Machine Learning applied to the analysis of quantum phases in a quantum simulation of the Agassi model

ECT* workshop Many-body quantum physics with machine learning

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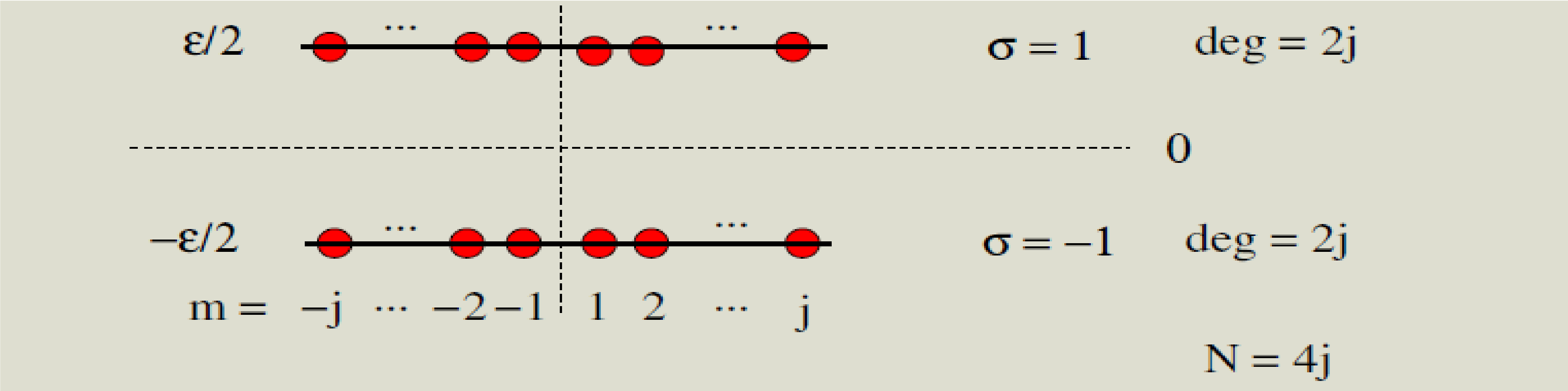
The extended Agassi Model. Why?

- It is a solvable many-body model that allows to mimic the main characteristics of the pairing-plus-quadrupole model.
- It can be exactly solved even in the case of large systems.
- It is used to benchmark many-body approximations because of its great flexibility and simplicity to be solved for large systems.
- The model owns a very rich phase diagram and even presents shape coexistence.
- The model is, somehow, an extension of the two-level Lipkin-Meshkov-Glick model that incorporates pairing interaction.
- It is a model slightly more complex than the used ones in Quantum Information Science (e.g. Lipkin, Dicke, Tavis-Cumming or Hubbard models) and, therefore, of great interest.



The extended Agassi Model

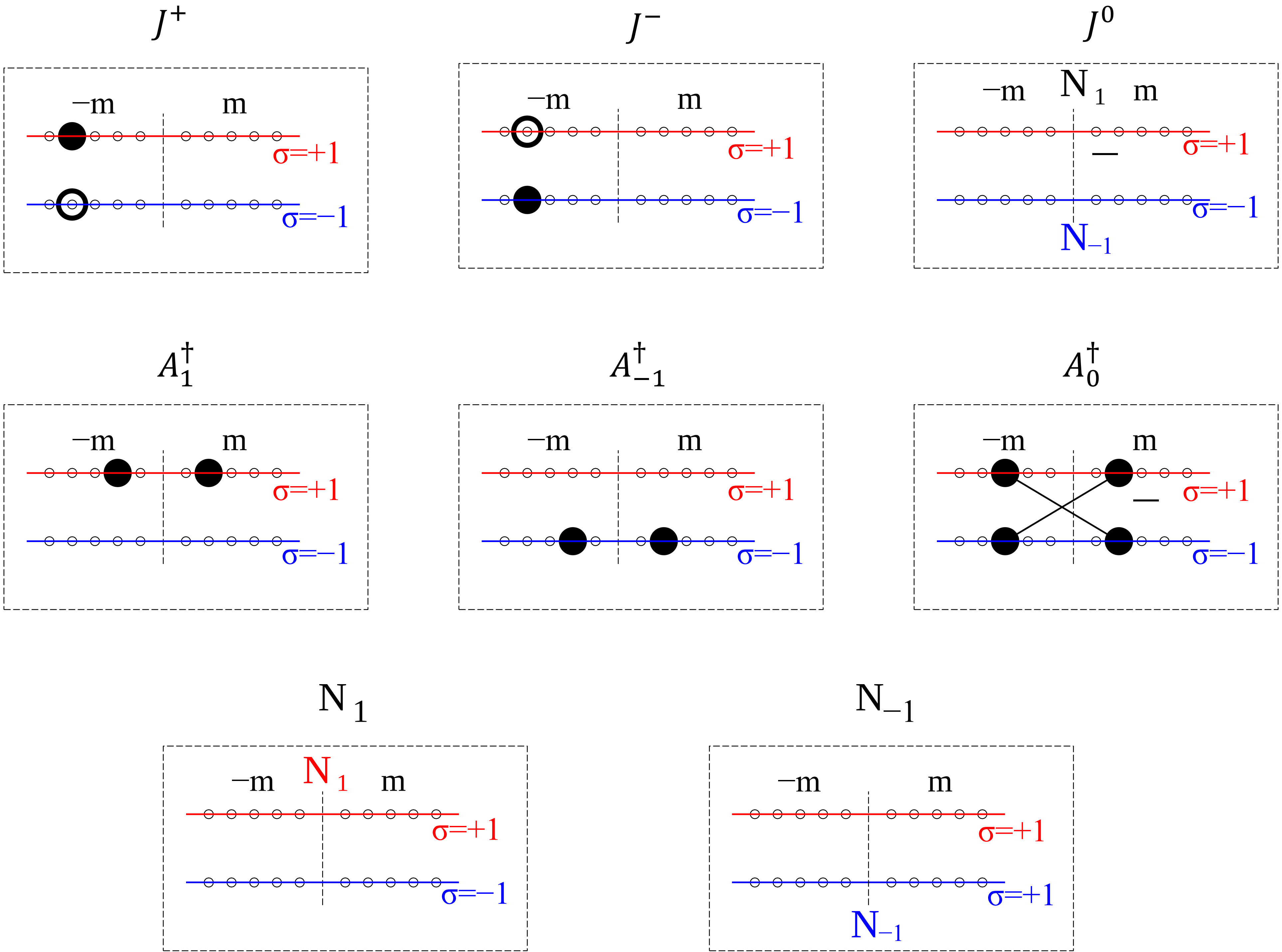
$$H = \varepsilon J^0 - g \sum_{\sigma,\sigma'} A_\sigma^\dagger A_{\sigma'} - \frac{V}{2}[(J^+)^2 + (J^-)^2] - 2h A_0^\dagger A_0$$

$$J^+ = \sum_{m=-j}^{j} c_{1,m}^\dagger c_{-1,m} \qquad J^0 = \frac{1}{2}\sum_{m=-j}^{j} (c_{1,m}^\dagger c_{1,m} - c_{-1,m}^\dagger c_{-1,m})$$

$$A_1^\dagger = \sum_{m=1}^{j} c_{1,m}^\dagger c_{1,-m}^\dagger \qquad A_{-1}^\dagger = \sum_{m=1}^{j} c_{-1,m}^\dagger c_{-1,-m}^\dagger$$

Spectrum Generator Algebra $O(5)$

$$A_0^\dagger = \frac{1}{2}\sum_{m=1}^{j} (c_{-1,m}^\dagger c_{1,-m}^\dagger - c_{-1,-m}^\dagger c_{1,m}^\dagger) \qquad N_\sigma = \sum_{m=-j}^{j} c_{\sigma,m}^\dagger c_{\sigma,m} \qquad N = N_1 + N_{-1}$$



J+
−m
m
σ=+1
σ=−1
J−
−m
m
σ=+1
σ=−1
J0
−m
N1
m
σ=+1
σ=−1
N−1
A†1
−m
m
σ=+1
σ=−1
A†−1
−m
m
σ=+1
σ=−1
A†0
−m
m
σ=+1
σ=−1
N1
−m
N1
m
σ=+1
σ=−1
N−1
−m
m
σ=+1
σ=+1
N−1

Quantum Simulation of the model

The Jordan-Wigner Transformation

- It is a non-local transformation that maps the fermion creation/annihilation operators into spin operators
- It is usual to relabel the fermion index, i.e., $\sigma, m \rightarrow i$

$$\begin{cases} \boldsymbol{c}^{\dagger}_{\boldsymbol{\sigma},\boldsymbol{m}} \rightarrow \boldsymbol{c}^{\dagger}_{\boldsymbol{i}} = \boldsymbol{I}_{\mathbf{1}} \otimes \cdots \otimes \boldsymbol{I}_{\boldsymbol{i}-\mathbf{1}} \otimes \boldsymbol{\sigma}^{+}_{\boldsymbol{i}} \otimes \boldsymbol{\sigma}^{\boldsymbol{z}}_{\boldsymbol{i}+\mathbf{1}} \otimes \cdots \otimes \boldsymbol{\sigma}^{\boldsymbol{z}}_{\boldsymbol{N}} \\ \boldsymbol{c}_{\boldsymbol{\sigma},\boldsymbol{m}} \rightarrow \boldsymbol{c}_{\boldsymbol{i}} = \boldsymbol{I}_{\mathbf{1}} \otimes \cdots \otimes \boldsymbol{I}_{\boldsymbol{i}-\mathbf{1}} \otimes \boldsymbol{\sigma}^{-}_{\boldsymbol{i}} \otimes \boldsymbol{\sigma}^{\boldsymbol{z}}_{\boldsymbol{i}+\mathbf{1}} \otimes \cdots \otimes \boldsymbol{\sigma}^{\boldsymbol{z}}_{\boldsymbol{N}} \end{cases}$$

$$\sigma^{+} = \frac{\sigma^{x} + i\sigma^{y}}{2} \qquad \sigma^{-} = \frac{\sigma^{x} - i\sigma^{y}}{2}$$

Pauli Matrices

$$\sigma^{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma^{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Quantum Simulation of the model

J=2: the case of 8 sites

$c_{1,2} \rightarrow c_1$ $\quad c_{-1,2} \rightarrow c_5$

$c_{1,1} \rightarrow c_2$ $\quad c_{-1,1} \rightarrow c_6$

$c_{1,-1} \rightarrow c_3$ $\quad c_{-1,-1} \rightarrow c_7$

$c_{1,-2} \rightarrow c_4$ $\quad c_{-1,-2} \rightarrow c_8$

For example:

$$\boldsymbol{A_1 = \sigma_2^- \otimes \sigma_3^- + \sigma_1^- \otimes \sigma_2^z \otimes \sigma_3^z \otimes \sigma_4^-}$$

The Hamiltonian

$$\boldsymbol{H = H_1 + H_2 + H_3 + H_4 + H_5 + H_6}$$

$$\boldsymbol{[H_i, H_j] \neq 0 \qquad i \neq j = 1 \dots 6}$$

Quantum Simulation of the model

The evolution operator

$$U(t) = e^{-itH}$$

Digital quantum simulation

LIE-TROTTER-SUZUKI (TROTTER) EXPANSION

Trotter Steps

$$U(t, n_T) = \left(\prod_{k=1}^{6} e^{-itH_k/n_T} \right)^{n_T} + \mathcal{O}\left(\frac{t^2}{n_T} \right)$$

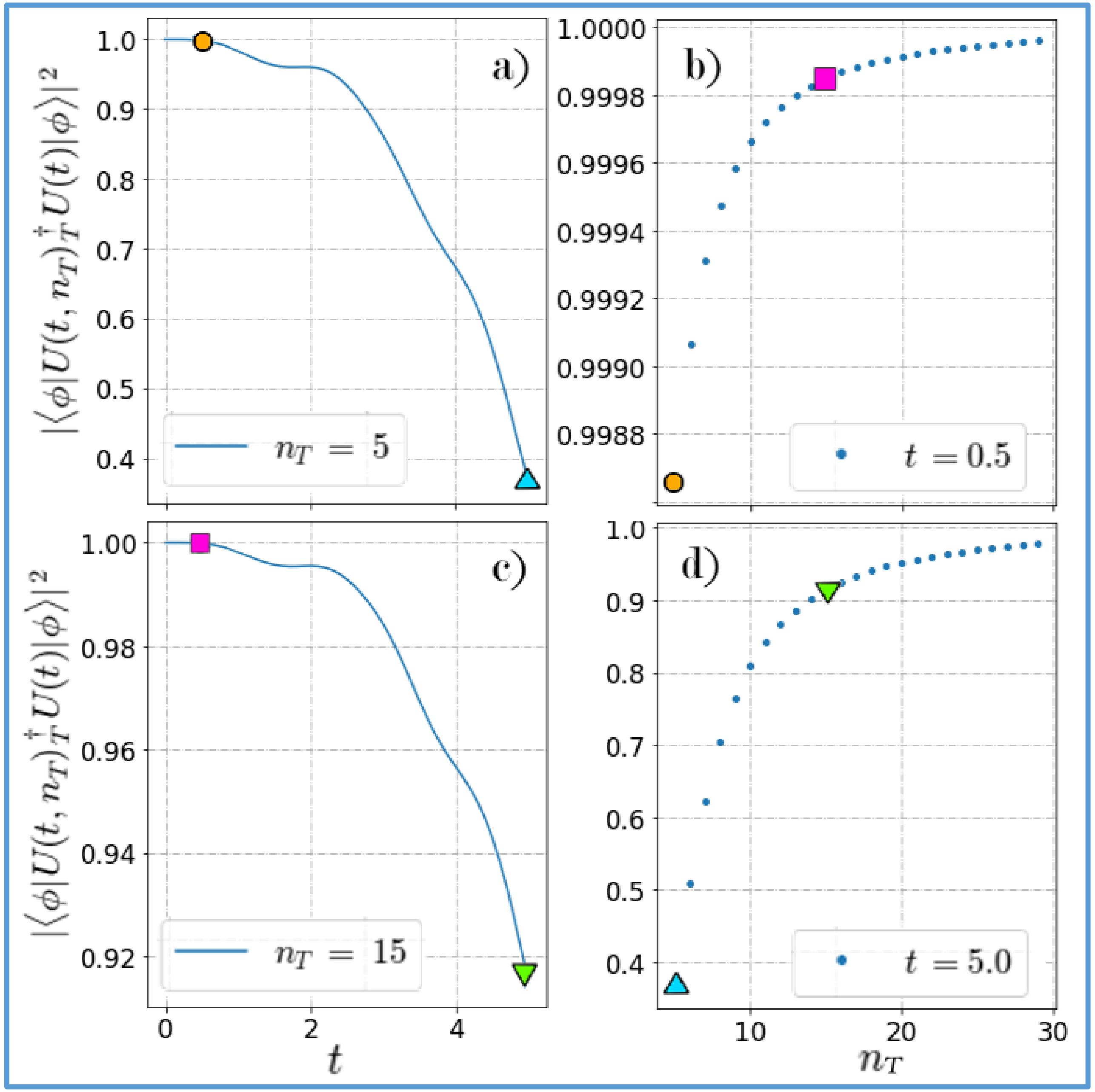
How good is the Trotter approach?

Check the Fidelity

$$F(t, n_T) = |\langle\phi|U(t, n_T)^{\dagger}U(t)|\phi\rangle|^2$$

Initial state: $|\phi\rangle = |\downarrow_1\downarrow_2\downarrow_3\downarrow_4\uparrow_5\uparrow_6\uparrow_7\uparrow_8\rangle$
(With mínimum value of $\langle J^0\rangle = -2$**)**

Parameters: $\varepsilon = 1, g = 0.25,$
$V = 0.25, h = 0.25$

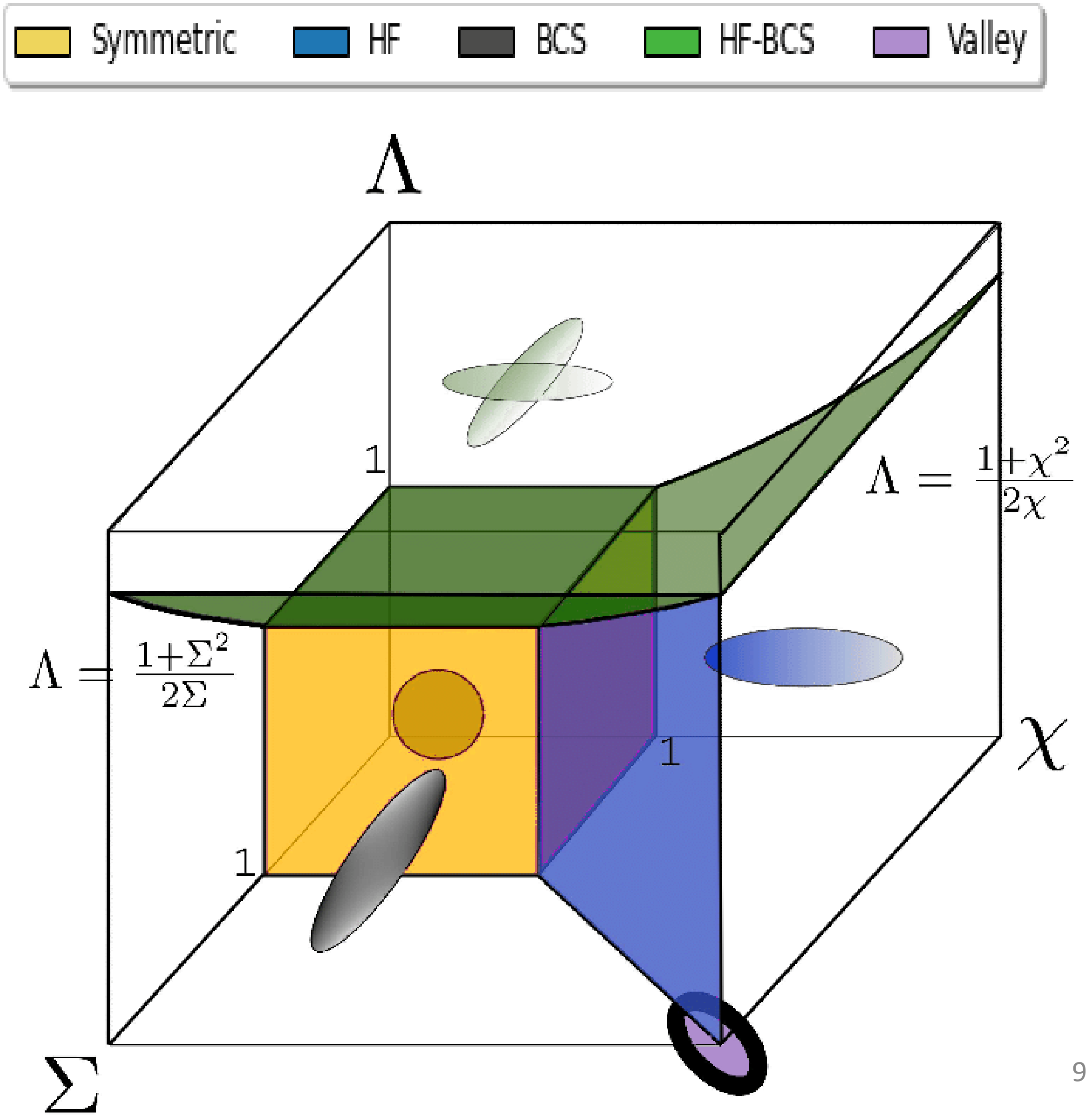


Exploring Quantum Phase Transitions (QPTs)

Quantum Phase Diagram

- Symmetric phase
- Hartree-Fock phase (HF)
- Bardeen-Cooper-Schrieffer phase (BCS)
- Combined HF-BCS phase
- Closed Valley solution

$g = \frac{\varepsilon\Sigma}{2j-1}$ $V = \frac{\varepsilon\chi}{2j-1}$ $h = \frac{\varepsilon\lambda}{2j-1}$



Exploring Quantum Phase Transitions (QPTs)

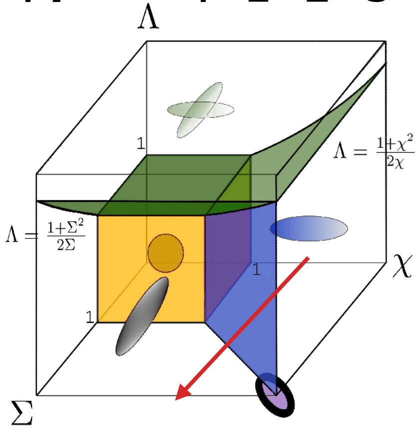
Correlation Functions

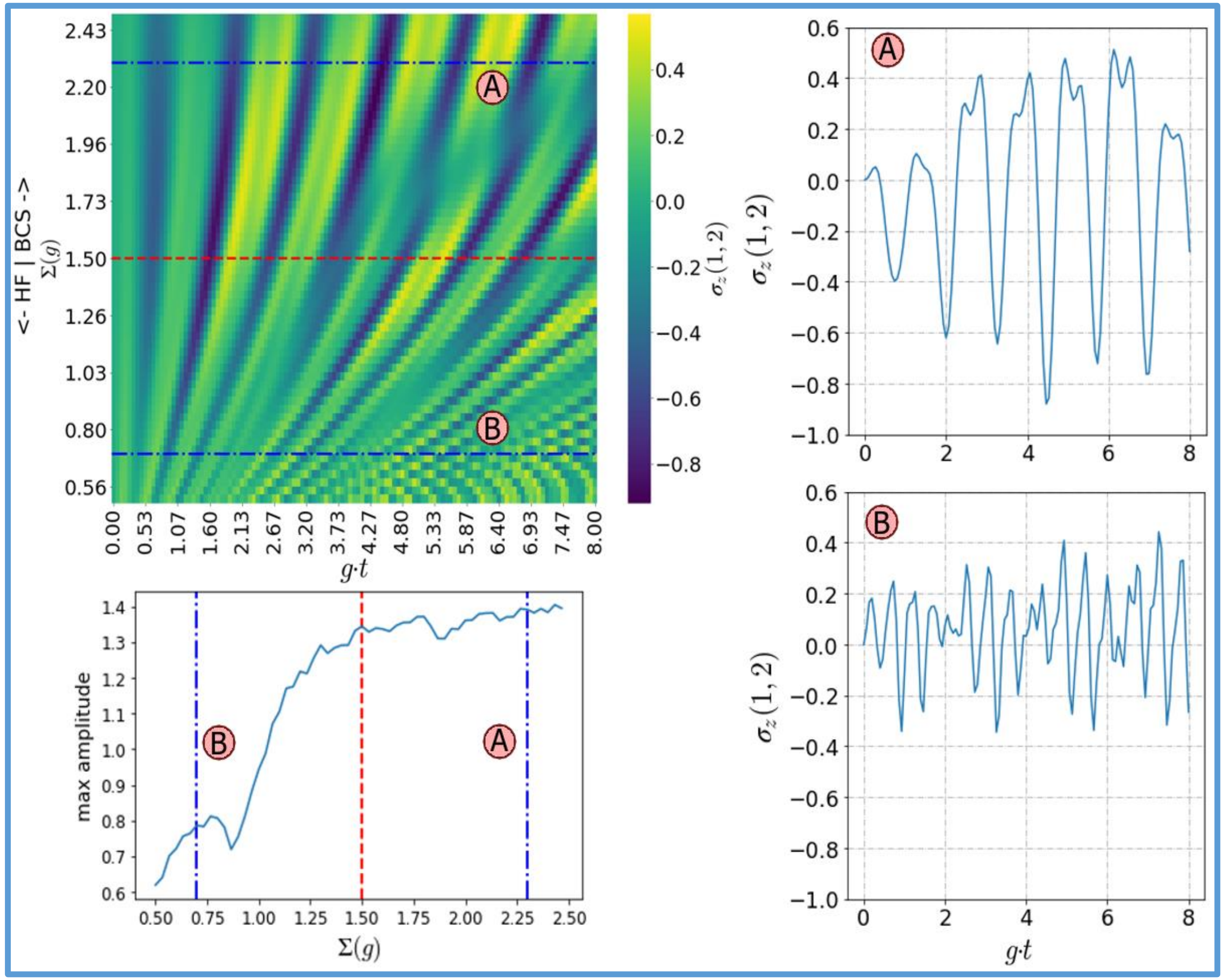
$$C_{\alpha,\beta}(i,j) = \left\langle \sigma_i^{\alpha} \otimes \sigma_j^{\beta} \right\rangle - \langle \sigma_i^{\alpha} \rangle \left\langle \sigma_j^{\beta} \right\rangle$$

Particular case

$$C_z(1,2) = \langle \sigma_1^z \otimes \sigma_2^z \rangle - \langle \sigma_1^z \rangle \langle \sigma_2^z \rangle$$

Initial state: $|\phi\rangle = |\downarrow_1 \downarrow_2 \downarrow_3 \downarrow_4 \uparrow_5 \uparrow_6 \uparrow_7 \uparrow_8\rangle$





From HF phase to BCS phase

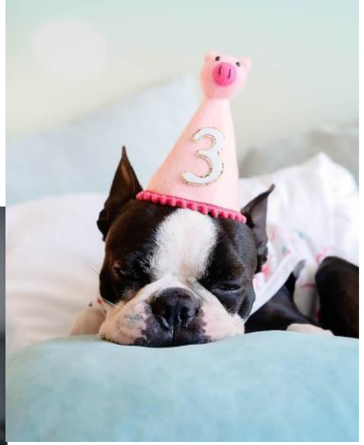
Machine Learning - How to train your AI

We know how a dog looks like, but,
how do we explain that to a computer?

WE DON'T

DOG

On its side, but
definitely a dog



Clearly a cute
dog with a
cute party hat

This is not a dog. This is a cat

Machine Learning - How to train your AI

A lot of different methods

- Regression
- Clustering
- Decision Trees
- Reinforced Learning
- Genetic Algorithms
- Multilayer Perceptro
- Neural Networks

Supervised VS Unsupervised

Exploration VS Exploitation

Accuracy VS Efficiency

Underfitting VS Overfitting

Training VS Testing

“No Free Lunch” theorem

Machine Learning - How to train your AI

AI in two steps - Step #1: Train

Data
(With labels)

→ scikit learn →

Model that fits
that data

AI in two steps - Step #2: Predict

Data
(Without labels)

→ scikit learn →

Predicted label
for that data

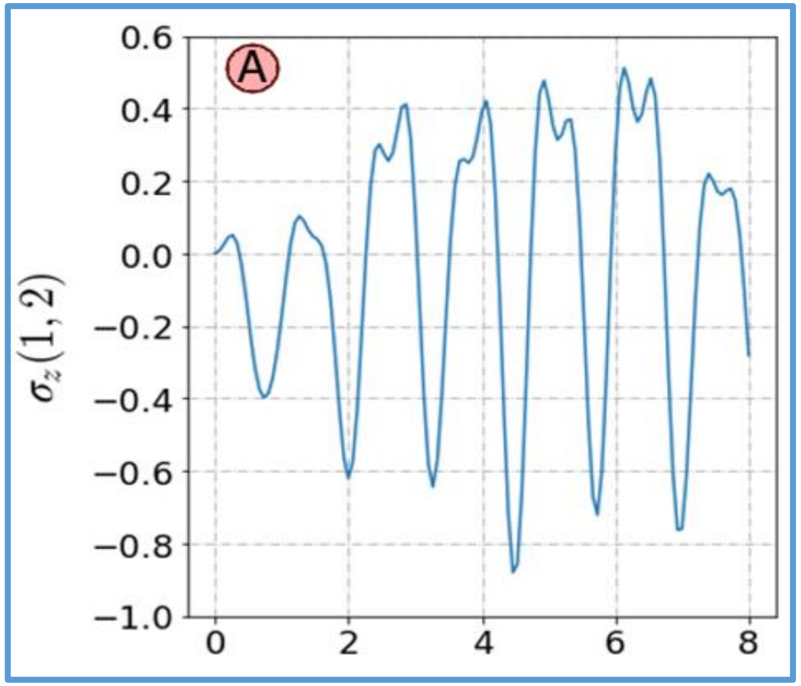
Deep Learning - Results

$$C_z(1,2) = \langle \sigma_1^z \otimes \sigma_2^z \rangle - \langle \sigma_1^z \rangle \langle \sigma_2^z \rangle$$

$$U(t) = e^{-itH} \approx \left(\prod_{k=1}^{6} e^{-itH_k/n_T} \right)^{n_T}$$

$$f(t) = \langle \phi(t) | \sigma_1^z \otimes \sigma_2^z | \phi(t) \rangle - \langle \phi(t) | \sigma_1^z | \phi(t) \rangle \langle \phi(t) | \sigma_2^z | \phi(t) \rangle$$

Input:



Input= $f(t)$ → CNN (scikit learn)

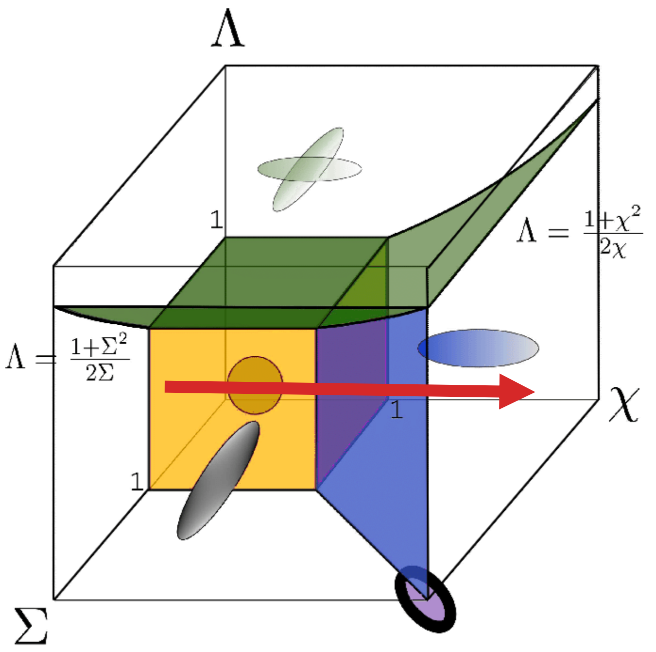
Output= $[P(y_1), P(y_2), P(y_3), P(y_4), P(y_5)]$

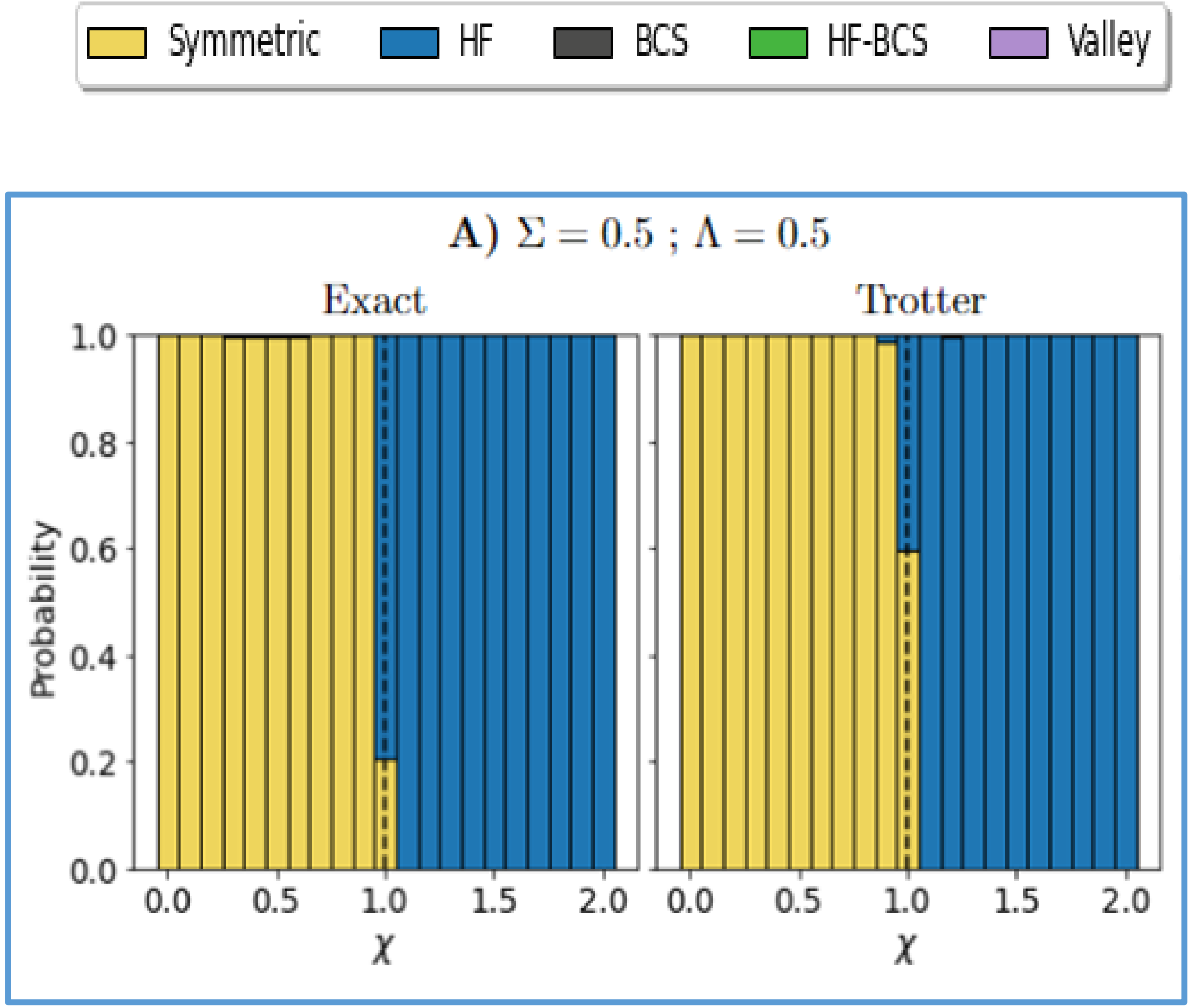
Output:

- **Symmetric= 0.00**
- **HF= 0.04**
- **BCS= 0.94**
- **Hf-BCS= 0.01**
- **Closed Valley= 0.01**

Convolutional Neural Network (CNN)- Results

98.35% Categorical Accuracy





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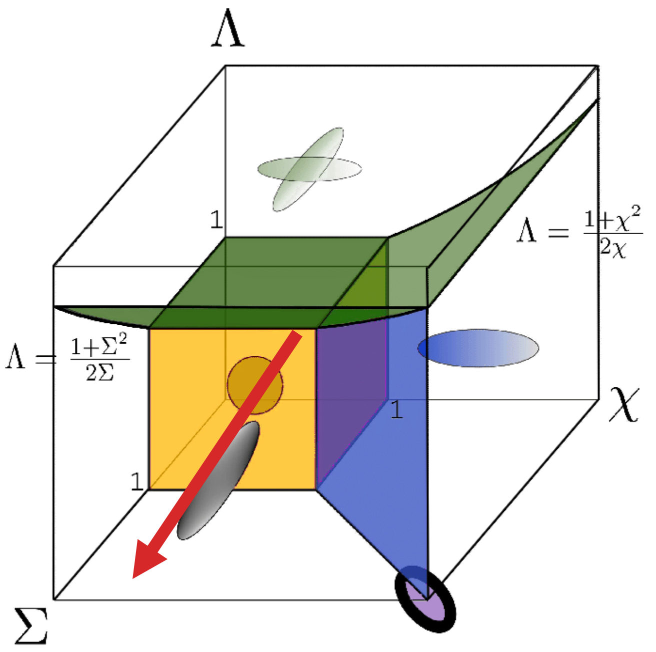

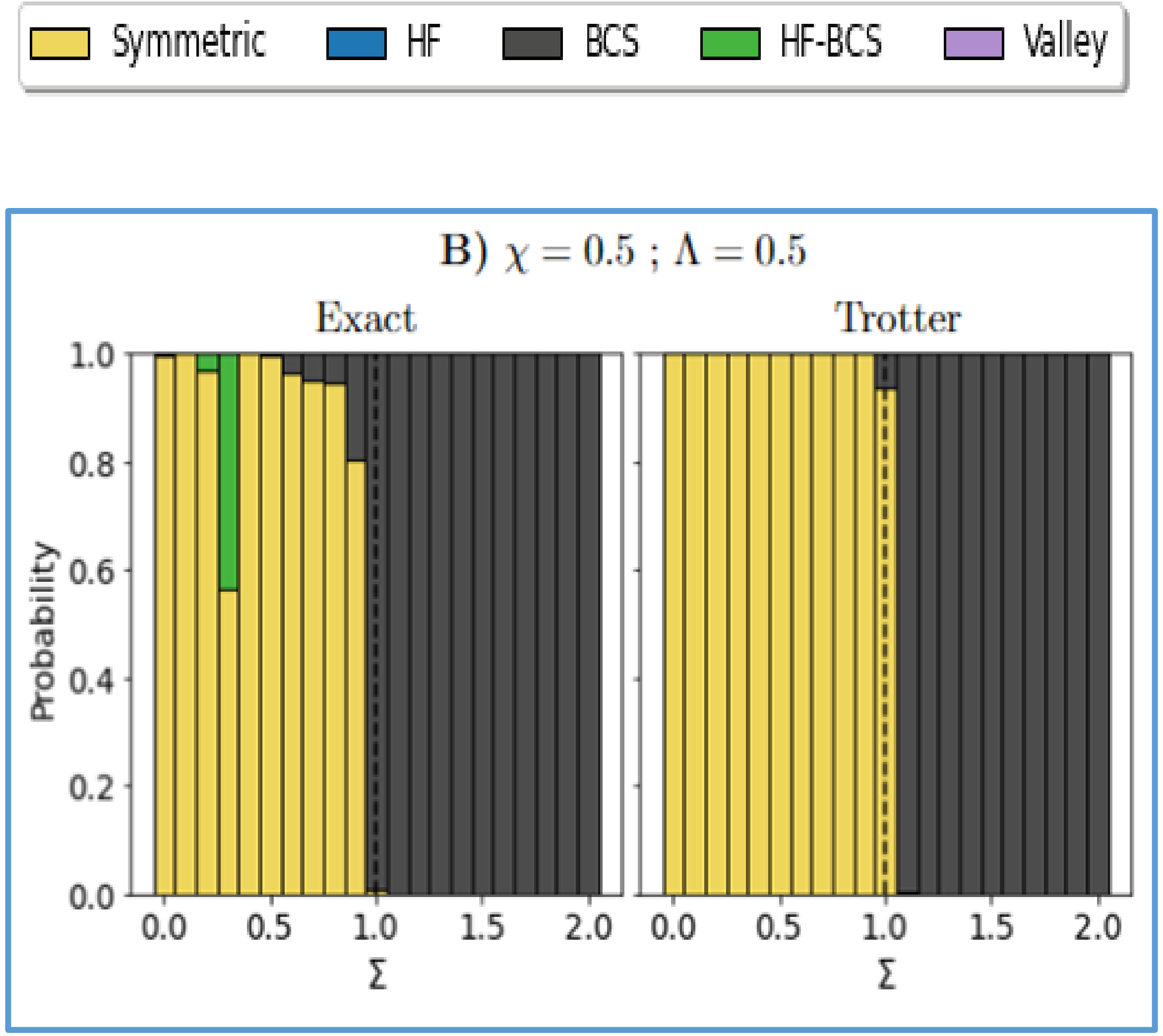

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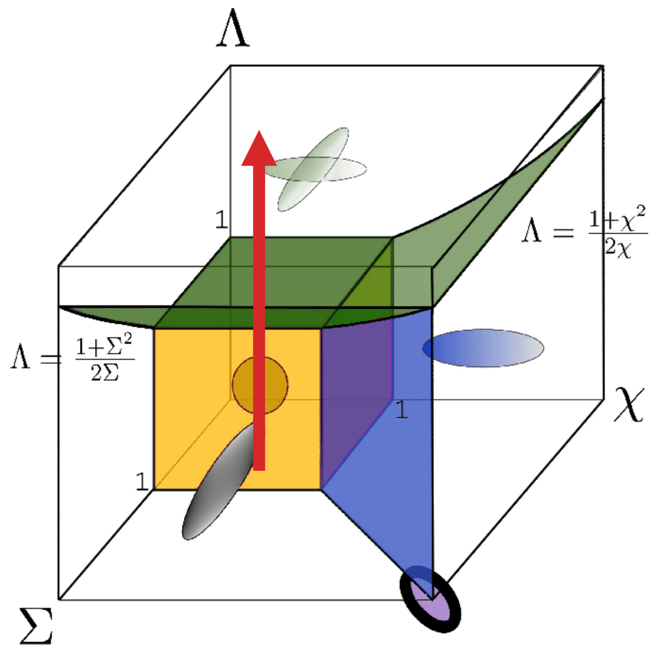

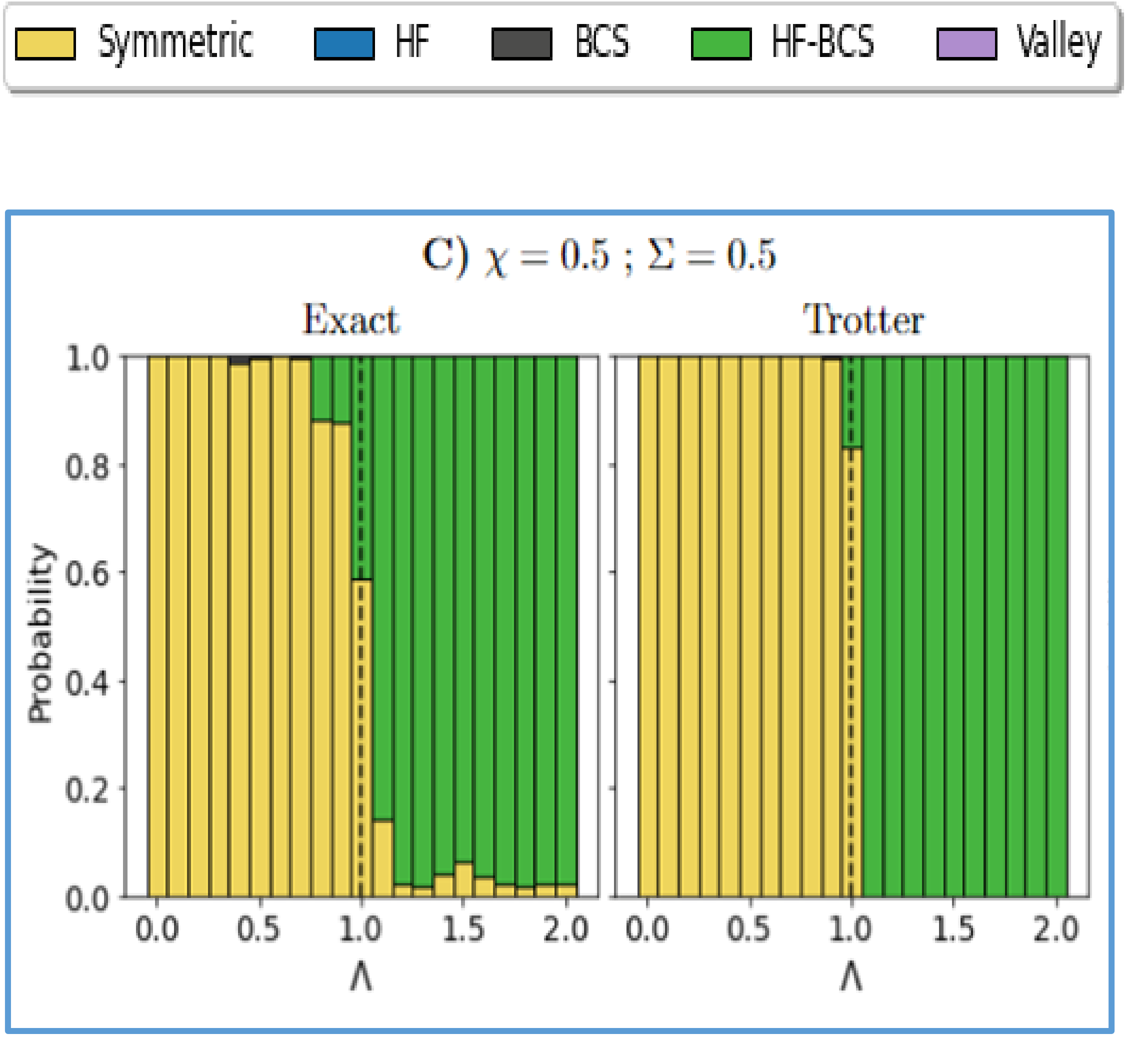

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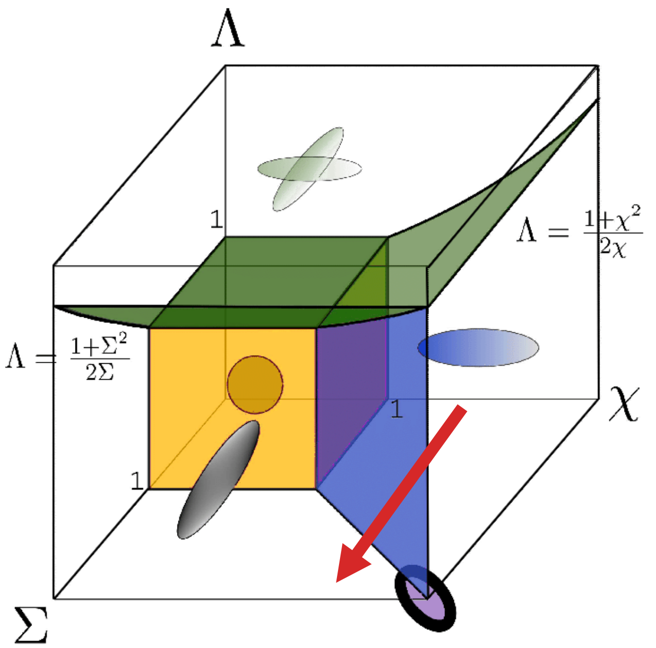

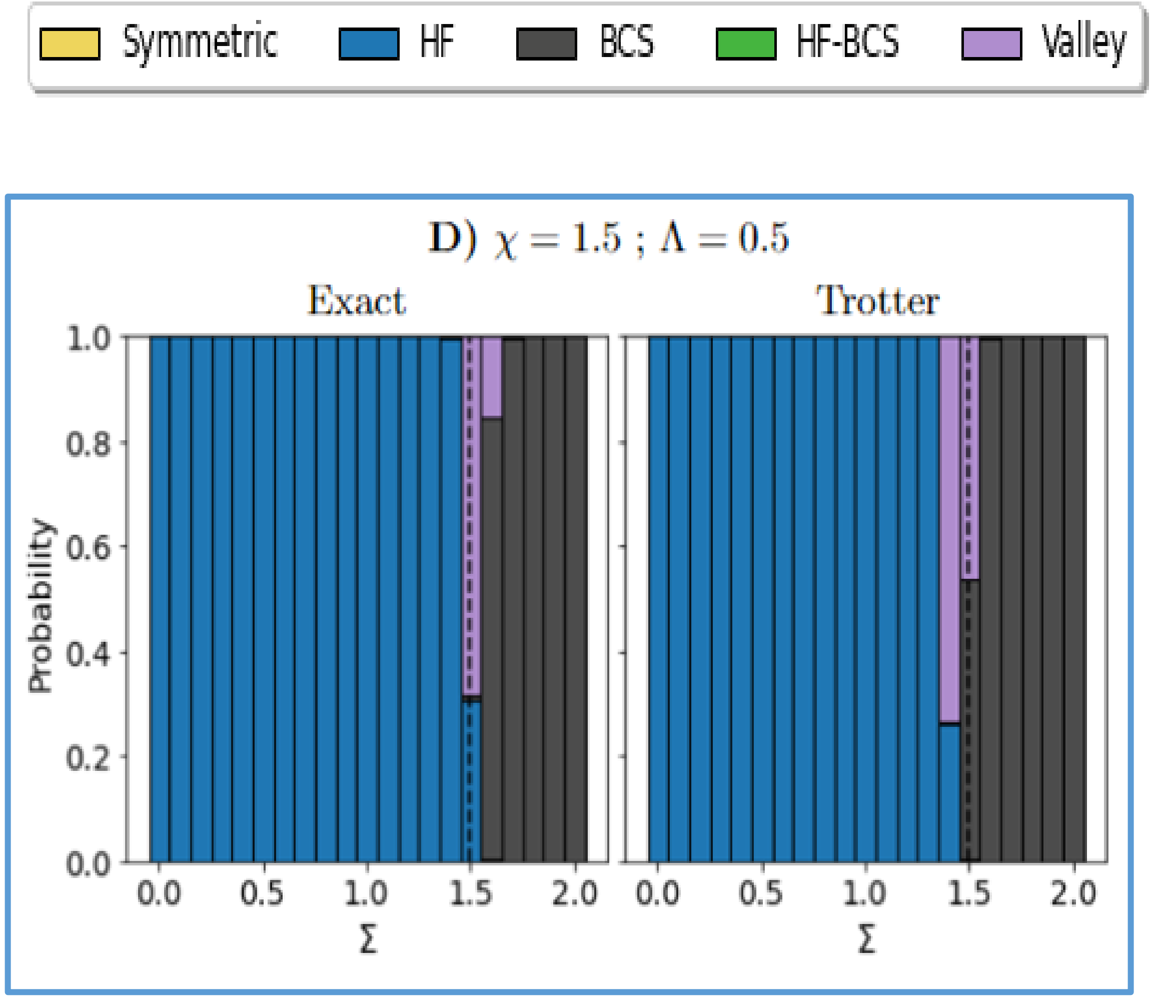

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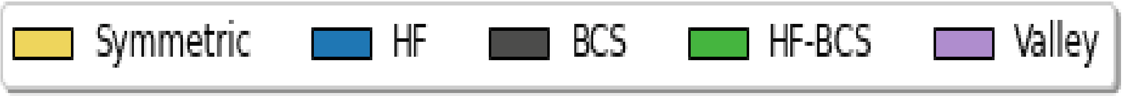

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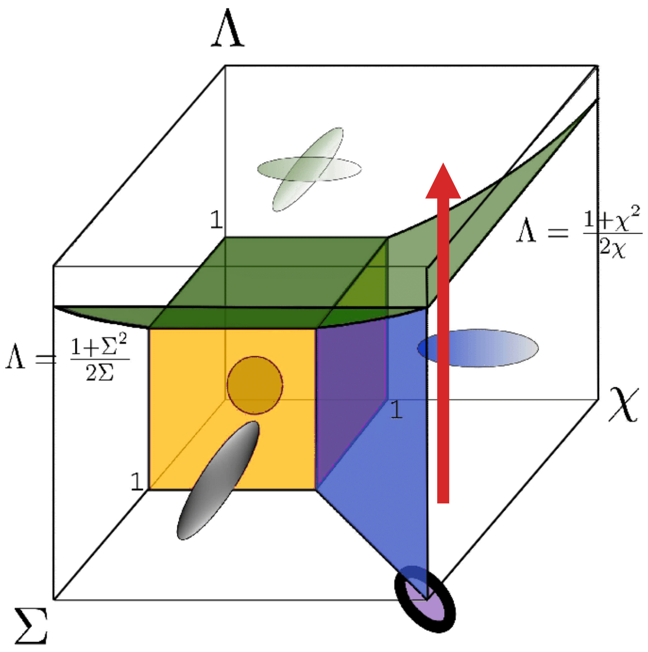

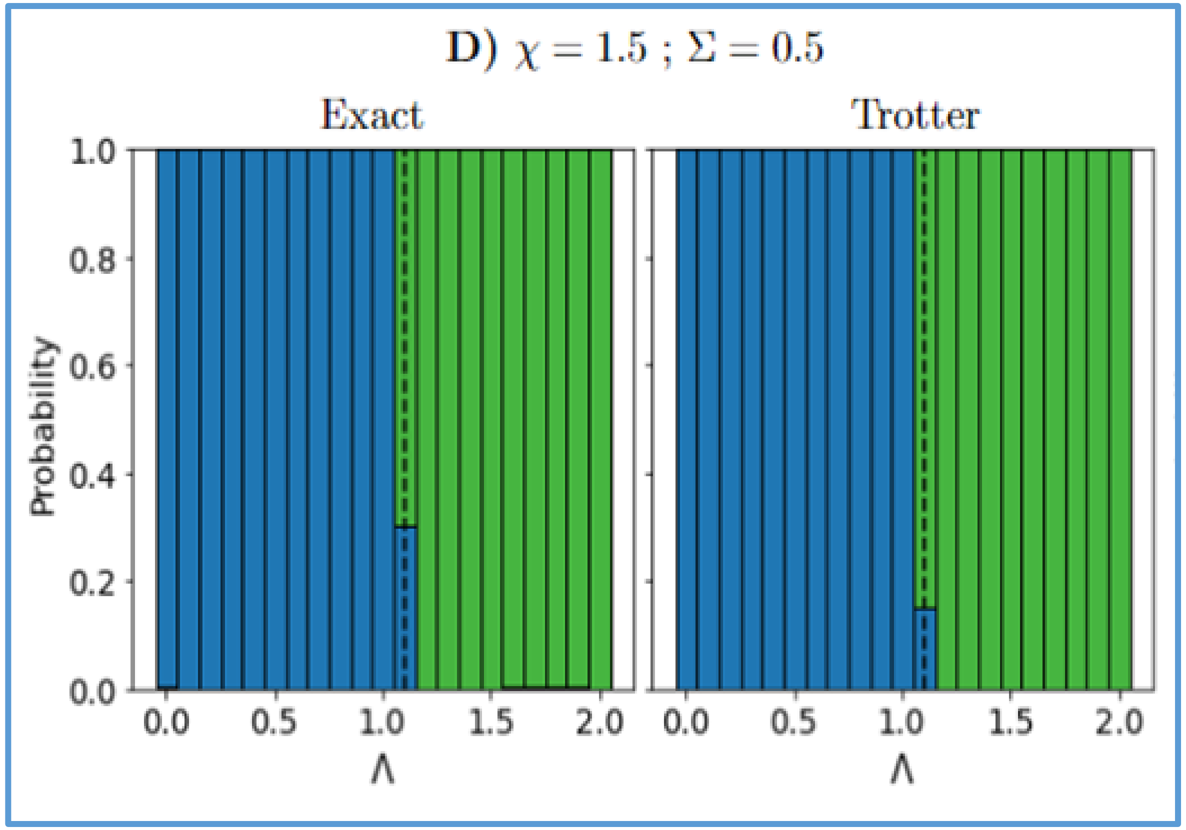

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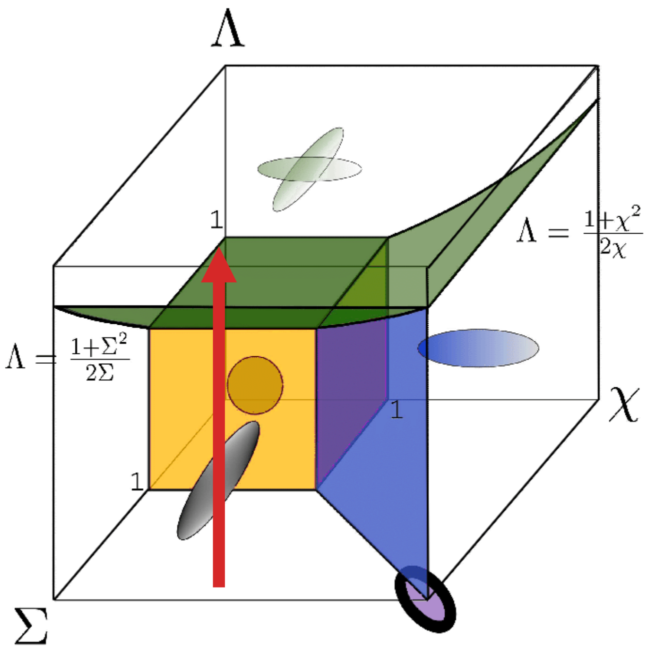

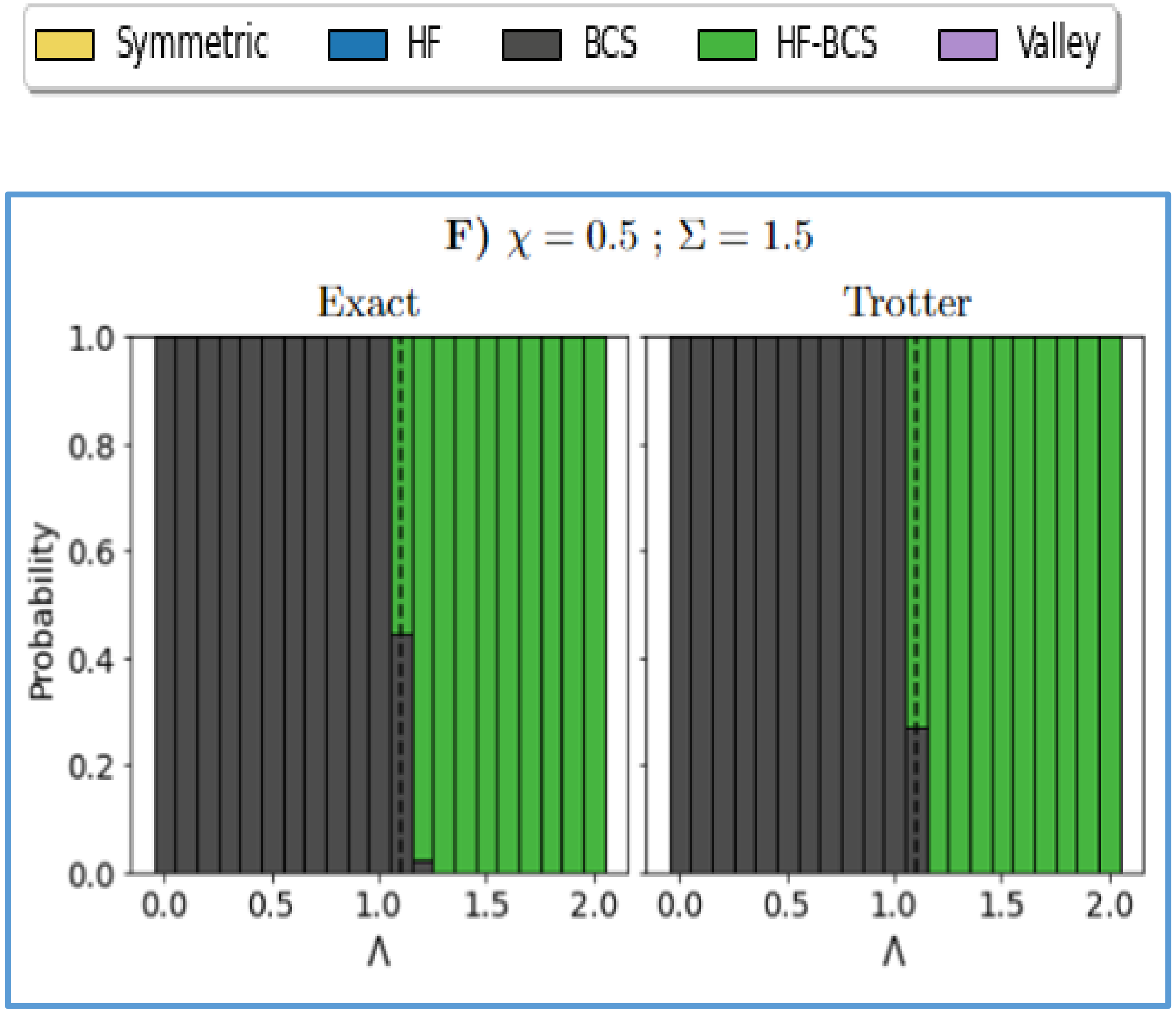

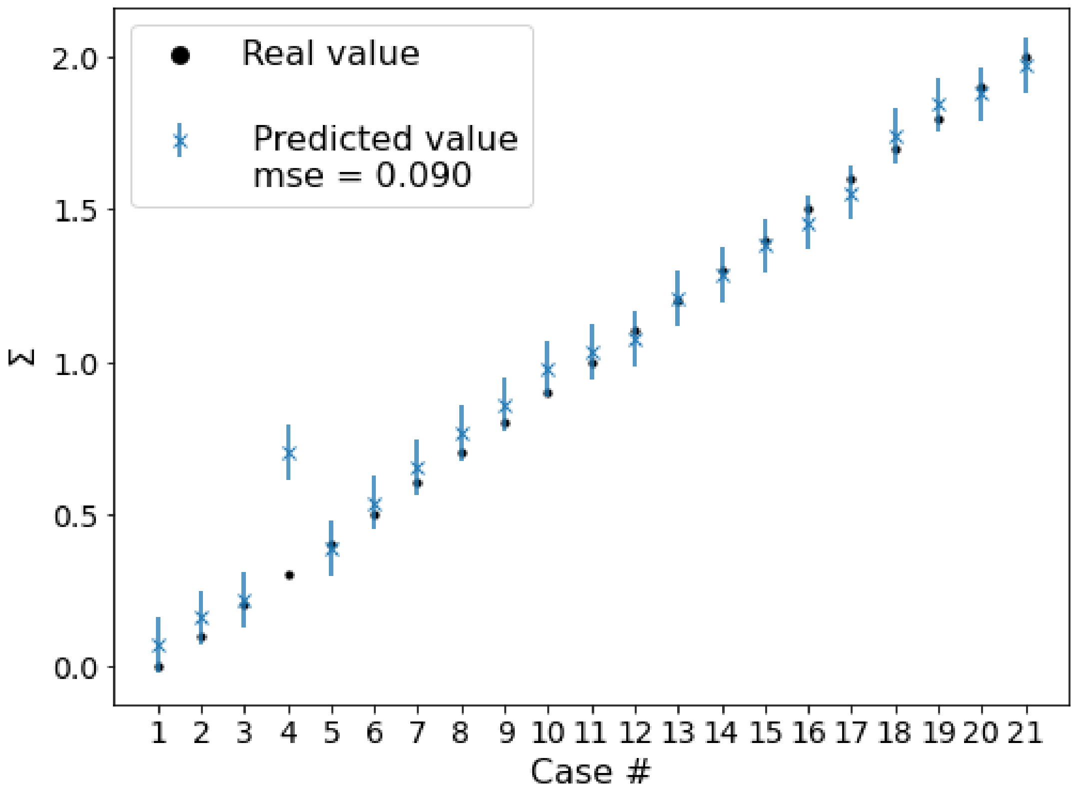

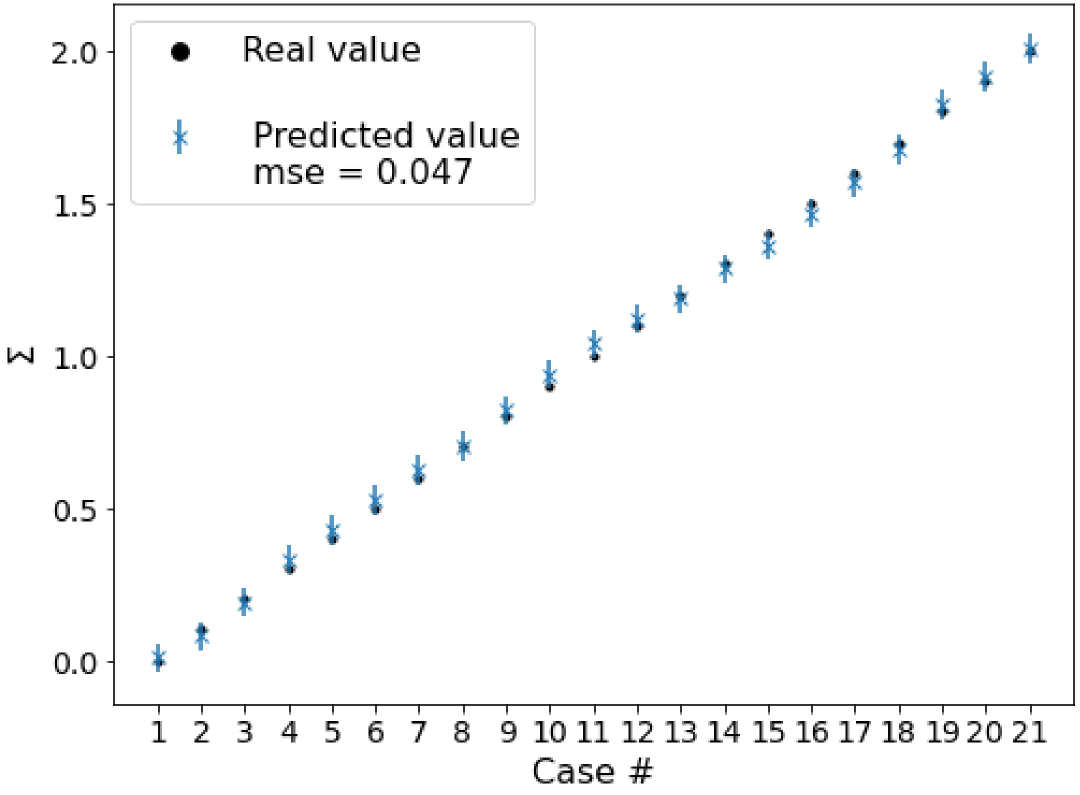

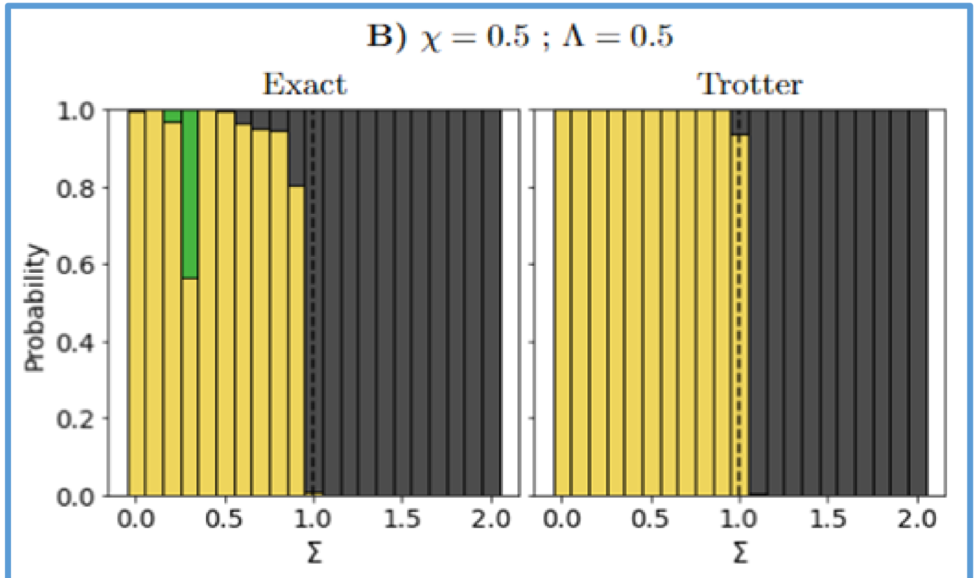

Mean error smaller than the step size (0.1)

Conclusions

- The quantum simulation is feasible with polynomial resources.
- Observables can be measured with this experimental setup.
- These observables can provide information about the phase/shape of the system.
- Machine Learning methods can make use of this information to extract the Quantum Phases of the system.
- These methods are robust against introduced errors.
- It’s fast and very accurate. Easily tailored to specific cases and different Hamiltonians, as long as there is data.

A. Sáiz et. al. PRC 106, 064322 (2022)