Tackling Quantum Many-Body systems with Artificial Neural Networks

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Introduction

Systems involving a large no. of interacting particles whose detailed behaviour and properties can be studied using quantum mechanics. E.g- superconductors, nano-materials, nuclei

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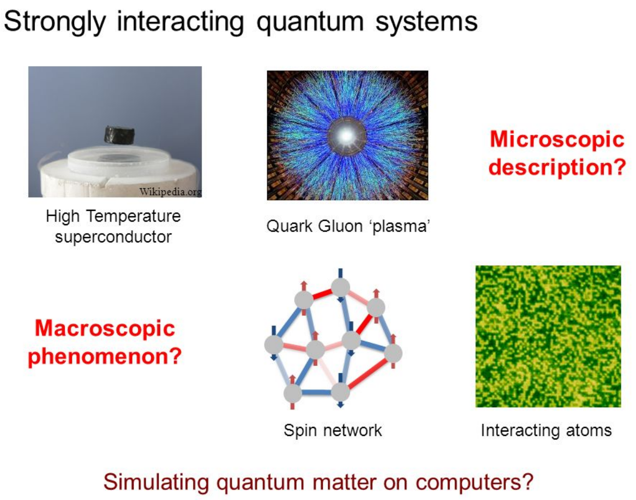
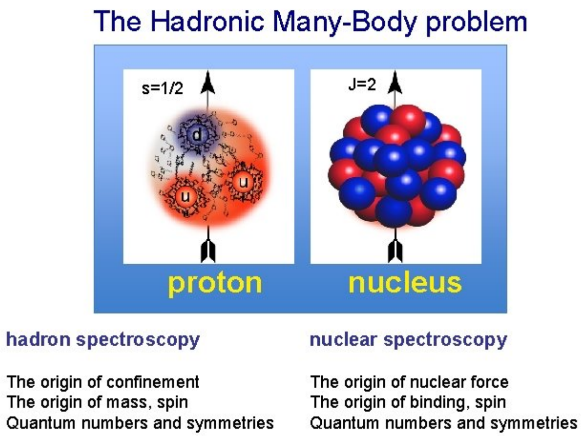




Schrödinger eqn. $H|\psi\rangle = E|\psi\rangle$

$$|\psi\rangle = c_{\uparrow\uparrow\uparrow\uparrow.....}|\uparrow\uparrow\uparrow\uparrow\ .....\rangle + c_{\downarrow\uparrow\uparrow\uparrow.....}|\downarrow\uparrow\uparrow\uparrow\ .....\rangle + ... + c_{\downarrow\downarrow\downarrow\downarrow.....}|\downarrow\downarrow\downarrow\downarrow\ .....\rangle$$

Hilbert space increases exponentially with increase in no. of particles

Artificial Neural Networks (ANN)

Simplification of a Biological Neural Network (BNN)

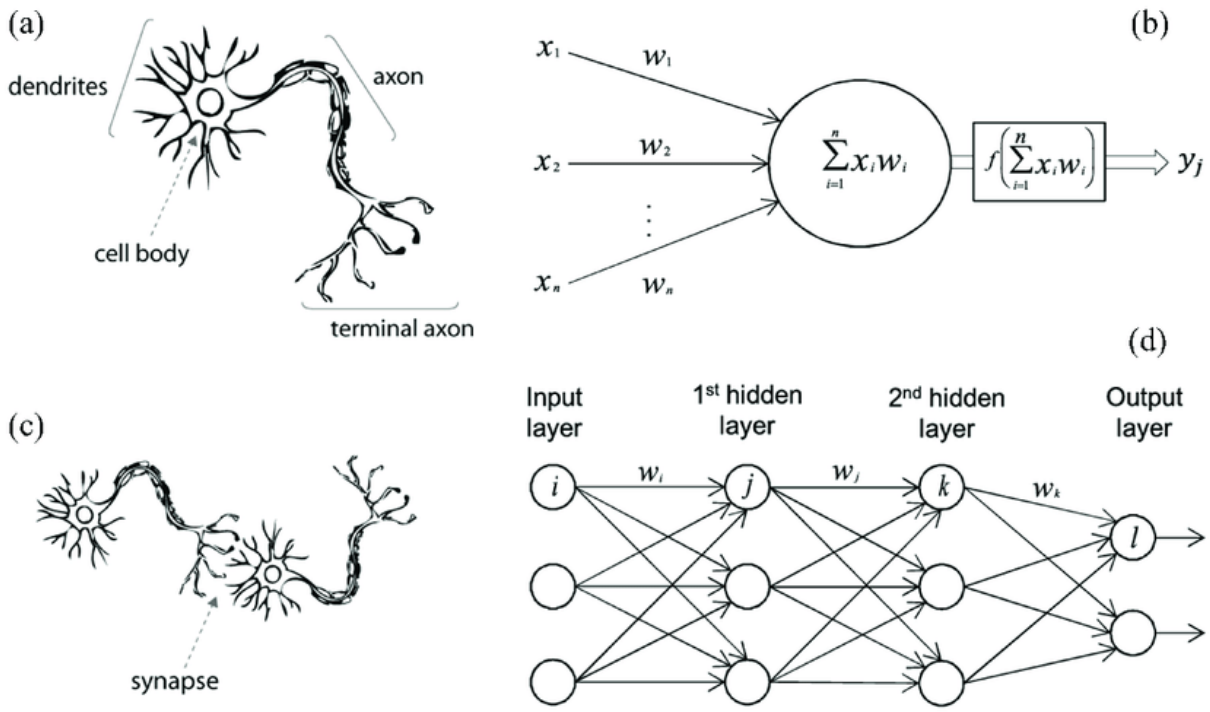


Figure: Image credit:'Using a Data Driven Approach to Predict Waves Generated by Gravity Driven Mass Flows'

Dendrites, Synapses, Cell body and Axon terminals are mimicked by the Input layer, Weights, Activation functions, and the Output layer respectively

Used for pattern recognition and classification in Machine Learning

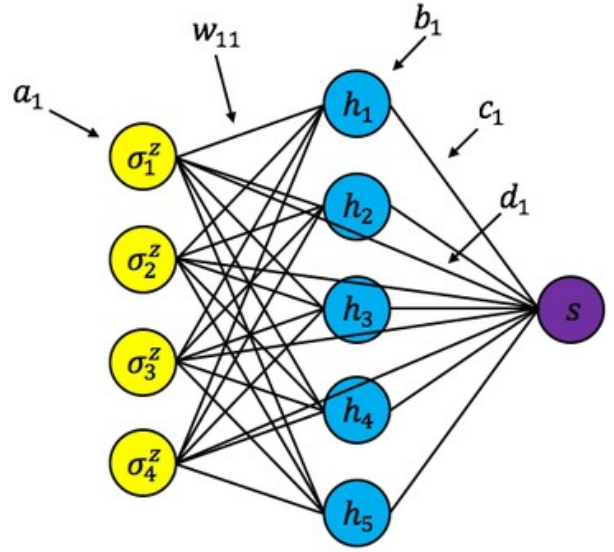
Neural Network Quantum States (NQS)

We use a type of ANN called Restricted Boltzmann Machine (RBM)[1]

Figure- Restricted Boltzmann Machine

- N body spin configuration
  $\mathcal{S} = \left(\sigma_1^z, \sigma_2^z, \ldots\ldots \sigma_N^z\right)$
- $\Psi_M(\mathcal{S};\mathcal{W}) = \sum_{\{h_i\}} e^{\sum_j a_j \sigma_j^z + \sum_i b_i h_i + \sum_{ij} w_{ij} h_i \sigma_j^z}$
  where $h_i = \{-1, 1\}$
  a_i and $b_i \longrightarrow$ visible and hidden biases
  $w_{ij} \longrightarrow$ weights

Figure: RBM with input nodes σ_i^z, hidden layer nodes h_i, and output node s

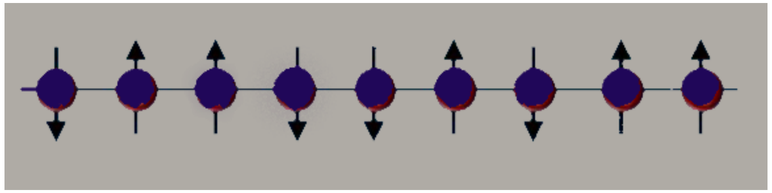


[1] Carleo and Troyer, Science **355**, 602 (2017)

1D Quantum Ising Model

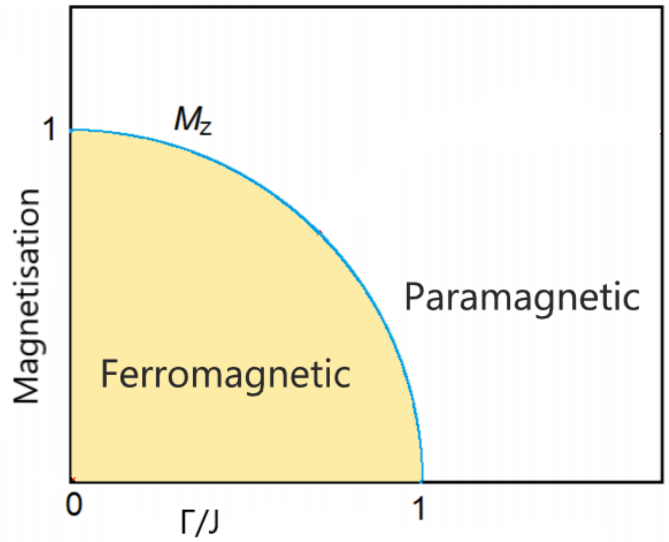
system of interacting spins-$\frac{1}{2}$ in a chain

transverse magnetic field applied in x-direction



(a) 1D spin chain

$$\boxed{\hat{H} = -J\sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - \Gamma \sum_i \hat{\sigma}_i^x}$$



(b) Phase Diagram for a 1D Transverse Field Ising model

$J > 0 \rightarrow$ Ferromagnetic interactions

$|\frac{\Gamma}{J}| = 1 \rightarrow$ Quantum phase transition

Method and Software: NetKet

open source framework developed by Carleo *et al.*[2] for solving quantum many-body systems using Machine Learning techniques

finds ground state properties of a discrete lattice model using an inbuilt Hamiltonian and a custom-built Hamiltonian on any non-trivial lattice graph

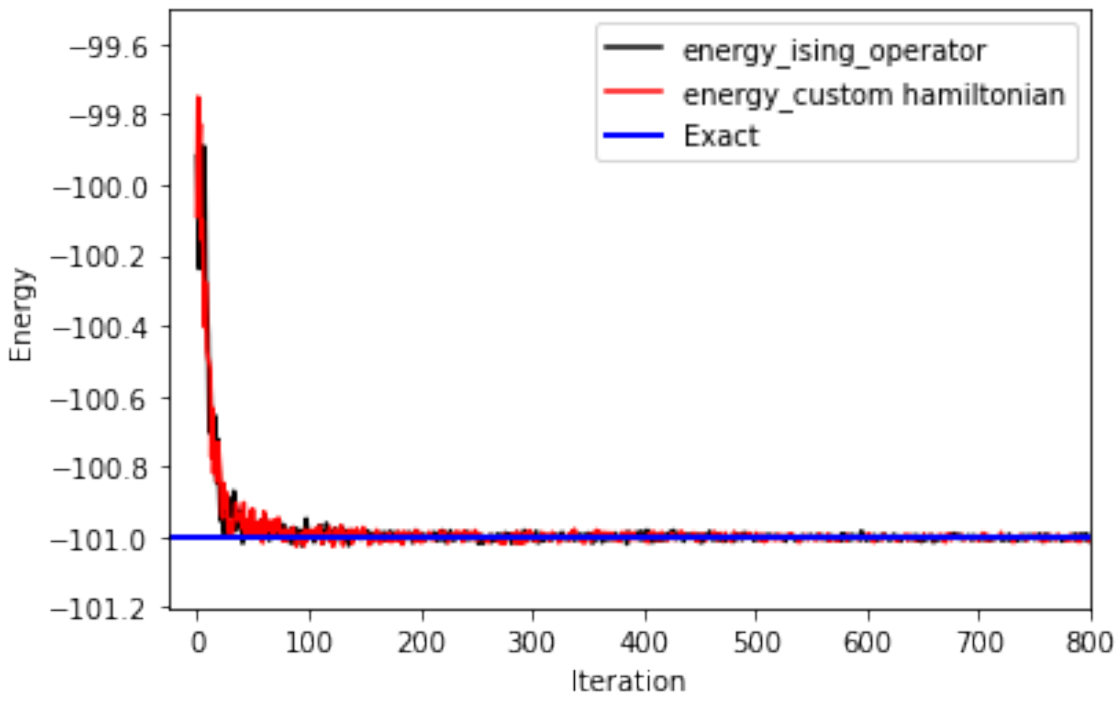


Figure: Convergence of the ground state energy to the exact value for $|\frac{\Gamma}{J}| > 1$

[2]Elsevier: doi.org/10.1016/j.softx.2019.100311

Results for the Ground state problem

$$E(N) = \frac{\langle \psi_M | \hat{H} | \psi_M \rangle}{\langle \psi_M | \psi_M \rangle} >= E_0, \; E_0 \rightarrow \text{exact ground state energy}$$

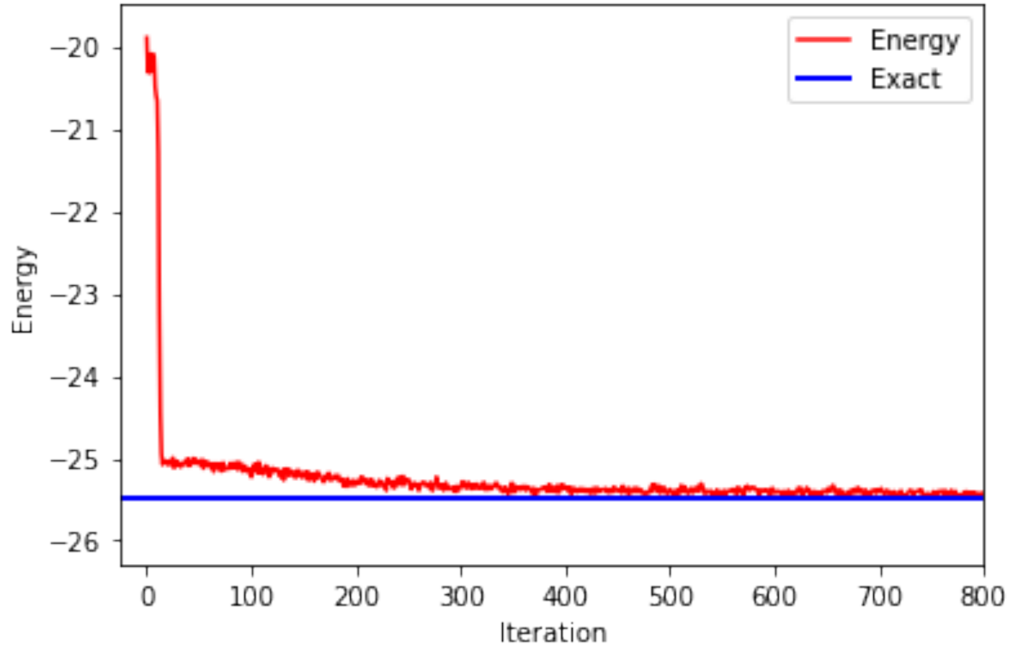


Figure: Convergence of the Ground state energy for Γ=1, J=1 using RBM, to the result obtained using Exact Diagonalization for N=20 lattice sites

minimization of ground state energy using variational sampling

Exact Diagonalization (ED) is limited to small system sizes due to Hilbert space growing exponentially with system size

Error Analysis

$$\boxed{\epsilon_{rel} = \frac{E_{RBM}(\alpha) - E_{exact}}{|E_{exact}|}} \quad \alpha = M/N$$

M$\rightarrow$No. of hidden nodes of RBM

N$\rightarrow$No. of visible nodes

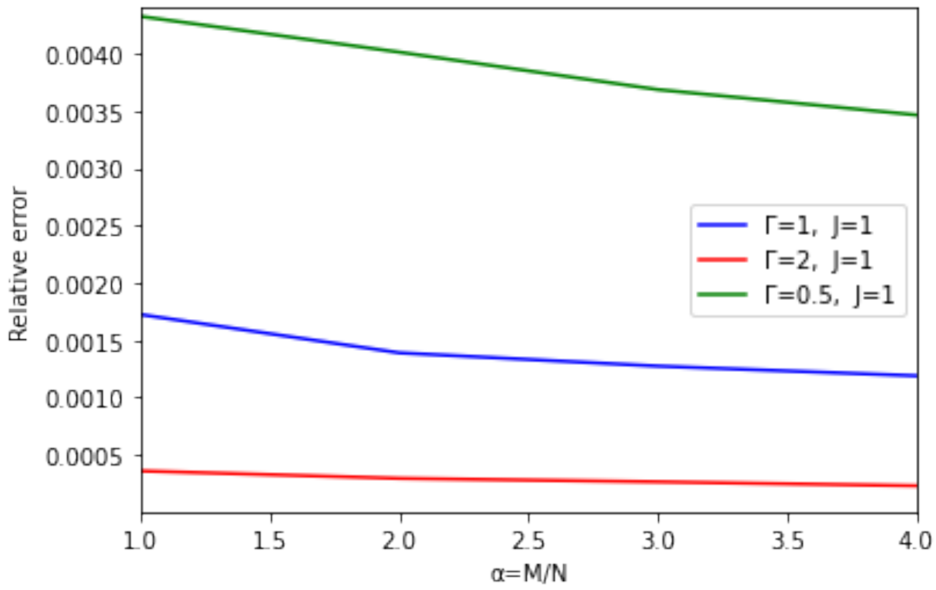


Figure: Relative error in the ground state energy of the 1D TFI model using a RBM as compared to that calculated using Exact Diagonalization for different values of Γ/J ratio

Supervised Learning

Exact Target wavefunction is given: $|\psi_{target}\rangle$
Variational Neural Network quantum state is chosen: $|\psi_{NQS}\rangle$

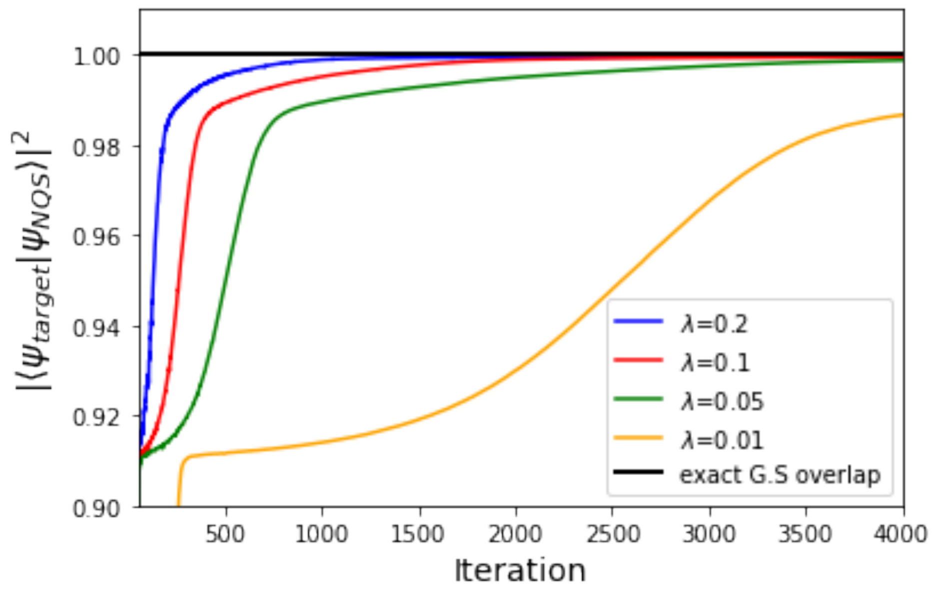


Figure: Overlap between the target and the variational wavefunction for 4000 iterations for different learning rates.

$$\mathcal{L}(\alpha) = -\log \frac{\langle\Psi_{\text{target}}|\Psi_{\text{NQS}}(\alpha)\rangle}{\langle\Psi_{\text{target}}|\Psi_{\text{target}}\rangle} \frac{\langle\Psi_{\text{NQS}}(\alpha)|\Psi_{\text{target}}\rangle}{\langle\Psi_{\text{NQS}}(\alpha)|\Psi_{\text{NQS}}(\alpha)\rangle}, \; \alpha \to \alpha - \lambda\nabla_\alpha \mathcal{L}$$

where $\nabla_\alpha \mathcal{L} \to$ gradient of loss function, $\lambda \to$ learning rate

Optimized ground state can be used to predict excited states [3]

[3] H.Kawai Y.O. Nakagawa Mach. Learn.: Sci. Technol. 1 (2020)

Magnetization

Transverse Magnetization $= \frac{1}{N} \sum_j \left\langle \psi_0 \middle| \sigma_j^x \middle| \psi_0 \right\rangle$,

$|\psi_0\rangle \longrightarrow$ ground state wavefunction.

Analytical soln. worked out by Pfeuty: $M_x = \frac{1}{\pi} \int_0^\pi \frac{1 + \frac{J}{\Gamma} \cos(q)}{\sqrt{1 + \frac{J^2}{\Gamma^2} + \frac{2J}{\Gamma} \cos(q)}} \, \mathrm{d}q$

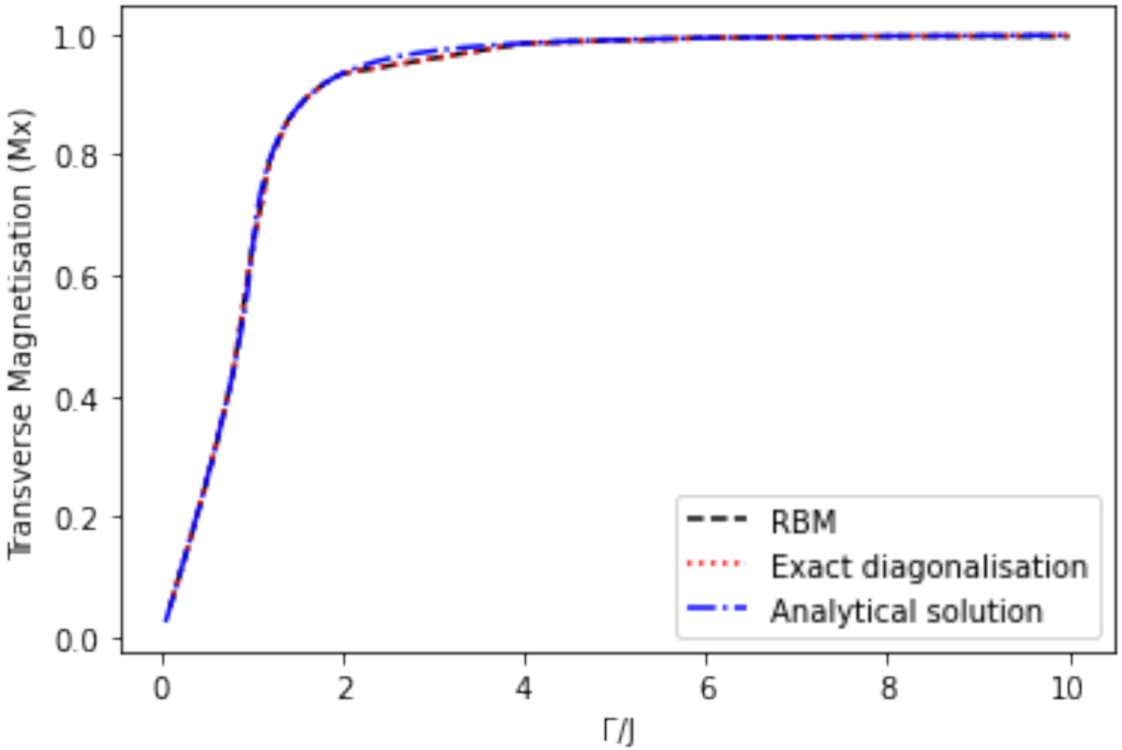


Figure: Transverse magnetization vs $\frac{\Gamma}{J}$ ratio using RBM, Exact Diagonalisation and the analytical solution

Magnetization

Longitudinal Magnetization $= \frac{1}{N} \sum_j \left\langle \psi_0 \middle| \sigma_j^z \middle| \psi_0 \right\rangle$

Analytical soln. : $M_z = \begin{cases} \left(1 - \frac{\Gamma^2}{J^2}\right)^{\frac{1}{8}} & , \quad J \geq \Gamma \\ 0 & , \quad J < \Gamma \end{cases}$

However, the Hamiltonian is slightly modified

$$\boxed{\hat{H} = -J \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - \Gamma \sum_i \hat{\sigma}_i^x - \Gamma_1 \sum_i \hat{\sigma}_i^z}$$

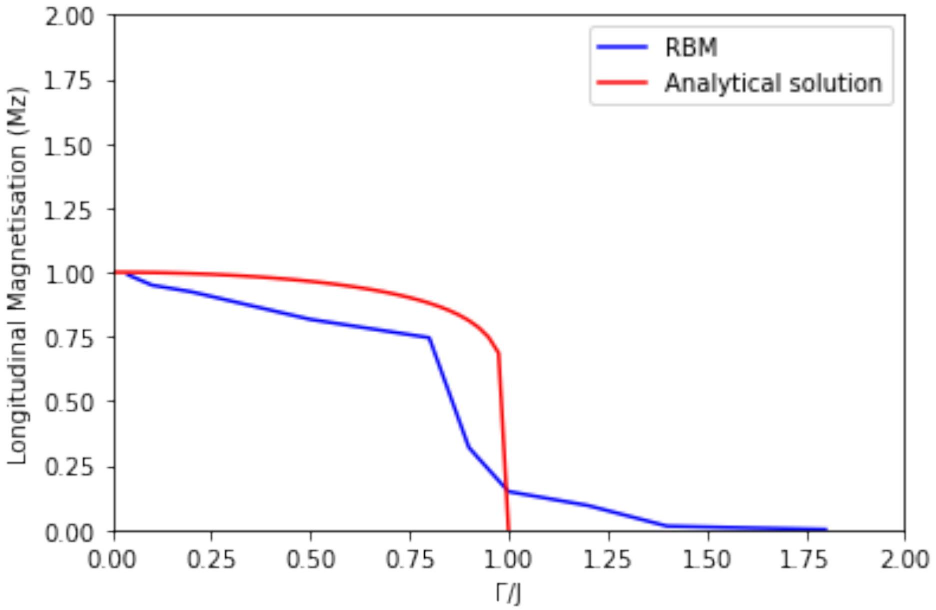


Figure: Longitudinal magnetization vs $\frac{\Gamma}{J}$ ratio using RBM and the analytical solution

Spin-Spin Correlation functions

- is a measure of the probability to what extent the spin at site i is aligned with the spin at site j
- Longitudinal correlation function: $\langle \sigma_i^z \sigma_j^z \rangle$
- Transverse correlation function: $\langle \sigma_i^x \sigma_j^x \rangle$
- obtain an exponential decay with increasing n

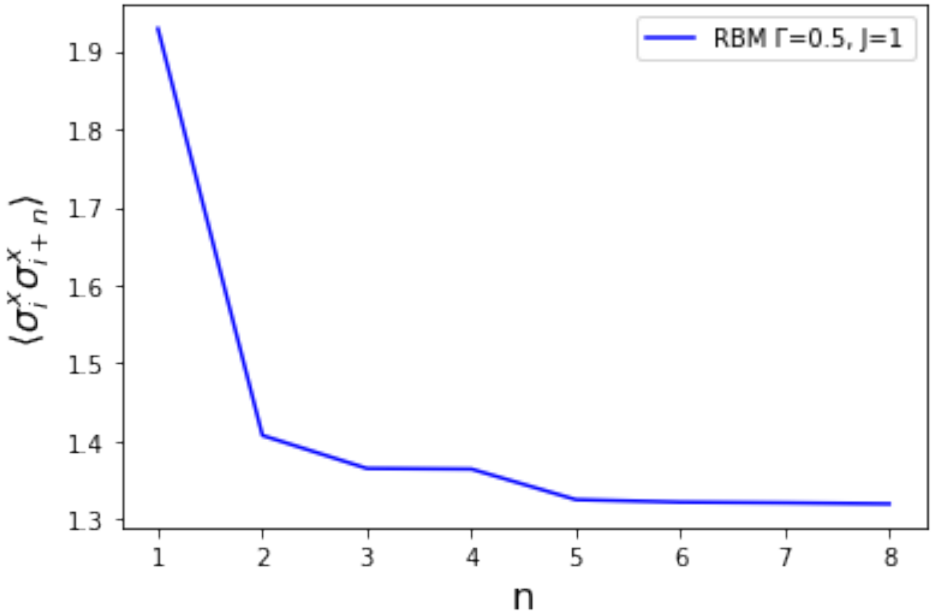


Figure: x-x correlation function with different neighbour interactions

Result comparison

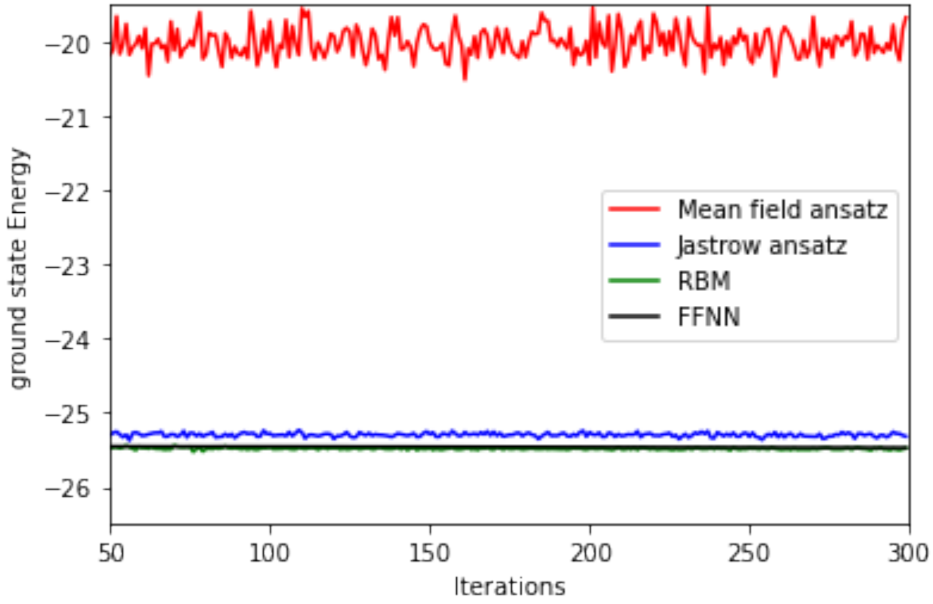


Figure: Caption

Mean field ansatz:

$$\langle \sigma_1^z, \ldots, \sigma_N^z | \Psi_{mf} \rangle = \prod_{i=1}^{N} \Phi(\sigma_i^z)$$

Jastrow ansatz:

$$\langle \sigma_1^z, \ldots, \sigma_N^z | \Psi_{jas} \rangle = exp(\sum_i J_1 \sigma_i^z \sigma_{i+1}^z + J_2 \sigma_i^z \sigma_{i+2}^z)$$

Conclusion - The 'Ising' on the cake

Advantages:

- compact representation of quantum many body states on ANN
- applies even to highly entangled states
- extends to high dimensional systems

Current Research and future possibilities:

- apply more advanced neural networks
- look at dynamic observables, frustrated(J1-J2), dissipative, and time-dependent models
- quantum enhanced machine learning

Thank You