Solving the quantum many-body problem with artificial neural networks

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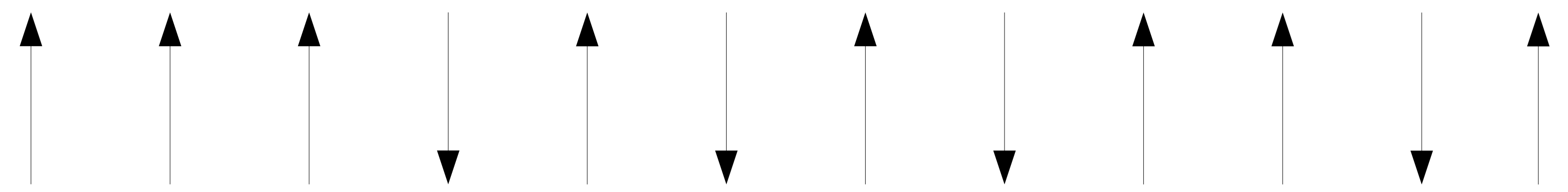
Carleo et al., Science 355, 602–606 (2017)

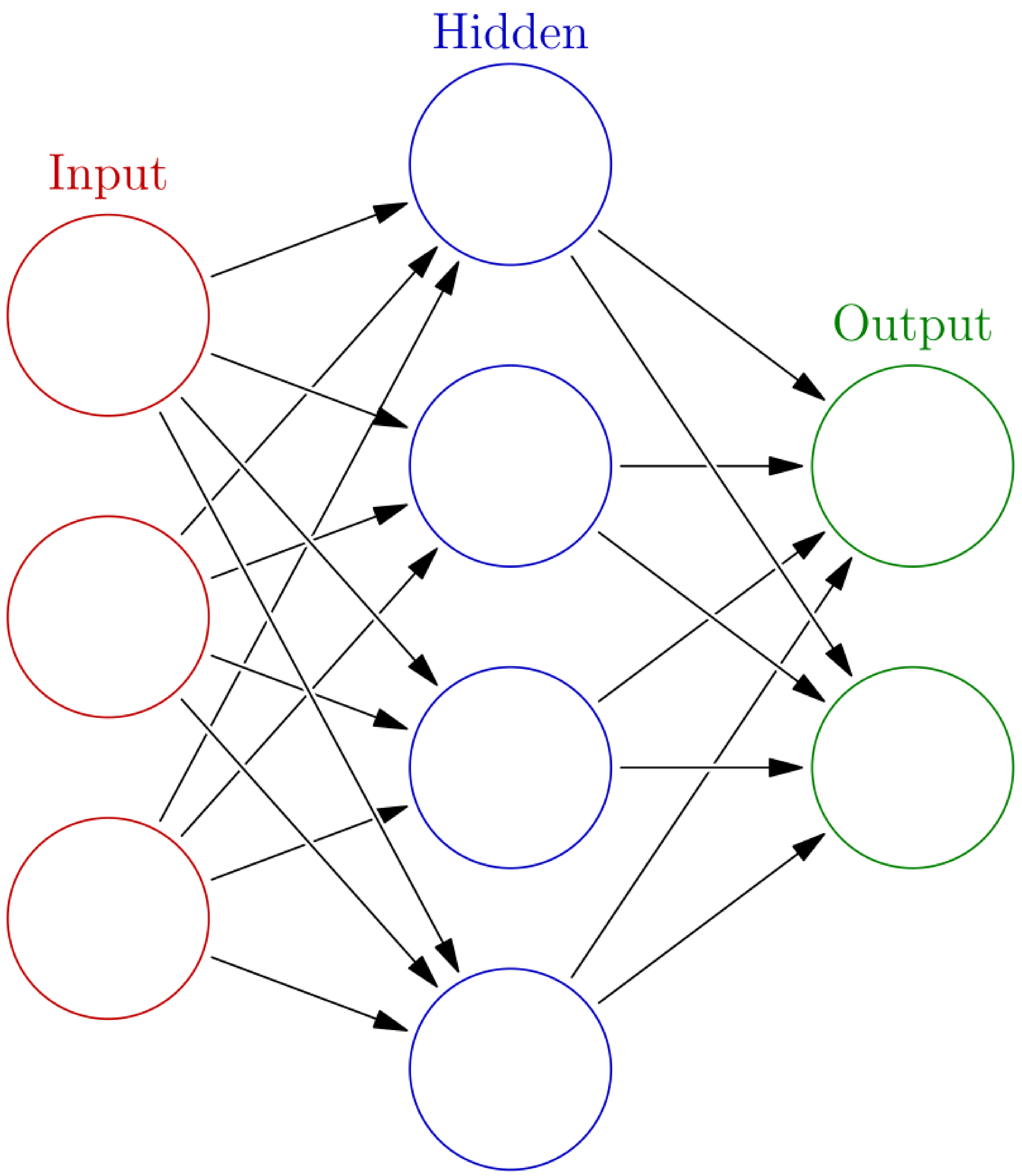
Quantum problem complexity

N spins → 2^N basis states



Limited by size of RAM → modern computers can solve systems up to ~40 spins

Neural networks



Neural-network Quantum States

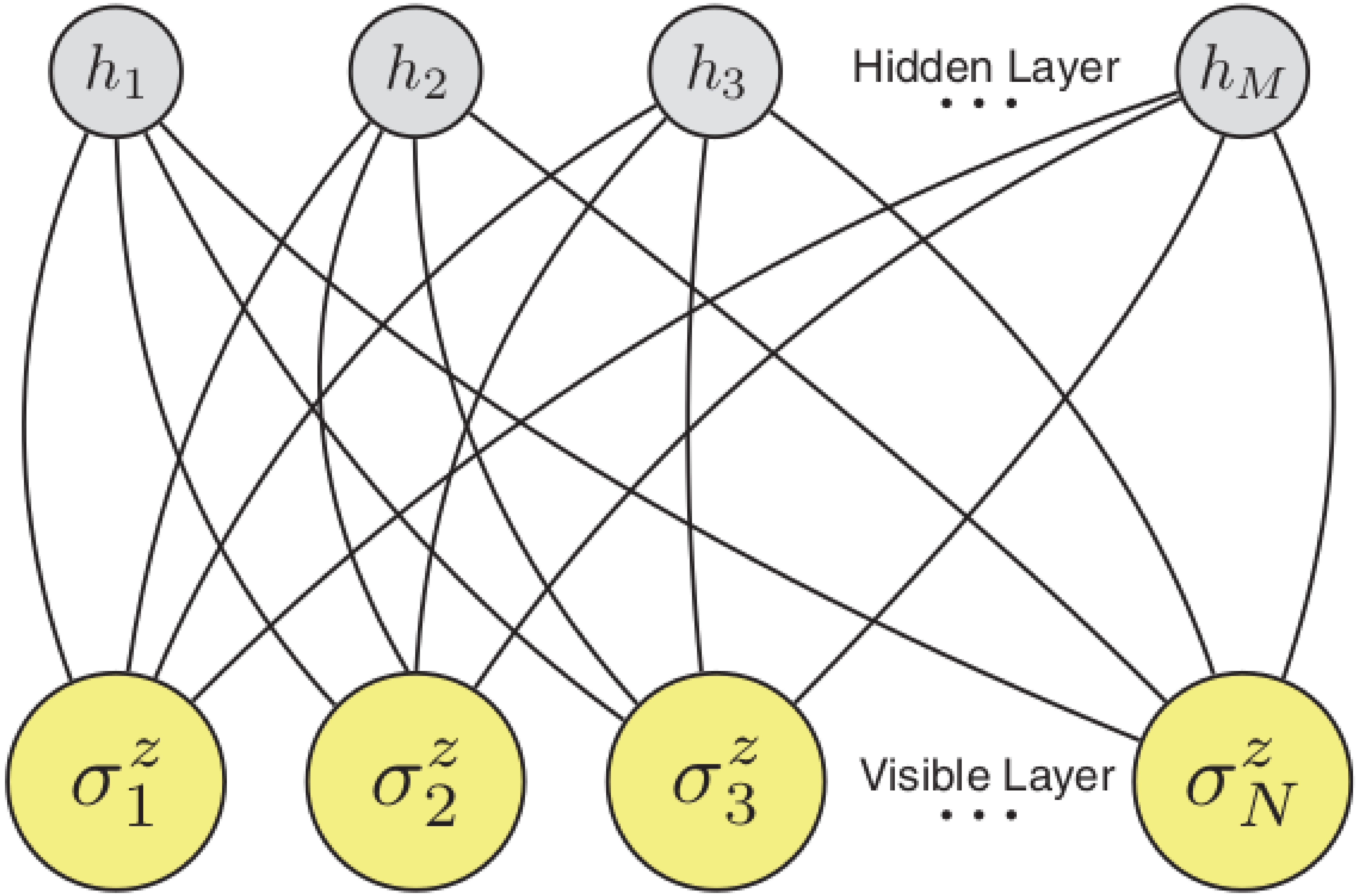


Fig. 1. Artificial neural network encoding a many-body quantum state of *N* spins. A restricted Boltzmann machine architecture that features a set of *N* visible artificial neurons (yellow dots) and a set of *M* hidden neurons (gray dots) is shown. For each value of the many-body spin configuration $\mathcal{S} = (\sigma_1^z, \sigma_2^z, \ldots, \sigma_N^z)$, the artificial neural network computes the value of the wave function $\Psi(\mathcal{S})$.

Wave function ansatz

$$\Psi_M(\mathcal{S};\mathcal{W}) = \sum_{\{h_i\}} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$

$$\Psi(\mathcal{S};\mathcal{W}) = e^{\sum_j a_j \sigma_j^z} \times \ \Pi_{i=1}^{M} F_i(S)$$

$$F_i(\mathcal{S}) = 2\cosh\left[b_i + \sum_j W_{ij} \sigma_j^z\right]$$

Optimization

$$\Psi_M(\mathcal{S};\mathcal{W}) = \sum_{\{h_i\}} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$

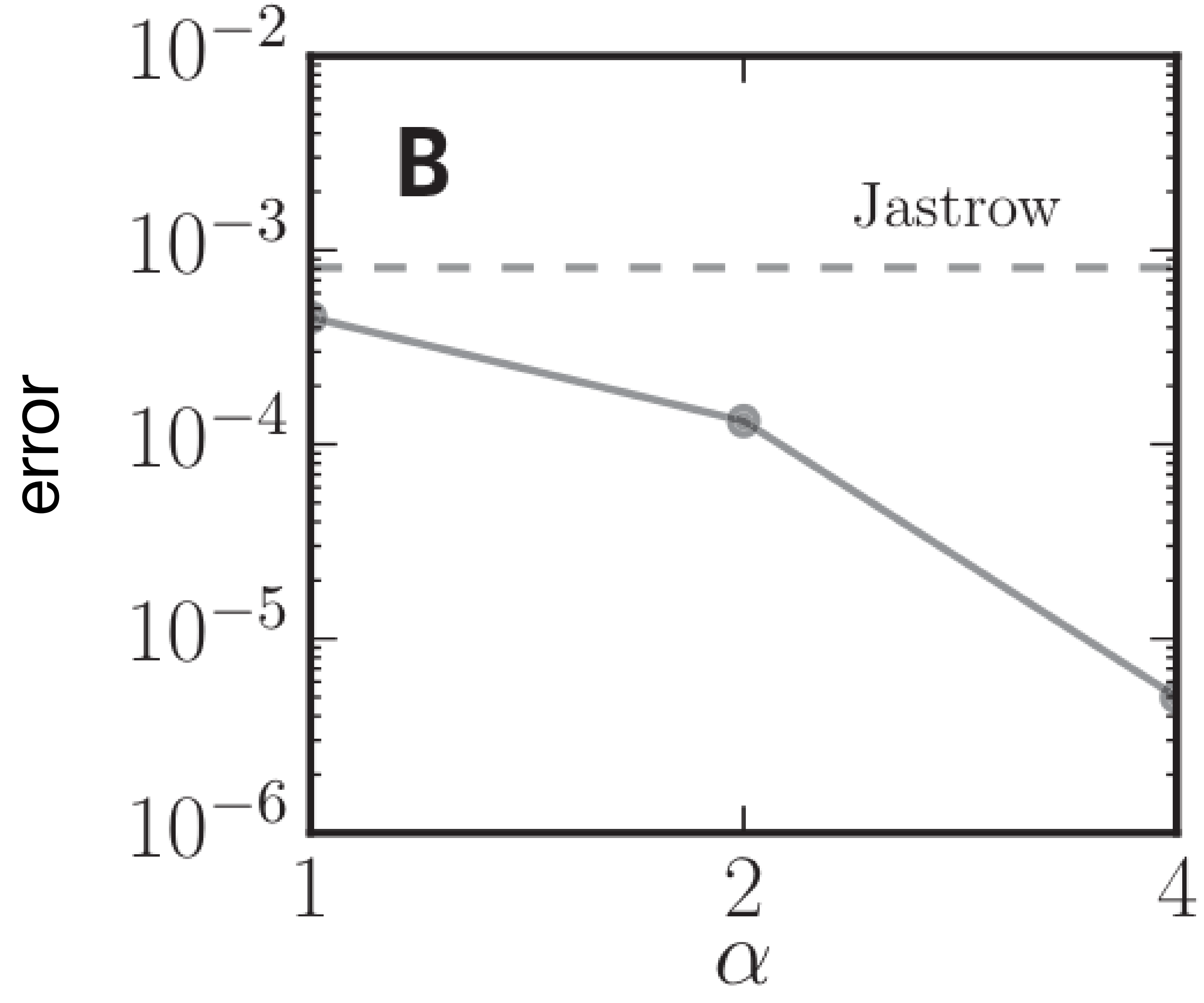
$$\mathcal{W} = \{a, b, W\}$$

$$E(\mathcal{W}) = \langle \Psi_M | \mathcal{H} | \Psi_M \rangle / \langle \Psi_M | \Psi_M \rangle$$

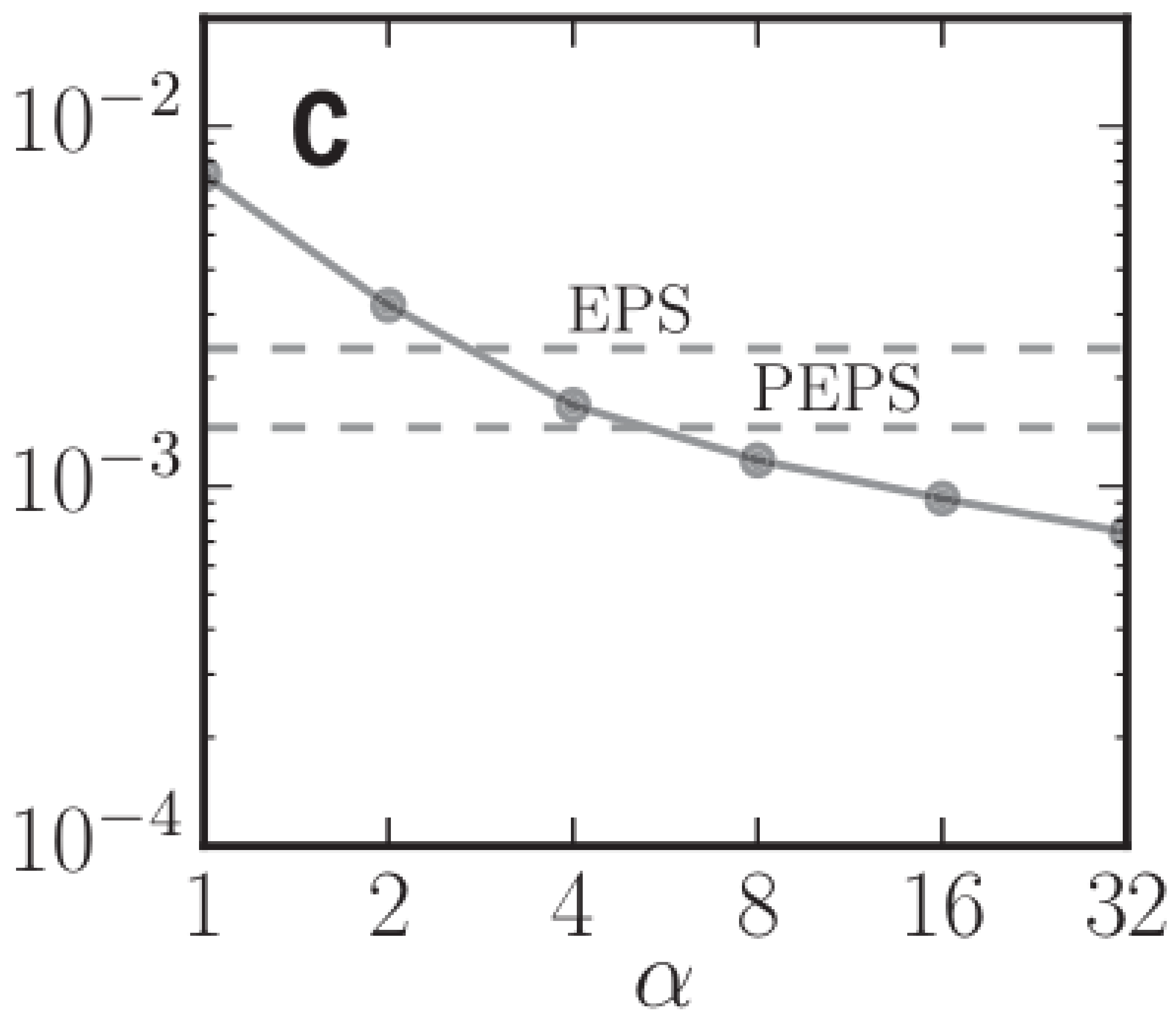
At each iteration k, a Monte Carlo sampling of |psi|^2 is realized for a given set of parameters Wk . At the same time, stochastic estimates of the energy gradient are obtained. These are then used to propose a next set of weights W k+1 with an improved gradient-descent optimization (32).

Ground state energy

$$\mathcal{H}_{\text{AFH}} = \sum_{ij} \sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y + \sigma_i^z \sigma_j^z$$



80-spin chain with PBCs



10-by-10 square lattice with PBCs

$$\alpha = M/N$$