The Use of Restricted Boltzmann Machines for Modeling a Many-body Quantum System

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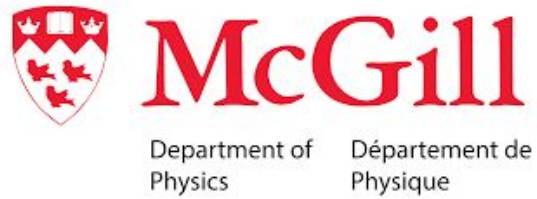

Motivation

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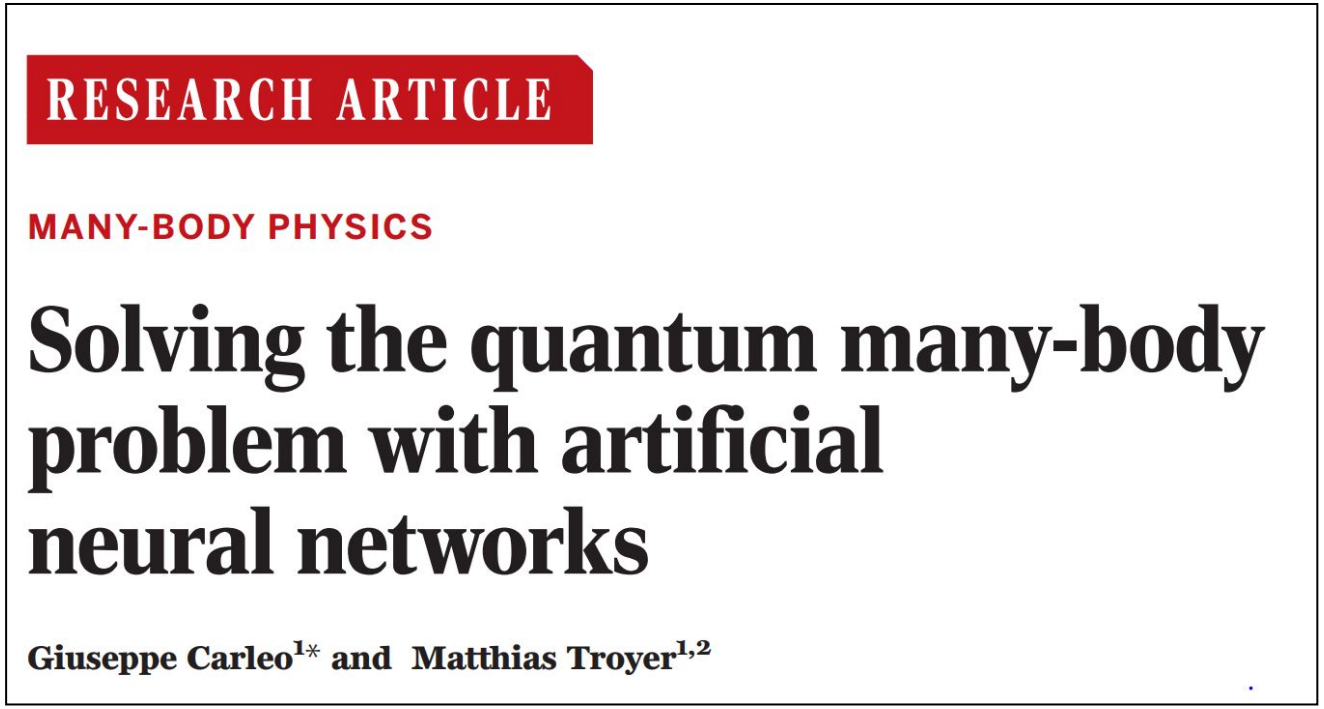


RESEARCH ARTICLE

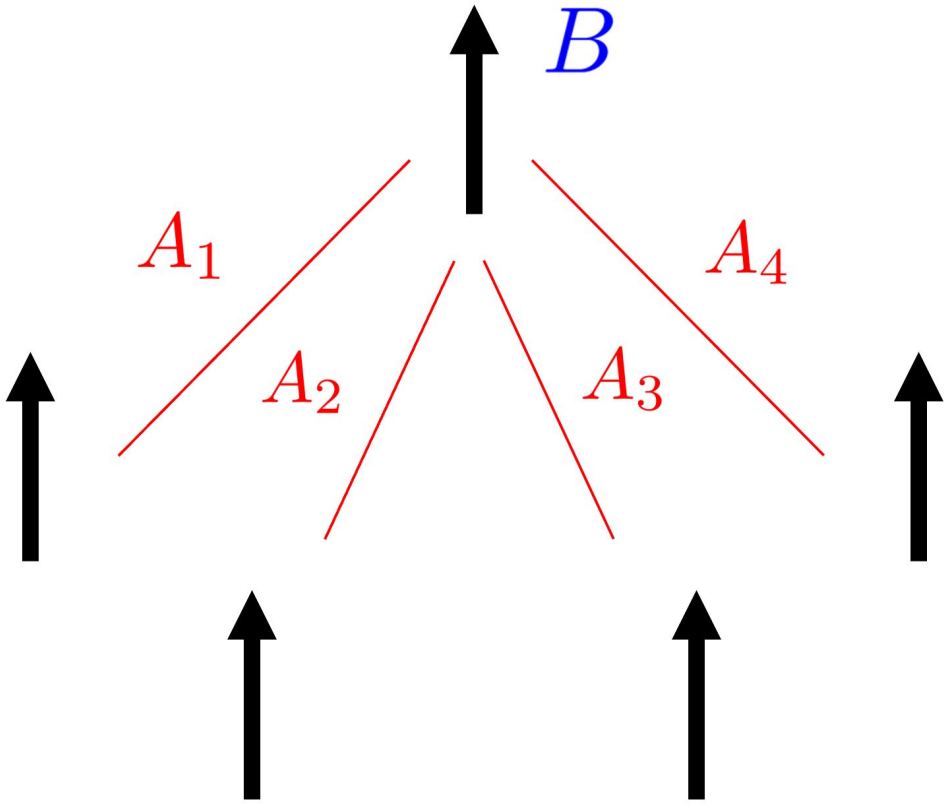
MANY-BODY PHYSICS

Solving the quantum many-body problem with artificial neural networks

Giuseppe Carleo[1]* and Matthias Troyer[1,2]

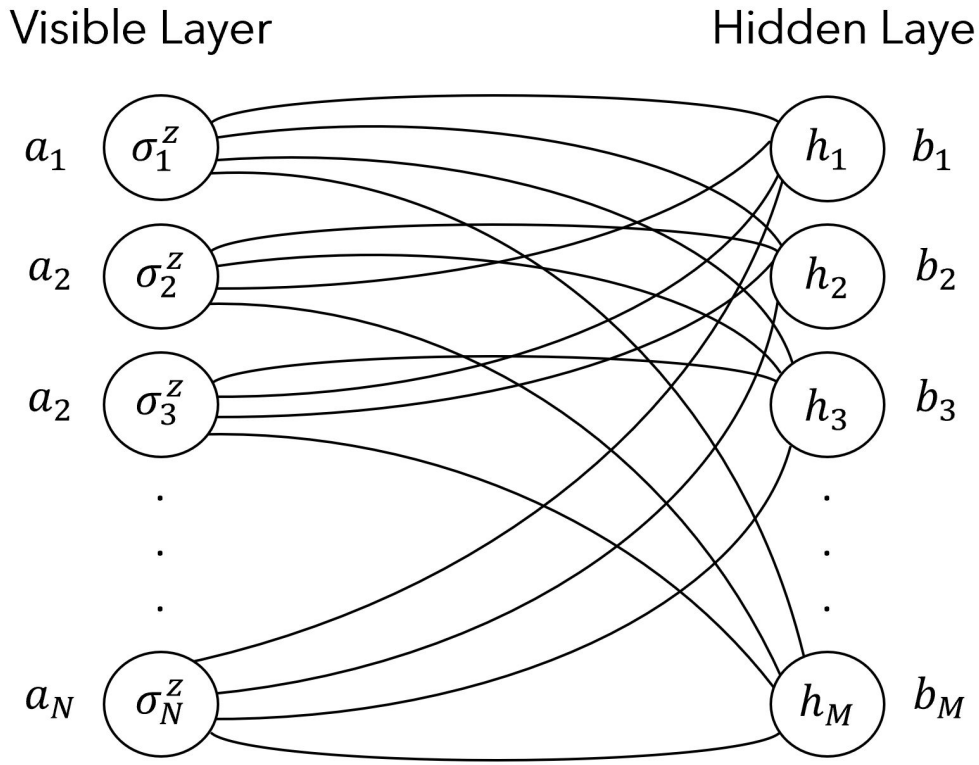
(Carleo and Troyer, Science 355, 602 (2017))

Central Spin Model



$$H = BS_0^z + \sum_{k=1}^{N-1} A_k \mathbf{S}_0 \cdot \mathbf{S}_k$$

Restricted Boltzmann Machine



Model Parameters:

a_j	(N elements)
b_i	(M elements)
W_{ij}	(N×M elements)

$$\Psi(S;\mathbf{a},\mathbf{b},\mathbf{W}) = \sum_{\{h_i\}} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} W_{ij} h_i \sigma_j^z}$$

Ground State Determination

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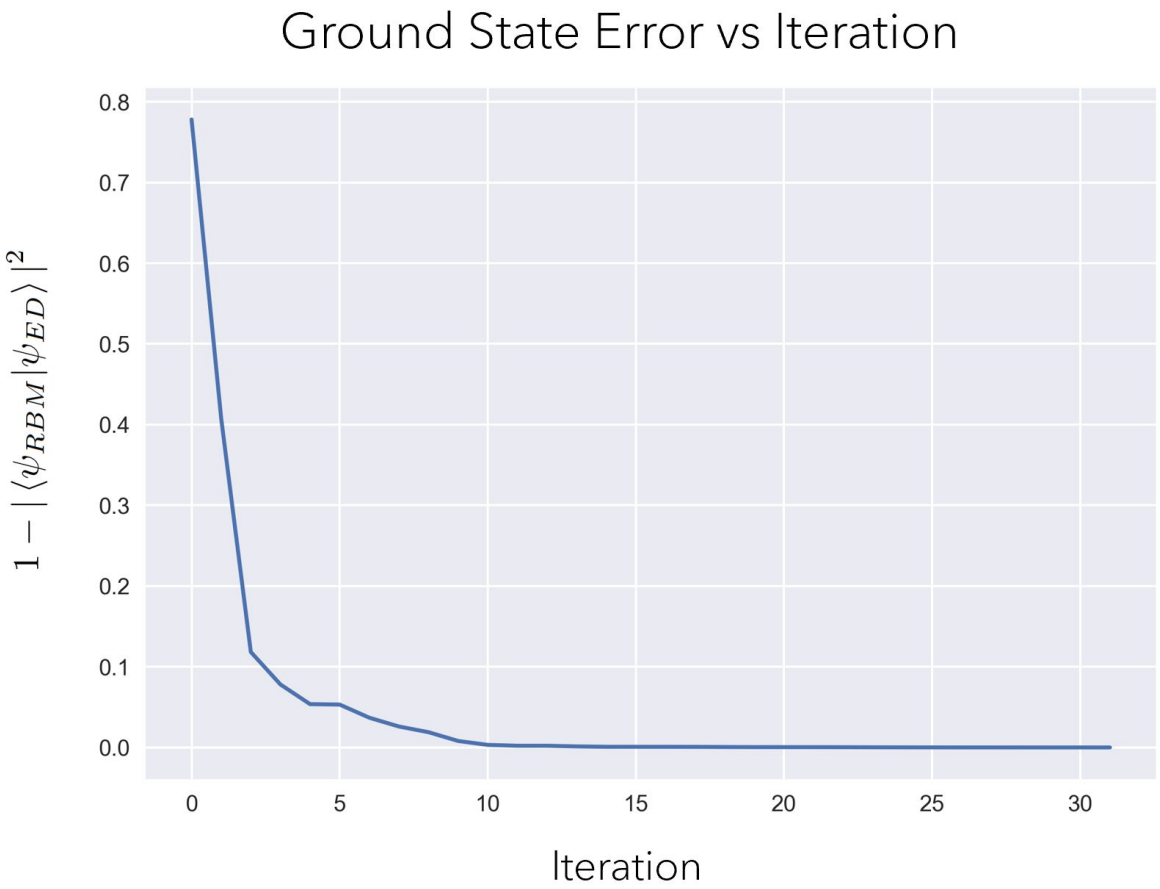
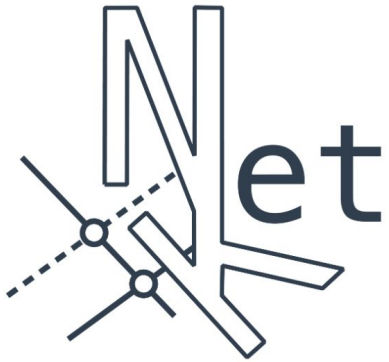


$$E(\mathbf{a}, \mathbf{b}, \mathbf{W}) = \frac{\langle \psi_{RBM} | H | \psi_{RBM} \rangle}{\langle \psi_{RBM} | \psi_{RBM} \rangle}$$

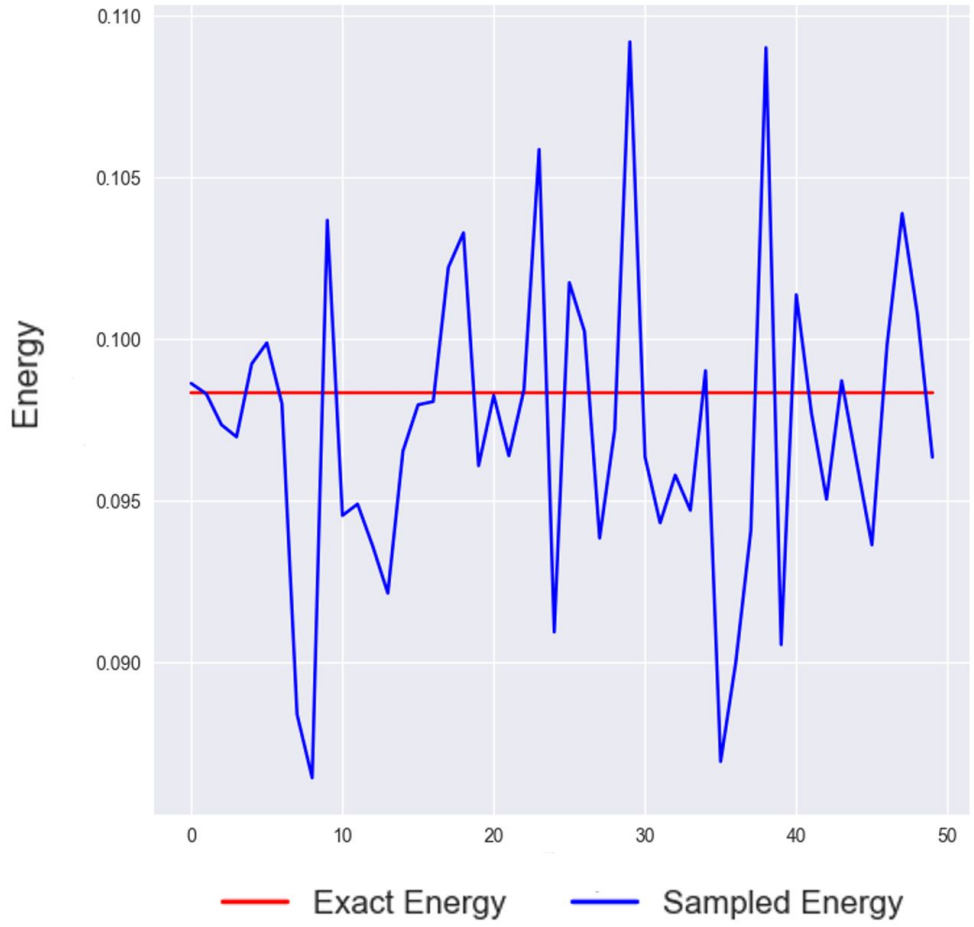
Monte Carlo Sampling

$$\langle \psi_{\mathrm{RBM}} | \, H \, | \psi_{\mathrm{RBM}} \rangle \approx \langle \psi_{\mathrm{RBM}} | \, H \, | \psi_{\mathrm{RBM}} \rangle_{\tilde{\sigma}}$$

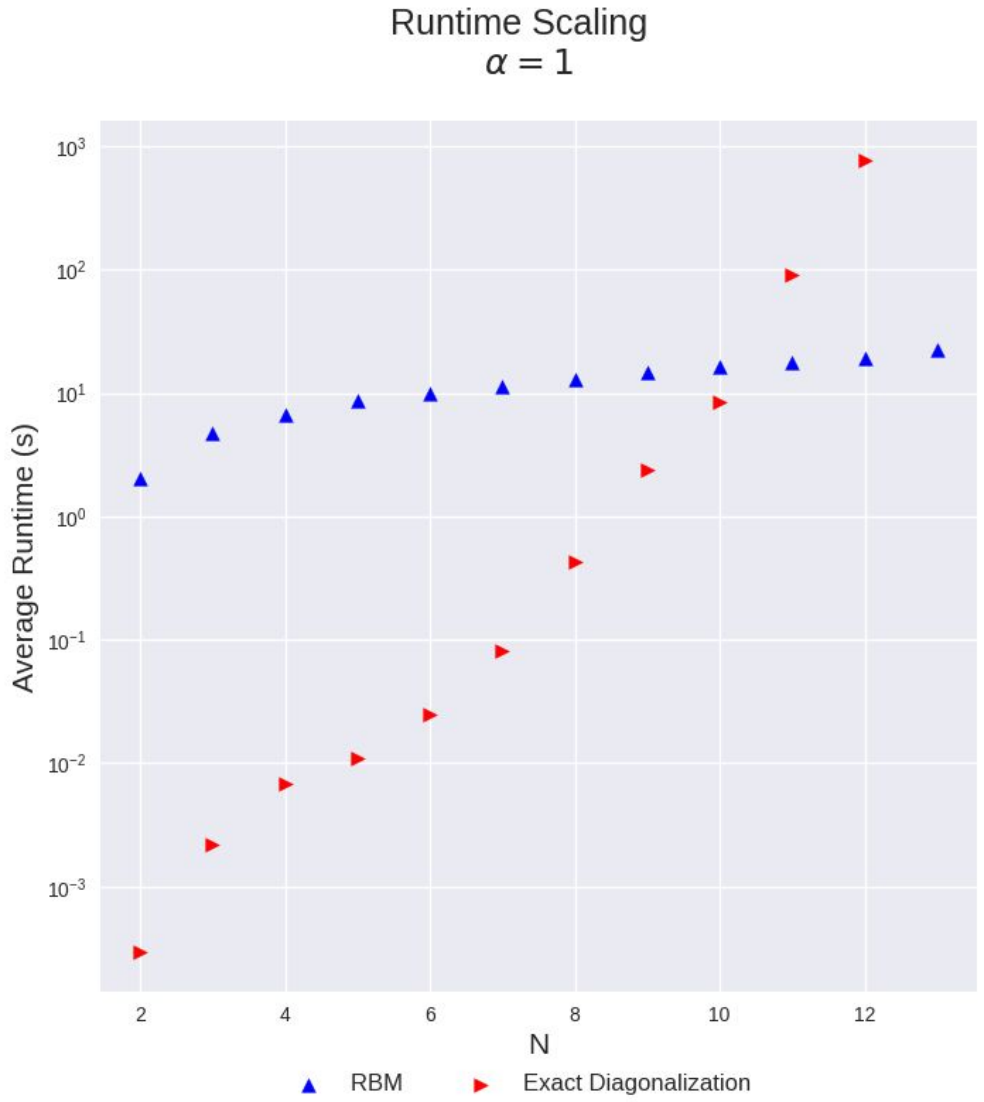


(Carleo, Giuseppe et al. SoftwareX10, 100311 (2019))

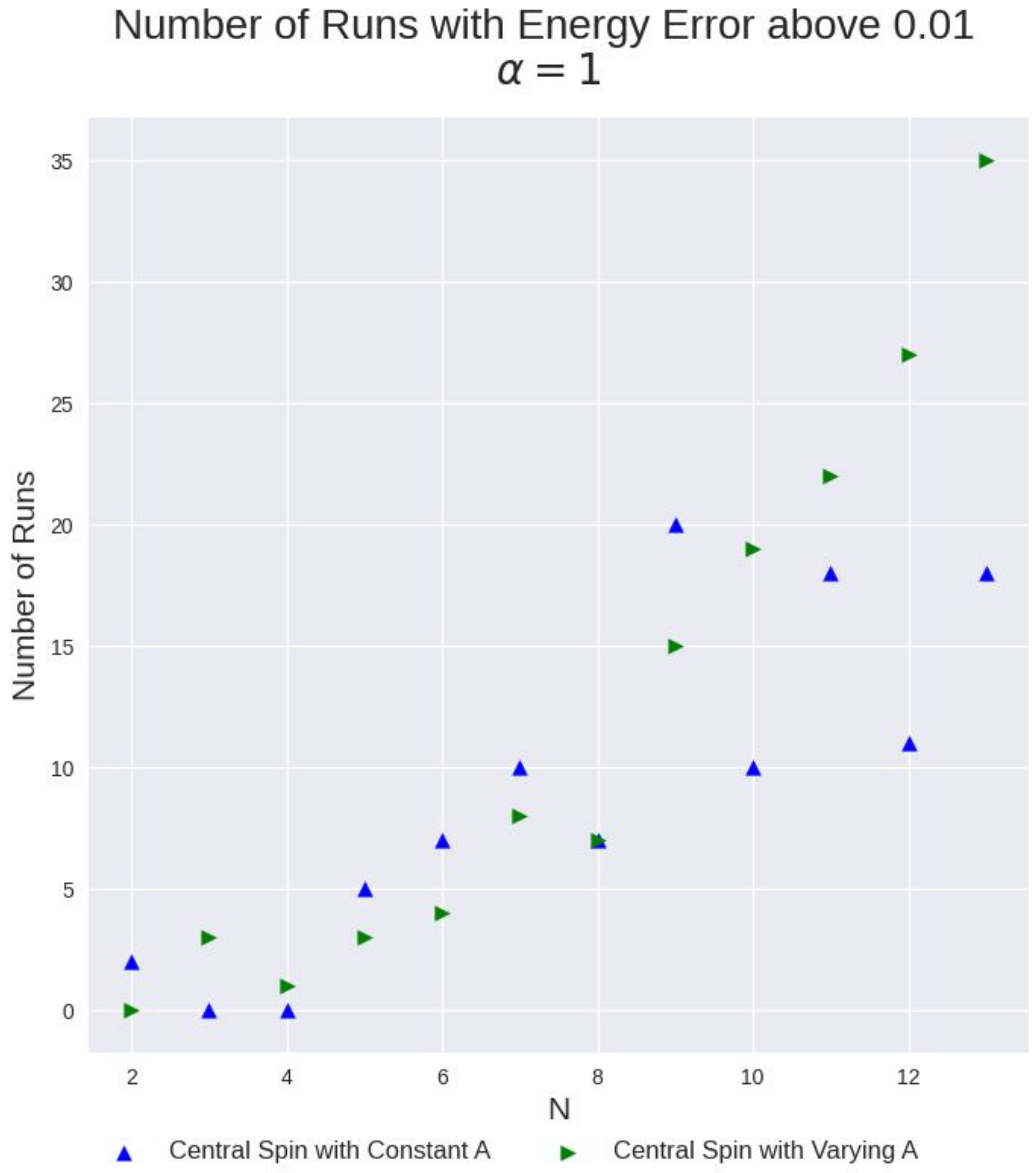
Metropolis Hastings Energy Sampling



Runtime Scaling Comparison



Hamiltonian Comparison



$$H = BS_0^z + \sum_{k=1}^{N-1} A_k \mathbf{S}_0 \cdot \mathbf{S}_k$$

- Constant coupling

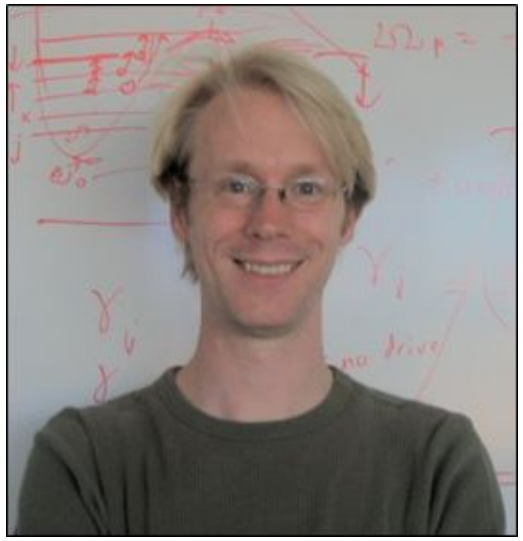
$$A_k = 1 \ \forall k, \ B = 1$$

- Varying coupling

$$A_k = \frac{A}{N_0} e^{\frac{-k}{N_0}}$$

$$A = \frac{N}{2}, \ B = \frac{N}{2}, \ N_0 = \frac{N}{2}$$

Acknowledgments



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References

1. G. Carleo and M. Troyer, Solving the quantum many-body problem with artificial neural networks, Science **355**, 602 (2017)
2. G. Carleo, K. Choo, D. Hofmann, J. E. Smith, T. Westerhout, F. Alet, E. J. Davis, S. Efthymiou,I. Glasser, S.-H. Lin, M. Mauri, G. Mazzola, C. B. Mendl, E. van Nieuwenburg, O. O'Reilly, H. Theveniaut,G. Torlai, F. Vicentini, and A. Wietek, Netket: A machine learning toolkit for many-body quantum systems, SoftwareX10, 100311 (2019).