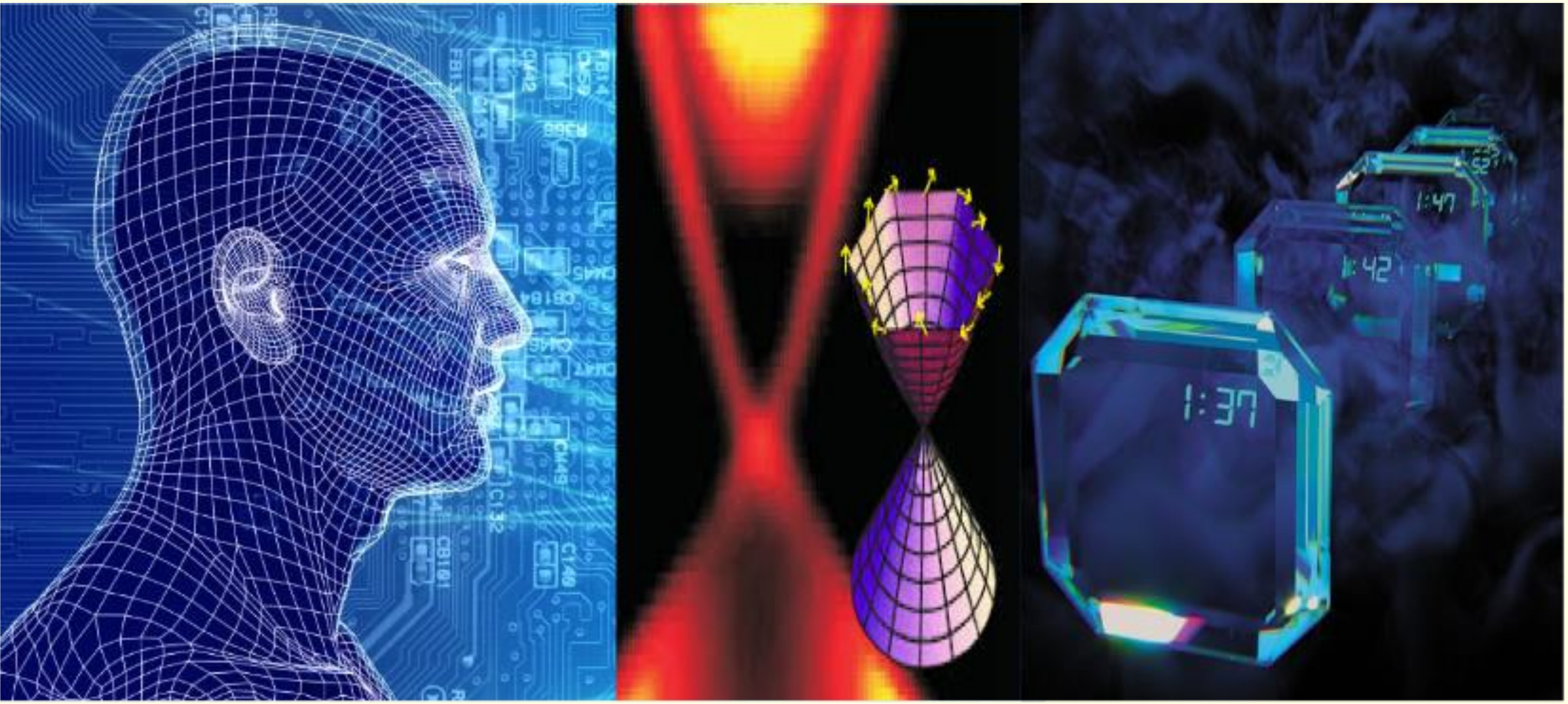
Look forward: a self-learning robot that teaches physicists physics?



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Thank you!

*Images shown found online